



Full wwPDB EM Validation Report ⓘ

Mar 31, 2025 – 07:34 PM JST

PDB ID : 6L4U / pdb_00006l4u
EMDB ID : EMD-0835
Title : Structure of the PSI-FCPI supercomplex from diatom
Authors : Nagao, R.; Kato, K.; Miyazaki, N.; Akita, F.; Shen, J.R.
Deposited on : 2019-10-21
Resolution : 2.40 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.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

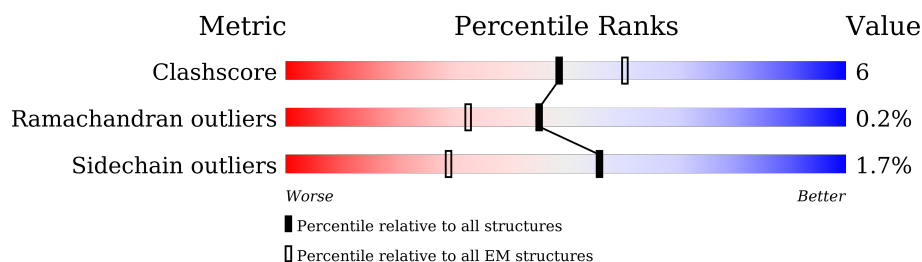
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.40 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	751	87% 11% .
2	B	733	90% 10%
3	C	81	83% 14% ...
4	D	139	82% 12% . 6%
5	E	67	85% . 10%
6	F	185	81% 6% 13%
7	I	36	94% . .
8	J	41	76% 24%
9	L	151	83% 7% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	M	30	
11	1u	130	
12	2u	121	
13	1	227	
14	2	205	
15	3	200	
16	4	215	
17	5	266	
18	6	208	
19	7	296	
20	8	270	
21	9	214	
22	10	207	
23	11	229	
24	12	204	
25	13	244	
26	14	249	
27	15	281	
28	16	218	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CL0	A	801	X	-	-	-
30	CLA	1	301	X	-	-	-
30	CLA	1	302	X	-	-	-
30	CLA	1	303	X	-	-	-
30	CLA	1	304	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	1	305	X	-	-	-
30	CLA	10	303	X	-	-	-
30	CLA	10	304	X	-	-	-
30	CLA	10	305	X	-	-	-
30	CLA	10	307	X	-	-	-
30	CLA	10	308	X	-	-	-
30	CLA	10	309	X	-	-	-
30	CLA	11	304	X	-	-	-
30	CLA	11	306	X	-	-	-
30	CLA	11	308	X	-	-	-
30	CLA	11	310	X	-	-	-
30	CLA	12	303	X	-	-	-
30	CLA	12	304	X	-	-	-
30	CLA	12	306	X	-	-	-
30	CLA	12	307	X	-	-	-
30	CLA	12	308	X	-	-	-
30	CLA	12	312	X	-	-	-
30	CLA	12	321	X	-	-	-
30	CLA	13	301	X	-	-	-
30	CLA	13	302	X	-	-	-
30	CLA	13	307	X	-	-	-
30	CLA	13	309	X	-	-	-
30	CLA	14	302	X	-	-	-
30	CLA	14	303	X	-	-	-
30	CLA	14	304	X	-	-	-
30	CLA	14	305	X	-	-	-
30	CLA	14	309	X	-	-	-
30	CLA	14	310	X	-	-	-
30	CLA	14	313	X	-	-	-
30	CLA	15	303	X	-	-	-
30	CLA	15	304	X	-	-	-
30	CLA	15	305	X	-	-	-
30	CLA	15	306	X	-	-	-
30	CLA	15	307	X	-	-	-
30	CLA	15	308	X	-	-	-
30	CLA	15	310	X	-	-	-
30	CLA	15	311	X	-	-	-
30	CLA	15	312	X	-	-	-
30	CLA	16	302	X	-	-	-
30	CLA	16	303	X	-	-	-
30	CLA	16	305	X	-	-	-
30	CLA	16	306	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	16	307	X	-	-	-
30	CLA	16	308	X	-	-	-
30	CLA	16	310	X	-	-	-
30	CLA	2	301	X	-	-	-
30	CLA	2	304	X	-	-	-
30	CLA	2	305	X	-	-	-
30	CLA	2	307	X	-	-	-
30	CLA	2	309	X	-	-	-
30	CLA	2	310	X	-	-	-
30	CLA	2u	202	X	-	-	-
30	CLA	3	301	X	-	-	-
30	CLA	3	302	X	-	-	-
30	CLA	3	303	X	-	-	-
30	CLA	3	305	X	-	-	-
30	CLA	3	306	X	-	-	-
30	CLA	3	307	X	-	-	-
30	CLA	4	301	X	-	-	-
30	CLA	4	302	X	-	-	-
30	CLA	4	303	X	-	-	-
30	CLA	4	304	X	-	-	-
30	CLA	4	305	X	-	-	-
30	CLA	4	306	X	-	-	-
30	CLA	4	309	X	-	-	-
30	CLA	4	311	X	-	-	-
30	CLA	5	302	X	-	-	-
30	CLA	5	303	X	-	-	-
30	CLA	5	304	X	-	-	-
30	CLA	5	307	X	-	-	-
30	CLA	5	309	X	-	-	-
30	CLA	5	311	X	-	-	-
30	CLA	6	304	X	-	-	-
30	CLA	6	305	X	-	-	-
30	CLA	6	306	X	-	-	-
30	CLA	6	307	X	-	-	-
30	CLA	6	309	X	-	-	-
30	CLA	6	310	X	-	-	-
30	CLA	6	315	X	-	-	-
30	CLA	6	316	X	-	-	-
30	CLA	6	317	X	-	-	-
30	CLA	7	303	X	-	-	-
30	CLA	7	304	X	-	-	-
30	CLA	7	305	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	7	306	X	-	-	-
30	CLA	7	309	X	-	-	-
30	CLA	7	311	X	-	-	-
30	CLA	7	312	X	-	-	-
30	CLA	8	301	X	-	-	-
30	CLA	8	302	X	-	-	-
30	CLA	8	304	X	-	-	-
30	CLA	8	308	X	-	-	-
30	CLA	9	301	X	-	-	-
30	CLA	9	302	X	-	-	-
30	CLA	9	305	X	-	-	-
30	CLA	9	306	X	-	-	-
30	CLA	9	307	X	-	-	-
30	CLA	9	308	X	-	-	-
30	CLA	9	309	X	-	-	-
30	CLA	A	802	X	-	-	-
30	CLA	A	803	X	-	-	-
30	CLA	A	804	X	-	-	-
30	CLA	A	805	X	-	-	-
30	CLA	A	806	X	-	-	-
30	CLA	A	807	X	-	-	-
30	CLA	A	808	X	-	-	-
30	CLA	A	809	X	-	-	-
30	CLA	A	810	X	-	-	-
30	CLA	A	811	X	-	-	-
30	CLA	A	812	X	-	-	-
30	CLA	A	813	X	-	-	-
30	CLA	A	814	X	-	-	-
30	CLA	A	815	X	-	-	-
30	CLA	A	816	X	-	-	-
30	CLA	A	820	X	-	-	-
30	CLA	A	821	X	-	-	-
30	CLA	A	822	X	-	-	-
30	CLA	A	824	X	-	-	-
30	CLA	A	825	X	-	-	-
30	CLA	A	826	X	-	-	-
30	CLA	A	827	X	-	-	-
30	CLA	A	828	X	-	-	-
30	CLA	A	829	X	-	-	-
30	CLA	A	830	X	-	-	-
30	CLA	A	831	X	-	-	-
30	CLA	A	833	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	A	834	X	-	-	-
30	CLA	A	835	X	-	-	-
30	CLA	A	836	X	-	-	-
30	CLA	A	837	X	-	-	-
30	CLA	A	838	X	-	-	-
30	CLA	A	839	X	-	-	-
30	CLA	A	840	X	-	-	-
30	CLA	A	841	X	-	-	-
30	CLA	A	842	X	-	-	-
30	CLA	A	843	X	-	-	-
30	CLA	A	844	X	-	-	-
30	CLA	B	801	X	-	-	-
30	CLA	B	802	X	-	-	-
30	CLA	B	803	X	-	-	-
30	CLA	B	804	X	-	-	-
30	CLA	B	805	X	-	-	-
30	CLA	B	806	X	-	-	-
30	CLA	B	807	X	-	-	-
30	CLA	B	808	X	-	-	-
30	CLA	B	809	X	-	-	-
30	CLA	B	810	X	-	-	-
30	CLA	B	811	X	-	-	-
30	CLA	B	812	X	-	-	-
30	CLA	B	813	X	-	-	-
30	CLA	B	814	X	-	-	-
30	CLA	B	815	X	-	-	-
30	CLA	B	817	X	-	-	-
30	CLA	B	818	X	-	-	-
30	CLA	B	819	X	-	-	-
30	CLA	B	821	X	-	-	-
30	CLA	B	823	X	-	-	-
30	CLA	B	824	X	-	-	-
30	CLA	B	825	X	-	-	-
30	CLA	B	826	X	-	-	-
30	CLA	B	827	X	-	-	-
30	CLA	B	828	X	-	-	-
30	CLA	B	829	X	-	-	-
30	CLA	B	830	X	-	-	-
30	CLA	B	832	X	-	-	-
30	CLA	B	833	X	-	-	-
30	CLA	B	834	X	-	-	-
30	CLA	B	835	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	B	836	X	-	-	-
30	CLA	B	837	X	-	-	-
30	CLA	B	838	X	-	-	-
30	CLA	B	839	X	-	-	-
30	CLA	F	201	X	-	-	-
30	CLA	F	202	X	-	-	-
30	CLA	F	203	X	-	-	-
30	CLA	J	101	X	-	-	-
30	CLA	L	202	X	-	-	-
30	CLA	L	203	X	-	-	-

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 62199 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 Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	741	Total	C	N	O	S	0	0
			5841	3816	991	1005	29		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	731	Total	C	N	O	S	0	0
			5801	3814	977	992	18		

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			599	368	103	118	10		

- Molecule 4 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	131	Total	C	N	O	S	0	0
			1037	663	177	194	3		

- Molecule 5 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	60	Total	C	N	O	0	0
			478	302	86	90		

- Molecule 6 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	161	Total	C	N	O	S	0	0
			1257	806	213	234	4		

- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	35	Total	C	N	O	S	0	0
			273	190	37	44	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	41	Total	C	N	O	S	0	0
			344	236	50	55	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	137	Total	C	N	O	S	0	0
			1030	680	169	179	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	30	Total	C	N	O	S	0	0
			227	151	35	40	1		

- Molecule 11 is a protein called Unknown protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1u	130	Total	C	N	O		0	0
			650	390	130	130			

- Molecule 12 is a protein called Photosystem I reaction center subunit Ps28.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	2u	89	Total	C	N	O	S	0	0
			674	438	110	120	6		

- Molecule 13 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1	141	Total	C	N	O	S	0	0
			1086	692	184	201	9		

- Molecule 14 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	2	172	Total	C	N	O	S	0	0
			1310	846	216	238	10		

- Molecule 15 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	3	164	Total	C	N	O	S	0	0
			1275	825	213	232	5		

- Molecule 16 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	4	179	Total	C	N	O	S	0	0
			1368	878	227	250	13		

- Molecule 17 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	5	169	Total	C	N	O	S	0	0
			1304	834	222	236	12		

- Molecule 18 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	6	174	Total	C	N	O	S	0	0
			1354	884	216	246	8		

- Molecule 19 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr10.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	7	188	Total	C	N	O	S	0	0
			1416	894	240	266	16		

- Molecule 20 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	8	213	Total	C	N	O	S	0	0
			1660	1075	274	302	9		

- Molecule 21 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcf6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	9	163	Total	C	N	O	S	0	0
			1267	816	211	233	7		

- Molecule 22 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	10	169	Total	C	N	O	S	0	0
			1302	849	212	233	8		

- Molecule 23 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq13.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	11	191	Total	C	N	O	S	0	0
			1479	958	243	270	8		

- Molecule 24 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	12	173	Total	C	N	O	S	0	0
			1274	814	209	243	8		

- Molecule 25 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq11.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	13	150	Total	C	N	O	S	0	0
			1148	736	203	204	5		

- Molecule 26 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq10.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	14	208	Total	C	N	O	S	0	0
			1609	1049	262	292	6		

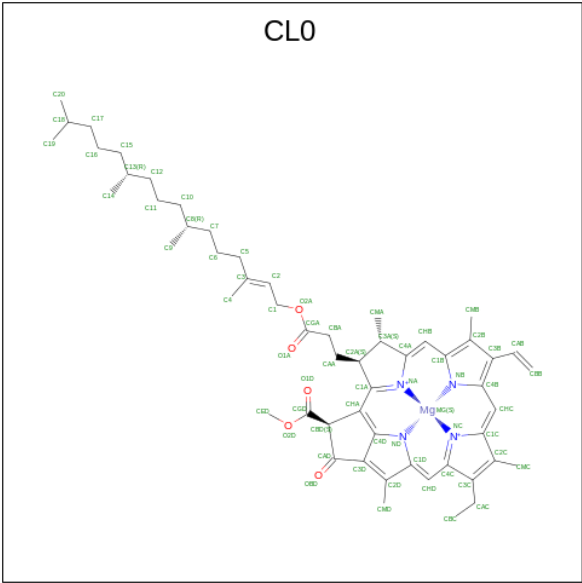
- Molecule 27 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq8.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	15	211	Total	C	N	O	S	0	0
			1654	1077	273	298	6		

- Molecule 28 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq5.

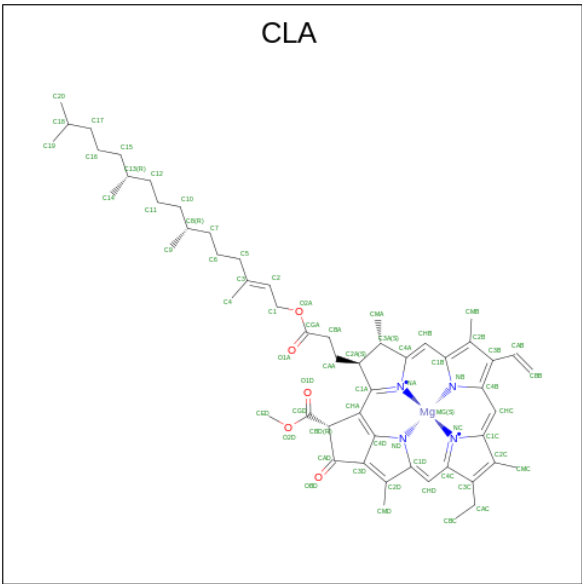
Mol	Chain	Residues	Atoms					AltConf	Trace
28	16	174	Total	C	N	O	S	0	0
			1313	846	217	242	8		

- Molecule 29 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 30 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
30	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	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
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	F	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
30	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	2u	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	2	1	Total 45	C 35	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
30	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
30	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	3	1	Total 62	C 52	Mg 1	N 4	O 5	0
30	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	4	1	Total 49	C 39	Mg 1	N 4	O 5	0
30	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
30	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
30	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	5	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
30	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	7	1	Total 46	C 36	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
30	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	8	1	Total 58	C 48	Mg 1	N 4	O 5	0
30	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	8	1	Total 47	C 37	Mg 1	N 4	O 5	0
30	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	9	1	Total 51	C 41	Mg 1	N 4	O 5	0
30	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	10	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	10	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	10	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	10	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	10	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
30	10	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	11	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	11	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	11	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	11	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	11	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	12	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	13	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	13	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	13	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	13	1	Total 45	C 35	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

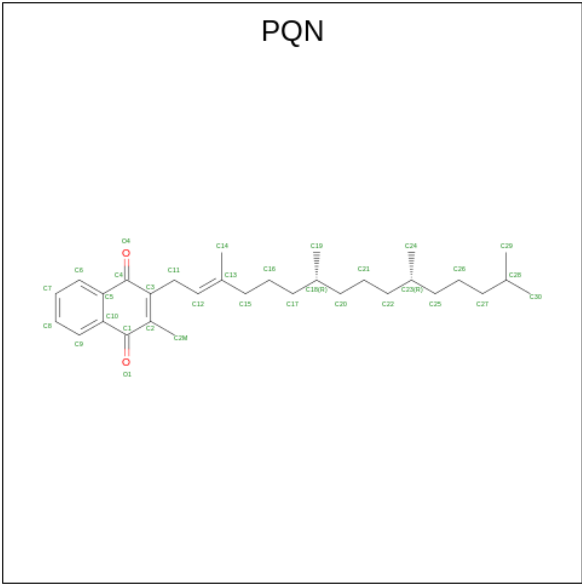
Mol	Chain	Residues	Atoms					AltConf
30	14	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	14	1	Total 57	C 47	Mg 1	N 4	O 5	0
30	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	14	1	Total 50	C 40	Mg 1	N 4	O 5	0
30	14	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	14	1	Total 50	C 40	Mg 1	N 4	O 5	0
30	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	14	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	15	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	15	1	Total 60	C 50	Mg 1	N 4	O 5	0
30	15	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	15	1	Total 50	C 40	Mg 1	N 4	O 5	0
30	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	15	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	15	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
30	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 31 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



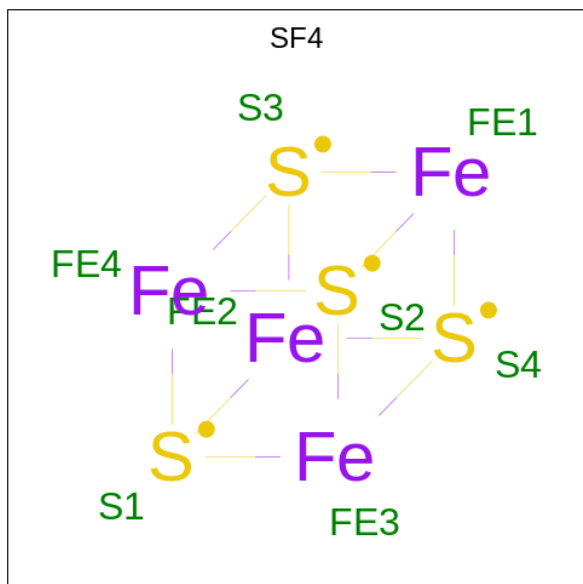
Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			33	31	2	

Continued on next page...

Continued from previous page...

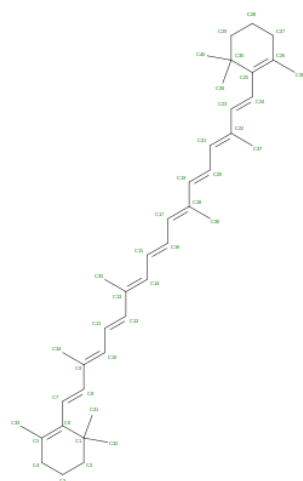
Mol	Chain	Residues	Atoms			AltConf
31	B	1	Total	C	O	0
			33	31	2	

- Molecule 32 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 33 is BETA-CAROTENE (CCD ID: BCR) (formula: $\text{C}_{40}\text{H}_{56}$).

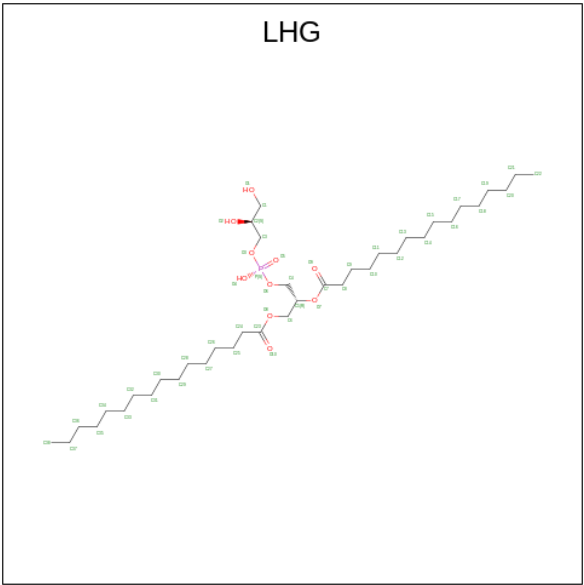


Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
33	J	1	Total C 40 40	0
33	L	1	Total C 40 40	0
33	L	1	Total C 40 40	0
33	L	1	Total C 40 40	0
33	M	1	Total C 40 40	0
33	2u	1	Total C 40 40	0

- Molecule 34 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



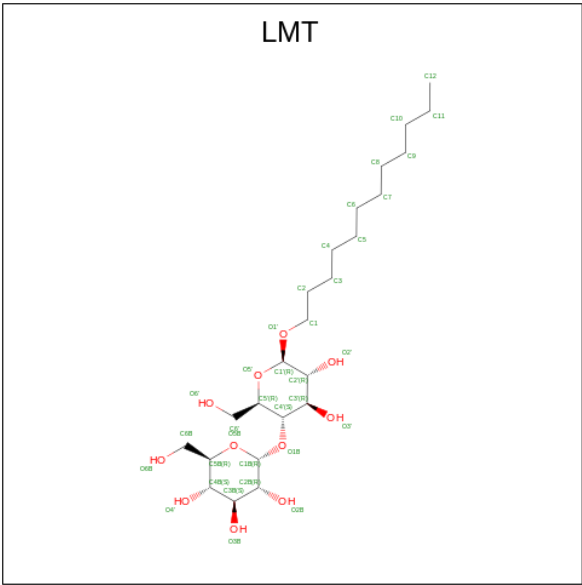
Mol	Chain	Residues	Atoms	AltConf
34	A	1	Total C O P 49 38 10 1	0
34	A	1	Total C O P 27 16 10 1	0
34	B	1	Total C O P 27 16 10 1	0
34	2	1	Total C O P 27 16 10 1	0
34	5	1	Total C O P 27 16 10 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
34	6	1	Total	C	O	P	0
			27	16	10	1	
34	9	1	Total	C	O	P	0
			34	23	10	1	

- Molecule 35 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



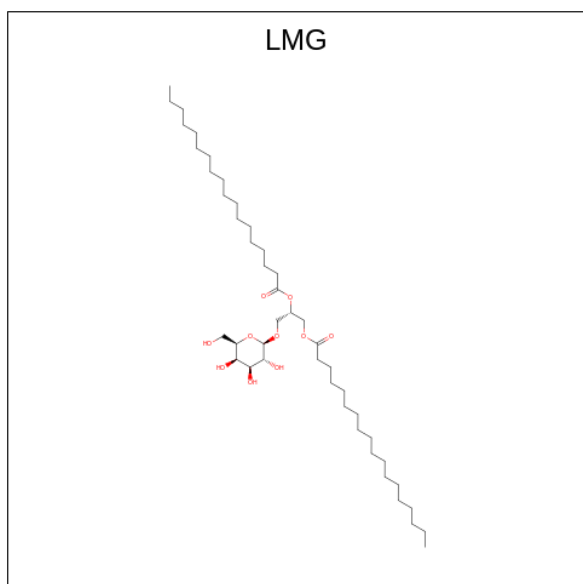
Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	C	O		0
			35	24	11		
35	A	1	Total	C	O		0
			35	24	11		
35	A	1	Total	C	O		0
			35	24	11		
35	B	1	Total	C	O		0
			35	24	11		
35	B	1	Total	C	O		0
			35	24	11		
35	1	1	Total	C	O		0
			35	24	11		
35	6	1	Total	C	O		0
			31	20	11		
35	7	1	Total	C	O		0
			35	24	11		
35	7	1	Total	C	O		0
			35	24	11		

Continued on next page...

Continued from previous page...

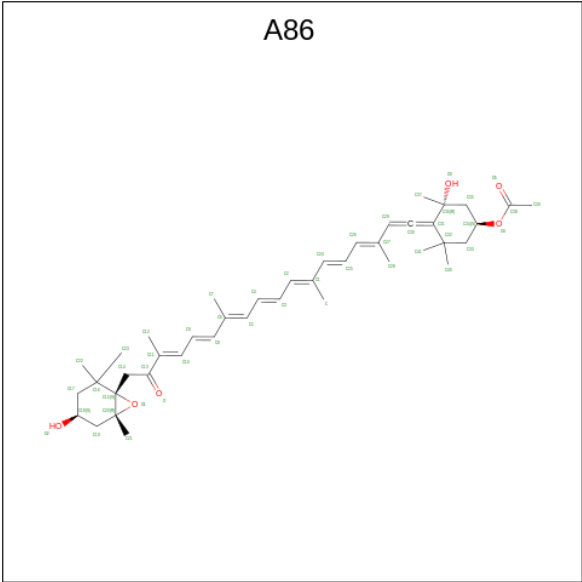
Mol	Chain	Residues	Atoms			AltConf
35	8	1	Total	C	O	0
			35	24	11	
35	9	1	Total	C	O	0
			32	21	11	
35	11	1	Total	C	O	0
			35	24	11	
35	11	1	Total	C	O	0
			35	24	11	
35	11	1	Total	C	O	0
			35	24	11	
35	11	1	Total	C	O	0
			35	24	11	
35	12	1	Total	C	O	0
			35	24	11	
35	12	1	Total	C	O	0
			35	24	11	
35	12	1	Total	C	O	0
			35	24	11	
35	12	1	Total	C	O	0
			35	24	11	
35	15	1	Total	C	O	0
			35	24	11	
35	16	1	Total	C	O	0
			35	24	11	

- Molecule 36 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
36	A	1	Total	C	O	0
			34	24	10	
36	B	1	Total	C	O	0
			55	45	10	
36	B	1	Total	C	O	0
			43	33	10	
36	F	1	Total	C	O	0
			27	17	10	
36	2u	1	Total	C	O	0
			31	21	10	
36	3	1	Total	C	O	0
			37	27	10	
36	5	1	Total	C	O	0
			33	23	10	
36	6	1	Total	C	O	0
			33	23	10	
36	7	1	Total	C	O	0
			37	27	10	
36	8	1	Total	C	O	0
			37	27	10	
36	8	1	Total	C	O	0
			42	32	10	
36	8	1	Total	C	O	0
			29	19	10	
36	14	1	Total	C	O	0
			38	28	10	

- Molecule 37 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'-yl acetate (CCD ID: A86) (formula: C₄₂H₅₈O₆).



Mol	Chain	Residues	Atoms			AltConf
37	2u	1	Total	C	O	0
			48	42	6	
37	2u	1	Total	C	O	0
			48	42	6	
37	1	1	Total	C	O	0
			48	42	6	
37	2	1	Total	C	O	0
			48	42	6	
37	2	1	Total	C	O	0
			48	42	6	
37	2	1	Total	C	O	0
			48	42	6	
37	3	1	Total	C	O	0
			48	42	6	
37	3	1	Total	C	O	0
			48	42	6	
37	4	1	Total	C	O	0
			48	42	6	
37	4	1	Total	C	O	0
			48	42	6	
37	4	1	Total	C	O	0
			48	42	6	
37	4	1	Total	C	O	0
			48	42	6	
37	5	1	Total	C	O	0
			48	42	6	
37	5	1	Total	C	O	0
			48	42	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
37	5	1	Total	C	O	0
			48	42	6	
37	6	1	Total	C	O	0
			48	42	6	
37	7	1	Total	C	O	0
			48	42	6	
37	7	1	Total	C	O	0
			48	42	6	
37	7	1	Total	C	O	0
			48	42	6	
37	8	1	Total	C	O	0
			48	42	6	
37	8	1	Total	C	O	0
			48	42	6	
37	9	1	Total	C	O	0
			48	42	6	
37	9	1	Total	C	O	0
			48	42	6	
37	9	1	Total	C	O	0
			48	42	6	
37	10	1	Total	C	O	0
			48	42	6	
37	10	1	Total	C	O	0
			48	42	6	
37	10	1	Total	C	O	0
			48	42	6	
37	10	1	Total	C	O	0
			48	42	6	
37	10	1	Total	C	O	0
			48	42	6	
37	11	1	Total	C	O	0
			48	42	6	
37	11	1	Total	C	O	0
			48	42	6	
37	11	1	Total	C	O	0
			48	42	6	
37	11	1	Total	C	O	0
			48	42	6	
37	12	1	Total	C	O	0
			48	42	6	
37	12	1	Total	C	O	0
			48	42	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
37	13	1	Total	C	O	0
			45	40	5	
37	13	1	Total	C	O	0
			48	42	6	
37	14	1	Total	C	O	0
			48	42	6	
37	14	1	Total	C	O	0
			48	42	6	
37	14	1	Total	C	O	0
			48	42	6	
37	14	1	Total	C	O	0
			48	42	6	
37	14	1	Total	C	O	0
			48	42	6	
37	14	1	Total	C	O	0
			48	42	6	
37	14	1	Total	C	O	0
			48	42	6	
37	15	1	Total	C	O	0
			48	42	6	
37	15	1	Total	C	O	0
			48	42	6	
37	15	1	Total	C	O	0
			48	42	6	
37	15	1	Total	C	O	0
			48	42	6	
37	15	1	Total	C	O	0
			48	42	6	
37	15	1	Total	C	O	0
			48	42	6	
37	16	1	Total	C	O	0
			48	42	6	
37	16	1	Total	C	O	0
			48	42	6	

- Molecule 38 is Chlorophyll c1 (CCD ID: KC1) (formula: $C_{35}H_{30}MgN_4O_5$).



Continued on next page...

Continued from previous page...

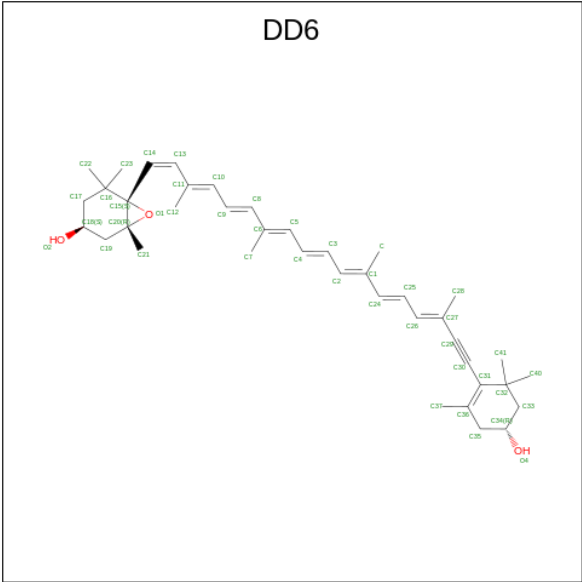
Mol	Chain	Residues	Atoms					AltConf
38	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	10	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	10	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	10	1	Total 45	C 35	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
38	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 39 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene -3,3'-diol (CCD ID: DD6) (formula: C₄₀H₅₄O₃).



Mol	Chain	Residues	Atoms			AltConf
39	1	1	Total	C	O	0
			43	40	3	
39	2	1	Total	C	O	0
			43	40	3	
39	2	1	Total	C	O	0
			43	40	3	
39	2	1	Total	C	O	0
			43	40	3	
39	3	1	Total	C	O	0
			43	40	3	
39	3	1	Total	C	O	0
			43	40	3	
39	3	1	Total	C	O	0
			43	40	3	
39	4	1	Total	C	O	0
			43	40	3	
39	4	1	Total	C	O	0
			43	40	3	
39	5	1	Total	C	O	0
			43	40	3	
39	5	1	Total	C	O	0
			43	40	3	
39	6	1	Total	C	O	0
			43	40	3	
39	6	1	Total	C	O	0
			43	40	3	
39	6	1	Total	C	O	0
			43	40	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
39	6	1	Total	C	O	0
			43	40	3	
39	7	1	Total	C	O	0
			43	40	3	
39	7	1	Total	C	O	0
			43	40	3	
39	7	1	Total	C	O	0
			43	40	3	
39	7	1	Total	C	O	0
			43	40	3	
39	8	1	Total	C	O	0
			43	40	3	
39	8	1	Total	C	O	0
			43	40	3	
39	9	1	Total	C	O	0
			43	40	3	
39	10	1	Total	C	O	0
			43	40	3	
39	10	1	Total	C	O	0
			43	40	3	
39	11	1	Total	C	O	0
			43	40	3	
39	12	1	Total	C	O	0
			43	40	3	
39	12	1	Total	C	O	0
			43	40	3	
39	13	1	Total	C	O	0
			43	40	3	
39	15	1	Total	C	O	0
			43	40	3	
39	15	1	Total	C	O	0
			43	40	3	
39	16	1	Total	C	O	0
			43	40	3	

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		AltConf
40	A	42	Total	O	0
			42	42	
40	B	53	Total	O	0
			53	53	

Continued on next page...

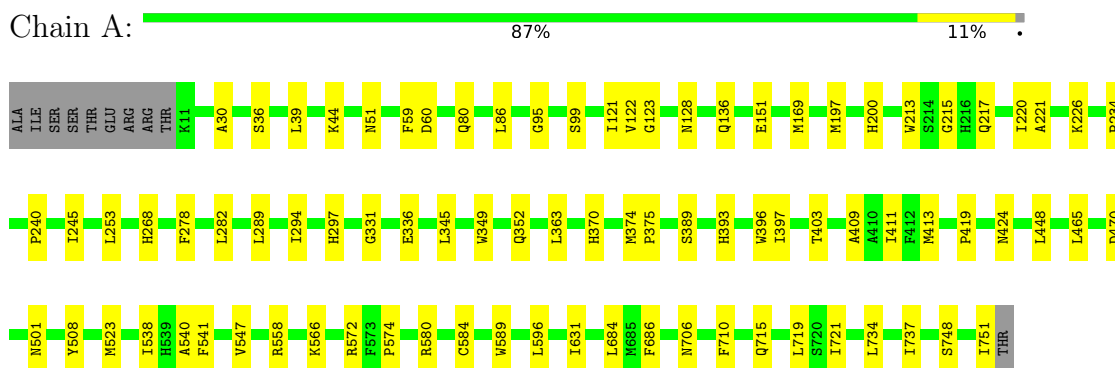
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
40	C	15	Total 15	O 15	0
40	D	13	Total 13	O 13	0
40	E	3	Total 3	O 3	0
40	F	3	Total 3	O 3	0
40	I	1	Total 1	O 1	0
40	L	8	Total 8	O 8	0
40	1	1	Total 1	O 1	0
40	2	2	Total 2	O 2	0
40	3	1	Total 1	O 1	0
40	5	1	Total 1	O 1	0
40	6	2	Total 2	O 2	0
40	7	2	Total 2	O 2	0
40	8	4	Total 4	O 4	0
40	9	1	Total 1	O 1	0
40	10	1	Total 1	O 1	0
40	11	1	Total 1	O 1	0
40	12	2	Total 2	O 2	0

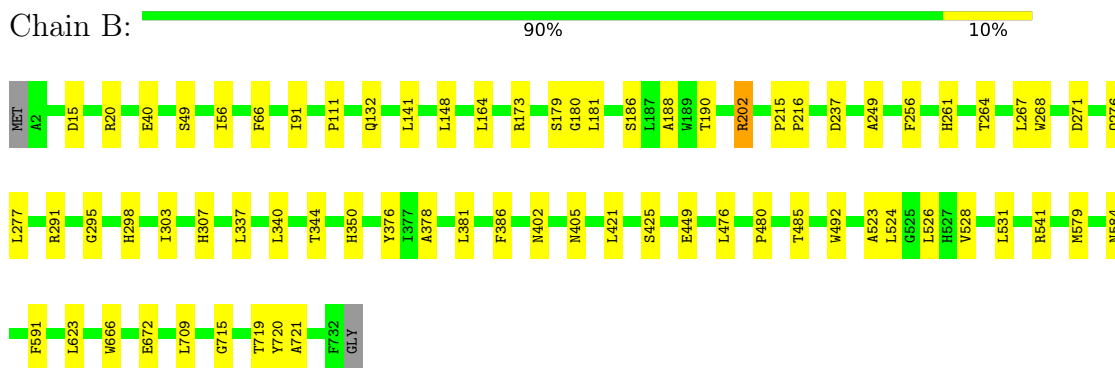
3 Residue-property plots

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. 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. 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.

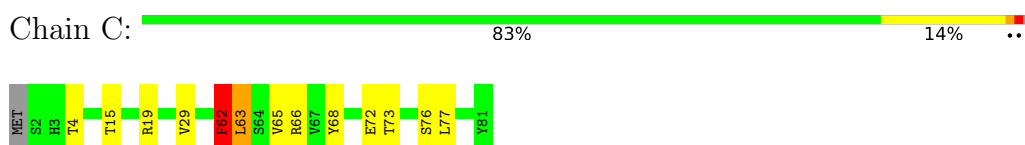
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



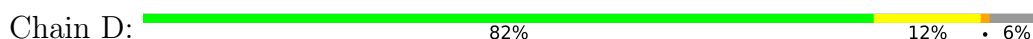
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 3: Photosystem I iron-sulfur center



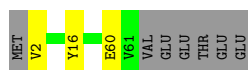
- Molecule 4: Photosystem I reaction center subunit II





- Molecule 5: Photosystem I reaction center subunit IV

Chain E: 85% 10%



- Molecule 6: Photosystem I reaction center subunit III

Chain F: 81% 6% 13%



- Molecule 7: Photosystem I reaction center subunit VIII

Chain I: 94% 1% 1%



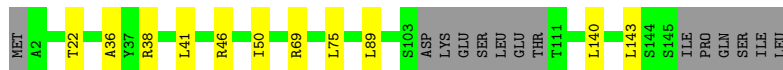
- Molecule 8: Photosystem I reaction center subunit IX

Chain J: 76% 24%



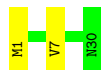
- Molecule 9: Photosystem I reaction center subunit XI

Chain L: 83% 7% 9%



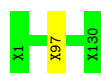
- Molecule 10: Photosystem I reaction center subunit XII

Chain M: 93% 7%



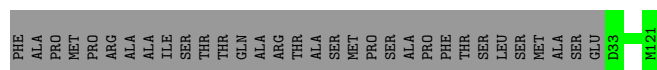
- Molecule 11: Unknown protein 1

Chain 1u: 99% 1%



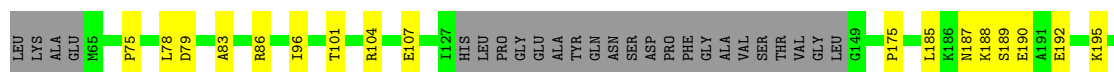
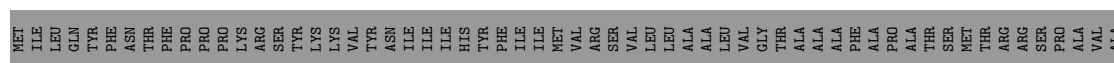
- Molecule 12: Photosystem I reaction center subunit Psa28

Chain 2u: 74% 26%



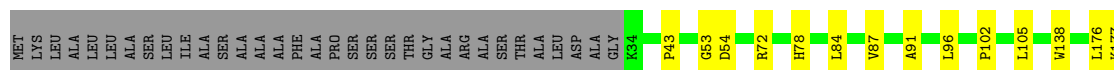
- Molecule 13: Fucoxanthin chlorophyll a/c-binding protein Lhcr15

Chain 1: 53% 9% 38%



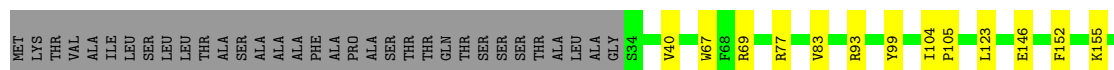
- Molecule 14: Fucoxanthin chlorophyll a/c-binding protein Lhcr8

Chain 2: 77% 7% 16%



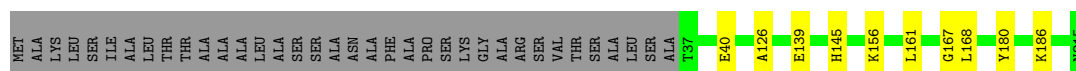
- Molecule 15: Fucoxanthin chlorophyll a/c-binding protein Lhcr2

Chain 3: 74% 8% 18%

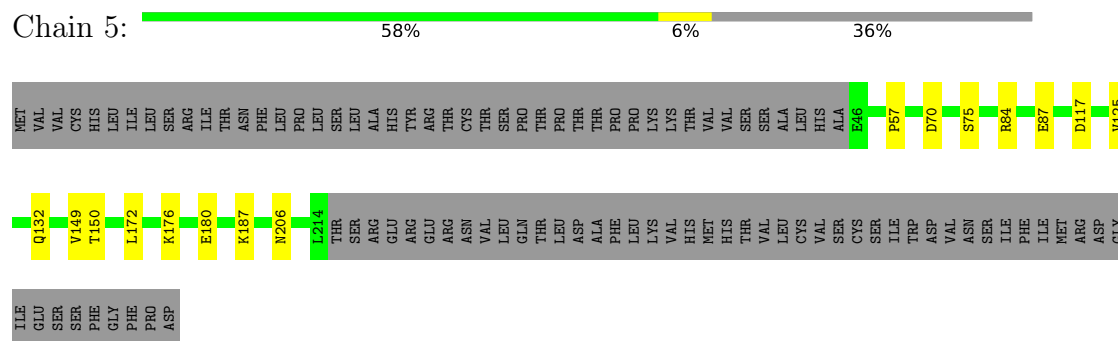


- Molecule 16: Fucoxanthin chlorophyll a/c-binding protein Lhcr9

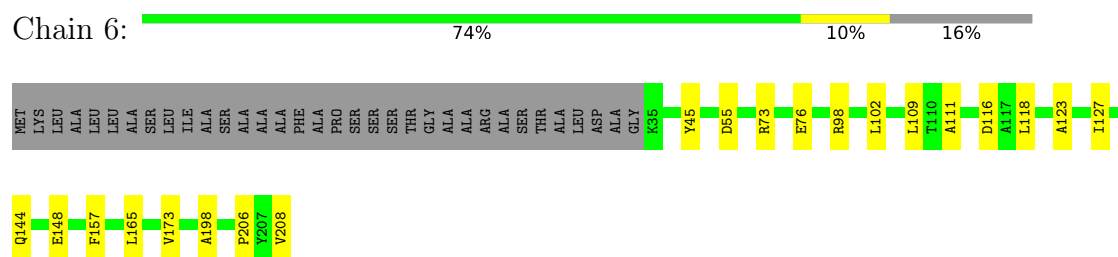
Chain 4: 79% 5% 17%



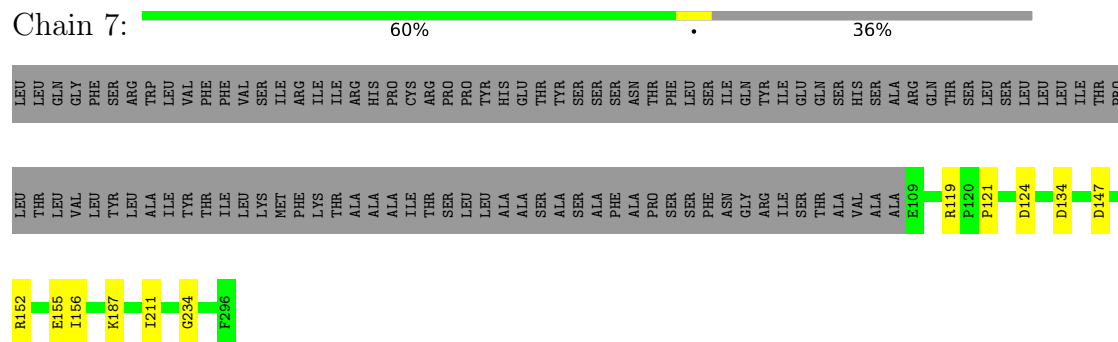
- Molecule 17: Fucoxanthin chlorophyll a/c-binding protein Lhcr11



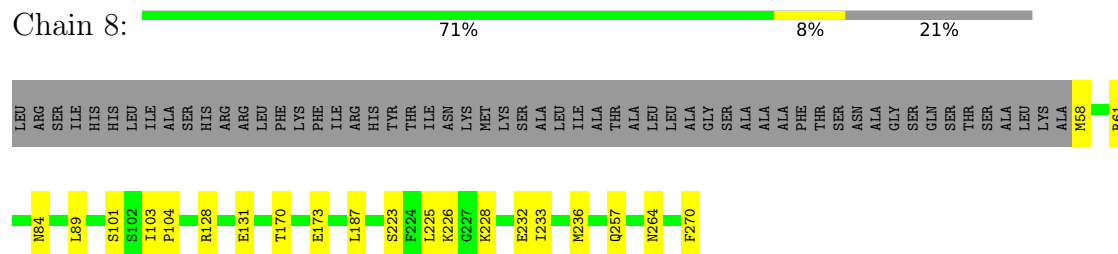
- Molecule 18: Fucoxanthin chlorophyll a/c-binding protein Lhcr12



- Molecule 19: Fucoxanthin chlorophyll a/c-binding protein Lhcr10

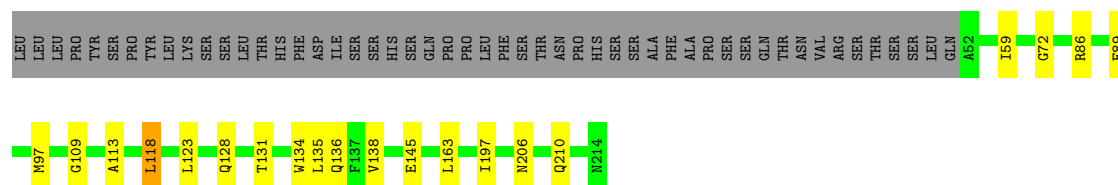


- Molecule 20: Fucoxanthin chlorophyll a/c-binding protein Lhcr4



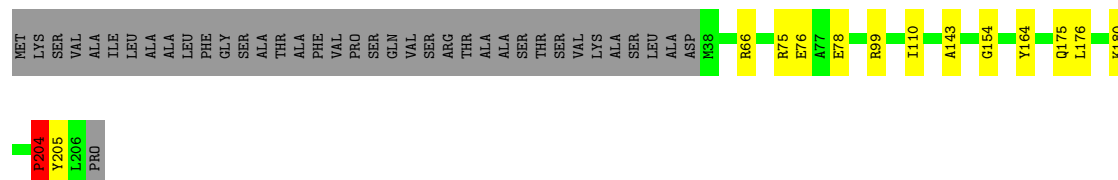
- Molecule 21: Fucoxanthin chlorophyll a/c-binding protein Lhcf6





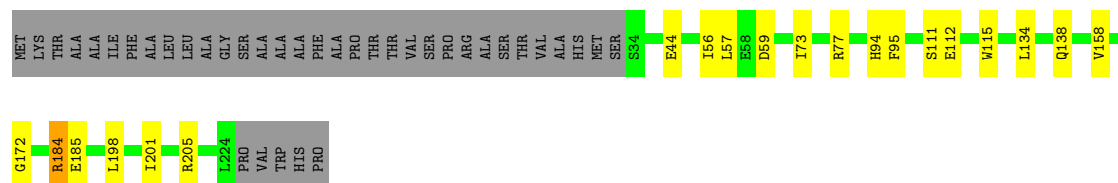
- Molecule 22: Fucoxanthin chlorophyll a/c-binding protein Lhc3

Chain 10: 75% 6% 18%



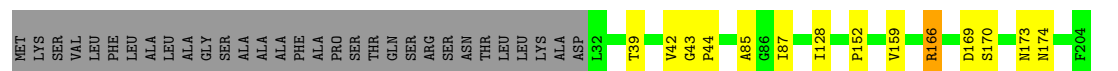
- Molecule 23: Fucoxanthin chlorophyll a/c-binding protein Lhcq13

Chain 11: 75% 8% 17%



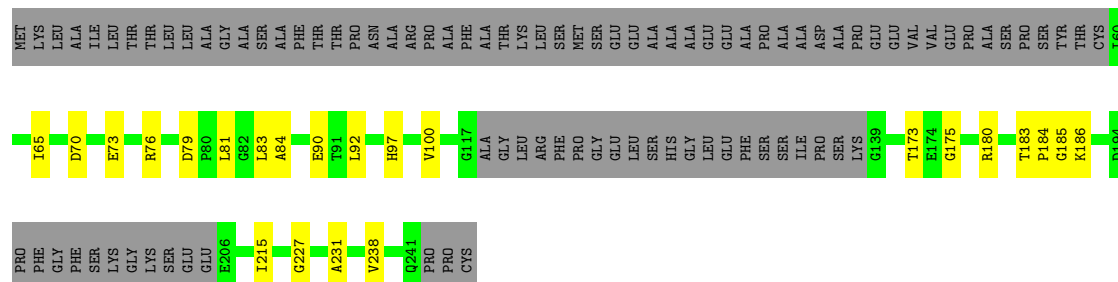
- Molecule 24: Fucoxanthin chlorophyll a/c-binding protein Lhcq3

Chain 12: 78% 6% 15%



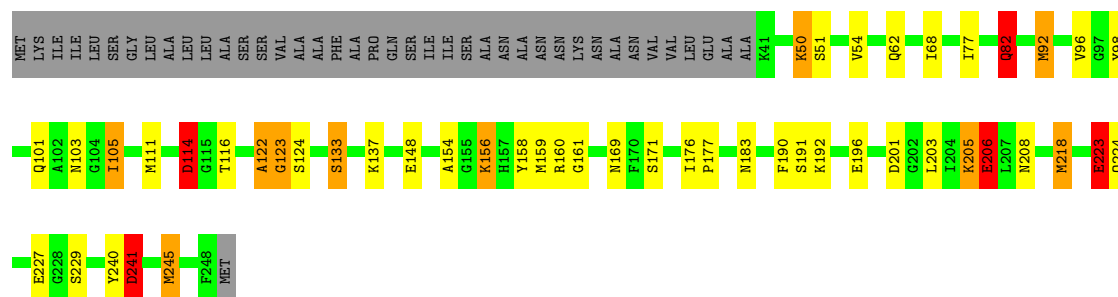
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcq11

Chain 13: 52% 9% 39%

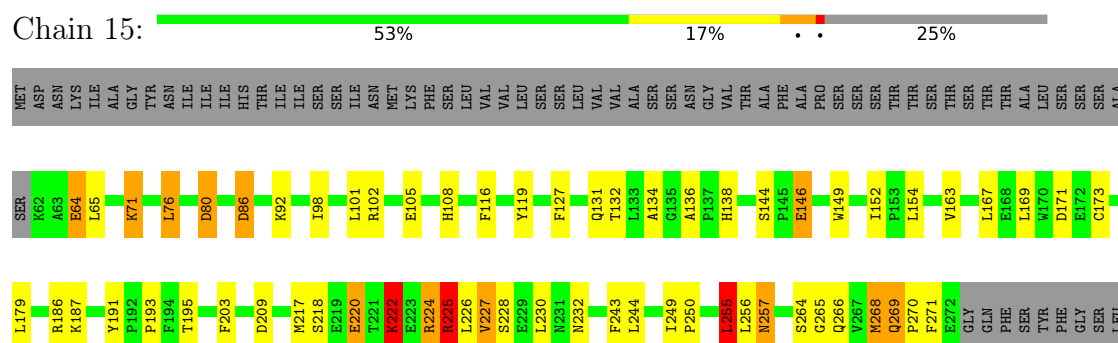


- Molecule 26: Fucoxanthin chlorophyll a/c-binding protein Lhcq10

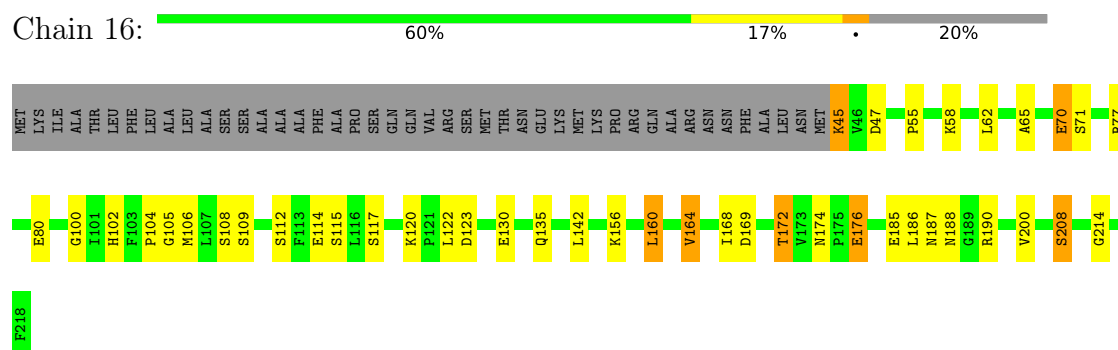
Chain 14: 63% 14% 16%



- Molecule 27: Fucoxanthin chlorophyll a/c-binding protein Lhcq8



- Molecule 28: Fucoxanthin chlorophyll a/c-binding protein Lhcq5



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	470801	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: KC1, PQN, DD6, LMG, A86, LMT, CLA, BCR, SF4, CL0, LHG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.39	0/6039	0.50	0/8220
2	B	0.38	0/6011	0.51	0/8209
3	C	0.44	0/609	0.63	1/826 (0.1%)
4	D	0.38	0/1064	0.62	0/1437
5	E	0.37	0/486	0.53	0/656
6	F	0.36	0/1287	0.50	0/1745
7	I	0.37	0/281	0.60	0/383
8	J	0.34	0/355	0.56	0/480
9	L	0.34	0/1054	0.49	0/1432
10	M	0.32	0/229	0.48	0/313
12	2u	0.32	0/696	0.45	0/948
13	1	0.30	0/1106	0.45	0/1490
14	2	0.35	0/1344	0.55	0/1818
15	3	0.32	0/1309	0.57	2/1767 (0.1%)
16	4	0.35	0/1404	0.51	0/1897
17	5	0.33	0/1336	0.52	0/1804
18	6	0.36	0/1391	0.48	0/1886
19	7	0.33	0/1445	0.48	0/1952
20	8	0.35	0/1706	0.49	0/2310
21	9	0.32	0/1302	0.54	1/1769 (0.1%)
22	10	0.32	0/1344	0.51	0/1824
23	11	0.30	0/1522	0.52	0/2070
24	12	0.32	0/1305	0.51	0/1776
25	13	0.31	0/1177	0.52	0/1592
26	14	0.55	4/1660 (0.2%)	1.29	23/2255 (1.0%)
27	15	0.61	2/1705 (0.1%)	1.46	33/2319 (1.4%)
28	16	0.48	1/1347 (0.1%)	0.98	12/1833 (0.7%)
All	All	0.38	7/40514 (0.0%)	0.65	72/55011 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1
11	1u	0	1
16	4	0	1
21	9	0	2
22	10	0	1
26	14	0	7
27	15	0	8
28	16	0	1
All	All	0	22

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	15	146	GLU	CB-CG	-10.73	1.31	1.52
28	16	70	GLU	CB-CG	-7.53	1.37	1.52
26	14	50	LYS	CD-CE	-6.61	1.34	1.51
26	14	206	GLU	CG-CD	-5.84	1.43	1.51
27	15	224	ARG	CB-CG	-5.79	1.36	1.52
26	14	227	GLU	CB-CG	-5.79	1.41	1.52
26	14	245	MET	CB-CG	-5.58	1.33	1.51

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	92	MET	CA-CB-CG	25.47	156.60	113.30
27	15	224	ARG	NE-CZ-NH1	-23.93	108.33	120.30
27	15	224	ARG	NE-CZ-NH2	22.70	131.65	120.30
27	15	146	GLU	CA-CB-CG	16.51	149.72	113.40
26	14	92	MET	CB-CG-SD	13.82	153.87	112.40
26	14	105	ILE	CG1-CB-CG2	-11.41	86.29	111.40
26	14	241	ASP	CB-CG-OD1	11.01	128.20	118.30
27	15	169	LEU	CB-CG-CD1	-10.09	93.85	111.00
26	14	241	ASP	CB-CG-OD2	-9.91	109.38	118.30
28	16	70	GLU	CA-CB-CG	9.74	134.83	113.40
27	15	269	GLN	CA-CB-CG	9.66	134.64	113.40
28	16	169	ASP	CB-CG-OD1	9.61	126.95	118.30
27	15	179	LEU	CB-CG-CD2	9.55	127.23	111.00
27	15	224	ARG	CD-NE-CZ	9.27	136.57	123.60
27	15	92	LYS	CD-CE-NZ	9.04	132.50	111.70
26	14	227	GLU	CA-CB-CG	8.99	133.18	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	15	225	ARG	CD-NE-CZ	8.79	135.91	123.60
26	14	245	MET	CG-SD-CE	-8.75	86.19	100.20
26	14	206	GLU	CA-CB-CG	8.56	132.23	113.40
27	15	71	LYS	CD-CE-NZ	8.53	131.33	111.70
28	16	214	GLY	C-N-CA	8.51	142.98	121.70
28	16	164	VAL	CG1-CB-CG2	-8.22	97.75	110.90
26	14	156	LYS	CB-CG-CD	-8.13	90.47	111.60
26	14	206	GLU	CG-CD-OE2	-7.72	102.86	118.30
26	14	206	GLU	OE1-CD-OE2	-7.60	114.18	123.30
27	15	255	LEU	CB-CG-CD2	7.42	123.61	111.00
26	14	92	MET	CB-CA-C	7.27	124.95	110.40
28	16	70	GLU	N-CA-CB	7.18	123.52	110.60
28	16	123	ASP	CB-CG-OD1	-7.13	111.88	118.30
28	16	176	GLU	CA-CB-CG	7.02	128.84	113.40
26	14	156	LYS	CD-CE-NZ	-6.98	95.65	111.70
27	15	203	PHE	CB-CG-CD2	-6.91	115.97	120.80
27	15	179	LEU	CA-CB-CG	6.86	131.08	115.30
26	14	218	MET	CG-SD-CE	6.77	111.04	100.20
28	16	160	LEU	CB-CG-CD1	6.60	122.21	111.00
15	3	77	ARG	NE-CZ-NH1	6.55	123.57	120.30
27	15	222	LYS	CB-CA-C	-6.36	97.68	110.40
21	9	118	LEU	CA-CB-CG	6.32	129.83	115.30
26	14	96	VAL	CG1-CB-CG2	-6.31	100.81	110.90
15	3	77	ARG	NE-CZ-NH2	-6.30	117.15	120.30
27	15	225	ARG	CB-CG-CD	-6.23	95.40	111.60
27	15	154	LEU	CB-CG-CD2	-6.17	100.52	111.00
27	15	92	LYS	CA-CB-CG	6.09	126.80	113.40
26	14	156	LYS	CA-CB-CG	5.95	126.48	113.40
27	15	209	ASP	CB-CG-OD1	5.94	123.65	118.30
26	14	114	ASP	CB-CA-C	-5.94	98.53	110.40
27	15	76	LEU	CB-CG-CD2	-5.92	100.94	111.00
27	15	224	ARG	CB-CG-CD	5.89	126.93	111.60
28	16	142	LEU	CB-CG-CD2	5.87	120.97	111.00
27	15	257	ASN	N-CA-CB	-5.79	100.18	110.60
27	15	98	ILE	CG1-CB-CG2	-5.75	98.75	111.40
26	14	227	GLU	CB-CA-C	5.74	121.89	110.40
27	15	203	PHE	CB-CG-CD1	5.74	124.82	120.80
28	16	123	ASP	CB-CG-OD2	5.71	123.44	118.30
27	15	152	ILE	C-N-CD	-5.65	108.17	120.60
27	15	102	ARG	CG-CD-NE	-5.50	100.26	111.80
26	14	218	MET	CB-CG-SD	5.47	128.80	112.40
26	14	223	GLU	CA-CB-CG	-5.40	101.53	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	15	220	GLU	CB-CA-C	-5.35	99.71	110.40
27	15	225	ARG	CG-CD-NE	5.31	122.95	111.80
27	15	86	ASP	CB-CG-OD1	5.30	123.07	118.30
27	15	225	ARG	NE-CZ-NH2	-5.28	117.66	120.30
28	16	168	ILE	C-N-CA	5.26	134.84	121.70
27	15	209	ASP	CB-CG-OD2	-5.24	113.58	118.30
27	15	265	GLY	N-CA-C	5.21	126.14	113.10
27	15	86	ASP	CB-CG-OD2	-5.21	113.61	118.30
27	15	271	PHE	N-CA-CB	5.15	119.87	110.60
3	C	62	PHE	C-N-CA	5.15	134.56	121.70
26	14	116	THR	CA-CB-CG2	5.12	119.56	112.40
26	14	122	ALA	C-N-CA	5.10	133.01	122.30
26	14	82	GLN	CB-CG-CD	5.08	124.82	111.60
28	16	45	LYS	CB-CG-CD	5.08	124.80	111.60

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	10	204	PRO	Peptide
26	14	123	GLY	Peptide
26	14	124	SER	Peptide
26	14	154	ALA	Peptide
26	14	161	GLY	Peptide
26	14	206	GLU	Sidechain
26	14	223	GLU	Sidechain
26	14	241	ASP	Sidechain
27	15	119	TYR	Sidechain
27	15	136	ALA	Peptide
27	15	225	ARG	Sidechain
27	15	257	ASN	Sidechain
27	15	264	SER	Peptide
27	15	268	MET	Peptide
27	15	270	PRO	Peptide
27	15	64	GLU	Sidechain
28	16	130	GLU	Sidechain
11	1u	97	UNK	Peptide
16	4	145	HIS	Sidechain
21	9	109	GLY	Peptide
21	9	113	ALA	Peptide
4	D	91	GLU	Peptide

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	5841	0	5666	71	0
2	B	5801	0	5614	50	0
3	C	599	0	579	6	0
4	D	1037	0	1023	10	0
5	E	478	0	473	2	0
6	F	1257	0	1259	11	0
7	I	273	0	285	1	0
8	J	344	0	351	10	0
9	L	1030	0	1063	11	0
10	M	227	0	247	2	0
11	1u	650	0	138	0	0
12	2u	674	0	658	0	0
13	1	1086	0	1089	13	0
14	2	1310	0	1287	13	0
15	3	1275	0	1239	9	0
16	4	1368	0	1344	8	0
17	5	1304	0	1286	10	0
18	6	1354	0	1328	13	0
19	7	1416	0	1379	8	0
20	8	1660	0	1625	16	0
21	9	1267	0	1210	12	0
22	10	1302	0	1274	8	0
23	11	1479	0	1452	16	0
24	12	1274	0	1267	10	0
25	13	1148	0	1130	16	0
26	14	1609	0	1568	22	0
27	15	1654	0	1613	21	0
28	16	1313	0	1309	22	0
29	A	65	0	72	3	0
30	1	390	0	425	12	0
30	10	435	0	465	7	0
30	11	315	0	337	11	0
30	12	566	0	604	12	0
30	13	350	0	354	11	0
30	14	468	0	400	8	0
30	15	685	0	589	16	0
30	16	478	0	429	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	2	620	0	649	16	0
30	2u	65	0	72	0	0
30	3	472	0	474	8	0
30	4	484	0	495	14	0
30	5	455	0	499	12	0
30	6	620	0	656	13	0
30	7	566	0	609	14	0
30	8	420	0	427	8	0
30	9	486	0	503	12	0
30	A	2614	0	2694	105	0
30	B	2465	0	2570	91	0
30	F	175	0	177	9	0
30	J	45	0	33	1	0
30	L	110	0	105	7	0
31	A	33	0	46	5	0
31	B	33	0	46	1	0
32	A	8	0	0	0	0
32	C	16	0	0	0	0
33	2u	40	0	56	0	0
33	A	200	0	280	13	0
33	B	240	0	336	12	0
33	F	40	0	56	3	0
33	I	40	0	56	2	0
33	J	80	0	112	7	0
33	L	120	0	168	10	0
33	M	40	0	56	3	0
34	2	27	0	24	0	0
34	5	27	0	24	1	0
34	6	27	0	24	0	0
34	9	34	0	38	0	0
34	A	76	0	98	2	0
34	B	27	0	24	0	0
35	1	35	0	46	0	0
35	11	140	0	184	5	0
35	12	140	0	184	4	0
35	15	35	0	46	0	0
35	16	35	0	46	0	0
35	6	31	0	35	2	0
35	7	70	0	91	2	0
35	8	35	0	46	0	0
35	9	32	0	37	0	0
35	A	105	0	138	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	B	70	0	92	0	0
36	14	38	0	46	2	0
36	2u	31	0	31	0	0
36	3	37	0	44	2	0
36	5	33	0	36	0	0
36	6	33	0	34	1	0
36	7	37	0	44	0	0
36	8	108	0	123	1	0
36	A	34	0	38	2	0
36	B	98	0	141	3	0
36	F	27	0	24	0	0
37	1	48	0	0	0	0
37	10	240	0	0	0	0
37	11	192	0	0	2	0
37	12	96	0	0	0	0
37	13	93	0	0	0	0
37	14	384	0	0	2	0
37	15	336	0	0	0	0
37	16	96	0	0	0	0
37	2	144	0	0	0	0
37	2u	96	0	0	0	0
37	3	96	0	0	0	0
37	4	192	0	0	1	0
37	5	144	0	0	1	0
37	6	48	0	0	0	0
37	7	144	0	0	1	0
37	8	96	0	0	1	0
37	9	144	0	0	1	0
38	1	90	0	0	0	0
38	10	135	0	0	0	0
38	11	180	0	0	0	0
38	12	180	0	0	1	0
38	13	270	0	0	0	0
38	14	135	0	0	0	0
38	16	90	0	0	1	0
38	2	135	0	0	0	0
38	3	135	0	0	1	0
38	4	135	0	0	1	0
38	5	180	0	0	2	0
38	6	180	0	0	0	0
38	7	90	0	0	0	0
38	8	315	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	9	180	0	0	0	0
39	1	43	0	0	0	0
39	10	86	0	0	1	0
39	11	43	0	0	0	0
39	12	86	0	0	0	0
39	13	43	0	0	1	0
39	15	86	0	0	0	0
39	16	43	0	0	0	0
39	2	129	0	0	0	0
39	3	129	0	0	0	0
39	4	86	0	0	0	0
39	5	86	0	0	0	0
39	6	172	0	0	3	0
39	7	172	0	0	0	0
39	8	86	0	0	0	0
39	9	43	0	0	0	0
40	1	1	0	0	0	0
40	10	1	0	0	0	0
40	11	1	0	0	0	0
40	12	2	0	0	0	0
40	2	2	0	0	0	0
40	3	1	0	0	0	0
40	5	1	0	0	0	0
40	6	2	0	0	0	0
40	7	2	0	0	0	0
40	8	4	0	0	0	0
40	9	1	0	0	0	0
40	A	42	0	0	2	0
40	B	53	0	0	0	0
40	C	15	0	0	0	0
40	D	13	0	0	0	0
40	E	3	0	0	0	0
40	F	3	0	0	0	0
40	I	1	0	0	0	0
40	L	8	0	0	0	0
All	All	62199	0	55344	644	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 6.

All (644) 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)
26:14:101:GLN:OE1	30:14:303:CLA:NA	2.01	0.94
23:11:44:GLU:OE1	30:11:310:CLA:NC	2.10	0.84
25:13:73:GLU:OE1	30:13:307:CLA:NC	2.11	0.83
27:15:105:GLU:OE1	30:15:302:CLA:NB	2.21	0.74
30:B:815:CLA:HBB1	33:B:841:BCR:H333	1.74	0.70
2:B:202:ARG:HG3	2:B:249:ALA:HB1	1.73	0.70
30:4:306:CLA:H42	30:4:306:CLA:HAA1	1.76	0.68
30:A:810:CLA:HBB1	33:J:102:BCR:HC7	1.76	0.68
30:A:802:CLA:H201	30:B:809:CLA:H2	1.75	0.68
27:15:127:PHE:O	27:15:138:HIS:NE2	2.26	0.67
4:D:42:GLU:H	4:D:72:GLN:HE22	1.41	0.66
2:B:402:ASN:HD22	2:B:405:ASN:HD21	1.43	0.66
21:9:59:ILE:O	21:9:86:ARG:NH2	2.29	0.66
30:3:302:CLA:HAC1	30:3:310:CLA:HAB	1.78	0.65
9:L:38:ARG:O	9:L:46:ARG:NH1	2.31	0.64
16:4:126:ALA:HB2	30:4:309:CLA:HBB1	1.79	0.64
30:A:843:CLA:H122	33:L:204:BCR:H19C	1.81	0.63
30:B:806:CLA:H162	30:B:827:CLA:HBB2	1.79	0.63
30:B:803:CLA:H13	33:I:101:BCR:H281	1.79	0.63
28:16:77:ARG:HG3	28:16:160:LEU:HD21	1.80	0.63
13:1:83:ALA:O	13:1:104:ARG:NH2	2.32	0.62
21:9:86:ARG:NH1	21:9:89:GLU:OE1	2.33	0.62
30:16:302:CLA:H202	30:16:302:CLA:HBB1	1.80	0.62
18:6:127:ILE:HB	30:6:314:CLA:HBC1	1.81	0.61
13:1:104:ARG:NH1	13:1:107:GLU:OE1	2.33	0.61
14:2:138:TRP:HB3	30:2:301:CLA:H2	1.81	0.61
18:6:73:ARG:NH2	18:6:76:GLU:OE1	2.33	0.61
15:3:123:LEU:HB2	30:3:310:CLA:HBC1	1.82	0.61
13:1:188:LYS:HE3	13:1:192:GLU:HG3	1.81	0.61
28:16:55:PRO:HB3	30:16:307:CLA:HBB1	1.82	0.61
30:A:834:CLA:H142	33:B:846:BCR:H15C	1.82	0.61
26:14:224:GLN:HB3	26:14:240:TYR:HB3	1.81	0.61
30:A:816:CLA:HBB1	33:A:847:BCR:H333	1.83	0.61
3:C:73:THR:H	3:C:76:SER:HB3	1.66	0.61
22:10:75:ARG:NH2	22:10:78:GLU:OE1	2.34	0.61
27:15:217:MET:SD	27:15:225:ARG:NH2	2.74	0.60
17:5:84:ARG:NH1	17:5:87:GLU:OE1	2.34	0.60
30:B:836:CLA:HBC3	30:4:301:CLA:HAC1	1.83	0.60
20:8:58:MET:SD	20:8:58:MET:N	2.75	0.60
30:A:802:CLA:H13	33:B:846:BCR:H10C	1.83	0.60
30:A:822:CLA:HMB2	30:A:826:CLA:HMA3	1.83	0.60
25:13:84:ALA:HB2	30:13:301:CLA:HBA1	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:734:LEU:HD22	30:A:842:CLA:HMA1	1.83	0.60
30:B:825:CLA:H112	33:B:844:BCR:H17C	1.83	0.60
23:11:56:ILE:HG13	23:11:57:LEU:HG	1.84	0.60
30:A:806:CLA:H12	30:A:807:CLA:HBB1	1.84	0.59
20:8:128:ARG:NH1	20:8:131:GLU:OE1	2.35	0.59
26:14:245:MET:HG2	30:14:312:CLA:HBB1	1.85	0.59
30:7:309:CLA:H52	25:13:83:LEU:HD22	1.84	0.59
30:B:811:CLA:HAA2	13:1:96:ILE:HD13	1.85	0.58
26:14:101:GLN:OE1	30:14:303:CLA:C1A	2.50	0.58
27:15:232:ASN:ND2	30:15:309:CLA:OBD	2.36	0.58
2:B:337:LEU:HD21	30:B:828:CLA:HAB	1.85	0.58
14:2:72:ARG:NH1	30:2:303:CLA:O1D	2.37	0.58
30:B:809:CLA:H202	33:I:101:BCR:H353	1.85	0.58
1:A:715:GLN:NE2	5:E:16:TYR:OH	2.36	0.58
18:6:144:GLN:HA	18:6:148:GLU:HB2	1.86	0.58
23:11:134:LEU:O	23:11:138:GLN:NE2	2.37	0.58
14:2:91:ALA:HB1	14:2:96:LEU:HD23	1.86	0.57
30:A:842:CLA:H172	8:J:23:ALA:HB2	1.86	0.57
20:8:89:LEU:HB3	20:8:128:ARG:HH21	1.70	0.57
30:B:819:CLA:HMB2	30:B:823:CLA:HMA3	1.87	0.57
17:5:125:VAL:HG11	30:5:304:CLA:HAA2	1.86	0.57
30:A:804:CLA:H203	30:A:804:CLA:H101	1.86	0.57
1:A:30:ALA:HB1	8:J:6:LYS:HD2	1.88	0.56
30:A:842:CLA:H101	8:J:16:THR:HG23	1.88	0.56
30:A:839:CLA:H203	30:L:202:CLA:H171	1.88	0.56
30:7:309:CLA:H92	30:7:309:CLA:H2	1.87	0.56
20:8:187:LEU:HG	30:8:303:CLA:H12	1.88	0.56
36:A:856:LMG:HC62	8:J:3:ASN:HD22	1.71	0.56
2:B:15:ASP:HB3	2:B:20:ARG:HB2	1.87	0.56
26:14:98:TYR:OH	26:14:224:GLN:NE2	2.36	0.56
3:C:15:THR:OG1	3:C:19:ARG:NH1	2.39	0.56
28:16:135:GLN:OE1	38:16:304:KC1:ND	2.39	0.56
30:13:301:CLA:H71	30:13:302:CLA:HMA1	1.88	0.56
1:A:540:ALA:HB1	30:A:839:CLA:HMB3	1.88	0.55
30:A:816:CLA:H8	33:A:848:BCR:H402	1.88	0.55
2:B:56:ILE:HD11	33:M:101:BCR:HC7	1.88	0.55
30:F:202:CLA:HED2	30:5:303:CLA:H93	1.88	0.55
17:5:57:PRO:HB3	17:5:70:ASP:HB3	1.89	0.55
36:8:319:LMG:HC8	36:8:321:LMG:H292	1.88	0.55
28:16:185:GLU:OE1	30:16:306:CLA:NA	2.39	0.55
6:F:158:TYR:HE1	30:5:307:CLA:HMB2	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:TRP:HB3	30:A:806:CLA:HAC1	1.88	0.55
30:A:804:CLA:H11	30:F:201:CLA:HMB2	1.89	0.55
20:8:264:ASN:ND2	20:8:270:PHE:O	2.39	0.55
26:14:208:ASN:ND2	30:14:307:CLA:O1D	2.39	0.55
30:B:811:CLA:H171	30:1:303:CLA:H121	1.87	0.55
27:15:191:TYR:HB2	30:15:308:CLA:HMD1	1.89	0.55
20:8:61:ARG:HH22	22:10:143:ALA:HB1	1.70	0.55
18:6:118:LEU:HB3	18:6:123:ALA:HB3	1.89	0.55
2:B:721:ALA:HB2	30:B:826:CLA:HBB1	1.87	0.55
18:6:98:ARG:NH2	18:6:109:LEU:O	2.40	0.55
1:A:121:ILE:O	1:A:123:GLY:N	2.40	0.54
2:B:190:THR:HG21	2:B:277:LEU:HB2	1.89	0.54
30:B:806:CLA:H102	30:B:806:CLA:H172	1.89	0.54
30:A:810:CLA:HAB	30:B:831:CLA:HMD2	1.89	0.54
2:B:584:ASN:HB2	30:B:802:CLA:HBC2	1.89	0.54
1:A:60:ASP:N	1:A:60:ASP:OD1	2.40	0.54
1:A:540:ALA:HB2	30:A:839:CLA:HMA1	1.90	0.54
4:D:62:ARG:NH2	4:D:64:GLU:OE2	2.39	0.54
26:14:159:MET:O	26:14:160:ARG:NH2	2.40	0.54
30:B:821:CLA:HHC	30:B:839:CLA:HED1	1.89	0.54
21:9:135:LEU:HA	21:9:138:VAL:HB	1.90	0.54
6:F:117:ILE:HG23	30:F:202:CLA:HAA1	1.90	0.54
18:6:165:LEU:HD22	18:6:173:VAL:HG12	1.89	0.54
2:B:180:GLY:HA3	30:B:813:CLA:HBB1	1.90	0.54
30:B:804:CLA:H2	33:M:101:BCR:HC21	1.91	0.54
1:A:151:GLU:HG2	1:A:213:TRP:HH2	1.73	0.53
30:A:836:CLA:H2	33:A:851:BCR:H383	1.91	0.53
28:16:80:GLU:OE1	30:16:301:CLA:NA	2.41	0.53
6:F:155:THR:HG21	30:5:303:CLA:HED2	1.91	0.53
30:B:838:CLA:HAC2	33:B:846:BCR:H23C	1.91	0.53
25:13:70:ASP:OD1	25:13:70:ASP:N	2.40	0.53
25:13:183:THR:HG22	25:13:185:GLY:H	1.74	0.53
30:A:811:CLA:H172	30:A:813:CLA:H203	1.89	0.53
4:D:85:ARG:HB3	4:D:93:GLN:HB2	1.90	0.53
25:13:173:THR:HG22	25:13:175:GLY:H	1.73	0.53
36:A:856:LMG:H142	35:6:302:LMT:H2'	1.91	0.53
14:2:87:VAL:HG12	30:2:305:CLA:HBC2	1.91	0.53
17:5:75:SER:HB3	30:5:302:CLA:HBA1	1.91	0.53
19:7:124:ASP:OD1	19:7:124:ASP:N	2.42	0.53
30:7:306:CLA:HHC	30:7:306:CLA:HBB1	1.91	0.53
1:A:336:GLU:HG2	1:A:424:ASN:HB3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:11:318:LMT:H51	35:12:301:LMT:H62	1.91	0.52
33:B:845:BCR:H381	30:F:201:CLA:HMC2	1.91	0.52
15:3:152:PHE:HB2	30:3:306:CLA:HMD1	1.91	0.52
1:A:501:ASN:HB2	30:A:837:CLA:HED2	1.91	0.52
2:B:173:ARG:HB2	30:B:813:CLA:HBC2	1.90	0.52
2:B:541:ARG:NH2	4:D:125:ASN:OD1	2.39	0.52
1:A:363:LEU:HD11	30:A:820:CLA:H71	1.89	0.52
30:A:805:CLA:HAB	30:A:812:CLA:H121	1.91	0.52
36:3:317:LMG:HC91	30:4:311:CLA:HAB	1.92	0.52
13:1:75:PRO:HB2	13:1:78:LEU:HB2	1.92	0.52
30:7:309:CLA:H122	30:13:301:CLA:H8	1.90	0.52
1:A:572:ARG:NH2	34:A:852:LHG:O2	2.42	0.52
2:B:66:PHE:HZ	10:M:7:VAL:HG13	1.75	0.52
23:11:158:VAL:HG22	35:11:303:LMT:H42	1.92	0.52
26:14:148:GLU:OE1	30:14:305:CLA:NA	2.43	0.52
30:A:820:CLA:HAB	30:A:820:CLA:H8	1.92	0.52
30:A:829:CLA:H161	30:A:842:CLA:H43	1.92	0.51
2:B:298:HIS:HB3	2:B:303:ILE:HD11	1.92	0.51
16:4:139:GLU:OE1	37:4:315:A86:O2	2.26	0.51
27:15:171:ASP:OD1	27:15:186:ARG:NH1	2.43	0.51
1:A:403:THR:HG21	1:A:596:LEU:HG	1.93	0.51
20:8:84:ASN:ND2	20:8:101:SER:O	2.43	0.51
23:11:205:ARG:NH2	30:11:304:CLA:O1D	2.42	0.51
30:A:832:CLA:H42	30:9:308:CLA:H52	1.91	0.51
2:B:720:TYR:HB2	30:B:801:CLA:HED3	1.92	0.51
30:A:817:CLA:H2	30:A:817:CLA:HBD	1.92	0.51
30:B:806:CLA:H143	30:B:827:CLA:HBB2	1.92	0.51
4:D:116:ARG:HH22	4:D:138:GLU:HB2	1.75	0.51
13:1:101:THR:HG23	13:1:175:PRO:HG3	1.92	0.51
16:4:40:GLU:OE1	16:4:186:LYS:NZ	2.44	0.51
28:16:65:ALA:HB2	30:16:301:CLA:HBA1	1.93	0.51
30:A:813:CLA:H121	33:A:849:BCR:H343	1.93	0.51
14:2:54:ASP:HA	30:2:303:CLA:CGD	2.38	0.51
18:6:157:PHE:HB2	30:6:309:CLA:HMD1	1.91	0.51
22:10:176:LEU:HG	22:10:180:LYS:HE2	1.92	0.51
30:A:828:CLA:HMB3	30:A:836:CLA:H12	1.93	0.51
30:A:823:CLA:HMD2	33:A:847:BCR:H23C	1.92	0.51
30:A:833:CLA:H171	33:L:205:BCR:H333	1.92	0.51
30:B:817:CLA:H122	30:B:817:CLA:HMC2	1.92	0.51
36:6:301:LMG:HC92	30:6:316:CLA:HMB2	1.93	0.51
1:A:128:ASN:HB3	1:A:136:GLN:HB3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:833:CLA:H142	30:L:202:CLA:HAA2	1.92	0.51
18:6:45:TYR:OH	18:6:55:ASP:OD2	2.29	0.51
23:11:44:GLU:OE1	30:11:310:CLA:C4C	2.59	0.51
23:11:94:HIS:HB3	30:11:306:CLA:HED3	1.93	0.51
27:15:227:VAL:HG13	30:15:309:CLA:HED2	1.92	0.51
19:7:152:ARG:NH2	19:7:155:GLU:OE1	2.42	0.50
1:A:748:SER:HA	1:A:751:ILE:HG12	1.93	0.50
30:B:826:CLA:HBC3	36:B:847:LMG:H421	1.93	0.50
17:5:172:LEU:HD22	30:5:308:CLA:H11	1.93	0.50
1:A:396:TRP:HB3	30:A:829:CLA:HMC3	1.93	0.50
30:A:804:CLA:HHC	30:A:804:CLA:HBB1	1.94	0.50
2:B:523:ALA:HB2	30:B:835:CLA:HMA1	1.94	0.50
30:B:807:CLA:H92	30:B:807:CLA:HMC2	1.93	0.50
23:11:115:TRP:O	35:11:317:LMT:O6'	2.29	0.50
30:B:824:CLA:HBB1	30:B:836:CLA:HHB	1.94	0.50
17:5:176:LYS:HB3	17:5:180:GLU:HG3	1.93	0.50
30:A:821:CLA:HHC	30:A:821:CLA:HBB1	1.94	0.50
30:B:813:CLA:H112	30:B:818:CLA:H93	1.94	0.50
21:9:163:LEU:HD13	30:9:301:CLA:H91	1.94	0.50
9:L:36:ALA:HB2	30:L:202:CLA:HMD1	1.94	0.50
2:B:291:ARG:NH1	2:B:295:GLY:O	2.44	0.50
30:7:303:CLA:H142	30:7:304:CLA:H161	1.93	0.50
30:A:841:CLA:HBB1	30:F:201:CLA:HMD1	1.93	0.49
27:15:193:PRO:HB2	27:15:195:THR:HG23	1.94	0.49
30:A:803:CLA:H91	31:A:845:PQN:H292	1.94	0.49
22:10:164:TYR:OH	22:10:175:GLN:NE2	2.44	0.49
1:A:470:ASP:OD1	9:L:69:ARG:NH2	2.45	0.49
30:B:827:CLA:H202	33:B:843:BCR:H17C	1.93	0.49
18:6:98:ARG:HB3	18:6:102:LEU:HD13	1.94	0.49
20:8:236:MET:HE1	30:8:305:CLA:H43	1.94	0.49
21:9:206:ASN:HD22	21:9:210:GLN:HG3	1.77	0.49
1:A:282:LEU:HD21	1:A:375:PRO:HD2	1.93	0.49
1:A:547:VAL:HG11	30:A:840:CLA:HMB3	1.94	0.49
21:9:118:LEU:HG	21:9:128:GLN:HB2	1.93	0.49
28:16:208:SER:HB3	30:16:309:CLA:C4D	2.42	0.49
1:A:411:ILE:HD13	30:A:831:CLA:HED3	1.93	0.49
30:A:817:CLA:H41	35:A:855:LMT:H6D	1.95	0.49
23:11:198:LEU:HD23	30:11:310:CLA:HED2	1.95	0.49
2:B:181:LEU:HD13	30:B:813:CLA:HHB	1.94	0.49
25:13:73:GLU:OE1	30:13:307:CLA:C1C	2.61	0.49
26:14:54:VAL:HG12	36:14:321:LMG:HC92	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ILE:HD13	33:J:103:BCR:H313	1.94	0.49
30:10:305:CLA:H202	30:10:308:CLA:HMD2	1.95	0.49
1:A:396:TRP:CD1	30:A:829:CLA:HAB	2.47	0.49
9:L:143:LEU:HG	30:L:203:CLA:HED3	1.94	0.49
2:B:188:ALA:HA	30:B:815:CLA:HAB	1.95	0.48
2:B:340:LEU:HB3	2:B:381:LEU:HD13	1.95	0.48
13:1:187:ASN:ND2	13:1:192:GLU:OE2	2.46	0.48
22:10:76:GLU:OE1	22:10:154:GLY:N	2.40	0.48
26:14:101:GLN:OE1	30:14:303:CLA:C4A	2.62	0.48
30:A:806:CLA:H72	33:A:849:BCR:H23C	1.94	0.48
27:15:222:LYS:O	27:15:226:LEU:N	2.43	0.48
23:11:77:ARG:NH1	23:11:172:GLY:O	2.47	0.48
1:A:217:GLN:HA	1:A:221:ALA:HB3	1.95	0.48
30:A:839:CLA:H201	30:L:202:CLA:H102	1.95	0.48
30:B:807:CLA:HBB1	30:B:807:CLA:H111	1.96	0.48
4:D:40:ILE:HG12	4:D:50:ILE:HG12	1.95	0.48
20:8:257:GLN:NE2	37:8:315:A86:O2	2.45	0.48
1:A:737:ILE:HG21	30:A:829:CLA:HMC2	1.95	0.48
1:A:580:ARG:NH1	40:A:908:HOH:O	2.45	0.48
30:B:805:CLA:HBA1	30:B:805:CLA:H3A	1.74	0.48
30:B:817:CLA:HBC1	30:B:819:CLA:H193	1.96	0.48
36:B:849:LMG:H132	36:B:849:LMG:H301	1.96	0.48
13:1:86:ARG:NH2	13:1:198:GLU:OE2	2.44	0.48
27:15:228:SER:O	27:15:232:ASN:ND2	2.47	0.48
1:A:574:PRO:HB3	1:A:721:ILE:HB	1.96	0.47
8:J:20:THR:HG22	33:J:103:BCR:H15C	1.95	0.47
1:A:197:MET:HE2	30:A:814:CLA:HBC2	1.97	0.47
26:14:68:ILE:O	37:14:317:A86:O2	2.32	0.47
26:14:82:GLN:HG2	26:14:158:TYR:CD1	2.49	0.47
27:15:80:ASP:HB3	30:15:302:CLA:HBA2	1.96	0.47
30:15:307:CLA:HHC	30:15:307:CLA:HBB1	1.96	0.47
1:A:289:LEU:HD21	1:A:374:MET:HB3	1.97	0.47
30:B:831:CLA:H61	30:B:831:CLA:H41	1.69	0.47
14:2:177:LYS:HD2	30:2:310:CLA:HBD	1.96	0.47
28:16:122:LEU:HD11	28:16:200:VAL:HG12	1.96	0.47
20:8:270:PHE:HA	30:8:308:CLA:HED2	1.95	0.47
23:11:59:ASP:OD2	23:11:59:ASP:N	2.43	0.47
2:B:449:GLU:OE1	6:F:76:ARG:NE	2.42	0.47
30:A:829:CLA:H121	30:A:831:CLA:H18	1.97	0.47
30:A:839:CLA:H191	30:L:202:CLA:H72	1.96	0.47
14:2:53:GLY:HA2	14:2:176:LEU:HD13	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:7:311:CLA:H162	30:7:311:CLA:H122	1.67	0.47
28:16:187:ASN:HA	28:16:190:ARG:HD2	1.97	0.47
30:6:307:CLA:H61	30:6:307:CLA:H41	1.64	0.47
30:7:309:CLA:H52	30:7:309:CLA:H8	1.60	0.47
28:16:187:ASN:HA	28:16:190:ARG:HB2	1.95	0.47
30:A:833:CLA:H111	33:L:205:BCR:H312	1.97	0.47
17:5:187:LYS:NZ	38:5:310:KC1:O1A	2.39	0.47
30:A:836:CLA:H41	30:A:836:CLA:H62	1.73	0.47
30:B:808:CLA:H141	30:B:808:CLA:HBA2	1.96	0.47
30:B:851:CLA:H13	30:2:307:CLA:HBB1	1.97	0.47
24:12:39:THR:HG21	24:12:173:ASN:HD21	1.79	0.47
30:B:827:CLA:H3A	30:B:827:CLA:HBA2	1.64	0.46
4:D:23:ALA:HB1	4:D:28:LYS:HD2	1.97	0.46
13:1:205:ARG:NH2	30:1:301:CLA:O1D	2.47	0.46
30:12:310:CLA:H162	30:12:310:CLA:H122	1.69	0.46
1:A:538:ILE:HD12	29:A:801:CL0:H63	1.97	0.46
2:B:421:LEU:HD13	2:B:531:LEU:HA	1.97	0.46
30:B:811:CLA:HBA2	30:1:302:CLA:H52	1.98	0.46
15:3:93:ARG:HH12	15:3:104:ILE:HB	1.79	0.46
1:A:220:ILE:HG23	1:A:240:PRO:HB3	1.96	0.46
31:A:845:PQN:H141	30:F:201:CLA:HBB2	1.98	0.46
18:6:198:ALA:HA	18:6:208:VAL:HG12	1.97	0.46
25:13:97:HIS:ND1	25:13:184:PRO:O	2.49	0.46
26:14:51:SER:HB2	26:14:208:ASN:HD21	1.81	0.46
2:B:526:LEU:HD12	30:B:836:CLA:HED3	1.98	0.46
18:6:206:PRO:O	39:6:318:DD6:O2	2.33	0.46
26:14:114:ASP:OD2	26:14:114:ASP:N	2.45	0.46
30:B:806:CLA:HMB2	30:B:828:CLA:HBB2	1.96	0.46
30:B:830:CLA:H18	33:F:204:BCR:H17C	1.97	0.46
3:C:4:THR:HB	3:C:68:TYR:HB2	1.98	0.46
30:13:307:CLA:HHC	30:13:307:CLA:HBB1	1.97	0.46
1:A:508:TYR:HB2	1:A:523:MET:HG3	1.97	0.46
30:A:810:CLA:H152	30:A:812:CLA:H152	1.97	0.46
30:A:834:CLA:H161	30:B:838:CLA:HBA2	1.98	0.46
30:B:806:CLA:H41	30:B:806:CLA:H61	1.68	0.46
30:B:828:CLA:H192	30:B:838:CLA:H3A	1.98	0.46
30:B:838:CLA:H18	7:I:20:ALA:HB2	1.98	0.46
1:A:226:LYS:HG2	1:A:253:LEU:HD22	1.98	0.46
2:B:237:ASP:HB2	2:B:268:TRP:HZ3	1.81	0.46
30:2:303:CLA:HBA2	30:2:303:CLA:H3A	1.45	0.46
30:8:302:CLA:HMB1	30:8:302:CLA:HBB1	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:11:304:CLA:H41	30:11:304:CLA:H61	1.62	0.46
28:16:164:VAL:HG23	30:16:310:CLA:HED2	1.97	0.46
30:7:309:CLA:H162	25:13:81:LEU:HD11	1.98	0.46
35:12:320:LMT:H91	35:12:320:LMT:H62	1.79	0.46
1:A:370:HIS:ND1	30:A:819:CLA:OBD	2.49	0.46
30:A:804:CLA:H162	30:A:804:CLA:H122	1.72	0.46
2:B:350:HIS:ND1	30:B:817:CLA:OBD	2.46	0.46
30:B:835:CLA:H152	33:F:204:BCR:H23C	1.97	0.46
30:1:307:CLA:H162	30:1:307:CLA:H122	1.73	0.46
24:12:169:ASP:HB2	30:12:308:CLA:HED2	1.96	0.46
30:A:835:CLA:HHD	30:B:809:CLA:HBB2	1.98	0.45
9:L:41:LEU:HD21	30:9:302:CLA:HED1	1.97	0.45
14:2:78:HIS:CD2	30:2:307:CLA:HMD1	2.51	0.45
21:9:72:GLY:HA3	22:10:66:ARG:HB3	1.98	0.45
28:16:188:ASN:ND2	30:16:307:CLA:OBD	2.49	0.45
1:A:413:MET:O	1:A:558:ARG:NH1	2.39	0.45
1:A:719:LEU:HD21	31:A:845:PQN:H151	1.99	0.45
2:B:132:GLN:NE2	10:M:1:MET:O	2.46	0.45
25:13:65:ILE:HG21	25:13:92:LEU:HG	1.98	0.45
26:14:183:ASN:O	37:14:320:A86:O2	2.35	0.45
1:A:363:LEU:HD21	30:A:820:CLA:H93	1.98	0.45
2:B:307:HIS:HA	30:B:839:CLA:HMD1	1.97	0.45
14:2:43:PRO:HG3	15:3:146:GLU:HG3	1.98	0.45
19:7:134:ASP:OD1	37:7:315:A86:O2	2.33	0.45
37:9:316:A86:O2	37:9:316:A86:O	2.35	0.45
24:12:170:SER:O	24:12:174:ASN:ND2	2.42	0.45
1:A:289:LEU:HB2	1:A:294:ILE:HD11	1.98	0.45
30:A:826:CLA:H143	30:A:826:CLA:H111	1.82	0.45
6:F:156:THR:HG22	17:5:150:THR:HB	1.98	0.45
30:A:802:CLA:HBB1	30:A:802:CLA:HMB1	1.99	0.45
2:B:524:LEU:HD21	30:B:802:CLA:HBB1	1.99	0.45
6:F:31:LYS:NZ	6:F:81:SER:O	2.50	0.45
14:2:102:PRO:HG2	14:2:105:LEU:HD12	1.98	0.45
30:3:305:CLA:H61	30:3:305:CLA:H41	1.64	0.45
30:5:307:CLA:HBA2	30:5:307:CLA:H3A	1.65	0.45
24:12:159:VAL:HG13	26:14:62:GLN:HB2	1.97	0.45
9:L:75:LEU:HG	9:L:140:LEU:HD12	1.98	0.45
13:1:189:SER:OG	13:1:190:GLU:N	2.49	0.45
30:4:302:CLA:H3A	30:4:302:CLA:HBA2	1.76	0.45
25:13:90:GLU:OE1	25:13:180:ARG:NH1	2.48	0.45
28:16:77:ARG:NH2	30:16:301:CLA:O1D	2.44	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLY:O	1:A:99:SER:OG	2.28	0.45
31:B:840:PQN:H222	31:B:840:PQN:H261	1.75	0.45
5:E:2:VAL:HG12	5:E:60:GLU:HG2	1.98	0.45
13:1:195:LYS:HA	13:1:198:GLU:HB2	1.98	0.45
30:4:306:CLA:HMB2	30:4:306:CLA:H72	1.98	0.45
30:15:313:CLA:H61	30:15:313:CLA:H41	1.74	0.45
28:16:104:PRO:HA	28:16:105:GLY:HA2	1.65	0.45
35:A:855:LMT:H32	30:6:316:CLA:HMD2	1.98	0.45
30:B:820:CLA:HMB1	30:B:820:CLA:HBB1	1.99	0.45
30:F:202:CLA:H71	30:F:202:CLA:H111	1.65	0.45
30:6:316:CLA:H8	30:6:316:CLA:H52	1.79	0.45
30:12:321:CLA:HHC	30:12:321:CLA:HBB1	1.99	0.45
28:16:102:HIS:NE2	28:16:114:GLU:HG2	2.32	0.45
33:A:847:BCR:H20C	33:A:847:BCR:H361	1.75	0.45
2:B:215:PRO:HA	2:B:216:PRO:HD3	1.90	0.45
30:12:308:CLA:H41	30:12:308:CLA:H62	1.79	0.45
30:A:809:CLA:H3A	30:A:809:CLA:HBA2	1.62	0.44
33:L:204:BCR:H20C	33:L:204:BCR:H361	1.78	0.44
15:3:99:TYR:OH	38:3:304:KC1:OBD	2.33	0.44
37:11:316:A86:O2	35:11:318:LMT:O6'	2.33	0.44
26:14:190:PHE:HA	26:14:191:SER:HA	1.72	0.44
1:A:389:SER:HB3	30:A:829:CLA:HMA1	1.99	0.44
16:4:180:TYR:CD2	30:4:306:CLA:H2	2.51	0.44
18:6:116:ASP:OD1	39:6:321:DD6:O2	2.35	0.44
37:11:315:A86:O3	35:11:317:LMT:O6'	2.35	0.44
27:15:132:THR:HG23	27:15:134:ALA:H	1.82	0.44
2:B:386:PHE:HZ	30:B:824:CLA:HAB	1.83	0.44
30:1:304:CLA:HBA2	30:1:304:CLA:H3A	1.78	0.44
16:4:167:GLY:HA3	16:4:168:LEU:HG	1.99	0.44
19:7:119:ARG:HH21	19:7:121:PRO:HA	1.82	0.44
30:9:307:CLA:HBA2	30:9:307:CLA:H3A	1.61	0.44
1:A:121:ILE:HB	33:J:103:BCR:H322	1.99	0.44
1:A:686:PHE:HA	31:A:845:PQN:H9	1.99	0.44
30:A:835:CLA:H152	33:L:201:BCR:H372	1.98	0.44
33:L:205:BCR:H323	30:9:306:CLA:HBA1	1.99	0.44
25:13:231:ALA:HA	25:13:238:VAL:HB	2.00	0.44
27:15:167:LEU:HD23	30:15:313:CLA:H43	2.00	0.44
30:15:303:CLA:HHC	30:15:303:CLA:HBB1	1.99	0.44
30:A:812:CLA:H111	30:A:812:CLA:H72	1.80	0.44
30:B:833:CLA:HBA2	30:B:833:CLA:H3A	1.65	0.44
30:4:306:CLA:H141	30:4:306:CLA:H162	1.86	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:13:79:ASP:OD2	39:13:314:DD6:O4	2.36	0.44
27:15:255:LEU:HA	27:15:256:LEU:HA	1.71	0.44
1:A:215:GLY:HA3	30:A:816:CLA:HAB	1.99	0.44
30:A:826:CLA:HBA1	30:A:830:CLA:H193	2.00	0.44
2:B:49:SER:HB2	30:B:805:CLA:HBB1	1.99	0.44
14:2:138:TRP:CE3	30:2:307:CLA:HHB	2.53	0.44
15:3:40:VAL:O	15:3:69:ARG:NH2	2.39	0.44
30:10:303:CLA:HBA2	30:10:303:CLA:H3A	1.75	0.44
24:12:166:ARG:NH2	38:12:309:KC1:OBD	2.51	0.44
30:5:302:CLA:H102	30:5:303:CLA:HMB3	1.98	0.44
21:9:131:THR:HA	21:9:134:TRP:HB2	2.00	0.44
30:9:307:CLA:H112	30:9:307:CLA:H71	1.70	0.44
23:11:184:ARG:HD3	23:11:185:GLU:HG2	1.99	0.44
30:11:308:CLA:H41	30:11:308:CLA:H92	1.99	0.44
33:A:850:BCR:H20C	33:A:850:BCR:H361	1.78	0.44
8:J:28:GLU:OE1	8:J:31:ARG:NH2	2.51	0.44
15:3:67:TRP:HB2	36:3:317:LMG:HC61	1.99	0.44
16:4:180:TYR:CG	30:4:306:CLA:H2	2.53	0.44
38:4:310:KC1:O1A	17:5:132:GLN:NE2	2.50	0.44
37:5:315:A86:O2	37:5:315:A86:O	2.36	0.44
27:15:149:TRP:NE1	27:15:266:GLN:O	2.49	0.44
1:A:297:HIS:HE2	30:A:820:CLA:C2B	2.31	0.43
1:A:465:LEU:HG	30:B:809:CLA:HMC3	1.99	0.43
30:A:813:CLA:H41	30:A:813:CLA:H62	1.80	0.43
30:A:814:CLA:H41	30:A:814:CLA:H61	1.80	0.43
2:B:344:THR:HB	2:B:378:ALA:HB2	2.00	0.43
30:B:813:CLA:H42	33:B:842:BCR:H19C	2.00	0.43
6:F:144:ILE:HG12	8:J:10:THR:HG22	2.00	0.43
9:L:41:LEU:HB3	9:L:46:ARG:HG2	2.00	0.43
13:1:212:THR:HG22	30:1:307:CLA:HBC2	2.00	0.43
30:9:307:CLA:H61	30:9:307:CLA:H41	1.70	0.43
1:A:409:ALA:HB1	33:A:850:BCR:HC42	2.00	0.43
26:14:82:GLN:HG2	26:14:158:TYR:CG	2.52	0.43
28:16:58:LYS:HE2	28:16:58:LYS:HB3	1.68	0.43
1:A:169:MET:HG3	33:A:848:BCR:H322	2.00	0.43
30:A:821:CLA:H41	30:A:821:CLA:H62	1.63	0.43
30:B:837:CLA:H62	30:B:837:CLA:H41	1.83	0.43
6:F:90:ASP:OD2	6:F:90:ASP:N	2.45	0.43
28:16:186:LEU:O	28:16:190:ARG:N	2.50	0.43
1:A:86:LEU:HD22	30:A:810:CLA:H202	2.00	0.43
1:A:349:TRP:CD1	30:A:826:CLA:H202	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:4:305:CLA:H62	30:4:305:CLA:H41	1.68	0.43
30:A:810:CLA:H42	33:J:102:BCR:H21C	2.01	0.43
30:2:304:CLA:H2	30:2:304:CLA:HED2	2.01	0.43
30:10:303:CLA:H112	30:10:303:CLA:H151	1.68	0.43
30:10:309:CLA:H101	30:10:309:CLA:H62	1.73	0.43
1:A:51:ASN:ND2	40:A:909:HOH:O	2.50	0.43
1:A:393:HIS:CE1	30:A:829:CLA:ND	2.86	0.43
1:A:419:PRO:HG2	4:D:42:GLU:HB2	2.01	0.43
2:B:376:TYR:CD1	30:B:826:CLA:HAB	2.54	0.43
30:B:838:CLA:H62	30:B:838:CLA:H41	1.72	0.43
30:9:305:CLA:H91	30:9:305:CLA:H112	1.81	0.43
30:15:313:CLA:H122	30:15:313:CLA:H162	1.88	0.43
28:16:172:THR:HG22	28:16:174:ASN:H	1.83	0.43
1:A:268:HIS:NE2	35:A:857:LMT:O5B	2.47	0.43
30:B:824:CLA:H172	30:4:301:CLA:HBC1	2.00	0.43
23:11:95:PHE:N	30:11:306:CLA:OBD	2.48	0.43
24:12:85:ALA:HB3	24:12:87:ILE:HD12	2.00	0.43
30:16:301:CLA:H142	30:16:301:CLA:H112	1.85	0.43
1:A:566:LYS:NZ	2:B:672:GLU:OE2	2.47	0.43
30:A:833:CLA:H111	30:A:833:CLA:H91	1.91	0.43
19:7:211:ILE:HG21	30:7:306:CLA:HMC3	2.00	0.43
1:A:80:GLN:HB2	30:A:806:CLA:HMB2	2.00	0.43
1:A:200:HIS:CG	30:A:814:CLA:HMC2	2.54	0.43
1:A:631:ILE:HD13	1:A:751:ILE:HD12	2.01	0.43
29:A:801:CL0:C1A	30:B:801:CLA:HAB	2.49	0.43
30:A:830:CLA:HHC	30:A:830:CLA:HBB1	2.00	0.43
2:B:579:MET:HG3	2:B:709:LEU:HD21	2.01	0.43
30:B:804:CLA:H41	33:L:204:BCR:HC32	2.01	0.43
30:B:837:CLA:H52	30:B:838:CLA:H93	2.00	0.43
33:B:845:BCR:H361	33:B:845:BCR:H20C	1.77	0.43
30:3:303:CLA:H92	30:3:303:CLA:H61	1.84	0.43
30:16:301:CLA:H143	30:16:301:CLA:H161	1.88	0.43
30:7:311:CLA:H61	35:7:321:LMT:H42	2.01	0.43
20:8:170:THR:OG1	20:8:173:GLU:OE1	2.29	0.43
22:10:99:ARG:HH12	22:10:110:ILE:HG13	1.83	0.43
1:A:245:ILE:HG22	35:7:301:LMT:H51	2.01	0.42
29:A:801:CL0:H11	30:B:801:CLA:HAA1	2.01	0.42
30:A:841:CLA:H172	6:F:125:GLY:HA2	2.00	0.42
3:C:29:VAL:HG12	4:D:110:ARG:HB3	2.01	0.42
4:D:28:LYS:HB3	4:D:86:ILE:HB	2.01	0.42
30:6:309:CLA:H91	30:6:309:CLA:H112	1.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:11:308:CLA:H162	30:11:308:CLA:H122	1.68	0.42
24:12:174:ASN:ND2	30:12:308:CLA:OBD	2.52	0.42
30:A:811:CLA:H112	30:A:811:CLA:H72	1.75	0.42
30:2:311:CLA:H141	30:3:303:CLA:H171	2.00	0.42
18:6:111:ALA:O	39:6:319:DD6:O2	2.37	0.42
30:12:303:CLA:H2	30:12:303:CLA:HED3	2.01	0.42
30:13:307:CLA:H41	30:13:307:CLA:H62	1.86	0.42
27:15:64:GLU:HG2	27:15:65:LEU:N	2.33	0.42
1:A:589:TRP:CD1	30:A:831:CLA:HMD1	2.54	0.42
30:A:829:CLA:H143	30:A:829:CLA:H112	1.85	0.42
31:A:845:PQN:H18	31:A:845:PQN:H222	1.79	0.42
2:B:181:LEU:HD21	30:B:813:CLA:H12	2.00	0.42
30:B:806:CLA:H51	30:B:828:CLA:H92	2.01	0.42
30:3:301:CLA:H61	30:3:301:CLA:H41	1.91	0.42
30:12:312:CLA:H193	30:12:312:CLA:H161	1.89	0.42
28:16:108:SER:OG	28:16:109:SER:N	2.53	0.42
30:A:824:CLA:H52	30:A:824:CLA:H11	1.77	0.42
2:B:298:HIS:CE1	30:B:820:CLA:NA	2.87	0.42
30:B:812:CLA:HAC2	30:1:302:CLA:H13	2.01	0.42
30:2:308:CLA:HBA2	30:2:308:CLA:H3A	1.67	0.42
30:5:304:CLA:H3A	30:5:304:CLA:HBA2	1.74	0.42
30:6:314:CLA:H41	30:6:314:CLA:H62	1.57	0.42
26:14:133:SER:O	26:14:137:LYS:HE3	2.19	0.42
1:A:397:ILE:HG21	30:A:830:CLA:HHC	2.02	0.42
1:A:584:CYS:HB2	2:B:666:TRP:HB3	2.02	0.42
30:A:833:CLA:H61	30:A:833:CLA:H41	1.69	0.42
33:A:849:BCR:H15C	33:A:849:BCR:H351	1.86	0.42
17:5:117:ASP:OD2	17:5:206:ASN:ND2	2.51	0.42
30:6:309:CLA:H92	30:6:309:CLA:H62	1.85	0.42
20:8:223:SER:HB2	20:8:226:LYS:HB2	2.00	0.42
35:12:319:LMT:H6E	35:12:319:LMT:H5B	2.01	0.42
30:B:834:CLA:HMB1	30:B:834:CLA:HBB1	2.01	0.42
33:F:204:BCR:H353	30:4:301:CLA:H2	2.01	0.42
8:J:12:PRO:HB2	33:J:103:BCR:H391	2.01	0.42
30:10:304:CLA:H2	30:10:304:CLA:HED3	2.02	0.42
1:A:684:LEU:HB2	30:A:803:CLA:HMC3	2.00	0.42
30:7:306:CLA:H3A	30:7:306:CLA:HBA1	1.82	0.42
30:7:307:CLA:HBA2	30:7:307:CLA:H3A	1.66	0.42
20:8:225:LEU:HD13	20:8:233:ILE:HG12	2.01	0.42
27:15:163:VAL:O	27:15:167:LEU:N	2.47	0.42
30:A:805:CLA:H2	30:A:812:CLA:H92	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:811:CLA:H203	30:A:811:CLA:H161	1.89	0.42
2:B:715:GLY:O	2:B:719:THR:OG1	2.27	0.42
30:1:304:CLA:H101	30:1:304:CLA:H62	1.91	0.42
14:2:84:LEU:HD22	30:2:305:CLA:H93	2.01	0.42
30:2:309:CLA:H41	30:2:309:CLA:H62	1.75	0.42
30:3:306:CLA:H142	30:3:306:CLA:H111	1.88	0.42
30:7:307:CLA:H151	30:13:302:CLA:H8	2.00	0.42
23:11:111:SER:OG	23:11:112:GLU:N	2.53	0.42
28:16:106:MET:HA	28:16:112:SER:HA	2.00	0.42
30:A:822:CLA:HBC3	30:A:828:CLA:H193	2.02	0.42
2:B:91:ILE:HB	2:B:111:PRO:HB2	2.01	0.42
30:B:816:CLA:HBA2	30:B:816:CLA:H3A	1.70	0.42
33:B:844:BCR:H24C	33:B:844:BCR:H371	1.84	0.42
3:C:66:ARG:HA	3:C:66:ARG:HD2	1.86	0.42
30:F:201:CLA:H101	8:J:14:LEU:HD22	2.01	0.42
14:2:180:LYS:HD3	30:2:309:CLA:CAD	2.50	0.42
15:3:83:VAL:HG23	15:3:186:ILE:HD12	2.02	0.42
35:6:302:LMT:O3'	35:6:302:LMT:O2B	2.36	0.42
20:8:228:LYS:HB3	20:8:232:GLU:HG3	2.02	0.42
22:10:204:PRO:O	39:10:313:DD6:O2	2.36	0.42
26:14:122:ALA:H	26:14:123:GLY:HA2	1.83	0.42
30:A:805:CLA:HMC3	30:A:807:CLA:HED3	2.02	0.42
30:A:820:CLA:HBA2	30:A:820:CLA:H3A	1.88	0.42
30:A:829:CLA:H91	30:A:831:CLA:H192	2.02	0.42
8:J:31:ARG:NH2	30:J:101:CLA:O1D	2.53	0.42
30:2:303:CLA:H61	30:2:303:CLA:H41	1.88	0.42
19:7:187:LYS:HA	19:7:187:LYS:HD3	1.86	0.42
24:12:128:ILE:HG13	30:12:310:CLA:HMA1	2.02	0.42
30:15:304:CLA:H3A	30:15:304:CLA:HBA2	1.86	0.42
30:A:820:CLA:HAB	30:A:820:CLA:H111	2.01	0.41
30:B:834:CLA:HMB2	30:B:836:CLA:HED1	2.02	0.41
27:15:105:GLU:HA	27:15:108:HIS:HB2	2.00	0.41
1:A:44:LYS:HE3	1:A:44:LYS:HB2	1.81	0.41
1:A:59:PHE:CD1	30:A:806:CLA:HMC2	2.55	0.41
2:B:271:ASP:HB3	30:B:817:CLA:HMA1	2.02	0.41
2:B:480:PRO:HA	2:B:485:THR:HG21	2.02	0.41
30:B:830:CLA:H62	30:B:830:CLA:H2	1.75	0.41
25:13:183:THR:HB	25:13:186:LYS:HD3	2.00	0.41
30:13:301:CLA:H91	30:13:301:CLA:H112	1.85	0.41
30:15:302:CLA:H102	30:15:303:CLA:H61	2.01	0.41
2:B:141:LEU:HD21	33:B:843:BCR:H24C	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:476:LEU:O	2:B:485:THR:OG1	2.38	0.41
38:5:312:KC1:C4D	34:5:317:LHG:HC81	2.50	0.41
19:7:156:ILE:HG21	19:7:234:GLY:HA3	2.02	0.41
27:15:101:LEU:HD23	27:15:101:LEU:HA	1.89	0.41
30:15:313:CLA:HMA2	30:15:313:CLA:H2	2.03	0.41
28:16:100:GLY:O	28:16:102:HIS:ND1	2.51	0.41
9:L:89:LEU:HB3	33:L:204:BCR:H401	2.02	0.41
33:L:201:BCR:H20C	33:L:201:BCR:H361	1.86	0.41
30:L:203:CLA:HBA1	30:L:203:CLA:H3A	1.82	0.41
30:11:304:CLA:H3A	30:11:304:CLA:HBA2	1.82	0.41
30:12:302:CLA:H61	30:12:302:CLA:H41	1.65	0.41
1:A:710:PHE:HB3	6:F:126:ARG:HG3	2.03	0.41
30:A:833:CLA:HAA1	9:L:22:THR:HG22	2.02	0.41
33:A:849:BCR:H20C	33:A:849:BCR:H361	1.84	0.41
30:B:835:CLA:H142	30:B:835:CLA:H112	1.93	0.41
33:J:102:BCR:H15C	33:J:102:BCR:H351	1.90	0.41
24:12:152:PRO:HG3	30:12:321:CLA:H8	1.70	0.41
27:15:116:PHE:HE2	27:15:243:PHE:HE2	1.68	0.41
30:A:838:CLA:HBB1	30:A:838:CLA:HMB1	2.01	0.41
2:B:148:LEU:HD21	30:1:302:CLA:H201	2.01	0.41
2:B:261:HIS:HD2	2:B:264:THR:H	1.69	0.41
2:B:425:SER:HB3	2:B:528:VAL:HG22	2.01	0.41
30:5:302:CLA:H162	30:5:302:CLA:H122	1.81	0.41
30:8:305:CLA:H142	30:8:305:CLA:H112	1.85	0.41
21:9:145:GLU:OE1	30:9:307:CLA:NA	2.53	0.41
26:14:176:ILE:HA	26:14:177:PRO:HD3	1.86	0.41
36:14:321:LMG:HC71	27:15:173:CYS:SG	2.60	0.41
28:16:80:GLU:OE1	30:16:301:CLA:C4A	2.69	0.41
1:A:36:SER:HB3	1:A:39:LEU:HB2	2.02	0.41
1:A:393:HIS:HE2	30:A:830:CLA:C1B	2.34	0.41
30:A:819:CLA:HBA2	30:A:819:CLA:H3A	1.79	0.41
30:A:831:CLA:H142	30:A:831:CLA:H112	1.91	0.41
30:B:801:CLA:H102	30:B:801:CLA:H62	1.82	0.41
30:B:809:CLA:H101	30:B:826:CLA:H171	2.01	0.41
30:B:812:CLA:H121	30:B:812:CLA:H162	1.89	0.41
30:10:309:CLA:H41	30:10:309:CLA:H61	1.69	0.41
23:11:44:GLU:OE1	30:11:310:CLA:C1C	2.67	0.41
35:12:301:LMT:H71	35:12:301:LMT:H102	1.92	0.41
30:14:302:CLA:H3A	30:14:302:CLA:HBA2	1.86	0.41
30:A:817:CLA:H11	30:6:316:CLA:CGA	2.51	0.41
2:B:186:SER:OG	2:B:276:GLN:O	2.39	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:B:828:CLA:H142	36:B:847:LMG:H212	2.03	0.41
30:1:303:CLA:H143	30:1:303:CLA:H112	1.83	0.41
15:3:160:SER:OG	15:3:161:SER:N	2.52	0.41
30:10:303:CLA:H192	30:10:307:CLA:H203	2.03	0.41
30:13:301:CLA:HBA2	30:13:301:CLA:H3A	1.77	0.41
30:16:303:CLA:HMC1	30:16:303:CLA:H192	2.03	0.41
30:A:822:CLA:H101	33:A:851:BCR:H10C	2.02	0.41
30:B:806:CLA:H111	30:B:806:CLA:H72	1.79	0.41
30:B:808:CLA:H162	30:B:826:CLA:H201	2.03	0.41
16:4:156:LYS:NZ	30:4:311:CLA:OBD	2.54	0.41
30:5:303:CLA:H2	30:5:303:CLA:HED3	2.02	0.41
30:6:306:CLA:H3A	30:6:306:CLA:HBA2	1.83	0.41
30:6:316:CLA:C1C	30:6:316:CLA:H51	2.51	0.41
19:7:147:ASP:OD1	19:7:147:ASP:N	2.54	0.41
20:8:103:ILE:HA	20:8:104:PRO:HD3	1.91	0.41
30:8:302:CLA:H41	30:8:302:CLA:H61	1.71	0.41
21:9:97:MET:SD	30:9:308:CLA:HAB	2.61	0.41
24:12:43:GLY:HA2	24:12:44:PRO:HA	1.92	0.41
30:14:302:CLA:H62	30:14:302:CLA:H41	1.63	0.41
30:15:302:CLA:H93	30:15:302:CLA:H61	1.84	0.41
30:15:304:CLA:H111	30:15:304:CLA:H152	1.57	0.41
1:A:448:LEU:HB3	1:A:541:PHE:HB2	2.02	0.41
30:B:822:CLA:HMA1	30:B:839:CLA:CGD	2.51	0.41
9:L:41:LEU:HD23	9:L:41:LEU:HA	1.90	0.41
30:6:306:CLA:H93	30:6:306:CLA:H111	1.88	0.41
20:8:225:LEU:HA	20:8:228:LYS:HG3	2.02	0.41
1:A:331:GLY:N	34:A:853:LHG:HC32	2.36	0.40
30:A:829:CLA:H111	30:A:829:CLA:H72	1.77	0.40
30:A:843:CLA:H111	30:A:843:CLA:H72	1.93	0.40
2:B:40:GLU:HA	2:B:164:LEU:HD13	2.02	0.40
30:B:809:CLA:H111	30:B:809:CLA:H152	1.83	0.40
30:B:821:CLA:HBC2	30:B:822:CLA:HBA1	2.03	0.40
9:L:46:ARG:O	9:L:50:ILE:HG12	2.21	0.40
30:5:308:CLA:H203	30:5:308:CLA:H162	1.91	0.40
30:9:305:CLA:H161	30:9:305:CLA:H122	1.76	0.40
30:12:303:CLA:H151	30:12:303:CLA:H112	1.87	0.40
2:B:591:PHE:CE2	2:B:623:LEU:HD21	2.56	0.40
3:C:72:GLU:HB3	3:C:77:LEU:HG	2.04	0.40
33:M:101:BCR:H15C	33:M:101:BCR:H351	1.88	0.40
23:11:73:ILE:HG12	23:11:201:ILE:HG12	2.04	0.40
30:12:308:CLA:H142	30:12:308:CLA:H111	1.90	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:13:100:VAL:HG12	25:13:215:ILE:HG12	2.03	0.40
26:14:201:ASP:O	26:14:205:LYS:HG2	2.21	0.40
30:15:303:CLA:H72	30:15:303:CLA:H111	1.82	0.40
1:A:345:LEU:HB3	1:A:352:GLN:HE21	1.86	0.40
1:A:706:ASN:HB3	6:F:180:VAL:HG13	2.04	0.40
30:A:839:CLA:H92	30:A:839:CLA:H61	1.90	0.40
2:B:267:LEU:HD13	30:B:817:CLA:HMA2	2.02	0.40
30:B:809:CLA:H203	30:B:809:CLA:H161	1.88	0.40
33:B:846:BCR:H20C	33:B:846:BCR:H361	1.87	0.40
30:8:301:CLA:HBA2	30:8:301:CLA:H3A	1.71	0.40
30:8:303:CLA:H62	30:8:303:CLA:H41	1.80	0.40
30:B:813:CLA:H93	30:B:827:CLA:HBC1	2.02	0.40
30:B:816:CLA:H62	30:B:816:CLA:H41	1.79	0.40
33:L:205:BCR:H20C	33:L:205:BCR:H361	1.93	0.40
16:4:161:LEU:HB2	30:4:306:CLA:HMD1	2.03	0.40
21:9:123:LEU:HA	21:9:123:LEU:HD23	1.83	0.40
25:13:227:GLY:O	25:13:231:ALA:N	2.45	0.40
30:A:816:CLA:H71	30:A:816:CLA:H111	1.65	0.40
30:A:818:CLA:CHD	30:A:819:CLA:HBB2	2.51	0.40
30:A:844:CLA:H161	30:A:844:CLA:H121	1.94	0.40
30:B:811:CLA:H193	30:1:303:CLA:H61	2.03	0.40
30:B:835:CLA:HBB1	30:B:835:CLA:H72	2.02	0.40
30:B:838:CLA:H93	30:B:838:CLA:H111	1.95	0.40
30:F:201:CLA:H162	30:F:201:CLA:H122	1.80	0.40
13:1:79:ASP:OD1	13:1:79:ASP:N	2.54	0.40
30:1:301:CLA:C1B	30:1:301:CLA:H42	2.51	0.40
30:7:309:CLA:H62	30:13:302:CLA:H43	2.03	0.40
21:9:136:GLN:NE2	30:9:306:CLA:C4D	2.85	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%)	712 (96%)	25 (3%)	2 (0%)	37	51
2	B	729/733 (100%)	699 (96%)	29 (4%)	1 (0%)	48	65
3	C	78/81 (96%)	73 (94%)	3 (4%)	2 (3%)	4	4
4	D	129/139 (93%)	109 (84%)	18 (14%)	2 (2%)	8	11
5	E	58/67 (87%)	55 (95%)	3 (5%)	0	100	100
6	F	159/185 (86%)	152 (96%)	7 (4%)	0	100	100
7	I	33/36 (92%)	30 (91%)	3 (9%)	0	100	100
8	J	39/41 (95%)	39 (100%)	0	0	100	100
9	L	133/151 (88%)	128 (96%)	5 (4%)	0	100	100
10	M	28/30 (93%)	28 (100%)	0	0	100	100
12	2u	87/121 (72%)	87 (100%)	0	0	100	100
13	1	137/227 (60%)	130 (95%)	7 (5%)	0	100	100
14	2	170/205 (83%)	151 (89%)	19 (11%)	0	100	100
15	3	162/200 (81%)	151 (93%)	9 (6%)	2 (1%)	11	16
16	4	177/215 (82%)	167 (94%)	10 (6%)	0	100	100
17	5	167/266 (63%)	157 (94%)	10 (6%)	0	100	100
18	6	172/208 (83%)	167 (97%)	5 (3%)	0	100	100
19	7	186/296 (63%)	179 (96%)	7 (4%)	0	100	100
20	8	211/270 (78%)	203 (96%)	8 (4%)	0	100	100
21	9	161/214 (75%)	149 (92%)	12 (8%)	0	100	100
22	10	167/207 (81%)	157 (94%)	8 (5%)	2 (1%)	11	16
23	11	189/229 (82%)	173 (92%)	16 (8%)	0	100	100
24	12	171/204 (84%)	160 (94%)	11 (6%)	0	100	100
25	13	144/244 (59%)	133 (92%)	11 (8%)	0	100	100
26	14	206/249 (83%)	177 (86%)	29 (14%)	0	100	100
27	15	209/281 (74%)	171 (82%)	37 (18%)	1 (0%)	25	38
28	16	172/218 (79%)	157 (91%)	15 (9%)	0	100	100
All	All	5013/6068 (83%)	4694 (94%)	307 (6%)	12 (0%)	45	59

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	92	VAL
2	B	492	TRP
3	C	62	PHE
3	C	63	LEU
4	D	91	GLU
22	10	204	PRO
22	10	205	TYR
27	15	250	PRO
15	3	162	LYS
1	A	234	PRO
15	3	105	PRO

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	602/611 (98%)	601 (100%)	1 (0%)	92	97
2	B	592/593 (100%)	589 (100%)	3 (0%)	86	94
3	C	69/70 (99%)	66 (96%)	3 (4%)	25	42
4	D	111/119 (93%)	111 (100%)	0	100	100
5	E	51/58 (88%)	51 (100%)	0	100	100
6	F	132/153 (86%)	132 (100%)	0	100	100
7	I	29/29 (100%)	29 (100%)	0	100	100
8	J	37/37 (100%)	37 (100%)	0	100	100
9	L	107/121 (88%)	107 (100%)	0	100	100
10	M	24/24 (100%)	24 (100%)	0	100	100
12	2u	69/94 (73%)	69 (100%)	0	100	100
13	1	114/183 (62%)	113 (99%)	1 (1%)	75	88
14	2	134/154 (87%)	134 (100%)	0	100	100
15	3	128/154 (83%)	127 (99%)	1 (1%)	79	90
16	4	142/165 (86%)	142 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	5	137/228 (60%)	136 (99%)	1 (1%)	81	91
18	6	140/160 (88%)	140 (100%)	0	100	100
19	7	143/236 (61%)	143 (100%)	0	100	100
20	8	171/215 (80%)	171 (100%)	0	100	100
21	9	126/175 (72%)	125 (99%)	1 (1%)	79	90
22	10	133/161 (83%)	133 (100%)	0	100	100
23	11	154/181 (85%)	153 (99%)	1 (1%)	84	92
24	12	136/159 (86%)	134 (98%)	2 (2%)	60	77
25	13	112/184 (61%)	111 (99%)	1 (1%)	75	88
26	14	166/196 (85%)	145 (87%)	21 (13%)	3	4
27	15	171/231 (74%)	151 (88%)	20 (12%)	4	6
28	16	139/174 (80%)	127 (91%)	12 (9%)	8	14
All	All	4069/4865 (84%)	4001 (98%)	68 (2%)	56	75

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	278	PHE
2	B	179	SER
2	B	202	ARG
2	B	256	PHE
3	C	62	PHE
3	C	63	LEU
3	C	65	VAL
13	1	185	LEU
15	3	155	LYS
17	5	149	VAL
21	9	197	ILE
23	11	184	ARG
24	12	42	VAL
24	12	166	ARG
25	13	76	ARG
26	14	50	LYS
26	14	77	ILE
26	14	82	GLN
26	14	92	MET
26	14	103	ASN
26	14	105	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	14	111	MET
26	14	114	ASP
26	14	133	SER
26	14	156	LYS
26	14	169	ASN
26	14	171	SER
26	14	192	LYS
26	14	196	GLU
26	14	203	LEU
26	14	205	LYS
26	14	206	GLU
26	14	218	MET
26	14	223	GLU
26	14	229	SER
26	14	241	ASP
27	15	71	LYS
27	15	76	LEU
27	15	80	ASP
27	15	86	ASP
27	15	131	GLN
27	15	144	SER
27	15	146	GLU
27	15	187	LYS
27	15	218	SER
27	15	220	GLU
27	15	222	LYS
27	15	224	ARG
27	15	225	ARG
27	15	227	VAL
27	15	230	LEU
27	15	244	LEU
27	15	249	ILE
27	15	255	LEU
27	15	268	MET
27	15	269	GLN
28	16	45	LYS
28	16	47	ASP
28	16	62	LEU
28	16	70	GLU
28	16	71	SER
28	16	115	SER
28	16	117	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	16	120	LYS
28	16	156	LYS
28	16	172	THR
28	16	176	GLU
28	16	208	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	51	ASN
1	A	113	GLN
1	A	139	GLN
1	A	225	ASN
1	A	252	GLN
1	A	715	GLN
2	B	113	ASN
2	B	261	HIS
2	B	402	ASN
2	B	451	GLN
2	B	613	ASN
2	B	632	ASN
2	B	671	GLN
2	B	681	HIS
4	D	72	GLN
4	D	79	ASN
8	J	3	ASN
9	L	116	GLN
10	M	30	ASN
13	1	97	GLN
13	1	169	HIS
14	2	78	HIS
14	2	173	ASN
15	3	195	HIS
17	5	211	HIS
19	7	189	GLN
21	9	206	ASN
22	10	175	GLN
22	10	201	HIS
24	12	49	ASN
26	14	82	GLN
26	14	183	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	14	209	ASN
27	15	216	ASN
28	16	177	GLN
28	16	215	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

427 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	$\# Z > 2$
30	CLA	A	813	1	65,73,73	2.03	18 (27%)	76,113,113	2.68	27 (35%)
33	BCR	B	843	-	41,41,41	1.10	2 (4%)	56,56,56	1.26	6 (10%)
30	CLA	2	307	14	65,73,73	1.97	16 (24%)	76,113,113	2.62	27 (35%)
30	CLA	3	306	15	65,73,73	2.01	15 (23%)	76,113,113	2.65	29 (38%)
30	CLA	15	310	27	45,53,73	2.54	17 (37%)	52,89,113	3.22	23 (44%)
30	CLA	B	837	40	65,73,73	1.95	16 (24%)	76,113,113	2.68	26 (34%)
38	KC1	8	306	40	48,53,53	3.40	22 (45%)	55,89,89	3.75	27 (49%)
38	KC1	10	312	22	48,53,53	3.44	25 (52%)	55,89,89	3.83	28 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	12	310	40	65,73,73	1.98	16 (24%)	76,113,113	2.72	26 (34%)
38	KC1	2	314	40	48,53,53	3.43	24 (50%)	55,89,89	3.81	30 (54%)
30	CLA	A	824	1	51,59,73	2.23	17 (33%)	59,96,113	3.09	27 (45%)
38	KC1	2	312	14	48,53,53	3.42	25 (52%)	55,89,89	3.75	29 (52%)
30	CLA	7	310	19	65,73,73	2.02	16 (24%)	76,113,113	2.68	26 (34%)
39	DD6	9	314	-	39,45,45	6.65	22 (56%)	52,67,67	7.29	26 (50%)
30	CLA	A	834	1	65,73,73	1.96	17 (26%)	76,113,113	2.71	29 (38%)
30	CLA	A	843	40	65,73,73	1.94	16 (24%)	76,113,113	2.63	27 (35%)
30	CLA	14	302	26	65,73,73	2.05	16 (24%)	76,113,113	2.75	31 (40%)
39	DD6	12	315	30	39,45,45	6.70	22 (56%)	52,67,67	6.85	26 (50%)
39	DD6	2	316	-	39,45,45	6.62	22 (56%)	52,67,67	6.70	28 (53%)
30	CLA	1	301	13	65,73,73	2.00	17 (26%)	76,113,113	2.64	24 (31%)
37	A86	2	319	-	44,50,50	3.89	22 (50%)	51,76,76	7.61	18 (35%)
30	CLA	B	839	34	65,73,73	1.92	16 (24%)	76,113,113	2.86	27 (35%)
30	CLA	B	806	2	65,73,73	1.97	15 (23%)	76,113,113	2.67	27 (35%)
30	CLA	A	841	1	65,73,73	2.01	17 (26%)	76,113,113	2.62	28 (36%)
30	CLA	A	819	1	54,62,73	2.18	16 (29%)	62,99,113	2.95	27 (43%)
30	CLA	6	315	18	45,53,73	2.45	16 (35%)	52,89,113	3.17	24 (46%)
30	CLA	B	832	37,40	65,73,73	2.01	17 (26%)	76,113,113	2.69	28 (36%)
30	CLA	2	305	40	65,73,73	2.00	17 (26%)	76,113,113	2.77	28 (36%)
37	A86	5	301	-	44,50,50	4.06	24 (54%)	51,76,76	7.93	21 (41%)
39	DD6	3	312	-	39,45,45	6.71	23 (58%)	52,67,67	6.79	26 (50%)
33	BCR	L	204	-	41,41,41	1.09	1 (2%)	56,56,56	1.44	8 (14%)
34	LHG	5	317	30	26,26,48	0.84	1 (3%)	29,32,54	1.35	3 (10%)
38	KC1	12	313	24	48,53,53	3.45	22 (45%)	55,89,89	4.42	28 (50%)
30	CLA	J	101	8	45,53,73	2.42	17 (37%)	52,89,113	3.10	24 (46%)
37	A86	15	322	30	44,50,50	4.28	24 (54%)	51,76,76	8.43	21 (41%)
38	KC1	13	305	25	48,53,53	3.47	27 (56%)	55,89,89	3.85	31 (56%)
37	A86	2u	203	30	44,50,50	3.98	24 (54%)	51,76,76	8.18	21 (41%)
30	CLA	A	830	1	65,73,73	1.91	15 (23%)	76,113,113	2.61	29 (38%)
31	PQN	A	845	-	34,34,34	1.52	2 (5%)	42,45,45	1.10	3 (7%)
30	CLA	A	811	1	65,73,73	1.96	15 (23%)	76,113,113	2.70	25 (32%)
30	CLA	11	309	23	65,73,73	2.05	17 (26%)	76,113,113	2.70	28 (36%)
37	A86	16	314	-	44,50,50	4.12	23 (52%)	51,76,76	8.52	19 (37%)
30	CLA	A	802	40	65,73,73	1.97	15 (23%)	76,113,113	2.78	29 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	KC1	4	307	16	48,53,53	3.46	25 (52%)	55,89,89	3.70	29 (52%)
37	A86	14	301	26	44,50,50	4.10	23 (52%)	51,76,76	8.08	17 (33%)
38	KC1	13	306	25	48,53,53	3.47	26 (54%)	55,89,89	3.73	29 (52%)
30	CLA	14	312	37,26	45,53,73	2.47	16 (35%)	52,89,113	3.14	23 (44%)
30	CLA	A	842	1	65,73,73	1.97	17 (26%)	76,113,113	2.75	28 (36%)
30	CLA	B	810	2	65,73,73	1.95	17 (26%)	76,113,113	2.69	27 (35%)
38	KC1	5	312	17	48,53,53	3.38	23 (47%)	55,89,89	3.78	28 (50%)
30	CLA	1	305	40	65,73,73	2.06	18 (27%)	76,113,113	2.64	27 (35%)
33	BCR	J	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.19	6 (10%)
30	CLA	A	803	-	65,73,73	1.97	16 (24%)	76,113,113	2.68	30 (39%)
39	DD6	6	318	-	39,45,45	6.65	23 (58%)	52,67,67	6.55	29 (55%)
30	CLA	3	305	15	62,70,73	2.06	17 (27%)	72,109,113	2.74	30 (41%)
38	KC1	13	308	25	48,53,53	3.48	27 (56%)	55,89,89	3.91	29 (52%)
30	CLA	6	307	39,18	65,73,73	2.01	16 (24%)	76,113,113	2.57	30 (39%)
32	SF4	C	101	3	0,12,12	-	-	-	-	-
30	CLA	6	310	34	65,73,73	2.04	17 (26%)	76,113,113	2.62	26 (34%)
30	CLA	7	305	40,19	65,73,73	2.12	18 (27%)	76,113,113	2.78	29 (38%)
34	LHG	9	318	-	33,33,48	0.70	0	36,39,54	1.25	4 (11%)
30	CLA	12	304	24,39	65,73,73	2.04	18 (27%)	76,113,113	2.90	29 (38%)
30	CLA	16	307	-	46,54,73	2.44	17 (36%)	53,90,113	3.11	24 (45%)
39	DD6	5	313	-	39,45,45	6.74	23 (58%)	52,67,67	6.85	25 (48%)
37	A86	1	309	-	44,50,50	3.96	23 (52%)	51,76,76	8.68	21 (41%)
37	A86	7	315	-	44,50,50	3.90	23 (52%)	51,76,76	7.79	20 (39%)
30	CLA	A	814	1	60,68,73	2.06	16 (26%)	70,107,113	2.76	26 (37%)
35	LMT	11	303	-	36,36,36	0.40	0	47,47,47	0.84	0
39	DD6	8	317	-	39,45,45	6.64	22 (56%)	52,67,67	7.04	29 (55%)
33	BCR	L	201	-	41,41,41	1.15	2 (4%)	56,56,56	1.31	5 (8%)
30	CLA	A	826	40	65,73,73	1.99	18 (27%)	76,113,113	2.72	26 (34%)
30	CLA	14	305	26	50,58,73	2.32	16 (32%)	58,95,113	3.02	27 (46%)
38	KC1	8	312	38	48,53,53	3.43	24 (50%)	55,89,89	3.29	28 (50%)
30	CLA	12	302	24	65,73,73	2.00	17 (26%)	76,113,113	2.76	31 (40%)
30	CLA	B	831	2	58,66,73	2.10	16 (27%)	67,104,113	2.98	27 (40%)
37	A86	11	315	-	44,50,50	3.99	22 (50%)	51,76,76	7.49	22 (43%)
38	KC1	7	308	40	48,53,53	3.43	24 (50%)	55,89,89	3.70	28 (50%)
30	CLA	A	825	1	59,67,73	2.09	17 (28%)	68,105,113	2.76	26 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	BCR	M	101	-	41,41,41	1.11	3 (7%)	56,56,56	1.27	6 (10%)
39	DD6	7	314	-	39,45,45	6.64	21 (53%)	52,67,67	7.34	28 (53%)
30	CLA	9	301	34	65,73,73	1.99	17 (26%)	76,113,113	2.83	27 (35%)
30	CLA	A	829	30,1	65,73,73	1.99	17 (26%)	76,113,113	2.75	27 (35%)
35	LMT	A	854	-	36,36,36	0.45	0	47,47,47	1.19	5 (10%)
36	LMG	A	856	-	34,34,55	0.99	1 (2%)	42,42,63	1.19	3 (7%)
30	CLA	B	820	2	45,53,73	2.42	16 (35%)	52,89,113	3.39	22 (42%)
30	CLA	A	823	1	49,57,73	2.28	17 (34%)	55,93,113	3.16	26 (47%)
30	CLA	3	302	15	60,68,73	2.06	17 (28%)	70,107,113	2.78	30 (42%)
30	CLA	8	308	20	55,63,73	2.17	15 (27%)	64,101,113	2.92	27 (42%)
37	A86	2	318	-	44,50,50	4.04	23 (52%)	51,76,76	7.66	23 (45%)
30	CLA	7	303	19	65,73,73	1.95	15 (23%)	76,113,113	2.72	29 (38%)
30	CLA	B	830	2	65,73,73	1.93	17 (26%)	76,113,113	2.87	27 (35%)
34	LHG	6	322	30	26,26,48	0.88	1 (3%)	29,32,54	1.36	3 (10%)
30	CLA	B	816	2	55,63,73	2.12	16 (29%)	64,101,113	3.01	26 (40%)
37	A86	3	314	-	44,50,50	4.05	23 (52%)	51,76,76	8.17	19 (37%)
37	A86	14	319	30	44,50,50	4.09	22 (50%)	51,76,76	8.30	17 (33%)
30	CLA	A	805	30,1	59,67,73	2.11	15 (25%)	68,105,113	2.87	29 (42%)
30	CLA	3	303	15	65,73,73	2.09	18 (27%)	76,113,113	2.78	29 (38%)
39	DD6	1	310	-	39,45,45	6.70	23 (58%)	52,67,67	6.71	24 (46%)
38	KC1	6	308	18	48,53,53	3.36	23 (47%)	55,89,89	3.84	28 (50%)
30	CLA	10	309	22	65,73,73	2.05	17 (26%)	76,113,113	2.64	25 (32%)
30	CLA	A	809	30,1	65,73,73	1.97	17 (26%)	76,113,113	2.69	28 (36%)
30	CLA	14	313	26	46,54,73	2.42	16 (34%)	53,90,113	3.25	26 (49%)
30	CLA	4	311	16	50,58,73	2.33	17 (34%)	58,95,113	3.23	30 (51%)
33	BCR	B	842	-	41,41,41	1.07	2 (4%)	56,56,56	1.19	5 (8%)
37	A86	4	314	-	44,50,50	4.10	22 (50%)	51,76,76	8.17	22 (43%)
36	LMG	3	317	-	37,37,55	0.97	2 (5%)	45,45,63	1.42	7 (15%)
30	CLA	10	304	22	65,73,73	2.01	18 (27%)	76,113,113	2.66	26 (34%)
30	CLA	A	821	1	61,69,73	1.98	17 (27%)	71,108,113	2.73	28 (39%)
30	CLA	A	832	1	50,58,73	2.22	17 (34%)	58,95,113	3.05	28 (48%)
30	CLA	1	303	30,13	65,73,73	2.00	16 (24%)	76,113,113	2.69	27 (35%)
39	DD6	7	317	-	39,45,45	6.70	20 (51%)	52,67,67	6.69	29 (55%)
30	CLA	9	303	21	65,73,73	1.99	16 (24%)	76,113,113	2.69	27 (35%)
39	DD6	15	319	30	39,45,45	6.79	22 (56%)	52,67,67	6.92	30 (57%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	DD6	6	321	-	39,45,45	6.60	23 (58%)	52,67,67	6.79	28 (53%)
30	CLA	10	303	22	65,73,73	2.01	15 (23%)	76,113,113	2.64	26 (34%)
30	CLA	B	817	2	59,67,73	2.07	16 (27%)	68,105,113	2.94	26 (38%)
38	KC1	3	311	40	48,53,53	3.44	24 (50%)	55,89,89	3.97	27 (49%)
30	CLA	B	807	2	65,73,73	1.93	18 (27%)	76,113,113	2.77	28 (36%)
30	CLA	12	306	24	65,73,73	1.97	17 (26%)	76,113,113	2.59	27 (35%)
30	CLA	11	310	23	65,73,73	2.10	17 (26%)	76,113,113	2.66	28 (36%)
30	CLA	A	827	40	65,73,73	1.93	18 (27%)	76,113,113	2.90	29 (38%)
30	CLA	12	312	24	65,73,73	2.02	16 (24%)	76,113,113	2.69	27 (35%)
37	A86	4	317	-	44,50,50	3.99	23 (52%)	51,76,76	7.58	20 (39%)
38	KC1	9	311	21	48,53,53	3.47	25 (52%)	55,89,89	3.90	31 (56%)
39	DD6	7	302	-	39,45,45	6.75	24 (61%)	52,67,67	6.58	28 (53%)
37	A86	10	315	-	44,50,50	4.10	22 (50%)	51,76,76	8.25	16 (31%)
30	CLA	B	838	2	65,73,73	1.96	14 (21%)	76,113,113	2.72	26 (34%)
30	CLA	5	307	17	65,73,73	2.00	19 (29%)	76,113,113	2.68	30 (39%)
30	CLA	7	312	19	46,54,73	2.44	17 (36%)	53,90,113	3.12	24 (45%)
30	CLA	2	308	14	65,73,73	2.02	15 (23%)	76,113,113	2.71	27 (35%)
30	CLA	B	802	30,40	65,73,73	1.92	17 (26%)	76,113,113	2.87	29 (38%)
30	CLA	A	828	1	65,73,73	1.92	16 (24%)	76,113,113	2.84	28 (36%)
35	LMT	12	301	-	36,36,36	0.43	0	47,47,47	0.76	0
30	CLA	13	304	25	45,53,73	2.50	16 (35%)	52,89,113	3.22	25 (48%)
30	CLA	B	821	2	55,63,73	2.16	15 (27%)	64,101,113	2.84	27 (42%)
37	A86	14	320	-	44,50,50	4.14	23 (52%)	51,76,76	7.22	21 (41%)
30	CLA	7	311	19	65,73,73	2.00	17 (26%)	76,113,113	2.60	26 (34%)
37	A86	9	313	21	44,50,50	3.98	23 (52%)	51,76,76	7.51	20 (39%)
33	BCR	J	103	-	41,41,41	1.15	3 (7%)	56,56,56	1.16	5 (8%)
38	KC1	6	311	18	48,53,53	3.36	23 (47%)	55,89,89	3.98	30 (54%)
39	DD6	6	303	30	39,45,45	6.78	23 (58%)	52,67,67	6.69	28 (53%)
30	CLA	A	844	-	65,73,73	2.06	16 (24%)	76,113,113	2.61	29 (38%)
38	KC1	7	313	-	48,53,53	3.36	22 (45%)	55,89,89	3.79	30 (54%)
39	DD6	13	314	-	39,45,45	6.78	22 (56%)	52,67,67	7.25	31 (59%)
30	CLA	8	304	20	58,66,73	2.08	16 (27%)	67,104,113	3.00	32 (47%)
30	CLA	A	804	1	65,73,73	1.95	16 (24%)	76,113,113	2.74	28 (36%)
39	DD6	15	318	-	39,45,45	6.78	21 (53%)	52,67,67	6.98	31 (59%)
30	CLA	13	309	-	45,53,73	2.48	16 (35%)	52,89,113	3.22	24 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	B	828	2	65,73,73	2.02	18 (27%)	76,113,113	2.74	28 (36%)
30	CLA	15	307	27	50,58,73	2.32	18 (36%)	58,95,113	3.02	26 (44%)
30	CLA	A	808	1	51,59,73	2.22	16 (31%)	59,96,113	3.06	26 (44%)
30	CLA	10	308	22	65,73,73	2.01	16 (24%)	76,113,113	2.63	26 (34%)
30	CLA	12	308	40	65,73,73	2.02	18 (27%)	76,113,113	2.63	27 (35%)
30	CLA	9	307	21	65,73,73	1.99	16 (24%)	76,113,113	2.68	26 (34%)
30	CLA	14	304	26	45,53,73	2.48	16 (35%)	52,89,113	3.19	23 (44%)
30	CLA	B	823	40	54,62,73	2.16	17 (31%)	62,99,113	2.93	27 (43%)
30	CLA	B	826	2	65,73,73	1.96	18 (27%)	76,113,113	2.74	28 (36%)
30	CLA	1	307	13	65,73,73	2.05	18 (27%)	76,113,113	2.73	27 (35%)
38	KC1	11	312	-	48,53,53	3.44	24 (50%)	55,89,89	3.58	29 (52%)
30	CLA	15	303	30,37,27	60,68,73	2.11	17 (28%)	70,107,113	2.88	27 (38%)
30	CLA	B	803	-	65,73,73	1.91	17 (26%)	76,113,113	2.69	28 (36%)
33	BCR	B	841	-	41,41,41	1.13	2 (4%)	56,56,56	1.27	8 (14%)
30	CLA	3	310	15	45,53,73	2.40	17 (37%)	52,89,113	3.21	24 (46%)
30	CLA	8	302	20	65,73,73	2.02	18 (27%)	76,113,113	2.76	26 (34%)
30	CLA	8	305	20	65,73,73	1.99	18 (27%)	76,113,113	4.76	31 (40%)
30	CLA	A	815	1	65,73,73	2.03	16 (24%)	76,113,113	2.72	28 (36%)
37	A86	2	302	-	44,50,50	4.10	23 (52%)	51,76,76	8.41	18 (35%)
30	CLA	6	306	40	65,73,73	2.01	16 (24%)	76,113,113	2.70	27 (35%)
38	KC1	8	307	20	48,53,53	3.36	23 (47%)	55,89,89	3.88	30 (54%)
39	DD6	16	313	-	39,45,45	6.75	21 (53%)	52,67,67	7.13	30 (57%)
30	CLA	B	819	40	65,73,73	1.97	16 (24%)	76,113,113	2.43	28 (36%)
30	CLA	11	308	23	65,73,73	2.03	16 (24%)	76,113,113	2.66	27 (35%)
34	LHG	A	853	30	26,26,48	0.91	1 (3%)	29,32,54	1.29	3 (10%)
30	CLA	3	307	15	65,73,73	2.10	18 (27%)	76,113,113	2.64	26 (34%)
30	CLA	4	305	16	65,73,73	1.97	16 (24%)	76,113,113	2.69	27 (35%)
39	DD6	12	317	-	39,45,45	6.67	22 (56%)	52,67,67	7.20	28 (53%)
30	CLA	F	203	6	45,53,73	2.41	17 (37%)	52,89,113	3.19	26 (50%)
37	A86	15	315	27	44,50,50	4.30	23 (52%)	51,76,76	8.22	28 (54%)
38	KC1	11	305	23	48,53,53	3.42	25 (52%)	55,89,89	3.86	30 (54%)
30	CLA	15	311	37	45,53,73	2.49	16 (35%)	52,89,113	3.17	24 (46%)
30	CLA	A	833	1	65,73,73	2.02	19 (29%)	76,113,113	2.65	26 (34%)
30	CLA	14	309	26	45,53,73	2.50	17 (37%)	52,89,113	3.10	24 (46%)
30	CLA	2u	202	12	65,73,73	1.95	17 (26%)	76,113,113	2.73	29 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	BCR	A	847	-	41,41,41	1.17	3 (7%)	56,56,56	1.24	7 (12%)
38	KC1	16	311	28	48,53,53	3.48	25 (52%)	55,89,89	3.70	26 (47%)
30	CLA	6	317	-	65,73,73	2.04	17 (26%)	76,113,113	2.69	26 (34%)
38	KC1	13	311	25	48,53,53	3.48	27 (56%)	55,89,89	3.61	29 (52%)
39	DD6	3	316	-	39,45,45	6.75	24 (61%)	52,67,67	6.80	26 (50%)
34	LHG	B	848	30	26,26,48	0.93	1 (3%)	29,32,54	1.39	4 (13%)
38	KC1	5	310	17	48,53,53	3.42	24 (50%)	55,89,89	3.91	30 (54%)
36	LMG	F	205	-	27,27,55	1.02	1 (3%)	35,35,63	1.25	5 (14%)
30	CLA	13	303	-	65,73,73	2.07	17 (26%)	76,113,113	2.76	29 (38%)
36	LMG	8	319	36,20	37,37,55	0.93	0	45,45,63	1.28	5 (11%)
37	A86	4	315	-	44,50,50	4.00	23 (52%)	51,76,76	7.94	19 (37%)
30	CLA	15	305	37,27	45,53,73	2.48	16 (35%)	52,89,113	3.16	26 (50%)
30	CLA	2	311	14	65,73,73	2.06	17 (26%)	76,113,113	2.64	24 (31%)
30	CLA	6	314	18	65,73,73	1.96	15 (23%)	76,113,113	2.78	30 (39%)
36	LMG	5	318	-	33,33,55	0.92	0	41,41,63	1.22	5 (12%)
30	CLA	B	827	2	65,73,73	1.95	16 (24%)	76,113,113	2.60	28 (36%)
30	CLA	4	303	16	65,73,73	1.99	17 (26%)	76,113,113	2.68	26 (34%)
38	KC1	14	306	26	48,53,53	3.44	27 (56%)	55,89,89	3.84	30 (54%)
30	CLA	2	304	14	65,73,73	2.02	16 (24%)	76,113,113	2.74	28 (36%)
38	KC1	4	308	16	48,53,53	3.48	24 (50%)	55,89,89	3.60	29 (52%)
38	KC1	8	311	40	48,53,53	3.36	23 (47%)	55,89,89	3.75	29 (52%)
38	KC1	9	312	21	48,53,53	3.43	25 (52%)	55,89,89	3.75	28 (50%)
37	A86	15	316	30	44,50,50	4.14	24 (54%)	51,76,76	7.80	17 (33%)
30	CLA	8	303	40	65,73,73	1.97	16 (24%)	76,113,113	2.64	28 (36%)
35	LMT	11	318	-	36,36,36	0.43	0	47,47,47	0.88	2 (4%)
37	A86	9	315	-	44,50,50	4.10	23 (52%)	51,76,76	7.06	19 (37%)
36	LMG	7	320	-	37,37,55	1.00	3 (8%)	45,45,63	1.25	5 (11%)
38	KC1	9	310	21	48,53,53	3.37	24 (50%)	55,89,89	3.92	28 (50%)
39	DD6	3	313	-	39,45,45	6.73	23 (58%)	52,67,67	6.66	24 (46%)
38	KC1	8	314	40,38	48,53,53	3.43	25 (52%)	55,89,89	3.72	29 (52%)
38	KC1	12	309	24	48,53,53	3.45	24 (50%)	55,89,89	3.72	30 (54%)
37	A86	12	314	-	44,50,50	4.02	22 (50%)	51,76,76	8.11	18 (35%)
30	CLA	B	829	2	65,73,73	1.94	15 (23%)	76,113,113	2.65	25 (32%)
30	CLA	L	202	9	65,73,73	1.94	16 (24%)	76,113,113	2.84	27 (35%)
30	CLA	A	810	1	65,73,73	1.98	18 (27%)	76,113,113	2.70	30 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	B	813	2	65,73,73	1.98	17 (26%)	76,113,113	2.67	26 (34%)
30	CLA	L	203	40	45,53,73	2.46	18 (40%)	52,89,113	3.19	23 (44%)
38	KC1	10	310	22	48,53,53	3.42	26 (54%)	55,89,89	3.93	30 (54%)
35	LMT	12	318	-	36,36,36	0.41	0	47,47,47	0.76	0
37	A86	16	312	28	44,50,50	4.06	23 (52%)	51,76,76	8.15	23 (45%)
30	CLA	B	822	30,2	65,73,73	1.97	17 (26%)	76,113,113	2.87	30 (39%)
35	LMT	9	317	-	33,33,36	0.49	0	44,44,47	1.11	5 (11%)
39	DD6	4	313	-	39,45,45	6.71	22 (56%)	52,67,67	6.72	26 (50%)
30	CLA	9	305	-	65,73,73	2.02	17 (26%)	76,113,113	2.85	30 (39%)
37	A86	12	316	-	44,50,50	4.08	23 (52%)	51,76,76	8.38	17 (33%)
37	A86	14	317	-	44,50,50	4.03	23 (52%)	51,76,76	8.75	18 (35%)
30	CLA	7	306	19	65,73,73	1.97	18 (27%)	76,113,113	2.60	28 (36%)
35	LMT	B	850	-	36,36,36	0.39	0	47,47,47	0.92	3 (6%)
37	A86	3	315	-	44,50,50	4.12	24 (54%)	51,76,76	8.24	16 (31%)
35	LMT	16	315	-	36,36,36	0.41	0	47,47,47	0.65	0
37	A86	4	312	-	44,50,50	3.92	23 (52%)	51,76,76	8.64	21 (41%)
30	CLA	16	301	28	65,73,73	2.00	16 (24%)	76,113,113	2.76	28 (36%)
38	KC1	10	306	22	48,53,53	3.39	25 (52%)	55,89,89	3.95	31 (56%)
39	DD6	11	313	-	39,45,45	6.77	23 (58%)	52,67,67	6.83	29 (55%)
35	LMT	8	322	-	36,36,36	0.40	0	47,47,47	0.73	1 (2%)
38	KC1	6	312	18	48,53,53	3.39	25 (52%)	55,89,89	3.69	30 (54%)
30	CLA	9	309	40,21	65,73,73	1.99	16 (24%)	76,113,113	2.59	27 (35%)
30	CLA	10	311	-	45,53,73	2.45	18 (40%)	52,89,113	3.19	24 (46%)
30	CLA	B	824	40	65,73,73	2.01	17 (26%)	76,113,113	4.67	29 (38%)
30	CLA	3	309	15	45,53,73	2.48	17 (37%)	52,89,113	3.24	24 (46%)
33	BCR	B	845	-	41,41,41	1.08	2 (4%)	56,56,56	1.20	6 (10%)
37	A86	13	313	25	41,47,50	4.31	22 (53%)	49,72,76	8.60	17 (34%)
38	KC1	8	313	20	48,53,53	3.34	23 (47%)	55,89,89	3.80	29 (52%)
38	KC1	12	305	24	48,53,53	3.44	25 (52%)	55,89,89	3.81	30 (54%)
30	CLA	9	308	21	65,73,73	2.00	16 (24%)	76,113,113	2.83	31 (40%)
39	DD6	4	316	-	39,45,45	6.68	23 (58%)	52,67,67	7.33	26 (50%)
30	CLA	6	305	18	65,73,73	2.05	18 (27%)	76,113,113	2.69	27 (35%)
38	KC1	12	311	24	48,53,53	3.46	25 (52%)	55,89,89	3.91	34 (61%)
30	CLA	A	807	1	65,73,73	1.96	16 (24%)	76,113,113	2.75	29 (38%)
36	LMG	B	847	-	55,55,55	0.80	1 (1%)	63,63,63	1.37	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	KC1	6	313	18	48,53,53	3.41	23 (47%)	55,89,89	3.78	29 (52%)
30	CLA	2	303	14	55,63,73	2.42	16 (29%)	64,101,113	2.89	28 (43%)
37	A86	5	316	-	44,50,50	4.04	22 (50%)	51,76,76	8.02	17 (33%)
30	CLA	B	804	2	52,60,73	2.21	17 (32%)	60,97,113	3.07	29 (48%)
30	CLA	15	314	30,27	45,53,73	2.40	16 (35%)	52,89,113	3.30	24 (46%)
37	A86	10	316	-	44,50,50	3.92	24 (54%)	51,76,76	8.13	21 (41%)
37	A86	14	318	-	44,50,50	4.10	22 (50%)	51,76,76	8.48	16 (31%)
30	CLA	B	835	2	65,73,73	1.96	16 (24%)	76,113,113	2.74	29 (38%)
32	SF4	C	102	3	0,12,12	-	-	-	-	-
30	CLA	2	301	14,2	65,73,73	1.94	16 (24%)	76,113,113	2.83	26 (34%)
30	CLA	7	309	19	65,73,73	1.94	17 (26%)	76,113,113	2.65	24 (31%)
30	CLA	9	302	9,21	51,59,73	2.30	17 (33%)	59,96,113	3.16	28 (47%)
30	CLA	14	310	-	50,58,73	2.33	16 (32%)	58,95,113	3.09	26 (44%)
36	LMG	2u	204	12	31,31,55	1.12	3 (9%)	39,39,63	1.18	4 (10%)
38	KC1	3	304	15	48,53,53	3.43	26 (54%)	55,89,89	3.89	32 (58%)
30	CLA	A	835	1	65,73,73	1.99	17 (26%)	76,113,113	2.77	26 (34%)
38	KC1	1	306	13	48,53,53	3.45	25 (52%)	55,89,89	3.83	30 (54%)
38	KC1	16	304	28	48,53,53	3.50	25 (52%)	55,89,89	3.59	27 (49%)
33	BCR	B	844	-	41,41,41	1.13	2 (4%)	56,56,56	1.38	8 (14%)
30	CLA	4	302	16	65,73,73	1.98	17 (26%)	76,113,113	2.63	25 (32%)
30	CLA	A	822	40	65,73,73	1.97	16 (24%)	76,113,113	2.52	27 (35%)
35	LMT	6	302	-	32,32,36	0.36	0	43,43,47	0.92	1 (2%)
30	CLA	5	309	34	65,73,73	2.01	17 (26%)	76,113,113	2.63	27 (35%)
30	CLA	13	307	25	65,73,73	2.09	17 (26%)	76,113,113	2.69	27 (35%)
30	CLA	B	815	2	45,53,73	2.37	16 (35%)	52,89,113	3.17	24 (46%)
30	CLA	A	820	1	65,73,73	2.02	17 (26%)	76,113,113	2.69	29 (38%)
35	LMT	7	321	-	36,36,36	0.32	0	47,47,47	0.75	2 (4%)
30	CLA	B	836	2	47,55,73	2.27	17 (36%)	54,91,113	3.25	25 (46%)
30	CLA	15	313	27	65,73,73	2.07	17 (26%)	76,113,113	2.74	28 (36%)
30	CLA	B	809	2	65,73,73	1.90	15 (23%)	76,113,113	2.60	24 (31%)
37	A86	10	317	-	44,50,50	4.19	23 (52%)	51,76,76	8.16	15 (29%)
33	BCR	A	850	-	41,41,41	1.13	2 (4%)	56,56,56	1.34	9 (16%)
36	LMG	B	849	2	43,43,55	0.95	2 (4%)	51,51,63	1.18	3 (5%)
30	CLA	7	304	19	65,73,73	1.97	16 (24%)	76,113,113	2.70	28 (36%)
35	LMT	11	317	-	36,36,36	0.43	0	47,47,47	0.89	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	A86	14	314	-	44,50,50	4.09	22 (50%)	51,76,76	8.27	21 (41%)
35	LMT	15	301	-	36,36,36	0.51	0	47,47,47	1.13	3 (6%)
38	KC1	11	307	23	48,53,53	3.46	25 (52%)	55,89,89	3.79	30 (54%)
38	KC1	13	312	25	48,53,53	3.54	27 (56%)	55,89,89	3.77	29 (52%)
36	LMG	8	320	-	42,42,55	0.90	3 (7%)	50,50,63	1.31	5 (10%)
38	KC1	14	308	30,26	48,53,53	3.45	26 (54%)	55,89,89	3.77	30 (54%)
30	CLA	12	307	24	46,54,73	2.33	16 (34%)	53,90,113	3.17	25 (47%)
39	DD6	7	318	-	39,45,45	6.70	21 (53%)	52,67,67	6.91	29 (55%)
33	BCR	F	204	-	41,41,41	1.07	2 (4%)	56,56,56	1.28	8 (14%)
37	A86	13	315	-	44,50,50	4.18	23 (52%)	51,76,76	8.50	18 (35%)
30	CLA	A	816	1,35	65,73,73	1.96	17 (26%)	76,113,113	2.68	26 (34%)
30	CLA	B	834	2	60,68,73	2.11	18 (30%)	70,107,113	2.85	27 (38%)
39	DD6	6	319	-	39,45,45	6.71	23 (58%)	52,67,67	6.51	31 (59%)
30	CLA	3	301	15	65,73,73	1.97	17 (26%)	76,113,113	2.74	27 (35%)
30	CLA	1	302	30,13	65,73,73	2.00	16 (24%)	76,113,113	2.69	26 (34%)
30	CLA	A	839	1	65,73,73	1.96	15 (23%)	76,113,113	2.83	30 (39%)
30	CLA	12	303	24	65,73,73	2.04	19 (29%)	76,113,113	2.66	26 (34%)
37	A86	8	315	-	44,50,50	3.75	22 (50%)	51,76,76	8.45	20 (39%)
30	CLA	15	308	30,27	45,53,73	2.43	18 (40%)	52,89,113	3.11	26 (50%)
37	A86	14	316	-	44,50,50	4.03	23 (52%)	51,76,76	8.16	18 (35%)
30	CLA	B	825	2	65,73,73	1.99	18 (27%)	76,113,113	2.77	29 (38%)
30	CLA	11	306	40	55,63,73	2.19	16 (29%)	64,101,113	3.02	30 (46%)
30	CLA	A	806	1	65,73,73	1.98	17 (26%)	76,113,113	2.92	29 (38%)
35	LMT	11	302	-	36,36,36	0.34	0	47,47,47	0.77	2 (4%)
37	A86	11	301	-	44,50,50	4.04	23 (52%)	51,76,76	8.20	21 (41%)
30	CLA	B	805	2	65,73,73	2.00	17 (26%)	76,113,113	2.72	27 (35%)
36	LMG	8	321	36	29,29,55	1.11	2 (6%)	37,37,63	1.27	5 (13%)
30	CLA	B	801	2	65,73,73	1.87	17 (26%)	76,113,113	2.81	31 (40%)
35	LMT	7	301	30	36,36,36	0.41	0	47,47,47	0.80	1 (2%)
39	DD6	2	315	-	39,45,45	6.74	23 (58%)	52,67,67	6.78	27 (51%)
30	CLA	B	808	2	65,73,73	1.94	16 (24%)	76,113,113	2.75	28 (36%)
37	A86	15	320	-	44,50,50	4.24	24 (54%)	51,76,76	8.23	19 (37%)
38	KC1	2	306	14	48,53,53	3.44	26 (54%)	55,89,89	3.90	31 (56%)
38	KC1	13	310	25	48,53,53	3.47	25 (52%)	55,89,89	3.83	29 (52%)
30	CLA	F	202	40	65,73,73	2.01	18 (27%)	76,113,113	2.70	27 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	LMG	14	321	-	38,38,55	1.03	3 (7%)	46,46,63	1.20	3 (6%)
30	CLA	A	817	40,36	49,57,73	2.30	15 (30%)	55,93,113	3.15	23 (41%)
38	KC1	9	304	21	48,53,53	3.40	23 (47%)	55,89,89	3.79	30 (54%)
30	CLA	2	310	14	65,73,73	2.03	16 (24%)	76,113,113	4.67	29 (38%)
30	CLA	16	305	28	50,58,73	2.28	19 (38%)	58,95,113	3.00	27 (46%)
30	CLA	10	305	40	65,73,73	1.99	16 (24%)	76,113,113	2.80	30 (39%)
38	KC1	8	310	20	48,53,53	3.35	23 (47%)	55,89,89	3.74	29 (52%)
33	BCR	B	846	-	41,41,41	1.13	2 (4%)	56,56,56	1.19	5 (8%)
30	CLA	A	838	1	51,59,73	2.27	17 (33%)	59,96,113	3.10	26 (44%)
35	LMT	A	857	-	36,36,36	0.37	0	47,47,47	0.78	0
30	CLA	B	833	30,40	65,73,73	1.97	18 (27%)	76,113,113	2.64	26 (34%)
37	A86	7	319	-	44,50,50	4.10	23 (52%)	51,76,76	8.25	22 (43%)
38	KC1	4	310	16	48,53,53	3.46	26 (54%)	55,89,89	3.91	29 (52%)
30	CLA	15	304	30,39,27	65,73,73	2.09	16 (24%)	76,113,113	2.75	26 (34%)
35	LMT	12	319	-	36,36,36	0.40	0	47,47,47	0.86	0
30	CLA	B	818	2	60,68,73	2.04	14 (23%)	70,107,113	2.88	29 (41%)
30	CLA	1	304	13	65,73,73	1.99	16 (24%)	76,113,113	2.59	27 (35%)
38	KC1	14	311	26	48,53,53	3.44	25 (52%)	55,89,89	3.80	29 (52%)
30	CLA	9	306	37,21	45,53,73	2.48	15 (33%)	52,89,113	3.21	26 (50%)
38	KC1	5	306	17	48,53,53	3.41	24 (50%)	55,89,89	4.11	30 (54%)
30	CLA	8	309	20	47,55,73	2.38	17 (36%)	54,91,113	3.05	24 (44%)
37	A86	10	301	22	44,50,50	3.86	23 (52%)	51,76,76	7.28	23 (45%)
37	A86	15	321	27	44,50,50	4.11	23 (52%)	51,76,76	8.63	19 (37%)
30	CLA	6	316	40	55,63,73	2.22	17 (30%)	64,101,113	2.80	25 (39%)
30	CLA	5	311	40,17	65,73,73	2.05	18 (27%)	76,113,113	2.80	26 (34%)
30	CLA	A	836	1	54,62,73	2.17	16 (29%)	62,99,113	2.85	29 (46%)
34	LHG	2	320	30	26,26,48	0.87	1 (3%)	29,32,54	1.30	3 (10%)
39	DD6	5	314	-	39,45,45	6.56	24 (61%)	52,67,67	7.17	30 (57%)
32	SF4	A	846	1,2	0,12,12	-	-	-	-	-
30	CLA	B	811	30,2	65,73,73	1.97	17 (26%)	76,113,113	2.62	31 (40%)
30	CLA	10	307	22	65,73,73	1.96	17 (26%)	76,113,113	2.61	27 (35%)
33	BCR	A	848	-	41,41,41	1.05	2 (4%)	56,56,56	1.21	4 (7%)
35	LMT	A	855	-	36,36,36	0.39	0	47,47,47	0.89	3 (6%)
30	CLA	5	304	17	65,73,73	2.08	18 (27%)	76,113,113	2.72	29 (38%)
35	LMT	1	311	-	36,36,36	0.40	0	47,47,47	0.78	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	15	302	30,27	65,73,73	2.06	16 (24%)	76,113,113	2.93	29 (38%)
30	CLA	5	303	17	65,73,73	1.98	17 (26%)	76,113,113	2.64	28 (36%)
35	LMT	B	852	-	36,36,36	0.36	0	47,47,47	1.12	2 (4%)
38	KC1	1	308	13	48,53,53	3.44	26 (54%)	55,89,89	3.81	28 (50%)
30	CLA	15	309	27	65,73,73	2.09	17 (26%)	76,113,113	2.68	26 (34%)
38	KC1	5	305	17	48,53,53	3.42	25 (52%)	55,89,89	3.80	29 (52%)
30	CLA	F	201	40	65,73,73	1.92	17 (26%)	76,113,113	2.65	27 (35%)
30	CLA	2	313	14	45,53,73	2.47	16 (35%)	52,89,113	3.21	25 (48%)
37	A86	6	320	-	44,50,50	3.90	23 (52%)	51,76,76	7.09	20 (39%)
37	A86	10	302	-	44,50,50	4.06	23 (52%)	51,76,76	8.39	17 (33%)
30	CLA	A	831	1	65,73,73	1.98	16 (24%)	76,113,113	2.83	28 (36%)
33	BCR	A	849	-	41,41,41	1.14	2 (4%)	56,56,56	1.38	9 (16%)
37	A86	11	314	-	44,50,50	4.09	23 (52%)	51,76,76	8.59	18 (35%)
39	DD6	2	317	-	39,45,45	6.77	22 (56%)	52,67,67	6.58	28 (53%)
30	CLA	16	302	28	65,73,73	1.99	17 (26%)	76,113,113	2.69	26 (34%)
37	A86	7	316	-	44,50,50	3.75	22 (50%)	51,76,76	7.71	27 (52%)
39	DD6	10	313	-	39,45,45	6.78	24 (61%)	52,67,67	7.12	30 (57%)
30	CLA	14	307	38	65,73,73	2.05	16 (24%)	76,113,113	2.81	24 (31%)
30	CLA	B	814	2	55,63,73	2.16	17 (30%)	64,101,113	2.84	27 (42%)
30	CLA	11	304	23	65,73,73	2.04	16 (24%)	76,113,113	2.69	25 (32%)
30	CLA	16	309	28	45,53,73	2.48	17 (37%)	52,89,113	3.26	24 (46%)
39	DD6	10	314	-	39,45,45	6.73	23 (58%)	52,67,67	6.78	28 (53%)
38	KC1	3	308	15	48,53,53	3.38	25 (52%)	55,89,89	3.81	29 (52%)
30	CLA	16	308	28	45,53,73	2.47	17 (37%)	52,89,113	3.21	25 (48%)
30	CLA	16	310	28	45,53,73	2.46	18 (40%)	52,89,113	3.21	26 (50%)
30	CLA	6	304	18	65,73,73	1.98	16 (24%)	76,113,113	2.75	28 (36%)
37	A86	2u	205	-	44,50,50	4.13	23 (52%)	51,76,76	7.47	22 (43%)
37	A86	9	316	30	44,50,50	4.22	22 (50%)	51,76,76	8.44	16 (31%)
30	CLA	16	303	28	65,73,73	2.01	15 (23%)	76,113,113	2.86	28 (36%)
30	CLA	5	308	17	65,73,73	2.00	16 (24%)	76,113,113	2.70	28 (36%)
30	CLA	4	304	-	60,68,73	2.08	15 (25%)	70,107,113	2.78	28 (40%)
30	CLA	B	851	14,2	65,73,73	1.98	17 (26%)	76,113,113	2.67	30 (39%)
30	CLA	16	306	28	52,60,73	2.26	18 (34%)	60,97,113	2.95	28 (46%)
33	BCR	L	205	-	41,41,41	1.06	2 (4%)	56,56,56	1.24	5 (8%)
30	CLA	12	321	24,26	65,73,73	2.04	17 (26%)	76,113,113	2.63	27 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	15	306	-	45,53,73	2.47	17 (37%)	52,89,113	3.29	23 (44%)
37	A86	15	317	30	44,50,50	4.15	23 (52%)	51,76,76	8.44	15 (29%)
30	CLA	4	301	16,2	49,57,73	2.25	18 (36%)	55,93,113	3.13	24 (43%)
29	CL0	A	801	1	65,73,73	1.92	17 (26%)	76,113,113	2.76	29 (38%)
30	CLA	14	303	26	57,65,73	2.19	16 (28%)	66,103,113	2.88	29 (43%)
30	CLA	8	301	20	65,73,73	2.00	17 (26%)	76,113,113	2.71	29 (38%)
33	BCR	2u	201	-	41,41,41	1.22	4 (9%)	56,56,56	1.38	7 (12%)
30	CLA	6	309	18	65,73,73	2.00	15 (23%)	76,113,113	2.68	31 (40%)
30	CLA	15	312	27	45,53,73	2.47	16 (35%)	52,89,113	3.33	28 (53%)
30	CLA	A	837	1	45,53,73	2.43	17 (37%)	52,89,113	3.15	24 (46%)
30	CLA	A	840	1	47,55,73	2.31	17 (36%)	54,91,113	3.27	26 (48%)
30	CLA	5	302	17	65,73,73	1.98	16 (24%)	76,113,113	2.66	27 (35%)
30	CLA	B	812	2	65,73,73	2.05	17 (26%)	76,113,113	2.57	26 (34%)
37	A86	8	318	-	44,50,50	3.98	24 (54%)	51,76,76	10.85	23 (45%)
30	CLA	13	301	25	65,73,73	1.99	16 (24%)	76,113,113	2.81	26 (34%)
30	CLA	4	309	-	65,73,73	2.09	17 (26%)	76,113,113	2.70	28 (36%)
33	BCR	I	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.29	5 (8%)
37	A86	14	315	26	44,50,50	3.99	23 (52%)	51,76,76	8.87	22 (43%)
34	LHG	A	852	-	48,48,48	0.64	1 (2%)	51,54,54	1.20	5 (9%)
36	LMG	6	301	30	33,33,55	0.95	1 (3%)	41,41,63	1.21	4 (9%)
30	CLA	A	812	30,1	65,73,73	1.93	18 (27%)	76,113,113	2.79	26 (34%)
38	KC1	11	311	23	48,53,53	3.49	26 (54%)	55,89,89	3.81	29 (52%)
37	A86	15	323	-	44,50,50	4.19	23 (52%)	51,76,76	8.39	17 (33%)
30	CLA	13	302	25	65,73,73	2.03	17 (26%)	76,113,113	2.62	27 (35%)
33	BCR	A	851	-	41,41,41	1.18	2 (4%)	56,56,56	1.25	6 (10%)
37	A86	11	316	-	44,50,50	4.05	23 (52%)	51,76,76	8.21	16 (31%)
30	CLA	7	307	19	65,73,73	1.97	16 (24%)	76,113,113	2.69	25 (32%)
30	CLA	4	306	16	65,73,73	2.00	16 (24%)	76,113,113	2.68	28 (36%)
31	PQN	B	840	-	34,34,34	1.50	2 (5%)	42,45,45	1.09	4 (9%)
35	LMT	12	320	-	36,36,36	0.39	0	47,47,47	0.71	0
30	CLA	A	818	1	54,62,73	2.11	16 (29%)	62,99,113	3.04	27 (43%)
37	A86	5	315	-	44,50,50	4.05	23 (52%)	51,76,76	8.37	18 (35%)
39	DD6	8	316	-	39,45,45	6.57	22 (56%)	52,67,67	6.80	30 (57%)
30	CLA	2	309	14,34	65,73,73	2.03	17 (26%)	76,113,113	2.67	28 (36%)

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
30	CLA	A	813	1	1/1/15/20	13/37/115/115	-
33	BCR	B	843	-	-	9/29/63/63	0/2/2/2
30	CLA	2	307	14	1/1/15/20	7/37/115/115	-
30	CLA	3	306	15	1/1/15/20	8/37/115/115	-
30	CLA	15	310	27	1/1/11/20	6/13/91/115	-
30	CLA	B	837	40	1/1/15/20	5/37/115/115	-
38	KC1	8	306	40	-	8/15/71/71	-
38	KC1	10	312	22	-	5/15/71/71	-
30	CLA	12	310	40	-	8/37/115/115	-
38	KC1	2	314	40	-	7/15/71/71	-
30	CLA	A	824	1	1/1/12/20	3/21/99/115	-
38	KC1	2	312	14	-	2/15/71/71	-
30	CLA	7	310	19	-	11/37/115/115	-
39	DD6	9	314	-	-	11/26/80/80	0/3/3/3
30	CLA	A	834	1	1/1/15/20	10/37/115/115	-
30	CLA	A	843	40	1/1/15/20	7/37/115/115	-
30	CLA	14	302	26	1/1/15/20	14/37/115/115	-
39	DD6	12	315	30	-	9/26/80/80	0/3/3/3
39	DD6	2	316	-	-	12/26/80/80	0/3/3/3
30	CLA	1	301	13	1/1/15/20	13/37/115/115	-
37	A86	2	319	-	-	12/34/90/90	0/3/3/3
30	CLA	B	839	34	1/1/15/20	4/37/115/115	-
30	CLA	B	806	2	1/1/15/20	9/37/115/115	-
30	CLA	A	841	1	1/1/15/20	10/37/115/115	-
30	CLA	A	819	1	-	6/24/102/115	-
30	CLA	6	315	18	1/1/11/20	3/13/91/115	-
30	CLA	B	832	37,40	1/1/15/20	5/37/115/115	-
30	CLA	2	305	40	1/1/15/20	9/37/115/115	-
37	A86	5	301	-	-	11/34/90/90	0/3/3/3
39	DD6	3	312	-	-	12/26/80/80	0/3/3/3
33	BCR	L	204	-	-	11/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LHG	5	317	30	-	4/31/31/53	-
38	KC1	12	313	24	-	7/15/71/71	-
30	CLA	J	101	8	1/1/11/20	3/13/91/115	-
37	A86	15	322	30	-	15/34/90/90	0/3/3/3
38	KC1	13	305	25	-	8/15/71/71	-
37	A86	2u	203	30	-	15/34/90/90	0/3/3/3
30	CLA	A	830	1	1/1/15/20	9/37/115/115	-
31	PQN	A	845	-	-	7/23/43/43	0/2/2/2
30	CLA	A	811	1	1/1/15/20	12/37/115/115	-
30	CLA	11	309	23	-	16/37/115/115	-
37	A86	16	314	-	-	11/34/90/90	0/3/3/3
30	CLA	A	802	40	1/1/15/20	6/37/115/115	-
38	KC1	4	307	16	-	6/15/71/71	-
37	A86	14	301	26	-	8/34/90/90	0/3/3/3
38	KC1	13	306	25	-	9/15/71/71	-
30	CLA	14	312	37,26	-	7/13/91/115	-
30	CLA	A	842	1	1/1/15/20	10/37/115/115	-
30	CLA	B	810	2	1/1/15/20	10/37/115/115	-
38	KC1	5	312	17	-	4/15/71/71	-
30	CLA	1	305	40	1/1/15/20	9/37/115/115	-
33	BCR	J	102	-	-	12/29/63/63	0/2/2/2
30	CLA	A	803	-	1/1/15/20	8/37/115/115	-
39	DD6	6	318	-	-	11/26/80/80	0/3/3/3
30	CLA	3	305	15	1/1/14/20	12/34/112/115	-
38	KC1	13	308	25	-	10/15/71/71	-
30	CLA	6	307	39,18	1/1/15/20	11/37/115/115	-
32	SF4	C	101	3	-	-	0/6/5/5
30	CLA	6	310	34	1/1/15/20	8/37/115/115	-
30	CLA	7	305	40,19	1/1/15/20	8/37/115/115	-
34	LHG	9	318	-	-	21/38/38/53	-
30	CLA	12	304	24,39	1/1/15/20	14/37/115/115	-
30	CLA	16	307	-	1/1/11/20	7/15/93/115	-
39	DD6	5	313	-	-	9/26/80/80	0/3/3/3
37	A86	1	309	-	-	8/34/90/90	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	A86	7	315	-	-	15/34/90/90	0/3/3/3
30	CLA	A	814	1	1/1/14/20	10/31/109/115	-
35	LMT	11	303	-	-	11/21/61/61	0/2/2/2
39	DD6	8	317	-	-	10/26/80/80	0/3/3/3
33	BCR	L	201	-	-	12/29/63/63	0/2/2/2
30	CLA	A	826	40	1/1/15/20	14/37/115/115	-
30	CLA	14	305	26	1/1/12/20	2/19/97/115	-
38	KC1	8	312	38	-	9/15/71/71	-
30	CLA	12	302	24	-	13/37/115/115	-
30	CLA	B	831	2	-	8/29/107/115	-
37	A86	11	315	-	-	13/34/90/90	0/3/3/3
38	KC1	7	308	40	-	7/15/71/71	-
30	CLA	A	825	1	1/1/13/20	13/30/108/115	-
33	BCR	M	101	-	-	11/29/63/63	0/2/2/2
39	DD6	7	314	-	-	11/26/80/80	0/3/3/3
30	CLA	9	301	34	1/1/15/20	10/37/115/115	-
30	CLA	A	829	30,1	1/1/15/20	14/37/115/115	-
35	LMT	A	854	-	-	15/21/61/61	0/2/2/2
36	LMG	A	856	-	-	15/29/49/70	0/1/1/1
30	CLA	B	820	2	-	2/13/91/115	-
30	CLA	3	302	15	1/1/14/20	7/31/109/115	-
30	CLA	A	823	1	-	6/18/96/115	-
30	CLA	8	308	20	1/1/13/20	10/25/103/115	-
37	A86	2	318	-	-	8/34/90/90	0/3/3/3
30	CLA	7	303	19	1/1/15/20	11/37/115/115	-
30	CLA	B	830	2	1/1/15/20	12/37/115/115	-
34	LHG	6	322	30	-	12/31/31/53	-
30	CLA	B	816	2	-	7/25/103/115	-
37	A86	3	314	-	-	9/34/90/90	0/3/3/3
37	A86	14	319	30	-	11/34/90/90	0/3/3/3
30	CLA	A	805	30,1	1/1/13/20	9/30/108/115	-
30	CLA	3	303	15	1/1/15/20	14/37/115/115	-
39	DD6	1	310	-	-	13/26/80/80	0/3/3/3
38	KC1	6	308	18	-	6/15/71/71	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	10	309	22	1/1/15/20	10/37/115/115	-
30	CLA	A	809	30,1	1/1/15/20	15/37/115/115	-
30	CLA	14	313	26	1/1/11/20	4/15/93/115	-
30	CLA	4	311	16	1/1/12/20	1/19/97/115	-
33	BCR	B	842	-	-	10/29/63/63	0/2/2/2
37	A86	4	314	-	-	11/34/90/90	0/3/3/3
36	LMG	3	317	-	-	18/32/52/70	0/1/1/1
30	CLA	10	304	22	1/1/15/20	3/37/115/115	-
30	CLA	A	821	1	1/1/14/20	11/33/111/115	-
30	CLA	A	832	1	-	5/19/97/115	-
30	CLA	1	303	30,13	1/1/15/20	13/37/115/115	-
39	DD6	7	317	-	-	10/26/80/80	0/3/3/3
30	CLA	9	303	21	-	9/37/115/115	-
39	DD6	15	319	30	-	13/26/80/80	0/3/3/3
39	DD6	6	321	-	-	12/26/80/80	0/3/3/3
30	CLA	10	303	22	1/1/15/20	13/37/115/115	-
30	CLA	B	817	2	1/1/13/20	5/30/108/115	-
38	KC1	3	311	40	-	6/15/71/71	-
30	CLA	B	807	2	1/1/15/20	9/37/115/115	-
30	CLA	12	306	24	1/1/15/20	6/37/115/115	-
30	CLA	11	310	23	1/1/15/20	15/37/115/115	-
30	CLA	A	827	40	1/1/15/20	5/37/115/115	-
30	CLA	12	312	24	1/1/15/20	12/37/115/115	-
37	A86	4	317	-	-	6/34/90/90	0/3/3/3
38	KC1	9	311	21	-	8/15/71/71	-
39	DD6	7	302	-	-	12/26/80/80	0/3/3/3
37	A86	10	315	-	-	13/34/90/90	0/3/3/3
30	CLA	B	838	2	1/1/15/20	17/37/115/115	-
30	CLA	5	307	17	1/1/15/20	14/37/115/115	-
30	CLA	7	312	19	1/1/11/20	6/15/93/115	-
30	CLA	2	308	14	-	9/37/115/115	-
30	CLA	B	802	30,40	1/1/15/20	10/37/115/115	-
30	CLA	A	828	1	1/1/15/20	13/37/115/115	-
35	LMT	12	301	-	-	4/21/61/61	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	13	304	25	-	7/13/91/115	-
30	CLA	B	821	2	1/1/13/20	14/25/103/115	-
37	A86	14	320	-	-	9/34/90/90	0/3/3/3
30	CLA	7	311	19	1/1/15/20	12/37/115/115	-
37	A86	9	313	21	-	8/34/90/90	0/3/3/3
33	BCR	J	103	-	-	9/29/63/63	0/2/2/2
38	KC1	6	311	18	-	10/15/71/71	-
39	DD6	6	303	30	-	10/26/80/80	0/3/3/3
30	CLA	A	844	-	1/1/15/20	12/37/115/115	-
38	KC1	7	313	-	-	4/15/71/71	-
39	DD6	13	314	-	-	13/26/80/80	0/3/3/3
30	CLA	8	304	20	1/1/13/20	9/29/107/115	-
30	CLA	A	804	1	1/1/15/20	11/37/115/115	-
39	DD6	15	318	-	-	13/26/80/80	0/3/3/3
30	CLA	13	309	-	1/1/11/20	8/13/91/115	-
30	CLA	B	828	2	1/1/15/20	14/37/115/115	-
30	CLA	15	307	27	1/1/12/20	7/19/97/115	-
30	CLA	A	808	1	1/1/12/20	3/21/99/115	-
30	CLA	10	308	22	1/1/15/20	11/37/115/115	-
30	CLA	12	308	40	1/1/15/20	11/37/115/115	-
30	CLA	9	307	21	1/1/15/20	9/37/115/115	-
30	CLA	14	304	26	1/1/11/20	4/13/91/115	-
30	CLA	B	823	40	1/1/12/20	3/24/102/115	-
30	CLA	B	826	2	1/1/15/20	14/37/115/115	-
30	CLA	1	307	13	-	17/37/115/115	-
38	KC1	11	312	-	-	5/15/71/71	-
30	CLA	15	303	30,37,27	1/1/14/20	9/31/109/115	-
30	CLA	B	803	-	1/1/15/20	6/37/115/115	-
33	BCR	B	841	-	-	10/29/63/63	0/2/2/2
30	CLA	8	302	20	1/1/15/20	8/37/115/115	-
30	CLA	3	310	15	-	4/13/91/115	-
30	CLA	8	305	20	-	13/37/115/115	-
30	CLA	A	815	1	1/1/15/20	7/37/115/115	-
37	A86	2	302	-	-	11/34/90/90	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	6	306	40	1/1/15/20	9/37/115/115	-
38	KC1	8	307	20	-	8/15/71/71	-
39	DD6	16	313	-	-	13/26/80/80	0/3/3/3
30	CLA	B	819	40	1/1/15/20	9/37/115/115	-
30	CLA	11	308	23	1/1/15/20	10/37/115/115	-
34	LHG	A	853	30	-	9/31/31/53	-
30	CLA	3	307	15	1/1/15/20	14/37/115/115	-
30	CLA	4	305	16	1/1/15/20	9/37/115/115	-
39	DD6	12	317	-	-	13/26/80/80	0/3/3/3
30	CLA	F	203	6	1/1/11/20	6/13/91/115	-
37	A86	15	315	27	-	9/34/90/90	0/3/3/3
38	KC1	11	305	23	-	7/15/71/71	-
30	CLA	15	311	37	1/1/11/20	7/13/91/115	-
30	CLA	A	833	1	1/1/15/20	13/37/115/115	-
30	CLA	14	309	26	1/1/11/20	3/13/91/115	-
30	CLA	2u	202	12	1/1/15/20	14/37/115/115	-
33	BCR	A	847	-	-	12/29/63/63	0/2/2/2
38	KC1	16	311	28	-	6/15/71/71	-
30	CLA	6	317	-	1/1/15/20	14/37/115/115	-
38	KC1	13	311	25	-	3/15/71/71	-
39	DD6	3	316	-	-	12/26/80/80	0/3/3/3
34	LHG	B	848	30	-	18/31/31/53	-
38	KC1	5	310	17	-	6/15/71/71	-
36	LMG	F	205	-	-	14/21/41/70	0/1/1/1
30	CLA	13	303	-	-	8/37/115/115	-
36	LMG	8	319	36,20	-	17/32/52/70	0/1/1/1
37	A86	4	315	-	-	5/34/90/90	0/3/3/3
30	CLA	15	305	37,27	1/1/11/20	8/13/91/115	-
30	CLA	2	311	14	-	11/37/115/115	-
30	CLA	6	314	18	-	16/37/115/115	-
36	LMG	5	318	-	-	10/28/48/70	0/1/1/1
30	CLA	B	827	2	1/1/15/20	5/37/115/115	-
30	CLA	4	303	16	1/1/15/20	4/37/115/115	-
38	KC1	14	306	26	-	7/15/71/71	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	2	304	14	1/1/15/20	13/37/115/115	-
38	KC1	4	308	16	-	2/15/71/71	-
38	KC1	8	311	40	-	5/15/71/71	-
38	KC1	9	312	21	-	6/15/71/71	-
37	A86	15	316	30	-	14/34/90/90	0/3/3/3
30	CLA	8	303	40	-	10/37/115/115	-
35	LMT	11	318	-	-	1/21/61/61	0/2/2/2
37	A86	9	315	-	-	10/34/90/90	0/3/3/3
36	LMG	7	320	-	-	14/32/52/70	0/1/1/1
38	KC1	9	310	21	-	7/15/71/71	-
39	DD6	3	313	-	-	9/26/80/80	0/3/3/3
38	KC1	8	314	40,38	-	7/15/71/71	-
38	KC1	12	309	24	-	8/15/71/71	-
37	A86	12	314	-	-	13/34/90/90	0/3/3/3
30	CLA	B	829	2	1/1/15/20	11/37/115/115	-
30	CLA	L	202	9	1/1/15/20	7/37/115/115	-
30	CLA	A	810	1	1/1/15/20	10/37/115/115	-
30	CLA	B	813	2	1/1/15/20	21/37/115/115	-
30	CLA	L	203	40	1/1/11/20	2/13/91/115	-
38	KC1	10	310	22	-	7/15/71/71	-
35	LMT	12	318	-	-	3/21/61/61	0/2/2/2
37	A86	16	312	28	-	13/34/90/90	0/3/3/3
30	CLA	B	822	30,2	-	12/37/115/115	-
35	LMT	9	317	-	-	5/18/58/61	0/2/2/2
39	DD6	4	313	-	-	14/26/80/80	0/3/3/3
30	CLA	9	305	-	1/1/15/20	13/37/115/115	-
37	A86	12	316	-	-	16/34/90/90	0/3/3/3
37	A86	14	317	-	-	15/34/90/90	0/3/3/3
30	CLA	7	306	19	1/1/15/20	8/37/115/115	-
35	LMT	B	850	-	-	1/21/61/61	0/2/2/2
37	A86	3	315	-	-	14/34/90/90	0/3/3/3
35	LMT	16	315	-	-	5/21/61/61	0/2/2/2
37	A86	4	312	-	-	11/34/90/90	0/3/3/3
30	CLA	16	301	28	-	12/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	KC1	10	306	22	-	8/15/71/71	-
39	DD6	11	313	-	-	11/26/80/80	0/3/3/3
35	LMT	8	322	-	-	3/21/61/61	0/2/2/2
38	KC1	6	312	18	-	6/15/71/71	-
30	CLA	9	309	40,21	1/1/15/20	9/37/115/115	-
30	CLA	10	311	-	-	7/13/91/115	-
30	CLA	B	824	40	1/1/15/20	5/37/115/115	-
30	CLA	3	309	15	-	4/13/91/115	-
33	BCR	B	845	-	-	13/29/63/63	0/2/2/2
37	A86	13	313	25	-	11/30/86/90	0/3/3/3
38	KC1	8	313	20	-	5/15/71/71	-
38	KC1	12	305	24	-	7/15/71/71	-
30	CLA	9	308	21	1/1/15/20	16/37/115/115	-
39	DD6	4	316	-	-	14/26/80/80	0/3/3/3
30	CLA	6	305	18	1/1/15/20	5/37/115/115	-
38	KC1	12	311	24	-	6/15/71/71	-
30	CLA	A	807	1	1/1/15/20	13/37/115/115	-
36	LMG	B	847	-	-	25/50/70/70	0/1/1/1
38	KC1	6	313	18	-	5/15/71/71	-
30	CLA	2	303	14	-	13/25/103/115	-
37	A86	5	316	-	-	6/34/90/90	0/3/3/3
30	CLA	B	804	2	1/1/12/20	6/22/100/115	-
30	CLA	15	314	30,27	-	4/13/91/115	-
37	A86	10	316	-	-	11/34/90/90	0/3/3/3
37	A86	14	318	-	-	17/34/90/90	0/3/3/3
30	CLA	B	835	2	1/1/15/20	6/37/115/115	-
32	SF4	C	102	3	-	-	0/6/5/5
30	CLA	2	301	14,2	1/1/15/20	12/37/115/115	-
30	CLA	7	309	19	1/1/15/20	10/37/115/115	-
30	CLA	9	302	9,21	1/1/12/20	7/21/99/115	-
30	CLA	14	310	-	1/1/12/20	5/19/97/115	-
36	LMG	2u	204	12	-	14/26/46/70	0/1/1/1
38	KC1	3	304	15	-	6/15/71/71	-
30	CLA	A	835	1	1/1/15/20	9/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	KC1	1	306	13	-	8/15/71/71	-
38	KC1	16	304	28	-	8/15/71/71	-
33	BCR	B	844	-	-	9/29/63/63	0/2/2/2
30	CLA	4	302	16	1/1/15/20	10/37/115/115	-
30	CLA	A	822	40	1/1/15/20	8/37/115/115	-
35	LMT	6	302	-	-	3/17/57/61	0/2/2/2
30	CLA	5	309	34	1/1/15/20	9/37/115/115	-
30	CLA	13	307	25	1/1/15/20	9/37/115/115	-
30	CLA	B	815	2	1/1/11/20	1/13/91/115	-
30	CLA	A	820	1	1/1/15/20	16/37/115/115	-
35	LMT	7	321	-	-	4/21/61/61	0/2/2/2
30	CLA	B	836	2	1/1/11/20	3/16/94/115	-
30	CLA	15	313	27	-	11/37/115/115	-
30	CLA	B	809	2	1/1/15/20	10/37/115/115	-
37	A86	10	317	-	-	12/34/90/90	0/3/3/3
33	BCR	A	850	-	-	11/29/63/63	0/2/2/2
36	LMG	B	849	2	-	15/38/58/70	0/1/1/1
30	CLA	7	304	19	1/1/15/20	7/37/115/115	-
35	LMT	11	317	-	-	2/21/61/61	0/2/2/2
37	A86	14	314	-	-	13/34/90/90	0/3/3/3
35	LMT	15	301	-	-	6/21/61/61	0/2/2/2
38	KC1	11	307	23	-	10/15/71/71	-
38	KC1	13	312	25	-	9/15/71/71	-
36	LMG	8	320	-	-	20/37/57/70	0/1/1/1
38	KC1	14	308	30,26	-	9/15/71/71	-
30	CLA	12	307	24	1/1/11/20	4/15/93/115	-
39	DD6	7	318	-	-	13/26/80/80	0/3/3/3
33	BCR	F	204	-	-	10/29/63/63	0/2/2/2
37	A86	13	315	-	-	13/34/90/90	0/3/3/3
30	CLA	A	816	1,35	1/1/15/20	17/37/115/115	-
30	CLA	B	834	2	1/1/14/20	8/31/109/115	-
39	DD6	6	319	-	-	11/26/80/80	0/3/3/3
30	CLA	3	301	15	1/1/15/20	7/37/115/115	-
30	CLA	1	302	30,13	1/1/15/20	10/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	A	839	1	1/1/15/20	14/37/115/115	-
30	CLA	12	303	24	1/1/15/20	6/37/115/115	-
37	A86	8	315	-	-	7/34/90/90	0/3/3/3
30	CLA	15	308	30,27	1/1/11/20	7/13/91/115	-
37	A86	14	316	-	-	11/34/90/90	0/3/3/3
30	CLA	B	825	2	1/1/15/20	7/37/115/115	-
30	CLA	11	306	40	1/1/13/20	8/25/103/115	-
30	CLA	A	806	1	1/1/15/20	15/37/115/115	-
35	LMT	11	302	-	-	0/21/61/61	0/2/2/2
37	A86	11	301	-	-	14/34/90/90	0/3/3/3
30	CLA	B	805	2	1/1/15/20	9/37/115/115	-
36	LMG	8	321	36	-	5/24/44/70	0/1/1/1
30	CLA	B	801	2	1/1/15/20	8/37/115/115	-
35	LMT	7	301	30	-	3/21/61/61	0/2/2/2
39	DD6	2	315	-	-	13/26/80/80	0/3/3/3
30	CLA	B	808	2	1/1/15/20	14/37/115/115	-
37	A86	15	320	-	-	15/34/90/90	0/3/3/3
38	KC1	2	306	14	-	6/15/71/71	-
38	KC1	13	310	25	-	5/15/71/71	-
30	CLA	F	202	40	1/1/15/20	18/37/115/115	-
36	LMG	14	321	-	-	13/33/53/70	0/1/1/1
30	CLA	A	817	40,36	-	4/18/96/115	-
38	KC1	9	304	21	-	6/15/71/71	-
30	CLA	2	310	14	1/1/15/20	6/37/115/115	-
30	CLA	16	305	28	1/1/12/20	3/19/97/115	-
30	CLA	10	305	40	1/1/15/20	10/37/115/115	-
38	KC1	8	310	20	-	6/15/71/71	-
33	BCR	B	846	-	-	7/29/63/63	0/2/2/2
30	CLA	A	838	1	1/1/12/20	4/21/99/115	-
35	LMT	A	857	-	-	3/21/61/61	0/2/2/2
30	CLA	B	833	30,40	1/1/15/20	11/37/115/115	-
37	A86	7	319	-	-	10/34/90/90	0/3/3/3
38	KC1	4	310	16	-	4/15/71/71	-
30	CLA	15	304	30,39,27	1/1/15/20	20/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LMT	12	319	-	-	0/21/61/61	0/2/2/2
30	CLA	B	818	2	1/1/14/20	6/31/109/115	-
30	CLA	1	304	13	1/1/15/20	11/37/115/115	-
38	KC1	14	311	26	-	5/15/71/71	-
30	CLA	9	306	37,21	1/1/11/20	6/13/91/115	-
38	KC1	5	306	17	-	10/15/71/71	-
30	CLA	8	309	20	-	3/16/94/115	-
37	A86	10	301	22	-	6/34/90/90	0/3/3/3
37	A86	15	321	27	-	13/34/90/90	0/3/3/3
30	CLA	6	316	40	1/1/13/20	7/25/103/115	-
30	CLA	5	311	40,17	1/1/15/20	15/37/115/115	-
30	CLA	A	836	1	1/1/12/20	7/24/102/115	-
34	LHG	2	320	30	-	12/31/31/53	-
39	DD6	5	314	-	-	10/26/80/80	0/3/3/3
32	SF4	A	846	1,2	-	-	0/6/5/5
30	CLA	B	811	30,2	1/1/15/20	10/37/115/115	-
30	CLA	10	307	22	1/1/15/20	10/37/115/115	-
33	BCR	A	848	-	-	10/29/63/63	0/2/2/2
35	LMT	A	855	-	-	4/21/61/61	0/2/2/2
30	CLA	5	304	17	1/1/15/20	12/37/115/115	-
35	LMT	1	311	-	-	4/21/61/61	0/2/2/2
30	CLA	15	302	30,27	-	15/37/115/115	-
30	CLA	5	303	17	1/1/15/20	6/37/115/115	-
35	LMT	B	852	-	-	8/21/61/61	0/2/2/2
38	KC1	1	308	13	-	5/15/71/71	-
30	CLA	15	309	27	-	10/37/115/115	-
38	KC1	5	305	17	-	5/15/71/71	-
30	CLA	F	201	40	1/1/15/20	10/37/115/115	-
30	CLA	2	313	14	-	3/13/91/115	-
37	A86	6	320	-	-	9/34/90/90	0/3/3/3
37	A86	10	302	-	-	13/34/90/90	0/3/3/3
30	CLA	A	831	1	1/1/15/20	9/37/115/115	-
33	BCR	A	849	-	-	12/29/63/63	0/2/2/2
37	A86	11	314	-	-	14/34/90/90	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	DD6	2	317	-	-	14/26/80/80	0/3/3/3
30	CLA	16	302	28	1/1/15/20	9/37/115/115	-
37	A86	7	316	-	-	7/34/90/90	0/3/3/3
39	DD6	10	313	-	-	11/26/80/80	0/3/3/3
30	CLA	14	307	38	-	10/37/115/115	-
30	CLA	B	814	2	1/1/13/20	5/25/103/115	-
30	CLA	11	304	23	1/1/15/20	9/37/115/115	-
30	CLA	16	309	28	-	4/13/91/115	-
39	DD6	10	314	-	-	9/26/80/80	0/3/3/3
38	KC1	3	308	15	-	8/15/71/71	-
30	CLA	16	308	28	1/1/11/20	6/13/91/115	-
30	CLA	16	310	28	1/1/11/20	7/13/91/115	-
30	CLA	6	304	18	1/1/15/20	10/37/115/115	-
37	A86	2u	205	-	-	11/34/90/90	0/3/3/3
37	A86	9	316	30	-	11/34/90/90	0/3/3/3
30	CLA	16	303	28	1/1/15/20	19/37/115/115	-
30	CLA	5	308	17	-	14/37/115/115	-
30	CLA	4	304	-	1/1/14/20	9/31/109/115	-
30	CLA	B	851	14,2	-	14/37/115/115	-
30	CLA	16	306	28	1/1/12/20	13/22/100/115	-
33	BCR	L	205	-	-	8/29/63/63	0/2/2/2
30	CLA	12	321	24,26	1/1/15/20	4/37/115/115	-
30	CLA	15	306	-	1/1/11/20	6/13/91/115	-
37	A86	15	317	30	-	16/34/90/90	0/3/3/3
30	CLA	4	301	16,2	1/1/11/20	7/18/96/115	-
29	CL0	A	801	1	3/3/20/25	4/37/135/135	-
30	CLA	14	303	26	1/1/13/20	7/28/106/115	-
30	CLA	8	301	20	1/1/15/20	20/37/115/115	-
33	BCR	2u	201	-	-	11/29/63/63	0/2/2/2
30	CLA	6	309	18	1/1/15/20	12/37/115/115	-
30	CLA	15	312	27	1/1/11/20	5/13/91/115	-
30	CLA	A	837	1	1/1/11/20	7/13/91/115	-
30	CLA	A	840	1	1/1/11/20	5/16/94/115	-
30	CLA	5	302	17	1/1/15/20	13/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	B	812	2	1/1/15/20	8/37/115/115	-
37	A86	8	318	-	-	15/34/90/90	0/3/3/3
30	CLA	13	301	25	1/1/15/20	15/37/115/115	-
30	CLA	4	309	-	1/1/15/20	9/37/115/115	-
33	BCR	I	101	-	-	5/29/63/63	0/2/2/2
37	A86	14	315	26	-	11/34/90/90	0/3/3/3
34	LHG	A	852	-	-	25/53/53/53	-
36	LMG	6	301	30	-	16/28/48/70	0/1/1/1
30	CLA	A	812	30,1	1/1/15/20	14/37/115/115	-
38	KC1	11	311	23	-	10/15/71/71	-
37	A86	15	323	-	-	15/34/90/90	0/3/3/3
30	CLA	13	302	25	1/1/15/20	16/37/115/115	-
33	BCR	A	851	-	-	7/29/63/63	0/2/2/2
37	A86	11	316	-	-	12/34/90/90	0/3/3/3
30	CLA	7	307	19	-	19/37/115/115	-
30	CLA	4	306	16	1/1/15/20	10/37/115/115	-
31	PQN	B	840	-	-	6/23/43/43	0/2/2/2
35	LMT	12	320	-	-	1/21/61/61	0/2/2/2
30	CLA	A	818	1	-	7/24/102/115	-
37	A86	5	315	-	-	6/34/90/90	0/3/3/3
39	DD6	8	316	-	-	13/26/80/80	0/3/3/3
30	CLA	2	309	14,34	1/1/15/20	11/37/115/115	-

All (7031) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	2	315	DD6	C10-C11	26.29	1.70	1.35
39	11	313	DD6	C10-C11	25.97	1.70	1.35
39	6	303	DD6	C10-C11	25.93	1.70	1.35
39	15	318	DD6	C10-C11	25.83	1.70	1.35
39	10	313	DD6	C10-C11	25.83	1.70	1.35
39	3	313	DD6	C10-C11	25.79	1.70	1.35
39	13	314	DD6	C10-C11	25.74	1.69	1.35
39	15	319	DD6	C10-C11	25.72	1.69	1.35
39	10	314	DD6	C10-C11	25.68	1.69	1.35
39	5	313	DD6	C10-C11	25.68	1.69	1.35
39	7	318	DD6	C10-C11	25.66	1.69	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	2	317	DD6	C10-C11	25.63	1.69	1.35
39	7	302	DD6	C10-C11	25.55	1.69	1.35
39	3	316	DD6	C10-C11	25.50	1.69	1.35
39	12	315	DD6	C10-C11	25.49	1.69	1.35
39	3	312	DD6	C10-C11	25.49	1.69	1.35
39	1	310	DD6	C10-C11	25.47	1.69	1.35
39	4	313	DD6	C10-C11	25.46	1.69	1.35
39	12	317	DD6	C10-C11	25.45	1.69	1.35
39	16	313	DD6	C10-C11	25.42	1.69	1.35
39	7	317	DD6	C10-C11	25.38	1.69	1.35
39	6	318	DD6	C10-C11	25.12	1.69	1.35
39	8	317	DD6	C10-C11	25.11	1.69	1.35
39	7	314	DD6	C10-C11	25.09	1.69	1.35
39	4	316	DD6	C10-C11	25.08	1.69	1.35
39	6	319	DD6	C10-C11	25.06	1.69	1.35
39	5	314	DD6	C10-C11	25.02	1.69	1.35
39	9	314	DD6	C10-C11	25.01	1.68	1.35
39	6	321	DD6	C10-C11	24.90	1.68	1.35
39	2	316	DD6	C10-C11	24.86	1.68	1.35
39	8	316	DD6	C10-C11	24.78	1.68	1.35
39	6	319	DD6	C5-C6	18.16	1.59	1.35
39	4	313	DD6	C5-C6	18.01	1.59	1.35
39	13	314	DD6	C5-C6	17.83	1.59	1.35
39	2	316	DD6	C5-C6	17.81	1.59	1.35
39	7	317	DD6	C5-C6	17.67	1.59	1.35
39	16	313	DD6	C5-C6	17.66	1.59	1.35
39	3	316	DD6	C5-C6	17.56	1.59	1.35
39	2	317	DD6	C5-C6	17.56	1.59	1.35
39	10	314	DD6	C5-C6	17.55	1.59	1.35
39	3	313	DD6	C5-C6	17.53	1.59	1.35
39	5	313	DD6	C5-C6	17.52	1.59	1.35
39	11	313	DD6	C5-C6	17.49	1.59	1.35
39	6	318	DD6	C5-C6	17.46	1.58	1.35
39	10	313	DD6	C5-C6	17.46	1.58	1.35
39	12	317	DD6	C5-C6	17.43	1.58	1.35
39	9	314	DD6	C5-C6	17.42	1.58	1.35
39	6	303	DD6	C5-C6	17.41	1.58	1.35
39	8	316	DD6	C5-C6	17.40	1.58	1.35
39	3	312	DD6	C5-C6	17.39	1.58	1.35
39	7	302	DD6	C5-C6	17.38	1.58	1.35
39	7	314	DD6	C5-C6	17.37	1.58	1.35
39	15	319	DD6	C5-C6	17.32	1.58	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	7	318	DD6	C5-C6	17.29	1.58	1.35
39	12	315	DD6	C5-C6	17.27	1.58	1.35
39	15	318	DD6	C5-C6	17.22	1.58	1.35
39	2	315	DD6	C5-C6	17.22	1.58	1.35
39	6	321	DD6	C5-C6	17.22	1.58	1.35
39	1	310	DD6	C5-C6	17.18	1.58	1.35
39	4	316	DD6	C5-C6	17.18	1.58	1.35
39	8	317	DD6	C5-C6	17.17	1.58	1.35
39	5	314	DD6	C5-C6	16.97	1.58	1.35
37	15	322	A86	C14-C13	15.15	1.69	1.51
37	15	315	A86	C14-C13	14.79	1.69	1.51
37	9	313	A86	C14-C13	14.53	1.68	1.51
37	16	314	A86	C14-C13	14.49	1.68	1.51
37	10	317	A86	C14-C13	14.35	1.68	1.51
37	2u	205	A86	C14-C13	14.34	1.68	1.51
37	15	320	A86	C14-C13	14.33	1.68	1.51
37	15	321	A86	C14-C13	14.27	1.68	1.51
37	9	316	A86	C14-C13	14.16	1.68	1.51
37	14	320	A86	C14-C13	14.14	1.68	1.51
37	13	315	A86	C14-C13	14.10	1.68	1.51
39	4	316	DD6	C36-C31	14.08	1.50	1.34
39	15	319	DD6	C36-C31	14.07	1.50	1.34
37	5	301	A86	C14-C13	14.07	1.68	1.51
37	7	319	A86	C14-C13	14.06	1.68	1.51
37	4	317	A86	C14-C13	14.05	1.68	1.51
37	14	301	A86	C14-C13	14.04	1.68	1.51
37	3	315	A86	C14-C13	14.02	1.68	1.51
37	2	318	A86	C14-C13	14.01	1.68	1.51
37	15	316	A86	C14-C13	13.99	1.68	1.51
37	5	315	A86	C14-C13	13.99	1.68	1.51
37	11	315	A86	C14-C13	13.98	1.68	1.51
37	11	314	A86	C14-C13	13.94	1.68	1.51
37	5	316	A86	C14-C13	13.94	1.68	1.51
37	4	315	A86	C14-C13	13.93	1.68	1.51
37	9	315	A86	C14-C13	13.87	1.68	1.51
39	3	316	DD6	C36-C31	13.86	1.50	1.34
37	14	318	A86	C14-C13	13.86	1.68	1.51
37	10	315	A86	C14-C13	13.84	1.68	1.51
37	8	318	A86	C14-C13	13.83	1.67	1.51
37	15	323	A86	C14-C13	13.82	1.67	1.51
37	14	316	A86	C14-C13	13.81	1.67	1.51
37	15	317	A86	C14-C13	13.81	1.67	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	2	319	A86	C14-C13	13.76	1.67	1.51
37	2	302	A86	C14-C13	13.75	1.67	1.51
37	14	315	A86	C14-C13	13.74	1.67	1.51
39	7	302	DD6	C36-C31	13.73	1.50	1.34
37	12	316	A86	C14-C13	13.71	1.67	1.51
37	14	317	A86	C14-C13	13.71	1.67	1.51
39	1	310	DD6	C36-C31	13.70	1.50	1.34
37	16	312	A86	C14-C13	13.69	1.67	1.51
39	6	321	DD6	C36-C31	13.69	1.50	1.34
37	12	314	A86	C14-C13	13.69	1.67	1.51
39	8	317	DD6	C36-C31	13.68	1.50	1.34
39	5	313	DD6	C36-C31	13.66	1.50	1.34
37	11	316	A86	C14-C13	13.64	1.67	1.51
39	13	314	DD6	C36-C31	13.63	1.50	1.34
39	6	319	DD6	C36-C31	13.62	1.50	1.34
37	13	313	A86	C14-C13	13.62	1.67	1.51
37	14	319	A86	C14-C13	13.61	1.67	1.51
39	7	317	DD6	C36-C31	13.59	1.50	1.34
37	10	301	A86	C14-C13	13.59	1.67	1.51
37	4	314	A86	C14-C13	13.58	1.67	1.51
37	10	316	A86	C14-C13	13.58	1.67	1.51
37	14	314	A86	C14-C13	13.58	1.67	1.51
37	3	314	A86	C14-C13	13.56	1.67	1.51
39	2	316	DD6	C36-C31	13.56	1.50	1.34
39	10	313	DD6	C36-C31	13.53	1.50	1.34
39	9	314	DD6	C36-C31	13.51	1.50	1.34
39	12	315	DD6	C36-C31	13.48	1.49	1.34
39	16	313	DD6	C36-C31	13.47	1.49	1.34
39	10	314	DD6	C36-C31	13.46	1.49	1.34
37	10	302	A86	C14-C13	13.43	1.67	1.51
39	11	313	DD6	C36-C31	13.39	1.49	1.34
39	3	312	DD6	C36-C31	13.37	1.49	1.34
37	4	312	A86	C14-C13	13.34	1.67	1.51
39	15	318	DD6	C36-C31	13.33	1.49	1.34
37	2u	203	A86	C14-C13	13.33	1.67	1.51
39	7	318	DD6	C36-C31	13.32	1.49	1.34
39	3	313	DD6	C36-C31	13.29	1.49	1.34
37	7	315	A86	C14-C13	13.26	1.67	1.51
37	1	309	A86	C14-C13	13.25	1.67	1.51
39	2	317	DD6	C36-C31	13.25	1.49	1.34
39	4	313	DD6	C36-C31	13.24	1.49	1.34
39	8	316	DD6	C36-C31	13.22	1.49	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	11	301	A86	C14-C13	13.21	1.67	1.51
37	7	316	A86	C14-C13	13.20	1.67	1.51
39	6	303	DD6	C36-C31	13.19	1.49	1.34
39	2	315	DD6	C36-C31	13.18	1.49	1.34
39	7	314	DD6	C36-C31	13.14	1.49	1.34
39	5	314	DD6	C36-C31	13.09	1.49	1.34
37	6	320	A86	C14-C13	13.02	1.67	1.51
39	6	318	DD6	C36-C31	12.98	1.49	1.34
39	12	317	DD6	C36-C31	12.97	1.49	1.34
37	8	315	A86	C14-C13	12.72	1.66	1.51
38	13	312	KC1	C1D-ND	10.26	1.44	1.35
38	13	311	KC1	C1D-ND	10.15	1.44	1.35
38	12	313	KC1	C1D-ND	10.10	1.44	1.35
38	13	306	KC1	C1D-ND	10.03	1.44	1.35
38	16	304	KC1	C1D-ND	9.99	1.44	1.35
38	13	308	KC1	C1D-ND	9.94	1.44	1.35
38	12	311	KC1	C1D-ND	9.90	1.44	1.35
38	11	311	KC1	C1D-ND	9.89	1.44	1.35
38	4	308	KC1	C1D-ND	9.89	1.44	1.35
38	8	314	KC1	C1D-ND	9.85	1.44	1.35
38	3	304	KC1	C1D-ND	9.85	1.44	1.35
38	11	312	KC1	C1D-ND	9.85	1.44	1.35
38	9	312	KC1	C1D-ND	9.84	1.44	1.35
38	12	309	KC1	C1D-ND	9.82	1.44	1.35
38	11	307	KC1	C1D-ND	9.79	1.43	1.35
38	9	311	KC1	C1D-ND	9.73	1.43	1.35
38	13	310	KC1	C1D-ND	9.72	1.43	1.35
38	16	311	KC1	C1D-ND	9.71	1.43	1.35
38	8	306	KC1	C1D-ND	9.70	1.43	1.35
38	11	305	KC1	C1D-ND	9.70	1.43	1.35
38	5	310	KC1	C1D-ND	9.69	1.43	1.35
38	4	310	KC1	C1D-ND	9.69	1.43	1.35
38	7	308	KC1	C1D-ND	9.68	1.43	1.35
38	14	311	KC1	C1D-ND	9.68	1.43	1.35
38	2	306	KC1	C1D-ND	9.68	1.43	1.35
38	10	310	KC1	C1D-ND	9.67	1.43	1.35
38	4	307	KC1	C1D-ND	9.66	1.43	1.35
38	3	311	KC1	C1D-ND	9.65	1.43	1.35
38	8	312	KC1	C1D-ND	9.65	1.43	1.35
38	12	305	KC1	C1D-ND	9.64	1.43	1.35
38	14	308	KC1	C1D-ND	9.64	1.43	1.35
38	1	306	KC1	C1D-ND	9.60	1.43	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	5	306	KC1	C1D-ND	9.59	1.43	1.35
38	13	305	KC1	C1D-ND	9.53	1.43	1.35
38	5	305	KC1	C1D-ND	9.53	1.43	1.35
38	10	312	KC1	C1D-ND	9.53	1.43	1.35
38	6	313	KC1	C1D-ND	9.52	1.43	1.35
38	10	306	KC1	C1D-ND	9.47	1.43	1.35
37	13	313	A86	C30-C29	9.47	1.47	1.32
38	8	310	KC1	C1D-ND	9.45	1.43	1.35
38	2	314	KC1	C1D-ND	9.42	1.43	1.35
38	9	304	KC1	C1D-ND	9.42	1.43	1.35
38	3	308	KC1	C1D-ND	9.39	1.43	1.35
38	8	307	KC1	C1D-ND	9.39	1.43	1.35
37	9	316	A86	C30-C29	9.38	1.47	1.32
38	6	311	KC1	C1D-ND	9.37	1.43	1.35
38	6	312	KC1	C1D-ND	9.34	1.43	1.35
38	2	312	KC1	C1D-ND	9.34	1.43	1.35
38	14	306	KC1	C1D-ND	9.32	1.43	1.35
37	15	317	A86	C30-C29	9.30	1.47	1.32
37	10	317	A86	C30-C29	9.28	1.47	1.32
37	15	322	A86	C30-C29	9.28	1.47	1.32
37	9	315	A86	C30-C29	9.27	1.47	1.32
37	15	320	A86	C30-C29	9.26	1.47	1.32
38	7	313	KC1	C1D-ND	9.26	1.43	1.35
37	15	323	A86	C30-C29	9.23	1.47	1.32
38	9	310	KC1	C1D-ND	9.23	1.43	1.35
37	13	315	A86	C30-C29	9.16	1.47	1.32
38	1	308	KC1	C1D-ND	9.16	1.43	1.35
37	3	314	A86	C30-C29	9.15	1.47	1.32
37	7	319	A86	C30-C29	9.11	1.47	1.32
37	3	315	A86	C30-C29	9.10	1.47	1.32
37	2	302	A86	C30-C29	9.09	1.47	1.32
37	15	315	A86	C30-C29	9.07	1.47	1.32
37	14	320	A86	C30-C29	9.07	1.47	1.32
37	14	317	A86	C30-C29	9.07	1.47	1.32
37	14	316	A86	C30-C29	9.05	1.47	1.32
38	6	308	KC1	C1D-ND	9.04	1.43	1.35
37	14	301	A86	C30-C29	9.03	1.47	1.32
37	10	315	A86	C30-C29	9.01	1.47	1.32
37	14	318	A86	C30-C29	9.00	1.47	1.32
37	16	312	A86	C30-C29	8.99	1.46	1.32
37	4	317	A86	C30-C29	8.97	1.46	1.32
37	10	302	A86	C30-C29	8.96	1.46	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	5	301	A86	C30-C29	8.93	1.46	1.32
37	12	316	A86	C30-C29	8.93	1.46	1.32
38	8	311	KC1	C1D-ND	8.91	1.43	1.35
39	15	319	DD6	C23-C16	8.91	1.71	1.53
37	4	315	A86	C30-C29	8.91	1.46	1.32
37	6	320	A86	C30-C29	8.90	1.46	1.32
37	14	314	A86	C30-C29	8.90	1.46	1.32
37	11	314	A86	C30-C29	8.89	1.46	1.32
37	11	316	A86	C30-C29	8.88	1.46	1.32
37	4	314	A86	C30-C29	8.88	1.46	1.32
39	2	317	DD6	C23-C16	8.86	1.71	1.53
37	15	316	A86	C30-C29	8.86	1.46	1.32
37	5	315	A86	C30-C29	8.84	1.46	1.32
37	15	321	A86	C30-C29	8.84	1.46	1.32
37	5	316	A86	C30-C29	8.83	1.46	1.32
37	11	301	A86	C30-C29	8.83	1.46	1.32
38	5	312	KC1	C1D-ND	8.82	1.43	1.35
39	12	315	DD6	C23-C16	8.80	1.71	1.53
39	6	321	DD6	C13-C11	-8.80	1.27	1.45
37	12	314	A86	C30-C29	8.76	1.46	1.32
38	8	313	KC1	C1D-ND	8.76	1.43	1.35
37	16	314	A86	C30-C29	8.75	1.46	1.32
39	10	313	DD6	C23-C16	8.74	1.70	1.53
37	14	319	A86	C30-C29	8.73	1.46	1.32
37	11	315	A86	C30-C29	8.73	1.46	1.32
37	10	316	A86	C30-C29	8.69	1.46	1.32
39	5	314	DD6	C13-C11	-8.68	1.27	1.45
37	2	318	A86	C30-C29	8.68	1.46	1.32
37	2u	205	A86	C30-C29	8.66	1.46	1.32
39	1	310	DD6	C23-C16	8.63	1.70	1.53
39	15	318	DD6	C23-C16	8.63	1.70	1.53
39	3	312	DD6	C23-C16	8.61	1.70	1.53
37	1	309	A86	C30-C29	8.61	1.46	1.32
39	5	313	DD6	C13-C11	-8.58	1.27	1.45
37	8	318	A86	C30-C29	8.56	1.46	1.32
37	10	301	A86	C30-C29	8.54	1.46	1.32
39	1	310	DD6	C13-C11	-8.54	1.27	1.45
39	2	317	DD6	C13-C11	-8.54	1.27	1.45
37	4	312	A86	C30-C29	8.53	1.46	1.32
37	14	315	A86	C30-C29	8.53	1.46	1.32
39	6	303	DD6	C23-C16	8.51	1.70	1.53
39	5	314	DD6	C23-C16	8.48	1.70	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	8	317	DD6	C13-C11	-8.48	1.27	1.45
39	3	312	DD6	C13-C11	-8.47	1.27	1.45
39	5	313	DD6	C23-C16	8.45	1.70	1.53
39	6	318	DD6	C13-C11	-8.44	1.27	1.45
39	10	314	DD6	C13-C11	-8.44	1.27	1.45
39	7	318	DD6	C13-C11	-8.44	1.27	1.45
39	3	316	DD6	C23-C16	8.43	1.70	1.53
39	3	313	DD6	C23-C16	8.42	1.70	1.53
30	2	303	CLA	OBD-CAD	8.42	1.37	1.22
39	15	319	DD6	C13-C11	-8.42	1.27	1.45
39	15	318	DD6	C2-C1	8.42	1.46	1.35
37	2u	203	A86	C30-C29	8.42	1.46	1.32
39	7	317	DD6	C13-C11	-8.41	1.27	1.45
39	9	314	DD6	C13-C11	-8.39	1.27	1.45
39	2	315	DD6	C23-C16	8.39	1.70	1.53
39	16	313	DD6	C13-C11	-8.38	1.27	1.45
37	9	313	A86	C30-C29	8.38	1.45	1.32
39	12	317	DD6	C13-C11	-8.38	1.27	1.45
39	9	314	DD6	C23-C16	8.37	1.70	1.53
39	4	316	DD6	C23-C16	8.37	1.70	1.53
39	6	303	DD6	C13-C11	-8.36	1.28	1.45
39	12	315	DD6	C13-C11	-8.36	1.28	1.45
39	4	313	DD6	C13-C11	-8.34	1.28	1.45
39	11	313	DD6	C19-C20	8.34	1.63	1.52
39	6	318	DD6	C23-C16	8.30	1.70	1.53
39	15	318	DD6	C13-C11	-8.29	1.28	1.45
39	11	313	DD6	C23-C16	8.29	1.70	1.53
39	7	302	DD6	C2-C1	8.28	1.46	1.35
39	8	317	DD6	C23-C16	8.27	1.69	1.53
37	8	315	A86	C30-C29	8.26	1.45	1.32
39	7	318	DD6	C23-C16	8.25	1.69	1.53
39	7	314	DD6	C23-C16	8.25	1.69	1.53
39	12	317	DD6	C19-C20	8.24	1.63	1.52
39	13	314	DD6	C23-C16	8.24	1.69	1.53
39	4	316	DD6	C13-C11	-8.24	1.28	1.45
39	10	313	DD6	C2-C1	8.22	1.46	1.35
39	4	313	DD6	C23-C16	8.21	1.69	1.53
39	7	317	DD6	C23-C16	8.19	1.69	1.53
39	2	316	DD6	C23-C16	8.19	1.69	1.53
37	2	319	A86	C30-C29	8.17	1.45	1.32
39	6	319	DD6	C2-C1	8.16	1.46	1.35
37	7	316	A86	C30-C29	8.16	1.45	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	3	316	DD6	C13-C11	-8.15	1.28	1.45
39	10	313	DD6	C13-C11	-8.15	1.28	1.45
39	13	314	DD6	C2-C1	8.14	1.46	1.35
39	10	313	DD6	C19-C20	8.12	1.63	1.52
39	6	303	DD6	C19-C20	8.12	1.63	1.52
39	2	317	DD6	C2-C1	8.12	1.46	1.35
39	3	313	DD6	C2-C1	8.11	1.46	1.35
39	6	303	DD6	C2-C1	8.11	1.46	1.35
37	7	315	A86	C30-C29	8.10	1.45	1.32
39	11	313	DD6	C13-C11	-8.10	1.28	1.45
39	2	316	DD6	C13-C11	-8.08	1.28	1.45
39	6	321	DD6	C23-C16	8.06	1.69	1.53
39	12	317	DD6	C23-C16	8.06	1.69	1.53
39	10	314	DD6	C2-C1	8.05	1.46	1.35
39	7	302	DD6	C19-C20	8.05	1.63	1.52
39	6	318	DD6	C19-C20	8.04	1.63	1.52
39	5	313	DD6	C2-C1	8.03	1.46	1.35
39	6	319	DD6	C19-C20	8.03	1.63	1.52
39	13	314	DD6	C19-C20	8.03	1.63	1.52
39	6	318	DD6	C2-C1	8.02	1.46	1.35
39	8	316	DD6	C23-C16	8.02	1.69	1.53
39	3	313	DD6	C13-C11	-8.01	1.28	1.45
39	7	314	DD6	C13-C11	-8.01	1.28	1.45
37	2u	205	A86	C8-C6	8.00	1.63	1.45
39	10	314	DD6	C23-C16	7.99	1.69	1.53
39	2	316	DD6	C2-C1	7.99	1.46	1.35
39	7	314	DD6	C19-C20	7.98	1.63	1.52
37	4	314	A86	C8-C6	7.97	1.63	1.45
39	3	312	DD6	C2-C1	7.96	1.46	1.35
38	8	314	KC1	C2A-C3A	7.95	1.53	1.37
37	10	302	A86	C8-C6	7.94	1.63	1.45
39	7	318	DD6	C19-C20	7.93	1.63	1.52
39	11	313	DD6	C2-C1	7.91	1.46	1.35
39	12	315	DD6	C2-C1	7.90	1.46	1.35
39	7	302	DD6	C23-C16	7.88	1.69	1.53
39	16	313	DD6	C19-C20	7.88	1.63	1.52
37	14	314	A86	C4-C5	7.88	1.67	1.43
39	6	319	DD6	C13-C11	-7.86	1.29	1.45
39	7	314	DD6	C2-C1	7.86	1.46	1.35
37	11	301	A86	C8-C6	7.86	1.62	1.45
39	2	315	DD6	C2-C1	7.85	1.46	1.35
39	16	313	DD6	C2-C1	7.85	1.46	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	2	315	DD6	C13-C11	-7.84	1.29	1.45
39	7	302	DD6	C13-C11	-7.84	1.29	1.45
37	15	315	A86	C8-C6	7.84	1.62	1.45
39	13	314	DD6	C13-C11	-7.83	1.29	1.45
39	12	317	DD6	C2-C1	7.83	1.46	1.35
39	4	316	DD6	C2-C1	7.83	1.46	1.35
37	15	315	A86	C4-C5	7.83	1.67	1.43
38	11	312	KC1	C2A-C3A	7.81	1.53	1.37
39	10	314	DD6	C19-C20	7.81	1.63	1.52
38	4	308	KC1	C2A-C3A	7.81	1.53	1.37
39	7	317	DD6	C2-C1	7.81	1.46	1.35
39	3	316	DD6	C2-C1	7.80	1.46	1.35
37	2u	203	A86	C8-C6	7.80	1.62	1.45
37	13	313	A86	C4-C5	7.78	1.67	1.43
39	7	318	DD6	C2-C1	7.77	1.46	1.35
39	15	318	DD6	C19-C20	7.77	1.63	1.52
39	8	317	DD6	C2-C1	7.75	1.46	1.35
39	11	313	DD6	C9-C10	7.74	1.67	1.43
39	1	310	DD6	C2-C1	7.74	1.46	1.35
38	16	311	KC1	C2A-C3A	7.73	1.52	1.37
39	8	316	DD6	C13-C11	-7.72	1.29	1.45
39	2	317	DD6	C19-C20	7.72	1.63	1.52
39	3	313	DD6	C9-C10	7.71	1.67	1.43
37	15	320	A86	C4-C5	7.67	1.67	1.43
39	9	314	DD6	C2-C1	7.67	1.45	1.35
37	15	322	A86	C4-C5	7.66	1.67	1.43
39	15	319	DD6	C19-C20	7.65	1.63	1.52
37	15	320	A86	C8-C6	7.65	1.62	1.45
39	7	302	DD6	C9-C10	7.65	1.67	1.43
39	1	310	DD6	C19-C20	7.65	1.62	1.52
37	14	320	A86	C4-C5	7.64	1.67	1.43
39	8	316	DD6	C2-C1	7.64	1.45	1.35
39	13	314	DD6	C9-C10	7.64	1.67	1.43
37	9	316	A86	C8-C6	7.64	1.62	1.45
37	9	316	A86	C4-C5	7.63	1.67	1.43
39	4	313	DD6	C2-C1	7.62	1.45	1.35
37	13	313	A86	C8-C6	7.62	1.62	1.45
37	8	318	A86	C4-C5	7.62	1.67	1.43
39	12	317	DD6	C9-C10	7.62	1.67	1.43
39	6	319	DD6	C9-C10	7.61	1.67	1.43
39	3	316	DD6	C9-C10	7.60	1.67	1.43
39	2	317	DD6	C9-C10	7.60	1.67	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	7	317	DD6	C19-C20	7.60	1.62	1.52
39	16	313	DD6	C21-C20	-7.59	1.39	1.51
39	6	319	DD6	C23-C16	7.59	1.68	1.53
39	5	313	DD6	C9-C10	7.58	1.66	1.43
37	10	317	A86	C4-C5	7.58	1.66	1.43
37	16	312	A86	C4-C5	7.57	1.66	1.43
39	16	313	DD6	C23-C16	7.57	1.68	1.53
39	16	313	DD6	C9-C10	7.57	1.66	1.43
37	14	319	A86	C4-C5	7.57	1.66	1.43
37	13	315	A86	C4-C5	7.56	1.66	1.43
39	15	319	DD6	C2-C1	7.56	1.45	1.35
37	3	314	A86	C4-C5	7.56	1.66	1.43
38	14	308	KC1	C2A-C3A	7.55	1.52	1.37
37	15	323	A86	C4-C5	7.55	1.66	1.43
39	4	316	DD6	C19-C20	7.54	1.62	1.52
39	10	314	DD6	C9-C10	7.54	1.66	1.43
37	9	315	A86	C4-C5	7.54	1.66	1.43
39	7	318	DD6	C9-C10	7.54	1.66	1.43
39	3	313	DD6	C19-C20	7.54	1.62	1.52
39	3	312	DD6	C9-C10	7.53	1.66	1.43
37	15	317	A86	C4-C5	7.53	1.66	1.43
38	14	311	KC1	C2A-C3A	7.53	1.52	1.37
37	12	316	A86	C4-C5	7.53	1.66	1.43
39	12	315	DD6	C9-C10	7.53	1.66	1.43
39	7	317	DD6	C9-C10	7.52	1.66	1.43
37	15	316	A86	C4-C5	7.51	1.66	1.43
39	15	318	DD6	C9-C10	7.51	1.66	1.43
39	15	319	DD6	C9-C10	7.51	1.66	1.43
39	6	318	DD6	C9-C10	7.51	1.66	1.43
37	10	315	A86	C4-C5	7.51	1.66	1.43
39	5	314	DD6	C2-C1	7.51	1.45	1.35
38	12	309	KC1	C2A-C3A	7.50	1.52	1.37
37	15	323	A86	C8-C6	7.50	1.62	1.45
37	14	317	A86	C4-C5	7.50	1.66	1.43
39	6	303	DD6	C9-C10	7.50	1.66	1.43
37	14	318	A86	C4-C5	7.49	1.66	1.43
37	11	314	A86	C4-C5	7.49	1.66	1.43
38	13	312	KC1	C2A-C3A	7.48	1.52	1.37
39	10	313	DD6	C9-C10	7.48	1.66	1.43
39	3	312	DD6	C19-C20	7.48	1.62	1.52
38	16	304	KC1	C2A-C3A	7.47	1.52	1.37
39	1	310	DD6	C9-C10	7.47	1.66	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	13	315	A86	C8-C6	7.47	1.62	1.45
39	4	316	DD6	C9-C10	7.47	1.66	1.43
37	12	314	A86	C4-C5	7.47	1.66	1.43
37	5	316	A86	C4-C5	7.47	1.66	1.43
37	3	315	A86	C4-C5	7.47	1.66	1.43
39	9	314	DD6	C19-C20	7.46	1.62	1.52
37	15	322	A86	C8-C6	7.46	1.62	1.45
37	5	301	A86	C4-C5	7.45	1.66	1.43
39	3	316	DD6	C19-C20	7.44	1.62	1.52
37	2	302	A86	C4-C5	7.43	1.66	1.43
37	14	314	A86	C8-C6	7.43	1.61	1.45
37	14	301	A86	C4-C5	7.42	1.66	1.43
31	A	845	PQN	C3-C2	7.42	1.48	1.35
38	8	306	KC1	C2A-C3A	7.42	1.52	1.37
37	11	316	A86	C4-C5	7.41	1.66	1.43
37	1	309	A86	C4-C5	7.41	1.66	1.43
39	8	317	DD6	C9-C10	7.41	1.66	1.43
37	9	316	A86	C19-C20	7.41	1.62	1.52
37	16	314	A86	C19-C20	7.41	1.62	1.52
38	11	311	KC1	C2A-C3A	7.40	1.52	1.37
37	10	317	A86	C8-C6	7.40	1.61	1.45
37	10	302	A86	C4-C5	7.40	1.66	1.43
39	6	321	DD6	C9-C10	7.40	1.66	1.43
37	4	314	A86	C4-C5	7.39	1.66	1.43
37	9	315	A86	C8-C6	7.39	1.61	1.45
37	5	315	A86	C4-C5	7.39	1.66	1.43
38	7	308	KC1	C2A-C3A	7.39	1.52	1.37
39	4	313	DD6	C9-C10	7.39	1.66	1.43
37	14	320	A86	C8-C6	7.38	1.61	1.45
39	9	314	DD6	C9-C10	7.37	1.66	1.43
37	7	315	A86	C4-C5	7.37	1.66	1.43
38	13	310	KC1	C2A-C3A	7.37	1.52	1.37
39	7	314	DD6	C9-C10	7.37	1.66	1.43
37	5	316	A86	C8-C6	7.36	1.61	1.45
37	16	314	A86	C4-C5	7.36	1.66	1.43
37	7	319	A86	C8-C6	7.36	1.61	1.45
37	10	315	A86	C8-C6	7.36	1.61	1.45
38	3	308	KC1	C2A-C3A	7.35	1.52	1.37
39	6	321	DD6	C2-C1	7.35	1.45	1.35
38	4	307	KC1	C2A-C3A	7.35	1.52	1.37
37	11	315	A86	C4-C5	7.35	1.66	1.43
37	2	319	A86	C4-C5	7.34	1.66	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	14	315	A86	C4-C5	7.34	1.66	1.43
37	14	316	A86	C4-C5	7.34	1.66	1.43
37	13	315	A86	C19-C20	7.34	1.62	1.52
39	8	317	DD6	C19-C20	7.34	1.62	1.52
39	6	321	DD6	C19-C20	7.34	1.62	1.52
37	4	312	A86	C4-C5	7.34	1.66	1.43
37	2	318	A86	C4-C5	7.33	1.66	1.43
37	11	301	A86	C4-C5	7.33	1.66	1.43
37	2u	205	A86	C4-C5	7.33	1.66	1.43
37	15	321	A86	C4-C5	7.33	1.66	1.43
39	8	316	DD6	C9-C10	7.33	1.66	1.43
39	2	315	DD6	C9-C10	7.33	1.66	1.43
37	15	317	A86	C8-C6	7.32	1.61	1.45
37	14	319	A86	C8-C6	7.31	1.61	1.45
38	13	308	KC1	C2A-C3A	7.31	1.52	1.37
39	2	315	DD6	C19-C20	7.31	1.62	1.52
38	11	307	KC1	C2A-C3A	7.30	1.52	1.37
37	5	315	A86	C8-C6	7.30	1.61	1.45
39	5	313	DD6	C19-C20	7.29	1.62	1.52
37	2	302	A86	C8-C6	7.28	1.61	1.45
38	8	310	KC1	C2A-C3A	7.28	1.52	1.37
37	15	321	A86	C19-C20	7.28	1.62	1.52
39	7	302	DD6	C24-C1	7.28	1.61	1.45
37	11	314	A86	C8-C6	7.28	1.61	1.45
37	12	316	A86	C8-C6	7.28	1.61	1.45
38	2	312	KC1	C2A-C3A	7.28	1.52	1.37
37	15	316	A86	C8-C6	7.28	1.61	1.45
39	5	314	DD6	C9-C10	7.27	1.66	1.43
38	14	306	KC1	C2A-C3A	7.26	1.52	1.37
37	16	312	A86	C8-C6	7.26	1.61	1.45
37	3	315	A86	C8-C6	7.26	1.61	1.45
38	12	311	KC1	C2A-C3A	7.25	1.52	1.37
37	10	316	A86	C4-C5	7.25	1.65	1.43
37	15	323	A86	C19-C20	7.25	1.62	1.52
37	4	317	A86	C4-C5	7.25	1.65	1.43
37	7	319	A86	C4-C5	7.25	1.65	1.43
38	4	310	KC1	C2A-C3A	7.25	1.52	1.37
38	12	305	KC1	C2A-C3A	7.24	1.51	1.37
37	2u	203	A86	C4-C5	7.24	1.65	1.43
37	14	301	A86	C8-C6	7.23	1.61	1.45
39	4	313	DD6	C19-C20	7.23	1.62	1.52
38	8	312	KC1	C2A-C3A	7.23	1.51	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	4	315	A86	C4-C5	7.23	1.65	1.43
39	2	316	DD6	C9-C10	7.22	1.65	1.43
37	3	314	A86	C8-C6	7.22	1.61	1.45
37	6	320	A86	C4-C5	7.21	1.65	1.43
37	14	319	A86	C19-C20	7.21	1.62	1.52
37	13	313	A86	C25-C26	7.20	1.65	1.43
37	16	314	A86	C8-C6	7.20	1.61	1.45
38	1	308	KC1	C2A-C3A	7.20	1.51	1.37
38	5	310	KC1	C2A-C3A	7.20	1.51	1.37
37	14	318	A86	C8-C6	7.19	1.61	1.45
37	14	318	A86	C19-C20	7.19	1.62	1.52
39	12	315	DD6	C19-C20	7.19	1.62	1.52
37	15	321	A86	C8-C6	7.19	1.61	1.45
37	5	301	A86	C8-C6	7.18	1.61	1.45
37	15	322	A86	C19-C20	7.18	1.62	1.52
38	3	304	KC1	C2A-C3A	7.17	1.51	1.37
39	2	317	DD6	C24-C1	7.17	1.61	1.45
31	B	840	PQN	C3-C2	7.17	1.48	1.35
37	13	313	A86	C19-C20	7.17	1.62	1.52
37	3	315	A86	C19-C20	7.17	1.62	1.52
37	14	317	A86	C8-C6	7.16	1.61	1.45
38	2	314	KC1	C2A-C3A	7.14	1.51	1.37
37	9	313	A86	C4-C5	7.14	1.65	1.43
37	10	317	A86	C19-C20	7.14	1.62	1.52
38	9	310	KC1	C2A-C3A	7.13	1.51	1.37
38	13	311	KC1	C2A-C3A	7.13	1.51	1.37
37	11	315	A86	C8-C6	7.13	1.61	1.45
37	15	320	A86	C19-C20	7.12	1.62	1.52
37	11	316	A86	C8-C6	7.11	1.61	1.45
37	1	309	A86	C19-C20	7.10	1.62	1.52
38	8	311	KC1	C2A-C3A	7.10	1.51	1.37
38	6	312	KC1	C2A-C3A	7.10	1.51	1.37
38	13	306	KC1	C2A-C3A	7.10	1.51	1.37
38	10	310	KC1	C2A-C3A	7.09	1.51	1.37
39	6	319	DD6	C24-C1	7.09	1.61	1.45
38	6	313	KC1	C2A-C3A	7.09	1.51	1.37
38	9	304	KC1	C2A-C3A	7.09	1.51	1.37
38	13	305	KC1	C2A-C3A	7.09	1.51	1.37
39	4	313	DD6	C24-C1	7.09	1.61	1.45
37	2	318	A86	C8-C6	7.08	1.61	1.45
38	10	312	KC1	C2A-C3A	7.07	1.51	1.37
39	2	315	DD6	C24-C1	7.07	1.61	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	14	315	A86	C19-C20	7.07	1.62	1.52
38	5	305	KC1	C2A-C3A	7.07	1.51	1.37
38	1	306	KC1	C2A-C3A	7.06	1.51	1.37
39	8	316	DD6	C21-C20	-7.06	1.40	1.51
38	6	311	KC1	C2A-C3A	7.06	1.51	1.37
39	15	318	DD6	C24-C1	7.06	1.61	1.45
39	15	319	DD6	C24-C1	7.05	1.61	1.45
37	15	317	A86	C19-C20	7.05	1.62	1.52
37	7	319	A86	C19-C20	7.05	1.62	1.52
37	11	316	A86	C19-C20	7.04	1.62	1.52
39	6	318	DD6	C24-C1	7.04	1.61	1.45
38	2	306	KC1	C2A-C3A	7.04	1.51	1.37
38	7	313	KC1	C2A-C3A	7.04	1.51	1.37
39	13	314	DD6	C24-C1	7.04	1.61	1.45
37	10	301	A86	C4-C5	7.03	1.65	1.43
37	8	318	A86	C19-C20	7.03	1.62	1.52
37	14	315	A86	C8-C6	7.02	1.61	1.45
37	14	316	A86	C8-C6	7.02	1.61	1.45
39	3	316	DD6	C24-C1	7.02	1.61	1.45
37	14	314	A86	C19-C20	7.02	1.62	1.52
37	4	312	A86	C8-C6	7.01	1.61	1.45
39	12	315	DD6	C24-C1	7.01	1.61	1.45
37	14	301	A86	C19-C20	7.00	1.62	1.52
37	2	319	A86	C8-C6	7.00	1.61	1.45
38	3	311	KC1	C2A-C3A	6.99	1.51	1.37
37	2	302	A86	C19-C20	6.99	1.62	1.52
38	5	312	KC1	C2A-C3A	6.99	1.51	1.37
39	4	316	DD6	C30-C29	6.99	1.40	1.20
37	11	314	A86	C19-C20	6.98	1.62	1.52
37	6	320	A86	C8-C6	6.98	1.60	1.45
37	12	316	A86	C19-C20	6.98	1.62	1.52
37	1	309	A86	C8-C6	6.98	1.60	1.45
39	7	317	DD6	C24-C1	6.98	1.60	1.45
37	15	316	A86	C19-C20	6.98	1.62	1.52
37	15	323	A86	C25-C26	6.98	1.65	1.43
39	2	316	DD6	C19-C20	6.98	1.62	1.52
39	6	303	DD6	C24-C1	6.97	1.60	1.45
39	3	313	DD6	C24-C1	6.96	1.60	1.45
37	12	314	A86	C19-C20	6.96	1.62	1.52
38	6	308	KC1	C2A-C3A	6.96	1.51	1.37
37	10	316	A86	C8-C6	6.95	1.60	1.45
39	8	317	DD6	C24-C1	6.95	1.60	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	8	315	A86	C4-C5	6.95	1.65	1.43
39	5	313	DD6	C24-C1	6.95	1.60	1.45
39	2	316	DD6	C24-C1	6.95	1.60	1.45
37	15	320	A86	C25-C26	6.94	1.65	1.43
37	15	316	A86	C25-C26	6.94	1.65	1.43
37	2	318	A86	C25-C26	6.94	1.64	1.43
39	3	312	DD6	C24-C1	6.94	1.60	1.45
37	4	315	A86	C8-C6	6.93	1.60	1.45
37	15	317	A86	C25-C26	6.93	1.64	1.43
37	2u	203	A86	C19-C20	6.93	1.61	1.52
37	14	317	A86	C19-C20	6.93	1.61	1.52
37	15	315	A86	C19-C20	6.93	1.61	1.52
37	3	315	A86	C25-C26	6.93	1.64	1.43
37	9	316	A86	C25-C26	6.92	1.64	1.43
39	10	314	DD6	C24-C1	6.91	1.60	1.45
37	4	317	A86	C8-C6	6.91	1.60	1.45
38	11	305	KC1	C2A-C3A	6.91	1.51	1.37
39	4	316	DD6	C24-C1	6.91	1.60	1.45
39	15	318	DD6	C30-C29	6.91	1.40	1.20
38	12	313	KC1	C2A-C3A	6.90	1.51	1.37
39	16	313	DD6	C24-C1	6.89	1.60	1.45
37	7	316	A86	C4-C5	6.89	1.64	1.43
39	9	314	DD6	C24-C1	6.89	1.60	1.45
37	5	315	A86	C19-C20	6.89	1.61	1.52
39	13	314	DD6	C30-C29	6.89	1.40	1.20
39	8	316	DD6	C19-C20	6.88	1.61	1.52
38	8	307	KC1	C2A-C3A	6.87	1.51	1.37
39	7	314	DD6	C24-C1	6.87	1.60	1.45
37	10	302	A86	C25-C26	6.86	1.64	1.43
38	10	306	KC1	C2A-C3A	6.86	1.51	1.37
37	10	315	A86	C19-C20	6.86	1.61	1.52
38	9	311	KC1	C2A-C3A	6.86	1.51	1.37
39	6	321	DD6	C24-C1	6.85	1.60	1.45
37	16	312	A86	C19-C20	6.85	1.61	1.52
39	7	318	DD6	C24-C1	6.85	1.60	1.45
37	15	321	A86	C25-C26	6.85	1.64	1.43
37	9	315	A86	C25-C26	6.84	1.64	1.43
38	12	311	KC1	CBA-CAA	6.84	1.53	1.33
39	5	314	DD6	C19-C20	6.84	1.61	1.52
39	12	317	DD6	C24-C1	6.84	1.60	1.45
37	10	317	A86	C25-C26	6.84	1.64	1.43
39	1	310	DD6	C24-C1	6.84	1.60	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	15	319	DD6	C30-C29	6.84	1.40	1.20
39	16	313	DD6	C30-C29	6.83	1.40	1.20
38	13	305	KC1	CBA-CAA	6.83	1.53	1.33
37	7	315	A86	C8-C6	6.83	1.60	1.45
39	10	313	DD6	C24-C1	6.82	1.60	1.45
37	11	316	A86	C25-C26	6.82	1.64	1.43
37	15	315	A86	C25-C26	6.82	1.64	1.43
38	5	306	KC1	C2A-C3A	6.82	1.51	1.37
37	15	322	A86	C25-C26	6.82	1.64	1.43
39	11	313	DD6	C24-C1	6.82	1.60	1.45
39	3	316	DD6	C30-C29	6.82	1.40	1.20
37	13	315	A86	C25-C26	6.82	1.64	1.43
39	2	315	DD6	C30-C29	6.81	1.40	1.20
37	12	314	A86	C8-C6	6.81	1.60	1.45
37	7	315	A86	C25-C26	6.81	1.64	1.43
39	12	315	DD6	C21-C20	-6.80	1.41	1.51
37	10	315	A86	C25-C26	6.80	1.64	1.43
37	3	314	A86	C25-C26	6.80	1.64	1.43
37	4	314	A86	C19-C20	6.79	1.61	1.52
37	14	317	A86	C25-C26	6.78	1.64	1.43
38	8	313	KC1	C2A-C3A	6.78	1.51	1.37
37	12	316	A86	C25-C26	6.78	1.64	1.43
37	9	313	A86	C8-C6	6.77	1.60	1.45
37	14	320	A86	C25-C26	6.77	1.64	1.43
37	14	318	A86	C25-C26	6.77	1.64	1.43
39	8	316	DD6	C24-C1	6.77	1.60	1.45
39	5	313	DD6	C30-C29	6.75	1.40	1.20
37	7	319	A86	C25-C26	6.75	1.64	1.43
37	11	301	A86	C19-C20	6.75	1.61	1.52
37	11	314	A86	C25-C26	6.75	1.64	1.43
39	6	303	DD6	C30-C29	6.75	1.40	1.20
37	5	301	A86	C25-C26	6.74	1.64	1.43
39	7	302	DD6	C30-C29	6.74	1.39	1.20
39	5	314	DD6	C24-C1	6.73	1.60	1.45
39	1	310	DD6	C30-C29	6.73	1.39	1.20
39	3	312	DD6	C30-C29	6.72	1.39	1.20
37	4	315	A86	C25-C26	6.72	1.64	1.43
37	12	314	A86	C25-C26	6.72	1.64	1.43
38	8	312	KC1	CBA-CAA	6.72	1.53	1.33
39	8	317	DD6	C30-C29	6.71	1.39	1.20
37	4	314	A86	C25-C26	6.71	1.64	1.43
39	4	313	DD6	C21-C20	-6.71	1.41	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	13	306	KC1	CBA-CAA	6.71	1.53	1.33
37	8	318	A86	C8-C6	6.71	1.60	1.45
37	4	312	A86	C19-C20	6.71	1.61	1.52
37	14	319	A86	C25-C26	6.71	1.64	1.43
38	6	308	KC1	CBA-CAA	6.70	1.53	1.33
39	2	317	DD6	C30-C29	6.70	1.39	1.20
38	11	312	KC1	CBA-CAA	6.70	1.53	1.33
38	14	308	KC1	CBA-CAA	6.70	1.53	1.33
39	10	313	DD6	C30-C29	6.69	1.39	1.20
37	14	316	A86	C25-C26	6.69	1.64	1.43
39	9	314	DD6	C30-C29	6.68	1.39	1.20
37	2	302	A86	C25-C26	6.68	1.64	1.43
39	10	314	DD6	C30-C29	6.68	1.39	1.20
37	6	320	A86	C25-C26	6.68	1.64	1.43
39	5	314	DD6	C21-C20	-6.67	1.41	1.51
37	4	315	A86	C19-C20	6.67	1.61	1.52
39	12	315	DD6	C30-C29	6.67	1.39	1.20
39	7	302	DD6	C21-C20	-6.67	1.41	1.51
38	12	305	KC1	CBA-CAA	6.66	1.53	1.33
39	7	317	DD6	C30-C29	6.66	1.39	1.20
37	5	315	A86	C25-C26	6.66	1.64	1.43
38	11	311	KC1	CBA-CAA	6.66	1.53	1.33
37	4	317	A86	C25-C26	6.66	1.64	1.43
38	5	310	KC1	CBA-CAA	6.65	1.53	1.33
39	3	313	DD6	C30-C29	6.65	1.39	1.20
39	9	314	DD6	C21-C20	-6.65	1.41	1.51
37	14	314	A86	C25-C26	6.65	1.64	1.43
38	16	304	KC1	CBA-CAA	6.64	1.53	1.33
37	11	301	A86	C25-C26	6.64	1.64	1.43
37	14	301	A86	C25-C26	6.64	1.64	1.43
39	11	313	DD6	C30-C29	6.64	1.39	1.20
38	7	313	KC1	CBA-CAA	6.63	1.53	1.33
38	9	312	KC1	CBA-CAA	6.63	1.53	1.33
38	9	312	KC1	C2A-C3A	6.63	1.50	1.37
37	11	315	A86	C25-C26	6.62	1.64	1.43
37	5	316	A86	C25-C26	6.62	1.64	1.43
37	16	312	A86	C25-C26	6.62	1.64	1.43
38	13	310	KC1	CBA-CAA	6.62	1.53	1.33
39	6	319	DD6	C30-C29	6.62	1.39	1.20
38	3	311	KC1	CBA-CAA	6.61	1.53	1.33
38	2	314	KC1	CBA-CAA	6.60	1.53	1.33
38	12	309	KC1	CBA-CAA	6.60	1.53	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	10	301	A86	C8-C6	6.60	1.60	1.45
37	10	301	A86	C25-C26	6.60	1.63	1.43
39	4	313	DD6	C30-C29	6.59	1.39	1.20
38	6	311	KC1	CBA-CAA	6.59	1.53	1.33
38	8	311	KC1	CBA-CAA	6.59	1.53	1.33
37	1	309	A86	C25-C26	6.59	1.63	1.43
37	10	316	A86	C25-C26	6.59	1.63	1.43
37	16	314	A86	C25-C26	6.59	1.63	1.43
38	4	310	KC1	CBA-CAA	6.58	1.53	1.33
39	8	316	DD6	C30-C29	6.58	1.39	1.20
38	5	305	KC1	CBA-CAA	6.58	1.53	1.33
38	4	307	KC1	CBA-CAA	6.58	1.53	1.33
37	2u	205	A86	C25-C26	6.57	1.63	1.43
37	14	315	A86	C25-C26	6.57	1.63	1.43
38	5	306	KC1	CBA-CAA	6.57	1.52	1.33
38	6	312	KC1	CBA-CAA	6.57	1.52	1.33
38	1	308	KC1	CBA-CAA	6.56	1.52	1.33
39	3	316	DD6	C21-C20	-6.56	1.41	1.51
37	9	313	A86	C19-C20	6.55	1.61	1.52
37	8	315	A86	C8-C6	6.55	1.60	1.45
38	8	307	KC1	CBA-CAA	6.55	1.52	1.33
39	2	316	DD6	C30-C29	6.54	1.39	1.20
38	12	313	KC1	CBA-CAA	6.54	1.52	1.33
39	7	318	DD6	C30-C29	6.54	1.39	1.20
38	13	308	KC1	CBA-CAA	6.54	1.52	1.33
39	6	321	DD6	C30-C29	6.54	1.39	1.20
39	7	314	DD6	C30-C29	6.54	1.39	1.20
38	16	311	KC1	CBA-CAA	6.53	1.52	1.33
38	10	310	KC1	CBA-CAA	6.53	1.52	1.33
39	12	317	DD6	C30-C29	6.53	1.39	1.20
38	14	311	KC1	CBA-CAA	6.53	1.52	1.33
38	4	308	KC1	CBA-CAA	6.53	1.52	1.33
38	11	307	KC1	CBA-CAA	6.52	1.52	1.33
38	10	312	KC1	CBA-CAA	6.52	1.52	1.33
38	2	306	KC1	CBA-CAA	6.51	1.52	1.33
38	3	308	KC1	CBA-CAA	6.51	1.52	1.33
38	14	306	KC1	CBA-CAA	6.51	1.52	1.33
38	9	310	KC1	CBA-CAA	6.51	1.52	1.33
37	5	316	A86	C19-C20	6.50	1.61	1.52
38	5	312	KC1	CBA-CAA	6.50	1.52	1.33
38	1	306	KC1	CBA-CAA	6.50	1.52	1.33
39	6	318	DD6	C30-C29	6.49	1.39	1.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	8	318	A86	C25-C26	6.49	1.63	1.43
37	4	312	A86	C25-C26	6.49	1.63	1.43
38	7	308	KC1	CBA-CAA	6.48	1.52	1.33
37	8	315	A86	C19-C20	6.48	1.61	1.52
39	7	317	DD6	C21-C20	-6.48	1.41	1.51
38	8	306	KC1	CBA-CAA	6.48	1.52	1.33
37	2u	203	A86	C25-C26	6.48	1.63	1.43
39	6	319	DD6	C21-C20	-6.48	1.41	1.51
30	15	310	CLA	C3B-C2B	6.48	1.49	1.40
37	14	316	A86	C19-C20	6.48	1.61	1.52
38	13	311	KC1	CBA-CAA	6.48	1.52	1.33
39	3	313	DD6	C21-C20	-6.47	1.41	1.51
39	7	318	DD6	C21-C20	-6.47	1.41	1.51
37	10	316	A86	C19-C20	6.47	1.61	1.52
38	13	312	KC1	CBA-CAA	6.46	1.52	1.33
38	3	304	KC1	CBA-CAA	6.46	1.52	1.33
39	5	314	DD6	C30-C29	6.44	1.39	1.20
30	9	301	CLA	C3B-C2B	6.44	1.49	1.40
30	L	203	CLA	C3B-C2B	6.44	1.49	1.40
38	9	304	KC1	CBA-CAA	6.43	1.52	1.33
38	9	311	KC1	CBA-CAA	6.43	1.52	1.33
38	2	312	KC1	CBA-CAA	6.43	1.52	1.33
38	8	313	KC1	CBA-CAA	6.42	1.52	1.33
38	8	310	KC1	CBA-CAA	6.42	1.52	1.33
38	10	306	KC1	CBA-CAA	6.42	1.52	1.33
39	7	314	DD6	C13-C14	6.42	1.46	1.32
39	1	310	DD6	C21-C20	-6.41	1.41	1.51
38	11	305	KC1	CBA-CAA	6.40	1.52	1.33
37	5	301	A86	C19-C20	6.39	1.61	1.52
37	9	313	A86	C25-C26	6.39	1.63	1.43
30	8	305	CLA	C3B-C2B	6.38	1.49	1.40
37	4	317	A86	C19-C20	6.38	1.61	1.52
37	10	302	A86	C19-C20	6.37	1.61	1.52
30	8	302	CLA	C3B-C2B	6.37	1.49	1.40
39	2	317	DD6	C30-C31	6.37	1.55	1.42
30	12	303	CLA	C3B-C2B	6.36	1.49	1.40
38	8	314	KC1	CBA-CAA	6.35	1.52	1.33
39	16	313	DD6	C13-C14	6.35	1.46	1.32
39	11	313	DD6	C21-C20	-6.34	1.41	1.51
38	12	313	KC1	C4A-C3A	6.34	1.56	1.44
39	15	318	DD6	C30-C31	6.34	1.55	1.42
37	8	315	A86	C25-C26	6.33	1.63	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	14	320	A86	C19-C20	6.33	1.61	1.52
30	F	202	CLA	C3B-C2B	6.33	1.49	1.40
39	2	317	DD6	C21-C20	-6.32	1.41	1.51
39	15	318	DD6	C21-C20	-6.31	1.42	1.51
37	2	318	A86	C19-C20	6.31	1.61	1.52
37	2	319	A86	C25-C26	6.31	1.63	1.43
30	B	834	CLA	C3B-C2B	6.30	1.49	1.40
37	7	316	A86	C19-C20	6.30	1.61	1.52
37	3	314	A86	C19-C20	6.30	1.61	1.52
39	5	313	DD6	C21-C20	-6.30	1.42	1.51
30	A	826	CLA	C3B-C2B	6.29	1.49	1.40
39	15	319	DD6	C30-C31	6.29	1.55	1.42
37	7	316	A86	C8-C6	6.28	1.59	1.45
39	7	314	DD6	C21-C20	-6.28	1.42	1.51
39	2	316	DD6	C21-C20	-6.28	1.42	1.51
37	2u	205	A86	C19-C20	6.27	1.61	1.52
37	7	316	A86	C25-C26	6.27	1.62	1.43
38	6	313	KC1	CBA-CAA	6.27	1.52	1.33
39	10	314	DD6	C21-C20	-6.26	1.42	1.51
39	6	321	DD6	C21-C20	-6.26	1.42	1.51
39	8	317	DD6	C21-C20	-6.25	1.42	1.51
39	15	319	DD6	C21-C20	-6.24	1.42	1.51
39	8	316	DD6	C13-C14	6.23	1.46	1.32
39	6	318	DD6	C21-C20	-6.22	1.42	1.51
30	A	838	CLA	C3B-C2B	6.21	1.49	1.40
30	5	307	CLA	C3B-C2B	6.21	1.49	1.40
30	2	310	CLA	C3B-C2B	6.21	1.49	1.40
37	2	319	A86	C19-C20	6.21	1.60	1.52
39	6	303	DD6	C30-C31	6.20	1.55	1.42
39	13	314	DD6	C30-C31	6.19	1.55	1.42
39	4	316	DD6	C30-C31	6.19	1.55	1.42
39	2	315	DD6	C21-C20	-6.19	1.42	1.51
37	7	315	A86	C19-C20	6.16	1.60	1.52
39	16	313	DD6	C30-C31	6.15	1.55	1.42
39	3	316	DD6	C30-C31	6.15	1.55	1.42
30	A	813	CLA	C3B-C2B	6.14	1.48	1.40
37	11	315	A86	C19-C20	6.14	1.60	1.52
30	7	305	CLA	C3B-C2B	6.13	1.48	1.40
30	B	812	CLA	C3B-C2B	6.12	1.48	1.40
30	A	806	CLA	C3B-C2B	6.11	1.48	1.40
39	3	312	DD6	C21-C20	-6.10	1.42	1.51
39	7	302	DD6	C30-C31	6.09	1.55	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	2	315	DD6	C30-C31	6.08	1.55	1.42
30	B	814	CLA	C3B-C2B	6.06	1.48	1.40
37	10	301	A86	C19-C20	6.06	1.60	1.52
30	6	305	CLA	C3B-C2B	6.04	1.48	1.40
39	10	313	DD6	C21-C20	-6.04	1.42	1.51
39	13	314	DD6	C13-C14	6.04	1.45	1.32
30	11	309	CLA	C3B-C2B	6.04	1.48	1.40
39	9	314	DD6	C30-C31	6.03	1.55	1.42
30	15	306	CLA	C3B-C2B	6.03	1.48	1.40
30	7	305	CLA	OBD-CAD	6.02	1.32	1.22
30	15	309	CLA	C3B-C2B	6.02	1.48	1.40
39	4	316	DD6	C21-C20	-6.01	1.42	1.51
30	4	309	CLA	C3B-C2B	6.01	1.48	1.40
39	8	317	DD6	C30-C31	5.99	1.55	1.42
38	3	311	KC1	O2A-CGA	5.98	1.46	1.30
30	8	301	CLA	C3B-C2B	5.98	1.48	1.40
38	1	308	KC1	O2A-CGA	5.98	1.45	1.30
39	3	312	DD6	C30-C31	5.98	1.55	1.42
30	2	304	CLA	C3B-C2B	5.97	1.48	1.40
38	8	313	KC1	O2A-CGA	5.97	1.45	1.30
30	11	310	CLA	C3B-C2B	5.97	1.48	1.40
38	13	312	KC1	O2A-CGA	5.97	1.45	1.30
30	13	307	CLA	C3B-C2B	5.97	1.48	1.40
38	2	306	KC1	O2A-CGA	5.97	1.45	1.30
39	12	317	DD6	C21-C20	-5.96	1.42	1.51
38	2	312	KC1	O2A-CGA	5.96	1.45	1.30
39	10	313	DD6	C13-C14	5.96	1.45	1.32
30	B	820	CLA	C3C-C2C	5.95	1.49	1.36
38	9	304	KC1	O2A-CGA	5.95	1.45	1.30
38	5	306	KC1	O2A-CGA	5.95	1.45	1.30
38	5	305	KC1	O2A-CGA	5.95	1.45	1.30
30	9	303	CLA	C3B-C2B	5.95	1.48	1.40
38	5	312	KC1	O2A-CGA	5.95	1.45	1.30
39	6	303	DD6	C21-C20	-5.95	1.42	1.51
38	12	311	KC1	O2A-CGA	5.95	1.45	1.30
38	6	308	KC1	O2A-CGA	5.95	1.45	1.30
37	9	315	A86	C19-C20	5.95	1.60	1.52
39	5	313	DD6	C30-C31	5.95	1.54	1.42
38	4	308	KC1	O2A-CGA	5.93	1.45	1.30
38	9	312	KC1	O2A-CGA	5.93	1.45	1.30
38	11	311	KC1	O2A-CGA	5.93	1.45	1.30
30	16	307	CLA	C3B-C2B	5.93	1.48	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	14	311	KC1	O2A-CGA	5.92	1.45	1.30
39	12	315	DD6	C30-C31	5.92	1.54	1.42
39	4	313	DD6	C13-C14	5.92	1.45	1.32
38	5	310	KC1	O2A-CGA	5.92	1.45	1.30
38	8	310	KC1	O2A-CGA	5.92	1.45	1.30
38	10	306	KC1	O2A-CGA	5.92	1.45	1.30
38	11	307	KC1	O2A-CGA	5.92	1.45	1.30
38	16	311	KC1	O2A-CGA	5.92	1.45	1.30
38	12	309	KC1	O2A-CGA	5.92	1.45	1.30
38	4	310	KC1	O2A-CGA	5.91	1.45	1.30
38	14	306	KC1	O2A-CGA	5.91	1.45	1.30
38	13	308	KC1	O2A-CGA	5.91	1.45	1.30
38	10	312	KC1	O2A-CGA	5.91	1.45	1.30
30	B	826	CLA	C3B-C2B	5.91	1.48	1.40
30	12	304	CLA	C3B-C2B	5.91	1.48	1.40
38	1	306	KC1	O2A-CGA	5.91	1.45	1.30
38	13	305	KC1	O2A-CGA	5.90	1.45	1.30
38	13	306	KC1	O2A-CGA	5.90	1.45	1.30
38	16	304	KC1	O2A-CGA	5.90	1.45	1.30
38	11	305	KC1	O2A-CGA	5.90	1.45	1.30
30	13	304	CLA	C3B-C2B	5.90	1.48	1.40
38	12	305	KC1	O2A-CGA	5.90	1.45	1.30
38	2	314	KC1	O2A-CGA	5.90	1.45	1.30
30	12	308	CLA	C3B-C2B	5.89	1.48	1.40
38	9	311	KC1	O2A-CGA	5.89	1.45	1.30
30	7	312	CLA	C3B-C2B	5.89	1.48	1.40
30	B	804	CLA	C3B-C2B	5.89	1.48	1.40
30	B	802	CLA	C3B-C2B	5.88	1.48	1.40
38	13	310	KC1	O2A-CGA	5.88	1.45	1.30
38	4	307	KC1	O2A-CGA	5.88	1.45	1.30
38	10	310	KC1	O2A-CGA	5.88	1.45	1.30
39	7	317	DD6	C30-C31	5.88	1.54	1.42
38	3	304	KC1	O2A-CGA	5.88	1.45	1.30
38	8	311	KC1	O2A-CGA	5.87	1.45	1.30
38	3	308	KC1	O2A-CGA	5.87	1.45	1.30
30	3	307	CLA	C3B-C2B	5.87	1.48	1.40
39	1	310	DD6	C30-C31	5.87	1.54	1.42
38	13	311	KC1	O2A-CGA	5.86	1.45	1.30
39	12	317	DD6	C13-C14	5.86	1.45	1.32
38	6	313	KC1	O2A-CGA	5.86	1.45	1.30
38	6	311	KC1	O2A-CGA	5.85	1.45	1.30
30	B	811	CLA	C3B-C2B	5.85	1.48	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	10	313	DD6	C30-C31	5.85	1.54	1.42
30	A	844	CLA	C3B-C2B	5.85	1.48	1.40
30	6	317	CLA	C3B-C2B	5.85	1.48	1.40
39	13	314	DD6	C21-C20	-5.84	1.42	1.51
30	9	306	CLA	C3B-C2B	5.84	1.48	1.40
30	14	304	CLA	C3B-C2B	5.84	1.48	1.40
39	10	314	DD6	C30-C31	5.84	1.54	1.42
30	B	828	CLA	C3B-C2B	5.84	1.48	1.40
30	16	310	CLA	C3B-C2B	5.84	1.48	1.40
39	15	319	DD6	C13-C14	5.83	1.45	1.32
39	15	318	DD6	C13-C14	5.83	1.45	1.32
30	A	829	CLA	C3B-C2B	5.83	1.48	1.40
39	2	316	DD6	C30-C31	5.82	1.54	1.42
38	12	313	KC1	O2A-CGA	5.82	1.45	1.30
30	14	309	CLA	C3B-C2B	5.81	1.48	1.40
39	4	313	DD6	C30-C31	5.81	1.54	1.42
39	3	313	DD6	C30-C31	5.81	1.54	1.42
30	15	311	CLA	C3B-C2B	5.81	1.48	1.40
30	A	809	CLA	C3B-C2B	5.81	1.48	1.40
30	A	805	CLA	C3B-C2B	5.81	1.48	1.40
38	8	307	KC1	O2A-CGA	5.80	1.45	1.30
38	9	310	KC1	O2A-CGA	5.80	1.45	1.30
30	B	825	CLA	C3B-C2B	5.80	1.48	1.40
30	10	311	CLA	C3B-C2B	5.80	1.48	1.40
30	13	303	CLA	C3B-C2B	5.80	1.48	1.40
30	10	309	CLA	C3B-C2B	5.80	1.48	1.40
39	7	318	DD6	C30-C31	5.80	1.54	1.42
38	6	312	KC1	O2A-CGA	5.79	1.45	1.30
30	14	313	CLA	C3B-C2B	5.79	1.48	1.40
38	8	306	KC1	O2A-CGA	5.78	1.45	1.30
30	2	313	CLA	C3B-C2B	5.78	1.48	1.40
30	16	309	CLA	C3B-C2B	5.78	1.48	1.40
30	12	312	CLA	C3B-C2B	5.78	1.48	1.40
39	6	321	DD6	C30-C31	5.78	1.54	1.42
30	16	306	CLA	C3B-C2B	5.77	1.48	1.40
30	15	307	CLA	C3B-C2B	5.77	1.48	1.40
30	3	309	CLA	C3B-C2B	5.77	1.48	1.40
30	15	305	CLA	C3B-C2B	5.77	1.48	1.40
38	7	308	KC1	O2A-CGA	5.77	1.45	1.30
39	6	319	DD6	C30-C31	5.76	1.54	1.42
30	B	820	CLA	C3B-C2B	5.76	1.48	1.40
38	7	313	KC1	O2A-CGA	5.75	1.45	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	7	318	DD6	C13-C14	5.75	1.45	1.32
38	8	312	KC1	O2A-CGA	5.75	1.45	1.30
30	A	823	CLA	C3B-C2B	5.75	1.48	1.40
30	15	313	CLA	C3B-C2B	5.75	1.48	1.40
30	16	308	CLA	C3B-C2B	5.74	1.48	1.40
30	6	315	CLA	C3B-C2B	5.74	1.48	1.40
38	4	308	KC1	C3B-C2B	5.74	1.48	1.37
30	6	316	CLA	C3B-C2B	5.74	1.48	1.40
39	6	318	DD6	C30-C31	5.72	1.54	1.42
30	1	307	CLA	C3B-C2B	5.72	1.48	1.40
39	11	313	DD6	C30-C31	5.72	1.54	1.42
30	1	305	CLA	C3B-C2B	5.72	1.48	1.40
37	6	320	A86	C19-C20	5.72	1.60	1.52
30	5	311	CLA	C3B-C2B	5.71	1.48	1.40
30	9	302	CLA	C3B-C2B	5.70	1.48	1.40
38	8	314	KC1	O2A-CGA	5.70	1.45	1.30
39	2	315	DD6	C13-C14	5.70	1.45	1.32
38	14	308	KC1	O2A-CGA	5.70	1.45	1.30
39	8	316	DD6	C30-C31	5.70	1.54	1.42
30	A	828	CLA	C3B-C2B	5.69	1.48	1.40
30	14	307	CLA	C3B-C2B	5.69	1.48	1.40
30	A	803	CLA	C3B-C2B	5.69	1.48	1.40
30	2	309	CLA	C3B-C2B	5.69	1.48	1.40
30	12	321	CLA	C3B-C2B	5.69	1.48	1.40
38	11	312	KC1	O2A-CGA	5.68	1.45	1.30
38	5	312	KC1	C3D-C2D	5.68	1.49	1.39
30	14	310	CLA	C3B-C2B	5.68	1.48	1.40
30	5	309	CLA	C3B-C2B	5.68	1.48	1.40
30	14	303	CLA	C3B-C2B	5.68	1.48	1.40
30	6	310	CLA	C3B-C2B	5.68	1.48	1.40
38	14	308	KC1	C3C-C2C	5.67	1.48	1.36
39	6	319	DD6	C13-C14	5.67	1.45	1.32
30	3	307	CLA	C3C-C2C	5.67	1.48	1.36
30	9	305	CLA	C3B-C2B	5.67	1.48	1.40
30	12	307	CLA	C3B-C2B	5.66	1.48	1.40
30	A	815	CLA	C3B-C2B	5.66	1.48	1.40
30	13	309	CLA	C3B-C2B	5.66	1.48	1.40
30	15	304	CLA	C3B-C2B	5.65	1.48	1.40
30	B	813	CLA	C3B-C2B	5.65	1.48	1.40
30	7	306	CLA	C3B-C2B	5.65	1.48	1.40
30	13	302	CLA	C3B-C2B	5.64	1.48	1.40
30	16	302	CLA	C3B-C2B	5.64	1.48	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	1	303	CLA	C3B-C2B	5.63	1.48	1.40
30	5	304	CLA	OBD-CAD	5.63	1.32	1.22
37	13	313	A86	C26-C27	5.63	1.43	1.35
30	B	805	CLA	C3B-C2B	5.62	1.48	1.40
39	12	317	DD6	C30-C31	5.62	1.54	1.42
30	A	819	CLA	C3B-C2B	5.62	1.48	1.40
30	J	101	CLA	C3B-C2B	5.62	1.48	1.40
30	16	305	CLA	C3B-C2B	5.62	1.48	1.40
38	1	308	KC1	C3D-C2D	5.62	1.49	1.39
30	3	302	CLA	C3B-C2B	5.62	1.48	1.40
30	3	305	CLA	C3B-C2B	5.62	1.48	1.40
38	11	311	KC1	C3B-C2B	5.62	1.48	1.37
38	14	306	KC1	C3D-C2D	5.62	1.49	1.39
30	2	301	CLA	C3B-C2B	5.61	1.48	1.40
30	11	304	CLA	C3B-C2B	5.61	1.48	1.40
30	L	202	CLA	C3B-C2B	5.61	1.48	1.40
30	5	304	CLA	C3B-C2B	5.61	1.48	1.40
30	8	309	CLA	C3B-C2B	5.60	1.48	1.40
30	12	302	CLA	C3B-C2B	5.60	1.48	1.40
30	10	304	CLA	C3B-C2B	5.60	1.48	1.40
30	F	203	CLA	C3B-C2B	5.60	1.48	1.40
30	14	312	CLA	C3B-C2B	5.60	1.48	1.40
38	9	311	KC1	OBD-CAD	5.59	1.30	1.22
38	13	306	KC1	C3B-C2B	5.59	1.48	1.37
30	1	302	CLA	C3B-C2B	5.59	1.48	1.40
30	14	302	CLA	C3B-C2B	5.59	1.48	1.40
39	5	314	DD6	C30-C31	5.58	1.54	1.42
30	15	303	CLA	C3B-C2B	5.58	1.48	1.40
38	11	311	KC1	C3D-C2D	5.58	1.49	1.39
39	7	302	DD6	C13-C14	5.58	1.44	1.32
37	2u	205	A86	C9-C8	5.57	1.48	1.34
39	7	317	DD6	C13-C14	5.57	1.44	1.32
38	9	311	KC1	C3D-C2D	5.57	1.49	1.39
30	6	306	CLA	C3B-C2B	5.56	1.48	1.40
30	B	810	CLA	C3B-C2B	5.55	1.48	1.40
38	12	309	KC1	C3B-C2B	5.55	1.48	1.37
30	15	304	CLA	C3C-C2C	5.54	1.48	1.36
30	A	842	CLA	C3B-C2B	5.54	1.48	1.40
38	13	308	KC1	C3B-C2B	5.54	1.48	1.37
30	2	305	CLA	C3B-C2B	5.54	1.48	1.40
30	A	810	CLA	C3B-C2B	5.54	1.48	1.40
30	5	308	CLA	C3B-C2B	5.53	1.48	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	10	310	KC1	C3D-C2D	5.53	1.49	1.39
38	16	311	KC1	C3C-C2C	5.52	1.48	1.36
30	3	303	CLA	C3B-C2B	5.52	1.48	1.40
30	1	304	CLA	C3B-C2B	5.52	1.48	1.40
38	13	310	KC1	C3D-C2D	5.52	1.49	1.39
38	4	307	KC1	C3D-C2D	5.51	1.49	1.39
30	16	303	CLA	C3B-C2B	5.51	1.48	1.40
30	A	817	CLA	C3B-C2B	5.51	1.48	1.40
38	2	314	KC1	C3B-C2B	5.51	1.48	1.37
38	13	312	KC1	C3D-C2D	5.50	1.49	1.39
38	13	305	KC1	C3D-C2D	5.50	1.49	1.39
30	B	832	CLA	C3B-C2B	5.50	1.48	1.40
30	4	306	CLA	C3B-C2B	5.50	1.48	1.40
30	11	306	CLA	C3B-C2B	5.50	1.48	1.40
30	15	302	CLA	C3B-C2B	5.50	1.48	1.40
39	2	317	DD6	C13-C14	5.50	1.44	1.32
38	2	312	KC1	C3B-C2B	5.49	1.48	1.37
38	10	312	KC1	C3B-C2B	5.49	1.48	1.37
38	13	312	KC1	C3B-C2B	5.49	1.48	1.37
30	11	308	CLA	C3B-C2B	5.49	1.48	1.40
38	11	307	KC1	C3D-C2D	5.49	1.49	1.39
30	A	837	CLA	C3B-C2B	5.48	1.48	1.40
30	12	306	CLA	C3B-C2B	5.48	1.48	1.40
30	13	301	CLA	C3B-C2B	5.48	1.48	1.40
39	7	314	DD6	C30-C31	5.48	1.53	1.42
38	16	304	KC1	C3B-C2B	5.47	1.48	1.37
38	7	308	KC1	C3D-C2D	5.47	1.49	1.39
38	6	313	KC1	C3D-C2D	5.47	1.49	1.39
30	11	310	CLA	C3C-C2C	5.47	1.48	1.36
30	B	837	CLA	C3B-C2B	5.46	1.48	1.40
30	B	823	CLA	C3B-C2B	5.46	1.47	1.40
38	14	308	KC1	C3D-C2D	5.46	1.49	1.39
38	11	307	KC1	C3B-C2B	5.46	1.48	1.37
30	2	311	CLA	C3B-C2B	5.46	1.47	1.40
38	13	308	KC1	C3D-C2D	5.46	1.49	1.39
38	13	305	KC1	C3B-C2B	5.46	1.48	1.37
38	2	306	KC1	C3B-C2B	5.45	1.48	1.37
30	A	804	CLA	C3B-C2B	5.45	1.47	1.40
38	13	311	KC1	C3D-C2D	5.45	1.49	1.39
38	11	305	KC1	C3B-C2B	5.45	1.48	1.37
38	5	306	KC1	C3B-C2B	5.45	1.48	1.37
30	B	831	CLA	C3B-C2B	5.45	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	3	304	KC1	C3B-C2B	5.45	1.48	1.37
38	4	310	KC1	C3D-C2D	5.45	1.49	1.39
30	9	308	CLA	C3B-C2B	5.44	1.47	1.40
30	10	303	CLA	C3B-C2B	5.44	1.47	1.40
30	15	314	CLA	C3B-C2B	5.44	1.47	1.40
38	12	305	KC1	C3B-C2B	5.44	1.48	1.37
30	2	308	CLA	C3B-C2B	5.43	1.47	1.40
30	A	824	CLA	C3B-C2B	5.43	1.47	1.40
30	3	301	CLA	C3B-C2B	5.43	1.47	1.40
30	15	312	CLA	C3B-C2B	5.43	1.47	1.40
30	B	827	CLA	C3B-C2B	5.43	1.47	1.40
30	4	302	CLA	C3B-C2B	5.43	1.47	1.40
30	B	824	CLA	C3B-C2B	5.42	1.47	1.40
39	11	313	DD6	C13-C14	5.42	1.44	1.32
38	1	306	KC1	C3B-C2B	5.42	1.48	1.37
30	4	309	CLA	C1D-ND	5.42	1.44	1.37
30	6	309	CLA	C3B-C2B	5.42	1.47	1.40
30	A	802	CLA	C3B-C2B	5.42	1.47	1.40
39	3	316	DD6	C13-C14	5.42	1.44	1.32
30	7	307	CLA	C3B-C2B	5.42	1.47	1.40
39	10	314	DD6	C13-C14	5.42	1.44	1.32
37	10	302	A86	C9-C8	5.42	1.48	1.34
38	16	311	KC1	C3B-C2B	5.42	1.48	1.37
38	6	308	KC1	C3D-C2D	5.42	1.49	1.39
30	4	301	CLA	C3B-C2B	5.41	1.47	1.40
30	B	816	CLA	C3B-C2B	5.41	1.47	1.40
38	12	311	KC1	C3B-C2B	5.41	1.48	1.37
30	A	811	CLA	C3B-C2B	5.41	1.47	1.40
38	8	313	KC1	C3B-C2B	5.41	1.48	1.37
30	A	808	CLA	C3B-C2B	5.40	1.47	1.40
38	10	312	KC1	C3D-C2D	5.40	1.49	1.39
38	6	313	KC1	C3B-C2B	5.40	1.48	1.37
30	B	836	CLA	C3B-C2B	5.40	1.47	1.40
38	1	306	KC1	C3D-C2D	5.40	1.49	1.39
30	16	301	CLA	C3B-C2B	5.40	1.47	1.40
30	16	308	CLA	C3C-C2C	5.40	1.48	1.36
30	A	831	CLA	C3B-C2B	5.40	1.47	1.40
30	3	303	CLA	OBD-CAD	5.40	1.31	1.22
30	9	307	CLA	C3B-C2B	5.40	1.47	1.40
39	2	316	DD6	C13-C14	5.39	1.44	1.32
38	9	310	KC1	C3D-C2D	5.39	1.49	1.39
37	4	314	A86	C9-C8	5.39	1.48	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	12	310	CLA	C3B-C2B	5.39	1.47	1.40
38	13	310	KC1	C3B-C2B	5.39	1.48	1.37
38	6	311	KC1	C3D-C2D	5.39	1.49	1.39
30	A	840	CLA	C3B-C2B	5.38	1.47	1.40
30	13	304	CLA	C3C-C2C	5.38	1.48	1.36
30	14	305	CLA	C3B-C2B	5.38	1.47	1.40
30	A	827	CLA	C3B-C2B	5.38	1.47	1.40
30	15	309	CLA	C3C-C2C	5.38	1.48	1.36
30	B	830	CLA	C3C-C2C	5.38	1.48	1.36
30	15	308	CLA	C3C-C2C	5.37	1.48	1.36
30	15	304	CLA	O2D-CGD	5.37	1.46	1.33
30	5	303	CLA	C3B-C2B	5.37	1.47	1.40
38	12	305	KC1	C3D-C2D	5.37	1.49	1.39
38	2	306	KC1	C3D-C2D	5.36	1.49	1.39
30	B	817	CLA	C3B-C2B	5.36	1.47	1.40
38	16	304	KC1	C3C-C2C	5.36	1.48	1.36
38	12	311	KC1	C3D-C2D	5.36	1.49	1.39
30	B	803	CLA	C3B-C2B	5.36	1.47	1.40
30	15	310	CLA	C3C-C2C	5.36	1.48	1.36
38	3	311	KC1	C3C-C2C	5.36	1.48	1.36
38	2	314	KC1	C3D-C2D	5.36	1.49	1.39
30	B	806	CLA	C3B-C2B	5.36	1.47	1.40
30	A	833	CLA	C3B-C2B	5.36	1.47	1.40
38	8	312	KC1	C3B-C2B	5.36	1.48	1.37
38	2	312	KC1	C3D-C2D	5.36	1.49	1.39
30	F	201	CLA	C3B-C2B	5.35	1.47	1.40
30	15	311	CLA	C3C-C2C	5.35	1.48	1.36
38	3	311	KC1	C3B-C2B	5.35	1.48	1.37
38	8	307	KC1	C3D-C2D	5.35	1.49	1.39
30	15	306	CLA	C3C-C2C	5.35	1.48	1.36
38	7	308	KC1	C3B-C2B	5.34	1.48	1.37
38	13	311	KC1	C3B-C2B	5.34	1.48	1.37
30	1	303	CLA	C3C-C2C	5.34	1.48	1.36
38	14	308	KC1	C3B-C2B	5.34	1.48	1.37
38	5	310	KC1	C3B-C2B	5.34	1.48	1.37
30	16	310	CLA	O2D-CGD	5.34	1.46	1.33
30	5	311	CLA	C3C-C2C	5.34	1.48	1.36
30	15	312	CLA	C3C-C2C	5.34	1.48	1.36
30	14	309	CLA	C3C-C2C	5.34	1.48	1.36
38	4	307	KC1	C3B-C2B	5.34	1.48	1.37
30	15	309	CLA	C1D-ND	5.34	1.44	1.37
39	3	313	DD6	C13-C14	5.33	1.44	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	11	308	CLA	C3C-C2C	5.33	1.48	1.36
30	2	303	CLA	O2D-CGD	5.33	1.46	1.33
38	5	306	KC1	C3D-C2D	5.33	1.49	1.39
30	14	310	CLA	C3C-C2C	5.33	1.48	1.36
38	8	313	KC1	C3D-C2D	5.33	1.49	1.39
30	B	834	CLA	C3C-C2C	5.33	1.48	1.36
30	10	308	CLA	C3B-C2B	5.33	1.47	1.40
30	A	844	CLA	C3C-C2C	5.33	1.48	1.36
30	7	312	CLA	C3C-C2C	5.33	1.48	1.36
30	7	310	CLA	C3C-C2C	5.32	1.48	1.36
38	10	306	KC1	C3B-C2B	5.32	1.48	1.37
38	10	310	KC1	C3B-C2B	5.32	1.48	1.37
30	B	824	CLA	C3C-C2C	5.32	1.48	1.36
30	15	305	CLA	C3C-C2C	5.32	1.48	1.36
30	13	307	CLA	C3C-C2C	5.32	1.48	1.36
30	16	303	CLA	C3C-C2C	5.32	1.48	1.36
38	5	312	KC1	C3B-C2B	5.32	1.48	1.37
30	11	304	CLA	C3C-C2C	5.32	1.48	1.36
38	11	305	KC1	C3D-C2D	5.32	1.49	1.39
30	B	820	CLA	CHC-C1C	5.32	1.48	1.35
38	9	304	KC1	C3B-C2B	5.32	1.48	1.37
38	8	314	KC1	C3D-C2D	5.32	1.49	1.39
30	8	303	CLA	C3B-C2B	5.32	1.47	1.40
38	9	312	KC1	C3C-C2C	5.32	1.48	1.36
38	5	310	KC1	C3D-C2D	5.31	1.49	1.39
30	3	309	CLA	C3C-C2C	5.31	1.48	1.36
30	16	309	CLA	C3C-C2C	5.31	1.48	1.36
30	8	308	CLA	C3B-C2B	5.31	1.47	1.40
30	15	313	CLA	C3C-C2C	5.31	1.48	1.36
38	9	304	KC1	C3D-C2D	5.31	1.49	1.39
30	3	306	CLA	C3B-C2B	5.31	1.47	1.40
30	14	312	CLA	C3C-C2C	5.31	1.48	1.36
30	13	309	CLA	O2D-CGD	5.31	1.46	1.33
38	9	311	KC1	C3B-C2B	5.30	1.48	1.37
38	3	308	KC1	C3D-C2D	5.30	1.48	1.39
30	8	309	CLA	C3C-C2C	5.30	1.48	1.36
38	1	308	KC1	C3B-C2B	5.30	1.48	1.37
30	14	313	CLA	C3C-C2C	5.30	1.48	1.36
39	6	318	DD6	C13-C14	5.30	1.44	1.32
30	B	835	CLA	C3C-C2C	5.30	1.48	1.36
30	15	311	CLA	C1D-ND	5.30	1.44	1.37
30	4	304	CLA	C3B-C2B	5.30	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	16	309	CLA	C1D-ND	5.29	1.44	1.37
30	B	832	CLA	C3C-C2C	5.29	1.48	1.36
30	13	304	CLA	C1D-ND	5.29	1.44	1.37
38	9	312	KC1	C3B-C2B	5.29	1.48	1.37
39	9	314	DD6	C13-C14	5.29	1.44	1.32
30	B	838	CLA	C3C-C2C	5.29	1.48	1.36
30	A	841	CLA	C3B-C2B	5.29	1.47	1.40
30	5	302	CLA	C3B-C2B	5.29	1.47	1.40
30	14	307	CLA	C3C-C2C	5.29	1.48	1.36
38	13	306	KC1	C3D-C2D	5.29	1.48	1.39
30	A	833	CLA	C3C-C2C	5.29	1.48	1.36
30	12	303	CLA	C3C-C2C	5.29	1.48	1.36
30	A	812	CLA	C3B-C2B	5.28	1.47	1.40
30	3	303	CLA	C3C-C2C	5.28	1.48	1.36
30	A	814	CLA	C3B-C2B	5.28	1.47	1.40
30	8	304	CLA	C3B-C2B	5.28	1.47	1.40
37	15	315	A86	C9-C8	5.28	1.48	1.34
38	1	308	KC1	C3C-C2C	5.28	1.47	1.36
30	13	303	CLA	C3C-C2C	5.28	1.47	1.36
30	A	807	CLA	C3B-C2B	5.27	1.47	1.40
38	9	311	KC1	C3C-C2C	5.27	1.47	1.36
38	13	308	KC1	C3C-C2C	5.27	1.47	1.36
30	11	306	CLA	CHC-C1C	5.27	1.48	1.35
37	9	316	A86	C26-C27	5.27	1.42	1.35
38	6	311	KC1	C3B-C2B	5.27	1.47	1.37
38	12	309	KC1	C3D-C2D	5.27	1.48	1.39
38	3	304	KC1	C3C-C2C	5.27	1.47	1.36
38	9	310	KC1	C3B-C2B	5.27	1.47	1.37
30	15	302	CLA	CHC-C1C	5.27	1.48	1.35
30	4	304	CLA	C3C-C2C	5.26	1.47	1.36
30	A	818	CLA	C3B-C2B	5.26	1.47	1.40
30	F	202	CLA	C3C-C2C	5.26	1.47	1.36
37	2u	203	A86	C9-C8	5.26	1.48	1.34
30	2	305	CLA	C3C-C2C	5.26	1.47	1.36
30	A	839	CLA	C3C-C2C	5.26	1.47	1.36
30	B	835	CLA	C3B-C2B	5.26	1.47	1.40
38	8	314	KC1	C3B-C2B	5.26	1.47	1.37
30	A	827	CLA	C3C-C2C	5.26	1.47	1.36
38	13	311	KC1	C3C-C2C	5.26	1.47	1.36
30	A	839	CLA	C3B-C2B	5.26	1.47	1.40
38	1	308	KC1	O2D-CGD	5.26	1.46	1.33
30	11	310	CLA	C1D-ND	5.26	1.44	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	4	301	CLA	C3C-C2C	5.26	1.47	1.36
30	10	309	CLA	C3C-C2C	5.26	1.47	1.36
39	6	303	DD6	C13-C14	5.25	1.44	1.32
30	B	815	CLA	C3B-C2B	5.25	1.47	1.40
30	6	310	CLA	C3C-C2C	5.25	1.47	1.36
38	2	306	KC1	C3C-C2C	5.25	1.47	1.36
38	13	312	KC1	C3C-C2C	5.25	1.47	1.36
38	4	307	KC1	C3C-C2C	5.25	1.47	1.36
38	16	311	KC1	C3D-C2D	5.25	1.48	1.39
30	13	307	CLA	C1D-ND	5.25	1.44	1.37
30	15	313	CLA	C1D-ND	5.25	1.44	1.37
30	1	305	CLA	C3C-C2C	5.25	1.47	1.36
30	B	830	CLA	C3B-C2B	5.25	1.47	1.40
30	14	309	CLA	C1D-ND	5.25	1.44	1.37
30	B	819	CLA	C3C-C2C	5.25	1.47	1.36
30	A	834	CLA	C3B-C2B	5.25	1.47	1.40
38	5	305	KC1	C3D-C2D	5.25	1.48	1.39
30	10	305	CLA	C3C-C2C	5.25	1.47	1.36
30	14	305	CLA	C3C-C2C	5.25	1.47	1.36
30	16	307	CLA	C3C-C2C	5.25	1.47	1.36
30	7	305	CLA	C3C-C2C	5.24	1.47	1.36
30	7	311	CLA	C3B-C2B	5.24	1.47	1.40
38	16	304	KC1	CHD-C4C	5.24	1.48	1.35
38	5	306	KC1	C3C-C2C	5.24	1.47	1.36
30	4	311	CLA	C3B-C2B	5.24	1.47	1.40
30	9	306	CLA	C3C-C2C	5.24	1.47	1.36
30	15	312	CLA	C1D-ND	5.24	1.44	1.37
30	15	302	CLA	C3C-C2C	5.24	1.47	1.36
38	14	306	KC1	C3B-C2B	5.24	1.47	1.37
37	15	315	A86	C26-C27	5.24	1.42	1.35
30	B	831	CLA	C3C-C2C	5.24	1.47	1.36
37	15	316	A86	C26-C27	5.24	1.42	1.35
38	7	308	KC1	C3C-C2C	5.24	1.47	1.36
30	14	304	CLA	C3C-C2C	5.24	1.47	1.36
30	4	305	CLA	C3C-C2C	5.24	1.47	1.36
38	4	310	KC1	C3B-C2B	5.23	1.47	1.37
39	1	310	DD6	C13-C14	5.23	1.44	1.32
38	6	312	KC1	C3B-C2B	5.23	1.47	1.37
30	15	303	CLA	C3C-C2C	5.23	1.47	1.36
38	4	310	KC1	C3C-C2C	5.23	1.47	1.36
39	6	303	DD6	C3-C2	5.23	1.59	1.43
30	10	304	CLA	C3C-C2C	5.23	1.47	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	13	312	KC1	CHD-C4C	5.23	1.48	1.35
38	5	305	KC1	C3B-C2B	5.23	1.47	1.37
38	6	308	KC1	C3B-C2B	5.23	1.47	1.37
38	2	314	KC1	C3C-C2C	5.23	1.47	1.36
38	8	312	KC1	C3C-C2C	5.23	1.47	1.36
30	B	821	CLA	C3B-C2B	5.23	1.47	1.40
30	9	309	CLA	C3B-C2B	5.23	1.47	1.40
30	10	311	CLA	C1D-ND	5.23	1.44	1.37
30	B	822	CLA	C3B-C2B	5.23	1.47	1.40
38	4	308	KC1	C3D-C2D	5.23	1.48	1.39
30	A	835	CLA	C3C-C2C	5.23	1.47	1.36
38	11	305	KC1	C3C-C2C	5.22	1.47	1.36
30	13	303	CLA	C1D-ND	5.22	1.44	1.37
30	12	304	CLA	C3C-C2C	5.22	1.47	1.36
30	15	310	CLA	C1D-ND	5.22	1.44	1.37
30	1	301	CLA	C3B-C2B	5.22	1.47	1.40
30	2	308	CLA	CHC-C1C	5.22	1.48	1.35
30	7	312	CLA	C1D-ND	5.22	1.44	1.37
30	A	813	CLA	C3C-C2C	5.22	1.47	1.36
38	3	311	KC1	CHD-C4C	5.22	1.48	1.35
38	14	306	KC1	CHD-C4C	5.22	1.48	1.35
30	16	308	CLA	C1D-ND	5.22	1.44	1.37
30	15	307	CLA	C3C-C2C	5.22	1.47	1.36
30	B	825	CLA	C3C-C2C	5.21	1.47	1.36
30	6	315	CLA	C3C-C2C	5.21	1.47	1.36
30	14	303	CLA	C3C-C2C	5.21	1.47	1.36
38	5	305	KC1	C3C-C2C	5.21	1.47	1.36
38	6	313	KC1	C3C-C2C	5.21	1.47	1.36
30	13	304	CLA	O2D-CGD	5.21	1.45	1.33
30	1	301	CLA	C3C-C2C	5.21	1.47	1.36
30	A	816	CLA	C3B-C2B	5.21	1.47	1.40
30	6	316	CLA	C3C-C2C	5.21	1.47	1.36
38	8	311	KC1	C3C-C2C	5.21	1.47	1.36
30	15	308	CLA	CHC-C1C	5.21	1.48	1.35
30	4	303	CLA	C3B-C2B	5.21	1.47	1.40
30	7	304	CLA	C3C-C2C	5.21	1.47	1.36
30	7	303	CLA	C3B-C2B	5.21	1.47	1.40
30	2	313	CLA	C3C-C2C	5.21	1.47	1.36
30	L	203	CLA	C3C-C2C	5.21	1.47	1.36
30	3	307	CLA	C1D-ND	5.21	1.44	1.37
30	7	304	CLA	C3B-C2B	5.21	1.47	1.40
38	5	306	KC1	CHD-C4C	5.20	1.48	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	12	315	DD6	C13-C14	5.20	1.43	1.32
30	11	304	CLA	CHC-C1C	5.20	1.48	1.35
38	8	306	KC1	C3C-C2C	5.20	1.47	1.36
30	4	309	CLA	O2D-CGD	5.20	1.45	1.33
38	8	312	KC1	C3D-C2D	5.20	1.48	1.39
30	A	844	CLA	O2D-CGD	5.20	1.45	1.33
38	13	305	KC1	C3C-C2C	5.20	1.47	1.36
30	4	303	CLA	C3C-C2C	5.20	1.47	1.36
30	6	307	CLA	C3C-C2C	5.20	1.47	1.36
30	8	302	CLA	C3C-C2C	5.20	1.47	1.36
38	13	312	KC1	O2D-CGD	5.20	1.45	1.33
38	6	312	KC1	C3D-C2D	5.20	1.48	1.39
38	11	312	KC1	C3D-C2D	5.20	1.48	1.39
30	12	321	CLA	C1D-ND	5.20	1.44	1.37
30	15	304	CLA	C1D-ND	5.20	1.44	1.37
38	11	311	KC1	C3C-C2C	5.19	1.47	1.36
30	3	306	CLA	C3C-C2C	5.19	1.47	1.36
30	16	310	CLA	C3C-C2C	5.19	1.47	1.36
38	4	307	KC1	CHD-C4C	5.19	1.48	1.35
30	12	321	CLA	C3C-C2C	5.19	1.47	1.36
30	14	302	CLA	CHC-C1C	5.19	1.48	1.35
38	13	308	KC1	CHD-C4C	5.19	1.48	1.35
30	4	309	CLA	C3C-C2C	5.19	1.47	1.36
30	11	309	CLA	C3C-C2C	5.19	1.47	1.36
30	15	306	CLA	C1D-ND	5.19	1.44	1.37
30	B	822	CLA	C3C-C2C	5.19	1.47	1.36
30	B	808	CLA	C3B-C2B	5.19	1.47	1.40
30	10	307	CLA	C3B-C2B	5.19	1.47	1.40
30	15	313	CLA	O2D-CGD	5.18	1.45	1.33
30	10	305	CLA	C3B-C2B	5.18	1.47	1.40
38	13	311	KC1	O2D-CGD	5.18	1.45	1.33
38	8	311	KC1	C3B-C2B	5.18	1.47	1.37
38	10	312	KC1	C3C-C2C	5.18	1.47	1.36
30	13	302	CLA	C3C-C2C	5.18	1.47	1.36
29	A	801	CL0	C3B-C2B	5.18	1.47	1.40
38	8	307	KC1	C3C-C2C	5.18	1.47	1.36
30	2	307	CLA	C3C-C2C	5.18	1.47	1.36
38	14	311	KC1	C3B-C2B	5.18	1.47	1.37
30	A	820	CLA	C3C-C2C	5.17	1.47	1.36
38	11	305	KC1	CHD-C4C	5.17	1.48	1.35
30	13	309	CLA	C3C-C2C	5.17	1.47	1.36
30	B	838	CLA	C3B-C2B	5.17	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	11	307	KC1	CHD-C4C	5.17	1.48	1.35
30	15	310	CLA	O2D-CGD	5.17	1.45	1.33
30	1	307	CLA	C3C-C2C	5.17	1.47	1.36
30	A	805	CLA	CHC-C1C	5.17	1.48	1.35
30	1	304	CLA	CHC-C1C	5.17	1.48	1.35
38	4	310	KC1	CHD-C4C	5.17	1.48	1.35
38	13	306	KC1	O2D-CGD	5.17	1.45	1.33
30	2	308	CLA	O2D-CGD	5.17	1.45	1.33
38	2	314	KC1	O2D-CGD	5.17	1.45	1.33
38	10	312	KC1	CHD-C4C	5.17	1.48	1.35
38	8	310	KC1	C3D-C2D	5.17	1.48	1.39
39	7	302	DD6	C3-C2	5.17	1.59	1.43
38	10	310	KC1	C3C-C2C	5.17	1.47	1.36
30	6	306	CLA	C3C-C2C	5.17	1.47	1.36
38	10	306	KC1	C3C-C2C	5.17	1.47	1.36
30	15	309	CLA	CHC-C1C	5.17	1.48	1.35
30	9	302	CLA	C3C-C2C	5.16	1.47	1.36
30	16	302	CLA	O2D-CGD	5.16	1.45	1.33
30	8	303	CLA	C3C-C2C	5.16	1.47	1.36
38	1	306	KC1	C3C-C2C	5.16	1.47	1.36
30	3	305	CLA	C3C-C2C	5.16	1.47	1.36
30	13	302	CLA	O2D-CGD	5.16	1.45	1.33
38	16	304	KC1	C3D-C2D	5.16	1.48	1.39
38	11	305	KC1	O2D-CGD	5.16	1.45	1.33
30	B	833	CLA	C3C-C2C	5.16	1.47	1.36
39	3	312	DD6	C13-C14	5.16	1.43	1.32
30	L	202	CLA	C3C-C2C	5.16	1.47	1.36
30	9	309	CLA	C3C-C2C	5.16	1.47	1.36
30	J	101	CLA	C3C-C2C	5.16	1.47	1.36
30	14	312	CLA	C1D-ND	5.16	1.44	1.37
30	12	310	CLA	C3C-C2C	5.16	1.47	1.36
30	B	815	CLA	C3C-C2C	5.16	1.47	1.36
30	A	834	CLA	C3C-C2C	5.16	1.47	1.36
38	3	308	KC1	C3B-C2B	5.16	1.47	1.37
30	3	302	CLA	C3C-C2C	5.15	1.47	1.36
30	14	302	CLA	C3C-C2C	5.15	1.47	1.36
30	7	309	CLA	C3B-C2B	5.15	1.47	1.40
30	14	304	CLA	C1D-ND	5.15	1.44	1.37
38	13	311	KC1	CHD-C4C	5.15	1.48	1.35
30	15	305	CLA	O2D-CGD	5.15	1.45	1.33
39	8	317	DD6	C13-C14	5.15	1.43	1.32
38	9	304	KC1	CHD-C4C	5.15	1.48	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	824	CLA	C3C-C2C	5.15	1.47	1.36
38	2	306	KC1	CHD-C4C	5.15	1.48	1.35
30	B	828	CLA	C3C-C2C	5.15	1.47	1.36
30	16	306	CLA	C3C-C2C	5.15	1.47	1.36
30	16	303	CLA	CHC-C1C	5.15	1.48	1.35
38	3	311	KC1	C3D-C2D	5.15	1.48	1.39
38	9	311	KC1	CHD-C4C	5.15	1.48	1.35
30	9	306	CLA	C1D-ND	5.15	1.44	1.37
38	11	311	KC1	O2D-CGD	5.14	1.45	1.33
30	8	308	CLA	C3C-C2C	5.14	1.47	1.36
30	A	838	CLA	C3C-C2C	5.14	1.47	1.36
30	B	829	CLA	C3C-C2C	5.14	1.47	1.36
30	13	307	CLA	O2D-CGD	5.14	1.45	1.33
30	9	305	CLA	C3C-C2C	5.14	1.47	1.36
38	8	313	KC1	O2D-CGD	5.14	1.45	1.33
38	9	312	KC1	C3D-C2D	5.14	1.48	1.39
30	A	822	CLA	C3C-C2C	5.14	1.47	1.36
30	6	305	CLA	C3C-C2C	5.14	1.47	1.36
30	14	302	CLA	O2D-CGD	5.14	1.45	1.33
37	15	320	A86	C26-C27	5.14	1.42	1.35
30	F	203	CLA	C3C-C2C	5.14	1.47	1.36
30	J	101	CLA	O2D-CGD	5.14	1.45	1.33
30	16	305	CLA	C3C-C2C	5.14	1.47	1.36
38	11	312	KC1	O2D-CGD	5.14	1.45	1.33
30	A	816	CLA	C3C-C2C	5.14	1.47	1.36
30	5	304	CLA	C3C-C2C	5.14	1.47	1.36
30	B	851	CLA	C3B-C2B	5.14	1.47	1.40
30	5	304	CLA	O2D-CGD	5.14	1.45	1.33
38	12	305	KC1	C3C-C2C	5.13	1.47	1.36
38	10	312	KC1	O2D-CGD	5.13	1.45	1.33
39	10	314	DD6	C3-C2	5.13	1.59	1.43
37	11	301	A86	C9-C8	5.13	1.47	1.34
30	15	311	CLA	O2D-CGD	5.13	1.45	1.33
30	11	306	CLA	C3C-C2C	5.13	1.47	1.36
39	5	313	DD6	C13-C14	5.13	1.43	1.32
30	5	309	CLA	C3C-C2C	5.13	1.47	1.36
30	14	309	CLA	O2D-CGD	5.13	1.45	1.33
38	3	308	KC1	O2D-CGD	5.13	1.45	1.33
30	2	313	CLA	C1D-ND	5.13	1.44	1.37
38	13	310	KC1	C3C-C2C	5.13	1.47	1.36
30	3	310	CLA	O2D-CGD	5.13	1.45	1.33
38	11	311	KC1	CHD-C4C	5.13	1.48	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	851	CLA	O2D-CGD	5.13	1.45	1.33
38	12	309	KC1	C3C-C2C	5.13	1.47	1.36
30	2	311	CLA	O2D-CGD	5.13	1.45	1.33
30	A	821	CLA	C3B-C2B	5.13	1.47	1.40
39	13	314	DD6	C3-C2	5.13	1.59	1.43
30	14	307	CLA	O2D-CGD	5.13	1.45	1.33
38	1	306	KC1	CHD-C4C	5.12	1.48	1.35
38	13	310	KC1	CHD-C4C	5.12	1.48	1.35
30	B	807	CLA	C3B-C2B	5.12	1.47	1.40
38	13	308	KC1	O2D-CGD	5.12	1.45	1.33
30	A	817	CLA	C3C-C2C	5.12	1.47	1.36
30	15	302	CLA	C1D-ND	5.12	1.44	1.37
38	9	312	KC1	CHD-C4C	5.12	1.48	1.35
38	13	305	KC1	CHD-C4C	5.12	1.48	1.35
37	15	315	A86	C2-C1	5.12	1.42	1.35
30	B	826	CLA	C3C-C2C	5.12	1.47	1.36
38	8	306	KC1	C3D-C2D	5.12	1.48	1.39
30	14	304	CLA	O2D-CGD	5.12	1.45	1.33
38	14	311	KC1	O2D-CGD	5.12	1.45	1.33
38	4	308	KC1	CHD-C4C	5.12	1.48	1.35
30	6	317	CLA	C3C-C2C	5.12	1.47	1.36
30	3	309	CLA	C1D-ND	5.12	1.44	1.37
38	5	305	KC1	CHD-C4C	5.12	1.48	1.35
30	9	306	CLA	O2D-CGD	5.12	1.45	1.33
30	15	314	CLA	C1D-ND	5.11	1.44	1.37
30	11	310	CLA	O2D-CGD	5.11	1.45	1.33
30	15	303	CLA	O2D-CGD	5.11	1.45	1.33
30	2	309	CLA	C3C-C2C	5.11	1.47	1.36
30	15	314	CLA	C3C-C2C	5.11	1.47	1.36
38	7	313	KC1	C3D-C2D	5.11	1.48	1.39
30	B	818	CLA	C3B-C2B	5.11	1.47	1.40
30	12	321	CLA	O2D-CGD	5.11	1.45	1.33
30	13	309	CLA	C1D-ND	5.11	1.44	1.37
30	7	312	CLA	O2D-CGD	5.11	1.45	1.33
30	3	306	CLA	CHC-C1C	5.11	1.48	1.35
30	16	309	CLA	O2D-CGD	5.11	1.45	1.33
30	7	303	CLA	C3C-C2C	5.11	1.47	1.36
30	4	304	CLA	CHC-C1C	5.11	1.48	1.35
38	16	311	KC1	CHD-C4C	5.11	1.48	1.35
30	A	819	CLA	C3C-C2C	5.11	1.47	1.36
30	F	201	CLA	C3C-C2C	5.11	1.47	1.36
38	11	307	KC1	O2D-CGD	5.11	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	2	314	KC1	CHD-C4C	5.11	1.48	1.35
30	5	303	CLA	C3C-C2C	5.10	1.47	1.36
38	7	313	KC1	CHD-C4C	5.10	1.48	1.35
30	16	302	CLA	C3C-C2C	5.10	1.47	1.36
30	3	310	CLA	C1D-ND	5.10	1.44	1.37
38	11	312	KC1	CHD-C4C	5.10	1.48	1.35
39	6	319	DD6	C3-C2	5.10	1.59	1.43
30	B	810	CLA	C3C-C2C	5.10	1.47	1.36
30	10	307	CLA	C3C-C2C	5.10	1.47	1.36
38	5	305	KC1	O2D-CGD	5.10	1.45	1.33
38	9	311	KC1	O2D-CGD	5.10	1.45	1.33
30	16	306	CLA	O2D-CGD	5.10	1.45	1.33
30	15	303	CLA	C1D-ND	5.10	1.44	1.37
30	B	836	CLA	C3C-C2C	5.10	1.47	1.36
30	B	829	CLA	CHC-C1C	5.10	1.48	1.35
30	16	307	CLA	C1D-ND	5.10	1.44	1.37
30	4	306	CLA	O2D-CGD	5.10	1.45	1.33
30	A	841	CLA	C3C-C2C	5.09	1.47	1.36
30	B	805	CLA	C3C-C2C	5.09	1.47	1.36
38	4	310	KC1	O2D-CGD	5.09	1.45	1.33
38	6	312	KC1	C3C-C2C	5.09	1.47	1.36
30	3	310	CLA	C3B-C2B	5.09	1.47	1.40
30	14	313	CLA	C1D-ND	5.09	1.44	1.37
30	3	301	CLA	C3C-C2C	5.09	1.47	1.36
38	10	310	KC1	CHD-C4C	5.09	1.48	1.35
30	A	836	CLA	C3C-C2C	5.09	1.47	1.36
30	14	302	CLA	C1D-ND	5.09	1.44	1.37
30	9	307	CLA	C3C-C2C	5.09	1.47	1.36
30	14	312	CLA	O2D-CGD	5.09	1.45	1.33
30	2	304	CLA	C3C-C2C	5.09	1.47	1.36
30	3	309	CLA	CHC-C1C	5.09	1.48	1.35
30	B	839	CLA	CHC-C1C	5.09	1.48	1.35
38	12	311	KC1	CHD-C4C	5.09	1.48	1.35
30	A	831	CLA	C3C-C2C	5.09	1.47	1.36
38	13	306	KC1	CHD-C4C	5.09	1.48	1.35
38	13	310	KC1	O2D-CGD	5.09	1.45	1.33
38	3	304	KC1	CHD-C4C	5.09	1.48	1.35
38	12	311	KC1	C3C-C2C	5.09	1.47	1.36
38	12	309	KC1	CHD-C4C	5.09	1.48	1.35
30	6	309	CLA	O2D-CGD	5.09	1.45	1.33
30	A	825	CLA	C3B-C2B	5.08	1.47	1.40
38	11	312	KC1	C3B-C2B	5.08	1.47	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	12	305	KC1	CHD-C4C	5.08	1.48	1.35
39	6	318	DD6	C3-C2	5.08	1.59	1.43
30	2	307	CLA	C3B-C2B	5.08	1.47	1.40
30	10	311	CLA	C3C-C2C	5.08	1.47	1.36
30	6	307	CLA	C3B-C2B	5.08	1.47	1.40
30	3	309	CLA	O2D-CGD	5.08	1.45	1.33
30	A	805	CLA	C3C-C2C	5.08	1.47	1.36
38	2	312	KC1	CHD-C4C	5.08	1.48	1.35
38	8	313	KC1	C3C-C2C	5.08	1.47	1.36
38	8	314	KC1	C3C-C2C	5.08	1.47	1.36
39	11	313	DD6	C3-C2	5.08	1.59	1.43
30	A	815	CLA	C3C-C2C	5.08	1.47	1.36
30	12	308	CLA	C3C-C2C	5.08	1.47	1.36
37	9	315	A86	C26-C27	5.08	1.42	1.35
38	3	311	KC1	O2D-CGD	5.08	1.45	1.33
30	16	308	CLA	O2D-CGD	5.08	1.45	1.33
30	1	305	CLA	C1D-ND	5.08	1.44	1.37
30	A	833	CLA	O2D-CGD	5.08	1.45	1.33
30	10	311	CLA	O2D-CGD	5.08	1.45	1.33
30	1	302	CLA	C3C-C2C	5.08	1.47	1.36
39	15	318	DD6	C3-C2	5.08	1.59	1.43
39	3	313	DD6	C3-C2	5.07	1.59	1.43
30	A	812	CLA	C3C-C2C	5.07	1.47	1.36
30	15	307	CLA	O2D-CGD	5.07	1.45	1.33
30	B	812	CLA	C3C-C2C	5.07	1.47	1.36
38	6	311	KC1	C3C-C2C	5.07	1.47	1.36
38	8	313	KC1	C1A-NA	-5.07	1.28	1.38
30	5	308	CLA	O2D-CGD	5.07	1.45	1.33
38	1	306	KC1	O2D-CGD	5.07	1.45	1.33
30	7	310	CLA	CHC-C1C	5.07	1.48	1.35
30	5	311	CLA	C1D-ND	5.07	1.44	1.37
30	A	830	CLA	C3B-C2B	5.07	1.47	1.40
38	8	306	KC1	CHD-C4C	5.07	1.48	1.35
38	8	311	KC1	CHD-C4C	5.07	1.48	1.35
30	6	317	CLA	C1D-ND	5.07	1.44	1.37
38	14	311	KC1	C3C-C2C	5.07	1.47	1.36
39	2	315	DD6	C3-C2	5.07	1.59	1.43
38	10	306	KC1	C3D-C2D	5.07	1.48	1.39
30	10	308	CLA	CHC-C1C	5.07	1.48	1.35
39	3	312	DD6	C3-C2	5.07	1.59	1.43
30	12	308	CLA	O2D-CGD	5.07	1.45	1.33
30	5	311	CLA	O2D-CGD	5.07	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	15	319	DD6	C3-C2	5.07	1.59	1.43
30	14	310	CLA	O2D-CGD	5.07	1.45	1.33
30	B	835	CLA	CHC-C1C	5.06	1.48	1.35
38	9	312	KC1	O2D-CGD	5.06	1.45	1.33
37	9	316	A86	C9-C8	5.06	1.47	1.34
30	B	817	CLA	CHC-C1C	5.06	1.47	1.35
30	6	315	CLA	C1D-ND	5.06	1.44	1.37
30	11	310	CLA	CHC-C1C	5.06	1.47	1.35
38	9	310	KC1	C3C-C2C	5.06	1.47	1.36
30	15	312	CLA	O2D-CGD	5.06	1.45	1.33
30	A	808	CLA	C3C-C2C	5.06	1.47	1.36
30	12	312	CLA	C3C-C2C	5.06	1.47	1.36
38	7	313	KC1	C3B-C2B	5.06	1.47	1.37
30	A	841	CLA	O2D-CGD	5.06	1.45	1.33
38	10	310	KC1	O2D-CGD	5.06	1.45	1.33
30	7	310	CLA	C3B-C2B	5.06	1.47	1.40
30	7	303	CLA	CHC-C1C	5.06	1.47	1.35
37	2	302	A86	C9-C8	5.06	1.47	1.34
30	14	307	CLA	CHC-C1C	5.06	1.47	1.35
30	14	303	CLA	O2D-CGD	5.06	1.45	1.33
39	10	313	DD6	C3-C2	5.06	1.59	1.43
30	2	313	CLA	O2D-CGD	5.06	1.45	1.33
30	6	314	CLA	C3B-C2B	5.05	1.47	1.40
30	15	309	CLA	O2D-CGD	5.05	1.45	1.33
38	8	314	KC1	CHD-C4C	5.05	1.47	1.35
30	B	827	CLA	C3C-C2C	5.05	1.47	1.36
30	10	303	CLA	C3C-C2C	5.05	1.47	1.36
30	3	306	CLA	O2D-CGD	5.05	1.45	1.33
38	14	308	KC1	O2D-CGD	5.05	1.45	1.33
38	6	312	KC1	CHD-C4C	5.05	1.47	1.35
30	10	309	CLA	O2D-CGD	5.05	1.45	1.33
38	4	308	KC1	O2D-CGD	5.05	1.45	1.33
38	6	311	KC1	C1A-NA	-5.05	1.28	1.38
30	12	307	CLA	O2D-CGD	5.05	1.45	1.33
38	3	308	KC1	C3C-C2C	5.05	1.47	1.36
39	16	313	DD6	C3-C2	5.05	1.59	1.43
30	A	844	CLA	C1D-ND	5.05	1.44	1.37
38	16	304	KC1	O2D-CGD	5.05	1.45	1.33
30	B	804	CLA	C3C-C2C	5.05	1.47	1.36
30	B	808	CLA	C3C-C2C	5.05	1.47	1.36
39	4	316	DD6	C3-C2	5.05	1.59	1.43
30	14	310	CLA	C1D-ND	5.05	1.44	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	5	302	CLA	CHC-C1C	5.04	1.47	1.35
37	15	323	A86	C26-C27	5.04	1.42	1.35
38	12	313	KC1	C3B-C2B	5.04	1.47	1.37
30	2	303	CLA	CHC-C1C	5.04	1.47	1.35
38	5	310	KC1	C3C-C2C	5.04	1.47	1.36
38	9	304	KC1	C3C-C2C	5.04	1.47	1.36
30	12	303	CLA	O2D-CGD	5.04	1.45	1.33
30	A	841	CLA	CHC-C1C	5.04	1.47	1.35
30	B	814	CLA	C3C-C2C	5.04	1.47	1.36
38	14	311	KC1	C3D-C2D	5.04	1.48	1.39
39	2	317	DD6	C3-C2	5.04	1.59	1.43
38	8	307	KC1	C3B-C2B	5.04	1.47	1.37
30	9	308	CLA	CHC-C1C	5.04	1.47	1.35
38	8	306	KC1	C3B-C2B	5.04	1.47	1.37
30	10	308	CLA	O2D-CGD	5.04	1.45	1.33
30	14	313	CLA	CHC-C1C	5.04	1.47	1.35
30	4	311	CLA	O2D-CGD	5.03	1.45	1.33
30	1	307	CLA	O2D-CGD	5.03	1.45	1.33
30	B	811	CLA	C3C-C2C	5.03	1.47	1.36
30	7	311	CLA	C3C-C2C	5.03	1.47	1.36
30	10	303	CLA	CHC-C1C	5.03	1.47	1.35
30	A	842	CLA	C3C-C2C	5.03	1.47	1.36
39	3	316	DD6	C3-C2	5.03	1.59	1.43
30	16	307	CLA	O2D-CGD	5.03	1.45	1.33
30	16	301	CLA	CHC-C1C	5.03	1.47	1.35
38	9	310	KC1	CHD-C4C	5.03	1.47	1.35
38	11	312	KC1	C3C-C2C	5.03	1.47	1.36
30	14	303	CLA	C1D-ND	5.03	1.44	1.37
30	14	313	CLA	O2D-CGD	5.03	1.45	1.33
38	8	307	KC1	CHD-C4C	5.03	1.47	1.35
30	A	836	CLA	C3B-C2B	5.03	1.47	1.40
38	9	304	KC1	O2D-CGD	5.03	1.45	1.33
30	1	303	CLA	CHC-C1C	5.03	1.47	1.35
30	6	315	CLA	O2D-CGD	5.03	1.45	1.33
30	16	301	CLA	O2D-CGD	5.03	1.45	1.33
30	11	306	CLA	O2D-CGD	5.03	1.45	1.33
38	7	313	KC1	C3C-C2C	5.03	1.47	1.36
39	12	315	DD6	C3-C2	5.03	1.59	1.43
30	15	304	CLA	CHC-C1C	5.03	1.47	1.35
30	2	311	CLA	C3C-C2C	5.02	1.47	1.36
30	2	309	CLA	O2D-CGD	5.02	1.45	1.33
30	13	303	CLA	O2D-CGD	5.02	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	13	301	CLA	C1D-ND	5.02	1.44	1.37
30	11	304	CLA	O2D-CGD	5.02	1.45	1.33
30	6	310	CLA	C1D-ND	5.02	1.44	1.37
30	1	304	CLA	O2D-CGD	5.02	1.45	1.33
30	3	303	CLA	CHC-C1C	5.02	1.47	1.35
38	8	310	KC1	C3B-C2B	5.02	1.47	1.37
38	3	308	KC1	CHD-C4C	5.02	1.47	1.35
30	B	839	CLA	C3C-C2C	5.02	1.47	1.36
37	3	315	A86	C9-C8	5.02	1.47	1.34
30	6	316	CLA	O2D-CGD	5.02	1.45	1.33
38	14	311	KC1	CHD-C4C	5.02	1.47	1.35
30	6	306	CLA	CHC-C1C	5.02	1.47	1.35
30	B	830	CLA	CHC-C1C	5.02	1.47	1.35
30	3	310	CLA	C3C-C2C	5.02	1.47	1.36
30	16	301	CLA	C3C-C2C	5.02	1.47	1.36
39	9	314	DD6	C3-C2	5.02	1.59	1.43
29	A	801	CL0	C3C-C2C	5.02	1.47	1.36
30	10	305	CLA	O2D-CGD	5.02	1.45	1.33
30	11	309	CLA	O2D-CGD	5.01	1.45	1.33
30	13	309	CLA	CHC-C1C	5.01	1.47	1.35
38	5	310	KC1	CHD-C4C	5.01	1.47	1.35
30	7	310	CLA	O2D-CGD	5.01	1.45	1.33
30	A	825	CLA	C3C-C2C	5.01	1.47	1.36
30	6	314	CLA	O2D-CGD	5.01	1.45	1.33
38	5	310	KC1	O2D-CGD	5.01	1.45	1.33
39	4	313	DD6	C3-C2	5.01	1.59	1.43
37	15	320	A86	C9-C8	5.01	1.47	1.34
30	7	304	CLA	O2D-CGD	5.01	1.45	1.33
30	12	306	CLA	C3C-C2C	5.01	1.47	1.36
30	2	310	CLA	O2D-CGD	5.01	1.45	1.33
30	A	828	CLA	C3C-C2C	5.01	1.47	1.36
30	2	313	CLA	CHC-C1C	5.01	1.47	1.35
38	1	308	KC1	CHD-C4C	5.01	1.47	1.35
30	A	823	CLA	C3C-C2C	5.01	1.47	1.36
38	8	312	KC1	O2D-CGD	5.01	1.45	1.33
30	A	837	CLA	C3C-C2C	5.01	1.47	1.36
30	15	305	CLA	C1D-ND	5.01	1.43	1.37
30	5	307	CLA	C3C-C2C	5.01	1.47	1.36
30	B	806	CLA	CHC-C1C	5.01	1.47	1.35
30	4	306	CLA	CHC-C1C	5.01	1.47	1.35
30	B	833	CLA	C3B-C2B	5.00	1.47	1.40
30	14	303	CLA	CHC-C1C	5.00	1.47	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	13	306	KC1	C3C-C2C	5.00	1.47	1.36
38	14	308	KC1	CHD-C4C	5.00	1.47	1.35
30	15	310	CLA	CHC-C1C	5.00	1.47	1.35
30	10	304	CLA	O2D-CGD	5.00	1.45	1.33
37	12	316	A86	C9-C8	5.00	1.47	1.34
37	15	322	A86	C9-C8	5.00	1.47	1.34
38	3	304	KC1	C3D-C2D	5.00	1.48	1.39
30	1	305	CLA	O2D-CGD	5.00	1.45	1.33
30	2u	202	CLA	C3C-C2C	5.00	1.47	1.36
37	15	317	A86	C26-C27	5.00	1.42	1.35
38	8	310	KC1	O2D-CGD	5.00	1.45	1.33
30	A	832	CLA	C3C-C2C	5.00	1.47	1.36
38	16	311	KC1	O2D-CGD	5.00	1.45	1.33
30	14	305	CLA	CHC-C1C	5.00	1.47	1.35
39	4	316	DD6	C13-C14	5.00	1.43	1.32
38	12	313	KC1	C3C-C2C	4.99	1.47	1.36
30	6	304	CLA	CHC-C1C	4.99	1.47	1.35
30	10	307	CLA	CHC-C1C	4.99	1.47	1.35
30	14	304	CLA	CHC-C1C	4.99	1.47	1.35
30	7	311	CLA	O2D-CGD	4.99	1.45	1.33
38	8	311	KC1	O2D-CGD	4.99	1.45	1.33
37	10	315	A86	C9-C8	4.99	1.47	1.34
37	13	313	A86	C9-C8	4.99	1.47	1.34
30	4	306	CLA	C3C-C2C	4.99	1.47	1.36
30	B	825	CLA	CHC-C1C	4.99	1.47	1.35
38	8	311	KC1	C3D-C2D	4.99	1.48	1.39
30	A	829	CLA	CHC-C1C	4.99	1.47	1.35
30	4	311	CLA	C3C-C2C	4.99	1.47	1.36
30	A	825	CLA	O2D-CGD	4.99	1.45	1.33
30	6	307	CLA	O2D-CGD	4.99	1.45	1.33
30	8	305	CLA	O2D-CGD	4.99	1.45	1.33
30	A	832	CLA	C3B-C2B	4.99	1.47	1.40
30	15	308	CLA	C3B-C2B	4.99	1.47	1.40
38	6	313	KC1	C1A-NA	-4.99	1.28	1.38
30	14	305	CLA	O2D-CGD	4.99	1.45	1.33
39	2	316	DD6	C3-C2	4.99	1.58	1.43
30	A	837	CLA	CHC-C1C	4.99	1.47	1.35
30	2	303	CLA	C3B-C2B	4.99	1.47	1.40
37	15	322	A86	C26-C27	4.99	1.42	1.35
30	9	309	CLA	O2D-CGD	4.99	1.45	1.33
38	12	311	KC1	O2D-CGD	4.99	1.45	1.33
30	16	303	CLA	O2D-CGD	4.99	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	7	306	CLA	C3C-C2C	4.99	1.47	1.36
38	2	312	KC1	C3C-C2C	4.99	1.47	1.36
39	5	313	DD6	C3-C2	4.99	1.58	1.43
37	11	316	A86	C26-C27	4.99	1.42	1.35
30	15	313	CLA	CHC-C1C	4.99	1.47	1.35
39	12	317	DD6	C3-C2	4.99	1.58	1.43
30	B	824	CLA	CHC-C1C	4.98	1.47	1.35
30	A	835	CLA	C3B-C2B	4.98	1.47	1.40
30	F	203	CLA	O2D-CGD	4.98	1.45	1.33
30	14	312	CLA	CHC-C1C	4.98	1.47	1.35
37	14	320	A86	C9-C8	4.98	1.47	1.34
30	A	804	CLA	C3C-C2C	4.98	1.47	1.36
30	12	304	CLA	O2D-CGD	4.98	1.45	1.33
30	A	810	CLA	C3C-C2C	4.98	1.47	1.36
38	12	305	KC1	O2D-CGD	4.98	1.45	1.33
30	12	310	CLA	O2D-CGD	4.98	1.45	1.33
38	4	308	KC1	C3C-C2C	4.98	1.47	1.36
30	14	310	CLA	CHC-C1C	4.98	1.47	1.35
38	8	312	KC1	CHD-C4C	4.98	1.47	1.35
30	A	817	CLA	O2D-CGD	4.98	1.45	1.33
30	10	308	CLA	C3C-C2C	4.98	1.47	1.36
37	2	318	A86	C26-C27	4.98	1.42	1.35
39	7	314	DD6	C3-C2	4.98	1.58	1.43
30	L	202	CLA	CHC-C1C	4.97	1.47	1.35
30	6	305	CLA	O2D-CGD	4.97	1.45	1.33
30	12	307	CLA	CHC-C1C	4.97	1.47	1.35
30	3	301	CLA	O2D-CGD	4.97	1.45	1.33
30	2	311	CLA	CHC-C1C	4.97	1.47	1.35
30	B	802	CLA	CHC-C1C	4.97	1.47	1.35
30	B	837	CLA	CHC-C1C	4.97	1.47	1.35
30	13	301	CLA	O2D-CGD	4.97	1.45	1.33
30	2	310	CLA	C3C-C2C	4.97	1.47	1.36
30	A	821	CLA	C3C-C2C	4.97	1.47	1.36
38	6	313	KC1	CHD-C4C	4.97	1.47	1.35
30	3	305	CLA	C1D-ND	4.97	1.43	1.37
30	A	803	CLA	C3C-C2C	4.97	1.47	1.36
38	11	307	KC1	C3C-C2C	4.97	1.47	1.36
30	13	307	CLA	CHC-C1C	4.97	1.47	1.35
30	4	302	CLA	O2D-CGD	4.97	1.45	1.33
30	11	308	CLA	CHC-C1C	4.97	1.47	1.35
30	A	833	CLA	CHC-C1C	4.97	1.47	1.35
37	7	319	A86	C26-C27	4.97	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	806	CLA	O2D-CGD	4.97	1.45	1.33
30	6	309	CLA	C3C-C2C	4.96	1.47	1.36
30	5	304	CLA	CHC-C1C	4.96	1.47	1.35
38	2	312	KC1	O2D-CGD	4.96	1.45	1.33
38	7	308	KC1	CHD-C4C	4.96	1.47	1.35
38	12	309	KC1	O2D-CGD	4.96	1.45	1.33
38	10	306	KC1	CHD-C4C	4.96	1.47	1.35
39	8	316	DD6	C3-C2	4.96	1.58	1.43
30	12	302	CLA	C3C-C2C	4.96	1.47	1.36
30	7	307	CLA	O2D-CGD	4.96	1.45	1.33
30	7	307	CLA	CHC-C1C	4.96	1.47	1.35
30	A	840	CLA	C1D-ND	4.96	1.43	1.37
38	7	313	KC1	C1A-NA	-4.96	1.28	1.38
37	13	315	A86	C9-C8	4.96	1.47	1.34
30	A	840	CLA	C3C-C2C	4.96	1.47	1.36
30	3	307	CLA	O2D-CGD	4.96	1.45	1.33
30	9	307	CLA	O2D-CGD	4.96	1.45	1.33
30	13	301	CLA	CHC-C1C	4.96	1.47	1.35
30	B	819	CLA	O2D-CGD	4.96	1.45	1.33
37	10	317	A86	C9-C8	4.96	1.47	1.34
38	6	311	KC1	O2D-CGD	4.95	1.45	1.33
30	A	811	CLA	C3C-C2C	4.95	1.47	1.36
30	6	317	CLA	O2D-CGD	4.95	1.45	1.33
30	16	307	CLA	CHC-C1C	4.95	1.47	1.35
30	A	844	CLA	CHC-C1C	4.95	1.47	1.35
30	B	821	CLA	C3C-C2C	4.95	1.47	1.36
30	5	302	CLA	C3C-C2C	4.95	1.47	1.36
30	12	312	CLA	O2D-CGD	4.95	1.45	1.33
30	15	312	CLA	CHC-C1C	4.95	1.47	1.35
30	B	822	CLA	O2D-CGD	4.95	1.45	1.33
30	9	305	CLA	CHC-C1C	4.95	1.47	1.35
30	16	301	CLA	C1D-ND	4.95	1.43	1.37
30	12	304	CLA	CHC-C1C	4.95	1.47	1.35
30	9	303	CLA	O2D-CGD	4.95	1.45	1.33
39	6	321	DD6	C13-C14	4.95	1.43	1.32
30	12	312	CLA	C1D-ND	4.95	1.43	1.37
38	10	312	KC1	C1A-NA	-4.95	1.28	1.38
38	6	308	KC1	C3C-C2C	4.95	1.47	1.36
30	A	837	CLA	C1D-ND	4.95	1.43	1.37
30	A	836	CLA	O2D-CGD	4.95	1.45	1.33
30	6	304	CLA	C3B-C2B	4.95	1.47	1.40
30	A	843	CLA	O2D-CGD	4.95	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	3	315	A86	C26-C27	4.95	1.42	1.35
30	4	302	CLA	CHC-C1C	4.95	1.47	1.35
30	15	305	CLA	CHC-C1C	4.94	1.47	1.35
30	15	307	CLA	C1D-ND	4.94	1.43	1.37
30	L	203	CLA	CHC-C1C	4.94	1.47	1.35
38	5	312	KC1	O2D-CGD	4.94	1.45	1.33
30	B	837	CLA	C3C-C2C	4.94	1.47	1.36
30	6	305	CLA	CHC-C1C	4.94	1.47	1.35
30	9	302	CLA	O2A-CGA	4.94	1.47	1.33
30	A	819	CLA	CHC-C1C	4.94	1.47	1.35
30	A	808	CLA	O2D-CGD	4.94	1.45	1.33
30	2	309	CLA	CHC-C1C	4.94	1.47	1.35
30	A	829	CLA	C3C-C2C	4.93	1.47	1.36
30	B	804	CLA	CHC-C1C	4.93	1.47	1.35
30	F	202	CLA	CHC-C1C	4.93	1.47	1.35
38	6	313	KC1	O2D-CGD	4.93	1.45	1.33
30	13	303	CLA	CHC-C1C	4.93	1.47	1.35
30	A	816	CLA	O2D-CGD	4.93	1.45	1.33
38	12	313	KC1	O2D-CGD	4.93	1.45	1.33
30	A	822	CLA	C3B-C2B	4.93	1.47	1.40
38	5	306	KC1	C1A-NA	-4.93	1.28	1.38
30	15	311	CLA	CHC-C1C	4.93	1.47	1.35
30	A	806	CLA	CHC-C1C	4.93	1.47	1.35
30	2	304	CLA	CHC-C1C	4.93	1.47	1.35
30	B	817	CLA	O2D-CGD	4.93	1.45	1.33
38	8	307	KC1	C1A-NA	-4.93	1.28	1.38
30	B	851	CLA	CHC-C1C	4.93	1.47	1.35
37	9	315	A86	C9-C8	4.93	1.47	1.34
37	15	321	A86	C26-C27	4.93	1.42	1.35
30	B	807	CLA	C3C-C2C	4.93	1.47	1.36
30	15	306	CLA	O2D-CGD	4.93	1.45	1.33
30	8	308	CLA	O2D-CGD	4.93	1.45	1.33
30	12	306	CLA	O2D-CGD	4.93	1.45	1.33
30	B	811	CLA	CHC-C1C	4.93	1.47	1.35
30	B	833	CLA	CHC-C1C	4.93	1.47	1.35
30	12	310	CLA	CHC-C1C	4.93	1.47	1.35
30	B	822	CLA	CHC-C1C	4.93	1.47	1.35
30	A	824	CLA	CHC-C1C	4.92	1.47	1.35
38	5	306	KC1	O2D-CGD	4.92	1.45	1.33
30	1	301	CLA	O2D-CGD	4.92	1.45	1.33
30	A	822	CLA	O2D-CGD	4.92	1.45	1.33
30	12	304	CLA	C1D-ND	4.92	1.43	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	14	320	A86	C26-C27	4.92	1.42	1.35
30	10	305	CLA	CHC-C1C	4.92	1.47	1.35
38	14	306	KC1	C3C-C2C	4.92	1.47	1.36
30	4	305	CLA	CHC-C1C	4.92	1.47	1.35
30	6	306	CLA	O2D-CGD	4.92	1.45	1.33
30	2	308	CLA	C3C-C2C	4.92	1.47	1.36
30	10	303	CLA	O2D-CGD	4.92	1.45	1.33
30	15	303	CLA	CHC-C1C	4.92	1.47	1.35
30	8	303	CLA	O2D-CGD	4.92	1.45	1.33
30	B	832	CLA	CHC-C1C	4.92	1.47	1.35
37	3	314	A86	C9-C8	4.92	1.47	1.34
38	5	312	KC1	CHD-C4C	4.92	1.47	1.35
30	2u	202	CLA	C3B-C2B	4.92	1.47	1.40
30	13	301	CLA	C3C-C2C	4.92	1.47	1.36
37	15	323	A86	C9-C8	4.92	1.47	1.34
30	2	305	CLA	CHC-C1C	4.92	1.47	1.35
30	6	307	CLA	CHC-C1C	4.92	1.47	1.35
30	A	807	CLA	C3C-C2C	4.91	1.47	1.36
30	9	303	CLA	CHC-C1C	4.91	1.47	1.35
30	B	820	CLA	O2D-CGD	4.91	1.45	1.33
30	2	303	CLA	C3C-C2C	4.91	1.47	1.36
30	8	305	CLA	C3C-C2C	4.91	1.47	1.36
30	1	301	CLA	CHC-C1C	4.91	1.47	1.35
30	3	302	CLA	O2D-CGD	4.91	1.45	1.33
39	7	317	DD6	C3-C2	4.91	1.58	1.43
30	A	839	CLA	CHC-C1C	4.91	1.47	1.35
30	5	303	CLA	CHC-C1C	4.91	1.47	1.35
30	A	807	CLA	CHC-C1C	4.91	1.47	1.35
30	5	309	CLA	C1D-ND	4.91	1.43	1.37
30	F	201	CLA	CHC-C1C	4.91	1.47	1.35
30	9	307	CLA	CHC-C1C	4.91	1.47	1.35
30	9	307	CLA	C1D-ND	4.91	1.43	1.37
30	3	305	CLA	CHC-C1C	4.91	1.47	1.35
30	4	303	CLA	CHC-C1C	4.91	1.47	1.35
39	7	318	DD6	C3-C2	4.90	1.58	1.43
38	8	310	KC1	C1A-NA	-4.90	1.28	1.38
38	9	304	KC1	C1A-NA	-4.90	1.28	1.38
38	9	311	KC1	C1A-NA	-4.90	1.28	1.38
30	B	817	CLA	C3C-C2C	4.90	1.47	1.36
30	B	819	CLA	CHC-C1C	4.90	1.47	1.35
30	A	818	CLA	O2D-CGD	4.90	1.45	1.33
30	B	831	CLA	O2D-CGD	4.90	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	818	CLA	CHC-C1C	4.90	1.47	1.35
30	4	301	CLA	CHC-C1C	4.90	1.47	1.35
30	B	826	CLA	O2D-CGD	4.90	1.45	1.33
38	4	307	KC1	O2D-CGD	4.90	1.45	1.33
30	16	309	CLA	CHC-C1C	4.90	1.47	1.35
30	A	826	CLA	C3C-C2C	4.90	1.47	1.36
30	6	304	CLA	C3C-C2C	4.90	1.47	1.36
30	4	309	CLA	CHC-C1C	4.90	1.47	1.35
30	1	302	CLA	C1D-ND	4.90	1.43	1.37
30	10	311	CLA	CHC-C1C	4.90	1.47	1.35
38	6	311	KC1	CHD-C4C	4.90	1.47	1.35
30	6	315	CLA	CHC-C1C	4.90	1.47	1.35
30	13	302	CLA	CHC-C1C	4.90	1.47	1.35
30	A	824	CLA	O2D-CGD	4.90	1.45	1.33
30	A	837	CLA	O2D-CGD	4.90	1.45	1.33
30	14	309	CLA	CHC-C1C	4.90	1.47	1.35
38	9	310	KC1	C1A-NA	-4.90	1.28	1.38
30	5	308	CLA	CHC-C1C	4.89	1.47	1.35
30	6	317	CLA	CHC-C1C	4.89	1.47	1.35
30	16	306	CLA	CHC-C1C	4.89	1.47	1.35
30	B	831	CLA	CHC-C1C	4.89	1.47	1.35
37	5	315	A86	C9-C8	4.89	1.47	1.34
30	2	304	CLA	O2D-CGD	4.89	1.45	1.33
30	10	309	CLA	CHC-C1C	4.89	1.47	1.35
30	16	305	CLA	O2D-CGD	4.89	1.45	1.33
30	A	830	CLA	C3C-C2C	4.89	1.47	1.36
30	A	819	CLA	O2D-CGD	4.89	1.45	1.33
30	13	304	CLA	CHC-C1C	4.89	1.47	1.35
30	9	308	CLA	C3C-C2C	4.89	1.47	1.36
30	6	306	CLA	C1D-ND	4.89	1.43	1.37
30	10	309	CLA	C1D-ND	4.89	1.43	1.37
30	8	309	CLA	O2D-CGD	4.89	1.45	1.33
39	6	321	DD6	C3-C2	4.89	1.58	1.43
30	2	311	CLA	C1D-ND	4.89	1.43	1.37
37	2	319	A86	C9-C8	4.89	1.47	1.34
30	11	309	CLA	CHC-C1C	4.89	1.47	1.35
30	A	808	CLA	CHC-C1C	4.89	1.47	1.35
30	16	302	CLA	CHC-C1C	4.89	1.47	1.35
30	B	837	CLA	O2D-CGD	4.89	1.45	1.33
30	5	309	CLA	CHC-C1C	4.89	1.47	1.35
30	8	308	CLA	CHC-C1C	4.89	1.47	1.35
38	1	306	KC1	C1A-NA	-4.88	1.28	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	5	308	CLA	C3C-C2C	4.88	1.47	1.36
38	14	306	KC1	O2D-CGD	4.88	1.45	1.33
30	A	823	CLA	O2D-CGD	4.88	1.45	1.33
30	5	309	CLA	O2D-CGD	4.88	1.45	1.33
30	3	302	CLA	CHC-C1C	4.88	1.47	1.35
30	A	820	CLA	C3B-C2B	4.88	1.47	1.40
37	14	319	A86	C9-C8	4.88	1.47	1.34
30	7	309	CLA	C3C-C2C	4.88	1.47	1.36
30	B	823	CLA	C3C-C2C	4.88	1.47	1.36
30	6	309	CLA	CHC-C1C	4.88	1.47	1.35
30	5	303	CLA	O2D-CGD	4.88	1.45	1.33
30	15	314	CLA	CHC-C1C	4.88	1.47	1.35
30	16	310	CLA	C1D-ND	4.88	1.43	1.37
30	5	311	CLA	CHC-C1C	4.88	1.47	1.35
37	15	317	A86	C9-C8	4.88	1.47	1.34
30	A	813	CLA	CHC-C1C	4.88	1.47	1.35
30	B	829	CLA	O2D-CGD	4.88	1.45	1.33
38	10	310	KC1	C1A-NA	-4.88	1.28	1.38
30	16	308	CLA	CHC-C1C	4.88	1.47	1.35
30	13	302	CLA	C1D-ND	4.88	1.43	1.37
30	8	301	CLA	CHC-C1C	4.88	1.47	1.35
39	1	310	DD6	C3-C2	4.87	1.58	1.43
30	6	316	CLA	CHC-C1C	4.87	1.47	1.35
30	B	823	CLA	CHC-C1C	4.87	1.47	1.35
30	A	822	CLA	CHC-C1C	4.87	1.47	1.35
37	5	316	A86	C9-C8	4.87	1.47	1.34
30	4	301	CLA	O2D-CGD	4.87	1.45	1.33
30	B	810	CLA	CHC-C1C	4.87	1.47	1.35
30	4	305	CLA	O2D-CGD	4.87	1.45	1.33
38	7	313	KC1	O2D-CGD	4.87	1.45	1.33
30	8	305	CLA	CHC-C1C	4.87	1.47	1.35
30	8	304	CLA	C3C-C2C	4.87	1.47	1.36
30	3	303	CLA	O2D-CGD	4.87	1.45	1.33
30	10	304	CLA	CHC-C1C	4.87	1.47	1.35
30	B	801	CLA	C3B-C2B	4.87	1.47	1.40
30	11	308	CLA	O2D-CGD	4.87	1.45	1.33
38	5	310	KC1	C1A-NA	-4.87	1.28	1.38
30	4	311	CLA	C1D-ND	4.87	1.43	1.37
30	6	310	CLA	O2D-CGD	4.87	1.45	1.33
30	1	307	CLA	C1D-ND	4.87	1.43	1.37
38	9	310	KC1	O2D-CGD	4.87	1.45	1.33
30	4	302	CLA	C3C-C2C	4.87	1.47	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	811	CLA	O2D-CGD	4.86	1.45	1.33
30	B	813	CLA	C3C-C2C	4.86	1.47	1.36
30	A	843	CLA	C3C-C2C	4.86	1.47	1.36
30	A	827	CLA	CHC-C1C	4.86	1.47	1.35
38	8	307	KC1	O2D-CGD	4.86	1.45	1.33
30	F	202	CLA	O2D-CGD	4.86	1.45	1.33
30	7	309	CLA	O2D-CGD	4.86	1.45	1.33
39	5	314	DD6	C3-C2	4.86	1.58	1.43
30	2	301	CLA	O2D-CGD	4.86	1.45	1.33
30	J	101	CLA	C1D-ND	4.86	1.43	1.37
30	A	817	CLA	CHC-C1C	4.86	1.47	1.35
30	3	305	CLA	O2D-CGD	4.86	1.45	1.33
30	8	302	CLA	O2D-CGD	4.86	1.45	1.33
30	A	802	CLA	CHC-C1C	4.86	1.47	1.35
38	2	314	KC1	C1A-NA	-4.85	1.28	1.38
38	6	308	KC1	CHD-C4C	4.85	1.47	1.35
30	2u	202	CLA	CHC-C1C	4.85	1.47	1.35
30	7	311	CLA	CHC-C1C	4.85	1.47	1.35
30	8	304	CLA	O2D-CGD	4.85	1.45	1.33
30	10	303	CLA	C1D-ND	4.85	1.43	1.37
39	8	317	DD6	C3-C2	4.85	1.58	1.43
30	4	305	CLA	C3B-C2B	4.85	1.47	1.40
38	13	311	KC1	CHC-C4B	4.85	1.47	1.38
30	11	308	CLA	C1D-ND	4.85	1.43	1.37
30	15	302	CLA	O2D-CGD	4.85	1.45	1.33
30	A	802	CLA	C3C-C2C	4.85	1.47	1.36
30	B	813	CLA	CHC-C1C	4.85	1.47	1.35
30	2	309	CLA	C1D-ND	4.85	1.43	1.37
30	8	302	CLA	CHC-C1C	4.85	1.47	1.35
38	5	312	KC1	C1A-NA	-4.85	1.28	1.38
37	16	312	A86	C9-C8	4.85	1.47	1.34
30	2	310	CLA	C1D-ND	4.85	1.43	1.37
30	3	303	CLA	C1D-ND	4.85	1.43	1.37
30	7	310	CLA	C1D-ND	4.85	1.43	1.37
30	B	832	CLA	O2D-CGD	4.85	1.45	1.33
30	B	833	CLA	O2D-CGD	4.85	1.45	1.33
30	8	304	CLA	CHC-C1C	4.84	1.47	1.35
30	A	803	CLA	O2D-CGD	4.84	1.45	1.33
30	B	827	CLA	CHC-C1C	4.84	1.47	1.35
30	A	803	CLA	CHC-C1C	4.84	1.47	1.35
30	A	825	CLA	C1D-ND	4.84	1.43	1.37
30	12	302	CLA	O2D-CGD	4.83	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	2u	205	A86	C17-C18	-4.83	1.45	1.52
30	7	305	CLA	CHC-C1C	4.83	1.47	1.35
30	4	304	CLA	O2D-CGD	4.83	1.45	1.33
30	9	301	CLA	C3C-C2C	4.83	1.47	1.36
30	1	305	CLA	CHC-C1C	4.83	1.47	1.35
30	9	305	CLA	C1D-ND	4.83	1.43	1.37
30	A	835	CLA	O2D-CGD	4.83	1.45	1.33
37	14	301	A86	C9-C8	4.83	1.47	1.34
30	12	312	CLA	CHC-C1C	4.83	1.47	1.35
38	11	305	KC1	C1A-NA	-4.83	1.28	1.38
38	1	308	KC1	C1A-NA	-4.83	1.28	1.38
30	A	823	CLA	CHC-C1C	4.83	1.47	1.35
30	B	821	CLA	O2D-CGD	4.83	1.45	1.33
30	2	310	CLA	CHC-C1C	4.82	1.47	1.35
30	B	825	CLA	O2D-CGD	4.82	1.45	1.33
30	11	304	CLA	C1D-ND	4.82	1.43	1.37
38	14	306	KC1	CHC-C4B	4.82	1.47	1.38
30	9	308	CLA	O2D-CGD	4.82	1.45	1.33
38	7	308	KC1	O2D-CGD	4.82	1.45	1.33
30	F	203	CLA	CHC-C1C	4.82	1.47	1.35
30	B	816	CLA	C3C-C2C	4.82	1.47	1.36
30	A	835	CLA	C1D-ND	4.82	1.43	1.37
38	5	312	KC1	C3C-C2C	4.82	1.47	1.36
30	16	310	CLA	CHC-C1C	4.82	1.47	1.35
37	7	319	A86	C9-C8	4.82	1.47	1.34
38	2	306	KC1	C1A-NA	-4.82	1.28	1.38
30	B	834	CLA	CHC-C1C	4.82	1.47	1.35
30	10	304	CLA	C1D-ND	4.82	1.43	1.37
38	12	313	KC1	CHD-C4C	4.82	1.47	1.35
30	7	309	CLA	C1D-ND	4.82	1.43	1.37
38	9	311	KC1	CHC-C4B	4.81	1.47	1.38
30	1	302	CLA	CHC-C1C	4.81	1.47	1.35
30	2u	202	CLA	O2D-CGD	4.81	1.44	1.33
30	A	832	CLA	CHC-C1C	4.81	1.47	1.35
38	7	308	KC1	C1A-NA	-4.81	1.28	1.38
38	11	311	KC1	C1A-NA	-4.81	1.28	1.38
30	8	301	CLA	C3C-C2C	4.81	1.47	1.36
38	6	312	KC1	O2D-CGD	4.81	1.44	1.33
30	7	312	CLA	CHC-C1C	4.81	1.47	1.35
37	11	315	A86	C9-C8	4.81	1.47	1.34
37	15	316	A86	C9-C8	4.81	1.47	1.34
30	14	305	CLA	C1D-ND	4.81	1.43	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	816	CLA	O2D-CGD	4.81	1.44	1.33
37	11	314	A86	C9-C8	4.81	1.47	1.34
30	A	821	CLA	O2D-CGD	4.81	1.44	1.33
30	A	842	CLA	O2D-CGD	4.81	1.44	1.33
30	A	830	CLA	CHC-C1C	4.81	1.47	1.35
30	A	811	CLA	CHC-C1C	4.80	1.47	1.35
30	A	834	CLA	CHC-C1C	4.80	1.47	1.35
30	B	806	CLA	C3C-C2C	4.80	1.46	1.36
38	10	306	KC1	O2D-CGD	4.80	1.44	1.33
30	A	810	CLA	CHC-C1C	4.80	1.47	1.35
30	12	303	CLA	CHC-C1C	4.80	1.47	1.35
30	2	307	CLA	CHC-C1C	4.80	1.47	1.35
30	7	307	CLA	C3C-C2C	4.80	1.46	1.36
30	A	811	CLA	O2D-CGD	4.80	1.44	1.33
30	7	305	CLA	C1D-ND	4.80	1.43	1.37
38	9	312	KC1	C1A-NA	-4.80	1.28	1.38
37	5	301	A86	C9-C8	4.80	1.46	1.34
38	4	307	KC1	C1A-NA	-4.80	1.28	1.38
37	11	301	A86	C17-C18	-4.80	1.45	1.52
38	13	306	KC1	CHC-C4B	4.80	1.47	1.38
30	16	305	CLA	C1D-ND	4.80	1.43	1.37
30	A	815	CLA	O2D-CGD	4.80	1.44	1.33
37	4	314	A86	C26-C27	4.79	1.42	1.35
30	B	821	CLA	CHC-C1C	4.79	1.47	1.35
30	A	840	CLA	O2D-CGD	4.79	1.44	1.33
30	B	836	CLA	O2D-CGD	4.79	1.44	1.33
37	14	316	A86	C17-C18	-4.79	1.45	1.52
30	3	307	CLA	CHC-C1C	4.79	1.47	1.35
30	12	308	CLA	CHC-C1C	4.79	1.47	1.35
30	8	309	CLA	CHC-C1C	4.79	1.47	1.35
38	8	312	KC1	CHB-C1B	4.79	1.47	1.38
39	5	314	DD6	C13-C14	4.79	1.43	1.32
30	B	803	CLA	O2D-CGD	4.79	1.44	1.33
30	16	302	CLA	C1D-ND	4.79	1.43	1.37
29	A	801	CL0	O2D-CGD	4.79	1.44	1.33
38	8	310	KC1	CHD-C4C	4.79	1.47	1.35
30	B	809	CLA	C3C-C2C	4.79	1.46	1.36
30	A	820	CLA	O2D-CGD	4.79	1.44	1.33
38	13	311	KC1	CHB-C1B	4.79	1.47	1.38
38	13	308	KC1	C1A-NA	-4.78	1.28	1.38
37	8	318	A86	C17-C18	-4.78	1.45	1.52
30	A	809	CLA	O2D-CGD	4.78	1.44	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	818	CLA	O2D-CGD	4.78	1.44	1.33
37	2u	205	A86	C26-C27	4.78	1.42	1.35
30	3	301	CLA	CHC-C1C	4.78	1.47	1.35
30	12	310	CLA	C1D-ND	4.78	1.43	1.37
30	12	321	CLA	CHC-C1C	4.78	1.47	1.35
37	10	317	A86	C26-C27	4.78	1.42	1.35
30	B	826	CLA	CHC-C1C	4.78	1.47	1.35
37	14	318	A86	C9-C8	4.78	1.46	1.34
30	A	842	CLA	CHC-C1C	4.78	1.47	1.35
30	5	307	CLA	O2D-CGD	4.78	1.44	1.33
30	B	814	CLA	CHC-C1C	4.78	1.47	1.35
37	9	313	A86	C17-C18	-4.77	1.45	1.52
30	B	807	CLA	O2D-CGD	4.77	1.44	1.33
30	B	818	CLA	CHC-C1C	4.77	1.47	1.35
37	12	316	A86	C26-C27	4.77	1.42	1.35
30	B	835	CLA	O2D-CGD	4.77	1.44	1.33
37	15	321	A86	C9-C8	4.77	1.46	1.34
30	A	804	CLA	CHC-C1C	4.77	1.47	1.35
30	7	305	CLA	O2D-CGD	4.77	1.44	1.33
30	A	813	CLA	O2D-CGD	4.77	1.44	1.33
30	A	814	CLA	CHC-C1C	4.77	1.47	1.35
30	10	307	CLA	O2D-CGD	4.77	1.44	1.33
38	8	313	KC1	CHD-C4C	4.77	1.47	1.35
30	4	303	CLA	O2D-CGD	4.77	1.44	1.33
30	5	307	CLA	C1D-ND	4.77	1.43	1.37
30	6	314	CLA	C1D-ND	4.77	1.43	1.37
30	B	808	CLA	O2D-CGD	4.77	1.44	1.33
37	13	315	A86	C26-C27	4.76	1.42	1.35
30	A	809	CLA	CHC-C1C	4.76	1.47	1.35
30	15	306	CLA	CHC-C1C	4.76	1.47	1.35
37	2	302	A86	C26-C27	4.76	1.42	1.35
30	1	304	CLA	C3C-C2C	4.76	1.46	1.36
30	B	818	CLA	C3C-C2C	4.76	1.46	1.36
30	B	851	CLA	C3C-C2C	4.76	1.46	1.36
30	8	309	CLA	C1D-ND	4.76	1.43	1.37
30	A	806	CLA	O2D-CGD	4.76	1.44	1.33
30	1	307	CLA	CHC-C1C	4.76	1.47	1.35
30	4	302	CLA	C1D-ND	4.76	1.43	1.37
38	6	308	KC1	O2D-CGD	4.76	1.44	1.33
38	8	306	KC1	C1A-NA	-4.76	1.28	1.38
30	B	851	CLA	C1D-ND	4.76	1.43	1.37
38	13	305	KC1	O2D-CGD	4.76	1.44	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	838	CLA	O2D-CGD	4.76	1.44	1.33
37	13	313	A86	C2-C1	4.76	1.42	1.35
30	B	827	CLA	O2D-CGD	4.76	1.44	1.33
30	B	814	CLA	O2D-CGD	4.76	1.44	1.33
30	L	202	CLA	O2D-CGD	4.76	1.44	1.33
30	B	839	CLA	C3B-C2B	4.76	1.47	1.40
38	6	308	KC1	CHC-C4B	4.76	1.47	1.38
30	B	802	CLA	C3C-C2C	4.76	1.46	1.36
37	10	315	A86	C26-C27	4.76	1.42	1.35
30	A	805	CLA	O2D-CGD	4.75	1.44	1.33
38	2	306	KC1	O2D-CGD	4.75	1.44	1.33
30	B	803	CLA	CHC-C1C	4.75	1.47	1.35
30	A	820	CLA	CHC-C1C	4.75	1.47	1.35
30	B	812	CLA	O2D-CGD	4.75	1.44	1.33
38	6	312	KC1	C1A-NA	-4.75	1.28	1.38
30	B	812	CLA	CHC-C1C	4.75	1.47	1.35
30	A	828	CLA	CHC-C1C	4.75	1.47	1.35
30	B	807	CLA	CHC-C1C	4.75	1.47	1.35
30	A	830	CLA	O2D-CGD	4.75	1.44	1.33
30	L	203	CLA	O2D-CGD	4.75	1.44	1.33
30	B	803	CLA	C3C-C2C	4.75	1.46	1.36
37	16	314	A86	C9-C8	4.75	1.46	1.34
30	6	314	CLA	C3C-C2C	4.75	1.46	1.36
38	11	307	KC1	C1A-NA	-4.75	1.28	1.38
30	8	308	CLA	C1D-ND	4.75	1.43	1.37
30	9	302	CLA	O2D-CGD	4.75	1.44	1.33
30	8	303	CLA	CHC-C1C	4.75	1.47	1.35
30	12	308	CLA	C1D-ND	4.75	1.43	1.37
37	14	318	A86	C26-C27	4.75	1.42	1.35
30	B	810	CLA	O2D-CGD	4.75	1.44	1.33
30	14	307	CLA	C1D-ND	4.75	1.43	1.37
30	8	301	CLA	O2D-CGD	4.75	1.44	1.33
30	A	814	CLA	C1D-ND	4.74	1.43	1.37
37	14	315	A86	C9-C8	4.74	1.46	1.34
37	10	315	A86	C2-C1	4.74	1.42	1.35
30	2	307	CLA	O2D-CGD	4.74	1.44	1.33
30	2	301	CLA	C3C-C2C	4.74	1.46	1.36
37	5	301	A86	C17-C18	-4.74	1.45	1.52
37	10	316	A86	C9-C8	4.74	1.46	1.34
37	14	317	A86	C9-C8	4.74	1.46	1.34
30	6	305	CLA	C1D-ND	4.74	1.43	1.37
37	7	315	A86	C26-C27	4.74	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	13	312	KC1	OBD-CAD	4.74	1.28	1.22
30	B	816	CLA	CHC-C1C	4.73	1.47	1.35
37	16	312	A86	C17-C18	-4.73	1.45	1.52
38	12	305	KC1	C1A-NA	-4.73	1.28	1.38
30	A	818	CLA	C3C-C2C	4.73	1.46	1.36
37	14	314	A86	C9-C8	4.73	1.46	1.34
30	16	305	CLA	CHC-C1C	4.73	1.47	1.35
30	A	828	CLA	O2D-CGD	4.73	1.44	1.33
30	B	828	CLA	CHC-C1C	4.73	1.47	1.35
38	3	311	KC1	C1A-NA	-4.73	1.28	1.38
30	B	836	CLA	CHC-C1C	4.73	1.47	1.35
30	A	816	CLA	CHC-C1C	4.73	1.47	1.35
30	A	825	CLA	CHC-C1C	4.73	1.47	1.35
38	8	311	KC1	C1A-NA	-4.73	1.28	1.38
38	14	306	KC1	C1A-NA	-4.73	1.28	1.38
38	8	310	KC1	C3C-C2C	4.73	1.46	1.36
38	2	312	KC1	C1A-NA	-4.72	1.28	1.38
30	A	829	CLA	O2D-CGD	4.72	1.44	1.33
30	A	812	CLA	O2D-CGD	4.72	1.44	1.33
38	8	306	KC1	O2D-CGD	4.72	1.44	1.33
30	J	101	CLA	CHC-C1C	4.72	1.47	1.35
38	13	305	KC1	CHC-C4B	4.72	1.47	1.38
30	4	311	CLA	CHC-C1C	4.72	1.47	1.35
30	A	832	CLA	O2D-CGD	4.72	1.44	1.33
30	A	807	CLA	O2D-CGD	4.72	1.44	1.33
30	A	838	CLA	CHC-C1C	4.72	1.47	1.35
30	B	805	CLA	CHC-C1C	4.72	1.47	1.35
30	7	304	CLA	CHC-C1C	4.71	1.47	1.35
30	A	809	CLA	C3C-C2C	4.71	1.46	1.36
38	13	310	KC1	CHC-C4B	4.71	1.47	1.38
38	4	310	KC1	C1A-NA	-4.71	1.28	1.38
30	L	203	CLA	C1D-ND	4.71	1.43	1.37
30	6	310	CLA	CHC-C1C	4.71	1.47	1.35
30	A	817	CLA	C1D-ND	4.71	1.43	1.37
30	A	812	CLA	CHC-C1C	4.70	1.47	1.35
30	9	306	CLA	CHC-C1C	4.70	1.47	1.35
38	3	304	KC1	O2D-CGD	4.70	1.44	1.33
30	A	815	CLA	C1D-ND	4.70	1.43	1.37
30	10	305	CLA	C1D-ND	4.70	1.43	1.37
37	15	323	A86	C2-C1	4.70	1.42	1.35
38	14	308	KC1	OBD-CAD	4.70	1.28	1.22
30	15	308	CLA	C1D-ND	4.70	1.43	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	9	302	CLA	CHC-C1C	4.70	1.47	1.35
30	10	308	CLA	C1D-ND	4.70	1.43	1.37
30	7	306	CLA	O2D-CGD	4.70	1.44	1.33
38	13	312	KC1	CHC-C4B	4.70	1.47	1.38
30	A	829	CLA	C1D-ND	4.70	1.43	1.37
30	6	314	CLA	CHC-C1C	4.70	1.47	1.35
30	F	203	CLA	C1D-ND	4.70	1.43	1.37
30	B	823	CLA	O2D-CGD	4.70	1.44	1.33
30	1	303	CLA	C1D-ND	4.70	1.43	1.37
38	1	306	KC1	CHC-C4B	4.69	1.47	1.38
37	14	319	A86	C26-C27	4.69	1.42	1.35
30	B	834	CLA	O2D-CGD	4.69	1.44	1.33
30	A	840	CLA	CHC-C1C	4.69	1.47	1.35
30	7	307	CLA	C1D-ND	4.69	1.43	1.37
30	A	827	CLA	O2D-CGD	4.69	1.44	1.33
30	A	838	CLA	O2D-CGD	4.69	1.44	1.33
30	12	303	CLA	C1D-ND	4.69	1.43	1.37
30	4	304	CLA	C1D-ND	4.68	1.43	1.37
30	A	810	CLA	O2D-CGD	4.68	1.44	1.33
30	B	805	CLA	O2D-CGD	4.68	1.44	1.33
30	B	809	CLA	O2D-CGD	4.68	1.44	1.33
30	12	307	CLA	C3C-C2C	4.68	1.46	1.36
30	B	804	CLA	O2D-CGD	4.68	1.44	1.33
30	9	309	CLA	CHC-C1C	4.68	1.47	1.35
30	B	833	CLA	C1D-ND	4.68	1.43	1.37
37	2	318	A86	C9-C8	4.67	1.46	1.34
38	2	306	KC1	CHC-C4B	4.67	1.47	1.38
30	B	812	CLA	C1D-ND	4.67	1.43	1.37
30	9	301	CLA	CHC-C1C	4.67	1.46	1.35
30	A	843	CLA	C3B-C2B	4.67	1.46	1.40
37	11	316	A86	C9-C8	4.67	1.46	1.34
30	12	302	CLA	CHC-C1C	4.67	1.46	1.35
38	12	305	KC1	OBD-CAD	4.67	1.28	1.22
30	B	806	CLA	C1D-ND	4.66	1.43	1.37
30	A	835	CLA	CHC-C1C	4.66	1.46	1.35
30	12	306	CLA	CHC-C1C	4.66	1.46	1.35
30	6	304	CLA	C1D-ND	4.66	1.43	1.37
30	B	824	CLA	O2D-CGD	4.66	1.44	1.33
30	A	843	CLA	CHC-C1C	4.66	1.46	1.35
37	12	314	A86	C9-C8	4.66	1.46	1.34
30	A	826	CLA	O2D-CGD	4.66	1.44	1.33
37	14	316	A86	C9-C8	4.66	1.46	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	8	314	KC1	O2D-CGD	4.66	1.44	1.33
30	B	816	CLA	C1D-ND	4.66	1.43	1.37
30	A	833	CLA	C1D-ND	4.66	1.43	1.37
30	2	304	CLA	C1D-ND	4.66	1.43	1.37
30	B	839	CLA	O2D-CGD	4.65	1.44	1.33
38	16	304	KC1	C1A-NA	-4.65	1.28	1.38
30	A	815	CLA	CHC-C1C	4.65	1.46	1.35
30	A	834	CLA	C1D-ND	4.65	1.43	1.37
30	2	303	CLA	O2A-CGA	4.65	1.46	1.33
30	F	201	CLA	O2D-CGD	4.65	1.44	1.33
30	3	310	CLA	CHC-C1C	4.65	1.46	1.35
38	13	305	KC1	C4D-ND	4.65	1.39	1.35
38	5	306	KC1	OBD-CAD	4.65	1.28	1.22
30	B	825	CLA	C1D-ND	4.65	1.43	1.37
37	10	302	A86	C26-C27	4.65	1.41	1.35
38	9	310	KC1	CHC-C4B	4.65	1.47	1.38
30	B	801	CLA	O2D-CGD	4.64	1.44	1.33
30	15	308	CLA	O2D-CGD	4.64	1.44	1.33
30	7	303	CLA	O2D-CGD	4.64	1.44	1.33
38	2	314	KC1	CHC-C4B	4.64	1.47	1.38
37	4	312	A86	C9-C8	4.64	1.46	1.34
37	15	320	A86	C2-C1	4.64	1.41	1.35
30	5	307	CLA	CHC-C1C	4.64	1.46	1.35
37	6	320	A86	C9-C8	4.64	1.46	1.34
38	5	306	KC1	CHC-C4B	4.63	1.47	1.38
38	10	312	KC1	CHC-C4B	4.63	1.47	1.38
30	A	831	CLA	CHC-C1C	4.63	1.46	1.35
30	5	303	CLA	C1D-ND	4.63	1.43	1.37
30	16	303	CLA	C1D-ND	4.63	1.43	1.37
30	B	815	CLA	O2D-CGD	4.63	1.44	1.33
30	2	311	CLA	OBD-CAD	4.63	1.30	1.22
30	B	815	CLA	CHC-C1C	4.63	1.46	1.35
30	15	307	CLA	CHC-C1C	4.63	1.46	1.35
30	B	801	CLA	CHC-C1C	4.63	1.46	1.35
38	3	311	KC1	OBD-CAD	4.63	1.28	1.22
38	2	312	KC1	CHC-C4B	4.62	1.47	1.38
30	B	832	CLA	C1D-ND	4.62	1.43	1.37
30	11	306	CLA	C1D-ND	4.62	1.43	1.37
37	11	314	A86	C26-C27	4.62	1.41	1.35
38	16	311	KC1	CHC-C4B	4.62	1.47	1.38
37	3	314	A86	C26-C27	4.62	1.41	1.35
30	9	303	CLA	C3C-C2C	4.62	1.46	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	6	308	KC1	C1A-NA	-4.62	1.29	1.38
30	9	308	CLA	C1D-ND	4.62	1.43	1.37
37	1	309	A86	C9-C8	4.62	1.46	1.34
37	14	314	A86	C26-C27	4.61	1.41	1.35
38	12	311	KC1	C1A-NA	-4.61	1.29	1.38
38	13	306	KC1	C1A-NA	-4.61	1.29	1.38
37	14	301	A86	C26-C27	4.61	1.41	1.35
38	10	312	KC1	OBD-CAD	4.61	1.28	1.22
38	12	311	KC1	CHC-C4B	4.61	1.47	1.38
30	5	304	CLA	C1D-ND	4.61	1.43	1.37
38	13	310	KC1	C1A-NA	-4.61	1.29	1.38
38	13	311	KC1	OBD-CAD	4.61	1.28	1.22
37	15	315	A86	C5-C6	4.61	1.41	1.35
37	15	315	A86	C17-C18	-4.61	1.45	1.52
30	B	815	CLA	C1D-ND	4.61	1.43	1.37
30	6	304	CLA	O2D-CGD	4.61	1.44	1.33
30	A	804	CLA	O2D-CGD	4.61	1.44	1.33
38	11	311	KC1	OBD-CAD	4.61	1.28	1.22
37	14	316	A86	C26-C27	4.60	1.41	1.35
30	12	302	CLA	C1D-ND	4.60	1.43	1.37
38	3	304	KC1	CHC-C4B	4.60	1.47	1.38
38	11	312	KC1	OBD-CAD	4.60	1.28	1.22
37	14	319	A86	C2-C1	4.60	1.41	1.35
37	15	316	A86	C2-C1	4.60	1.41	1.35
30	2	308	CLA	C1D-ND	4.60	1.43	1.37
37	4	317	A86	C9-C8	4.60	1.46	1.34
38	6	312	KC1	CHC-C4B	4.60	1.47	1.38
30	A	806	CLA	C3C-C2C	4.60	1.46	1.36
30	A	826	CLA	CHC-C1C	4.60	1.46	1.35
30	9	305	CLA	O2D-CGD	4.59	1.44	1.33
37	10	315	A86	O4-C38	4.59	1.45	1.35
30	B	834	CLA	C1D-ND	4.59	1.43	1.37
37	5	301	A86	C26-C27	4.59	1.41	1.35
38	6	313	KC1	CHC-C4B	4.59	1.47	1.38
30	2	305	CLA	O2D-CGD	4.59	1.44	1.33
38	12	305	KC1	CHC-C4B	4.59	1.47	1.38
37	4	317	A86	C17-C18	-4.59	1.45	1.52
38	3	308	KC1	C1A-NA	-4.59	1.29	1.38
30	B	831	CLA	C1D-ND	4.59	1.43	1.37
30	7	311	CLA	C1D-ND	4.59	1.43	1.37
30	B	801	CLA	C3C-C2C	4.59	1.46	1.36
30	A	818	CLA	C1D-ND	4.59	1.43	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	9	302	CLA	C1D-ND	4.58	1.43	1.37
38	5	305	KC1	CHC-C4B	4.58	1.47	1.38
37	8	315	A86	C17-C18	-4.58	1.45	1.52
38	11	307	KC1	OBD-CAD	4.58	1.28	1.22
30	3	302	CLA	C1D-ND	4.58	1.43	1.37
30	1	302	CLA	O2D-CGD	4.58	1.44	1.33
30	A	823	CLA	C1D-ND	4.58	1.43	1.37
38	3	311	KC1	CHC-C4B	4.58	1.47	1.38
38	12	309	KC1	C1A-NA	-4.57	1.29	1.38
37	8	318	A86	C9-C8	4.57	1.46	1.34
30	5	302	CLA	O2D-CGD	4.57	1.44	1.33
38	8	312	KC1	CHC-C4B	4.57	1.47	1.38
38	13	308	KC1	CHC-C4B	4.57	1.47	1.38
30	2u	202	CLA	C1D-ND	4.57	1.43	1.37
30	A	802	CLA	O2D-CGD	4.57	1.44	1.33
37	4	315	A86	C9-C8	4.57	1.46	1.34
38	8	313	KC1	CHC-C4B	4.57	1.47	1.38
30	1	304	CLA	C1D-ND	4.57	1.43	1.37
37	15	322	A86	C2-C1	4.57	1.41	1.35
37	9	313	A86	C9-C8	4.56	1.46	1.34
30	A	834	CLA	O2D-CGD	4.56	1.44	1.33
30	15	314	CLA	O2D-CGD	4.56	1.44	1.33
38	4	310	KC1	OBD-CAD	4.56	1.28	1.22
38	9	312	KC1	OBD-CAD	4.56	1.28	1.22
30	A	839	CLA	C1D-ND	4.56	1.43	1.37
30	5	302	CLA	C1D-ND	4.56	1.43	1.37
37	11	301	A86	C26-C27	4.56	1.41	1.35
38	16	304	KC1	OBD-CAD	4.56	1.28	1.22
30	B	808	CLA	CHC-C1C	4.56	1.46	1.35
31	A	845	PQN	C10-C5	4.56	1.48	1.40
30	1	301	CLA	C1D-ND	4.55	1.43	1.37
38	11	307	KC1	CHC-C4B	4.55	1.47	1.38
37	13	315	A86	C2-C1	4.55	1.41	1.35
30	11	309	CLA	C1D-ND	4.55	1.43	1.37
38	11	305	KC1	CHC-C4B	4.55	1.47	1.38
30	4	306	CLA	C1D-ND	4.55	1.43	1.37
30	14	309	CLA	CHD-C1D	4.55	1.47	1.38
38	4	310	KC1	CHC-C4B	4.55	1.47	1.38
30	A	836	CLA	CHC-C1C	4.54	1.46	1.35
37	7	315	A86	C2-C1	4.54	1.41	1.35
30	B	809	CLA	C3B-C2B	4.54	1.46	1.40
30	4	303	CLA	C1D-ND	4.54	1.43	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	8	306	KC1	OBD-CAD	4.54	1.28	1.22
37	7	315	A86	C9-C8	4.54	1.46	1.34
38	9	312	KC1	CHB-C1B	4.54	1.47	1.38
37	4	312	A86	C17-C18	-4.54	1.45	1.52
37	12	314	A86	C17-C18	-4.54	1.45	1.52
30	B	819	CLA	C3B-C2B	4.54	1.46	1.40
30	9	306	CLA	O2A-CGA	4.54	1.46	1.30
30	A	831	CLA	O2D-CGD	4.53	1.44	1.33
30	B	813	CLA	O2D-CGD	4.53	1.44	1.33
38	14	306	KC1	OBD-CAD	4.53	1.28	1.22
38	9	312	KC1	CHC-C4B	4.53	1.47	1.38
38	7	308	KC1	CHC-C4B	4.53	1.47	1.38
38	2	306	KC1	OBD-CAD	4.53	1.28	1.22
38	13	305	KC1	C1A-NA	-4.53	1.29	1.38
38	14	308	KC1	CHC-C4B	4.53	1.47	1.38
30	A	811	CLA	C1D-ND	4.53	1.43	1.37
38	1	306	KC1	OBD-CAD	4.53	1.28	1.22
37	14	314	A86	C2-C1	4.53	1.41	1.35
30	A	839	CLA	O2D-CGD	4.53	1.44	1.33
30	B	817	CLA	C1D-ND	4.53	1.43	1.37
37	5	316	A86	C26-C27	4.53	1.41	1.35
38	4	308	KC1	OBD-CAD	4.53	1.28	1.22
37	7	316	A86	C17-C18	-4.53	1.45	1.52
38	14	311	KC1	CHC-C4B	4.53	1.47	1.38
38	13	312	KC1	C4D-ND	4.53	1.39	1.35
30	11	310	CLA	CHD-C1D	4.52	1.47	1.38
38	1	308	KC1	CHC-C4B	4.52	1.47	1.38
30	A	814	CLA	C3C-C2C	4.52	1.46	1.36
37	9	316	A86	O4-C38	4.52	1.45	1.35
30	5	311	CLA	O2A-CGA	4.52	1.46	1.33
30	L	203	CLA	O2A-CGA	4.52	1.45	1.30
38	2	314	KC1	OBD-CAD	4.52	1.28	1.22
30	A	820	CLA	C1D-ND	4.52	1.43	1.37
38	16	304	KC1	CHC-C4B	4.51	1.47	1.38
37	5	316	A86	C17-C18	-4.51	1.45	1.52
30	9	303	CLA	C1D-ND	4.51	1.43	1.37
30	3	310	CLA	O2A-CGA	4.51	1.45	1.30
30	16	309	CLA	O2A-CGA	4.51	1.45	1.30
30	A	807	CLA	C1D-ND	4.51	1.43	1.37
38	5	310	KC1	OBD-CAD	4.51	1.28	1.22
30	14	309	CLA	O2A-CGA	4.51	1.45	1.30
38	10	306	KC1	C1A-NA	-4.51	1.29	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	14	311	KC1	OBD-CAD	4.51	1.28	1.22
30	A	816	CLA	C1D-ND	4.51	1.43	1.37
30	14	304	CLA	O2A-CGA	4.51	1.45	1.30
38	4	307	KC1	C4D-ND	4.51	1.39	1.35
38	5	305	KC1	C1A-NA	-4.51	1.29	1.38
30	10	311	CLA	O2A-CGA	4.50	1.45	1.30
30	B	809	CLA	CHC-C1C	4.50	1.46	1.35
30	7	306	CLA	CHC-C1C	4.50	1.46	1.35
30	15	314	CLA	O2A-CGA	4.50	1.45	1.30
30	13	304	CLA	O2A-CGA	4.50	1.45	1.30
38	13	310	KC1	OBD-CAD	4.50	1.28	1.22
38	8	307	KC1	CHC-C4B	4.50	1.47	1.38
30	4	305	CLA	C1D-ND	4.50	1.43	1.37
38	5	312	KC1	CHC-C4B	4.50	1.47	1.38
38	16	311	KC1	C1A-NA	-4.50	1.29	1.38
30	7	309	CLA	CHC-C1C	4.50	1.46	1.35
30	15	306	CLA	O2A-CGA	4.49	1.45	1.30
30	1	305	CLA	CHD-C1D	4.49	1.47	1.38
38	7	313	KC1	CHC-C4B	4.49	1.47	1.38
30	9	301	CLA	O2D-CGD	4.49	1.44	1.33
30	3	309	CLA	O2A-CGA	4.49	1.45	1.30
38	13	312	KC1	C1A-NA	-4.49	1.29	1.38
37	6	320	A86	C26-C27	4.49	1.41	1.35
38	10	306	KC1	OBD-CAD	4.49	1.28	1.22
30	6	316	CLA	C1D-ND	4.49	1.43	1.37
30	F	202	CLA	C1D-ND	4.49	1.43	1.37
30	B	823	CLA	C1D-ND	4.49	1.43	1.37
30	13	309	CLA	O2A-CGA	4.49	1.45	1.30
30	1	303	CLA	O2D-CGD	4.49	1.44	1.33
37	3	314	A86	O4-C38	4.49	1.45	1.35
38	1	308	KC1	C4D-ND	4.48	1.39	1.35
30	B	815	CLA	O2A-CGA	4.48	1.45	1.30
37	11	301	A86	C7-C6	4.48	1.60	1.50
38	14	308	KC1	C1A-NA	-4.48	1.29	1.38
30	2	313	CLA	O2A-CGA	4.48	1.45	1.30
38	5	312	KC1	OBD-CAD	4.48	1.28	1.22
30	15	311	CLA	O2A-CGA	4.48	1.45	1.30
30	2	301	CLA	O2A-CGA	4.48	1.46	1.33
30	16	303	CLA	O2A-CGA	4.48	1.46	1.33
38	2	312	KC1	OBD-CAD	4.48	1.28	1.22
37	2u	205	A86	O4-C38	4.48	1.45	1.35
30	A	810	CLA	C1D-ND	4.48	1.43	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	1	307	CLA	OBD-CAD	4.48	1.30	1.22
38	9	311	KC1	CHB-C1B	4.48	1.47	1.38
38	9	304	KC1	CHC-C4B	4.48	1.47	1.38
30	A	838	CLA	C1D-ND	4.48	1.43	1.37
37	2	319	A86	C17-C18	-4.48	1.45	1.52
37	10	317	A86	C2-C1	4.48	1.41	1.35
30	12	306	CLA	C1D-ND	4.48	1.43	1.37
37	9	315	A86	O4-C38	4.48	1.45	1.35
37	5	315	A86	C26-C27	4.48	1.41	1.35
38	8	311	KC1	CHC-C4B	4.48	1.47	1.38
38	10	306	KC1	CHC-C4B	4.48	1.47	1.38
30	6	315	CLA	O2A-CGA	4.47	1.45	1.30
30	14	312	CLA	O2A-CGA	4.47	1.45	1.30
38	9	304	KC1	OBD-CAD	4.47	1.28	1.22
38	13	311	KC1	C1A-NA	-4.47	1.29	1.38
38	9	311	KC1	C4D-ND	4.47	1.39	1.35
30	15	312	CLA	CHD-C1D	4.47	1.47	1.38
30	16	310	CLA	O2A-CGA	4.47	1.45	1.30
30	B	835	CLA	C1D-ND	4.47	1.43	1.37
30	B	812	CLA	O2A-CGA	4.47	1.46	1.33
30	15	305	CLA	O2A-CGA	4.47	1.45	1.30
38	13	305	KC1	OBD-CAD	4.47	1.28	1.22
29	A	801	CL0	CHC-C1C	4.46	1.46	1.35
37	5	316	A86	O4-C38	4.46	1.45	1.35
30	B	838	CLA	CHC-C1C	4.46	1.46	1.35
30	3	301	CLA	C1D-ND	4.46	1.43	1.37
38	12	313	KC1	CHC-C4B	4.46	1.47	1.38
37	6	320	A86	O4-C38	4.46	1.45	1.35
30	A	837	CLA	O2A-CGA	4.46	1.45	1.30
30	16	308	CLA	O2A-CGA	4.46	1.45	1.30
37	15	315	A86	C10-C11	4.46	1.47	1.34
37	9	315	A86	C2-C1	4.46	1.41	1.35
30	15	310	CLA	O2A-CGA	4.46	1.45	1.30
38	5	305	KC1	CHB-C1B	4.46	1.47	1.38
30	B	818	CLA	C1D-ND	4.46	1.43	1.37
30	15	312	CLA	O2A-CGA	4.46	1.45	1.30
38	11	311	KC1	CHC-C4B	4.45	1.47	1.38
37	3	315	A86	C17-C18	-4.45	1.45	1.52
38	8	314	KC1	CHC-C4B	4.45	1.47	1.38
38	13	308	KC1	OBD-CAD	4.45	1.28	1.22
30	15	308	CLA	O2A-CGA	4.45	1.45	1.30
38	12	313	KC1	C1A-CHA	4.45	1.52	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	13	312	KC1	CHB-C1B	4.45	1.47	1.38
30	A	821	CLA	CHC-C1C	4.45	1.46	1.35
30	10	307	CLA	C1D-ND	4.45	1.43	1.37
30	7	303	CLA	O2A-CGA	4.45	1.46	1.33
38	3	304	KC1	C1A-NA	-4.45	1.29	1.38
37	9	313	A86	O4-C38	4.45	1.45	1.35
38	10	306	KC1	C4D-ND	4.45	1.39	1.35
30	6	306	CLA	O2A-CGA	4.45	1.46	1.33
38	8	310	KC1	OBD-CAD	4.45	1.28	1.22
37	2	319	A86	O4-C38	4.45	1.45	1.35
30	J	101	CLA	O2A-CGA	4.45	1.45	1.30
37	8	315	A86	O4-C38	4.44	1.45	1.35
37	14	301	A86	O4-C38	4.44	1.45	1.35
30	9	301	CLA	C1D-ND	4.44	1.43	1.37
30	11	306	CLA	O2A-CGA	4.44	1.46	1.33
38	8	312	KC1	OBD-CAD	4.44	1.28	1.22
30	A	813	CLA	C1D-ND	4.44	1.43	1.37
38	4	308	KC1	C1B-NB	-4.44	1.32	1.37
30	2	301	CLA	CHC-C1C	4.44	1.46	1.35
30	B	829	CLA	C3B-C2B	4.44	1.46	1.40
30	B	837	CLA	C1D-ND	4.44	1.43	1.37
38	13	306	KC1	CHB-C1B	4.43	1.47	1.38
30	B	838	CLA	C1D-ND	4.43	1.43	1.37
38	12	309	KC1	OBD-CAD	4.43	1.28	1.22
30	B	820	CLA	O2A-CGA	4.43	1.45	1.30
30	B	828	CLA	O2D-CGD	4.43	1.44	1.33
30	F	203	CLA	O2A-CGA	4.43	1.45	1.30
38	5	312	KC1	C1B-NB	-4.43	1.32	1.37
37	14	320	A86	O4-C38	4.43	1.45	1.35
30	A	814	CLA	O2D-CGD	4.43	1.44	1.33
30	13	307	CLA	CHD-C1D	4.43	1.47	1.38
38	6	312	KC1	CHB-C1B	4.43	1.47	1.38
37	15	320	A86	O4-C38	4.43	1.45	1.35
37	2u	203	A86	C17-C18	-4.43	1.46	1.52
38	10	306	KC1	CHB-C1B	4.42	1.47	1.38
37	4	312	A86	O4-C38	4.42	1.45	1.35
37	14	315	A86	C17-C18	-4.42	1.46	1.52
37	2	302	A86	C7-C6	4.42	1.60	1.50
30	6	309	CLA	C1D-ND	4.42	1.43	1.37
37	9	316	A86	C2-C1	4.42	1.41	1.35
37	11	314	A86	O4-C38	4.42	1.45	1.35
37	11	315	A86	O4-C38	4.42	1.45	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	809	CLA	C1D-ND	4.42	1.43	1.37
38	8	312	KC1	C1A-NA	-4.42	1.29	1.38
38	11	305	KC1	CHB-C1B	4.42	1.47	1.38
37	12	314	A86	O4-C38	4.42	1.45	1.35
37	10	301	A86	C9-C8	4.42	1.46	1.34
37	11	316	A86	O4-C38	4.42	1.45	1.35
30	15	304	CLA	O2A-CGA	4.42	1.46	1.33
30	A	808	CLA	C1D-ND	4.42	1.43	1.37
37	3	314	A86	C2-C1	4.42	1.41	1.35
37	16	312	A86	O4-C38	4.42	1.45	1.35
37	10	316	A86	C17-C18	-4.41	1.46	1.52
30	B	830	CLA	O2A-CGA	4.41	1.46	1.33
30	15	302	CLA	O2A-CGA	4.41	1.46	1.33
38	12	313	KC1	C3D-C2D	4.41	1.47	1.39
38	11	307	KC1	CHB-C1B	4.41	1.47	1.38
37	10	301	A86	O4-C38	4.41	1.45	1.35
38	3	308	KC1	CHB-C1B	4.41	1.47	1.38
30	B	836	CLA	C1D-ND	4.41	1.43	1.37
37	7	319	A86	C2-C1	4.41	1.41	1.35
37	10	317	A86	O4-C38	4.41	1.45	1.35
38	6	313	KC1	CHB-C1B	4.41	1.46	1.38
37	15	317	A86	C2-C1	4.41	1.41	1.35
37	14	319	A86	O4-C38	4.41	1.45	1.35
30	3	306	CLA	C1D-ND	4.40	1.43	1.37
38	2	306	KC1	C4D-ND	4.40	1.39	1.35
30	13	304	CLA	CHD-C1D	4.40	1.46	1.38
30	B	802	CLA	O2D-CGD	4.40	1.43	1.33
38	1	306	KC1	CHB-C1B	4.40	1.46	1.38
30	3	307	CLA	CHD-C1D	4.40	1.46	1.38
38	7	308	KC1	CHB-C1B	4.40	1.46	1.38
30	6	316	CLA	O2A-CGA	4.40	1.46	1.33
30	8	302	CLA	C1D-ND	4.40	1.43	1.37
30	5	308	CLA	C1D-ND	4.40	1.43	1.37
38	4	307	KC1	CHC-C4B	4.40	1.46	1.38
37	2	302	A86	O4-C38	4.40	1.45	1.35
30	2	303	CLA	C3D-C2D	4.40	1.51	1.39
38	14	311	KC1	CHB-C1B	4.40	1.46	1.38
37	4	314	A86	C7-C6	4.39	1.60	1.50
30	6	307	CLA	C1D-ND	4.39	1.43	1.37
30	9	309	CLA	C1D-ND	4.39	1.43	1.37
30	16	306	CLA	C1D-ND	4.39	1.43	1.37
38	14	311	KC1	C1A-NA	-4.39	1.29	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	2	318	A86	C17-C18	-4.39	1.46	1.52
37	16	312	A86	C26-C27	4.39	1.41	1.35
37	5	315	A86	O4-C38	4.39	1.45	1.35
38	6	312	KC1	OBD-CAD	4.39	1.28	1.22
37	10	302	A86	O4-C38	4.39	1.45	1.35
30	B	804	CLA	C1D-ND	4.39	1.43	1.37
38	2	312	KC1	CHB-C1B	4.38	1.46	1.38
37	4	315	A86	C26-C27	4.38	1.41	1.35
38	11	312	KC1	C1A-NA	-4.38	1.29	1.38
37	7	319	A86	O4-C38	4.38	1.45	1.35
38	9	304	KC1	CHB-C1B	4.38	1.46	1.38
38	16	311	KC1	OBD-CAD	4.38	1.28	1.22
37	15	317	A86	C17-C18	-4.38	1.46	1.52
30	6	307	CLA	CHD-C1D	4.38	1.46	1.38
38	12	313	KC1	OBD-CAD	4.38	1.28	1.22
30	2	305	CLA	C1D-ND	4.38	1.43	1.37
38	3	304	KC1	C4D-ND	4.38	1.39	1.35
37	15	322	A86	C7-C6	4.37	1.59	1.50
38	6	313	KC1	OBD-CAD	4.37	1.28	1.22
38	12	309	KC1	CHC-C4B	4.37	1.46	1.38
37	14	319	A86	C7-C6	4.37	1.59	1.50
37	7	316	A86	C9-C8	4.37	1.45	1.34
30	4	309	CLA	CHD-C1D	4.37	1.46	1.38
37	11	314	A86	C2-C1	4.37	1.41	1.35
37	15	323	A86	C17-C18	-4.37	1.46	1.52
30	A	835	CLA	O2A-CGA	4.37	1.46	1.33
30	10	305	CLA	O2A-CGA	4.37	1.46	1.33
37	12	316	A86	C17-C18	-4.37	1.46	1.52
38	13	308	KC1	CHB-C1B	4.37	1.46	1.38
38	5	305	KC1	OBD-CAD	4.37	1.28	1.22
37	13	315	A86	O4-C38	4.36	1.45	1.35
37	8	315	A86	C9-C8	4.36	1.45	1.34
30	A	827	CLA	C1D-ND	4.36	1.43	1.37
30	B	813	CLA	C1D-ND	4.36	1.43	1.37
30	9	306	CLA	CHD-C1D	4.36	1.46	1.38
31	B	840	PQN	C10-C5	4.36	1.47	1.40
37	15	321	A86	C7-C6	4.36	1.59	1.50
37	14	314	A86	O4-C38	4.36	1.45	1.35
30	7	304	CLA	C1D-ND	4.36	1.43	1.37
30	13	303	CLA	CHD-C1D	4.36	1.46	1.38
37	14	320	A86	C2-C1	4.36	1.41	1.35
30	A	828	CLA	C1D-ND	4.36	1.43	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	5	304	CLA	O2A-CGA	4.36	1.46	1.33
37	15	317	A86	O4-C38	4.35	1.45	1.35
37	14	318	A86	O4-C38	4.35	1.45	1.35
30	5	303	CLA	O2A-CGA	4.35	1.46	1.33
30	14	307	CLA	O2A-CGA	4.35	1.46	1.33
38	4	307	KC1	OBD-CAD	4.35	1.28	1.22
38	5	310	KC1	CHC-C4B	4.35	1.46	1.38
38	7	313	KC1	OBD-CAD	4.35	1.28	1.22
38	12	311	KC1	OBD-CAD	4.35	1.28	1.22
38	8	310	KC1	CHC-C4B	4.35	1.46	1.38
30	14	312	CLA	CHD-C1D	4.35	1.46	1.38
30	B	824	CLA	C1D-ND	4.35	1.43	1.37
38	11	312	KC1	CHB-C1B	4.35	1.46	1.38
30	12	307	CLA	C1D-ND	4.35	1.43	1.37
30	12	321	CLA	O2A-CGA	4.35	1.46	1.33
37	2	318	A86	O4-C38	4.35	1.45	1.35
38	1	308	KC1	OBD-CAD	4.35	1.28	1.22
37	15	323	A86	O4-C38	4.35	1.45	1.35
37	14	317	A86	C17-C18	-4.34	1.46	1.52
30	A	841	CLA	C1D-ND	4.34	1.43	1.37
30	10	309	CLA	O2A-CGA	4.34	1.46	1.33
30	B	823	CLA	O2A-CGA	4.34	1.46	1.33
30	A	825	CLA	CHD-C1D	4.34	1.46	1.38
30	6	310	CLA	CHD-C1D	4.34	1.46	1.38
38	8	306	KC1	CHC-C4B	4.34	1.46	1.38
30	14	303	CLA	CHD-C1D	4.34	1.46	1.38
30	16	307	CLA	CHD-C1D	4.34	1.46	1.38
37	10	302	A86	C7-C6	4.34	1.59	1.50
37	14	320	A86	C7-C6	4.34	1.59	1.50
30	15	309	CLA	CHD-C1D	4.34	1.46	1.38
37	15	315	A86	O4-C38	4.34	1.45	1.35
30	15	311	CLA	CHD-C1D	4.33	1.46	1.38
30	A	820	CLA	CHD-C1D	4.33	1.46	1.38
30	13	303	CLA	O2A-CGA	4.33	1.46	1.33
38	10	310	KC1	CHC-C4B	4.33	1.46	1.38
30	A	832	CLA	C1D-ND	4.33	1.43	1.37
37	2u	203	A86	C7-C6	4.33	1.59	1.50
30	A	815	CLA	O2A-CGA	4.33	1.46	1.33
38	13	305	KC1	CHB-C1B	4.33	1.46	1.38
37	14	301	A86	C2-C1	4.33	1.41	1.35
37	15	323	A86	C7-C6	4.33	1.59	1.50
37	4	315	A86	O4-C38	4.33	1.45	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	2	303	CLA	CHD-C1D	4.33	1.46	1.38
30	7	310	CLA	CHD-C1D	4.32	1.46	1.38
30	B	805	CLA	C1D-ND	4.32	1.43	1.37
38	14	311	KC1	C4D-ND	4.32	1.39	1.35
30	15	303	CLA	O2A-CGA	4.32	1.46	1.33
30	2	308	CLA	O2A-CGA	4.32	1.46	1.33
30	16	309	CLA	CHD-C1D	4.32	1.46	1.38
38	13	310	KC1	C4D-ND	4.32	1.39	1.35
30	8	305	CLA	C1D-ND	4.32	1.43	1.37
37	16	314	A86	O4-C38	4.32	1.45	1.35
30	B	821	CLA	C1D-ND	4.32	1.43	1.37
37	15	317	A86	C7-C6	4.32	1.59	1.50
38	12	305	KC1	CHB-C1B	4.32	1.46	1.38
30	8	309	CLA	CHD-C1D	4.32	1.46	1.38
38	13	306	KC1	OBD-CAD	4.32	1.28	1.22
30	7	312	CLA	CHD-C1D	4.32	1.46	1.38
30	A	838	CLA	O2A-CGA	4.32	1.46	1.33
38	7	308	KC1	OBD-CAD	4.32	1.28	1.22
37	14	316	A86	O4-C38	4.31	1.44	1.35
37	4	317	A86	C26-C27	4.31	1.41	1.35
38	8	311	KC1	OBD-CAD	4.31	1.28	1.22
37	12	316	A86	C2-C1	4.31	1.41	1.35
38	3	304	KC1	CHB-C1B	4.31	1.46	1.38
30	7	306	CLA	C1D-ND	4.31	1.43	1.37
30	15	313	CLA	CHD-C1D	4.31	1.46	1.38
37	3	315	A86	O4-C38	4.31	1.44	1.35
30	11	308	CLA	O2A-CGA	4.31	1.45	1.33
38	3	308	KC1	CHC-C4B	4.31	1.46	1.38
37	12	316	A86	O4-C38	4.31	1.44	1.35
30	1	305	CLA	O2A-CGA	4.31	1.45	1.33
30	A	844	CLA	CHD-C1D	4.30	1.46	1.38
30	A	819	CLA	C1D-ND	4.30	1.43	1.37
38	13	311	KC1	C4D-ND	4.30	1.39	1.35
37	11	315	A86	C26-C27	4.30	1.41	1.35
37	11	316	A86	C7-C6	4.30	1.59	1.50
30	2	309	CLA	O2A-CGA	4.30	1.45	1.33
30	8	309	CLA	O2A-CGA	4.30	1.45	1.33
30	B	827	CLA	O2A-CGA	4.30	1.45	1.33
30	4	303	CLA	O2A-CGA	4.30	1.45	1.33
37	5	316	A86	C2-C1	4.30	1.41	1.35
30	1	301	CLA	O2A-CGA	4.30	1.45	1.33
30	9	305	CLA	O2A-CGA	4.30	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	815	CLA	CHD-C1D	4.30	1.46	1.38
37	9	316	A86	C7-C6	4.30	1.59	1.50
30	3	309	CLA	CHD-C1D	4.30	1.46	1.38
38	9	310	KC1	OBD-CAD	4.30	1.28	1.22
30	16	306	CLA	O2A-CGA	4.30	1.45	1.33
30	A	837	CLA	CHD-C1D	4.29	1.46	1.38
30	1	304	CLA	O2A-CGA	4.29	1.45	1.33
30	B	820	CLA	C1D-ND	4.29	1.43	1.37
37	11	316	A86	C17-C18	-4.29	1.46	1.52
38	14	308	KC1	CHB-C1B	4.29	1.46	1.38
30	8	301	CLA	C1D-ND	4.29	1.43	1.37
30	B	807	CLA	C1D-ND	4.29	1.43	1.37
37	14	318	A86	C17-C18	-4.29	1.46	1.52
30	A	805	CLA	C1D-ND	4.29	1.43	1.37
37	12	314	A86	C26-C27	4.29	1.41	1.35
30	3	303	CLA	CHD-C1D	4.29	1.46	1.38
30	A	842	CLA	C1D-ND	4.29	1.43	1.37
37	11	314	A86	C7-C6	4.29	1.59	1.50
30	14	304	CLA	CHD-C1D	4.29	1.46	1.38
30	B	812	CLA	CHD-C1D	4.29	1.46	1.38
30	A	843	CLA	C1D-ND	4.28	1.43	1.37
30	A	813	CLA	O2A-CGA	4.28	1.45	1.33
30	7	305	CLA	O2A-CGA	4.28	1.45	1.33
30	A	804	CLA	O2A-CGA	4.28	1.45	1.33
38	16	304	KC1	CHB-C1B	4.28	1.46	1.38
38	8	310	KC1	CHB-C1B	4.28	1.46	1.38
30	3	306	CLA	CHD-C1D	4.28	1.46	1.38
37	4	317	A86	O4-C38	4.28	1.44	1.35
30	15	307	CLA	O2A-CGA	4.28	1.45	1.33
37	15	322	A86	O4-C38	4.28	1.44	1.35
30	2	305	CLA	O2A-CGA	4.28	1.45	1.33
30	B	810	CLA	C1D-ND	4.28	1.43	1.37
38	13	310	KC1	CHB-C1B	4.28	1.46	1.38
37	15	315	A86	C7-C6	4.28	1.59	1.50
30	A	822	CLA	O2A-CGA	4.28	1.45	1.33
30	B	816	CLA	O2A-CGA	4.28	1.45	1.33
37	14	315	A86	C7-C6	4.28	1.59	1.50
37	14	317	A86	O4-C38	4.28	1.44	1.35
30	14	305	CLA	CHD-C1D	4.28	1.46	1.38
38	11	311	KC1	CHB-C1B	4.28	1.46	1.38
30	6	315	CLA	CHD-C1D	4.28	1.46	1.38
37	11	316	A86	C2-C1	4.28	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	11	308	CLA	CHD-C1D	4.28	1.46	1.38
30	A	835	CLA	CHD-C1D	4.27	1.46	1.38
37	13	315	A86	C7-C6	4.27	1.59	1.50
37	11	301	A86	O4-C38	4.27	1.44	1.35
37	10	301	A86	C17-C18	-4.27	1.46	1.52
30	2	311	CLA	CHD-C1D	4.27	1.46	1.38
30	A	825	CLA	O2A-CGA	4.27	1.45	1.33
30	B	814	CLA	O2A-CGA	4.27	1.45	1.33
30	14	302	CLA	CHD-C1D	4.27	1.46	1.38
30	14	305	CLA	O2A-CGA	4.27	1.45	1.33
37	14	318	A86	C2-C1	4.27	1.41	1.35
30	A	826	CLA	C1D-ND	4.27	1.43	1.37
38	8	311	KC1	CHB-C1B	4.27	1.46	1.38
37	4	314	A86	C2-C1	4.27	1.41	1.35
30	2	307	CLA	O2A-CGA	4.27	1.45	1.33
30	2	311	CLA	O2A-CGA	4.27	1.45	1.33
30	13	302	CLA	O2A-CGA	4.27	1.45	1.33
37	15	320	A86	C7-C6	4.27	1.59	1.50
30	12	303	CLA	O2A-CGA	4.27	1.45	1.33
30	14	313	CLA	CHD-C1D	4.27	1.46	1.38
38	2	306	KC1	CHB-C1B	4.27	1.46	1.38
37	5	301	A86	O4-C38	4.27	1.44	1.35
30	B	834	CLA	O2A-CGA	4.27	1.45	1.33
30	15	310	CLA	CHD-C1D	4.27	1.46	1.38
30	12	321	CLA	CHD-C1D	4.26	1.46	1.38
30	13	309	CLA	CHD-C1D	4.26	1.46	1.38
37	14	301	A86	C7-C6	4.26	1.59	1.50
38	8	307	KC1	OBD-CAD	4.26	1.28	1.22
30	15	304	CLA	CHD-C1D	4.26	1.46	1.38
38	2	314	KC1	CHB-C1B	4.26	1.46	1.38
37	16	312	A86	C7-C6	4.26	1.59	1.50
30	11	304	CLA	O2A-CGA	4.26	1.45	1.33
37	1	309	A86	C26-C27	4.26	1.41	1.35
30	3	307	CLA	O2A-CGA	4.26	1.45	1.33
30	B	839	CLA	C1D-ND	4.26	1.43	1.37
30	14	303	CLA	O2A-CGA	4.26	1.45	1.33
37	4	315	A86	C7-C6	4.26	1.59	1.50
30	14	310	CLA	O2A-CGA	4.26	1.45	1.33
30	A	810	CLA	O2A-CGA	4.25	1.45	1.33
37	10	317	A86	C7-C6	4.25	1.59	1.50
37	15	316	A86	O4-C38	4.25	1.44	1.35
37	13	315	A86	C10-C11	4.25	1.46	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	4	301	CLA	C1D-ND	4.25	1.43	1.37
37	2u	203	A86	O4-C38	4.25	1.44	1.35
37	1	309	A86	O4-C38	4.25	1.44	1.35
37	16	314	A86	C7-C6	4.25	1.59	1.50
30	A	806	CLA	C1D-ND	4.25	1.43	1.37
38	4	307	KC1	CHB-C1B	4.25	1.46	1.38
30	8	304	CLA	O2A-CGA	4.25	1.45	1.33
37	15	316	A86	C7-C6	4.25	1.59	1.50
30	10	308	CLA	CHD-C1D	4.25	1.46	1.38
38	3	311	KC1	CHB-C1B	4.25	1.46	1.38
38	11	307	KC1	C4D-ND	4.25	1.39	1.35
30	15	306	CLA	CHD-C1D	4.25	1.46	1.38
38	3	304	KC1	OBD-CAD	4.25	1.28	1.22
37	4	314	A86	O4-C38	4.25	1.44	1.35
30	A	836	CLA	O2A-CGA	4.25	1.45	1.33
30	1	307	CLA	CHD-C1D	4.24	1.46	1.38
38	8	314	KC1	C1A-NA	-4.24	1.29	1.38
30	2	310	CLA	O2A-CGA	4.24	1.45	1.33
30	15	309	CLA	O2A-CGA	4.24	1.45	1.33
30	A	802	CLA	CHD-C1D	4.24	1.46	1.38
30	B	821	CLA	O2A-CGA	4.24	1.45	1.33
30	16	308	CLA	CHD-C1D	4.24	1.46	1.38
30	1	307	CLA	O2A-CGA	4.24	1.45	1.33
30	6	304	CLA	O2A-CGA	4.24	1.45	1.33
30	A	824	CLA	O2A-CGA	4.24	1.45	1.33
30	6	305	CLA	O2A-CGA	4.24	1.45	1.33
30	4	309	CLA	O2A-CGA	4.24	1.45	1.33
37	9	313	A86	C7-C6	4.24	1.59	1.50
37	13	315	A86	C17-C18	-4.24	1.46	1.52
37	14	301	A86	C21-C20	4.24	1.58	1.51
30	F	202	CLA	O2A-CGA	4.24	1.45	1.33
38	8	313	KC1	CHB-C1B	4.24	1.46	1.38
37	14	320	A86	C5-C6	4.24	1.41	1.35
30	9	309	CLA	O2A-CGA	4.24	1.45	1.33
30	A	804	CLA	C1D-ND	4.24	1.43	1.37
38	10	310	KC1	OBD-CAD	4.23	1.28	1.22
30	12	304	CLA	O2A-CGA	4.23	1.45	1.33
30	A	824	CLA	C1D-ND	4.23	1.43	1.37
30	9	308	CLA	O2A-CGA	4.23	1.45	1.33
38	8	306	KC1	CHB-C1B	4.23	1.46	1.38
30	A	841	CLA	CHD-C1D	4.23	1.46	1.38
30	10	303	CLA	O2A-CGA	4.23	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	16	314	A86	C26-C27	4.23	1.41	1.35
30	10	304	CLA	O2A-CGA	4.23	1.45	1.33
30	7	307	CLA	O2A-CGA	4.23	1.45	1.33
30	10	308	CLA	O2A-CGA	4.23	1.45	1.33
30	7	311	CLA	O2A-CGA	4.23	1.45	1.33
30	15	303	CLA	CHD-C1D	4.23	1.46	1.38
30	B	808	CLA	C1D-ND	4.22	1.43	1.37
30	A	803	CLA	O2A-CGA	4.22	1.45	1.33
38	14	306	KC1	C4D-ND	4.22	1.39	1.35
30	15	313	CLA	O2A-CGA	4.22	1.45	1.33
30	5	308	CLA	O2A-CGA	4.22	1.45	1.33
30	14	310	CLA	CHD-C1D	4.22	1.46	1.38
37	13	313	A86	C5-C6	4.22	1.41	1.35
38	4	308	KC1	C1A-CHA	4.22	1.51	1.40
30	L	202	CLA	O2A-CGA	4.22	1.45	1.33
37	15	320	A86	C5-C6	4.22	1.41	1.35
30	2	313	CLA	CHD-C1D	4.22	1.46	1.38
37	15	321	A86	C2-C1	4.22	1.41	1.35
30	13	307	CLA	O2A-CGA	4.22	1.45	1.33
38	14	306	KC1	CHB-C1B	4.22	1.46	1.38
37	2	302	A86	C2-C1	4.22	1.41	1.35
37	1	309	A86	C7-C6	4.22	1.59	1.50
30	A	817	CLA	O2A-CGA	4.22	1.45	1.33
38	4	308	KC1	C1A-NA	-4.22	1.29	1.38
30	2u	202	CLA	O2A-CGA	4.22	1.45	1.33
30	3	303	CLA	O2A-CGA	4.22	1.45	1.33
30	11	309	CLA	O2A-CGA	4.22	1.45	1.33
38	10	312	KC1	CHB-C1B	4.22	1.46	1.38
37	5	301	A86	C2-C1	4.21	1.41	1.35
38	1	308	KC1	C1B-NB	-4.21	1.32	1.37
30	5	309	CLA	O2A-CGA	4.21	1.45	1.33
37	4	317	A86	C7-C6	4.21	1.59	1.50
37	15	321	A86	O4-C38	4.21	1.44	1.35
30	4	304	CLA	O2A-CGA	4.21	1.45	1.33
30	6	314	CLA	O2A-CGA	4.21	1.45	1.33
37	14	319	A86	C17-C18	-4.21	1.46	1.52
38	12	311	KC1	C4D-ND	4.20	1.39	1.35
30	9	302	CLA	CHD-C1D	4.20	1.46	1.38
30	12	304	CLA	CHD-C1D	4.20	1.46	1.38
30	15	305	CLA	CHD-C1D	4.20	1.46	1.38
30	8	302	CLA	O2A-CGA	4.20	1.45	1.33
37	15	320	A86	C10-C11	4.20	1.46	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	4	302	CLA	O2A-CGA	4.20	1.45	1.33
38	4	310	KC1	C4D-ND	4.20	1.39	1.35
30	4	305	CLA	O2A-CGA	4.20	1.45	1.33
38	3	308	KC1	OBD-CAD	4.20	1.28	1.22
30	B	809	CLA	O2A-CGA	4.20	1.45	1.33
37	4	315	A86	C17-C18	-4.20	1.46	1.52
38	1	308	KC1	CHB-C1B	4.20	1.46	1.38
37	16	314	A86	C19-C18	4.20	1.58	1.52
30	7	311	CLA	CHD-C1D	4.20	1.46	1.38
30	B	832	CLA	CHD-C1D	4.20	1.46	1.38
30	12	308	CLA	O2A-CGA	4.20	1.45	1.33
30	6	317	CLA	CHD-C1D	4.20	1.46	1.38
37	14	317	A86	C7-C6	4.20	1.59	1.50
30	B	824	CLA	CHD-C1D	4.20	1.46	1.38
30	A	844	CLA	O2A-CGA	4.19	1.45	1.33
30	9	307	CLA	O2A-CGA	4.19	1.45	1.33
30	B	830	CLA	O2D-CGD	4.19	1.43	1.33
30	6	310	CLA	O2A-CGA	4.19	1.45	1.33
30	15	302	CLA	CHD-C1D	4.19	1.46	1.38
37	2u	205	A86	C7-C6	4.19	1.59	1.50
30	11	310	CLA	O2A-CGA	4.19	1.45	1.33
30	14	302	CLA	O2A-CGA	4.19	1.45	1.33
30	B	832	CLA	O2A-CGA	4.19	1.45	1.33
30	5	302	CLA	O2A-CGA	4.19	1.45	1.33
30	10	309	CLA	CHD-C1D	4.19	1.46	1.38
38	5	312	KC1	CHB-C1B	4.19	1.46	1.38
30	6	317	CLA	O2A-CGA	4.19	1.45	1.33
30	6	316	CLA	CHD-C1D	4.18	1.46	1.38
38	8	307	KC1	CHB-C1B	4.18	1.46	1.38
38	5	305	KC1	C4D-ND	4.18	1.38	1.35
30	3	310	CLA	CHD-C1D	4.18	1.46	1.38
30	12	312	CLA	O2A-CGA	4.18	1.45	1.33
38	6	311	KC1	CHB-C1B	4.18	1.46	1.38
37	15	316	A86	C19-C18	4.18	1.58	1.52
30	8	308	CLA	O2A-CGA	4.18	1.45	1.33
38	3	311	KC1	C4D-ND	4.18	1.38	1.35
30	B	821	CLA	CHD-C1D	4.18	1.46	1.38
37	10	316	A86	O4-C38	4.18	1.44	1.35
30	A	812	CLA	C1D-ND	4.18	1.42	1.37
30	13	301	CLA	O2A-CGA	4.18	1.45	1.33
30	B	836	CLA	O2A-CGA	4.18	1.45	1.33
37	16	312	A86	C10-C11	4.18	1.46	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	11	311	KC1	C4D-ND	4.18	1.38	1.35
37	14	315	A86	O4-C38	4.17	1.44	1.35
38	5	310	KC1	CHB-C1B	4.17	1.46	1.38
37	5	301	A86	C7-C6	4.17	1.59	1.50
37	14	301	A86	C17-C18	-4.17	1.46	1.52
30	10	305	CLA	CHD-C1D	4.17	1.46	1.38
30	A	820	CLA	O2A-CGA	4.17	1.45	1.33
30	10	303	CLA	CHD-C1D	4.17	1.46	1.38
37	12	316	A86	C7-C6	4.17	1.59	1.50
30	6	309	CLA	CHD-C1D	4.17	1.46	1.38
37	14	316	A86	C7-C6	4.17	1.59	1.50
30	3	305	CLA	O2A-CGA	4.17	1.45	1.33
37	9	315	A86	C7-C6	4.17	1.59	1.50
30	12	302	CLA	O2A-CGA	4.17	1.45	1.33
30	16	301	CLA	O2A-CGA	4.17	1.45	1.33
30	5	309	CLA	CHD-C1D	4.17	1.46	1.38
30	11	309	CLA	CHD-C1D	4.17	1.46	1.38
30	2	304	CLA	O2A-CGA	4.16	1.45	1.33
38	6	311	KC1	CHC-C4B	4.16	1.46	1.38
38	11	312	KC1	CHC-C4B	4.16	1.46	1.38
30	A	840	CLA	O2A-CGA	4.16	1.45	1.33
37	2	318	A86	C7-C6	4.16	1.59	1.50
30	B	831	CLA	O2A-CGA	4.16	1.45	1.33
30	8	304	CLA	C1D-ND	4.16	1.42	1.37
38	1	306	KC1	C4D-ND	4.16	1.38	1.35
30	12	310	CLA	O2A-CGA	4.16	1.45	1.33
30	7	305	CLA	CHD-C1D	4.16	1.46	1.38
37	4	314	A86	C21-C20	4.16	1.58	1.51
38	11	312	KC1	C1A-CHA	4.16	1.51	1.40
37	12	314	A86	C2-C1	4.16	1.41	1.35
30	2	307	CLA	C1D-ND	4.16	1.42	1.37
30	J	101	CLA	CHD-C1D	4.16	1.46	1.38
30	15	307	CLA	CHD-C1D	4.16	1.46	1.38
37	2u	205	A86	C10-C11	4.16	1.46	1.34
38	13	305	KC1	C1A-CHA	4.16	1.51	1.40
30	2	307	CLA	CHD-C1D	4.16	1.46	1.38
37	14	318	A86	C7-C6	4.15	1.59	1.50
37	6	320	A86	C7-C6	4.15	1.59	1.50
30	15	312	CLA	CHD-C4C	4.15	1.48	1.39
30	5	311	CLA	CHD-C1D	4.15	1.46	1.38
30	10	311	CLA	CHD-C1D	4.15	1.46	1.38
30	A	836	CLA	C1D-ND	4.15	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	L	202	CLA	C1D-ND	4.15	1.42	1.37
30	8	303	CLA	O2A-CGA	4.15	1.45	1.33
30	B	801	CLA	C1D-ND	4.15	1.42	1.37
30	4	304	CLA	CHD-C1D	4.15	1.46	1.38
30	7	310	CLA	O2A-CGA	4.15	1.45	1.33
30	10	307	CLA	O2A-CGA	4.15	1.45	1.33
37	13	313	A86	C7-C6	4.14	1.59	1.50
30	A	814	CLA	CHD-C1D	4.14	1.46	1.38
30	A	842	CLA	O2A-CGA	4.14	1.45	1.33
30	A	805	CLA	O2A-CGA	4.14	1.45	1.33
30	A	823	CLA	O2A-CGA	4.14	1.45	1.33
37	4	317	A86	C2-C1	4.14	1.41	1.35
30	7	312	CLA	O2A-CGA	4.14	1.46	1.33
37	14	320	A86	C21-C20	4.14	1.58	1.51
30	B	828	CLA	CHD-C1D	4.14	1.46	1.38
37	11	315	A86	C7-C6	4.14	1.59	1.50
37	3	315	A86	C7-C6	4.14	1.59	1.50
30	A	821	CLA	O2A-CGA	4.14	1.45	1.33
38	16	304	KC1	C4D-ND	4.14	1.38	1.35
30	A	836	CLA	CHD-C1D	4.14	1.46	1.38
30	B	828	CLA	O2A-CGA	4.13	1.45	1.33
38	16	311	KC1	C4D-ND	4.13	1.38	1.35
30	A	817	CLA	CHD-C1D	4.13	1.46	1.38
30	3	302	CLA	O2A-CGA	4.13	1.45	1.33
30	A	811	CLA	O2A-CGA	4.13	1.45	1.33
37	16	312	A86	C21-C20	4.13	1.58	1.51
37	10	316	A86	C7-C6	4.13	1.59	1.50
30	B	838	CLA	O2A-CGA	4.13	1.45	1.33
30	6	307	CLA	O2A-CGA	4.13	1.45	1.33
30	4	305	CLA	CHD-C1D	4.12	1.46	1.38
30	12	312	CLA	CHD-C1D	4.12	1.46	1.38
37	14	319	A86	C21-C20	4.12	1.58	1.51
38	6	308	KC1	CHB-C1B	4.12	1.46	1.38
30	9	305	CLA	CHD-C1D	4.12	1.46	1.38
38	12	311	KC1	CHB-C1B	4.12	1.46	1.38
37	2	302	A86	C19-C18	4.12	1.58	1.52
37	14	317	A86	C2-C1	4.12	1.41	1.35
30	1	303	CLA	O2A-CGA	4.12	1.45	1.33
37	2u	203	A86	C26-C27	4.12	1.41	1.35
30	5	308	CLA	CHD-C1D	4.12	1.46	1.38
30	B	851	CLA	CHD-C1D	4.12	1.46	1.38
30	4	301	CLA	O2A-CGA	4.12	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	818	CLA	O2A-CGA	4.12	1.45	1.33
30	6	305	CLA	CHD-C1D	4.12	1.46	1.38
30	16	305	CLA	O2A-CGA	4.12	1.45	1.33
37	3	314	A86	C7-C6	4.11	1.59	1.50
30	6	314	CLA	CHD-C1D	4.11	1.46	1.38
30	9	301	CLA	O2A-CGA	4.11	1.45	1.33
30	7	309	CLA	O2A-CGA	4.11	1.45	1.33
30	9	303	CLA	O2A-CGA	4.11	1.45	1.33
30	16	310	CLA	CHD-C1D	4.11	1.46	1.38
30	B	839	CLA	O2A-CGA	4.11	1.45	1.33
38	12	309	KC1	C1A-CHA	4.11	1.51	1.40
30	A	839	CLA	O2A-CGA	4.11	1.45	1.33
37	2u	203	A86	C10-C11	4.11	1.46	1.34
30	B	823	CLA	CHD-C1D	4.11	1.46	1.38
37	16	314	A86	C17-C18	-4.11	1.46	1.52
37	11	301	A86	C21-C20	4.11	1.58	1.51
30	2	304	CLA	CHD-C1D	4.11	1.46	1.38
38	9	312	KC1	C4D-ND	4.11	1.38	1.35
30	5	304	CLA	CHD-C1D	4.11	1.46	1.38
30	3	306	CLA	CHD-C4C	4.11	1.48	1.39
37	10	301	A86	C7-C6	4.11	1.59	1.50
37	13	313	A86	C17-C18	-4.10	1.46	1.52
38	6	313	KC1	C4D-ND	4.10	1.38	1.35
37	7	316	A86	C7-C6	4.10	1.59	1.50
38	11	305	KC1	OBD-CAD	4.10	1.28	1.22
30	9	309	CLA	CHD-C1D	4.10	1.46	1.38
30	A	832	CLA	O2A-CGA	4.10	1.45	1.33
30	8	308	CLA	CHD-C1D	4.10	1.46	1.38
38	10	310	KC1	CHB-C1B	4.10	1.46	1.38
30	B	830	CLA	C1D-ND	4.10	1.42	1.37
30	A	819	CLA	O2A-CGA	4.10	1.45	1.33
30	B	817	CLA	O2A-CGA	4.10	1.45	1.33
37	14	318	A86	C21-C20	4.10	1.58	1.51
37	14	314	A86	C21-C20	4.10	1.58	1.51
30	3	306	CLA	O2A-CGA	4.10	1.45	1.33
30	4	306	CLA	O2A-CGA	4.10	1.45	1.33
30	8	305	CLA	O2A-CGA	4.10	1.45	1.33
38	12	313	KC1	C4D-ND	4.10	1.38	1.35
37	12	314	A86	C21-C20	4.10	1.58	1.51
30	13	302	CLA	CHD-C1D	4.10	1.46	1.38
30	B	819	CLA	O2A-CGA	4.10	1.45	1.33
30	6	304	CLA	CHD-C1D	4.09	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	12	308	CLA	CHD-C1D	4.09	1.46	1.38
30	9	307	CLA	CHD-C1D	4.09	1.46	1.38
30	B	829	CLA	O2A-CGA	4.09	1.45	1.33
38	5	306	KC1	CHB-C1B	4.09	1.46	1.38
30	A	806	CLA	O2A-CGA	4.09	1.45	1.33
30	12	306	CLA	O2A-CGA	4.09	1.45	1.33
30	A	833	CLA	O2A-CGA	4.09	1.45	1.33
37	14	315	A86	C2-C1	4.09	1.41	1.35
38	13	308	KC1	C4D-ND	4.09	1.38	1.35
30	2	310	CLA	CHD-C1D	4.09	1.46	1.38
37	15	323	A86	C21-C20	4.09	1.58	1.51
30	A	843	CLA	CHD-C1D	4.09	1.46	1.38
37	2	302	A86	C5-C6	4.09	1.41	1.35
37	3	315	A86	C2-C1	4.09	1.41	1.35
37	13	313	A86	C10-C11	4.09	1.46	1.34
38	3	308	KC1	C4D-ND	4.09	1.38	1.35
38	5	312	KC1	C4D-ND	4.09	1.38	1.35
30	B	829	CLA	CHD-C1D	4.09	1.46	1.38
37	10	315	A86	C7-C6	4.09	1.59	1.50
37	11	301	A86	C2-C1	4.09	1.41	1.35
30	A	822	CLA	CHD-C1D	4.09	1.46	1.38
30	16	306	CLA	CHD-C1D	4.09	1.46	1.38
30	B	825	CLA	O2A-CGA	4.08	1.45	1.33
30	B	826	CLA	C1D-ND	4.08	1.42	1.37
38	7	308	KC1	C1B-NB	-4.08	1.32	1.37
30	A	816	CLA	O2A-CGA	4.08	1.45	1.33
38	8	311	KC1	C1B-NB	-4.08	1.32	1.37
30	12	306	CLA	CHD-C1D	4.08	1.46	1.38
30	B	806	CLA	O2A-CGA	4.08	1.45	1.33
38	12	313	KC1	C1B-NB	-4.08	1.32	1.37
30	1	301	CLA	CHD-C1D	4.08	1.46	1.38
37	14	315	A86	C21-C20	4.08	1.58	1.51
37	5	315	A86	C7-C6	4.08	1.59	1.50
37	15	321	A86	C17-C18	-4.08	1.46	1.52
37	14	314	A86	C5-C6	4.08	1.41	1.35
30	A	838	CLA	CHD-C1D	4.08	1.46	1.38
30	3	301	CLA	O2A-CGA	4.08	1.45	1.33
37	14	319	A86	C10-C11	4.08	1.46	1.34
37	7	315	A86	O4-C38	4.07	1.44	1.35
30	A	843	CLA	O2A-CGA	4.07	1.45	1.33
30	2	309	CLA	CHD-C1D	4.07	1.46	1.38
37	14	316	A86	C2-C1	4.07	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	804	CLA	O2A-CGA	4.07	1.45	1.33
30	B	829	CLA	C1D-ND	4.07	1.42	1.37
30	5	307	CLA	O2A-CGA	4.07	1.45	1.33
37	15	317	A86	C21-C20	4.07	1.58	1.51
30	14	309	CLA	CHD-C4C	4.07	1.48	1.39
30	10	304	CLA	CHD-C1D	4.07	1.46	1.38
30	4	311	CLA	O2A-CGA	4.07	1.45	1.33
30	B	828	CLA	C1D-ND	4.07	1.42	1.37
30	F	203	CLA	CHD-C1D	4.07	1.46	1.38
37	1	309	A86	C17-C18	-4.07	1.46	1.52
38	9	310	KC1	CHB-C1B	4.07	1.46	1.38
30	16	302	CLA	O2A-CGA	4.07	1.45	1.33
37	8	315	A86	C7-C6	4.07	1.59	1.50
38	9	304	KC1	C4D-ND	4.06	1.38	1.35
30	15	302	CLA	CHD-C4C	4.06	1.48	1.39
30	A	826	CLA	O2A-CGA	4.06	1.45	1.33
30	12	303	CLA	CHD-C1D	4.06	1.46	1.38
37	2u	205	A86	C9-C10	4.06	1.56	1.43
38	11	312	KC1	C1B-NB	-4.06	1.32	1.37
37	2	318	A86	C21-C20	4.06	1.58	1.51
37	11	314	A86	C17-C18	-4.06	1.46	1.52
30	A	810	CLA	CHD-C1D	4.06	1.46	1.38
38	13	312	KC1	C1A-CHA	4.06	1.51	1.40
30	4	311	CLA	CHD-C1D	4.06	1.46	1.38
37	14	314	A86	C19-C18	4.06	1.58	1.52
37	2	318	A86	C2-C1	4.05	1.41	1.35
30	8	303	CLA	CHD-C1D	4.05	1.46	1.38
30	16	307	CLA	O2A-CGA	4.05	1.45	1.33
38	4	308	KC1	CHC-C4B	4.05	1.46	1.38
37	13	313	A86	C21-C20	4.05	1.58	1.51
37	14	314	A86	C10-C11	4.05	1.46	1.34
38	6	308	KC1	C1A-CHA	4.05	1.51	1.40
30	6	306	CLA	CHD-C1D	4.05	1.46	1.38
30	13	304	CLA	CHD-C4C	4.05	1.48	1.39
38	5	310	KC1	C1B-NB	-4.05	1.32	1.37
30	B	815	CLA	CHD-C1D	4.05	1.46	1.38
38	7	313	KC1	CHB-C1B	4.05	1.46	1.38
38	8	313	KC1	OBD-CAD	4.05	1.28	1.22
37	11	315	A86	C21-C20	4.05	1.58	1.51
30	B	818	CLA	CHD-C1D	4.05	1.46	1.38
30	B	833	CLA	O2A-CGA	4.05	1.45	1.33
37	15	322	A86	C10-C11	4.05	1.46	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	16	305	CLA	CHD-C1D	4.05	1.46	1.38
30	7	310	CLA	CHD-C4C	4.05	1.48	1.39
30	B	811	CLA	O2A-CGA	4.05	1.45	1.33
37	11	315	A86	C2-C1	4.05	1.41	1.35
30	A	808	CLA	O2A-CGA	4.04	1.45	1.33
37	9	316	A86	C9-C10	4.04	1.56	1.43
37	15	316	A86	C21-C20	4.04	1.58	1.51
37	7	319	A86	C19-C18	4.04	1.58	1.52
30	A	809	CLA	O2A-CGA	4.04	1.45	1.33
30	A	832	CLA	CHD-C1D	4.04	1.46	1.38
30	11	310	CLA	CHD-C4C	4.04	1.48	1.39
30	B	813	CLA	O2A-CGA	4.04	1.45	1.33
38	8	314	KC1	C1A-CHA	4.04	1.51	1.40
30	4	309	CLA	CHD-C4C	4.04	1.48	1.39
30	1	302	CLA	CHD-C1D	4.04	1.46	1.38
30	15	309	CLA	CHD-C4C	4.04	1.48	1.39
38	11	305	KC1	C4D-ND	4.03	1.38	1.35
30	7	306	CLA	CHD-C1D	4.03	1.46	1.38
30	F	201	CLA	O2A-CGA	4.03	1.45	1.33
38	6	308	KC1	OBD-CAD	4.03	1.27	1.22
38	6	311	KC1	C1B-NB	-4.03	1.32	1.37
37	10	317	A86	C19-C18	4.03	1.58	1.52
37	14	314	A86	C9-C10	4.03	1.55	1.43
37	14	320	A86	C10-C11	4.03	1.46	1.34
30	13	303	CLA	CHD-C4C	4.03	1.48	1.39
37	2	319	A86	C7-C6	4.03	1.59	1.50
30	A	814	CLA	O2A-CGA	4.03	1.45	1.33
30	B	851	CLA	O2A-CGA	4.03	1.45	1.33
30	A	831	CLA	O2A-CGA	4.03	1.45	1.33
30	4	303	CLA	CHD-C1D	4.03	1.46	1.38
30	14	307	CLA	CHD-C1D	4.02	1.46	1.38
30	B	838	CLA	CHD-C1D	4.02	1.46	1.38
30	B	813	CLA	CHD-C1D	4.02	1.46	1.38
38	12	309	KC1	CHB-C1B	4.02	1.46	1.38
37	10	317	A86	C10-C11	4.02	1.46	1.34
37	15	321	A86	C21-C20	4.02	1.58	1.51
38	3	304	KC1	C1A-CHA	4.02	1.51	1.40
37	8	318	A86	O4-C38	4.02	1.44	1.35
30	16	302	CLA	CHD-C1D	4.02	1.46	1.38
38	14	311	KC1	C1A-CHA	4.02	1.51	1.40
30	15	310	CLA	CHD-C4C	4.02	1.48	1.39
38	12	305	KC1	C4D-ND	4.02	1.38	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	4	314	A86	C9-C10	4.02	1.55	1.43
38	10	312	KC1	C4D-ND	4.02	1.38	1.35
37	2u	205	A86	C2-C1	4.02	1.41	1.35
37	2	319	A86	C21-C20	4.02	1.58	1.51
30	13	309	CLA	CHD-C4C	4.02	1.48	1.39
30	A	840	CLA	CHD-C1D	4.02	1.46	1.38
30	15	308	CLA	CHD-C1D	4.02	1.46	1.38
30	7	309	CLA	CHD-C1D	4.01	1.46	1.38
38	10	310	KC1	C4D-ND	4.01	1.38	1.35
37	14	315	A86	C26-C27	4.01	1.41	1.35
30	B	805	CLA	CHD-C1D	4.01	1.46	1.38
30	9	308	CLA	CHD-C1D	4.01	1.46	1.38
30	12	310	CLA	CHD-C1D	4.01	1.46	1.38
30	A	829	CLA	O2A-CGA	4.01	1.45	1.33
37	9	313	A86	C26-C27	4.01	1.41	1.35
37	7	319	A86	C7-C6	4.01	1.59	1.50
30	A	821	CLA	C1D-ND	4.01	1.42	1.37
37	4	312	A86	C2-C1	4.01	1.41	1.35
30	B	810	CLA	O2A-CGA	4.01	1.45	1.33
37	2u	203	A86	C21-C20	4.01	1.58	1.51
37	3	314	A86	C21-C20	4.01	1.58	1.51
37	14	319	A86	C9-C10	4.01	1.55	1.43
37	10	301	A86	C26-C27	4.01	1.41	1.35
30	14	313	CLA	CHD-C4C	4.01	1.48	1.39
37	1	309	A86	C21-C20	4.01	1.58	1.51
30	7	312	CLA	CHD-C4C	4.00	1.48	1.39
30	A	839	CLA	CHD-C1D	4.00	1.46	1.38
30	B	814	CLA	C1D-ND	4.00	1.42	1.37
37	10	317	A86	C21-C20	4.00	1.58	1.51
38	8	310	KC1	C1A-CHA	4.00	1.51	1.40
30	A	834	CLA	O2A-CGA	4.00	1.45	1.33
30	A	834	CLA	CHD-C1D	4.00	1.46	1.38
30	B	811	CLA	CHD-C1D	4.00	1.46	1.38
30	3	307	CLA	CHD-C4C	4.00	1.48	1.39
30	14	302	CLA	CHD-C4C	4.00	1.48	1.39
38	16	311	KC1	C1A-CHA	4.00	1.51	1.40
38	12	309	KC1	C4D-ND	4.00	1.38	1.35
37	15	323	A86	C10-C11	4.00	1.46	1.34
30	11	306	CLA	CHD-C1D	4.00	1.46	1.38
30	16	308	CLA	CHD-C4C	4.00	1.48	1.39
37	10	315	A86	C21-C20	4.00	1.58	1.51
38	11	307	KC1	C1A-CHA	4.00	1.51	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	2	312	KC1	C4D-ND	4.00	1.38	1.35
30	A	831	CLA	C1B-NB	-3.99	1.31	1.35
37	15	320	A86	C21-C20	3.99	1.58	1.51
37	13	315	A86	C9-C10	3.99	1.55	1.43
30	4	306	CLA	CHD-C1D	3.99	1.46	1.38
30	15	308	CLA	CHD-C4C	3.99	1.48	1.39
30	12	302	CLA	CHD-C1D	3.99	1.46	1.38
38	4	308	KC1	CHB-C1B	3.99	1.46	1.38
30	8	301	CLA	O2A-CGA	3.99	1.45	1.33
30	11	308	CLA	CHD-C4C	3.99	1.48	1.39
30	15	304	CLA	CHD-C4C	3.99	1.48	1.39
37	9	316	A86	C5-C6	3.99	1.41	1.35
30	14	304	CLA	CHD-C4C	3.99	1.48	1.39
37	1	309	A86	C2-C1	3.99	1.41	1.35
38	12	311	KC1	C1A-CHA	3.99	1.51	1.40
37	16	314	A86	C2-C1	3.99	1.41	1.35
30	10	308	CLA	CHD-C4C	3.99	1.48	1.39
30	A	816	CLA	CHD-C1D	3.98	1.46	1.38
38	4	310	KC1	CHB-C1B	3.98	1.46	1.38
30	B	822	CLA	O2A-CGA	3.98	1.45	1.33
38	12	313	KC1	C1A-NA	-3.98	1.30	1.38
30	3	310	CLA	CHD-C4C	3.98	1.48	1.39
30	2	303	CLA	CHD-C4C	3.98	1.48	1.39
37	8	318	A86	C7-C6	3.98	1.59	1.50
30	A	833	CLA	CHD-C1D	3.98	1.46	1.38
37	15	323	A86	C5-C6	3.98	1.41	1.35
30	9	306	CLA	CHD-C4C	3.98	1.48	1.39
30	8	303	CLA	C1D-ND	3.98	1.42	1.37
38	14	308	KC1	C1A-CHA	3.98	1.51	1.40
30	A	812	CLA	O2A-CGA	3.98	1.45	1.33
30	14	313	CLA	O2A-CGA	3.98	1.45	1.33
30	B	807	CLA	O2A-CGA	3.98	1.45	1.33
30	3	303	CLA	CHD-C4C	3.98	1.48	1.39
30	A	807	CLA	O2A-CGA	3.98	1.45	1.33
30	B	802	CLA	O2A-CGA	3.98	1.45	1.33
37	7	316	A86	C21-C20	3.98	1.58	1.51
30	A	844	CLA	CHD-C4C	3.98	1.48	1.39
30	11	304	CLA	CHD-C1D	3.98	1.46	1.38
30	B	826	CLA	O2A-CGA	3.98	1.45	1.33
30	2	305	CLA	CHD-C1D	3.98	1.46	1.38
30	3	305	CLA	CHD-C1D	3.97	1.46	1.38
30	14	312	CLA	CHD-C4C	3.97	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	4	312	A86	C7-C6	3.97	1.59	1.50
30	14	303	CLA	CHD-C4C	3.97	1.48	1.39
37	11	316	A86	C21-C20	3.97	1.58	1.51
38	4	310	KC1	C1B-NB	-3.97	1.32	1.37
37	13	315	A86	C21-C20	3.97	1.58	1.51
37	4	312	A86	C26-C27	3.97	1.41	1.35
30	A	828	CLA	O2A-CGA	3.97	1.44	1.33
30	1	305	CLA	CHD-C4C	3.97	1.48	1.39
37	9	315	A86	C9-C10	3.97	1.55	1.43
38	16	311	KC1	C1B-NB	-3.97	1.32	1.37
38	6	311	KC1	OBD-CAD	3.97	1.27	1.22
30	B	837	CLA	O2A-CGA	3.97	1.44	1.33
38	8	313	KC1	C1B-NB	-3.97	1.32	1.37
37	15	317	A86	C5-C6	3.96	1.41	1.35
37	15	315	A86	C9-C10	3.96	1.55	1.43
30	14	310	CLA	CHD-C4C	3.96	1.48	1.39
30	7	304	CLA	CHD-C1D	3.96	1.46	1.38
37	2	302	A86	C10-C11	3.96	1.46	1.34
38	8	314	KC1	C1B-NB	-3.96	1.32	1.37
30	7	306	CLA	O2A-CGA	3.96	1.44	1.33
37	3	314	A86	C10-C11	3.96	1.46	1.34
37	7	319	A86	C10-C11	3.96	1.46	1.34
30	11	309	CLA	CHD-C4C	3.96	1.48	1.39
30	A	802	CLA	C1D-ND	3.96	1.42	1.37
37	12	316	A86	C10-C11	3.96	1.46	1.34
38	8	306	KC1	C4D-ND	3.96	1.38	1.35
30	2	308	CLA	CHD-C1D	3.96	1.46	1.38
37	14	320	A86	C17-C18	-3.96	1.46	1.52
37	2u	203	A86	C9-C10	3.96	1.55	1.43
38	8	314	KC1	CHB-C1B	3.96	1.46	1.38
30	2	313	CLA	CHD-C4C	3.96	1.48	1.39
38	5	312	KC1	C1A-CHA	3.96	1.51	1.40
30	B	808	CLA	CHD-C1D	3.96	1.46	1.38
30	2u	202	CLA	CHD-C1D	3.95	1.46	1.38
37	15	320	A86	C9-C10	3.95	1.55	1.43
30	5	303	CLA	CHD-C1D	3.95	1.46	1.38
37	3	314	A86	C17-C18	-3.95	1.46	1.52
37	14	316	A86	C21-C20	3.95	1.58	1.51
30	3	302	CLA	CHD-C1D	3.95	1.46	1.38
38	8	314	KC1	OBD-CAD	3.95	1.27	1.22
37	5	315	A86	C2-C1	3.95	1.41	1.35
38	8	310	KC1	C1B-NB	-3.95	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	15	314	CLA	CHD-C1D	3.95	1.46	1.38
38	13	310	KC1	C1A-CHA	3.95	1.51	1.40
30	15	305	CLA	CHD-C4C	3.95	1.48	1.39
30	A	811	CLA	CHD-C1D	3.95	1.46	1.38
30	1	303	CLA	CHD-C1D	3.95	1.46	1.38
30	2	301	CLA	C1D-ND	3.95	1.42	1.37
38	14	306	KC1	CHC-C1C	3.95	1.48	1.39
38	5	310	KC1	C4D-ND	3.94	1.38	1.35
38	9	310	KC1	C4D-ND	3.94	1.38	1.35
30	15	311	CLA	CHD-C4C	3.94	1.48	1.39
30	B	805	CLA	O2A-CGA	3.94	1.44	1.33
30	16	309	CLA	CHD-C4C	3.94	1.48	1.39
38	8	311	KC1	C1A-CHA	3.94	1.51	1.40
37	7	315	A86	C7-C6	3.94	1.59	1.50
37	15	322	A86	C5-C6	3.94	1.41	1.35
30	2	309	CLA	CHD-C4C	3.94	1.48	1.39
30	A	831	CLA	CHD-C1D	3.94	1.46	1.38
37	4	312	A86	C21-C20	3.94	1.58	1.51
30	11	304	CLA	CHD-C4C	3.94	1.48	1.39
30	5	302	CLA	CHD-C1D	3.94	1.46	1.38
30	12	321	CLA	CHD-C4C	3.93	1.48	1.39
38	5	305	KC1	C1A-CHA	3.93	1.51	1.40
30	A	807	CLA	CHD-C1D	3.93	1.46	1.38
38	7	308	KC1	C1A-CHA	3.93	1.51	1.40
38	5	306	KC1	C4D-ND	3.93	1.38	1.35
30	1	304	CLA	CHD-C1D	3.93	1.46	1.38
30	9	303	CLA	CHD-C1D	3.93	1.46	1.38
30	6	307	CLA	CHD-C4C	3.93	1.48	1.39
37	5	315	A86	C21-C20	3.93	1.58	1.51
37	10	302	A86	C2-C1	3.93	1.41	1.35
37	11	301	A86	C9-C10	3.93	1.55	1.43
30	15	303	CLA	CHD-C4C	3.93	1.48	1.39
30	14	307	CLA	CHD-C4C	3.93	1.48	1.39
37	8	318	A86	C21-C20	3.93	1.58	1.51
37	5	315	A86	C17-C18	-3.93	1.46	1.52
30	B	819	CLA	CHD-C1D	3.93	1.46	1.38
37	13	313	A86	C9-C10	3.93	1.55	1.43
30	B	816	CLA	CHD-C1D	3.93	1.46	1.38
30	1	302	CLA	O2A-CGA	3.92	1.44	1.33
38	4	307	KC1	C1A-CHA	3.92	1.51	1.40
38	3	304	KC1	C1B-NB	-3.92	1.33	1.37
30	13	307	CLA	CHD-C4C	3.92	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	7	304	CLA	O2A-CGA	3.92	1.44	1.33
38	10	306	KC1	C1A-CHA	3.92	1.51	1.40
37	9	315	A86	C21-C20	3.92	1.58	1.51
30	15	313	CLA	CHD-C4C	3.92	1.48	1.39
29	A	801	CL0	O2A-CGA	3.92	1.44	1.33
30	B	804	CLA	CHD-C1D	3.92	1.46	1.38
37	7	319	A86	C9-C10	3.92	1.55	1.43
38	6	308	KC1	C1B-NB	-3.92	1.33	1.37
30	14	305	CLA	CHD-C4C	3.92	1.48	1.39
37	11	301	A86	C10-C11	3.92	1.45	1.34
37	10	316	A86	C26-C27	3.92	1.41	1.35
37	9	316	A86	C19-C18	3.92	1.58	1.52
37	15	317	A86	C10-C11	3.92	1.45	1.34
30	B	824	CLA	CHD-C4C	3.92	1.48	1.39
37	5	316	A86	C9-C10	3.92	1.55	1.43
37	10	317	A86	C9-C10	3.91	1.55	1.43
30	6	310	CLA	CHD-C4C	3.91	1.48	1.39
30	12	307	CLA	O2A-CGA	3.91	1.45	1.33
30	4	302	CLA	CHD-C1D	3.91	1.46	1.38
30	11	306	CLA	CHD-C4C	3.91	1.48	1.39
30	B	818	CLA	O2A-CGA	3.91	1.44	1.33
30	8	304	CLA	CHD-C1D	3.91	1.46	1.38
38	6	313	KC1	C1A-CHA	3.91	1.51	1.40
30	B	835	CLA	CHD-C1D	3.91	1.46	1.38
38	8	306	KC1	C1B-NB	-3.91	1.33	1.37
30	B	828	CLA	C1B-NB	-3.91	1.31	1.35
37	9	313	A86	C21-C20	3.91	1.58	1.51
30	A	824	CLA	CHD-C1D	3.91	1.46	1.38
38	6	312	KC1	C1B-NB	-3.91	1.33	1.37
38	4	307	KC1	C1B-NB	-3.91	1.33	1.37
30	B	833	CLA	CHD-C1D	3.91	1.46	1.38
30	B	803	CLA	C1D-ND	3.90	1.42	1.37
30	16	307	CLA	CHD-C4C	3.90	1.48	1.39
37	11	314	A86	C21-C20	3.90	1.57	1.51
38	3	311	KC1	C1A-CHA	3.90	1.51	1.40
38	11	311	KC1	C1A-CHA	3.90	1.51	1.40
37	2	319	A86	C2-C1	3.90	1.41	1.35
30	B	835	CLA	CHD-C4C	3.90	1.48	1.39
38	6	312	KC1	C4D-ND	3.90	1.38	1.35
30	8	309	CLA	CHD-C4C	3.90	1.48	1.39
38	2	306	KC1	C1A-CHA	3.90	1.51	1.40
37	9	316	A86	C10-C11	3.90	1.45	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	6	309	CLA	O2A-CGA	3.90	1.44	1.33
37	1	309	A86	C10-C11	3.90	1.45	1.34
30	B	806	CLA	CHD-C1D	3.90	1.46	1.38
37	11	315	A86	C17-C18	-3.90	1.46	1.52
30	6	316	CLA	CHD-C4C	3.90	1.48	1.39
37	10	315	A86	C19-C18	3.90	1.57	1.52
37	15	320	A86	C19-C18	3.90	1.57	1.52
38	12	305	KC1	C1A-CHA	3.90	1.51	1.40
37	9	315	A86	C10-C11	3.90	1.45	1.34
30	L	203	CLA	CHD-C1D	3.90	1.46	1.38
30	B	831	CLA	CHD-C1D	3.90	1.46	1.38
30	A	837	CLA	CHD-C4C	3.90	1.48	1.39
37	7	316	A86	O4-C38	3.89	1.44	1.35
30	A	822	CLA	C1D-ND	3.89	1.42	1.37
37	12	316	A86	C9-C10	3.89	1.55	1.43
30	B	802	CLA	C3D-C2D	3.89	1.49	1.39
38	10	312	KC1	C1B-NB	-3.89	1.33	1.37
30	10	309	CLA	CHD-C4C	3.89	1.48	1.39
37	15	316	A86	C10-C11	3.89	1.45	1.34
38	10	306	KC1	C1B-NB	-3.89	1.33	1.37
30	15	314	CLA	CHD-C4C	3.89	1.48	1.39
30	16	301	CLA	CHD-C1D	3.89	1.45	1.38
37	13	315	A86	C5-C6	3.89	1.40	1.35
37	15	322	A86	C9-C10	3.89	1.55	1.43
38	8	314	KC1	C4D-ND	3.89	1.38	1.35
38	2	312	KC1	C1A-CHA	3.89	1.51	1.40
38	16	304	KC1	C1A-CHA	3.89	1.51	1.40
30	B	808	CLA	O2A-CGA	3.89	1.44	1.33
37	10	302	A86	C21-C20	3.89	1.57	1.51
30	10	303	CLA	CHD-C4C	3.89	1.48	1.39
38	8	307	KC1	C4D-ND	3.89	1.38	1.35
30	A	809	CLA	CHD-C1D	3.89	1.45	1.38
37	15	323	A86	C9-C10	3.89	1.55	1.43
30	B	835	CLA	O2A-CGA	3.89	1.44	1.33
30	A	815	CLA	CHD-C4C	3.88	1.48	1.39
37	4	315	A86	C21-C20	3.88	1.57	1.51
30	12	312	CLA	CHD-C4C	3.88	1.48	1.39
37	11	314	A86	C5-C6	3.88	1.40	1.35
30	3	301	CLA	CHD-C1D	3.88	1.45	1.38
30	12	307	CLA	CHD-C1D	3.88	1.45	1.38
30	13	301	CLA	CHD-C1D	3.88	1.45	1.38
30	3	309	CLA	CHD-C4C	3.88	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	15	306	CLA	CHD-C4C	3.88	1.48	1.39
37	5	316	A86	C7-C6	3.88	1.58	1.50
37	10	317	A86	C5-C6	3.88	1.40	1.35
30	1	302	CLA	CHD-C4C	3.88	1.48	1.39
30	B	801	CLA	O2A-CGA	3.88	1.44	1.33
30	A	813	CLA	CHD-C1D	3.88	1.45	1.38
30	6	315	CLA	CHD-C4C	3.88	1.48	1.39
38	10	310	KC1	C1B-NB	-3.87	1.33	1.37
38	14	306	KC1	C1B-NB	-3.87	1.33	1.37
30	A	842	CLA	CHD-C1D	3.87	1.45	1.38
37	15	316	A86	C5-C6	3.87	1.40	1.35
30	4	306	CLA	CHD-C4C	3.87	1.48	1.39
30	B	824	CLA	O2A-CGA	3.87	1.44	1.33
37	11	314	A86	C9-C10	3.87	1.55	1.43
30	A	830	CLA	O2A-CGA	3.87	1.44	1.33
30	2	311	CLA	CHD-C4C	3.87	1.48	1.39
30	A	831	CLA	C1D-ND	3.87	1.42	1.37
38	3	311	KC1	C1B-NB	-3.87	1.33	1.37
30	A	802	CLA	O2A-CGA	3.87	1.44	1.33
30	A	835	CLA	CHD-C4C	3.86	1.48	1.39
30	A	820	CLA	CHD-C4C	3.86	1.48	1.39
38	3	308	KC1	C1A-CHA	3.86	1.51	1.40
37	5	316	A86	C10-C11	3.86	1.45	1.34
30	4	311	CLA	CHD-C4C	3.86	1.48	1.39
37	14	320	A86	C9-C10	3.86	1.55	1.43
37	14	319	A86	C5-C6	3.86	1.40	1.35
30	3	306	CLA	C3D-C2D	3.86	1.49	1.39
38	7	313	KC1	C1A-CHA	3.86	1.50	1.40
38	9	312	KC1	C1A-CHA	3.86	1.50	1.40
30	B	822	CLA	CHD-C4C	3.86	1.48	1.39
30	2	301	CLA	CHD-C4C	3.85	1.48	1.39
30	A	808	CLA	CHD-C1D	3.85	1.45	1.38
38	8	307	KC1	C1B-NB	-3.85	1.33	1.37
30	8	301	CLA	CHD-C1D	3.85	1.45	1.38
30	5	307	CLA	CHD-C1D	3.85	1.45	1.38
30	5	311	CLA	CHD-C4C	3.85	1.48	1.39
30	7	304	CLA	CHD-C4C	3.85	1.48	1.39
37	10	302	A86	C9-C10	3.85	1.55	1.43
30	6	317	CLA	CHD-C4C	3.85	1.48	1.39
38	2	312	KC1	C1B-NB	-3.85	1.33	1.37
30	A	820	CLA	C1B-NB	-3.85	1.31	1.35
30	B	805	CLA	CHD-C4C	3.85	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	10	315	A86	C9-C10	3.85	1.55	1.43
30	B	837	CLA	CHD-C1D	3.85	1.45	1.38
38	9	310	KC1	C1B-NB	-3.85	1.33	1.37
30	B	811	CLA	C1D-ND	3.85	1.42	1.37
30	12	304	CLA	CHD-C4C	3.85	1.48	1.39
30	4	303	CLA	CHD-C4C	3.84	1.48	1.39
30	A	805	CLA	CHD-C1D	3.84	1.45	1.38
30	A	825	CLA	CHD-C4C	3.84	1.48	1.39
30	5	308	CLA	C3D-C2D	3.84	1.49	1.39
37	12	314	A86	C5-C6	3.84	1.40	1.35
38	8	306	KC1	C1A-CHA	3.84	1.50	1.40
37	6	320	A86	C2-C1	3.84	1.40	1.35
38	4	310	KC1	C1A-CHA	3.84	1.50	1.40
30	A	827	CLA	O2A-CGA	3.84	1.44	1.33
38	8	313	KC1	CHC-C1C	3.84	1.48	1.39
37	12	314	A86	C10-C11	3.84	1.45	1.34
38	13	310	KC1	CHC-C1C	3.84	1.48	1.39
38	13	308	KC1	C1A-CHA	3.84	1.50	1.40
30	A	833	CLA	CHD-C4C	3.83	1.48	1.39
37	14	317	A86	C26-C27	3.83	1.40	1.35
38	1	308	KC1	C1A-CHA	3.83	1.50	1.40
30	B	814	CLA	CHD-C1D	3.83	1.45	1.38
30	6	305	CLA	CHD-C4C	3.83	1.48	1.39
37	15	317	A86	C9-C10	3.83	1.55	1.43
30	2	304	CLA	CHD-C4C	3.83	1.48	1.39
38	2	314	KC1	C1B-NB	-3.83	1.33	1.37
38	7	308	KC1	C4D-ND	3.83	1.38	1.35
38	1	306	KC1	C1B-NB	-3.83	1.33	1.37
30	B	851	CLA	CHD-C4C	3.83	1.48	1.39
30	A	818	CLA	CHD-C1D	3.83	1.45	1.38
37	16	312	A86	C5-C6	3.83	1.40	1.35
30	A	829	CLA	CHD-C1D	3.83	1.45	1.38
38	1	306	KC1	C1A-CHA	3.83	1.50	1.40
37	16	314	A86	C21-C20	3.83	1.57	1.51
38	13	306	KC1	C1A-CHA	3.83	1.50	1.40
38	12	313	KC1	CHB-C1B	3.83	1.45	1.38
30	1	307	CLA	CHD-C4C	3.83	1.48	1.39
30	7	305	CLA	CHD-C4C	3.83	1.48	1.39
30	A	804	CLA	CHD-C1D	3.83	1.45	1.38
37	12	314	A86	C9-C10	3.83	1.55	1.43
37	16	312	A86	C2-C1	3.82	1.40	1.35
37	2	302	A86	C9-C10	3.82	1.55	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	10	311	CLA	CHD-C4C	3.82	1.48	1.39
30	J	101	CLA	CHD-C4C	3.82	1.48	1.39
37	12	314	A86	C7-C6	3.82	1.58	1.50
37	14	301	A86	C10-C11	3.82	1.45	1.34
30	A	817	CLA	CHD-C4C	3.82	1.48	1.39
30	1	301	CLA	CHD-C4C	3.82	1.48	1.39
38	8	312	KC1	C4D-ND	3.82	1.38	1.35
38	13	306	KC1	C4D-ND	3.82	1.38	1.35
37	16	314	A86	C9-C10	3.82	1.55	1.43
30	A	834	CLA	CHD-C4C	3.82	1.47	1.39
30	B	834	CLA	CHD-C1D	3.82	1.45	1.38
38	4	308	KC1	C4D-ND	3.82	1.38	1.35
37	10	302	A86	C19-C18	3.82	1.57	1.52
30	6	314	CLA	CHD-C4C	3.81	1.47	1.39
37	1	309	A86	C9-C10	3.81	1.55	1.43
30	B	812	CLA	CHD-C4C	3.81	1.47	1.39
30	15	310	CLA	C3D-C2D	3.81	1.49	1.39
30	B	821	CLA	CHD-C4C	3.81	1.47	1.39
37	16	312	A86	C9-C10	3.81	1.55	1.43
37	11	314	A86	C10-C11	3.81	1.45	1.34
30	6	304	CLA	CHD-C4C	3.81	1.47	1.39
30	6	309	CLA	C3D-C2D	3.81	1.49	1.39
30	5	309	CLA	CHD-C4C	3.81	1.47	1.39
30	6	309	CLA	CHD-C4C	3.81	1.47	1.39
37	10	315	A86	C10-C11	3.81	1.45	1.34
38	12	309	KC1	C1B-NB	-3.81	1.33	1.37
30	3	301	CLA	CHD-C4C	3.81	1.47	1.39
30	14	309	CLA	C3D-C2D	3.81	1.49	1.39
30	B	827	CLA	C1D-ND	3.81	1.42	1.37
38	8	312	KC1	C1A-CHA	3.80	1.50	1.40
30	9	305	CLA	CHD-C4C	3.80	1.47	1.39
38	10	312	KC1	CHC-C1C	3.80	1.47	1.39
37	3	314	A86	C9-C10	3.80	1.55	1.43
38	2	314	KC1	C1A-CHA	3.80	1.50	1.40
37	3	315	A86	C10-C11	3.80	1.45	1.34
30	10	305	CLA	CHD-C4C	3.80	1.47	1.39
38	7	313	KC1	C4D-ND	3.80	1.38	1.35
38	13	306	KC1	C1B-NB	-3.80	1.33	1.37
30	4	304	CLA	CHD-C4C	3.80	1.47	1.39
37	7	315	A86	C21-C20	3.80	1.57	1.51
30	3	302	CLA	CHD-C4C	3.80	1.47	1.39
30	13	302	CLA	CHD-C4C	3.80	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	11	312	KC1	C4D-ND	3.80	1.38	1.35
30	A	802	CLA	C3D-C2D	3.80	1.49	1.39
30	8	308	CLA	CHD-C4C	3.79	1.47	1.39
37	3	315	A86	C9-C10	3.79	1.55	1.43
37	15	316	A86	C9-C10	3.79	1.55	1.43
30	4	305	CLA	CHD-C4C	3.79	1.47	1.39
30	2	307	CLA	C3D-C2D	3.79	1.49	1.39
30	4	309	CLA	C3D-C2D	3.79	1.49	1.39
30	16	302	CLA	CHD-C4C	3.79	1.47	1.39
30	B	822	CLA	CHD-C1D	3.79	1.45	1.38
30	10	307	CLA	CHD-C1D	3.79	1.45	1.38
30	A	802	CLA	CHD-C4C	3.79	1.47	1.39
29	A	801	CL0	C1D-ND	3.79	1.42	1.37
30	A	843	CLA	CHD-C4C	3.79	1.47	1.39
30	16	303	CLA	CHD-C4C	3.79	1.47	1.39
38	6	313	KC1	C1B-NB	-3.79	1.33	1.37
30	B	832	CLA	CHD-C4C	3.79	1.47	1.39
38	13	312	KC1	CHC-C1C	3.79	1.47	1.39
30	A	823	CLA	CHD-C4C	3.79	1.47	1.39
30	L	203	CLA	CHD-C4C	3.79	1.47	1.39
30	2	305	CLA	CHD-C4C	3.79	1.47	1.39
37	2u	205	A86	C21-C20	3.79	1.57	1.51
37	5	315	A86	C10-C11	3.79	1.45	1.34
37	14	318	A86	C10-C11	3.78	1.45	1.34
30	13	302	CLA	C3D-C2D	3.78	1.49	1.39
30	2	310	CLA	CHD-C4C	3.78	1.47	1.39
30	5	302	CLA	CHD-C4C	3.78	1.47	1.39
30	B	817	CLA	CHD-C1D	3.78	1.45	1.38
38	9	311	KC1	C1A-CHA	3.78	1.50	1.40
38	13	311	KC1	C1A-CHA	3.78	1.50	1.40
38	11	305	KC1	C1A-CHA	3.78	1.50	1.40
30	B	818	CLA	CHD-C4C	3.77	1.47	1.39
37	11	315	A86	C10-C11	3.77	1.45	1.34
30	A	819	CLA	CHD-C1D	3.77	1.45	1.38
30	13	304	CLA	OBD-CAD	3.77	1.29	1.22
37	5	301	A86	C10-C11	3.77	1.45	1.34
37	10	301	A86	C21-C20	3.77	1.57	1.51
30	15	307	CLA	C3D-C2D	3.77	1.49	1.39
30	16	306	CLA	CHD-C4C	3.77	1.47	1.39
37	14	317	A86	C21-C20	3.77	1.57	1.51
30	A	802	CLA	C1B-NB	-3.77	1.31	1.35
38	4	310	KC1	CHC-C1C	3.77	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	12	316	A86	C5-C6	3.77	1.40	1.35
30	12	308	CLA	CHD-C4C	3.77	1.47	1.39
38	14	306	KC1	C1A-CHA	3.77	1.50	1.40
30	15	308	CLA	C3D-C2D	3.77	1.49	1.39
38	16	311	KC1	CHB-C1B	3.77	1.45	1.38
37	14	318	A86	C5-C6	3.77	1.40	1.35
30	5	308	CLA	CHD-C4C	3.77	1.47	1.39
30	13	303	CLA	OBD-CAD	3.76	1.29	1.22
30	13	303	CLA	C3D-C2D	3.76	1.49	1.39
38	12	311	KC1	C1B-NB	-3.76	1.33	1.37
30	B	812	CLA	C3D-C2D	3.76	1.49	1.39
37	15	315	A86	C21-C20	3.76	1.57	1.51
38	5	305	KC1	C1B-NB	-3.76	1.33	1.37
30	15	311	CLA	OBD-CAD	3.76	1.29	1.22
30	B	828	CLA	CHD-C4C	3.76	1.47	1.39
37	10	302	A86	C17-C18	-3.76	1.46	1.52
37	4	314	A86	C19-C18	3.76	1.57	1.52
30	B	822	CLA	C1D-ND	3.76	1.42	1.37
30	14	309	CLA	OBD-CAD	3.76	1.29	1.22
30	14	305	CLA	C3D-C2D	3.76	1.49	1.39
30	A	826	CLA	CHD-C1D	3.76	1.45	1.38
37	14	301	A86	C5-C6	3.76	1.40	1.35
38	12	305	KC1	C1B-NB	-3.76	1.33	1.37
30	B	810	CLA	CHD-C1D	3.76	1.45	1.38
37	14	318	A86	C9-C10	3.76	1.55	1.43
37	5	315	A86	C9-C10	3.76	1.55	1.43
37	8	318	A86	C26-C27	3.76	1.40	1.35
38	11	305	KC1	C1B-NB	-3.76	1.33	1.37
30	10	304	CLA	CHD-C4C	3.76	1.47	1.39
37	8	315	A86	C21-C20	3.75	1.57	1.51
30	6	315	CLA	C3D-C2D	3.75	1.49	1.39
38	8	311	KC1	C4D-ND	3.75	1.38	1.35
30	5	304	CLA	CHD-C4C	3.75	1.47	1.39
37	15	322	A86	C19-C18	3.75	1.57	1.52
30	4	302	CLA	CHD-C4C	3.75	1.47	1.39
30	A	841	CLA	O2A-CGA	3.75	1.44	1.33
37	4	314	A86	C10-C11	3.75	1.45	1.34
30	2	308	CLA	CHD-C4C	3.75	1.47	1.39
30	2	305	CLA	C3D-C2D	3.75	1.49	1.39
38	6	312	KC1	C1A-CHA	3.75	1.50	1.40
37	15	321	A86	C10-C11	3.75	1.45	1.34
30	9	303	CLA	CHD-C4C	3.75	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	9	306	CLA	C3D-C2D	3.75	1.49	1.39
30	B	816	CLA	CHD-C4C	3.75	1.47	1.39
37	9	313	A86	C2-C1	3.75	1.40	1.35
30	15	310	CLA	OBD-CAD	3.75	1.28	1.22
30	14	312	CLA	C3D-C2D	3.75	1.49	1.39
30	9	302	CLA	CHD-C4C	3.75	1.47	1.39
38	13	306	KC1	CHC-C1C	3.75	1.47	1.39
30	A	831	CLA	C3D-C2D	3.75	1.49	1.39
30	A	821	CLA	CHD-C1D	3.74	1.45	1.38
30	15	304	CLA	C3D-C2D	3.74	1.49	1.39
30	8	304	CLA	C3D-C2D	3.74	1.49	1.39
30	1	303	CLA	CHD-C4C	3.74	1.47	1.39
30	16	310	CLA	CHD-C4C	3.74	1.47	1.39
30	15	314	CLA	OBD-CAD	3.74	1.28	1.22
30	A	803	CLA	C3D-C2D	3.74	1.49	1.39
37	5	301	A86	C21-C20	3.74	1.57	1.51
30	6	306	CLA	CHD-C4C	3.74	1.47	1.39
30	15	307	CLA	OBD-CAD	3.74	1.28	1.22
30	9	309	CLA	CHD-C4C	3.74	1.47	1.39
30	14	304	CLA	OBD-CAD	3.74	1.28	1.22
30	10	311	CLA	C3D-C2D	3.74	1.49	1.39
30	15	308	CLA	OBD-CAD	3.74	1.28	1.22
38	9	311	KC1	CHC-C1C	3.74	1.47	1.39
30	7	306	CLA	C3D-C2D	3.74	1.49	1.39
30	15	302	CLA	OBD-CAD	3.74	1.28	1.22
38	10	310	KC1	C1A-CHA	3.73	1.50	1.40
30	16	305	CLA	C3D-C2D	3.73	1.49	1.39
39	15	319	DD6	C35-C34	3.73	1.58	1.52
30	3	305	CLA	CHD-C4C	3.73	1.47	1.39
38	8	313	KC1	C1A-CHA	3.73	1.50	1.40
30	15	309	CLA	C3D-C2D	3.73	1.49	1.39
37	2	319	A86	C10-C11	3.73	1.45	1.34
30	15	306	CLA	C3D-C2D	3.73	1.49	1.39
38	14	311	KC1	CHC-C1C	3.73	1.47	1.39
37	4	315	A86	C2-C1	3.73	1.40	1.35
38	5	310	KC1	C1A-CHA	3.73	1.50	1.40
30	A	823	CLA	CHD-C1D	3.73	1.45	1.38
30	L	202	CLA	CHD-C4C	3.73	1.47	1.39
30	6	310	CLA	C3D-C2D	3.73	1.49	1.39
30	7	307	CLA	CHD-C1D	3.73	1.45	1.38
37	15	321	A86	C9-C10	3.73	1.55	1.43
30	13	309	CLA	OBD-CAD	3.73	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	10	302	A86	C10-C11	3.73	1.45	1.34
30	B	809	CLA	CHD-C1D	3.73	1.45	1.38
30	A	839	CLA	CHD-C4C	3.73	1.47	1.39
37	10	316	A86	C21-C20	3.73	1.57	1.51
30	13	307	CLA	OBD-CAD	3.73	1.28	1.22
38	9	310	KC1	C1A-CHA	3.73	1.50	1.40
30	A	803	CLA	C1B-NB	-3.73	1.31	1.35
38	9	304	KC1	C1B-NB	-3.73	1.33	1.37
38	13	305	KC1	C1B-NB	-3.73	1.33	1.37
37	8	318	A86	C9-C10	3.72	1.55	1.43
37	12	316	A86	C21-C20	3.72	1.57	1.51
38	8	312	KC1	CHC-C1C	3.72	1.47	1.39
30	14	303	CLA	C3D-C2D	3.72	1.49	1.39
30	15	313	CLA	C3D-C2D	3.72	1.49	1.39
37	3	314	A86	C5-C6	3.72	1.40	1.35
38	9	304	KC1	C1A-CHA	3.72	1.50	1.40
38	8	311	KC1	CHC-C1C	3.72	1.47	1.39
30	A	841	CLA	C3D-C2D	3.72	1.49	1.39
30	7	303	CLA	C1D-ND	3.72	1.42	1.37
30	13	307	CLA	C3D-C2D	3.72	1.49	1.39
30	8	301	CLA	C3D-C2D	3.72	1.49	1.39
30	9	308	CLA	CHD-C4C	3.72	1.47	1.39
30	12	310	CLA	CHD-C4C	3.72	1.47	1.39
37	3	315	A86	C21-C20	3.72	1.57	1.51
30	B	803	CLA	CHD-C1D	3.72	1.45	1.38
37	9	316	A86	C21-C20	3.72	1.57	1.51
38	16	304	KC1	C1B-NB	-3.72	1.33	1.37
30	A	838	CLA	CHD-C4C	3.72	1.47	1.39
30	8	303	CLA	CHD-C4C	3.72	1.47	1.39
30	A	809	CLA	CHD-C4C	3.72	1.47	1.39
30	2	311	CLA	C3D-C2D	3.72	1.49	1.39
30	A	840	CLA	CHD-C4C	3.72	1.47	1.39
30	B	833	CLA	CHD-C4C	3.72	1.47	1.39
30	8	302	CLA	CHD-C4C	3.72	1.47	1.39
38	8	307	KC1	C1A-CHA	3.72	1.50	1.40
30	7	311	CLA	CHD-C4C	3.72	1.47	1.39
30	16	308	CLA	OBD-CAD	3.72	1.28	1.22
30	A	813	CLA	CHD-C4C	3.71	1.47	1.39
37	6	320	A86	C17-C18	-3.71	1.47	1.52
30	16	309	CLA	C3D-C2D	3.71	1.49	1.39
30	3	301	CLA	C3D-C2D	3.71	1.49	1.39
30	3	309	CLA	C3D-C2D	3.71	1.49	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	6	311	KC1	C4B-NB	-3.71	1.33	1.37
37	15	322	A86	C21-C20	3.71	1.57	1.51
38	5	306	KC1	CHC-C1C	3.71	1.47	1.39
30	9	307	CLA	CHD-C4C	3.71	1.47	1.39
37	14	315	A86	C9-C10	3.71	1.54	1.43
30	11	304	CLA	OBD-CAD	3.71	1.28	1.22
37	2	319	A86	C9-C10	3.71	1.54	1.43
38	7	313	KC1	C1B-NB	-3.71	1.33	1.37
37	8	318	A86	C5-C6	3.71	1.40	1.35
37	11	316	A86	C9-C10	3.71	1.54	1.43
30	5	311	CLA	C3D-C2D	3.71	1.49	1.39
30	2	313	CLA	OBD-CAD	3.71	1.28	1.22
37	5	301	A86	C9-C10	3.71	1.54	1.43
30	15	303	CLA	C3D-C2D	3.71	1.49	1.39
30	B	829	CLA	CHD-C4C	3.70	1.47	1.39
30	2	308	CLA	C3D-C2D	3.70	1.49	1.39
30	5	303	CLA	CHD-C4C	3.70	1.47	1.39
30	15	307	CLA	CHD-C4C	3.70	1.47	1.39
38	16	311	KC1	CHC-C1C	3.70	1.47	1.39
30	12	312	CLA	C3D-C2D	3.70	1.49	1.39
30	12	303	CLA	C3D-C2D	3.70	1.49	1.39
37	14	316	A86	C10-C11	3.70	1.45	1.34
30	15	302	CLA	C3D-C2D	3.70	1.49	1.39
30	15	311	CLA	C3D-C2D	3.70	1.49	1.39
30	3	310	CLA	C3D-C2D	3.70	1.49	1.39
30	13	304	CLA	C3D-C2D	3.70	1.49	1.39
30	13	309	CLA	C3D-C2D	3.70	1.49	1.39
30	14	307	CLA	C3D-C2D	3.70	1.49	1.39
37	14	301	A86	C9-C10	3.70	1.54	1.43
30	2	310	CLA	C3D-C2D	3.70	1.49	1.39
38	2	306	KC1	CHC-C1C	3.70	1.47	1.39
30	14	304	CLA	C3D-C2D	3.70	1.49	1.39
37	1	309	A86	C19-C18	3.70	1.57	1.52
30	3	302	CLA	C3D-C2D	3.70	1.49	1.39
30	15	305	CLA	C3D-C2D	3.70	1.49	1.39
30	B	830	CLA	CHD-C4C	3.70	1.47	1.39
30	6	317	CLA	C3D-C2D	3.70	1.49	1.39
30	7	307	CLA	CHD-C4C	3.70	1.47	1.39
30	8	302	CLA	CHD-C1D	3.70	1.45	1.38
30	12	321	CLA	C3D-C2D	3.70	1.49	1.39
37	11	315	A86	C9-C10	3.70	1.54	1.43
30	10	308	CLA	C3D-C2D	3.70	1.49	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	14	302	CLA	OBD-CAD	3.70	1.28	1.22
30	3	309	CLA	OBD-CAD	3.70	1.28	1.22
30	B	831	CLA	CHD-C4C	3.70	1.47	1.39
38	16	304	KC1	CHC-C1C	3.70	1.47	1.39
30	B	823	CLA	CHD-C4C	3.69	1.47	1.39
30	1	305	CLA	C3D-C2D	3.69	1.49	1.39
37	2	302	A86	C21-C20	3.69	1.57	1.51
38	2	314	KC1	C4D-ND	3.69	1.38	1.35
30	3	305	CLA	C3D-C2D	3.69	1.49	1.39
37	2	319	A86	C26-C27	3.69	1.40	1.35
37	11	316	A86	C10-C11	3.69	1.45	1.34
38	10	312	KC1	C1A-CHA	3.69	1.50	1.40
30	B	803	CLA	C3D-C2D	3.69	1.49	1.39
38	11	311	KC1	C1B-NB	-3.69	1.33	1.37
38	8	307	KC1	CHC-C1C	3.69	1.47	1.39
38	13	308	KC1	C1B-NB	-3.69	1.33	1.37
37	14	315	A86	C10-C11	3.69	1.45	1.34
38	2	314	KC1	CHC-C1C	3.69	1.47	1.39
37	4	314	A86	C17-C18	-3.69	1.47	1.52
30	B	813	CLA	C3D-C2D	3.69	1.49	1.39
30	10	307	CLA	C3D-C2D	3.69	1.49	1.39
30	16	307	CLA	C3D-C2D	3.68	1.49	1.39
30	B	809	CLA	C1B-NB	-3.68	1.31	1.35
30	10	307	CLA	CHD-C4C	3.68	1.47	1.39
30	2	304	CLA	C3D-C2D	3.68	1.49	1.39
30	16	307	CLA	OBD-CAD	3.68	1.28	1.22
30	A	836	CLA	C3D-C2D	3.68	1.49	1.39
30	16	301	CLA	CHD-C4C	3.68	1.47	1.39
30	B	804	CLA	CHD-C4C	3.68	1.47	1.39
30	12	303	CLA	CHD-C4C	3.68	1.47	1.39
30	A	811	CLA	CHD-C4C	3.68	1.47	1.39
37	2	302	A86	C17-C18	-3.68	1.47	1.52
37	14	317	A86	C9-C10	3.68	1.54	1.43
30	F	203	CLA	CHD-C4C	3.68	1.47	1.39
39	6	303	DD6	C35-C34	3.68	1.58	1.52
30	9	303	CLA	C3D-C2D	3.68	1.49	1.39
38	14	311	KC1	C1B-NB	-3.68	1.33	1.37
37	5	301	A86	C5-C6	3.68	1.40	1.35
30	5	309	CLA	C3D-C2D	3.68	1.49	1.39
30	4	309	CLA	OBD-CAD	3.68	1.28	1.22
38	5	306	KC1	C1A-CHA	3.68	1.50	1.40
30	12	306	CLA	CHD-C4C	3.68	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	3	310	CLA	OBD-CAD	3.68	1.28	1.22
30	A	814	CLA	CHD-C4C	3.68	1.47	1.39
38	9	310	KC1	CHC-C1C	3.68	1.47	1.39
30	B	806	CLA	CHD-C4C	3.67	1.47	1.39
38	6	308	KC1	CHC-C1C	3.67	1.47	1.39
30	B	825	CLA	CHD-C1D	3.67	1.45	1.38
37	9	316	A86	C17-C18	-3.67	1.47	1.52
30	12	304	CLA	C3D-C2D	3.67	1.49	1.39
30	9	301	CLA	CHD-C4C	3.67	1.47	1.39
30	14	313	CLA	C3D-C2D	3.67	1.49	1.39
30	A	805	CLA	CHD-C4C	3.67	1.47	1.39
30	A	841	CLA	CHD-C4C	3.67	1.47	1.39
30	10	311	CLA	OBD-CAD	3.67	1.28	1.22
37	2	318	A86	C10-C11	3.67	1.45	1.34
30	B	807	CLA	CHD-C1D	3.67	1.45	1.38
37	7	315	A86	C17-C18	-3.67	1.47	1.52
37	10	316	A86	C2-C1	3.67	1.40	1.35
38	11	311	KC1	CHC-C1C	3.67	1.47	1.39
30	9	308	CLA	C3D-C2D	3.67	1.49	1.39
30	11	309	CLA	OBD-CAD	3.67	1.28	1.22
30	16	305	CLA	CHD-C4C	3.67	1.47	1.39
30	10	304	CLA	C3D-C2D	3.67	1.49	1.39
30	14	313	CLA	OBD-CAD	3.67	1.28	1.22
37	16	314	A86	C10-C11	3.67	1.45	1.34
30	15	305	CLA	OBD-CAD	3.67	1.28	1.22
30	11	310	CLA	OBD-CAD	3.66	1.28	1.22
30	7	311	CLA	C3D-C2D	3.66	1.49	1.39
30	14	303	CLA	OBD-CAD	3.66	1.28	1.22
30	F	202	CLA	CHD-C1D	3.66	1.45	1.38
37	2	318	A86	C9-C10	3.66	1.54	1.43
38	9	311	KC1	C1B-NB	-3.66	1.33	1.37
30	B	810	CLA	CHD-C4C	3.66	1.47	1.39
37	14	317	A86	C5-C6	3.66	1.40	1.35
37	2u	203	A86	C2-C1	3.66	1.40	1.35
30	7	312	CLA	C3D-C2D	3.66	1.49	1.39
30	15	313	CLA	OBD-CAD	3.66	1.28	1.22
30	16	303	CLA	CHD-C1D	3.66	1.45	1.38
30	A	812	CLA	CHD-C1D	3.66	1.45	1.38
30	9	306	CLA	OBD-CAD	3.66	1.28	1.22
30	A	822	CLA	CHD-C4C	3.66	1.47	1.39
37	14	319	A86	C19-C18	3.66	1.57	1.52
30	B	838	CLA	CHD-C4C	3.66	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	16	301	CLA	C3D-C2D	3.66	1.49	1.39
30	10	303	CLA	C3D-C2D	3.65	1.49	1.39
30	B	829	CLA	C3D-C2D	3.65	1.49	1.39
38	7	313	KC1	CHC-C1C	3.65	1.47	1.39
30	11	308	CLA	C3D-C2D	3.65	1.49	1.39
37	9	315	A86	C5-C6	3.65	1.40	1.35
38	13	305	KC1	CHC-C1C	3.65	1.47	1.39
30	F	203	CLA	C3D-C2D	3.65	1.49	1.39
30	B	818	CLA	C3D-C2D	3.65	1.49	1.39
30	7	304	CLA	C3D-C2D	3.65	1.49	1.39
30	12	302	CLA	C3D-C2D	3.65	1.49	1.39
30	A	830	CLA	C3D-C2D	3.65	1.49	1.39
30	16	308	CLA	C3D-C2D	3.65	1.49	1.39
30	14	312	CLA	OBD-CAD	3.65	1.28	1.22
30	2	307	CLA	CHD-C4C	3.65	1.47	1.39
30	B	815	CLA	CHD-C4C	3.65	1.47	1.39
30	A	833	CLA	C3D-C2D	3.65	1.49	1.39
30	A	824	CLA	CHD-C4C	3.65	1.47	1.39
30	13	301	CLA	CHD-C4C	3.65	1.47	1.39
38	8	314	KC1	CHC-C1C	3.65	1.47	1.39
30	3	307	CLA	OBD-CAD	3.65	1.28	1.22
38	6	311	KC1	C4D-ND	3.65	1.38	1.35
38	13	308	KC1	CHC-C1C	3.65	1.47	1.39
37	7	319	A86	C21-C20	3.65	1.57	1.51
37	9	313	A86	C10-C11	3.64	1.45	1.34
30	1	302	CLA	C3D-C2D	3.64	1.49	1.39
30	B	807	CLA	CHD-C4C	3.64	1.47	1.39
30	A	843	CLA	C3D-C2D	3.64	1.49	1.39
30	F	201	CLA	C3D-C2D	3.64	1.49	1.39
30	4	305	CLA	C3D-C2D	3.64	1.49	1.39
38	2	312	KC1	CHC-C1C	3.64	1.47	1.39
30	16	309	CLA	OBD-CAD	3.64	1.28	1.22
30	B	802	CLA	C1D-ND	3.64	1.42	1.37
38	3	311	KC1	CHC-C1C	3.64	1.47	1.39
30	A	814	CLA	C3D-C2D	3.64	1.49	1.39
30	B	819	CLA	C1B-NB	-3.64	1.32	1.35
38	6	311	KC1	C1A-CHA	3.64	1.50	1.40
30	1	304	CLA	C3D-C2D	3.64	1.49	1.39
37	4	314	A86	C5-C6	3.64	1.40	1.35
30	B	817	CLA	CHD-C4C	3.64	1.47	1.39
38	12	309	KC1	CHC-C1C	3.64	1.47	1.39
30	3	303	CLA	C3D-C2D	3.64	1.49	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	1	308	KC1	CHC-C1C	3.64	1.47	1.39
38	5	306	KC1	C1B-NB	-3.64	1.33	1.37
30	B	805	CLA	C3D-C2D	3.64	1.49	1.39
30	B	804	CLA	C3D-C2D	3.64	1.49	1.39
38	6	312	KC1	CHC-C1C	3.63	1.47	1.39
38	13	311	KC1	CHC-C1C	3.63	1.47	1.39
30	B	827	CLA	CHD-C1D	3.63	1.45	1.38
30	A	832	CLA	CHD-C4C	3.63	1.47	1.39
37	14	316	A86	C9-C10	3.63	1.54	1.43
30	1	301	CLA	C3D-C2D	3.63	1.49	1.39
30	6	314	CLA	OBD-CAD	3.63	1.28	1.22
30	B	833	CLA	C3D-C2D	3.63	1.49	1.39
30	3	307	CLA	C3D-C2D	3.63	1.49	1.39
30	9	305	CLA	OBD-CAD	3.63	1.28	1.22
30	2	313	CLA	C3D-C2D	3.63	1.49	1.39
30	6	305	CLA	C3D-C2D	3.63	1.49	1.39
30	10	309	CLA	OBD-CAD	3.63	1.28	1.22
37	8	315	A86	C26-C27	3.63	1.40	1.35
38	2	306	KC1	C1B-NB	-3.63	1.33	1.37
30	15	306	CLA	OBD-CAD	3.62	1.28	1.22
30	15	312	CLA	OBD-CAD	3.62	1.28	1.22
37	10	315	A86	C17-C18	-3.62	1.47	1.52
30	B	807	CLA	C3D-C2D	3.62	1.49	1.39
30	A	807	CLA	C3D-C2D	3.62	1.49	1.39
37	14	315	A86	C5-C6	3.62	1.40	1.35
30	B	815	CLA	C3D-C2D	3.62	1.49	1.39
30	8	303	CLA	C3D-C2D	3.62	1.49	1.39
30	16	303	CLA	C3D-C2D	3.62	1.49	1.39
30	A	844	CLA	OBD-CAD	3.62	1.28	1.22
30	A	820	CLA	C3D-C2D	3.62	1.49	1.39
30	11	306	CLA	C3D-C2D	3.62	1.49	1.39
30	6	315	CLA	OBD-CAD	3.62	1.28	1.22
30	A	844	CLA	C3D-C2D	3.62	1.49	1.39
30	B	836	CLA	CHD-C4C	3.62	1.47	1.39
30	4	301	CLA	CHD-C4C	3.62	1.47	1.39
30	A	830	CLA	CHD-C1D	3.62	1.45	1.38
30	B	838	CLA	C3D-C2D	3.62	1.49	1.39
37	4	312	A86	C9-C10	3.62	1.54	1.43
37	7	315	A86	C9-C10	3.61	1.54	1.43
30	B	839	CLA	CHD-C1D	3.61	1.45	1.38
30	14	307	CLA	OBD-CAD	3.61	1.28	1.22
30	6	306	CLA	C3D-C2D	3.61	1.49	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	9	305	CLA	C3D-C2D	3.61	1.49	1.39
38	8	310	KC1	CHC-C1C	3.61	1.47	1.39
38	6	308	KC1	C4D-ND	3.61	1.38	1.35
37	15	323	A86	C19-C18	3.61	1.57	1.52
30	10	309	CLA	C3D-C2D	3.61	1.49	1.39
30	4	311	CLA	C3D-C2D	3.61	1.49	1.39
38	7	313	KC1	C4B-NB	-3.61	1.33	1.37
30	6	317	CLA	OBD-CAD	3.61	1.28	1.22
30	14	305	CLA	OBD-CAD	3.61	1.28	1.22
30	A	837	CLA	C3D-C2D	3.61	1.49	1.39
30	15	314	CLA	C3D-C2D	3.61	1.49	1.39
37	6	320	A86	C10-C11	3.61	1.45	1.34
30	1	303	CLA	C3D-C2D	3.61	1.49	1.39
30	B	803	CLA	O2A-CGA	3.61	1.43	1.33
30	A	816	CLA	C3D-C2D	3.61	1.49	1.39
30	6	316	CLA	C3D-C2D	3.61	1.49	1.39
30	12	308	CLA	OBD-CAD	3.61	1.28	1.22
30	14	310	CLA	OBD-CAD	3.61	1.28	1.22
30	13	301	CLA	OBD-CAD	3.61	1.28	1.22
30	F	202	CLA	CHD-C4C	3.61	1.47	1.39
38	6	313	KC1	CHC-C1C	3.61	1.47	1.39
30	5	307	CLA	CHD-C4C	3.61	1.47	1.39
30	2u	202	CLA	C3D-C2D	3.61	1.49	1.39
37	10	316	A86	C9-C10	3.60	1.54	1.43
30	7	306	CLA	CHD-C4C	3.60	1.47	1.39
30	B	808	CLA	CHD-C4C	3.60	1.47	1.39
30	A	823	CLA	C3D-C2D	3.60	1.49	1.39
37	5	315	A86	C19-C18	3.60	1.57	1.52
30	12	307	CLA	C3D-C2D	3.60	1.49	1.39
39	2	315	DD6	C35-C34	3.60	1.58	1.52
38	11	307	KC1	C1B-NB	-3.60	1.33	1.37
30	16	301	CLA	OBD-CAD	3.60	1.28	1.22
30	2u	202	CLA	CHD-C4C	3.60	1.47	1.39
30	7	303	CLA	C3D-C2D	3.60	1.48	1.39
30	2	309	CLA	C3D-C2D	3.60	1.48	1.39
30	15	304	CLA	OBD-CAD	3.60	1.28	1.22
30	A	808	CLA	CHD-C4C	3.60	1.47	1.39
37	15	321	A86	C5-C6	3.60	1.40	1.35
30	A	841	CLA	C1B-NB	-3.60	1.32	1.35
30	8	308	CLA	C3D-C2D	3.60	1.48	1.39
37	11	316	A86	C5-C6	3.59	1.40	1.35
30	8	309	CLA	C3D-C2D	3.59	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	12	306	CLA	C3D-C2D	3.59	1.48	1.39
37	7	315	A86	C10-C11	3.59	1.45	1.34
37	10	316	A86	C10-C11	3.59	1.45	1.34
30	16	302	CLA	C3D-C2D	3.59	1.48	1.39
30	12	302	CLA	OBD-CAD	3.59	1.28	1.22
30	B	809	CLA	C1D-ND	3.59	1.42	1.37
30	B	834	CLA	C3D-C2D	3.59	1.48	1.39
37	10	315	A86	C5-C6	3.59	1.40	1.35
30	9	309	CLA	C3D-C2D	3.59	1.48	1.39
30	8	301	CLA	CHD-C4C	3.59	1.47	1.39
30	A	816	CLA	CHD-C4C	3.59	1.47	1.39
37	4	312	A86	C10-C11	3.59	1.45	1.34
30	4	306	CLA	C3D-C2D	3.59	1.48	1.39
38	12	305	KC1	CHC-C1C	3.59	1.47	1.39
37	13	313	A86	C19-C18	3.59	1.57	1.52
30	A	836	CLA	CHD-C4C	3.59	1.47	1.39
30	A	813	CLA	C3D-C2D	3.59	1.48	1.39
30	A	803	CLA	CHD-C4C	3.58	1.47	1.39
30	F	201	CLA	C1D-ND	3.58	1.42	1.37
30	5	308	CLA	OBD-CAD	3.58	1.28	1.22
30	B	826	CLA	CHD-C1D	3.58	1.45	1.38
37	7	319	A86	C17-C18	-3.58	1.47	1.52
30	A	819	CLA	CHD-C4C	3.58	1.47	1.39
30	4	303	CLA	C3D-C2D	3.58	1.48	1.39
30	11	310	CLA	C3D-C2D	3.58	1.48	1.39
37	14	314	A86	C7-C6	3.58	1.58	1.50
30	A	810	CLA	CHD-C4C	3.58	1.47	1.39
30	B	837	CLA	CHD-C4C	3.58	1.47	1.39
30	7	312	CLA	OBD-CAD	3.57	1.28	1.22
37	4	315	A86	C9-C10	3.57	1.54	1.43
30	7	310	CLA	C3D-C2D	3.57	1.48	1.39
30	11	304	CLA	C3D-C2D	3.57	1.48	1.39
30	A	804	CLA	CHD-C4C	3.57	1.47	1.39
30	10	308	CLA	OBD-CAD	3.57	1.28	1.22
30	1	307	CLA	C3D-C2D	3.57	1.48	1.39
29	A	801	CL0	CHD-C1D	3.57	1.45	1.38
30	A	842	CLA	C3D-C2D	3.57	1.48	1.39
30	B	839	CLA	C3D-C2D	3.57	1.48	1.39
30	B	819	CLA	CHD-C4C	3.57	1.47	1.39
37	7	319	A86	C5-C6	3.56	1.40	1.35
37	4	317	A86	C10-C11	3.56	1.44	1.34
30	A	807	CLA	CHD-C4C	3.56	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	5	305	KC1	CHC-C1C	3.56	1.47	1.39
30	16	306	CLA	C3D-C2D	3.56	1.48	1.39
30	5	304	CLA	C3D-C2D	3.56	1.48	1.39
30	5	307	CLA	C3D-C2D	3.56	1.48	1.39
37	6	320	A86	C9-C10	3.56	1.54	1.43
30	B	816	CLA	C3D-C2D	3.56	1.48	1.39
30	A	812	CLA	CHD-C4C	3.56	1.47	1.39
30	6	307	CLA	C3D-C2D	3.56	1.48	1.39
30	1	304	CLA	OBD-CAD	3.56	1.28	1.22
30	A	806	CLA	CHD-C1D	3.56	1.45	1.38
30	A	826	CLA	CHD-C4C	3.56	1.47	1.39
38	1	306	KC1	CHC-C1C	3.56	1.47	1.39
30	A	806	CLA	CHD-C4C	3.56	1.47	1.39
30	15	309	CLA	OBD-CAD	3.56	1.28	1.22
30	A	809	CLA	C3D-C2D	3.56	1.48	1.39
30	A	835	CLA	C3D-C2D	3.55	1.48	1.39
30	9	307	CLA	C3D-C2D	3.55	1.48	1.39
30	14	310	CLA	C3D-C2D	3.55	1.48	1.39
30	7	303	CLA	CHD-C1D	3.55	1.45	1.38
30	A	825	CLA	C3D-C2D	3.55	1.48	1.39
30	B	834	CLA	CHD-C4C	3.55	1.47	1.39
30	11	309	CLA	C3D-C2D	3.55	1.48	1.39
30	A	842	CLA	CHD-C4C	3.55	1.47	1.39
30	B	851	CLA	OBD-CAD	3.55	1.28	1.22
30	12	312	CLA	OBD-CAD	3.55	1.28	1.22
37	13	315	A86	C19-C18	3.55	1.57	1.52
30	8	309	CLA	OBD-CAD	3.55	1.28	1.22
37	14	314	A86	C17-C18	-3.55	1.47	1.52
37	2u	205	A86	C5-C6	3.55	1.40	1.35
30	A	831	CLA	CHD-C4C	3.55	1.47	1.39
38	9	304	KC1	CHC-C1C	3.55	1.47	1.39
37	1	309	A86	C5-C6	3.55	1.40	1.35
37	4	315	A86	C10-C11	3.55	1.44	1.34
30	9	302	CLA	C3D-C2D	3.55	1.48	1.39
30	B	831	CLA	C3D-C2D	3.54	1.48	1.39
30	2	303	CLA	C1D-ND	3.54	1.42	1.37
30	A	805	CLA	C3D-C2D	3.54	1.48	1.39
30	A	811	CLA	C3D-C2D	3.54	1.48	1.39
30	B	809	CLA	C3D-C2D	3.54	1.48	1.39
37	14	317	A86	C10-C11	3.54	1.44	1.34
30	6	304	CLA	C3D-C2D	3.54	1.48	1.39
30	B	809	CLA	CHD-C4C	3.54	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	11	307	KC1	CHC-C1C	3.54	1.47	1.39
30	L	203	CLA	OBD-CAD	3.54	1.28	1.22
30	A	815	CLA	C3D-C2D	3.54	1.48	1.39
38	4	308	KC1	C4B-NB	-3.54	1.33	1.37
38	8	313	KC1	C4D-ND	3.54	1.38	1.35
37	5	315	A86	C5-C6	3.54	1.40	1.35
30	A	837	CLA	OBD-CAD	3.54	1.28	1.22
30	6	316	CLA	OBD-CAD	3.54	1.28	1.22
30	A	838	CLA	C3D-C2D	3.54	1.48	1.39
37	4	317	A86	C9-C10	3.54	1.54	1.43
30	4	301	CLA	CHD-C1D	3.54	1.45	1.38
30	10	305	CLA	C3D-C2D	3.53	1.48	1.39
30	1	304	CLA	CHD-C4C	3.53	1.47	1.39
30	7	303	CLA	CHD-C4C	3.53	1.47	1.39
37	15	322	A86	C17-C18	-3.53	1.47	1.52
30	B	839	CLA	CHD-C4C	3.53	1.47	1.39
38	8	306	KC1	CHC-C1C	3.53	1.47	1.39
38	10	310	KC1	CHC-C1C	3.53	1.47	1.39
30	L	202	CLA	C3D-C2D	3.53	1.48	1.39
38	10	306	KC1	CHC-C1C	3.53	1.47	1.39
30	7	309	CLA	C3D-C2D	3.53	1.48	1.39
37	8	318	A86	C2-C1	3.53	1.40	1.35
30	7	309	CLA	CHD-C4C	3.53	1.47	1.39
30	9	307	CLA	OBD-CAD	3.53	1.28	1.22
30	11	308	CLA	OBD-CAD	3.53	1.28	1.22
38	9	312	KC1	C1B-NB	-3.52	1.33	1.37
30	8	304	CLA	CHD-C4C	3.52	1.47	1.39
30	B	825	CLA	CHD-C4C	3.52	1.47	1.39
30	2	309	CLA	OBD-CAD	3.52	1.28	1.22
30	5	303	CLA	C3D-C2D	3.52	1.48	1.39
38	9	312	KC1	CHC-C1C	3.52	1.47	1.39
30	L	203	CLA	C3D-C2D	3.52	1.48	1.39
30	16	305	CLA	OBD-CAD	3.52	1.28	1.22
30	A	832	CLA	C3D-C2D	3.51	1.48	1.39
39	15	318	DD6	C35-C34	3.51	1.58	1.52
30	A	818	CLA	CHD-C4C	3.51	1.47	1.39
30	A	839	CLA	C3D-C2D	3.51	1.48	1.39
30	A	834	CLA	C3D-C2D	3.51	1.48	1.39
30	B	811	CLA	CHD-C4C	3.51	1.47	1.39
30	B	801	CLA	CHD-C1D	3.51	1.45	1.38
38	11	305	KC1	CHC-C1C	3.51	1.47	1.39
30	A	829	CLA	CHD-C4C	3.51	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	12	307	CLA	CHD-C4C	3.51	1.47	1.39
30	9	302	CLA	OBD-CAD	3.51	1.28	1.22
30	10	303	CLA	OBD-CAD	3.51	1.28	1.22
37	3	315	A86	C5-C6	3.51	1.40	1.35
30	16	310	CLA	C3D-C2D	3.51	1.48	1.39
38	5	312	KC1	CHC-C1C	3.51	1.47	1.39
37	9	315	A86	C17-C18	-3.50	1.47	1.52
38	14	308	KC1	CHC-C1C	3.50	1.47	1.39
30	B	835	CLA	C3D-C2D	3.50	1.48	1.39
30	12	308	CLA	C3D-C2D	3.50	1.48	1.39
30	F	201	CLA	CHD-C1D	3.50	1.45	1.38
30	12	302	CLA	CHD-C4C	3.50	1.47	1.39
30	12	310	CLA	C3D-C2D	3.50	1.48	1.39
30	14	302	CLA	C3D-C2D	3.50	1.48	1.39
38	14	308	KC1	C1B-NB	-3.50	1.33	1.37
30	F	202	CLA	C3D-C2D	3.50	1.48	1.39
30	A	817	CLA	C3D-C2D	3.50	1.48	1.39
30	4	302	CLA	C3D-C2D	3.50	1.48	1.39
37	14	318	A86	C19-C18	3.50	1.57	1.52
30	B	832	CLA	C3D-C2D	3.49	1.48	1.39
37	10	316	A86	C5-C6	3.49	1.40	1.35
30	7	307	CLA	C3D-C2D	3.49	1.48	1.39
30	B	836	CLA	CHD-C1D	3.49	1.45	1.38
30	4	304	CLA	OBD-CAD	3.49	1.28	1.22
30	13	302	CLA	OBD-CAD	3.48	1.28	1.22
30	B	806	CLA	C3D-C2D	3.48	1.48	1.39
38	4	307	KC1	CHC-C1C	3.48	1.47	1.39
37	14	301	A86	C19-C18	3.48	1.57	1.52
38	7	308	KC1	CHC-C1C	3.48	1.47	1.39
30	A	808	CLA	C3D-C2D	3.48	1.48	1.39
30	A	804	CLA	C3D-C2D	3.48	1.48	1.39
30	B	813	CLA	CHD-C4C	3.48	1.47	1.39
39	11	313	DD6	O2-C18	3.48	1.53	1.43
30	A	812	CLA	C3D-C2D	3.48	1.48	1.39
30	7	303	CLA	OBD-CAD	3.48	1.28	1.22
30	B	827	CLA	CHD-C4C	3.47	1.47	1.39
30	3	306	CLA	OBD-CAD	3.47	1.28	1.22
30	B	820	CLA	C3D-C2D	3.47	1.48	1.39
30	A	826	CLA	OBD-CAD	3.47	1.28	1.22
30	7	307	CLA	OBD-CAD	3.47	1.28	1.22
30	8	308	CLA	OBD-CAD	3.47	1.28	1.22
37	11	315	A86	C5-C6	3.47	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	814	CLA	CHD-C4C	3.47	1.47	1.39
30	A	826	CLA	C3D-C2D	3.47	1.48	1.39
30	2	305	CLA	OBD-CAD	3.46	1.28	1.22
30	15	312	CLA	C3D-C2D	3.46	1.48	1.39
30	B	802	CLA	CHD-C1D	3.46	1.45	1.38
37	14	316	A86	C5-C6	3.46	1.40	1.35
29	A	801	CL0	C3D-C2D	3.46	1.48	1.39
30	A	817	CLA	OBD-CAD	3.46	1.28	1.22
30	A	810	CLA	C3D-C2D	3.46	1.48	1.39
38	3	304	KC1	CHC-C1C	3.46	1.47	1.39
37	15	316	A86	C17-C18	-3.46	1.47	1.52
30	4	301	CLA	C3D-C2D	3.46	1.48	1.39
30	B	824	CLA	C3D-C2D	3.46	1.48	1.39
37	11	314	A86	C19-C18	3.46	1.57	1.52
30	1	301	CLA	OBD-CAD	3.46	1.28	1.22
37	4	317	A86	C21-C20	3.46	1.57	1.51
30	B	836	CLA	C3D-C2D	3.46	1.48	1.39
30	13	301	CLA	C3D-C2D	3.46	1.48	1.39
37	16	314	A86	C5-C6	3.46	1.40	1.35
38	13	310	KC1	C1B-NB	-3.46	1.33	1.37
37	15	321	A86	C19-C18	3.45	1.57	1.52
30	B	826	CLA	C3D-C2D	3.45	1.48	1.39
38	13	311	KC1	C1B-NB	-3.45	1.33	1.37
38	12	311	KC1	CHC-C1C	3.45	1.47	1.39
38	3	308	KC1	C1B-NB	-3.45	1.33	1.37
37	7	315	A86	C5-C6	3.45	1.40	1.35
39	2	317	DD6	C35-C34	3.45	1.58	1.52
30	B	828	CLA	OBD-CAD	3.45	1.28	1.22
39	15	318	DD6	C-C1	3.45	1.58	1.50
37	6	320	A86	C19-C18	3.45	1.57	1.52
38	8	313	KC1	C4B-NB	-3.45	1.33	1.37
30	A	822	CLA	C3D-C2D	3.45	1.48	1.39
30	9	301	CLA	C3D-C2D	3.45	1.48	1.39
37	10	302	A86	C5-C6	3.45	1.40	1.35
30	7	310	CLA	OBD-CAD	3.45	1.28	1.22
30	9	309	CLA	OBD-CAD	3.45	1.28	1.22
30	B	814	CLA	C3D-C2D	3.44	1.48	1.39
39	2	317	DD6	O2-C18	3.44	1.53	1.43
30	F	203	CLA	OBD-CAD	3.44	1.28	1.22
30	B	827	CLA	C3D-C2D	3.44	1.48	1.39
30	A	814	CLA	OBD-CAD	3.44	1.28	1.22
30	16	303	CLA	OBD-CAD	3.44	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	8	302	CLA	C3D-C2D	3.44	1.48	1.39
30	5	302	CLA	OBD-CAD	3.44	1.28	1.22
38	8	312	KC1	C1B-NB	-3.44	1.33	1.37
30	2	308	CLA	OBD-CAD	3.44	1.28	1.22
37	5	316	A86	C21-C20	3.44	1.57	1.51
37	6	320	A86	C21-C20	3.44	1.57	1.51
30	6	310	CLA	OBD-CAD	3.44	1.28	1.22
37	10	301	A86	C10-C11	3.44	1.44	1.34
30	B	805	CLA	OBD-CAD	3.44	1.28	1.22
30	A	830	CLA	C1D-ND	3.43	1.42	1.37
30	5	311	CLA	OBD-CAD	3.43	1.28	1.22
37	6	320	A86	C5-C6	3.43	1.40	1.35
30	2	301	CLA	C3D-C2D	3.43	1.48	1.39
30	A	828	CLA	C3D-C2D	3.43	1.48	1.39
30	4	311	CLA	OBD-CAD	3.43	1.28	1.22
30	9	303	CLA	OBD-CAD	3.43	1.28	1.22
30	L	202	CLA	CHD-C1D	3.43	1.45	1.38
37	7	316	A86	C10-C11	3.43	1.44	1.34
30	J	101	CLA	OBD-CAD	3.43	1.28	1.22
30	5	309	CLA	OBD-CAD	3.43	1.28	1.22
30	A	821	CLA	C3D-C2D	3.43	1.48	1.39
37	9	313	A86	C9-C10	3.43	1.54	1.43
37	14	315	A86	C19-C18	3.43	1.57	1.52
37	7	316	A86	C26-C27	3.42	1.40	1.35
30	A	827	CLA	CHD-C1D	3.42	1.45	1.38
30	B	830	CLA	OBD-CAD	3.42	1.28	1.22
30	2	301	CLA	CHD-C1D	3.42	1.45	1.38
30	B	808	CLA	OBD-CAD	3.42	1.28	1.22
30	B	804	CLA	OBD-CAD	3.42	1.28	1.22
30	1	302	CLA	OBD-CAD	3.42	1.28	1.22
30	1	305	CLA	OBD-CAD	3.42	1.28	1.22
37	8	318	A86	C10-C11	3.42	1.44	1.34
30	9	301	CLA	CHD-C1D	3.41	1.45	1.38
30	B	817	CLA	C3D-C2D	3.41	1.48	1.39
30	B	819	CLA	C1D-ND	3.41	1.42	1.37
38	6	313	KC1	C4B-NB	-3.41	1.33	1.37
30	3	305	CLA	OBD-CAD	3.41	1.28	1.22
39	7	318	DD6	O2-C18	3.41	1.53	1.43
30	B	851	CLA	C3D-C2D	3.41	1.48	1.39
39	12	317	DD6	O2-C18	3.41	1.53	1.43
37	15	320	A86	C17-C18	-3.41	1.47	1.52
30	B	802	CLA	CHD-C4C	3.41	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	5	310	KC1	CHC-C1C	3.41	1.47	1.39
37	10	301	A86	C9-C10	3.41	1.54	1.43
30	A	815	CLA	OBD-CAD	3.41	1.28	1.22
30	A	830	CLA	C1B-NB	-3.41	1.32	1.35
30	J	101	CLA	C3D-C2D	3.41	1.48	1.39
30	A	808	CLA	OBD-CAD	3.41	1.28	1.22
37	8	315	A86	C2-C1	3.40	1.40	1.35
30	A	805	CLA	OBD-CAD	3.40	1.28	1.22
39	3	312	DD6	C-C1	3.40	1.57	1.50
38	4	308	KC1	CHC-C1C	3.40	1.47	1.39
39	6	303	DD6	O2-C18	3.40	1.53	1.43
30	6	309	CLA	OBD-CAD	3.40	1.28	1.22
30	B	814	CLA	OBD-CAD	3.40	1.28	1.22
30	4	302	CLA	OBD-CAD	3.40	1.28	1.22
30	4	306	CLA	OBD-CAD	3.40	1.28	1.22
37	10	301	A86	C19-C18	3.39	1.57	1.52
30	B	826	CLA	CHD-C4C	3.39	1.47	1.39
37	12	314	A86	C19-C18	3.39	1.57	1.52
37	11	315	A86	C19-C18	3.39	1.57	1.52
37	4	312	A86	C5-C6	3.39	1.40	1.35
37	4	315	A86	C5-C6	3.39	1.40	1.35
30	A	842	CLA	OBD-CAD	3.39	1.28	1.22
30	6	304	CLA	OBD-CAD	3.39	1.28	1.22
30	2	310	CLA	OBD-CAD	3.39	1.28	1.22
30	A	830	CLA	CHD-C4C	3.39	1.47	1.39
30	A	811	CLA	OBD-CAD	3.39	1.28	1.22
38	12	313	KC1	CHC-C1C	3.38	1.47	1.39
38	8	310	KC1	C4B-NB	-3.38	1.33	1.37
30	A	822	CLA	C1B-NB	-3.38	1.32	1.35
30	A	827	CLA	CHD-C4C	3.38	1.47	1.39
30	6	314	CLA	C3D-C2D	3.38	1.48	1.39
37	8	315	A86	C9-C10	3.38	1.53	1.43
38	13	312	KC1	C1B-NB	-3.38	1.33	1.37
30	1	303	CLA	OBD-CAD	3.38	1.28	1.22
37	5	316	A86	C5-C6	3.38	1.40	1.35
30	6	307	CLA	OBD-CAD	3.38	1.28	1.22
39	3	312	DD6	C35-C34	3.38	1.58	1.52
30	B	811	CLA	C3D-C2D	3.38	1.48	1.39
30	A	818	CLA	C3D-C2D	3.38	1.48	1.39
39	13	314	DD6	O2-C18	3.37	1.53	1.43
30	A	821	CLA	CHD-C4C	3.37	1.46	1.39
39	3	312	DD6	O2-C18	3.37	1.53	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	803	CLA	CHD-C1D	3.37	1.44	1.38
30	L	202	CLA	OBD-CAD	3.37	1.28	1.22
37	3	314	A86	C19-C18	3.37	1.57	1.52
30	A	829	CLA	C3D-C2D	3.37	1.48	1.39
38	5	312	KC1	C4B-NB	-3.37	1.33	1.37
30	B	821	CLA	C3D-C2D	3.37	1.48	1.39
37	7	316	A86	C9-C10	3.37	1.53	1.43
30	B	837	CLA	C3D-C2D	3.37	1.48	1.39
29	A	801	CL0	CHD-C4C	3.37	1.46	1.39
30	B	819	CLA	OBD-CAD	3.37	1.28	1.22
30	B	820	CLA	CHD-C1D	3.36	1.44	1.38
30	8	303	CLA	OBD-CAD	3.36	1.28	1.22
39	1	310	DD6	O2-C18	3.36	1.53	1.43
37	14	320	A86	C19-C18	3.36	1.57	1.52
30	5	302	CLA	C3D-C2D	3.36	1.48	1.39
30	8	305	CLA	CHD-C4C	3.36	1.46	1.39
37	15	322	A86	C14-C15	3.36	1.59	1.52
30	10	305	CLA	OBD-CAD	3.36	1.28	1.22
30	4	304	CLA	C3D-C2D	3.36	1.48	1.39
30	B	829	CLA	OBD-CAD	3.36	1.28	1.22
39	15	318	DD6	O2-C18	3.36	1.53	1.43
30	8	301	CLA	OBD-CAD	3.36	1.28	1.22
38	2	312	KC1	C4B-NB	-3.36	1.33	1.37
38	2	314	KC1	C4B-NB	-3.36	1.33	1.37
30	8	305	CLA	CHD-C1D	3.36	1.44	1.38
30	10	307	CLA	OBD-CAD	3.35	1.28	1.22
37	15	317	A86	C19-C18	3.35	1.57	1.52
37	9	315	A86	C19-C18	3.35	1.57	1.52
30	2	307	CLA	OBD-CAD	3.35	1.28	1.22
38	8	314	KC1	C4B-NB	-3.35	1.33	1.37
30	A	810	CLA	OBD-CAD	3.35	1.28	1.22
39	7	317	DD6	O2-C18	3.35	1.53	1.43
37	8	318	A86	C19-C18	3.35	1.57	1.52
30	A	813	CLA	OBD-CAD	3.35	1.28	1.22
38	11	311	KC1	C4B-NB	-3.35	1.33	1.37
30	A	816	CLA	OBD-CAD	3.34	1.28	1.22
30	9	301	CLA	OBD-CAD	3.34	1.28	1.22
37	8	315	A86	C10-C11	3.34	1.44	1.34
30	A	843	CLA	OBD-CAD	3.34	1.28	1.22
30	A	819	CLA	C3D-C2D	3.34	1.48	1.39
30	B	823	CLA	C3D-C2D	3.34	1.48	1.39
30	12	304	CLA	OBD-CAD	3.34	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	826	CLA	OBD-CAD	3.34	1.28	1.22
30	A	834	CLA	OBD-CAD	3.33	1.28	1.22
38	7	308	KC1	C4B-NB	-3.33	1.33	1.37
30	A	836	CLA	OBD-CAD	3.33	1.28	1.22
30	B	812	CLA	OBD-CAD	3.33	1.28	1.22
30	A	806	CLA	OBD-CAD	3.33	1.28	1.22
30	B	820	CLA	OBD-CAD	3.33	1.28	1.22
30	7	305	CLA	C3D-C2D	3.33	1.48	1.39
30	B	817	CLA	OBD-CAD	3.33	1.28	1.22
30	7	311	CLA	OBD-CAD	3.33	1.28	1.22
38	8	311	KC1	C4B-NB	-3.33	1.33	1.37
37	13	313	A86	C25-C24	3.33	1.43	1.34
37	15	320	A86	C25-C24	3.33	1.43	1.34
38	10	312	KC1	C4B-NB	-3.32	1.33	1.37
38	12	309	KC1	C4B-NB	-3.32	1.33	1.37
30	A	803	CLA	OBD-CAD	3.32	1.28	1.22
39	7	302	DD6	C-C1	3.32	1.57	1.50
30	2u	202	CLA	OBD-CAD	3.32	1.28	1.22
30	B	839	CLA	OBD-CAD	3.32	1.28	1.22
30	A	840	CLA	C3D-C2D	3.32	1.48	1.39
30	B	825	CLA	C3D-C2D	3.31	1.48	1.39
37	10	317	A86	C17-C18	-3.31	1.47	1.52
39	15	319	DD6	O2-C18	3.31	1.53	1.43
39	10	314	DD6	O2-C18	3.31	1.53	1.43
30	B	824	CLA	OBD-CAD	3.31	1.28	1.22
30	A	819	CLA	C1B-NB	-3.31	1.32	1.35
30	B	820	CLA	CHD-C4C	3.31	1.46	1.39
38	3	308	KC1	CHC-C1C	3.31	1.46	1.39
38	4	310	KC1	C4B-NB	-3.31	1.33	1.37
30	B	816	CLA	OBD-CAD	3.31	1.28	1.22
38	16	311	KC1	C4B-NB	-3.31	1.33	1.37
39	3	316	DD6	C35-C34	3.30	1.57	1.52
37	16	312	A86	C19-C18	3.30	1.57	1.52
30	A	823	CLA	OBD-CAD	3.30	1.28	1.22
37	7	315	A86	C19-C18	3.30	1.57	1.52
30	A	827	CLA	C3D-C2D	3.30	1.48	1.39
39	3	316	DD6	O2-C18	3.30	1.53	1.43
39	5	313	DD6	O2-C18	3.30	1.53	1.43
39	9	314	DD6	C-C1	3.30	1.57	1.50
30	A	821	CLA	OBD-CAD	3.29	1.28	1.22
30	A	822	CLA	OBD-CAD	3.29	1.28	1.22
39	15	319	DD6	C-C1	3.29	1.57	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	12	315	DD6	O2-C18	3.29	1.53	1.43
30	B	822	CLA	OBD-CAD	3.29	1.28	1.22
30	A	824	CLA	C3D-C2D	3.28	1.48	1.39
30	F	201	CLA	CHD-C4C	3.28	1.46	1.39
38	11	312	KC1	CHC-C1C	3.28	1.46	1.39
39	9	314	DD6	O2-C18	3.28	1.53	1.43
30	4	311	CLA	CAA-C2A	3.28	1.60	1.54
38	8	307	KC1	C4B-NB	-3.28	1.33	1.37
30	4	305	CLA	OBD-CAD	3.28	1.28	1.22
37	2	318	A86	C5-C6	3.28	1.40	1.35
30	2	304	CLA	OBD-CAD	3.28	1.28	1.22
30	12	306	CLA	OBD-CAD	3.28	1.28	1.22
33	A	847	BCR	C1-C6	-3.28	1.49	1.53
30	12	310	CLA	OBD-CAD	3.28	1.28	1.22
30	A	828	CLA	CHD-C1D	3.28	1.44	1.38
39	4	316	DD6	O2-C18	3.28	1.53	1.43
37	9	315	A86	C25-C24	3.27	1.43	1.34
30	2	301	CLA	OBD-CAD	3.27	1.28	1.22
30	B	822	CLA	C3D-C2D	3.27	1.48	1.39
37	9	316	A86	C25-C24	3.27	1.43	1.34
38	6	311	KC1	CHC-C1C	3.27	1.46	1.39
38	3	304	KC1	C4B-NB	-3.27	1.33	1.37
39	6	318	DD6	O2-C18	3.27	1.53	1.43
38	16	304	KC1	C4B-NB	-3.27	1.33	1.37
39	3	313	DD6	O2-C18	3.27	1.53	1.43
37	10	301	A86	C2-C1	3.27	1.40	1.35
30	A	830	CLA	OBD-CAD	3.27	1.28	1.22
30	B	818	CLA	OBD-CAD	3.27	1.28	1.22
30	5	307	CLA	OBD-CAD	3.26	1.28	1.22
38	8	310	KC1	C4D-ND	3.26	1.38	1.35
30	B	801	CLA	CHD-C4C	3.26	1.46	1.39
37	4	317	A86	C5-C6	3.26	1.40	1.35
38	2	306	KC1	C4B-NB	-3.26	1.33	1.37
37	15	323	A86	C25-C24	3.26	1.43	1.34
30	12	321	CLA	OBD-CAD	3.26	1.28	1.22
39	7	314	DD6	O2-C18	3.26	1.53	1.43
38	11	305	KC1	C4B-NB	-3.26	1.33	1.37
39	3	313	DD6	C-C1	3.26	1.57	1.50
39	10	313	DD6	O2-C18	3.26	1.53	1.43
30	4	303	CLA	OBD-CAD	3.25	1.28	1.22
38	12	305	KC1	C4B-NB	-3.25	1.33	1.37
30	A	806	CLA	C3D-C2D	3.25	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	810	CLA	C3D-C2D	3.25	1.48	1.39
30	A	820	CLA	OBD-CAD	3.25	1.28	1.22
38	8	306	KC1	C4B-NB	-3.25	1.33	1.37
30	A	833	CLA	OBD-CAD	3.25	1.28	1.22
38	14	308	KC1	C4D-ND	3.25	1.38	1.35
38	13	310	KC1	C4B-NB	-3.25	1.33	1.37
30	B	813	CLA	OBD-CAD	3.25	1.28	1.22
39	7	302	DD6	O2-C18	3.25	1.53	1.43
39	6	321	DD6	O2-C18	3.25	1.53	1.43
37	7	319	A86	C25-C24	3.25	1.42	1.34
37	15	322	A86	C25-C24	3.25	1.42	1.34
38	3	308	KC1	C4B-NB	-3.24	1.33	1.37
30	B	801	CLA	C3D-C2D	3.24	1.48	1.39
39	2	315	DD6	O2-C18	3.24	1.53	1.43
37	2u	205	A86	C25-C24	3.24	1.42	1.34
38	9	312	KC1	C4B-NB	-3.24	1.33	1.37
30	16	310	CLA	OBD-CAD	3.24	1.28	1.22
39	16	313	DD6	C-C1	3.24	1.57	1.50
30	8	305	CLA	C3D-C2D	3.24	1.48	1.39
30	B	819	CLA	C3D-C2D	3.24	1.48	1.39
30	F	201	CLA	OBD-CAD	3.24	1.28	1.22
30	A	812	CLA	OBD-CAD	3.24	1.28	1.22
38	9	304	KC1	C4B-NB	-3.24	1.33	1.37
30	B	810	CLA	OBD-CAD	3.23	1.28	1.22
30	A	818	CLA	OBD-CAD	3.23	1.28	1.22
30	B	832	CLA	OBD-CAD	3.23	1.28	1.22
39	16	313	DD6	O2-C18	3.23	1.53	1.43
30	B	830	CLA	C3D-C2D	3.23	1.47	1.39
30	A	803	CLA	C1D-ND	3.23	1.41	1.37
38	11	312	KC1	C4B-NB	-3.23	1.33	1.37
30	A	804	CLA	OBD-CAD	3.23	1.28	1.22
38	5	305	KC1	C4B-NB	-3.23	1.33	1.37
30	7	306	CLA	OBD-CAD	3.22	1.28	1.22
30	B	821	CLA	OBD-CAD	3.22	1.28	1.22
30	9	308	CLA	OBD-CAD	3.22	1.28	1.22
39	7	302	DD6	C35-C34	3.22	1.57	1.52
30	A	831	CLA	OBD-CAD	3.22	1.28	1.22
38	4	307	KC1	C4B-NB	-3.22	1.33	1.37
30	A	825	CLA	OBD-CAD	3.21	1.28	1.22
33	2u	201	BCR	C1-C6	-3.21	1.49	1.53
30	B	821	CLA	C1B-NB	-3.21	1.32	1.35
37	14	317	A86	C19-C18	3.21	1.56	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	6	319	DD6	O2-C18	3.21	1.53	1.43
39	7	317	DD6	C-C1	3.21	1.57	1.50
37	13	315	A86	C25-C24	3.20	1.42	1.34
37	3	315	A86	C19-C18	3.20	1.56	1.52
30	B	811	CLA	OBD-CAD	3.20	1.28	1.22
33	J	103	BCR	C1-C6	-3.20	1.49	1.53
39	6	319	DD6	C-C1	3.20	1.57	1.50
37	14	320	A86	C25-C24	3.20	1.42	1.34
30	B	803	CLA	CHD-C4C	3.20	1.46	1.39
30	B	838	CLA	OBD-CAD	3.20	1.28	1.22
39	7	318	DD6	C-C1	3.20	1.57	1.50
39	2	315	DD6	C-C1	3.20	1.57	1.50
33	B	841	BCR	C1-C6	-3.20	1.49	1.53
39	12	317	DD6	C35-C34	3.19	1.57	1.52
38	12	313	KC1	C4B-NB	-3.19	1.33	1.37
38	13	311	KC1	C4A-C3A	3.19	1.50	1.44
39	13	314	DD6	C-C1	3.19	1.57	1.50
37	15	317	A86	C25-C24	3.19	1.42	1.34
30	B	803	CLA	OBD-CAD	3.19	1.28	1.22
37	11	316	A86	C25-C24	3.19	1.42	1.34
30	A	835	CLA	OBD-CAD	3.19	1.28	1.22
30	10	304	CLA	OBD-CAD	3.19	1.28	1.22
38	6	308	KC1	C4B-NB	-3.18	1.33	1.37
38	5	306	KC1	C4B-NB	-3.18	1.33	1.37
37	2u	203	A86	C19-C18	3.18	1.56	1.52
37	10	317	A86	C25-C24	3.18	1.42	1.34
37	4	314	A86	C25-C24	3.18	1.42	1.34
30	B	809	CLA	OBD-CAD	3.18	1.28	1.22
30	A	805	CLA	C1B-NB	-3.18	1.32	1.35
37	7	316	A86	C2-C1	3.18	1.40	1.35
30	B	801	CLA	OBD-CAD	3.18	1.28	1.22
38	9	310	KC1	C4B-NB	-3.18	1.33	1.37
30	A	841	CLA	OBD-CAD	3.17	1.27	1.22
39	12	315	DD6	C-C1	3.17	1.57	1.50
39	10	313	DD6	C9-C8	3.17	1.42	1.34
37	2	318	A86	C19-C18	3.17	1.56	1.52
39	1	310	DD6	C-C1	3.17	1.57	1.50
30	2	301	CLA	C1B-NB	-3.17	1.32	1.35
38	8	312	KC1	C4A-C3A	3.17	1.50	1.44
39	12	317	DD6	C-C1	3.17	1.57	1.50
30	A	828	CLA	CHD-C4C	3.17	1.46	1.39
37	11	301	A86	C5-C6	3.17	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	809	CLA	OBD-CAD	3.17	1.27	1.22
38	3	311	KC1	C4B-NB	-3.16	1.33	1.37
37	13	313	A86	C24-C1	3.16	1.52	1.45
38	5	310	KC1	C4B-NB	-3.16	1.33	1.37
39	8	317	DD6	O2-C18	3.16	1.52	1.43
39	4	316	DD6	C-C1	3.16	1.57	1.50
37	3	315	A86	C25-C24	3.16	1.42	1.34
39	8	317	DD6	C-C1	3.16	1.57	1.50
37	10	302	A86	C25-C24	3.15	1.42	1.34
38	11	307	KC1	C4B-NB	-3.15	1.33	1.37
38	10	310	KC1	C4B-NB	-3.15	1.33	1.37
30	B	827	CLA	OBD-CAD	3.15	1.27	1.22
39	13	314	DD6	C9-C8	3.15	1.42	1.34
37	12	316	A86	C19-C18	3.15	1.56	1.52
37	12	316	A86	C25-C24	3.15	1.42	1.34
38	8	312	KC1	C4B-NB	-3.15	1.33	1.37
39	6	303	DD6	C-C1	3.14	1.57	1.50
30	A	824	CLA	OBD-CAD	3.14	1.27	1.22
30	6	305	CLA	OBD-CAD	3.14	1.27	1.22
30	16	306	CLA	OBD-CAD	3.14	1.27	1.22
39	10	313	DD6	C-C1	3.14	1.57	1.50
37	11	316	A86	C19-C18	3.14	1.56	1.52
39	11	313	DD6	C-C1	3.14	1.57	1.50
30	B	830	CLA	CHD-C1D	3.13	1.44	1.38
37	5	301	A86	C25-C24	3.13	1.42	1.34
37	4	312	A86	C19-C18	3.13	1.56	1.52
37	14	318	A86	C25-C24	3.13	1.42	1.34
39	3	316	DD6	C-C1	3.13	1.57	1.50
37	15	315	A86	C25-C24	3.12	1.42	1.34
30	B	808	CLA	C3D-C2D	3.12	1.47	1.39
37	2u	203	A86	C5-C6	3.12	1.39	1.35
30	B	823	CLA	OBD-CAD	3.12	1.27	1.22
30	A	815	CLA	C1B-NB	-3.12	1.32	1.35
30	11	306	CLA	OBD-CAD	3.12	1.27	1.22
37	11	301	A86	C19-C18	3.12	1.56	1.52
38	1	308	KC1	C4B-NB	-3.11	1.34	1.37
30	7	309	CLA	OBD-CAD	3.11	1.27	1.22
30	B	807	CLA	OBD-CAD	3.11	1.27	1.22
39	10	314	DD6	C-C1	3.11	1.57	1.50
30	B	827	CLA	C1B-NB	-3.11	1.32	1.35
39	11	313	DD6	C35-C34	3.11	1.57	1.52
39	4	313	DD6	O2-C18	3.11	1.52	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	833	CLA	OBD-CAD	3.11	1.27	1.22
30	B	837	CLA	OBD-CAD	3.11	1.27	1.22
39	8	316	DD6	O2-C18	3.11	1.52	1.43
30	15	303	CLA	OBD-CAD	3.10	1.27	1.22
39	5	313	DD6	C-C1	3.10	1.57	1.50
37	15	316	A86	C25-C24	3.10	1.42	1.34
29	A	801	CL0	OBD-CAD	3.10	1.27	1.22
30	B	818	CLA	C1B-NB	-3.10	1.32	1.35
37	15	321	A86	C25-C24	3.10	1.42	1.34
30	8	305	CLA	C1B-NB	-3.10	1.32	1.35
33	J	102	BCR	C1-C6	-3.09	1.49	1.53
39	2	317	DD6	C-C1	3.09	1.57	1.50
39	6	321	DD6	C35-C34	3.09	1.57	1.52
30	8	304	CLA	OBD-CAD	3.09	1.27	1.22
33	B	841	BCR	C30-C25	-3.09	1.49	1.53
39	6	321	DD6	C-C1	3.09	1.57	1.50
30	B	828	CLA	C3D-C2D	3.09	1.47	1.39
37	15	315	A86	C19-C18	3.08	1.56	1.52
37	3	314	A86	C25-C24	3.08	1.42	1.34
38	4	308	KC1	C2A-C1A	3.08	1.54	1.44
37	14	314	A86	C25-C24	3.08	1.42	1.34
39	11	313	DD6	C9-C8	3.07	1.42	1.34
37	14	319	A86	C25-C24	3.07	1.42	1.34
30	B	819	CLA	C3D-C4D	-3.07	1.37	1.44
30	8	302	CLA	OBD-CAD	3.07	1.27	1.22
39	7	318	DD6	C35-C34	3.07	1.57	1.52
39	7	314	DD6	C-C1	3.07	1.57	1.50
39	4	313	DD6	C-C1	3.07	1.57	1.50
37	2	318	A86	C25-C24	3.06	1.42	1.34
39	5	314	DD6	C-C1	3.06	1.57	1.50
30	B	831	CLA	OBD-CAD	3.06	1.27	1.22
39	2	316	DD6	C-C1	3.06	1.57	1.50
30	A	819	CLA	OBD-CAD	3.06	1.27	1.22
39	7	314	DD6	C26-C27	-3.05	1.30	1.37
37	8	315	A86	C19-C18	3.05	1.56	1.52
38	14	311	KC1	C4B-NB	-3.05	1.34	1.37
39	10	314	DD6	C9-C8	3.05	1.42	1.34
30	12	307	CLA	C1B-NB	-3.05	1.32	1.35
37	16	312	A86	C25-C24	3.05	1.42	1.34
30	A	832	CLA	OBD-CAD	3.05	1.27	1.22
30	A	838	CLA	C1B-NB	-3.05	1.32	1.35
38	10	306	KC1	C4B-NB	-3.05	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	6	319	DD6	C9-C8	3.05	1.42	1.34
39	5	314	DD6	O2-C18	3.05	1.52	1.43
30	3	301	CLA	OBD-CAD	3.04	1.27	1.22
30	B	815	CLA	OBD-CAD	3.03	1.27	1.22
37	2	319	A86	C5-C6	3.03	1.39	1.35
30	A	824	CLA	C1B-NB	-3.03	1.32	1.35
39	2	316	DD6	O2-C18	3.03	1.52	1.43
39	8	316	DD6	C-C1	3.03	1.57	1.50
39	16	313	DD6	C9-C8	3.03	1.42	1.34
39	6	318	DD6	C-C1	3.03	1.57	1.50
30	A	807	CLA	OBD-CAD	3.03	1.27	1.22
39	4	316	DD6	C35-C34	3.03	1.57	1.52
37	11	301	A86	C25-C24	3.02	1.42	1.34
30	9	309	CLA	C1B-NB	-3.02	1.32	1.35
37	14	316	A86	C25-C24	3.02	1.42	1.34
33	B	845	BCR	C30-C25	-3.02	1.49	1.53
39	8	317	DD6	C35-C34	3.02	1.57	1.52
37	10	315	A86	C25-C24	3.02	1.42	1.34
30	8	304	CLA	C1B-NB	-3.02	1.32	1.35
37	14	301	A86	C25-C24	3.01	1.42	1.34
30	B	803	CLA	C1C-NC	-3.01	1.33	1.37
29	A	801	CL0	C1B-NB	-3.01	1.32	1.35
38	12	311	KC1	C4B-NB	-3.01	1.34	1.37
30	A	804	CLA	C1B-NB	-3.01	1.32	1.35
37	2	318	A86	C14-C15	3.00	1.58	1.52
37	9	316	A86	C14-C15	3.00	1.58	1.52
37	5	315	A86	C25-C24	3.00	1.42	1.34
39	9	314	DD6	C9-C8	3.00	1.42	1.34
30	B	833	CLA	C1B-NB	-3.00	1.32	1.35
30	6	307	CLA	C1B-NB	-3.00	1.32	1.35
37	5	316	A86	C25-C24	2.99	1.42	1.34
33	M	101	BCR	C1-C6	-2.99	1.49	1.53
38	9	311	KC1	C4B-NB	-2.99	1.34	1.37
39	3	312	DD6	C9-C8	2.99	1.42	1.34
30	9	308	CLA	C1B-NB	-2.99	1.32	1.35
37	15	315	A86	C14-C15	2.99	1.58	1.52
30	12	307	CLA	OBD-CAD	2.98	1.27	1.22
39	7	302	DD6	C9-C8	2.98	1.42	1.34
30	5	303	CLA	OBD-CAD	2.98	1.27	1.22
37	9	315	A86	O-C13	-2.98	1.17	1.23
30	4	301	CLA	OBD-CAD	2.98	1.27	1.22
37	15	315	A86	C24-C1	2.98	1.52	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	806	CLA	C1B-NB	-2.98	1.32	1.35
30	6	304	CLA	C1B-NB	-2.98	1.32	1.35
37	4	315	A86	C25-C24	2.98	1.42	1.34
38	6	312	KC1	C4B-NB	-2.98	1.34	1.37
38	13	308	KC1	C4B-NB	-2.98	1.34	1.37
39	6	303	DD6	C9-C8	2.97	1.42	1.34
37	12	314	A86	C25-C24	2.97	1.42	1.34
37	13	313	A86	C-C1	2.97	1.57	1.50
30	B	802	CLA	OBD-CAD	2.97	1.27	1.22
30	6	306	CLA	OBD-CAD	2.97	1.27	1.22
37	11	314	A86	C25-C24	2.97	1.42	1.34
37	9	313	A86	C14-C15	2.97	1.58	1.52
37	2	302	A86	C25-C24	2.96	1.42	1.34
39	2	317	DD6	C9-C8	2.96	1.42	1.34
39	5	313	DD6	C9-C8	2.96	1.42	1.34
39	13	314	DD6	C35-C34	2.96	1.57	1.52
39	2	315	DD6	C9-C8	2.96	1.42	1.34
30	4	311	CLA	C1B-NB	-2.96	1.32	1.35
37	4	317	A86	C25-C24	2.96	1.42	1.34
33	L	204	BCR	C30-C25	-2.95	1.49	1.53
30	B	806	CLA	C1B-NB	-2.95	1.32	1.35
30	B	806	CLA	OBD-CAD	2.95	1.27	1.22
30	A	814	CLA	C1B-NB	-2.95	1.32	1.35
37	9	313	A86	C5-C6	2.95	1.39	1.35
30	A	827	CLA	C1B-NB	-2.95	1.32	1.35
30	B	802	CLA	C1B-NB	-2.95	1.32	1.35
33	A	849	BCR	C1-C6	-2.95	1.49	1.53
37	11	315	A86	C25-C24	2.95	1.42	1.34
39	1	310	DD6	C35-C34	2.95	1.57	1.52
30	A	812	CLA	C1B-NB	-2.94	1.32	1.35
37	5	316	A86	C19-C18	2.94	1.56	1.52
37	2u	205	A86	C19-C18	2.94	1.56	1.52
30	A	828	CLA	C1C-NC	-2.94	1.33	1.37
30	B	825	CLA	C1B-NB	-2.94	1.32	1.35
37	6	320	A86	C25-C24	2.94	1.42	1.34
33	J	103	BCR	C30-C25	-2.94	1.49	1.53
37	9	315	A86	C14-C15	2.94	1.58	1.52
30	8	301	CLA	C4B-NB	-2.93	1.32	1.35
37	8	318	A86	O-C13	-2.93	1.17	1.23
37	9	315	A86	C24-C1	2.93	1.52	1.45
39	7	314	DD6	C35-C34	2.93	1.57	1.52
37	15	320	A86	C24-C1	2.93	1.52	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	3	313	DD6	C9-C8	2.93	1.42	1.34
39	12	317	DD6	C9-C8	2.93	1.42	1.34
37	7	315	A86	C25-C24	2.93	1.42	1.34
30	16	302	CLA	OBD-CAD	2.93	1.27	1.22
37	4	315	A86	C19-C18	2.93	1.56	1.52
37	2	319	A86	C19-C18	2.92	1.56	1.52
37	9	313	A86	C19-C18	2.92	1.56	1.52
37	14	316	A86	C19-C18	2.92	1.56	1.52
37	6	320	A86	O-C13	-2.92	1.17	1.23
30	B	838	CLA	C1B-NB	-2.92	1.32	1.35
30	B	805	CLA	C1B-NB	-2.92	1.32	1.35
33	A	850	BCR	C30-C25	-2.92	1.49	1.53
30	8	303	CLA	C1B-NB	-2.92	1.32	1.35
38	8	314	KC1	C2A-C1A	2.92	1.53	1.44
30	7	303	CLA	C1B-NB	-2.92	1.32	1.35
30	B	814	CLA	C1B-NB	-2.91	1.32	1.35
39	15	318	DD6	C9-C8	2.91	1.42	1.34
39	3	316	DD6	C9-C8	2.91	1.42	1.34
30	A	826	CLA	C1B-NB	-2.91	1.32	1.35
30	2	305	CLA	C1B-NB	-2.91	1.32	1.35
30	A	829	CLA	OBD-CAD	2.91	1.27	1.22
30	7	304	CLA	C1B-NB	-2.91	1.32	1.35
30	B	834	CLA	C4B-NB	-2.91	1.32	1.35
30	8	305	CLA	C3D-C4D	-2.90	1.37	1.44
39	15	319	DD6	C9-C8	2.90	1.42	1.34
30	B	836	CLA	C1B-NB	-2.90	1.32	1.35
39	10	313	DD6	C35-C34	2.90	1.57	1.52
37	15	323	A86	C24-C1	2.90	1.52	1.45
30	5	308	CLA	C1B-NB	-2.89	1.32	1.35
37	15	322	A86	C24-C1	2.89	1.52	1.45
37	8	315	A86	C5-C6	2.89	1.39	1.35
39	1	310	DD6	C9-C8	2.89	1.42	1.34
37	14	317	A86	C25-C24	2.89	1.42	1.34
39	4	313	DD6	C9-C8	2.88	1.42	1.34
38	13	312	KC1	C4B-NB	-2.88	1.34	1.37
39	4	316	DD6	C9-C8	2.88	1.42	1.34
30	6	309	CLA	C1B-NB	-2.88	1.32	1.35
37	16	314	A86	C14-C15	2.88	1.58	1.52
39	16	313	DD6	C35-C34	2.88	1.57	1.52
38	4	310	KC1	CHB-C4A	-2.88	1.32	1.39
37	9	316	A86	C24-C1	2.87	1.52	1.45
33	L	201	BCR	C1-C6	-2.87	1.49	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	1	309	A86	C25-C24	2.87	1.42	1.34
39	6	318	DD6	C9-C8	2.87	1.42	1.34
30	A	832	CLA	C1B-NB	-2.87	1.32	1.35
37	10	301	A86	C25-C24	2.87	1.42	1.34
33	A	847	BCR	C30-C25	-2.87	1.49	1.53
37	2u	203	A86	C25-C24	2.87	1.42	1.34
33	A	851	BCR	C30-C25	-2.87	1.49	1.53
30	A	840	CLA	OBD-CAD	2.87	1.27	1.22
37	16	314	A86	C25-C24	2.87	1.42	1.34
30	B	808	CLA	C1B-NB	-2.87	1.32	1.35
30	7	311	CLA	C1B-NB	-2.86	1.32	1.35
30	9	301	CLA	C1B-NB	-2.86	1.32	1.35
38	13	306	KC1	C4B-NB	-2.86	1.34	1.37
30	7	306	CLA	C1B-NB	-2.86	1.32	1.35
30	A	813	CLA	C1B-NB	-2.86	1.32	1.35
30	6	305	CLA	C1B-NB	-2.86	1.32	1.35
39	7	317	DD6	C26-C27	-2.85	1.31	1.37
39	12	315	DD6	C9-C8	2.85	1.41	1.34
39	3	313	DD6	C35-C34	2.85	1.57	1.52
39	7	317	DD6	C9-C8	2.85	1.41	1.34
39	8	317	DD6	C9-C8	2.85	1.41	1.34
33	A	851	BCR	C1-C6	-2.85	1.49	1.53
33	B	846	BCR	C30-C25	-2.85	1.49	1.53
39	8	316	DD6	C9-C8	2.85	1.41	1.34
30	B	834	CLA	C1B-NB	-2.85	1.32	1.35
38	4	308	KC1	C4A-C3A	2.85	1.50	1.44
30	A	821	CLA	C1B-NB	-2.84	1.32	1.35
30	B	822	CLA	C1B-NB	-2.84	1.32	1.35
30	B	828	CLA	C3D-C4D	-2.84	1.37	1.44
37	2	318	A86	O-C13	-2.84	1.17	1.23
39	7	314	DD6	C9-C8	2.84	1.41	1.34
33	A	848	BCR	C1-C6	-2.84	1.49	1.53
30	14	307	CLA	C4C-C3C	2.83	1.49	1.45
38	1	308	KC1	CHB-C4A	-2.83	1.32	1.39
38	9	312	KC1	C4A-C3A	2.82	1.50	1.44
38	14	306	KC1	C4C-C3C	2.82	1.49	1.45
30	4	303	CLA	C1B-NB	-2.82	1.32	1.35
37	10	317	A86	C24-C1	2.82	1.52	1.45
37	10	317	A86	C14-C15	2.81	1.58	1.52
30	B	839	CLA	C1B-NB	-2.81	1.32	1.35
38	13	312	KC1	C4A-C3A	2.81	1.50	1.44
37	15	316	A86	C24-C1	2.81	1.52	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	10	316	A86	C25-C24	2.81	1.41	1.34
30	A	829	CLA	C1B-NB	-2.81	1.32	1.35
30	A	811	CLA	C1B-NB	-2.81	1.32	1.35
38	14	308	KC1	C4C-C3C	2.80	1.49	1.45
37	14	315	A86	C25-C24	2.80	1.41	1.34
38	14	306	KC1	CHB-C4A	-2.80	1.32	1.39
30	A	803	CLA	C4B-NB	-2.80	1.32	1.35
38	16	311	KC1	C2A-C1A	2.80	1.53	1.44
30	A	840	CLA	C3D-C4D	-2.80	1.37	1.44
30	A	827	CLA	C3D-C4D	-2.80	1.37	1.44
37	15	322	A86	C-C1	2.80	1.56	1.50
30	9	303	CLA	C1B-NB	-2.80	1.32	1.35
38	16	304	KC1	C4A-C3A	2.80	1.50	1.44
30	A	842	CLA	C1B-NB	-2.79	1.32	1.35
37	13	315	A86	C24-C1	2.79	1.51	1.45
37	14	320	A86	C24-C1	2.79	1.51	1.45
38	6	308	KC1	CAA-C2A	2.79	1.55	1.46
39	5	314	DD6	C9-C8	2.79	1.41	1.34
37	7	316	A86	C5-C6	2.79	1.39	1.35
38	10	310	KC1	CHB-C4A	-2.79	1.32	1.39
30	A	836	CLA	C1B-NB	-2.78	1.32	1.35
37	15	317	A86	C24-C1	2.78	1.51	1.45
30	B	825	CLA	C3D-C4D	-2.78	1.37	1.44
39	12	315	DD6	C35-C34	2.78	1.57	1.52
33	B	843	BCR	C1-C6	-2.78	1.49	1.53
37	4	312	A86	C25-C24	2.78	1.41	1.34
30	F	201	CLA	C1B-NB	-2.78	1.32	1.35
30	5	302	CLA	C1B-NB	-2.78	1.32	1.35
30	B	824	CLA	C3D-C4D	-2.78	1.37	1.44
38	10	312	KC1	CHB-C4A	-2.78	1.32	1.39
39	5	313	DD6	C35-C34	2.78	1.57	1.52
30	A	808	CLA	C1B-NB	-2.78	1.32	1.35
30	A	810	CLA	C1B-NB	-2.78	1.32	1.35
30	A	843	CLA	C1B-NB	-2.78	1.32	1.35
39	12	317	DD6	C26-C27	-2.78	1.31	1.37
30	B	834	CLA	C3D-C4D	-2.77	1.37	1.44
38	11	312	KC1	C2A-C1A	2.77	1.53	1.44
37	4	317	A86	C14-C15	2.77	1.58	1.52
38	12	313	KC1	CAA-C2A	2.77	1.55	1.46
30	A	828	CLA	OBD-CAD	2.77	1.27	1.22
30	A	838	CLA	C3D-C4D	-2.77	1.37	1.44
39	9	314	DD6	C35-C34	2.77	1.57	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	L	205	BCR	C1-C6	-2.77	1.50	1.53
39	5	314	DD6	C26-C27	-2.77	1.31	1.37
30	A	807	CLA	C1B-NB	-2.76	1.32	1.35
37	9	315	A86	C-C1	2.76	1.56	1.50
37	14	320	A86	C-C1	2.76	1.56	1.50
30	A	839	CLA	C1B-NB	-2.76	1.32	1.35
37	9	313	A86	O-C13	-2.76	1.17	1.23
30	B	811	CLA	C3D-C4D	-2.76	1.37	1.44
38	5	306	KC1	CHB-C4A	-2.76	1.32	1.39
39	7	317	DD6	C35-C34	2.76	1.57	1.52
30	B	817	CLA	C1B-NB	-2.76	1.32	1.35
30	16	306	CLA	C1B-NB	-2.76	1.32	1.35
39	6	318	DD6	C35-C34	2.76	1.57	1.52
37	10	301	A86	C-C1	2.76	1.56	1.50
30	8	302	CLA	C4B-NB	-2.76	1.32	1.35
39	8	316	DD6	C35-C34	2.75	1.57	1.52
30	B	825	CLA	OBD-CAD	2.75	1.27	1.22
30	A	824	CLA	C3D-C4D	-2.75	1.38	1.44
37	4	315	A86	O-C13	-2.75	1.17	1.23
30	A	827	CLA	OBD-CAD	2.75	1.27	1.22
30	7	304	CLA	OBD-CAD	2.75	1.27	1.22
30	B	811	CLA	C1B-NB	-2.75	1.32	1.35
37	15	316	A86	C14-C15	2.75	1.58	1.52
30	A	822	CLA	C3D-C4D	-2.75	1.38	1.44
30	B	824	CLA	C1B-NB	-2.74	1.32	1.35
30	3	307	CLA	C4C-C3C	2.74	1.49	1.45
39	7	318	DD6	C9-C8	2.74	1.41	1.34
37	14	301	A86	C-C1	2.74	1.56	1.50
30	A	840	CLA	C1B-NB	-2.74	1.32	1.35
37	16	314	A86	O-C13	-2.74	1.17	1.23
36	14	321	LMG	O7-C8	-2.74	1.39	1.46
37	2u	205	A86	C24-C1	2.74	1.51	1.45
37	10	315	A86	C24-C1	2.73	1.51	1.45
38	1	306	KC1	C4B-NB	-2.73	1.34	1.37
37	4	317	A86	C19-C18	2.73	1.56	1.52
38	13	305	KC1	CAA-C2A	2.73	1.55	1.46
30	2	308	CLA	C1B-NB	-2.73	1.32	1.35
30	3	307	CLA	C4D-CHA	2.73	1.48	1.38
37	14	316	A86	C-C1	2.73	1.56	1.50
38	14	308	KC1	C4A-C3A	2.73	1.49	1.44
38	16	311	KC1	CHB-C4A	-2.73	1.33	1.39
39	2	316	DD6	C35-C34	2.73	1.56	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	6	308	KC1	CHB-C4A	-2.72	1.33	1.39
37	2	302	A86	C24-C1	2.72	1.51	1.45
37	10	315	A86	C-C1	2.72	1.56	1.50
37	7	316	A86	C19-C18	2.72	1.56	1.52
38	5	312	KC1	CHB-C4A	-2.72	1.33	1.39
30	15	306	CLA	C4D-CHA	2.72	1.48	1.38
37	7	315	A86	C24-C1	2.72	1.51	1.45
37	7	319	A86	C14-C15	2.72	1.58	1.52
30	A	828	CLA	C3D-C4D	-2.72	1.38	1.44
33	A	850	BCR	C1-C6	-2.72	1.50	1.53
37	15	317	A86	C-C1	2.72	1.56	1.50
38	14	311	KC1	C2A-C1A	2.72	1.53	1.44
39	2	316	DD6	C9-C8	2.72	1.41	1.34
37	15	323	A86	C-C1	2.72	1.56	1.50
30	8	305	CLA	C4B-NB	-2.72	1.32	1.35
38	14	306	KC1	C3B-C4B	2.71	1.51	1.46
37	13	315	A86	C-C1	2.71	1.56	1.50
38	3	308	KC1	C4A-C3A	2.71	1.49	1.44
37	3	314	A86	C24-C1	2.71	1.51	1.45
30	B	815	CLA	C4B-NB	-2.71	1.32	1.35
30	4	309	CLA	C4D-CHA	2.71	1.48	1.38
30	12	302	CLA	C1B-NB	-2.71	1.32	1.35
39	10	314	DD6	C35-C34	2.71	1.56	1.52
30	15	303	CLA	C4D-CHA	2.70	1.48	1.38
30	15	308	CLA	C4D-CHA	2.70	1.48	1.38
30	A	838	CLA	C4B-NB	-2.70	1.32	1.35
39	6	303	DD6	C26-C27	-2.70	1.31	1.37
38	8	313	KC1	CHB-C4A	-2.70	1.33	1.39
30	15	311	CLA	C4D-CHA	2.70	1.48	1.38
30	B	822	CLA	C3D-C4D	-2.70	1.38	1.44
37	3	315	A86	C24-C1	2.70	1.51	1.45
30	6	314	CLA	C1B-NB	-2.70	1.32	1.35
30	14	309	CLA	C4D-CHA	2.70	1.48	1.38
30	9	306	CLA	C4D-CHA	2.70	1.48	1.38
38	6	311	KC1	CHB-C4A	-2.70	1.33	1.39
38	6	308	KC1	C2A-C1A	2.70	1.52	1.44
39	8	316	DD6	C26-C27	-2.69	1.31	1.37
37	10	316	A86	C19-C18	2.69	1.56	1.52
38	9	310	KC1	CHB-C4A	-2.69	1.33	1.39
39	6	321	DD6	C26-C27	-2.69	1.31	1.37
38	14	311	KC1	C4A-C3A	2.69	1.49	1.44
37	7	319	A86	C24-C1	2.69	1.51	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	826	CLA	C1B-NB	-2.69	1.32	1.35
30	A	806	CLA	C3D-C4D	-2.69	1.38	1.44
37	9	313	A86	C25-C24	2.69	1.41	1.34
37	5	301	A86	C24-C1	2.69	1.51	1.45
30	B	813	CLA	C1B-NB	-2.69	1.32	1.35
37	10	301	A86	C24-C1	2.69	1.51	1.45
30	A	835	CLA	C3D-C4D	-2.69	1.38	1.44
37	15	320	A86	C-C1	2.69	1.56	1.50
38	14	308	KC1	C4B-NB	-2.69	1.34	1.37
30	1	305	CLA	C4D-CHA	2.68	1.47	1.38
37	7	315	A86	O-C13	-2.68	1.17	1.23
30	A	802	CLA	OBD-CAD	2.68	1.27	1.22
30	13	309	CLA	C4D-CHA	2.68	1.47	1.38
38	7	313	KC1	CHB-C4A	-2.68	1.33	1.39
30	A	829	CLA	C4B-NB	-2.68	1.32	1.35
30	2	303	CLA	C1B-NB	-2.68	1.32	1.35
30	8	308	CLA	C1B-NB	-2.68	1.32	1.35
38	2	314	KC1	CHB-C4A	-2.68	1.33	1.39
37	10	301	A86	O-C13	-2.68	1.17	1.23
38	12	309	KC1	C2A-C1A	2.68	1.52	1.44
30	6	315	CLA	C4D-CHA	2.68	1.47	1.38
37	15	320	A86	C14-C15	2.68	1.58	1.52
30	B	820	CLA	C4B-CHC	2.68	1.48	1.41
30	16	307	CLA	C4D-CHA	2.68	1.47	1.38
37	14	318	A86	C24-C1	2.68	1.51	1.45
30	A	814	CLA	C1C-NC	-2.68	1.33	1.37
37	4	317	A86	C-C1	2.68	1.56	1.50
30	B	835	CLA	C1B-NB	-2.68	1.32	1.35
38	5	310	KC1	CHB-C4A	-2.68	1.33	1.39
30	B	821	CLA	C3D-C4D	-2.68	1.38	1.44
38	16	304	KC1	CHB-C4A	-2.67	1.33	1.39
30	15	305	CLA	C4D-CHA	2.67	1.47	1.38
37	5	315	A86	C-C1	2.67	1.56	1.50
33	B	846	BCR	C1-C6	-2.67	1.50	1.53
39	7	318	DD6	C26-C27	-2.67	1.31	1.37
37	12	316	A86	C24-C1	2.67	1.51	1.45
38	8	307	KC1	CHB-C4A	-2.67	1.33	1.39
37	11	301	A86	O-C13	-2.67	1.17	1.23
37	10	301	A86	C5-C6	2.67	1.39	1.35
33	B	842	BCR	C1-C6	-2.67	1.50	1.53
36	F	205	LMG	C1-C2	2.67	1.60	1.52
38	13	310	KC1	C2A-C1A	2.67	1.52	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	835	CLA	C3D-C4D	-2.67	1.38	1.44
37	7	316	A86	O-C13	-2.66	1.17	1.23
30	11	309	CLA	C1B-NB	-2.66	1.32	1.35
30	B	837	CLA	C3D-C4D	-2.66	1.38	1.44
37	8	315	A86	C25-C24	2.66	1.41	1.34
29	A	801	CL0	C3D-C4D	-2.66	1.38	1.44
30	A	806	CLA	C4B-NB	-2.66	1.32	1.35
30	8	302	CLA	C1B-NB	-2.66	1.32	1.35
37	15	316	A86	C-C1	2.66	1.56	1.50
30	4	301	CLA	C1B-NB	-2.66	1.32	1.35
39	6	318	DD6	C26-C27	-2.66	1.31	1.37
37	2u	203	A86	O-C13	-2.66	1.17	1.23
30	A	842	CLA	C3D-C4D	-2.66	1.38	1.44
30	A	809	CLA	C1B-NB	-2.66	1.32	1.35
30	A	825	CLA	C4D-CHA	2.66	1.47	1.38
37	3	315	A86	C14-C15	2.66	1.57	1.52
30	1	301	CLA	C1B-NB	-2.66	1.32	1.35
38	4	307	KC1	CHB-C4A	-2.66	1.33	1.39
30	14	303	CLA	C4D-CHA	2.65	1.47	1.38
39	1	310	DD6	C26-C27	-2.65	1.31	1.37
38	13	305	KC1	C4B-NB	-2.65	1.34	1.37
38	14	306	KC1	C4A-C3A	2.65	1.49	1.44
30	3	306	CLA	C4D-CHA	2.65	1.47	1.38
37	14	318	A86	C-C1	2.65	1.56	1.50
37	4	315	A86	C-C1	2.65	1.56	1.50
30	15	309	CLA	C4D-CHA	2.65	1.47	1.38
38	16	311	KC1	C4A-C3A	2.65	1.49	1.44
30	A	838	CLA	C4D-CHA	2.65	1.47	1.38
30	16	310	CLA	O1D-CGD	2.65	1.27	1.21
30	B	803	CLA	C1B-NB	-2.65	1.32	1.35
30	7	312	CLA	C4D-CHA	2.65	1.47	1.38
38	11	307	KC1	C4A-C3A	2.65	1.49	1.44
30	A	819	CLA	C3D-C4D	-2.65	1.38	1.44
30	B	837	CLA	C1B-NB	-2.65	1.32	1.35
37	2	302	A86	C-C1	2.65	1.56	1.50
30	F	202	CLA	OBD-CAD	2.65	1.27	1.22
38	13	308	KC1	C4A-C3A	2.65	1.49	1.44
37	10	316	A86	C-C1	2.65	1.56	1.50
38	11	311	KC1	C4A-C3A	2.65	1.49	1.44
30	A	836	CLA	C4B-NB	-2.65	1.32	1.35
30	A	807	CLA	C3D-C4D	-2.65	1.38	1.44
30	A	831	CLA	C3D-C4D	-2.65	1.38	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	829	CLA	C3D-C4D	-2.65	1.38	1.44
30	8	305	CLA	OBD-CAD	2.65	1.27	1.22
30	3	301	CLA	C1B-NB	-2.65	1.32	1.35
30	6	310	CLA	C1B-NB	-2.65	1.32	1.35
30	B	823	CLA	C1B-NB	-2.64	1.32	1.35
30	6	314	CLA	C3D-C4D	-2.64	1.38	1.44
30	A	833	CLA	C1B-NB	-2.64	1.32	1.35
38	8	314	KC1	CHB-C4A	-2.64	1.33	1.39
30	9	305	CLA	C4D-CHA	2.64	1.47	1.38
30	14	312	CLA	C4D-CHA	2.64	1.47	1.38
30	B	813	CLA	C1C-NC	-2.64	1.33	1.37
30	3	302	CLA	C4D-CHA	2.64	1.47	1.38
37	3	315	A86	C-C1	2.64	1.56	1.50
30	B	817	CLA	C3D-C4D	-2.64	1.38	1.44
30	4	306	CLA	C1B-NB	-2.64	1.32	1.35
38	4	307	KC1	C4A-C3A	2.64	1.49	1.44
30	B	823	CLA	C4D-CHA	2.64	1.47	1.38
30	5	303	CLA	C1B-NB	-2.64	1.32	1.35
37	8	318	A86	C25-C24	2.64	1.41	1.34
37	3	314	A86	C-C1	2.63	1.56	1.50
30	A	817	CLA	C3D-C4D	-2.63	1.38	1.44
39	2	317	DD6	C26-C27	-2.63	1.31	1.37
30	B	838	CLA	C1C-NC	-2.63	1.33	1.37
30	B	815	CLA	C4D-CHA	2.63	1.47	1.38
39	13	314	DD6	C4-C5	2.63	1.51	1.43
30	2	313	CLA	C4D-CHA	2.63	1.47	1.38
30	12	321	CLA	C4D-CHA	2.63	1.47	1.38
39	3	313	DD6	C26-C27	-2.63	1.31	1.37
38	12	309	KC1	CHB-C4A	-2.63	1.33	1.39
30	B	812	CLA	C1B-NB	-2.63	1.32	1.35
30	A	841	CLA	C4D-CHA	2.63	1.47	1.38
30	16	305	CLA	C4D-CHA	2.63	1.47	1.38
37	15	321	A86	C-C1	2.63	1.56	1.50
37	7	319	A86	O-C13	-2.63	1.17	1.23
30	B	808	CLA	C3D-C4D	-2.63	1.38	1.44
30	12	303	CLA	C4D-CHA	2.63	1.47	1.38
30	A	820	CLA	C3D-C4D	-2.63	1.38	1.44
37	12	314	A86	C-C1	2.63	1.56	1.50
37	5	315	A86	C24-C1	2.63	1.51	1.45
30	8	304	CLA	C3D-C4D	-2.63	1.38	1.44
30	4	302	CLA	C4D-CHA	2.63	1.47	1.38
37	11	316	A86	C-C1	2.63	1.56	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	831	CLA	C4D-CHA	2.63	1.47	1.38
38	1	306	KC1	CHB-C4A	-2.63	1.33	1.39
37	2	319	A86	C25-C24	2.63	1.41	1.34
39	6	321	DD6	C9-C8	2.63	1.41	1.34
30	13	302	CLA	C4D-CHA	2.63	1.47	1.38
39	11	313	DD6	C26-C27	-2.63	1.31	1.37
30	B	838	CLA	C3D-C4D	-2.63	1.38	1.44
37	16	314	A86	C-C1	2.63	1.56	1.50
37	8	315	A86	O-C13	-2.62	1.17	1.23
39	5	313	DD6	C26-C27	-2.62	1.31	1.37
30	15	310	CLA	C4D-CHA	2.62	1.47	1.38
30	B	814	CLA	C3D-C4D	-2.62	1.38	1.44
30	8	303	CLA	C3D-C4D	-2.62	1.38	1.44
37	8	318	A86	C-C1	2.62	1.56	1.50
30	3	310	CLA	C4D-CHA	2.62	1.47	1.38
30	13	304	CLA	C4D-CHA	2.62	1.47	1.38
30	A	832	CLA	C3D-C4D	-2.62	1.38	1.44
30	A	826	CLA	C4D-CHA	2.62	1.47	1.38
30	13	307	CLA	C4D-CHA	2.62	1.47	1.38
37	14	317	A86	C24-C1	2.62	1.51	1.45
30	B	806	CLA	C3D-C4D	-2.62	1.38	1.44
30	6	310	CLA	C4D-CHA	2.62	1.47	1.38
30	A	837	CLA	C1B-NB	-2.62	1.32	1.35
38	8	312	KC1	C2A-C1A	2.62	1.52	1.44
30	12	302	CLA	C4B-NB	-2.62	1.32	1.35
30	14	310	CLA	C4D-CHA	2.61	1.47	1.38
37	8	318	A86	C14-C15	2.61	1.57	1.52
38	8	310	KC1	CHB-C4A	-2.61	1.33	1.39
30	4	301	CLA	C3D-C4D	-2.61	1.38	1.44
30	11	310	CLA	C4D-CHA	2.61	1.47	1.38
37	5	301	A86	C-C1	2.61	1.56	1.50
30	8	302	CLA	C3D-C4D	-2.61	1.38	1.44
38	3	311	KC1	CHB-C4A	-2.61	1.33	1.39
38	13	308	KC1	CHB-C4A	-2.61	1.33	1.39
30	A	825	CLA	C3D-C4D	-2.61	1.38	1.44
30	1	301	CLA	C4D-CHA	2.61	1.47	1.38
30	15	308	CLA	C4C-C3C	2.61	1.49	1.45
37	7	315	A86	C-C1	2.61	1.56	1.50
38	9	304	KC1	C4A-C3A	2.61	1.49	1.44
30	A	814	CLA	C4B-NB	-2.61	1.32	1.35
37	14	301	A86	C24-C1	2.61	1.51	1.45
37	10	316	A86	C14-C15	2.61	1.57	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	9	316	A86	C-C1	2.61	1.56	1.50
39	4	313	DD6	C35-C34	2.61	1.56	1.52
38	6	312	KC1	CHB-C4A	-2.61	1.33	1.39
30	A	837	CLA	C4D-CHA	2.61	1.47	1.38
30	15	304	CLA	C4D-CHA	2.61	1.47	1.38
30	F	203	CLA	C1B-NB	-2.61	1.32	1.35
30	2	304	CLA	C1B-NB	-2.61	1.32	1.35
30	12	303	CLA	C1B-NB	-2.61	1.32	1.35
38	12	311	KC1	CHB-C4A	-2.61	1.33	1.39
30	B	810	CLA	C3D-C4D	-2.60	1.38	1.44
37	4	314	A86	C24-C1	2.60	1.51	1.45
38	7	308	KC1	CHB-C4A	-2.60	1.33	1.39
37	12	316	A86	C-C1	2.60	1.56	1.50
30	4	311	CLA	C3D-C4D	-2.60	1.38	1.44
30	6	305	CLA	C3D-C4D	-2.60	1.38	1.44
38	12	309	KC1	C4A-C3A	2.60	1.49	1.44
30	5	311	CLA	C4D-CHA	2.60	1.47	1.38
37	10	302	A86	C24-C1	2.60	1.51	1.45
30	A	807	CLA	C4D-CHA	2.60	1.47	1.38
30	B	804	CLA	C4D-CHA	2.60	1.47	1.38
30	A	839	CLA	OBD-CAD	2.60	1.27	1.22
30	8	308	CLA	C4D-CHA	2.60	1.47	1.38
38	8	311	KC1	CHB-C4A	-2.60	1.33	1.39
30	B	833	CLA	C4D-CHA	2.60	1.47	1.38
37	10	302	A86	C-C1	2.60	1.56	1.50
37	12	314	A86	C24-C1	2.60	1.51	1.45
30	15	313	CLA	C4D-CHA	2.60	1.47	1.38
30	B	815	CLA	C1C-NC	-2.60	1.33	1.37
30	7	303	CLA	C3D-C4D	-2.60	1.38	1.44
30	1	304	CLA	C4D-CHA	2.60	1.47	1.38
30	16	309	CLA	C4D-CHA	2.60	1.47	1.38
37	4	314	A86	O-C13	-2.60	1.17	1.23
30	A	844	CLA	C4D-CHA	2.60	1.47	1.38
37	11	315	A86	C-C1	2.60	1.56	1.50
30	A	808	CLA	C3D-C4D	-2.60	1.38	1.44
37	4	315	A86	C14-C15	2.60	1.57	1.52
30	5	308	CLA	C4D-CHA	2.60	1.47	1.38
38	2	306	KC1	CHB-C4A	-2.60	1.33	1.39
30	15	307	CLA	C4D-CHA	2.60	1.47	1.38
30	2	301	CLA	C3D-C4D	-2.60	1.38	1.44
30	B	831	CLA	C3D-C4D	-2.60	1.38	1.44
30	A	828	CLA	C4D-CHA	2.60	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	7	307	CLA	C4D-CHA	2.60	1.47	1.38
30	9	307	CLA	C4D-CHA	2.60	1.47	1.38
38	11	312	KC1	C4A-C3A	2.59	1.49	1.44
30	7	304	CLA	C3D-C4D	-2.59	1.38	1.44
37	14	314	A86	C24-C1	2.59	1.51	1.45
38	7	308	KC1	C4A-C3A	2.59	1.49	1.44
30	11	308	CLA	C4D-CHA	2.59	1.47	1.38
30	6	316	CLA	C4D-CHA	2.59	1.47	1.38
38	13	312	KC1	C2A-C1A	2.59	1.52	1.44
30	B	820	CLA	C1C-C2C	2.59	1.49	1.44
30	6	306	CLA	C4D-CHA	2.59	1.47	1.38
37	2	302	A86	C14-C15	2.59	1.57	1.52
30	9	308	CLA	C4D-CHA	2.59	1.47	1.38
30	A	815	CLA	C4D-CHA	2.59	1.47	1.38
30	14	305	CLA	C4D-CHA	2.59	1.47	1.38
30	B	812	CLA	C4D-CHA	2.59	1.47	1.38
30	12	303	CLA	OBD-CAD	2.59	1.26	1.22
30	A	809	CLA	C4B-NB	-2.59	1.32	1.35
39	2	316	DD6	C26-C27	-2.59	1.31	1.37
30	B	807	CLA	C3D-C4D	-2.59	1.38	1.44
38	13	306	KC1	C4A-C3A	2.59	1.49	1.44
37	5	316	A86	C-C1	2.59	1.56	1.50
30	A	833	CLA	C3D-C4D	-2.59	1.38	1.44
30	16	301	CLA	C4D-CHA	2.59	1.47	1.38
30	A	821	CLA	C1C-NC	-2.59	1.33	1.37
37	14	315	A86	C-C1	2.59	1.56	1.50
30	A	815	CLA	C1C-NC	-2.59	1.33	1.37
30	A	809	CLA	C4D-CHA	2.59	1.47	1.38
38	1	306	KC1	C4A-C3A	2.59	1.49	1.44
30	16	308	CLA	C4D-CHA	2.58	1.47	1.38
37	11	301	A86	C-C1	2.58	1.56	1.50
30	8	309	CLA	C1B-NB	-2.58	1.32	1.35
30	5	303	CLA	C4D-CHA	2.58	1.47	1.38
39	3	316	DD6	C26-C27	-2.58	1.31	1.37
30	B	805	CLA	C4D-CHA	2.58	1.47	1.38
30	A	804	CLA	C1C-NC	-2.58	1.34	1.37
30	16	302	CLA	C4D-CHA	2.58	1.47	1.38
30	A	802	CLA	C3D-C4D	-2.58	1.38	1.44
30	16	310	CLA	C3D-C4D	-2.58	1.38	1.44
30	2	305	CLA	C4D-CHA	2.58	1.47	1.38
38	13	310	KC1	C4A-C3A	2.58	1.49	1.44
30	B	818	CLA	C4D-CHA	2.58	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	836	CLA	C4D-CHA	2.58	1.47	1.38
38	1	306	KC1	C3B-C4B	2.58	1.50	1.46
39	6	303	DD6	O1-C20	2.58	1.50	1.46
30	3	305	CLA	C4D-CHA	2.58	1.47	1.38
30	B	810	CLA	C1B-NB	-2.58	1.32	1.35
30	12	306	CLA	C1B-NB	-2.58	1.32	1.35
30	A	815	CLA	C3D-C4D	-2.58	1.38	1.44
30	A	820	CLA	C4D-CHA	2.58	1.47	1.38
30	8	309	CLA	C3D-C4D	-2.57	1.38	1.44
37	5	315	A86	C14-C15	2.57	1.57	1.52
30	10	307	CLA	C4D-CHA	2.57	1.47	1.38
30	4	303	CLA	C4C-C3C	2.57	1.49	1.45
30	3	309	CLA	C4D-CHA	2.57	1.47	1.38
30	10	303	CLA	C4D-CHA	2.57	1.47	1.38
30	B	816	CLA	C3D-C4D	-2.57	1.38	1.44
30	15	312	CLA	C4D-CHA	2.57	1.47	1.38
30	9	301	CLA	C4B-NB	-2.57	1.32	1.35
30	F	202	CLA	C4D-CHA	2.57	1.47	1.38
37	5	301	A86	C19-C18	2.57	1.56	1.52
37	11	316	A86	C24-C1	2.57	1.51	1.45
38	13	306	KC1	C2A-C1A	2.57	1.52	1.44
38	3	304	KC1	CHB-C4A	-2.57	1.33	1.39
30	B	836	CLA	C3D-C4D	-2.57	1.38	1.44
30	10	304	CLA	C4D-CHA	2.57	1.47	1.38
30	A	819	CLA	C4D-CHA	2.57	1.47	1.38
37	7	316	A86	C25-C24	2.57	1.41	1.34
37	2	318	A86	C24-C1	2.57	1.51	1.45
30	B	805	CLA	C4B-NB	-2.57	1.32	1.35
30	6	316	CLA	C1B-NB	-2.57	1.32	1.35
30	A	805	CLA	C4D-CHA	2.57	1.47	1.38
38	13	306	KC1	CHB-C4A	-2.57	1.33	1.39
38	11	305	KC1	CHB-C4A	-2.57	1.33	1.39
38	2	312	KC1	CHB-C4A	-2.57	1.33	1.39
30	2	310	CLA	C1B-NB	-2.57	1.32	1.35
37	13	315	A86	C14-C15	2.57	1.57	1.52
30	12	303	CLA	C3D-C4D	-2.57	1.38	1.44
38	14	306	KC1	C4B-NB	-2.57	1.34	1.37
30	B	813	CLA	C4D-CHA	2.57	1.47	1.38
30	12	308	CLA	C4D-CHA	2.57	1.47	1.38
37	10	317	A86	C-C1	2.57	1.56	1.50
30	2	304	CLA	C4D-CHA	2.57	1.47	1.38
30	B	804	CLA	C1B-NB	-2.56	1.32	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	801	CLA	C3D-C4D	-2.56	1.38	1.44
30	9	309	CLA	C3D-C4D	-2.56	1.38	1.44
30	12	312	CLA	C4D-CHA	2.56	1.47	1.38
30	A	816	CLA	C4D-CHA	2.56	1.47	1.38
30	B	807	CLA	C1B-NB	-2.56	1.32	1.35
37	7	316	A86	O4-C34	-2.56	1.40	1.46
30	3	303	CLA	C4D-CHA	2.56	1.47	1.38
30	6	309	CLA	C4D-CHA	2.56	1.47	1.38
30	10	308	CLA	C1B-NB	-2.56	1.32	1.35
30	16	306	CLA	C3D-C4D	-2.56	1.38	1.44
37	14	316	A86	C24-C1	2.56	1.51	1.45
30	4	311	CLA	C4D-CHA	2.56	1.47	1.38
37	5	301	A86	O-C13	-2.56	1.17	1.23
30	6	307	CLA	C4D-CHA	2.56	1.47	1.38
38	12	313	KC1	C2A-C1A	2.56	1.52	1.44
38	13	311	KC1	C2A-C1A	2.56	1.52	1.44
30	B	829	CLA	C3D-C4D	-2.56	1.38	1.44
37	14	319	A86	C-C1	2.56	1.56	1.50
30	13	303	CLA	C4D-CHA	2.56	1.47	1.38
30	12	306	CLA	C4D-CHA	2.56	1.47	1.38
30	J	101	CLA	C3D-C4D	-2.56	1.38	1.44
30	2	310	CLA	C4D-CHA	2.55	1.47	1.38
30	6	307	CLA	C3D-C4D	-2.55	1.38	1.44
30	6	317	CLA	C4D-CHA	2.55	1.47	1.38
37	4	315	A86	C24-C1	2.55	1.51	1.45
30	3	301	CLA	C4D-CHA	2.55	1.47	1.38
30	B	836	CLA	OBD-CAD	2.55	1.26	1.22
30	1	307	CLA	C4D-CHA	2.55	1.47	1.38
37	7	316	A86	C14-C15	2.55	1.57	1.52
30	A	813	CLA	C4D-CHA	2.55	1.47	1.38
30	7	311	CLA	C4D-CHA	2.55	1.47	1.38
38	16	304	KC1	C2A-C1A	2.55	1.52	1.44
37	9	316	A86	O-C13	-2.55	1.17	1.23
33	A	849	BCR	C30-C25	-2.55	1.50	1.53
33	2u	201	BCR	C30-C25	-2.55	1.50	1.53
30	2	308	CLA	C4D-CHA	2.55	1.47	1.38
30	F	203	CLA	C4D-CHA	2.55	1.47	1.38
30	J	101	CLA	C4D-CHA	2.55	1.47	1.38
30	4	306	CLA	C4D-CHA	2.55	1.47	1.38
38	13	311	KC1	C4B-NB	-2.55	1.34	1.37
37	14	317	A86	O-C13	-2.55	1.17	1.23
38	9	312	KC1	CAA-C2A	2.55	1.54	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	13	312	KC1	CAA-C2A	2.55	1.54	1.46
37	1	309	A86	C-C1	2.55	1.56	1.50
38	2	312	KC1	C4A-C3A	2.55	1.49	1.44
30	10	309	CLA	C4D-CHA	2.55	1.47	1.38
30	11	310	CLA	C4C-C3C	2.55	1.49	1.45
38	8	306	KC1	CHB-C4A	-2.54	1.33	1.39
38	12	311	KC1	CAA-C2A	2.54	1.54	1.46
37	3	315	A86	O-C13	-2.54	1.17	1.23
30	A	839	CLA	C3D-C4D	-2.54	1.38	1.44
37	11	301	A86	C24-C1	2.54	1.51	1.45
37	11	315	A86	C24-C1	2.54	1.51	1.45
30	B	838	CLA	C4D-CHA	2.54	1.47	1.38
30	1	303	CLA	C4D-CHA	2.54	1.47	1.38
30	15	312	CLA	C1B-NB	-2.54	1.32	1.35
30	A	832	CLA	C4D-CHA	2.54	1.47	1.38
30	B	809	CLA	C3D-C4D	-2.54	1.38	1.44
38	6	312	KC1	C4A-C3A	2.54	1.49	1.44
30	B	832	CLA	C3D-C4D	-2.54	1.38	1.44
30	A	810	CLA	C3D-C4D	-2.54	1.38	1.44
37	7	316	A86	C-C1	2.54	1.56	1.50
30	B	806	CLA	C4D-CHA	2.54	1.47	1.38
37	6	320	A86	O1-C15	2.54	1.50	1.45
30	9	303	CLA	C4D-CHA	2.54	1.47	1.38
30	7	306	CLA	C4D-CHA	2.54	1.47	1.38
30	4	305	CLA	C1B-NB	-2.54	1.32	1.35
30	3	302	CLA	C3D-C4D	-2.54	1.38	1.44
39	10	313	DD6	C26-C27	-2.54	1.31	1.37
30	12	304	CLA	C4D-CHA	2.54	1.47	1.38
39	6	303	DD6	C4-C5	2.53	1.51	1.43
30	15	305	CLA	C4C-C3C	2.53	1.49	1.45
38	16	304	KC1	C4C-C3C	2.53	1.49	1.45
38	12	305	KC1	CHB-C4A	-2.53	1.33	1.39
34	A	853	LHG	O7-C5	-2.53	1.40	1.46
30	A	814	CLA	C4D-CHA	2.53	1.47	1.38
38	13	305	KC1	CHB-C4A	-2.53	1.33	1.39
37	11	314	A86	C24-C1	2.53	1.51	1.45
30	2	309	CLA	C4D-CHA	2.53	1.47	1.38
37	11	315	A86	O-C13	-2.53	1.18	1.23
30	A	816	CLA	C1B-NB	-2.53	1.33	1.35
30	A	828	CLA	C1B-NB	-2.53	1.33	1.35
30	B	834	CLA	C4D-CHA	2.53	1.47	1.38
30	2u	202	CLA	C3D-C4D	-2.53	1.38	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	9	301	CLA	C1C-NC	-2.53	1.34	1.37
30	5	309	CLA	C4D-CHA	2.53	1.47	1.38
38	9	311	KC1	CHB-C4A	-2.53	1.33	1.39
30	A	810	CLA	C4D-CHA	2.53	1.47	1.38
30	B	801	CLA	C1C-NC	-2.53	1.34	1.37
38	6	313	KC1	CHB-C4A	-2.53	1.33	1.39
30	B	824	CLA	C4D-CHA	2.53	1.47	1.38
37	15	321	A86	C24-C1	2.53	1.51	1.45
30	A	812	CLA	C3D-C4D	-2.53	1.38	1.44
30	15	304	CLA	C4C-C3C	2.53	1.49	1.45
33	B	845	BCR	C1-C6	-2.53	1.50	1.53
39	9	314	DD6	C26-C27	-2.53	1.31	1.37
30	6	305	CLA	C4D-CHA	2.53	1.47	1.38
38	3	311	KC1	CAA-C2A	2.53	1.54	1.46
30	7	304	CLA	C4D-CHA	2.53	1.47	1.38
30	B	832	CLA	C1B-NB	-2.52	1.33	1.35
30	2	307	CLA	C4D-CHA	2.52	1.47	1.38
38	4	310	KC1	C2A-C1A	2.52	1.52	1.44
38	11	311	KC1	CHB-C4A	-2.52	1.33	1.39
39	7	302	DD6	C26-C27	-2.52	1.31	1.37
30	B	816	CLA	C4D-CHA	2.52	1.47	1.38
30	4	305	CLA	C4D-CHA	2.52	1.47	1.38
38	5	305	KC1	C4A-C3A	2.52	1.49	1.44
30	10	311	CLA	C4D-CHA	2.52	1.47	1.38
37	5	315	A86	O-C13	-2.52	1.18	1.23
30	7	307	CLA	C1B-NB	-2.52	1.33	1.35
30	B	836	CLA	C4D-CHA	2.52	1.47	1.38
30	B	808	CLA	C1C-NC	-2.52	1.34	1.37
37	2u	205	A86	O-C13	-2.52	1.18	1.23
37	12	314	A86	O-C13	-2.52	1.18	1.23
38	9	304	KC1	CHB-C4A	-2.52	1.33	1.39
30	5	307	CLA	C4D-CHA	2.52	1.47	1.38
37	15	322	A86	O-C13	-2.52	1.18	1.23
30	B	832	CLA	C4D-CHA	2.52	1.47	1.38
30	2	311	CLA	C4D-CHA	2.52	1.47	1.38
37	2	319	A86	C14-C15	2.52	1.57	1.52
38	4	308	KC1	CHB-C4A	-2.52	1.33	1.39
30	5	304	CLA	C4D-CHA	2.52	1.47	1.38
29	A	801	CL0	C4D-CHA	2.52	1.47	1.38
30	12	307	CLA	C3D-C4D	-2.52	1.38	1.44
30	B	813	CLA	C3D-C4D	-2.52	1.38	1.44
37	10	302	A86	O-C13	-2.52	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	10	315	A86	C14-C15	2.52	1.57	1.52
37	15	321	A86	C14-C15	2.52	1.57	1.52
38	13	310	KC1	CHB-C4A	-2.52	1.33	1.39
30	10	308	CLA	C4D-CHA	2.51	1.47	1.38
33	B	844	BCR	C1-C6	-2.51	1.50	1.53
37	4	317	A86	O-C13	-2.51	1.18	1.23
30	B	812	CLA	C4B-NB	-2.51	1.33	1.35
30	B	835	CLA	C4D-CHA	2.51	1.47	1.38
37	14	317	A86	C-C1	2.51	1.56	1.50
38	14	308	KC1	C2A-C1A	2.51	1.52	1.44
39	4	316	DD6	C26-C27	-2.51	1.31	1.37
30	B	825	CLA	C4D-CHA	2.51	1.47	1.38
30	15	314	CLA	C4D-CHA	2.51	1.47	1.38
30	A	813	CLA	C4B-NB	-2.51	1.33	1.35
38	2	306	KC1	C4A-C3A	2.51	1.49	1.44
37	6	320	A86	C-C1	2.51	1.56	1.50
37	6	320	A86	C24-C1	2.51	1.51	1.45
30	16	308	CLA	C4C-C3C	2.51	1.49	1.45
30	A	818	CLA	C1B-NB	-2.51	1.33	1.35
30	15	302	CLA	C4D-CHA	2.51	1.47	1.38
30	A	826	CLA	C4B-NB	-2.51	1.33	1.35
30	14	304	CLA	C4D-CHA	2.51	1.47	1.38
30	A	823	CLA	C3D-C4D	-2.51	1.38	1.44
30	B	830	CLA	C3D-C4D	-2.51	1.38	1.44
30	14	307	CLA	C4D-CHA	2.51	1.47	1.38
30	9	305	CLA	C1B-NB	-2.51	1.33	1.35
30	B	830	CLA	C4B-CHC	2.51	1.48	1.41
30	A	804	CLA	C3D-C4D	-2.51	1.38	1.44
30	A	809	CLA	C3D-C4D	-2.51	1.38	1.44
38	5	310	KC1	C4A-C3A	2.51	1.49	1.44
38	9	312	KC1	C4C-C3C	2.51	1.49	1.45
30	8	309	CLA	C4D-CHA	2.50	1.47	1.38
37	10	317	A86	O-C13	-2.50	1.18	1.23
37	10	302	A86	C14-C15	2.50	1.57	1.52
30	13	301	CLA	C4D-CHA	2.50	1.47	1.38
30	A	821	CLA	C3D-C4D	-2.50	1.38	1.44
37	14	320	A86	C14-C15	2.50	1.57	1.52
30	A	831	CLA	C1C-NC	-2.50	1.34	1.37
30	14	302	CLA	C4D-CHA	2.50	1.47	1.38
30	B	823	CLA	C3D-C4D	-2.50	1.38	1.44
30	A	840	CLA	C4D-CHA	2.50	1.47	1.38
37	11	314	A86	C14-C15	2.50	1.57	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	5	316	A86	C24-C1	2.50	1.51	1.45
38	3	304	KC1	C2A-C1A	2.50	1.52	1.44
38	10	310	KC1	C4A-C3A	2.50	1.49	1.44
30	7	310	CLA	C4D-CHA	2.50	1.47	1.38
30	A	833	CLA	C4D-CHA	2.50	1.47	1.38
30	7	309	CLA	C4D-CHA	2.50	1.47	1.38
30	8	304	CLA	C4D-CHA	2.50	1.47	1.38
30	B	839	CLA	C4B-CHC	2.50	1.47	1.41
30	2u	202	CLA	C4D-CHA	2.50	1.47	1.38
37	10	316	A86	O-C13	-2.50	1.18	1.23
38	5	305	KC1	CHB-C4A	-2.50	1.33	1.39
37	14	314	A86	O-C13	-2.50	1.18	1.23
37	5	316	A86	C14-C15	2.50	1.57	1.52
30	A	835	CLA	C4D-CHA	2.50	1.47	1.38
39	2	317	DD6	C4-C5	2.50	1.51	1.43
39	10	314	DD6	C26-C27	-2.50	1.31	1.37
30	6	304	CLA	C4D-CHA	2.50	1.47	1.38
38	3	304	KC1	C4A-C3A	2.50	1.49	1.44
33	L	201	BCR	C30-C25	-2.50	1.50	1.53
30	A	821	CLA	C4D-CHA	2.50	1.47	1.38
30	12	307	CLA	C4D-CHA	2.49	1.47	1.38
38	11	305	KC1	C4A-C3A	2.49	1.49	1.44
38	10	306	KC1	CHB-C4A	-2.49	1.33	1.39
38	6	313	KC1	C4A-C3A	2.49	1.49	1.44
36	A	856	LMG	O7-C8	-2.49	1.40	1.46
38	12	311	KC1	C2A-C1A	2.49	1.52	1.44
30	A	808	CLA	C4D-CHA	2.49	1.47	1.38
30	3	301	CLA	C3D-C4D	-2.49	1.38	1.44
30	15	302	CLA	C4B-CHC	2.49	1.47	1.41
39	6	319	DD6	C35-C34	2.49	1.56	1.52
38	12	305	KC1	C2A-C1A	2.49	1.52	1.44
30	B	821	CLA	C4D-CHA	2.49	1.47	1.38
37	1	309	A86	O-C13	-2.49	1.18	1.23
30	A	834	CLA	C4D-CHA	2.49	1.47	1.38
38	11	307	KC1	CHB-C4A	-2.49	1.33	1.39
37	12	316	A86	C14-C15	2.49	1.57	1.52
30	A	806	CLA	C1C-NC	-2.49	1.34	1.37
30	L	203	CLA	C3D-C4D	-2.49	1.38	1.44
30	9	301	CLA	C4D-CHA	2.49	1.47	1.38
30	4	304	CLA	C4D-CHA	2.49	1.47	1.38
38	14	308	KC1	CHB-C4A	-2.49	1.33	1.39
38	13	305	KC1	C2A-C1A	2.48	1.52	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	1	305	CLA	C4C-C3C	2.48	1.49	1.45
30	B	827	CLA	C3D-C4D	-2.48	1.38	1.44
30	B	851	CLA	C3D-C4D	-2.48	1.38	1.44
39	5	314	DD6	C35-C34	2.48	1.56	1.52
30	11	309	CLA	C3D-C4D	-2.48	1.38	1.44
37	11	314	A86	C-C1	2.48	1.56	1.50
30	8	308	CLA	C3D-C4D	-2.48	1.38	1.44
30	A	839	CLA	C4D-CHA	2.48	1.47	1.38
30	6	316	CLA	C3D-C4D	-2.48	1.38	1.44
30	16	310	CLA	C4D-CHA	2.48	1.47	1.38
30	A	836	CLA	C3D-C4D	-2.48	1.38	1.44
30	A	837	CLA	C3D-C4D	-2.48	1.38	1.44
30	9	302	CLA	C4D-CHA	2.48	1.47	1.38
30	4	303	CLA	C4D-CHA	2.48	1.47	1.38
30	A	818	CLA	C3D-C4D	-2.48	1.38	1.44
38	8	314	KC1	C4D-CHA	2.48	1.48	1.45
30	L	203	CLA	C4D-CHA	2.48	1.47	1.38
37	2	319	A86	O-C13	-2.48	1.18	1.23
30	B	818	CLA	C3D-C4D	-2.48	1.38	1.44
39	3	316	DD6	C4-C5	2.48	1.51	1.43
37	14	301	A86	C14-C15	2.48	1.57	1.52
30	13	307	CLA	C4B-CHC	2.48	1.47	1.41
30	A	822	CLA	C4D-CHA	2.48	1.47	1.38
30	A	843	CLA	C4D-CHA	2.48	1.47	1.38
37	4	317	A86	C24-C1	2.48	1.51	1.45
30	2	304	CLA	C3D-C4D	-2.48	1.38	1.44
36	14	321	LMG	C4-C3	2.48	1.58	1.52
37	14	316	A86	O-C13	-2.48	1.18	1.23
38	2	314	KC1	C4A-C3A	2.48	1.49	1.44
30	B	826	CLA	C3D-C4D	-2.48	1.38	1.44
30	B	839	CLA	C1C-C2C	2.48	1.49	1.44
30	B	837	CLA	C4D-CHA	2.48	1.47	1.38
30	5	302	CLA	C4D-CHA	2.48	1.47	1.38
39	15	319	DD6	C4-C5	2.47	1.51	1.43
30	F	201	CLA	C1C-NC	-2.47	1.34	1.37
30	A	819	CLA	C4B-CHC	2.47	1.47	1.41
30	A	803	CLA	C4D-CHA	2.47	1.47	1.38
30	A	807	CLA	C1C-NC	-2.47	1.34	1.37
30	4	301	CLA	C4D-CHA	2.47	1.47	1.38
30	B	805	CLA	C3D-C4D	-2.47	1.38	1.44
30	A	813	CLA	C3D-C4D	-2.47	1.38	1.44
30	B	831	CLA	C4D-CHA	2.47	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	835	CLA	C1B-NB	-2.47	1.33	1.35
30	A	811	CLA	C3D-C4D	-2.47	1.38	1.44
30	7	305	CLA	C4D-CHA	2.47	1.47	1.38
30	11	304	CLA	C4D-CHA	2.47	1.47	1.38
30	1	302	CLA	C1B-NB	-2.47	1.33	1.35
38	13	312	KC1	CHB-C4A	-2.47	1.33	1.39
30	1	302	CLA	C4D-CHA	2.47	1.47	1.38
30	B	809	CLA	C4D-CHA	2.47	1.47	1.38
38	8	310	KC1	C4A-C3A	2.47	1.49	1.44
37	15	323	A86	O-C13	-2.47	1.18	1.23
30	B	835	CLA	OBD-CAD	2.47	1.26	1.22
30	A	814	CLA	C3D-C4D	-2.47	1.38	1.44
30	5	302	CLA	C3D-C4D	-2.47	1.38	1.44
38	4	310	KC1	CAA-C2A	2.47	1.54	1.46
30	B	817	CLA	C4B-CHC	2.47	1.47	1.41
38	11	311	KC1	C2A-C1A	2.47	1.52	1.44
30	A	823	CLA	C4D-CHA	2.47	1.47	1.38
30	A	829	CLA	C4D-CHA	2.47	1.47	1.38
39	3	313	DD6	C4-C5	2.47	1.51	1.43
39	6	319	DD6	C4-C5	2.47	1.51	1.43
38	12	305	KC1	C4A-C3A	2.47	1.49	1.44
30	A	817	CLA	C1B-NB	-2.47	1.33	1.35
30	B	839	CLA	C3D-C4D	-2.47	1.38	1.44
30	B	810	CLA	C1C-C2C	2.46	1.49	1.44
30	F	202	CLA	C1B-NB	-2.46	1.33	1.35
39	15	318	DD6	C26-C27	-2.46	1.31	1.37
37	15	315	A86	C-C1	2.46	1.56	1.50
30	B	807	CLA	C4D-CHA	2.46	1.47	1.38
30	7	306	CLA	C1C-NC	-2.46	1.34	1.37
36	6	301	LMG	O7-C8	-2.46	1.40	1.46
30	F	202	CLA	C3D-C4D	-2.46	1.38	1.44
30	B	819	CLA	C1C-NC	-2.46	1.34	1.37
30	1	303	CLA	C1B-NB	-2.46	1.33	1.35
37	14	320	A86	O-C13	-2.46	1.18	1.23
30	10	305	CLA	C3D-C4D	-2.46	1.38	1.44
30	A	818	CLA	C4D-CHA	2.46	1.47	1.38
39	13	314	DD6	C26-C27	-2.46	1.31	1.37
39	16	313	DD6	C4-C5	2.46	1.51	1.43
30	B	831	CLA	C1B-NB	-2.46	1.33	1.35
36	8	321	LMG	C3-C2	2.46	1.58	1.52
30	B	827	CLA	C4D-CHA	2.46	1.47	1.38
30	A	811	CLA	C4D-CHA	2.46	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	10	308	CLA	C3D-C4D	-2.46	1.38	1.44
30	9	309	CLA	C4D-CHA	2.46	1.47	1.38
37	4	314	A86	C14-C15	2.46	1.57	1.52
38	7	308	KC1	C2A-C1A	2.46	1.52	1.44
38	13	308	KC1	C2A-C1A	2.46	1.52	1.44
37	12	316	A86	O-C13	-2.45	1.18	1.23
37	14	315	A86	O-C13	-2.45	1.18	1.23
30	B	834	CLA	OBD-CAD	2.45	1.26	1.22
30	A	842	CLA	C4D-CHA	2.45	1.47	1.38
30	B	851	CLA	C4D-CHA	2.45	1.47	1.38
37	2	318	A86	C-C1	2.45	1.55	1.50
30	B	829	CLA	C4D-CHA	2.45	1.47	1.38
38	14	311	KC1	CHB-C4A	-2.45	1.33	1.39
37	10	316	A86	C24-C1	2.45	1.51	1.45
30	2	308	CLA	C3D-C4D	-2.45	1.38	1.44
30	8	303	CLA	C4D-CHA	2.45	1.47	1.38
39	3	312	DD6	C26-C27	-2.45	1.31	1.37
30	5	303	CLA	C3D-C4D	-2.45	1.38	1.44
38	3	311	KC1	C4C-C3C	2.45	1.49	1.45
30	7	310	CLA	C1B-NB	-2.45	1.33	1.35
38	11	312	KC1	CHB-C4A	-2.45	1.33	1.39
30	A	834	CLA	C3D-C4D	-2.45	1.38	1.44
30	A	830	CLA	C4D-CHA	2.45	1.47	1.38
30	1	302	CLA	C3D-C4D	-2.45	1.38	1.44
30	9	302	CLA	C1B-NB	-2.45	1.33	1.35
30	A	830	CLA	C3D-C4D	-2.45	1.38	1.44
30	6	316	CLA	C4B-NB	-2.45	1.33	1.35
39	12	315	DD6	C26-C27	-2.45	1.31	1.37
37	3	314	A86	O-C13	-2.45	1.18	1.23
30	A	826	CLA	C3D-C4D	-2.45	1.38	1.44
38	4	308	KC1	C4D-CHA	2.45	1.48	1.45
37	8	315	A86	C-C1	2.45	1.55	1.50
30	6	306	CLA	C1B-NB	-2.45	1.33	1.35
37	2u	205	A86	C14-C15	2.45	1.57	1.52
37	14	319	A86	C24-C1	2.45	1.51	1.45
39	8	317	DD6	C26-C27	-2.45	1.31	1.37
30	16	302	CLA	C3D-C4D	-2.45	1.38	1.44
38	2	312	KC1	C2A-C1A	2.44	1.52	1.44
39	15	319	DD6	C35-C36	2.44	1.54	1.51
30	8	301	CLA	C4D-CHA	2.44	1.47	1.38
37	2	302	A86	O-C13	-2.44	1.18	1.23
30	B	812	CLA	C3D-C4D	-2.44	1.38	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	13	309	CLA	C4C-C3C	2.44	1.49	1.45
37	14	314	A86	C-C1	2.44	1.55	1.50
37	5	316	A86	O-C13	-2.44	1.18	1.23
30	B	808	CLA	C4D-CHA	2.44	1.47	1.38
39	4	313	DD6	C26-C27	-2.44	1.31	1.37
38	9	311	KC1	C4A-C3A	2.44	1.49	1.44
36	2u	204	LMG	C4-C3	2.44	1.58	1.52
30	12	307	CLA	C4B-CHC	2.44	1.47	1.41
37	4	312	A86	C-C1	2.44	1.55	1.50
30	A	816	CLA	C3D-C4D	-2.44	1.38	1.44
30	B	819	CLA	C4D-CHA	2.44	1.47	1.38
37	10	301	A86	C14-C15	2.44	1.57	1.52
38	2	314	KC1	CAA-C2A	2.44	1.54	1.46
39	5	313	DD6	C4-C5	2.44	1.51	1.43
30	6	314	CLA	C4D-CHA	2.44	1.47	1.38
39	11	313	DD6	C4-C5	2.44	1.51	1.43
37	16	312	A86	O-C13	-2.44	1.18	1.23
30	A	812	CLA	C4D-CHA	2.44	1.47	1.38
30	12	310	CLA	C4D-CHA	2.44	1.47	1.38
30	7	310	CLA	C3D-C4D	-2.44	1.38	1.44
30	12	310	CLA	C3D-C4D	-2.44	1.38	1.44
30	13	303	CLA	C4C-C3C	2.44	1.49	1.45
38	4	307	KC1	C2A-C1A	2.44	1.52	1.44
30	2	301	CLA	C4D-CHA	2.44	1.47	1.38
30	B	814	CLA	C1C-NC	-2.44	1.34	1.37
30	14	305	CLA	C1B-NB	-2.44	1.33	1.35
38	9	312	KC1	CHB-C4A	-2.44	1.33	1.39
30	3	302	CLA	OBD-CAD	2.44	1.26	1.22
37	14	318	A86	O-C13	-2.44	1.18	1.23
30	1	301	CLA	C3D-C4D	-2.44	1.38	1.44
37	2u	203	A86	C14-C15	2.44	1.57	1.52
30	4	304	CLA	C3D-C4D	-2.43	1.38	1.44
39	10	314	DD6	C4-C5	2.43	1.51	1.43
38	8	310	KC1	C2A-C1A	2.43	1.52	1.44
33	F	204	BCR	C1-C6	-2.43	1.50	1.53
39	4	313	DD6	C4-C5	2.43	1.51	1.43
39	6	318	DD6	C4-C5	2.43	1.51	1.43
30	A	817	CLA	C4D-CHA	2.43	1.47	1.38
30	15	311	CLA	C4B-CHC	2.43	1.47	1.41
38	8	314	KC1	C4A-C3A	2.43	1.49	1.44
30	16	306	CLA	C4D-CHA	2.43	1.47	1.38
30	2	308	CLA	C4B-CHC	2.43	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	B	844	BCR	C30-C25	-2.43	1.50	1.53
30	B	820	CLA	C3D-C4D	-2.43	1.38	1.44
30	B	820	CLA	C4D-CHA	2.43	1.47	1.38
30	A	825	CLA	C1B-NB	-2.43	1.33	1.35
30	8	302	CLA	C4D-CHA	2.43	1.47	1.38
38	6	312	KC1	CAA-C2A	2.43	1.54	1.46
30	6	304	CLA	C3D-C4D	-2.43	1.38	1.44
30	B	814	CLA	C4D-CHA	2.43	1.47	1.38
30	8	305	CLA	C4D-CHA	2.43	1.47	1.38
39	6	319	DD6	C26-C27	-2.43	1.31	1.37
30	10	305	CLA	C4D-CHA	2.43	1.47	1.38
39	4	316	DD6	C4-C5	2.43	1.51	1.43
34	2	320	LHG	O7-C5	-2.43	1.40	1.46
34	5	317	LHG	O7-C5	-2.43	1.40	1.46
30	8	301	CLA	C1C-C2C	2.43	1.49	1.44
36	B	849	LMG	C7-C8	2.43	1.58	1.50
30	B	825	CLA	C4B-CHC	2.43	1.47	1.41
30	16	307	CLA	C4C-C3C	2.43	1.49	1.45
30	14	309	CLA	C4C-C3C	2.43	1.49	1.45
30	15	309	CLA	C4C-C3C	2.43	1.49	1.45
30	8	304	CLA	C1C-NC	-2.42	1.34	1.37
39	15	319	DD6	C26-C27	-2.42	1.31	1.37
30	15	303	CLA	C4B-CHC	2.42	1.47	1.41
38	11	307	KC1	C2A-C1A	2.42	1.52	1.44
30	16	305	CLA	C1B-NB	-2.42	1.33	1.35
36	B	847	LMG	O7-C8	-2.42	1.40	1.46
38	6	312	KC1	C2A-C1A	2.42	1.52	1.44
38	10	312	KC1	C4A-C3A	2.42	1.49	1.44
30	6	309	CLA	C3D-C4D	-2.42	1.38	1.44
38	5	312	KC1	C4A-C3A	2.42	1.49	1.44
30	4	306	CLA	C3D-C4D	-2.42	1.38	1.44
30	7	311	CLA	C3D-C4D	-2.42	1.38	1.44
37	16	314	A86	C24-C1	2.42	1.51	1.45
30	B	830	CLA	C1B-NB	-2.42	1.33	1.35
38	10	310	KC1	C2A-C1A	2.42	1.52	1.44
30	11	306	CLA	C4B-CHC	2.42	1.47	1.41
30	11	309	CLA	C4D-CHA	2.42	1.47	1.38
30	15	310	CLA	C4C-C3C	2.42	1.49	1.45
37	11	316	A86	O-C13	-2.42	1.18	1.23
37	11	314	A86	O-C13	-2.42	1.18	1.23
39	11	313	DD6	O1-C20	2.42	1.49	1.46
30	2u	202	CLA	C1B-NB	-2.42	1.33	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	10	304	CLA	C3D-C4D	-2.42	1.38	1.44
30	13	301	CLA	C1C-C2C	2.42	1.49	1.44
30	3	306	CLA	C4B-CHC	2.42	1.47	1.41
38	1	306	KC1	C4C-C3C	2.42	1.49	1.45
37	15	320	A86	O-C13	-2.42	1.18	1.23
37	14	318	A86	C14-C15	2.42	1.57	1.52
30	7	305	CLA	C1B-NB	-2.42	1.33	1.35
39	16	313	DD6	C26-C27	-2.42	1.31	1.37
30	F	201	CLA	C4D-CHA	2.42	1.47	1.38
30	4	303	CLA	C3D-C4D	-2.42	1.38	1.44
38	3	311	KC1	C2A-C1A	2.42	1.52	1.44
30	10	307	CLA	C1B-NB	-2.42	1.33	1.35
30	A	804	CLA	C4D-CHA	2.42	1.47	1.38
38	11	307	KC1	C4C-C3C	2.42	1.49	1.45
39	10	313	DD6	C4-C5	2.42	1.50	1.43
30	A	842	CLA	C4B-CHC	2.42	1.47	1.41
30	A	827	CLA	C4D-CHA	2.42	1.47	1.38
30	9	303	CLA	C3D-C4D	-2.41	1.38	1.44
38	4	308	KC1	CAA-C2A	2.41	1.54	1.46
38	7	313	KC1	CAA-C2A	2.41	1.54	1.46
38	5	310	KC1	C2A-C1A	2.41	1.52	1.44
37	5	301	A86	C14-C15	2.41	1.57	1.52
30	11	306	CLA	C4D-CHA	2.41	1.47	1.38
30	J	101	CLA	C1B-NB	-2.41	1.33	1.35
30	4	302	CLA	C1B-NB	-2.41	1.33	1.35
30	8	305	CLA	C1C-NC	-2.41	1.34	1.37
30	2	313	CLA	C4B-CHC	2.41	1.47	1.41
30	1	304	CLA	C1C-C2C	2.41	1.49	1.44
30	12	302	CLA	C4D-CHA	2.41	1.47	1.38
30	A	803	CLA	C1C-NC	-2.41	1.34	1.37
37	10	315	A86	O-C13	-2.41	1.18	1.23
30	B	839	CLA	C4D-CHA	2.41	1.47	1.38
37	2	319	A86	C-C1	2.41	1.55	1.50
30	A	841	CLA	C3D-C4D	-2.41	1.38	1.44
30	A	838	CLA	OBD-CAD	2.41	1.26	1.22
30	11	306	CLA	C1C-C2C	2.41	1.49	1.44
30	1	304	CLA	C4B-CHC	2.41	1.47	1.41
38	8	306	KC1	C2A-C1A	2.41	1.52	1.44
38	3	308	KC1	C4C-C3C	2.41	1.49	1.45
30	B	813	CLA	C4B-NB	-2.41	1.33	1.35
39	3	312	DD6	O1-C20	2.41	1.49	1.46
30	15	302	CLA	C1C-C2C	2.41	1.49	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	843	CLA	C3D-C4D	-2.41	1.38	1.44
38	10	306	KC1	C4A-C3A	2.41	1.49	1.44
36	B	849	LMG	O1-C1	2.41	1.44	1.40
33	I	101	BCR	C1-C6	-2.41	1.50	1.53
37	14	319	A86	O-C13	-2.40	1.18	1.23
30	A	844	CLA	C3D-C4D	-2.40	1.38	1.44
38	3	308	KC1	C2A-C1A	2.40	1.52	1.44
30	16	309	CLA	C4C-C3C	2.40	1.49	1.45
38	13	305	KC1	C4C-C3C	2.40	1.49	1.45
33	B	843	BCR	C30-C25	-2.40	1.50	1.53
38	13	310	KC1	C1C-C2C	2.40	1.49	1.44
30	3	309	CLA	C4B-CHC	2.40	1.47	1.41
30	16	306	CLA	C4C-C3C	2.40	1.49	1.45
30	A	830	CLA	C1C-C2C	2.40	1.49	1.44
37	13	313	A86	O-C13	-2.40	1.18	1.23
39	10	313	DD6	C22-C16	-2.40	1.49	1.53
30	B	833	CLA	C4B-CHC	2.40	1.47	1.41
30	A	805	CLA	C3D-C4D	-2.40	1.38	1.44
38	6	311	KC1	C2A-C1A	2.40	1.51	1.44
30	15	313	CLA	C4B-CHC	2.40	1.47	1.41
30	A	823	CLA	C1B-NB	-2.40	1.33	1.35
38	6	311	KC1	C4A-C3A	2.40	1.49	1.44
30	7	309	CLA	C1B-NB	-2.40	1.33	1.35
30	B	810	CLA	C4B-CHC	2.39	1.47	1.41
30	A	828	CLA	C4B-NB	-2.39	1.33	1.35
30	B	829	CLA	C1B-NB	-2.39	1.33	1.35
30	14	304	CLA	C4B-CHC	2.39	1.47	1.41
30	15	308	CLA	C1C-C2C	2.39	1.49	1.44
30	F	203	CLA	C3D-C4D	-2.39	1.38	1.44
30	7	309	CLA	C3D-C4D	-2.39	1.38	1.44
38	8	311	KC1	C4A-C3A	2.39	1.49	1.44
38	16	311	KC1	C1C-C2C	2.39	1.49	1.44
38	5	312	KC1	C2A-C1A	2.39	1.51	1.44
30	3	306	CLA	C3D-C4D	-2.39	1.38	1.44
30	16	301	CLA	C4B-CHC	2.39	1.47	1.41
30	5	307	CLA	C1B-CHB	2.39	1.47	1.41
39	5	313	DD6	O1-C20	2.39	1.49	1.46
33	F	204	BCR	C30-C25	-2.39	1.50	1.53
37	3	314	A86	C14-C15	2.39	1.57	1.52
38	5	305	KC1	C2A-C1A	2.39	1.51	1.44
30	9	305	CLA	C3D-C4D	-2.39	1.38	1.44
30	16	301	CLA	C1C-C2C	2.39	1.49	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	830	CLA	C4B-CHC	2.39	1.47	1.41
30	16	303	CLA	C4D-CHA	2.39	1.46	1.38
37	11	315	A86	C14-C15	2.39	1.57	1.52
30	12	306	CLA	C3D-C4D	-2.39	1.38	1.44
30	7	310	CLA	C1C-C2C	2.39	1.49	1.44
30	4	304	CLA	C1B-NB	-2.39	1.33	1.35
37	4	312	A86	O-C13	-2.39	1.18	1.23
39	2	316	DD6	C4-C5	2.39	1.50	1.43
30	15	308	CLA	C4B-CHC	2.39	1.47	1.41
30	7	312	CLA	C4C-C3C	2.39	1.49	1.45
30	A	818	CLA	C4B-CHC	2.39	1.47	1.41
30	11	304	CLA	C4B-CHC	2.39	1.47	1.41
30	14	307	CLA	C4B-CHC	2.39	1.47	1.41
37	14	301	A86	O-C13	-2.39	1.18	1.23
37	15	317	A86	C14-C15	2.39	1.57	1.52
30	10	309	CLA	C4C-C3C	2.39	1.49	1.45
30	F	201	CLA	C3D-C4D	-2.39	1.38	1.44
30	A	805	CLA	C4B-CHC	2.38	1.47	1.41
30	11	306	CLA	C3D-C4D	-2.38	1.38	1.44
38	8	313	KC1	C4A-C3A	2.38	1.49	1.44
30	14	302	CLA	C3D-C4D	-2.38	1.38	1.44
30	14	302	CLA	C4B-CHC	2.38	1.47	1.41
39	6	321	DD6	C35-C36	2.38	1.54	1.51
30	A	802	CLA	C4D-CHA	2.38	1.46	1.38
38	1	308	KC1	CAA-C2A	2.38	1.53	1.46
30	B	810	CLA	C4D-CHA	2.38	1.46	1.38
39	7	302	DD6	C4-C5	2.38	1.50	1.43
30	15	302	CLA	C1B-NB	-2.38	1.33	1.35
30	12	302	CLA	C3D-C4D	-2.38	1.38	1.44
37	7	315	A86	O4-C34	-2.38	1.40	1.46
30	14	313	CLA	C4D-CHA	2.38	1.46	1.38
38	3	308	KC1	CHB-C4A	-2.38	1.33	1.39
30	16	306	CLA	C4B-CHC	2.38	1.47	1.41
30	B	803	CLA	C4D-CHA	2.38	1.46	1.38
37	14	315	A86	C14-C15	2.38	1.57	1.52
34	A	852	LHG	O7-C5	-2.38	1.40	1.46
39	3	312	DD6	C4-C5	2.38	1.50	1.43
30	15	306	CLA	C4C-C3C	2.38	1.49	1.45
29	A	801	CL0	C4B-NB	-2.38	1.33	1.35
37	11	316	A86	C14-C15	2.38	1.57	1.52
30	B	817	CLA	C4D-CHA	2.38	1.46	1.38
30	7	303	CLA	C4D-CHA	2.38	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	851	CLA	C1B-NB	-2.38	1.33	1.35
37	7	319	A86	C-C1	2.38	1.55	1.50
38	14	311	KC1	C1C-C2C	2.38	1.49	1.44
30	15	311	CLA	C4C-C3C	2.37	1.49	1.45
30	2	303	CLA	C3D-CAD	2.37	1.53	1.45
30	6	305	CLA	C4B-NB	-2.37	1.33	1.35
39	15	318	DD6	C4-C5	2.37	1.50	1.43
30	B	826	CLA	C4D-CHA	2.37	1.46	1.38
30	9	306	CLA	C4C-C3C	2.37	1.49	1.45
30	8	301	CLA	C1C-NC	-2.37	1.34	1.37
30	9	302	CLA	C1C-NC	-2.37	1.34	1.37
38	5	305	KC1	CAA-C2A	2.37	1.53	1.46
30	A	844	CLA	C4B-CHC	2.37	1.47	1.41
30	16	308	CLA	C4B-CHC	2.37	1.47	1.41
30	10	304	CLA	C1B-NB	-2.37	1.33	1.35
30	B	831	CLA	C1C-NC	-2.37	1.34	1.37
38	14	306	KC1	C2A-C1A	2.37	1.51	1.44
30	L	202	CLA	C4D-CHA	2.37	1.46	1.38
37	15	316	A86	O-C13	-2.37	1.18	1.23
30	15	313	CLA	C4C-C3C	2.37	1.49	1.45
30	F	201	CLA	C4B-CHC	2.37	1.47	1.41
30	B	801	CLA	C1B-NB	-2.37	1.33	1.35
30	10	303	CLA	C1B-NB	-2.37	1.33	1.35
38	10	306	KC1	C2A-C1A	2.37	1.51	1.44
30	16	307	CLA	C4B-CHC	2.37	1.47	1.41
30	8	301	CLA	C3D-C4D	-2.37	1.38	1.44
38	10	310	KC1	C4C-C3C	2.36	1.49	1.45
38	8	311	KC1	C2A-C1A	2.36	1.51	1.44
38	8	306	KC1	C4A-C3A	2.36	1.49	1.44
38	4	310	KC1	C4D-CHA	2.36	1.48	1.45
30	2	307	CLA	C1B-NB	-2.36	1.33	1.35
30	F	201	CLA	C1C-C2C	2.36	1.49	1.44
30	A	805	CLA	C1C-C2C	2.36	1.49	1.44
30	7	306	CLA	C3D-C4D	-2.36	1.38	1.44
30	1	303	CLA	C4B-CHC	2.36	1.47	1.41
30	15	302	CLA	C3D-C4D	-2.36	1.38	1.44
30	A	843	CLA	C1B-CHB	2.36	1.47	1.41
30	12	302	CLA	C1C-NC	-2.36	1.34	1.37
39	7	317	DD6	C4-C5	2.36	1.50	1.43
30	6	306	CLA	C3D-C4D	-2.36	1.38	1.44
38	3	304	KC1	CAA-C2A	2.36	1.53	1.46
38	8	311	KC1	CAA-C2A	2.36	1.53	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	837	CLA	C4B-CHC	2.36	1.47	1.41
30	7	312	CLA	C3D-C4D	-2.36	1.38	1.44
30	B	834	CLA	C4B-CHC	2.36	1.47	1.41
38	5	306	KC1	C4C-C3C	2.36	1.49	1.45
39	5	314	DD6	C29-C27	-2.36	1.38	1.42
39	2	315	DD6	C4-C5	2.36	1.50	1.43
30	F	202	CLA	C1B-CHB	2.36	1.47	1.41
30	8	308	CLA	C4B-CHC	2.36	1.47	1.41
30	1	305	CLA	C1B-NB	-2.36	1.33	1.35
30	16	303	CLA	C3D-C4D	-2.36	1.38	1.44
30	A	827	CLA	C4B-CHC	2.35	1.47	1.41
30	5	308	CLA	C3D-C4D	-2.35	1.38	1.44
30	12	304	CLA	C3D-C4D	-2.35	1.38	1.44
37	15	320	A86	C35-C34	2.35	1.56	1.51
37	16	312	A86	C24-C1	2.35	1.51	1.45
39	7	318	DD6	C4-C5	2.35	1.50	1.43
37	2u	203	A86	C24-C1	2.35	1.51	1.45
30	A	833	CLA	C4B-NB	-2.35	1.33	1.35
38	13	305	KC1	C4A-C3A	2.35	1.49	1.44
30	B	814	CLA	C4B-NB	-2.35	1.33	1.35
38	12	311	KC1	C4C-C3C	2.35	1.49	1.45
30	7	303	CLA	C1C-C2C	2.35	1.49	1.44
30	2	309	CLA	C1B-NB	-2.35	1.33	1.35
30	A	824	CLA	C4D-CHA	2.35	1.46	1.38
30	B	811	CLA	C4D-CHA	2.35	1.46	1.38
30	11	304	CLA	C3D-C4D	-2.35	1.38	1.44
38	11	312	KC1	C4C-C3C	2.35	1.49	1.45
37	14	314	A86	C14-C15	2.35	1.57	1.52
38	5	305	KC1	C4C-C3C	2.35	1.49	1.45
30	B	801	CLA	C4D-CHA	2.35	1.46	1.38
30	B	802	CLA	C4D-CHA	2.35	1.46	1.38
39	9	314	DD6	C4-C5	2.35	1.50	1.43
39	5	314	DD6	C22-C16	-2.35	1.49	1.53
30	8	301	CLA	C1B-NB	-2.35	1.33	1.35
30	A	808	CLA	C1C-C2C	2.35	1.49	1.44
30	1	307	CLA	C3D-C4D	-2.35	1.38	1.44
30	14	312	CLA	C4C-C3C	2.35	1.49	1.45
30	3	309	CLA	C1C-C2C	2.35	1.49	1.44
30	15	307	CLA	C4B-CHC	2.35	1.47	1.41
30	3	310	CLA	C3D-C4D	-2.34	1.38	1.44
30	J	101	CLA	C4B-CHC	2.34	1.47	1.41
30	B	822	CLA	C1C-NC	-2.34	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	L	202	CLA	C1B-NB	-2.34	1.33	1.35
38	9	312	KC1	C2A-C1A	2.34	1.51	1.44
30	2	310	CLA	C3D-C4D	-2.34	1.38	1.44
30	B	836	CLA	C4B-CHC	2.34	1.47	1.41
30	13	304	CLA	C4C-C3C	2.34	1.49	1.45
30	13	307	CLA	C4C-C3C	2.34	1.49	1.45
30	A	815	CLA	C4B-NB	-2.34	1.33	1.35
30	7	307	CLA	C3D-C4D	-2.34	1.38	1.44
30	A	820	CLA	C4C-C3C	2.34	1.49	1.45
30	2	307	CLA	C3D-C4D	-2.34	1.38	1.44
30	A	819	CLA	C1C-NC	-2.34	1.34	1.37
30	A	842	CLA	C1C-NC	-2.34	1.34	1.37
38	13	306	KC1	C4D-CHA	2.34	1.48	1.45
30	A	813	CLA	C1C-NC	-2.34	1.34	1.37
39	3	316	DD6	C35-C36	2.34	1.54	1.51
39	4	316	DD6	O1-C20	2.34	1.49	1.46
30	A	836	CLA	C1C-NC	-2.34	1.34	1.37
38	5	312	KC1	CAA-C2A	2.34	1.53	1.46
33	J	102	BCR	C30-C25	-2.34	1.50	1.53
38	8	310	KC1	CAA-C2A	2.34	1.53	1.46
38	13	305	KC1	C4D-CHA	2.34	1.48	1.45
30	7	303	CLA	C4B-CHC	2.34	1.47	1.41
30	13	301	CLA	C4B-CHC	2.34	1.47	1.41
30	B	815	CLA	C1B-NB	-2.34	1.33	1.35
30	16	303	CLA	C1C-C2C	2.34	1.49	1.44
30	A	811	CLA	C1C-NC	-2.34	1.34	1.37
29	A	801	CL0	C1C-NC	-2.34	1.34	1.37
30	2	311	CLA	C4B-CHC	2.34	1.47	1.41
30	11	310	CLA	C4B-CHC	2.34	1.47	1.41
30	A	823	CLA	C4B-NB	-2.34	1.33	1.35
30	B	832	CLA	C4B-NB	-2.34	1.33	1.35
37	7	315	A86	C14-C15	2.34	1.57	1.52
38	11	305	KC1	C4C-C3C	2.34	1.49	1.45
30	5	304	CLA	C1A-CHA	2.34	1.52	1.43
30	A	824	CLA	C4B-CHC	2.33	1.47	1.41
29	A	801	CL0	C1B-CHB	2.33	1.47	1.41
30	15	311	CLA	C1C-C2C	2.33	1.49	1.44
30	4	309	CLA	C4B-CHC	2.33	1.47	1.41
38	13	311	KC1	CHB-C4A	-2.33	1.33	1.39
30	2	309	CLA	C3D-C4D	-2.33	1.38	1.44
30	9	308	CLA	C3D-C4D	-2.33	1.38	1.44
39	6	319	DD6	C22-C16	-2.33	1.49	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	3	316	DD6	O1-C20	2.33	1.49	1.46
30	6	317	CLA	C4B-CHC	2.33	1.47	1.41
30	12	308	CLA	C4B-CHC	2.33	1.47	1.41
30	15	312	CLA	C3D-C4D	-2.33	1.38	1.44
30	3	307	CLA	C1C-NC	-2.33	1.34	1.37
39	7	302	DD6	C22-C16	-2.33	1.49	1.53
30	15	314	CLA	C1C-C2C	2.33	1.49	1.44
30	6	315	CLA	C4B-CHC	2.33	1.47	1.41
36	7	320	LMG	C4-C5	2.33	1.57	1.53
38	2	314	KC1	C2A-C1A	2.32	1.51	1.44
39	3	313	DD6	O1-C20	2.32	1.49	1.46
30	F	203	CLA	C4B-CHC	2.32	1.47	1.41
30	7	311	CLA	C4B-CHC	2.32	1.47	1.41
37	11	301	A86	C14-C15	2.32	1.57	1.52
30	2	313	CLA	C4C-C3C	2.32	1.49	1.45
30	11	308	CLA	C4B-CHC	2.32	1.47	1.41
30	10	309	CLA	C3D-C4D	-2.32	1.38	1.44
30	7	309	CLA	C1C-NC	-2.32	1.34	1.37
39	11	313	DD6	C35-C36	2.32	1.54	1.51
30	12	321	CLA	C4B-CHC	2.32	1.47	1.41
37	1	309	A86	C24-C1	2.32	1.50	1.45
30	13	301	CLA	C3D-C4D	-2.32	1.38	1.44
30	10	309	CLA	C4B-CHC	2.32	1.47	1.41
30	4	305	CLA	C3D-C4D	-2.32	1.38	1.44
30	A	835	CLA	C4B-NB	-2.32	1.33	1.35
38	13	312	KC1	C4C-C3C	2.32	1.49	1.45
30	14	313	CLA	C4B-CHC	2.32	1.47	1.41
30	1	305	CLA	C3D-C4D	-2.32	1.38	1.44
30	14	313	CLA	C3D-C4D	-2.32	1.38	1.44
30	B	802	CLA	C3D-C4D	-2.32	1.38	1.44
30	A	834	CLA	C1B-NB	-2.31	1.33	1.35
30	L	203	CLA	C1B-NB	-2.31	1.33	1.35
30	9	302	CLA	C4C-C3C	2.31	1.49	1.45
30	14	313	CLA	C1B-CHB	2.31	1.47	1.41
30	5	309	CLA	C3D-C4D	-2.31	1.39	1.44
37	15	321	A86	O-C13	-2.31	1.18	1.23
30	15	314	CLA	C4C-C3C	2.31	1.49	1.45
30	9	308	CLA	C4B-CHC	2.31	1.47	1.41
30	14	303	CLA	C4B-CHC	2.31	1.47	1.41
30	1	307	CLA	C1B-NB	-2.31	1.33	1.35
30	2	308	CLA	C1C-C2C	2.31	1.49	1.44
37	4	312	A86	C14-C15	2.31	1.57	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	5	311	CLA	C3D-C4D	-2.31	1.39	1.44
30	A	837	CLA	C4B-CHC	2.31	1.47	1.41
30	16	303	CLA	C4B-CHC	2.31	1.47	1.41
30	14	309	CLA	C4B-CHC	2.31	1.47	1.41
30	B	815	CLA	C3D-C4D	-2.31	1.39	1.44
30	14	312	CLA	C3D-C4D	-2.31	1.39	1.44
37	2u	203	A86	C-C1	2.31	1.55	1.50
30	13	302	CLA	C4B-CHC	2.31	1.47	1.41
30	14	310	CLA	C4B-CHC	2.31	1.47	1.41
30	10	303	CLA	C3D-C4D	-2.31	1.39	1.44
36	2u	204	LMG	C4-C5	2.31	1.57	1.53
38	13	308	KC1	C4C-C3C	2.31	1.49	1.45
30	12	312	CLA	C3D-C4D	-2.31	1.39	1.44
37	14	317	A86	C14-C15	2.31	1.57	1.52
30	14	304	CLA	C4C-C3C	2.31	1.49	1.45
30	12	306	CLA	C1C-NC	-2.31	1.34	1.37
30	15	305	CLA	C4B-CHC	2.31	1.47	1.41
30	15	309	CLA	C4B-CHC	2.31	1.47	1.41
30	13	303	CLA	C4B-CHC	2.31	1.47	1.41
30	L	202	CLA	C3D-C4D	-2.31	1.39	1.44
39	9	314	DD6	O1-C20	2.31	1.49	1.46
39	4	316	DD6	C22-C16	-2.31	1.49	1.53
39	15	318	DD6	C22-C16	-2.31	1.49	1.53
30	13	307	CLA	C1B-NB	-2.31	1.33	1.35
37	12	314	A86	C14-C15	2.31	1.57	1.52
30	14	310	CLA	C4C-C3C	2.30	1.49	1.45
37	15	323	A86	C14-C15	2.30	1.57	1.52
30	2	305	CLA	C3D-C4D	-2.30	1.39	1.44
30	10	308	CLA	C4B-CHC	2.30	1.47	1.41
30	13	309	CLA	C4B-CHC	2.30	1.47	1.41
30	B	836	CLA	C1C-NC	-2.30	1.34	1.37
39	6	318	DD6	C29-C27	-2.30	1.38	1.42
30	A	844	CLA	C4C-C3C	2.30	1.49	1.45
30	4	305	CLA	C4B-CHC	2.30	1.47	1.41
30	B	830	CLA	C4D-CHA	2.30	1.46	1.38
30	4	302	CLA	C3D-C4D	-2.30	1.39	1.44
39	7	314	DD6	C4-C5	2.30	1.50	1.43
30	1	302	CLA	C4B-CHC	2.30	1.47	1.41
37	9	313	A86	C-C1	2.30	1.55	1.50
36	8	320	LMG	O8-C9	-2.30	1.39	1.45
30	14	312	CLA	C4B-CHC	2.30	1.47	1.41
30	13	302	CLA	C1C-C2C	2.30	1.49	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	9	302	CLA	C3D-C4D	-2.30	1.39	1.44
37	13	313	A86	C14-C15	2.30	1.57	1.52
37	15	317	A86	O-C13	-2.30	1.18	1.23
30	6	316	CLA	C4C-C3C	2.30	1.49	1.45
30	9	307	CLA	C1C-C2C	2.30	1.49	1.44
38	8	312	KC1	C1C-C2C	2.30	1.49	1.44
30	13	302	CLA	C1B-CHB	2.30	1.47	1.41
30	B	832	CLA	C1C-NC	-2.30	1.34	1.37
30	7	307	CLA	C4B-CHC	2.30	1.47	1.41
30	3	303	CLA	C1B-NB	-2.30	1.33	1.35
30	10	311	CLA	C4B-CHC	2.30	1.47	1.41
30	11	310	CLA	C3D-C4D	-2.30	1.39	1.44
30	10	309	CLA	C1C-C2C	2.30	1.49	1.44
30	11	304	CLA	C1C-C2C	2.30	1.49	1.44
38	12	311	KC1	C3B-C4B	2.30	1.50	1.46
30	5	309	CLA	C4C-C3C	2.30	1.49	1.45
38	1	306	KC1	C2A-C1A	2.30	1.51	1.44
38	13	311	KC1	C1C-C2C	2.30	1.49	1.44
30	B	831	CLA	C4B-NB	-2.29	1.33	1.35
39	12	317	DD6	C4-C5	2.29	1.50	1.43
30	15	310	CLA	C1C-C2C	2.29	1.49	1.44
30	B	826	CLA	C1C-NC	-2.29	1.34	1.37
30	1	302	CLA	C1C-NC	-2.29	1.34	1.37
30	15	304	CLA	C4B-CHC	2.29	1.47	1.41
30	B	824	CLA	C4B-NB	-2.29	1.33	1.35
30	1	303	CLA	C1C-C2C	2.29	1.49	1.44
30	13	304	CLA	C4B-CHC	2.29	1.47	1.41
30	14	303	CLA	C4C-C3C	2.29	1.49	1.45
30	14	313	CLA	C1C-C2C	2.29	1.49	1.44
30	9	302	CLA	C4B-CHC	2.29	1.47	1.41
39	1	310	DD6	O1-C20	2.29	1.49	1.46
30	1	303	CLA	C3D-C4D	-2.29	1.39	1.44
38	4	310	KC1	C4A-C3A	2.29	1.49	1.44
30	5	302	CLA	C4B-CHC	2.29	1.47	1.41
33	B	842	BCR	C30-C25	-2.29	1.50	1.53
30	A	841	CLA	C4B-CHC	2.29	1.47	1.41
38	5	306	KC1	CAA-C2A	2.29	1.53	1.46
38	16	311	KC1	C4D-CHA	2.29	1.47	1.45
30	3	307	CLA	C4B-CHC	2.29	1.47	1.41
38	2	306	KC1	C2A-C1A	2.29	1.51	1.44
30	B	805	CLA	C1C-NC	-2.29	1.34	1.37
37	13	315	A86	O-C13	-2.28	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	2	309	CLA	C4B-CHC	2.28	1.47	1.41
30	6	317	CLA	C1C-C2C	2.28	1.49	1.44
30	B	828	CLA	C4D-CHA	2.28	1.46	1.38
30	B	833	CLA	C3D-C4D	-2.28	1.39	1.44
39	12	315	DD6	C4-C5	2.28	1.50	1.43
30	14	310	CLA	C1C-C2C	2.28	1.49	1.44
30	10	304	CLA	C4B-CHC	2.28	1.47	1.41
38	12	311	KC1	C4D-CHA	2.28	1.47	1.45
30	10	307	CLA	C1C-C2C	2.28	1.49	1.44
38	3	304	KC1	C4D-CHA	2.28	1.47	1.45
38	13	305	KC1	C3B-C4B	2.28	1.50	1.46
30	B	834	CLA	C1C-C2C	2.28	1.49	1.44
38	9	310	KC1	C4A-C3A	2.28	1.49	1.44
30	15	304	CLA	C3D-C4D	-2.28	1.39	1.44
37	2u	203	A86	O4-C34	-2.28	1.40	1.46
30	A	810	CLA	C1B-CHB	2.28	1.47	1.41
30	9	307	CLA	C4B-CHC	2.28	1.47	1.41
36	14	321	LMG	O4-C4	-2.28	1.37	1.43
39	8	316	DD6	C22-C16	-2.28	1.49	1.53
38	8	307	KC1	C2A-C1A	2.28	1.51	1.44
38	2	306	KC1	C4C-C3C	2.28	1.49	1.45
38	12	309	KC1	C4D-CHA	2.28	1.47	1.45
38	4	307	KC1	C4C-C3C	2.28	1.49	1.45
30	2	313	CLA	C1C-C2C	2.28	1.49	1.44
38	13	312	KC1	C1C-C2C	2.27	1.49	1.44
30	15	305	CLA	C1C-C2C	2.27	1.49	1.44
37	14	319	A86	C14-C15	2.27	1.57	1.52
38	10	306	KC1	CAA-C2A	2.27	1.53	1.46
30	A	826	CLA	C1C-NC	-2.27	1.34	1.37
39	10	314	DD6	O1-C20	2.27	1.49	1.46
30	8	309	CLA	C4C-C3C	2.27	1.49	1.45
30	12	321	CLA	C4C-C3C	2.27	1.49	1.45
38	2	312	KC1	C4C-C3C	2.27	1.49	1.45
30	3	305	CLA	C1B-NB	-2.27	1.33	1.35
37	4	314	A86	C-C1	2.27	1.55	1.50
30	1	304	CLA	C3D-C4D	-2.27	1.39	1.44
30	A	839	CLA	C1C-NC	-2.27	1.34	1.37
30	15	307	CLA	C4C-C3C	2.27	1.49	1.45
30	7	310	CLA	C4B-CHC	2.27	1.47	1.41
36	3	317	LMG	C1-C2	2.27	1.59	1.52
30	5	303	CLA	C4B-CHC	2.27	1.47	1.41
30	15	314	CLA	C4B-CHC	2.27	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	830	CLA	C4C-C3C	2.27	1.48	1.45
39	3	313	DD6	C22-C16	-2.27	1.49	1.53
37	15	315	A86	O-C13	-2.27	1.18	1.23
30	14	303	CLA	C1B-NB	-2.27	1.33	1.35
30	15	307	CLA	C1B-NB	-2.27	1.33	1.35
30	5	307	CLA	C3D-C4D	-2.27	1.39	1.44
30	14	304	CLA	C3D-C4D	-2.27	1.39	1.44
30	14	303	CLA	C1C-C2C	2.27	1.49	1.44
30	16	309	CLA	C3D-C4D	-2.27	1.39	1.44
30	A	806	CLA	C4D-CHA	2.27	1.46	1.38
38	10	310	KC1	C3B-C4B	2.27	1.50	1.46
30	11	308	CLA	C3D-C4D	-2.27	1.39	1.44
30	A	816	CLA	C1C-NC	-2.27	1.34	1.37
30	4	301	CLA	C1C-NC	-2.26	1.34	1.37
30	9	301	CLA	C4C-C3C	2.26	1.48	1.45
30	3	305	CLA	C4B-CHC	2.26	1.47	1.41
38	13	312	KC1	C4D-CHA	2.26	1.47	1.45
30	A	807	CLA	C4B-NB	-2.26	1.33	1.35
30	1	304	CLA	C1B-NB	-2.26	1.33	1.35
30	5	304	CLA	C1B-NB	-2.26	1.33	1.35
30	14	302	CLA	C1B-NB	-2.26	1.33	1.35
30	B	812	CLA	C4C-C3C	2.26	1.48	1.45
38	13	306	KC1	C4C-C3C	2.26	1.48	1.45
30	3	305	CLA	C3D-C4D	-2.26	1.39	1.44
30	A	829	CLA	C4B-CHC	2.26	1.47	1.41
30	1	301	CLA	C4C-C3C	2.26	1.48	1.45
30	B	807	CLA	C4B-NB	-2.26	1.33	1.35
38	1	308	KC1	C2A-C1A	2.26	1.51	1.44
30	13	303	CLA	C3D-C4D	-2.26	1.39	1.44
38	1	308	KC1	C4A-C3A	2.26	1.48	1.44
30	15	313	CLA	C3D-C4D	-2.26	1.39	1.44
30	B	815	CLA	C4C-C3C	2.26	1.48	1.45
30	6	307	CLA	C4C-C3C	2.26	1.48	1.45
30	10	305	CLA	C1B-CHB	2.26	1.47	1.41
30	B	822	CLA	C4D-CHA	2.26	1.46	1.38
38	2	312	KC1	CAA-C2A	2.26	1.53	1.46
30	4	301	CLA	C4B-NB	-2.26	1.33	1.35
38	11	305	KC1	C4D-CHA	2.26	1.47	1.45
30	B	801	CLA	C1B-CHB	2.26	1.47	1.41
30	12	310	CLA	C4B-CHC	2.26	1.47	1.41
39	4	316	DD6	C35-C36	2.25	1.54	1.51
30	6	310	CLA	C4B-CHC	2.25	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	811	CLA	C1B-CHB	2.25	1.47	1.41
30	A	842	CLA	C1C-C2C	2.25	1.48	1.44
30	14	302	CLA	C1C-C2C	2.25	1.48	1.44
30	2	303	CLA	C4D-CHA	2.25	1.46	1.38
39	12	315	DD6	O1-C20	2.25	1.49	1.46
30	15	309	CLA	C1C-C2C	2.25	1.48	1.44
30	4	309	CLA	C4C-C3C	2.25	1.48	1.45
39	8	317	DD6	C35-C36	2.25	1.54	1.51
30	13	301	CLA	C1B-CHB	2.25	1.47	1.41
38	13	306	KC1	C3B-C4B	2.25	1.50	1.46
30	12	310	CLA	C1C-C2C	2.25	1.48	1.44
30	2	309	CLA	C4C-C3C	2.25	1.48	1.45
39	12	317	DD6	C29-C27	-2.25	1.38	1.42
38	10	312	KC1	C2A-C1A	2.25	1.51	1.44
30	B	819	CLA	C4B-NB	-2.25	1.33	1.35
30	16	302	CLA	C4B-CHC	2.25	1.47	1.41
30	14	305	CLA	C4C-C3C	2.25	1.48	1.45
30	13	304	CLA	C1C-C2C	2.25	1.48	1.44
38	3	311	KC1	C4A-C3A	2.25	1.48	1.44
30	2	311	CLA	C3D-C4D	-2.25	1.39	1.44
38	9	310	KC1	C2A-C1A	2.25	1.51	1.44
37	16	312	A86	C14-C15	2.25	1.57	1.52
39	2	315	DD6	O1-C20	2.24	1.49	1.46
30	6	309	CLA	C4B-CHC	2.24	1.47	1.41
38	14	306	KC1	CAA-C2A	2.24	1.53	1.46
30	9	301	CLA	C3D-C4D	-2.24	1.39	1.44
30	9	306	CLA	C3D-C4D	-2.24	1.39	1.44
30	14	304	CLA	C1B-CHB	2.24	1.47	1.41
30	11	304	CLA	C4C-C3C	2.24	1.48	1.45
30	3	302	CLA	C1B-NB	-2.24	1.33	1.35
30	3	309	CLA	C3D-C4D	-2.24	1.39	1.44
30	12	308	CLA	C3D-C4D	-2.24	1.39	1.44
30	16	305	CLA	C4B-CHC	2.24	1.47	1.41
30	15	311	CLA	C1B-CHB	2.24	1.47	1.41
30	15	303	CLA	C1C-C2C	2.24	1.48	1.44
39	13	314	DD6	O1-C20	2.24	1.49	1.46
30	A	832	CLA	C4B-NB	-2.24	1.33	1.35
38	4	310	KC1	C4C-C3C	2.24	1.48	1.45
30	F	203	CLA	C1C-NC	-2.24	1.34	1.37
30	2	303	CLA	C1A-CHA	2.24	1.52	1.43
30	11	309	CLA	C4C-C3C	2.24	1.48	1.45
30	2	313	CLA	C3D-C4D	-2.24	1.39	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	13	304	CLA	C3D-C4D	-2.24	1.39	1.44
30	13	307	CLA	C1C-C2C	2.24	1.48	1.44
30	4	306	CLA	C4B-CHC	2.24	1.47	1.41
38	8	313	KC1	C2A-C1A	2.23	1.51	1.44
30	4	304	CLA	C4B-CHC	2.23	1.47	1.41
30	6	310	CLA	C3D-C4D	-2.23	1.39	1.44
30	B	802	CLA	C1C-C2C	2.23	1.48	1.44
39	8	316	DD6	C4-C5	2.23	1.50	1.43
30	16	302	CLA	C1B-CHB	2.23	1.47	1.41
30	15	310	CLA	C4B-CHC	2.23	1.47	1.41
30	16	310	CLA	C4B-CHC	2.23	1.47	1.41
30	B	824	CLA	C4C-C3C	2.23	1.48	1.45
38	13	306	KC1	CAA-C2A	2.23	1.53	1.46
30	B	810	CLA	C1C-NC	-2.23	1.34	1.37
30	A	804	CLA	C4B-CHC	2.23	1.47	1.41
38	5	306	KC1	C1C-C2C	2.23	1.48	1.44
30	3	309	CLA	C4C-C3C	2.23	1.48	1.45
39	6	303	DD6	C35-C36	2.23	1.54	1.51
30	B	824	CLA	C1C-NC	-2.23	1.34	1.37
30	B	835	CLA	C4B-CHC	2.23	1.47	1.41
30	8	308	CLA	C1C-C2C	2.23	1.48	1.44
39	10	313	DD6	C35-C36	2.23	1.54	1.51
30	2	311	CLA	C1B-NB	-2.23	1.33	1.35
30	10	307	CLA	C4B-CHC	2.23	1.47	1.41
37	16	312	A86	C-C1	2.23	1.55	1.50
30	6	315	CLA	C3D-C4D	-2.23	1.39	1.44
30	B	801	CLA	C4B-NB	-2.23	1.33	1.35
30	12	303	CLA	C4B-NB	-2.23	1.33	1.35
39	5	313	DD6	C22-C16	-2.23	1.49	1.53
30	B	821	CLA	C1C-NC	-2.23	1.34	1.37
30	A	821	CLA	C1B-CHB	2.23	1.47	1.41
30	10	304	CLA	C4C-C3C	2.23	1.48	1.45
38	3	304	KC1	C4C-C3C	2.23	1.48	1.45
37	10	302	A86	O4-C34	-2.23	1.41	1.46
38	5	306	KC1	C2A-C1A	2.23	1.51	1.44
30	4	303	CLA	C4B-CHC	2.23	1.47	1.41
30	F	202	CLA	C4B-CHC	2.23	1.47	1.41
36	8	320	LMG	O7-C8	-2.23	1.41	1.46
38	8	312	KC1	CAA-C2A	2.23	1.53	1.46
39	6	321	DD6	C29-C27	-2.22	1.38	1.42
30	A	807	CLA	C4B-CHC	2.22	1.47	1.41
30	A	833	CLA	C4B-CHC	2.22	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	6	305	CLA	C4B-CHC	2.22	1.47	1.41
30	16	309	CLA	C4B-CHC	2.22	1.47	1.41
30	5	302	CLA	C1C-C2C	2.22	1.48	1.44
30	3	303	CLA	C4B-CHC	2.22	1.47	1.41
30	2	311	CLA	C1C-C2C	2.22	1.48	1.44
38	10	306	KC1	C1C-C2C	2.22	1.48	1.44
30	16	307	CLA	C3D-C4D	-2.22	1.39	1.44
30	15	313	CLA	C1B-NB	-2.22	1.33	1.35
30	16	306	CLA	C1C-C2C	2.22	1.48	1.44
30	15	303	CLA	C4C-C3C	2.22	1.48	1.45
38	8	311	KC1	C4C-C3C	2.22	1.48	1.45
30	8	309	CLA	C4B-CHC	2.22	1.47	1.41
38	5	305	KC1	C1C-C2C	2.22	1.48	1.44
30	B	802	CLA	C4B-CHC	2.22	1.47	1.41
30	A	820	CLA	C4B-NB	-2.22	1.33	1.35
30	16	307	CLA	C1C-C2C	2.22	1.48	1.44
30	12	312	CLA	C4B-CHC	2.22	1.47	1.41
37	8	318	A86	C24-C1	2.22	1.50	1.45
30	B	834	CLA	C1C-NC	-2.22	1.34	1.37
30	5	309	CLA	C4B-CHC	2.22	1.47	1.41
30	10	304	CLA	C1B-CHB	2.22	1.47	1.41
30	L	203	CLA	C1B-CHB	2.22	1.47	1.41
39	8	317	DD6	C4-C5	2.22	1.50	1.43
30	14	307	CLA	C1C-C2C	2.22	1.48	1.44
30	11	308	CLA	C1B-NB	-2.22	1.33	1.35
30	2	309	CLA	C1C-C2C	2.22	1.48	1.44
30	B	804	CLA	C4B-CHC	2.22	1.47	1.41
30	12	310	CLA	C1B-CHB	2.22	1.47	1.41
30	2u	202	CLA	C4B-CHC	2.22	1.47	1.41
30	9	308	CLA	C1C-C2C	2.22	1.48	1.44
30	1	307	CLA	C4C-C3C	2.22	1.48	1.45
38	1	306	KC1	CAA-C2A	2.22	1.53	1.46
30	15	313	CLA	C1C-C2C	2.22	1.48	1.44
38	13	308	KC1	C4D-CHA	2.22	1.47	1.45
39	3	316	DD6	C22-C16	-2.22	1.49	1.53
30	A	812	CLA	C1C-NC	-2.22	1.34	1.37
30	15	304	CLA	C1B-NB	-2.22	1.33	1.35
30	B	806	CLA	C4B-CHC	2.22	1.47	1.41
37	14	316	A86	C14-C15	2.22	1.57	1.52
37	4	312	A86	C24-C1	2.21	1.50	1.45
30	4	309	CLA	C3D-C4D	-2.21	1.39	1.44
30	12	312	CLA	C1B-CHB	2.21	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	14	302	CLA	C4C-C3C	2.21	1.48	1.45
30	6	310	CLA	C4C-C3C	2.21	1.48	1.45
30	4	305	CLA	C1C-C2C	2.21	1.48	1.44
39	7	318	DD6	C29-C27	-2.21	1.38	1.42
30	A	839	CLA	C4B-CHC	2.21	1.47	1.41
30	10	303	CLA	C4B-CHC	2.21	1.47	1.41
30	13	303	CLA	C1B-CHB	2.21	1.47	1.41
30	A	844	CLA	C1C-C2C	2.21	1.48	1.44
30	13	309	CLA	C1C-C2C	2.21	1.48	1.44
30	7	306	CLA	C4C-C3C	2.21	1.48	1.45
30	A	819	CLA	C1C-C2C	2.21	1.48	1.44
37	8	318	A86	C35-C34	2.21	1.55	1.51
30	A	808	CLA	C4B-CHC	2.21	1.47	1.41
30	12	321	CLA	C1C-NC	-2.21	1.34	1.37
38	4	307	KC1	C4D-CHA	2.21	1.47	1.45
30	A	824	CLA	C1C-NC	-2.21	1.34	1.37
30	10	311	CLA	C3D-C4D	-2.21	1.39	1.44
30	B	822	CLA	C3A-C2A	-2.21	1.48	1.54
39	8	316	DD6	C29-C27	-2.21	1.38	1.42
30	A	825	CLA	C4C-C3C	2.21	1.48	1.45
30	1	304	CLA	C1B-CHB	2.21	1.47	1.41
30	A	829	CLA	C1C-NC	-2.21	1.34	1.37
30	5	304	CLA	C1C-C2C	2.21	1.48	1.44
30	A	822	CLA	C1C-NC	-2.21	1.34	1.37
30	A	838	CLA	C1C-NC	-2.21	1.34	1.37
30	6	306	CLA	C4B-CHC	2.21	1.47	1.41
38	16	311	KC1	C4C-C3C	2.21	1.48	1.45
39	6	321	DD6	C4-C5	2.21	1.50	1.43
30	B	831	CLA	C4B-CHC	2.21	1.47	1.41
30	F	202	CLA	C4B-NB	-2.21	1.33	1.35
38	14	308	KC1	C1C-C2C	2.21	1.48	1.44
38	11	311	KC1	C4C-C3C	2.21	1.48	1.45
38	13	311	KC1	C4C-C3C	2.21	1.48	1.45
30	B	803	CLA	C4B-NB	-2.21	1.33	1.35
30	B	830	CLA	C1C-C2C	2.21	1.48	1.44
30	A	826	CLA	C1B-CHB	2.20	1.47	1.41
30	14	307	CLA	C3D-C4D	-2.20	1.39	1.44
30	14	312	CLA	C1C-C2C	2.20	1.48	1.44
30	A	836	CLA	C4C-C3C	2.20	1.48	1.45
30	J	101	CLA	C4C-C3C	2.20	1.48	1.45
30	10	307	CLA	C3D-C4D	-2.20	1.39	1.44
30	8	301	CLA	C4B-CHC	2.20	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	12	304	CLA	C4B-CHC	2.20	1.47	1.41
30	B	817	CLA	C1C-NC	-2.20	1.34	1.37
30	F	202	CLA	C1C-C2C	2.20	1.48	1.44
38	8	312	KC1	C4C-C3C	2.20	1.48	1.45
30	7	305	CLA	C3D-C4D	-2.20	1.39	1.44
30	7	306	CLA	C4B-CHC	2.20	1.47	1.41
30	10	311	CLA	C1B-CHB	2.20	1.47	1.41
30	7	311	CLA	C4C-C3C	2.20	1.48	1.45
33	L	205	BCR	C30-C25	-2.20	1.50	1.53
39	6	319	DD6	O1-C20	2.20	1.49	1.46
30	4	302	CLA	C4B-CHC	2.20	1.47	1.41
30	14	305	CLA	C4B-CHC	2.20	1.47	1.41
38	5	310	KC1	C3B-C4B	2.20	1.50	1.46
30	B	825	CLA	C1C-NC	-2.20	1.34	1.37
30	2	307	CLA	C1C-NC	-2.20	1.34	1.37
37	16	314	A86	C35-C34	2.20	1.55	1.51
30	9	305	CLA	C1C-C2C	2.20	1.48	1.44
30	2	303	CLA	C4B-CHC	2.20	1.47	1.41
30	A	815	CLA	C4C-C3C	2.20	1.48	1.45
30	B	827	CLA	C1C-NC	-2.20	1.34	1.37
38	6	308	KC1	C4A-C3A	2.20	1.48	1.44
30	12	308	CLA	C1B-NB	-2.20	1.33	1.35
30	15	302	CLA	C4C-C3C	2.20	1.48	1.45
30	13	302	CLA	C3D-C4D	-2.20	1.39	1.44
30	7	312	CLA	C4B-CHC	2.20	1.47	1.41
30	12	308	CLA	C1B-CHB	2.20	1.47	1.41
30	8	309	CLA	C1C-NC	-2.20	1.34	1.37
30	5	307	CLA	C1B-NB	-2.20	1.33	1.35
30	A	840	CLA	C4B-CHC	2.20	1.47	1.41
30	16	310	CLA	C1C-C2C	2.20	1.48	1.44
39	7	314	DD6	C29-C27	-2.20	1.38	1.42
30	B	822	CLA	C4B-NB	-2.19	1.33	1.35
30	5	304	CLA	C4B-CHC	2.19	1.47	1.41
30	13	309	CLA	C1B-CHB	2.19	1.47	1.41
30	11	308	CLA	C4C-C3C	2.19	1.48	1.45
36	7	320	LMG	O1-C7	-2.19	1.39	1.43
30	B	828	CLA	C1C-NC	-2.19	1.34	1.37
30	B	809	CLA	C1B-CHB	2.19	1.47	1.41
30	14	309	CLA	C3D-C4D	-2.19	1.39	1.44
38	12	305	KC1	C4C-C3C	2.19	1.48	1.45
30	16	302	CLA	C1C-C2C	2.19	1.48	1.44
30	2	304	CLA	C1C-C2C	2.19	1.48	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	2	305	CLA	C4C-C3C	2.19	1.48	1.45
30	15	304	CLA	C1C-C2C	2.19	1.48	1.44
30	B	820	CLA	C1B-CHB	2.19	1.47	1.41
39	9	314	DD6	C22-C16	-2.19	1.49	1.53
30	3	302	CLA	C1C-C2C	2.19	1.48	1.44
30	A	810	CLA	C1C-NC	-2.19	1.34	1.37
30	6	317	CLA	C3D-C4D	-2.19	1.39	1.44
39	8	317	DD6	C22-C16	-2.19	1.49	1.53
30	15	312	CLA	C1C-C2C	2.19	1.48	1.44
30	A	825	CLA	C1C-NC	-2.19	1.34	1.37
30	3	307	CLA	C1B-NB	-2.19	1.33	1.35
30	A	808	CLA	C1C-NC	-2.19	1.34	1.37
38	9	304	KC1	C2A-C1A	2.19	1.51	1.44
37	11	301	A86	O4-C34	-2.19	1.41	1.46
30	B	851	CLA	C4B-CHC	2.19	1.47	1.41
30	14	305	CLA	C3D-C4D	-2.18	1.39	1.44
30	B	829	CLA	C4B-CHC	2.18	1.47	1.41
30	13	307	CLA	C3D-C4D	-2.18	1.39	1.44
39	2	315	DD6	C35-C36	2.18	1.54	1.51
30	16	301	CLA	C1B-NB	-2.18	1.33	1.35
30	A	837	CLA	C4C-C3C	2.18	1.48	1.45
30	16	305	CLA	C3D-C4D	-2.18	1.39	1.44
30	1	305	CLA	C4B-CHC	2.18	1.47	1.41
30	B	826	CLA	C4B-NB	-2.18	1.33	1.35
30	5	307	CLA	C1A-CHA	2.18	1.52	1.43
39	2	317	DD6	C41-C32	-2.18	1.49	1.53
30	12	308	CLA	C1C-C2C	2.18	1.48	1.44
30	16	309	CLA	C1C-C2C	2.18	1.48	1.44
30	9	303	CLA	C4B-CHC	2.18	1.47	1.41
30	B	816	CLA	C1C-NC	-2.18	1.34	1.37
30	9	306	CLA	C4B-CHC	2.18	1.47	1.41
30	8	303	CLA	C1C-NC	-2.18	1.34	1.37
30	16	310	CLA	C1B-CHB	2.18	1.47	1.41
30	B	804	CLA	C3D-C4D	-2.18	1.39	1.44
37	14	315	A86	C24-C1	2.18	1.50	1.45
33	M	101	BCR	C30-C25	-2.18	1.50	1.53
30	13	309	CLA	C3D-C4D	-2.18	1.39	1.44
38	7	313	KC1	C2A-C1A	2.18	1.51	1.44
30	11	306	CLA	C1B-NB	-2.18	1.33	1.35
30	A	824	CLA	C1C-C2C	2.18	1.48	1.44
30	14	304	CLA	C1C-C2C	2.18	1.48	1.44
30	9	307	CLA	C1B-NB	-2.18	1.33	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	15	309	CLA	C3D-C4D	-2.18	1.39	1.44
30	16	309	CLA	C1B-CHB	2.18	1.47	1.41
38	2	306	KC1	C4D-CHA	2.18	1.47	1.45
30	B	823	CLA	C4B-CHC	2.18	1.47	1.41
30	3	302	CLA	C1B-CHB	2.18	1.47	1.41
30	5	311	CLA	C1B-CHB	2.18	1.47	1.41
30	B	828	CLA	C4C-C3C	2.18	1.48	1.45
30	12	307	CLA	C1C-C2C	2.18	1.48	1.44
33	A	847	BCR	C33-C5	-2.18	1.47	1.50
30	4	301	CLA	C4B-CHC	2.18	1.47	1.41
30	A	832	CLA	C1C-NC	-2.18	1.34	1.37
30	L	203	CLA	C4B-CHC	2.18	1.47	1.41
30	B	807	CLA	C1B-CHB	2.17	1.47	1.41
30	2	301	CLA	C1B-CHB	2.17	1.47	1.41
30	5	311	CLA	C4C-C3C	2.17	1.48	1.45
39	1	310	DD6	C4-C5	2.17	1.50	1.43
30	9	305	CLA	C4B-CHC	2.17	1.47	1.41
38	4	307	KC1	CAA-C2A	2.17	1.53	1.46
30	1	307	CLA	C4B-CHC	2.17	1.47	1.41
30	L	202	CLA	C4B-CHC	2.17	1.47	1.41
39	6	318	DD6	C22-C16	-2.17	1.49	1.53
38	9	310	KC1	C1C-C2C	2.17	1.48	1.44
38	12	313	KC1	C1C-C2C	2.17	1.48	1.44
38	10	306	KC1	C4D-CHA	2.17	1.47	1.45
38	11	307	KC1	CAA-C2A	2.17	1.53	1.46
30	10	309	CLA	C1B-CHB	2.17	1.47	1.41
30	3	307	CLA	C3D-C4D	-2.17	1.39	1.44
30	8	305	CLA	C4B-CHC	2.17	1.47	1.41
30	2	303	CLA	C4C-C3C	2.17	1.48	1.45
30	2	301	CLA	C1C-NC	-2.17	1.34	1.37
38	11	311	KC1	C1C-C2C	2.17	1.48	1.44
37	8	315	A86	O4-C34	-2.17	1.41	1.46
39	3	312	DD6	C35-C36	2.17	1.54	1.51
30	16	307	CLA	C1B-CHB	2.17	1.47	1.41
30	15	306	CLA	C4B-CHC	2.17	1.47	1.41
38	16	304	KC1	C1D-CHD	2.17	1.47	1.41
30	14	305	CLA	C1C-C2C	2.17	1.48	1.44
30	B	805	CLA	C4C-C3C	2.17	1.48	1.45
30	L	203	CLA	C1C-NC	-2.17	1.34	1.37
37	13	313	A86	C35-C34	2.16	1.55	1.52
38	8	312	KC1	CHB-C4A	-2.16	1.34	1.39
30	B	813	CLA	C4C-C3C	2.16	1.48	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	6	306	CLA	C1C-C2C	2.16	1.48	1.44
30	11	309	CLA	C4B-CHC	2.16	1.47	1.41
37	2	302	A86	C35-C34	2.16	1.55	1.51
30	15	306	CLA	C1B-CHB	2.16	1.47	1.41
30	2u	202	CLA	C1B-CHB	2.16	1.47	1.41
30	5	307	CLA	C1C-C2C	2.16	1.48	1.44
30	B	824	CLA	C4B-CHC	2.16	1.47	1.41
38	12	311	KC1	C4A-C3A	2.16	1.48	1.44
30	B	809	CLA	C1C-NC	-2.16	1.34	1.37
30	16	302	CLA	C1B-NB	-2.16	1.33	1.35
30	9	307	CLA	C3D-C4D	-2.16	1.39	1.44
30	16	301	CLA	C3D-C4D	-2.16	1.39	1.44
30	12	312	CLA	C4C-C3C	2.16	1.48	1.45
37	9	315	A86	C35-C34	2.16	1.55	1.51
30	B	807	CLA	C1C-C2C	2.16	1.48	1.44
30	6	315	CLA	C1C-C2C	2.16	1.48	1.44
30	10	304	CLA	C1C-C2C	2.16	1.48	1.44
37	11	314	A86	C35-C34	2.16	1.55	1.51
37	15	321	A86	O4-C34	-2.16	1.41	1.46
30	6	304	CLA	C4B-CHC	2.16	1.47	1.41
30	14	309	CLA	C1B-CHB	2.16	1.47	1.41
37	14	315	A86	O4-C34	-2.16	1.41	1.46
30	L	203	CLA	C4B-NB	-2.16	1.33	1.35
30	7	312	CLA	C1B-NB	-2.16	1.33	1.35
30	A	812	CLA	C4B-CHC	2.16	1.47	1.41
30	15	312	CLA	C4C-C3C	2.16	1.48	1.45
30	B	816	CLA	C1B-NB	-2.16	1.33	1.35
30	A	803	CLA	C4B-CHC	2.16	1.47	1.41
30	A	817	CLA	C4B-CHC	2.16	1.47	1.41
30	12	303	CLA	C4B-CHC	2.16	1.47	1.41
30	15	307	CLA	C1C-C2C	2.16	1.48	1.44
39	7	302	DD6	C35-C36	2.16	1.54	1.51
36	2u	204	LMG	O7-C8	-2.16	1.41	1.46
39	2	316	DD6	C22-C16	-2.16	1.49	1.53
30	14	313	CLA	C4C-C3C	2.16	1.48	1.45
30	16	305	CLA	C1C-NC	-2.16	1.34	1.37
30	A	840	CLA	C1C-C2C	2.16	1.48	1.44
30	9	303	CLA	C4B-NB	-2.16	1.33	1.35
30	12	321	CLA	C1B-NB	-2.16	1.33	1.35
38	11	305	KC1	C2A-C1A	2.16	1.51	1.44
39	5	314	DD6	O1-C20	2.16	1.49	1.46
30	3	303	CLA	C4C-C3C	2.16	1.48	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	6	319	DD6	C29-C27	-2.16	1.38	1.42
30	12	302	CLA	C1C-C2C	2.15	1.48	1.44
30	A	817	CLA	C1B-CHB	2.15	1.47	1.41
30	9	302	CLA	C4B-NB	-2.15	1.33	1.35
30	12	310	CLA	C1B-NB	-2.15	1.33	1.35
30	5	311	CLA	C4B-CHC	2.15	1.47	1.41
36	7	320	LMG	O8-C9	-2.15	1.40	1.45
30	6	315	CLA	C1B-CHB	2.15	1.47	1.41
30	3	306	CLA	C1C-C2C	2.15	1.48	1.44
39	1	310	DD6	C35-C36	2.15	1.54	1.51
30	A	841	CLA	C4B-NB	-2.15	1.33	1.35
38	2	314	KC1	C4C-C3C	2.15	1.48	1.45
30	F	203	CLA	C1C-C2C	2.15	1.48	1.44
30	3	301	CLA	C1C-NC	-2.15	1.34	1.37
39	6	303	DD6	C22-C16	-2.15	1.49	1.53
30	A	834	CLA	C4B-CHC	2.15	1.47	1.41
30	11	310	CLA	C1C-C2C	2.15	1.48	1.44
38	8	307	KC1	C4A-C3A	2.15	1.48	1.44
30	B	851	CLA	C1C-NC	-2.15	1.34	1.37
30	13	302	CLA	C4C-C3C	2.15	1.48	1.45
30	B	835	CLA	C1C-NC	-2.15	1.34	1.37
38	10	312	KC1	CAA-C2A	2.15	1.53	1.46
30	A	818	CLA	C1C-NC	-2.15	1.34	1.37
30	16	302	CLA	C4C-C3C	2.15	1.48	1.45
30	12	321	CLA	C3D-C4D	-2.15	1.39	1.44
30	15	303	CLA	C3D-C4D	-2.15	1.39	1.44
30	A	840	CLA	C1C-NC	-2.15	1.34	1.37
30	B	822	CLA	C4B-CHC	2.15	1.47	1.41
38	8	307	KC1	C1C-C2C	2.15	1.48	1.44
30	8	302	CLA	C1C-NC	-2.15	1.34	1.37
30	4	311	CLA	C4B-CHC	2.15	1.47	1.41
30	A	831	CLA	C4B-NB	-2.15	1.33	1.35
37	2	319	A86	O4-C34	-2.15	1.41	1.46
30	B	820	CLA	C1C-NC	-2.15	1.34	1.37
38	11	312	KC1	C4D-CHA	2.15	1.47	1.45
30	13	304	CLA	C1B-CHB	2.15	1.47	1.41
30	B	830	CLA	C1C-NC	-2.15	1.34	1.37
30	16	308	CLA	C3D-C4D	-2.15	1.39	1.44
30	9	309	CLA	C1C-NC	-2.15	1.34	1.37
30	4	309	CLA	C1C-C2C	2.15	1.48	1.44
38	6	308	KC1	C1C-C2C	2.15	1.48	1.44
38	11	311	KC1	CAA-C2A	2.15	1.53	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	15	310	CLA	C3D-C4D	-2.15	1.39	1.44
37	14	301	A86	C35-C34	2.15	1.55	1.51
38	13	308	KC1	C3B-C4B	2.15	1.49	1.46
30	4	311	CLA	C4C-C3C	2.15	1.48	1.45
38	2	306	KC1	C1C-C2C	2.15	1.48	1.44
30	B	832	CLA	C4B-CHC	2.15	1.47	1.41
30	6	317	CLA	C4C-C3C	2.14	1.48	1.45
30	15	310	CLA	C1B-CHB	2.14	1.47	1.41
30	15	311	CLA	C3D-C4D	-2.14	1.39	1.44
30	A	827	CLA	C4B-NB	-2.14	1.33	1.35
38	6	313	KC1	C1C-C2C	2.14	1.48	1.44
30	B	819	CLA	C4B-CHC	2.14	1.46	1.41
30	10	311	CLA	C1C-NC	-2.14	1.34	1.37
30	B	804	CLA	C1C-C2C	2.14	1.48	1.44
30	A	816	CLA	C1B-CHB	2.14	1.46	1.41
38	4	307	KC1	C1D-CHD	2.14	1.46	1.41
30	A	827	CLA	C1C-C2C	2.14	1.48	1.44
30	A	841	CLA	C1C-C2C	2.14	1.48	1.44
37	5	301	A86	C35-C34	2.14	1.55	1.51
30	7	305	CLA	C1A-CHA	2.14	1.52	1.43
30	A	810	CLA	C4B-NB	-2.14	1.33	1.35
30	15	305	CLA	C1B-CHB	2.14	1.46	1.41
39	2	316	DD6	C29-C27	-2.14	1.38	1.42
30	A	844	CLA	C1B-CHB	2.14	1.46	1.41
30	6	316	CLA	C4B-CHC	2.14	1.46	1.41
38	14	308	KC1	C1D-CHD	2.14	1.46	1.41
30	B	828	CLA	C4B-NB	-2.14	1.33	1.35
30	B	821	CLA	C4C-C3C	2.14	1.48	1.45
38	13	310	KC1	C4D-CHA	2.14	1.47	1.45
30	A	823	CLA	C4B-CHC	2.14	1.46	1.41
30	A	809	CLA	C1C-NC	-2.14	1.34	1.37
30	5	311	CLA	C1B-NB	-2.14	1.33	1.35
30	B	811	CLA	C1C-C2C	2.14	1.48	1.44
30	3	302	CLA	C4B-CHC	2.14	1.46	1.41
30	A	838	CLA	C4B-CHC	2.13	1.46	1.41
30	13	303	CLA	C1C-C2C	2.13	1.48	1.44
30	15	307	CLA	C1C-NC	-2.13	1.34	1.37
30	3	309	CLA	C1B-CHB	2.13	1.46	1.41
30	3	303	CLA	C3D-C4D	-2.13	1.39	1.44
38	7	313	KC1	C4A-C3A	2.13	1.48	1.44
30	4	304	CLA	C1C-C2C	2.13	1.48	1.44
30	B	825	CLA	C1C-C2C	2.13	1.48	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	15	305	CLA	C3D-C4D	-2.13	1.39	1.44
30	B	837	CLA	C1C-NC	-2.13	1.34	1.37
30	B	826	CLA	C1B-CHB	2.13	1.46	1.41
30	14	310	CLA	C3D-C4D	-2.13	1.39	1.44
30	12	304	CLA	C1B-NB	-2.13	1.33	1.35
30	A	825	CLA	C4B-CHC	2.13	1.46	1.41
30	A	838	CLA	C1C-C2C	2.13	1.48	1.44
30	F	202	CLA	C4C-C3C	2.13	1.48	1.45
30	2	304	CLA	C4B-CHC	2.13	1.46	1.41
38	10	312	KC1	C1C-C2C	2.13	1.48	1.44
38	13	312	KC1	C3B-C4B	2.13	1.49	1.46
30	B	807	CLA	C4B-CHC	2.13	1.46	1.41
37	6	320	A86	C14-C15	2.13	1.56	1.52
39	2	315	DD6	C22-C16	-2.13	1.49	1.53
38	14	311	KC1	CAA-C2A	2.13	1.53	1.46
30	B	801	CLA	C4B-CHC	2.13	1.46	1.41
33	A	848	BCR	C30-C25	-2.13	1.50	1.53
30	A	814	CLA	C4C-C3C	2.13	1.48	1.45
38	8	314	KC1	CAA-C2A	2.13	1.53	1.46
38	14	311	KC1	C4D-CHA	2.13	1.47	1.45
30	A	835	CLA	C1C-NC	-2.13	1.34	1.37
30	15	307	CLA	C3D-C4D	-2.12	1.39	1.44
39	3	312	DD6	C22-C16	-2.12	1.49	1.53
30	6	309	CLA	C4B-NB	-2.12	1.33	1.35
30	12	312	CLA	C1C-C2C	2.12	1.48	1.44
38	14	308	KC1	C3B-C4B	2.12	1.49	1.46
38	16	311	KC1	C1D-CHD	2.12	1.46	1.41
39	6	318	DD6	C35-C36	2.12	1.54	1.51
30	15	306	CLA	C1B-NB	-2.12	1.33	1.35
30	A	812	CLA	C4B-NB	-2.12	1.33	1.35
38	9	311	KC1	C1C-C2C	2.12	1.48	1.44
30	3	310	CLA	C4B-CHC	2.12	1.46	1.41
30	15	307	CLA	C1B-CHB	2.12	1.46	1.41
39	6	321	DD6	O1-C20	2.12	1.49	1.46
30	12	308	CLA	C4C-C3C	2.12	1.48	1.45
30	7	305	CLA	C4B-CHC	2.12	1.46	1.41
37	1	309	A86	C14-C15	2.12	1.56	1.52
30	A	833	CLA	C1C-C2C	2.12	1.48	1.44
30	2	311	CLA	C1B-CHB	2.12	1.46	1.41
30	A	826	CLA	C4C-C3C	2.12	1.48	1.45
38	11	307	KC1	C4D-CHA	2.12	1.47	1.45
30	1	301	CLA	C4B-CHC	2.12	1.46	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	2	307	CLA	C4B-CHC	2.12	1.46	1.41
30	4	311	CLA	C1C-NC	-2.12	1.34	1.37
33	J	103	BCR	C33-C5	-2.12	1.47	1.50
30	3	306	CLA	C1B-NB	-2.12	1.33	1.35
37	2u	205	A86	C-C1	2.12	1.55	1.50
30	15	306	CLA	C3D-C4D	-2.12	1.39	1.44
38	4	310	KC1	C1C-C2C	2.12	1.48	1.44
38	6	311	KC1	CAA-C2A	2.12	1.53	1.46
39	7	302	DD6	O1-C20	2.12	1.49	1.46
37	2u	205	A86	O4-C34	-2.12	1.41	1.46
30	5	307	CLA	C4B-CHC	2.12	1.46	1.41
30	8	303	CLA	C4B-NB	-2.12	1.33	1.35
38	5	310	KC1	CAA-C2A	2.12	1.53	1.46
30	4	309	CLA	C1B-CHB	2.12	1.46	1.41
30	5	308	CLA	C4B-CHC	2.12	1.46	1.41
38	13	310	KC1	C4C-C3C	2.11	1.48	1.45
30	B	806	CLA	C4B-NB	-2.11	1.33	1.35
30	9	303	CLA	C1C-C2C	2.11	1.48	1.44
38	2	312	KC1	C1C-C2C	2.11	1.48	1.44
38	14	308	KC1	CAA-C2A	2.11	1.53	1.46
30	A	802	CLA	C1C-NC	-2.11	1.34	1.37
38	6	313	KC1	C2A-C1A	2.11	1.51	1.44
38	7	308	KC1	CAA-C2A	2.11	1.53	1.46
30	15	314	CLA	C3D-C4D	-2.11	1.39	1.44
30	12	304	CLA	C4B-NB	-2.11	1.33	1.35
30	2	309	CLA	C1B-CHB	2.11	1.46	1.41
30	6	315	CLA	C4C-C3C	2.11	1.48	1.45
38	13	312	KC1	C1D-CHD	2.11	1.46	1.41
30	7	312	CLA	C1B-CHB	2.11	1.46	1.41
30	15	303	CLA	C1B-CHB	2.11	1.46	1.41
39	5	314	DD6	C4-C5	2.11	1.50	1.43
30	B	811	CLA	C4B-CHC	2.11	1.46	1.41
38	5	312	KC1	C4D-CHA	2.11	1.47	1.45
30	6	305	CLA	C4C-C3C	2.11	1.48	1.45
30	B	803	CLA	C4B-CHC	2.11	1.46	1.41
30	14	303	CLA	C3D-C4D	-2.11	1.39	1.44
30	5	304	CLA	C4C-C3C	2.11	1.48	1.45
30	1	307	CLA	C1B-CHB	2.11	1.46	1.41
30	12	302	CLA	C4B-CHC	2.11	1.46	1.41
33	M	101	BCR	C33-C5	-2.11	1.47	1.50
30	2	313	CLA	C1B-CHB	2.11	1.46	1.41
38	11	312	KC1	CAA-C2A	2.11	1.53	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	2	310	CLA	C4B-CHC	2.11	1.46	1.41
30	2u	202	CLA	C1C-NC	-2.11	1.34	1.37
30	A	806	CLA	C4B-CHC	2.11	1.46	1.41
39	16	313	DD6	C35-C36	2.11	1.54	1.51
30	A	802	CLA	C4B-NB	-2.11	1.33	1.35
30	5	309	CLA	C1B-NB	-2.11	1.33	1.35
37	13	315	A86	O4-C34	-2.11	1.41	1.46
39	10	313	DD6	O1-C20	2.11	1.49	1.46
30	12	308	CLA	C1C-NC	-2.11	1.34	1.37
30	B	803	CLA	C3D-C4D	-2.11	1.39	1.44
37	1	309	A86	O4-C34	-2.11	1.41	1.46
39	12	317	DD6	O1-C20	2.10	1.49	1.46
30	10	305	CLA	C1C-C2C	2.10	1.48	1.44
38	9	311	KC1	C1D-CHD	2.10	1.46	1.41
30	A	842	CLA	C1B-CHB	2.10	1.46	1.41
30	B	810	CLA	C1B-CHB	2.10	1.46	1.41
38	14	306	KC1	C1C-C2C	2.10	1.48	1.44
38	13	311	KC1	C3B-C4B	2.10	1.49	1.46
30	12	303	CLA	C1C-C2C	2.10	1.48	1.44
38	16	304	KC1	CAA-C2A	2.10	1.53	1.46
30	15	312	CLA	C4B-CHC	2.10	1.46	1.41
37	16	312	A86	C35-C34	2.10	1.55	1.51
30	7	309	CLA	C1B-CHB	2.10	1.46	1.41
38	2	306	KC1	CAA-C2A	2.10	1.53	1.46
39	2	315	DD6	C26-C27	-2.10	1.32	1.37
38	13	306	KC1	C1C-C2C	2.10	1.48	1.44
30	12	303	CLA	C1B-CHB	2.10	1.46	1.41
30	3	305	CLA	C1C-C2C	2.10	1.48	1.44
30	5	309	CLA	C1C-C2C	2.10	1.48	1.44
30	2	305	CLA	C1B-CHB	2.10	1.46	1.41
30	2	305	CLA	C4B-CHC	2.10	1.46	1.41
30	7	307	CLA	C1C-NC	-2.10	1.34	1.37
30	7	311	CLA	C1C-C2C	2.10	1.48	1.44
39	10	313	DD6	C29-C27	-2.10	1.38	1.42
30	12	306	CLA	C4B-CHC	2.10	1.46	1.41
30	7	307	CLA	C1C-C2C	2.10	1.48	1.44
30	12	304	CLA	C1C-C2C	2.10	1.48	1.44
38	9	310	KC1	CAA-C2A	2.10	1.53	1.46
30	16	308	CLA	C1C-C2C	2.10	1.48	1.44
38	11	305	KC1	C1C-C2C	2.10	1.48	1.44
30	A	803	CLA	C3D-C4D	-2.10	1.39	1.44
30	A	818	CLA	C1C-C2C	2.10	1.48	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	3	307	CLA	C1C-C2C	2.10	1.48	1.44
30	A	827	CLA	C1C-NC	-2.10	1.34	1.37
30	15	309	CLA	C1B-CHB	2.10	1.46	1.41
38	11	305	KC1	CAA-C2A	2.10	1.53	1.46
30	3	301	CLA	C4B-NB	-2.10	1.33	1.35
30	B	827	CLA	C4B-CHC	2.10	1.46	1.41
37	15	320	A86	C4-C3	2.10	1.41	1.36
38	9	311	KC1	CAA-C2A	2.10	1.53	1.46
30	6	317	CLA	C1B-CHB	2.10	1.46	1.41
30	16	305	CLA	C1C-C2C	2.09	1.48	1.44
30	A	823	CLA	C1B-CHB	2.09	1.46	1.41
30	B	813	CLA	C4B-CHC	2.09	1.46	1.41
30	A	832	CLA	C1C-C2C	2.09	1.48	1.44
30	B	812	CLA	C1C-NC	-2.09	1.34	1.37
30	2	311	CLA	C4C-C3C	2.09	1.48	1.45
30	B	807	CLA	C1C-NC	-2.09	1.34	1.37
30	11	309	CLA	C1C-NC	-2.09	1.34	1.37
30	B	837	CLA	C1C-C2C	2.09	1.48	1.44
30	11	310	CLA	C1B-CHB	2.09	1.46	1.41
30	15	306	CLA	C1C-C2C	2.09	1.48	1.44
30	16	301	CLA	C1B-CHB	2.09	1.46	1.41
38	8	314	KC1	C1C-C2C	2.09	1.48	1.44
30	9	308	CLA	C4B-NB	-2.09	1.33	1.35
38	3	308	KC1	C1C-C2C	2.09	1.48	1.44
30	A	822	CLA	C4B-CHC	2.09	1.46	1.41
30	B	825	CLA	C1B-CHB	2.09	1.46	1.41
30	8	302	CLA	C4B-CHC	2.09	1.46	1.41
30	B	833	CLA	C4C-C3C	2.09	1.48	1.45
38	9	312	KC1	C1C-C2C	2.09	1.48	1.44
30	A	820	CLA	C4B-CHC	2.09	1.46	1.41
38	13	305	KC1	C1C-C2C	2.09	1.48	1.44
34	6	322	LHG	O7-C5	-2.09	1.41	1.46
38	8	306	KC1	CAA-C2A	2.09	1.53	1.46
30	B	851	CLA	C4B-NB	-2.09	1.33	1.35
30	A	833	CLA	C1C-NC	-2.09	1.34	1.37
36	8	321	LMG	C4-C3	2.09	1.57	1.52
30	1	307	CLA	C1C-NC	-2.09	1.34	1.37
30	J	101	CLA	C1C-C2C	2.09	1.48	1.44
30	A	813	CLA	C4B-CHC	2.09	1.46	1.41
30	7	309	CLA	C4C-C3C	2.09	1.48	1.45
38	10	310	KC1	C4D-CHA	2.09	1.47	1.45
30	6	316	CLA	C1C-C2C	2.09	1.48	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	5	303	CLA	C1C-NC	-2.09	1.34	1.37
38	13	311	KC1	C4D-CHA	2.09	1.47	1.45
30	B	812	CLA	C4B-CHC	2.09	1.46	1.41
30	8	302	CLA	C1C-C2C	2.09	1.48	1.44
30	16	310	CLA	C4C-C3C	2.08	1.48	1.45
38	12	309	KC1	C1C-C2C	2.08	1.48	1.44
38	13	310	KC1	CAA-C2A	2.08	1.53	1.46
30	5	303	CLA	C1C-C2C	2.08	1.48	1.44
39	12	315	DD6	C22-C16	-2.08	1.49	1.53
34	B	848	LHG	O7-C5	-2.08	1.41	1.46
30	7	309	CLA	C4B-CHC	2.08	1.46	1.41
29	A	801	CL0	C1C-C2C	2.08	1.48	1.44
30	10	307	CLA	C1A-CHA	2.08	1.51	1.43
30	A	822	CLA	C4C-C3C	2.08	1.48	1.45
38	10	306	KC1	C4C-C3C	2.08	1.48	1.45
37	14	316	A86	C35-C34	2.08	1.55	1.51
38	8	314	KC1	C4C-C3C	2.08	1.48	1.45
38	9	304	KC1	C4C-C3C	2.08	1.48	1.45
30	A	832	CLA	C4B-CHC	2.08	1.46	1.41
30	5	309	CLA	C1B-CHB	2.08	1.46	1.41
30	6	307	CLA	C4B-CHC	2.08	1.46	1.41
30	2	310	CLA	C1B-CHB	2.08	1.46	1.41
30	6	304	CLA	C1C-C2C	2.08	1.48	1.44
30	8	304	CLA	C4B-NB	-2.08	1.33	1.35
30	8	305	CLA	C1B-CHB	2.08	1.46	1.41
30	10	305	CLA	C4C-C3C	2.08	1.48	1.45
30	12	304	CLA	C4C-C3C	2.08	1.48	1.45
30	16	306	CLA	C1C-NC	-2.08	1.34	1.37
30	15	313	CLA	C1B-CHB	2.08	1.46	1.41
30	4	305	CLA	C4C-C3C	2.08	1.48	1.45
30	B	814	CLA	C4B-CHC	2.08	1.46	1.41
30	A	843	CLA	C1C-NC	-2.08	1.34	1.37
30	2u	202	CLA	C1C-C2C	2.08	1.48	1.44
30	6	305	CLA	C1C-C2C	2.08	1.48	1.44
30	6	314	CLA	C4B-CHC	2.08	1.46	1.41
30	7	312	CLA	C1C-NC	-2.08	1.34	1.37
36	3	317	LMG	O6-C1	2.08	1.47	1.41
38	12	305	KC1	C4D-CHA	2.08	1.47	1.45
30	6	306	CLA	C4B-NB	-2.08	1.33	1.35
30	9	307	CLA	C1A-CHA	2.08	1.51	1.43
30	13	307	CLA	C1B-CHB	2.08	1.46	1.41
38	5	310	KC1	C4C-C3C	2.08	1.48	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	823	CLA	C1C-NC	-2.08	1.34	1.37
39	4	313	DD6	C22-C16	-2.07	1.49	1.53
38	4	310	KC1	C1D-CHD	2.07	1.46	1.41
37	11	316	A86	O4-C34	-2.07	1.41	1.46
30	16	306	CLA	C1B-CHB	2.07	1.46	1.41
30	3	301	CLA	C1C-C2C	2.07	1.48	1.44
30	5	303	CLA	C1B-CHB	2.07	1.46	1.41
30	12	307	CLA	C1B-CHB	2.07	1.46	1.41
38	6	313	KC1	C4C-C3C	2.07	1.48	1.45
37	5	301	A86	O4-C34	-2.07	1.41	1.46
30	8	305	CLA	C1C-C2C	2.07	1.48	1.44
30	10	308	CLA	C1C-C2C	2.07	1.48	1.44
38	2	314	KC1	C1C-C2C	2.07	1.48	1.44
30	1	302	CLA	C1B-CHB	2.07	1.46	1.41
39	15	319	DD6	C22-C16	-2.07	1.49	1.53
30	B	833	CLA	C1C-NC	-2.07	1.34	1.37
30	3	301	CLA	C4B-CHC	2.07	1.46	1.41
30	10	308	CLA	C4C-C3C	2.07	1.48	1.45
38	13	308	KC1	C1C-C2C	2.07	1.48	1.44
38	13	308	KC1	CAA-C2A	2.07	1.52	1.46
30	7	304	CLA	C4B-NB	-2.07	1.33	1.35
30	12	303	CLA	C4C-C3C	2.07	1.48	1.45
30	B	836	CLA	C1B-CHB	2.07	1.46	1.41
39	10	314	DD6	C22-C16	-2.07	1.49	1.53
30	10	305	CLA	C4B-CHC	2.07	1.46	1.41
33	I	101	BCR	C30-C25	-2.07	1.50	1.53
39	10	314	DD6	C35-C36	2.07	1.54	1.51
37	15	317	A86	C35-C34	2.07	1.55	1.51
30	1	307	CLA	C1C-C2C	2.07	1.48	1.44
38	1	306	KC1	C1C-C2C	2.07	1.48	1.44
37	9	313	A86	C24-C1	2.07	1.50	1.45
37	3	315	A86	C35-C34	2.07	1.55	1.51
30	12	303	CLA	C1C-NC	-2.07	1.34	1.37
30	3	303	CLA	C1C-C2C	2.07	1.48	1.44
30	B	834	CLA	C1B-CHB	2.07	1.46	1.41
30	A	824	CLA	C1B-CHB	2.07	1.46	1.41
30	5	304	CLA	C1B-CHB	2.07	1.46	1.41
30	3	310	CLA	C1B-NB	-2.07	1.33	1.35
30	11	306	CLA	C4C-C3C	2.07	1.48	1.45
30	A	809	CLA	C1C-C2C	2.07	1.48	1.44
30	4	303	CLA	C1B-CHB	2.07	1.46	1.41
30	8	304	CLA	C4B-CHC	2.07	1.46	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	841	CLA	C1C-NC	-2.07	1.34	1.37
30	A	828	CLA	C4B-CHC	2.07	1.46	1.41
30	11	308	CLA	C1C-C2C	2.07	1.48	1.44
30	10	311	CLA	C4C-C3C	2.07	1.48	1.45
30	9	306	CLA	C1C-C2C	2.07	1.48	1.44
38	6	311	KC1	C4C-C3C	2.07	1.48	1.45
38	9	304	KC1	CAA-C2A	2.07	1.52	1.46
30	A	835	CLA	C4C-C3C	2.07	1.48	1.45
30	5	307	CLA	C4B-NB	-2.06	1.33	1.35
30	16	307	CLA	C1B-NB	-2.06	1.33	1.35
30	2	301	CLA	C4B-CHC	2.06	1.46	1.41
30	6	304	CLA	C1C-NC	-2.06	1.34	1.37
38	13	311	KC1	CAA-C2A	2.06	1.52	1.46
37	10	301	A86	O4-C34	-2.06	1.41	1.46
39	4	313	DD6	C29-C27	-2.06	1.38	1.42
30	14	310	CLA	C1B-NB	-2.06	1.33	1.35
30	15	310	CLA	C1B-NB	-2.06	1.33	1.35
38	8	310	KC1	C4D-CHA	2.06	1.47	1.45
30	B	828	CLA	C1B-CHB	2.06	1.46	1.41
30	A	821	CLA	C4B-CHC	2.06	1.46	1.41
38	6	312	KC1	C1C-C2C	2.06	1.48	1.44
30	3	305	CLA	C1A-CHA	2.06	1.51	1.43
38	4	308	KC1	C4C-C3C	2.06	1.48	1.45
30	14	307	CLA	C1B-CHB	2.06	1.46	1.41
30	B	836	CLA	C1C-C2C	2.06	1.48	1.44
30	B	816	CLA	C1B-CHB	2.06	1.46	1.41
37	2u	203	A86	C39-C38	2.06	1.56	1.49
30	A	834	CLA	C1B-CHB	2.06	1.46	1.41
37	15	316	A86	O4-C34	-2.06	1.41	1.46
38	1	308	KC1	C4C-C3C	2.06	1.48	1.45
38	1	308	KC1	C4D-CHA	2.06	1.47	1.45
30	15	308	CLA	C1B-NB	-2.06	1.33	1.35
30	F	203	CLA	C1B-CHB	2.06	1.46	1.41
37	15	323	A86	C4-C3	2.06	1.41	1.36
30	B	839	CLA	C1C-NC	-2.06	1.34	1.37
39	5	314	DD6	C41-C32	-2.06	1.49	1.53
30	B	828	CLA	C4B-CHC	2.06	1.46	1.41
38	12	305	KC1	CAA-C2A	2.06	1.52	1.46
38	3	311	KC1	C1D-CHD	2.06	1.46	1.41
38	11	307	KC1	C1C-C2C	2.06	1.48	1.44
30	5	304	CLA	C3D-C4D	-2.06	1.39	1.44
37	12	316	A86	O4-C34	-2.06	1.41	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	3	310	CLA	C1B-CHB	2.06	1.46	1.41
30	16	305	CLA	C4C-C3C	2.06	1.48	1.45
30	5	308	CLA	C4B-NB	-2.06	1.33	1.35
38	3	308	KC1	C4D-CHA	2.06	1.47	1.45
37	4	312	A86	O4-C34	-2.06	1.41	1.46
37	14	317	A86	O4-C34	-2.06	1.41	1.46
30	16	308	CLA	C1B-NB	-2.06	1.33	1.35
30	9	309	CLA	C1B-CHB	2.05	1.46	1.41
30	B	825	CLA	C4B-NB	-2.05	1.33	1.35
30	6	310	CLA	C1C-C2C	2.05	1.48	1.44
30	3	310	CLA	C1C-NC	-2.05	1.34	1.37
38	9	311	KC1	C2A-C1A	2.05	1.50	1.44
30	12	321	CLA	C1B-CHB	2.05	1.46	1.41
38	8	313	KC1	CAA-C2A	2.05	1.52	1.46
38	10	310	KC1	CAA-C2A	2.05	1.52	1.46
30	A	820	CLA	C1C-NC	-2.05	1.34	1.37
30	9	301	CLA	C1B-CHB	2.05	1.46	1.41
38	2	306	KC1	C1D-CHD	2.05	1.46	1.41
30	B	826	CLA	C1C-C2C	2.05	1.48	1.44
37	9	313	A86	C35-C34	2.05	1.55	1.51
30	16	309	CLA	C1B-NB	-2.05	1.33	1.35
30	16	308	CLA	C1B-CHB	2.05	1.46	1.41
38	13	308	KC1	C1D-CHD	2.05	1.46	1.41
30	B	802	CLA	C4C-C3C	2.05	1.48	1.45
30	4	301	CLA	C1C-C2C	2.05	1.48	1.44
30	15	308	CLA	C3D-C4D	-2.05	1.39	1.44
38	12	309	KC1	C4C-C3C	2.05	1.48	1.45
30	10	311	CLA	C1C-C2C	2.05	1.48	1.44
30	F	201	CLA	C1B-CHB	2.05	1.46	1.41
38	3	304	KC1	C1C-C2C	2.05	1.48	1.44
37	4	315	A86	O4-C34	-2.05	1.41	1.46
30	B	818	CLA	C4B-CHC	2.05	1.46	1.41
30	5	302	CLA	C1B-CHB	2.05	1.46	1.41
30	10	309	CLA	C1B-NB	-2.05	1.33	1.35
30	A	813	CLA	C1C-C2C	2.05	1.48	1.44
30	7	306	CLA	C1A-CHA	2.05	1.51	1.43
30	16	303	CLA	C1B-CHB	2.05	1.46	1.41
38	5	306	KC1	C1D-CHD	2.05	1.46	1.41
30	A	831	CLA	C4C-C3C	2.05	1.48	1.45
38	16	304	KC1	C4D-CHA	2.05	1.47	1.45
37	10	316	A86	C35-C34	2.05	1.55	1.51
30	J	101	CLA	C1C-NC	-2.05	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	803	CLA	C1A-CHA	2.05	1.51	1.43
30	B	804	CLA	C1A-CHA	2.05	1.51	1.43
38	11	311	KC1	C4D-CHA	2.04	1.47	1.45
30	15	314	CLA	C1B-CHB	2.04	1.46	1.41
38	10	312	KC1	C4C-C3C	2.04	1.48	1.45
30	A	835	CLA	C4B-CHC	2.04	1.46	1.41
30	A	811	CLA	C4B-CHC	2.04	1.46	1.41
30	4	306	CLA	C1C-C2C	2.04	1.48	1.44
30	B	826	CLA	C4B-CHC	2.04	1.46	1.41
38	9	311	KC1	C4C-C3C	2.04	1.48	1.45
30	A	812	CLA	C1C-C2C	2.04	1.48	1.44
30	A	809	CLA	C1A-CHA	2.04	1.51	1.43
30	1	305	CLA	C1C-C2C	2.04	1.48	1.44
30	A	833	CLA	C4C-C3C	2.04	1.48	1.45
30	3	307	CLA	C1B-CHB	2.04	1.46	1.41
30	A	823	CLA	C1C-NC	-2.04	1.34	1.37
30	11	309	CLA	C4B-NB	-2.04	1.33	1.35
30	A	804	CLA	C1B-CHB	2.04	1.46	1.41
30	8	303	CLA	C1B-CHB	2.04	1.46	1.41
30	6	310	CLA	C1C-NC	-2.04	1.34	1.37
38	14	311	KC1	C4C-C3C	2.04	1.48	1.45
30	1	305	CLA	C1C-NC	-2.04	1.34	1.37
38	8	313	KC1	C4D-CHA	2.04	1.47	1.45
30	B	827	CLA	C1B-CHB	2.04	1.46	1.41
30	14	312	CLA	C1B-CHB	2.04	1.46	1.41
30	13	301	CLA	C4C-C3C	2.04	1.48	1.45
37	2	318	A86	O4-C34	-2.04	1.41	1.46
30	A	816	CLA	C4B-CHC	2.04	1.46	1.41
30	13	302	CLA	C1B-NB	-2.04	1.33	1.35
30	A	843	CLA	C4B-CHC	2.04	1.46	1.41
38	14	306	KC1	C4D-CHA	2.04	1.47	1.45
30	10	311	CLA	C1B-NB	-2.04	1.33	1.35
30	A	826	CLA	C1A-CHA	2.04	1.51	1.43
30	A	810	CLA	C4B-CHC	2.04	1.46	1.41
30	7	306	CLA	C1C-C2C	2.04	1.48	1.44
30	7	304	CLA	C1C-NC	-2.04	1.34	1.37
30	9	305	CLA	C4C-C3C	2.04	1.48	1.45
30	A	837	CLA	C1C-C2C	2.04	1.48	1.44
38	3	308	KC1	C1B-C2B	2.03	1.49	1.45
30	B	823	CLA	C1B-CHB	2.03	1.46	1.41
30	14	309	CLA	C1B-NB	-2.03	1.33	1.35
30	15	303	CLA	C1B-NB	-2.03	1.33	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	8	302	CLA	C1B-CHB	2.03	1.46	1.41
38	5	305	KC1	C4D-CHA	2.03	1.47	1.45
38	8	307	KC1	CAA-C2A	2.03	1.52	1.46
30	16	310	CLA	C1C-NC	-2.03	1.34	1.37
30	A	834	CLA	C1C-C2C	2.03	1.48	1.44
37	8	315	A86	C14-C15	2.03	1.56	1.52
38	6	312	KC1	C3B-C4B	2.03	1.49	1.46
37	15	322	A86	C35-C34	2.03	1.55	1.51
33	2u	201	BCR	C38-C26	-2.03	1.47	1.50
38	7	308	KC1	C1C-C2C	2.03	1.48	1.44
30	7	310	CLA	C4C-C3C	2.03	1.48	1.45
30	11	310	CLA	C1C-NC	-2.03	1.34	1.37
30	3	305	CLA	C4C-C3C	2.03	1.48	1.45
30	B	805	CLA	C4B-CHC	2.03	1.46	1.41
30	4	302	CLA	C1B-CHB	2.03	1.46	1.41
38	13	311	KC1	C1D-CHD	2.03	1.46	1.41
30	9	309	CLA	C4C-C3C	2.03	1.48	1.45
30	B	808	CLA	C4B-CHC	2.03	1.46	1.41
30	1	301	CLA	C1C-NC	-2.03	1.34	1.37
30	B	833	CLA	C1A-CHA	2.03	1.51	1.43
30	11	304	CLA	C1B-CHB	2.03	1.46	1.41
30	3	302	CLA	C4B-NB	-2.03	1.33	1.35
30	6	314	CLA	C4C-C3C	2.03	1.48	1.45
38	9	312	KC1	C1D-CHD	2.03	1.46	1.41
30	L	202	CLA	C1C-NC	-2.03	1.34	1.37
38	10	312	KC1	C1D-CHD	2.03	1.46	1.41
30	2	310	CLA	C4C-C3C	2.03	1.48	1.45
37	5	315	A86	O4-C34	-2.03	1.41	1.46
30	3	309	CLA	C1B-NB	-2.03	1.33	1.35
30	5	311	CLA	C4B-NB	-2.03	1.33	1.35
38	1	308	KC1	C1C-C2C	2.02	1.48	1.44
30	B	817	CLA	C1C-C2C	2.02	1.48	1.44
30	6	317	CLA	C1A-CHA	2.02	1.51	1.43
38	6	312	KC1	C4C-C3C	2.02	1.48	1.45
30	A	810	CLA	C4C-C3C	2.02	1.48	1.45
30	4	301	CLA	C4C-C3C	2.02	1.48	1.45
37	15	316	A86	C35-C34	2.02	1.55	1.51
39	11	313	DD6	C29-C27	-2.02	1.38	1.42
30	9	305	CLA	C1B-CHB	2.02	1.46	1.41
30	5	308	CLA	C4C-C3C	2.02	1.48	1.45
30	B	811	CLA	C1C-NC	-2.02	1.34	1.37
30	A	829	CLA	C1C-C2C	2.02	1.48	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	11	311	KC1	C1D-CHD	2.02	1.46	1.41
30	4	302	CLA	C1C-C2C	2.02	1.48	1.44
33	2u	201	BCR	C33-C5	-2.02	1.47	1.50
30	12	306	CLA	C4C-C3C	2.02	1.48	1.45
30	A	834	CLA	C1C-NC	-2.02	1.34	1.37
30	B	829	CLA	C1C-C2C	2.02	1.48	1.44
30	A	840	CLA	C1B-CHB	2.02	1.46	1.41
30	7	304	CLA	C4C-C3C	2.02	1.48	1.45
30	B	816	CLA	C4B-CHC	2.02	1.46	1.41
39	3	316	DD6	C41-C32	-2.02	1.49	1.53
30	4	303	CLA	C1C-C2C	2.02	1.48	1.44
37	8	318	A86	O4-C34	-2.02	1.41	1.46
30	7	311	CLA	C1B-CHB	2.02	1.46	1.41
30	16	305	CLA	C1A-CHA	2.02	1.51	1.43
37	15	322	A86	C4-C3	2.02	1.41	1.36
30	B	833	CLA	C1C-C2C	2.02	1.48	1.44
30	1	305	CLA	C1B-CHB	2.02	1.46	1.41
30	16	305	CLA	C1B-CHB	2.02	1.46	1.41
30	4	302	CLA	C1A-CHA	2.02	1.51	1.43
30	3	303	CLA	C1A-CHA	2.02	1.51	1.43
30	14	309	CLA	C1C-C2C	2.02	1.48	1.44
30	B	804	CLA	C1B-CHB	2.02	1.46	1.41
30	7	305	CLA	C1B-CHB	2.02	1.46	1.41
30	2	304	CLA	C4C-C3C	2.02	1.48	1.45
39	13	314	DD6	C35-C36	2.02	1.54	1.51
30	8	309	CLA	C1B-CHB	2.02	1.46	1.41
30	4	309	CLA	C1C-NC	-2.02	1.34	1.37
30	A	833	CLA	C1B-CHB	2.02	1.46	1.41
30	12	306	CLA	C1B-CHB	2.02	1.46	1.41
30	7	305	CLA	C1C-C2C	2.02	1.48	1.44
37	3	315	A86	O4-C34	-2.02	1.41	1.46
37	15	315	A86	O4-C34	-2.02	1.41	1.46
36	8	320	LMG	O4-C4	-2.02	1.38	1.43
39	2	317	DD6	C22-C16	-2.01	1.49	1.53
30	A	837	CLA	C1C-NC	-2.01	1.34	1.37
37	10	316	A86	O4-C34	-2.01	1.41	1.46
30	A	813	CLA	C1B-CHB	2.01	1.46	1.41
37	14	320	A86	O4-C34	-2.01	1.41	1.46
30	A	827	CLA	C1B-CHB	2.01	1.46	1.41
30	B	832	CLA	C4C-C3C	2.01	1.48	1.45
30	1	303	CLA	C1C-NC	-2.01	1.34	1.37
38	14	306	KC1	C1D-CHD	2.01	1.46	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	3	314	A86	O4-C34	-2.01	1.41	1.46
30	A	812	CLA	C4C-C3C	2.01	1.48	1.45
38	9	310	KC1	C4C-C3C	2.01	1.48	1.45
30	5	311	CLA	C1C-NC	-2.01	1.34	1.37
30	B	802	CLA	C1B-CHB	2.01	1.46	1.41
30	1	301	CLA	C1B-CHB	2.01	1.46	1.41
30	A	806	CLA	C1B-CHB	2.01	1.46	1.41
30	B	814	CLA	C1B-CHB	2.01	1.46	1.41
37	10	317	A86	O4-C34	-2.01	1.41	1.46
30	6	305	CLA	C1B-CHB	2.01	1.46	1.41
30	10	303	CLA	C1C-NC	-2.01	1.34	1.37
30	B	808	CLA	C4B-NB	-2.01	1.33	1.35
39	1	310	DD6	C22-C16	-2.01	1.49	1.53
39	3	313	DD6	C35-C36	2.01	1.54	1.51
30	15	309	CLA	C1D-C2D	2.01	1.49	1.45
30	15	308	CLA	C1A-CHA	2.01	1.51	1.43
30	15	308	CLA	C1B-CHB	2.01	1.46	1.41
38	7	308	KC1	C4D-CHA	2.01	1.47	1.45
30	L	203	CLA	C1C-C2C	2.01	1.48	1.44
38	3	304	KC1	C1D-CHD	2.01	1.46	1.41
38	10	310	KC1	C1D-CHD	2.01	1.46	1.41
38	13	305	KC1	C1D-CHD	2.01	1.46	1.41
30	A	816	CLA	C4C-C3C	2.01	1.48	1.45
30	B	835	CLA	C4B-NB	-2.01	1.33	1.35
30	13	303	CLA	C1D-C2D	2.00	1.49	1.45
30	A	821	CLA	C4C-C3C	2.00	1.48	1.45
30	10	304	CLA	C1C-NC	-2.00	1.34	1.37
30	L	202	CLA	C1C-C2C	2.00	1.48	1.44
30	3	310	CLA	C4C-C3C	2.00	1.48	1.45
30	6	307	CLA	C1B-CHB	2.00	1.46	1.41
38	1	308	KC1	C1D-CHD	2.00	1.46	1.41
39	7	302	DD6	C29-C27	-2.00	1.38	1.42
30	5	307	CLA	C1C-NC	-2.00	1.34	1.37
30	2	307	CLA	C4C-C3C	2.00	1.48	1.45
37	4	317	A86	C35-C34	2.00	1.55	1.51
39	5	313	DD6	C35-C36	2.00	1.54	1.51
30	2	305	CLA	C4B-NB	-2.00	1.33	1.35
30	4	306	CLA	C4B-NB	-2.00	1.33	1.35
30	12	304	CLA	C1C-NC	-2.00	1.34	1.37
30	B	823	CLA	C4C-C3C	2.00	1.48	1.45
30	B	851	CLA	C1B-CHB	2.00	1.46	1.41
30	10	307	CLA	C4C-C3C	2.00	1.48	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	7	305	CLA	C1C-NC	-2.00	1.34	1.37
38	2	312	KC1	C4D-CHA	2.00	1.47	1.45
30	A	825	CLA	C1B-CHB	2.00	1.46	1.41
37	7	319	A86	O4-C34	-2.00	1.41	1.46
38	12	305	KC1	C1C-C2C	2.00	1.48	1.44
30	3	303	CLA	C1B-CHB	2.00	1.46	1.41

All (9756) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	14	315	A86	O1-C20-C19	58.15	157.06	113.38
37	14	317	A86	O1-C20-C19	57.25	156.39	113.38
37	15	321	A86	O1-C20-C19	57.05	156.24	113.38
37	8	318	A86	O1-C20-C19	56.85	156.09	113.38
37	4	312	A86	O1-C20-C19	56.56	155.87	113.38
37	16	314	A86	O1-C20-C19	56.23	155.63	113.38
37	1	309	A86	O1-C20-C19	56.19	155.59	113.38
37	11	314	A86	O1-C20-C19	55.94	155.41	113.38
37	13	315	A86	O1-C20-C19	55.92	155.39	113.38
37	8	315	A86	O1-C20-C19	55.91	155.38	113.38
37	14	318	A86	O1-C20-C19	55.91	155.38	113.38
37	15	317	A86	O1-C20-C19	55.69	155.22	113.38
37	13	313	A86	O1-C20-C19	55.54	155.10	113.38
37	9	316	A86	O1-C20-C19	55.53	155.10	113.38
37	15	323	A86	O1-C20-C19	55.39	154.99	113.38
37	5	315	A86	O1-C20-C19	55.06	154.75	113.38
37	12	316	A86	O1-C20-C19	55.02	154.72	113.38
37	15	322	A86	O1-C20-C19	54.87	154.60	113.38
37	3	315	A86	O1-C20-C19	54.69	154.47	113.38
37	11	316	A86	O1-C20-C19	54.41	154.26	113.38
37	14	319	A86	O1-C20-C19	54.31	154.18	113.38
37	10	315	A86	O1-C20-C19	54.27	154.15	113.38
37	2	302	A86	O1-C20-C19	54.26	154.14	113.38
37	10	302	A86	O1-C20-C19	54.23	154.12	113.38
37	15	320	A86	O1-C20-C19	54.15	154.06	113.38
37	10	317	A86	O1-C20-C19	53.87	153.85	113.38
37	2u	203	A86	O1-C20-C19	53.66	153.69	113.38
37	7	319	A86	O1-C20-C19	53.65	153.68	113.38
37	14	301	A86	O1-C20-C19	53.44	153.53	113.38
37	14	316	A86	O1-C20-C19	53.38	153.48	113.38
37	11	301	A86	O1-C20-C19	53.33	153.45	113.38
37	4	314	A86	O1-C20-C19	53.32	153.44	113.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	12	314	A86	O1-C20-C19	53.16	153.32	113.38
37	14	314	A86	O1-C20-C19	53.10	153.28	113.38
37	10	316	A86	O1-C20-C19	52.91	153.13	113.38
37	3	314	A86	O1-C20-C19	52.35	152.71	113.38
37	5	316	A86	O1-C20-C19	52.31	152.68	113.38
37	16	312	A86	O1-C20-C19	51.84	152.32	113.38
37	4	315	A86	O1-C20-C19	51.67	152.20	113.38
37	15	315	A86	O1-C20-C19	51.53	152.09	113.38
37	5	301	A86	O1-C20-C19	51.51	152.08	113.38
37	15	316	A86	O1-C20-C19	51.24	151.88	113.38
37	7	315	A86	O1-C20-C19	50.24	151.12	113.38
37	7	316	A86	O1-C20-C19	49.35	150.45	113.38
37	4	317	A86	O1-C20-C19	48.76	150.01	113.38
37	2	319	A86	O1-C20-C19	48.74	150.00	113.38
37	2	318	A86	O1-C20-C19	48.64	149.92	113.38
37	9	313	A86	O1-C20-C19	48.16	149.56	113.38
37	11	315	A86	O1-C20-C19	47.43	149.01	113.38
37	2u	205	A86	O1-C20-C19	46.62	148.40	113.38
37	9	315	A86	O1-C20-C19	45.27	147.39	113.38
37	14	320	A86	O1-C20-C19	44.91	147.12	113.38
37	10	301	A86	O1-C20-C19	44.78	147.02	113.38
37	6	320	A86	O1-C20-C19	43.19	145.83	113.38
39	9	314	DD6	O1-C20-C19	34.40	139.22	113.38
39	4	316	DD6	O1-C20-C19	33.98	138.91	113.38
39	7	314	DD6	O1-C20-C19	33.53	138.57	113.38
37	8	318	A86	C-C1-C2	-33.04	76.65	122.92
39	13	314	DD6	O1-C20-C19	32.61	137.88	113.38
39	5	314	DD6	O1-C20-C19	32.03	137.44	113.38
39	8	317	DD6	O1-C20-C19	31.79	137.26	113.38
39	5	313	DD6	O1-C20-C19	31.24	136.85	113.38
39	12	317	DD6	O1-C20-C19	31.07	136.72	113.38
39	2	315	DD6	O1-C20-C19	31.07	136.72	113.38
39	16	313	DD6	O1-C20-C19	30.49	136.29	113.38
39	15	318	DD6	O1-C20-C19	30.45	136.26	113.38
39	10	313	DD6	O1-C20-C19	30.36	136.19	113.38
39	12	315	DD6	O1-C20-C19	30.13	136.01	113.38
39	2	316	DD6	O1-C20-C19	30.07	135.97	113.38
39	3	312	DD6	O1-C20-C19	29.96	135.89	113.38
39	3	316	DD6	O1-C20-C19	29.90	135.84	113.38
39	6	303	DD6	O1-C20-C19	29.75	135.73	113.38
39	8	316	DD6	O1-C20-C19	29.52	135.56	113.38
39	4	313	DD6	O1-C20-C19	29.25	135.35	113.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	6	319	DD6	O1-C20-C19	29.13	135.27	113.38
39	7	318	DD6	O1-C20-C19	28.61	134.87	113.38
39	11	313	DD6	O1-C20-C19	28.43	134.74	113.38
39	7	302	DD6	O1-C20-C19	28.25	134.61	113.38
39	10	314	DD6	O1-C20-C19	28.24	134.59	113.38
39	3	313	DD6	O1-C20-C19	27.98	134.40	113.38
39	1	310	DD6	O1-C20-C19	27.92	134.36	113.38
39	15	319	DD6	O1-C20-C19	27.58	134.10	113.38
39	6	321	DD6	O1-C20-C19	27.33	133.91	113.38
39	6	318	DD6	O1-C20-C19	27.20	133.81	113.38
39	2	317	DD6	O1-C20-C19	26.86	133.56	113.38
37	8	318	A86	C-C1-C24	-26.67	76.06	118.08
39	7	317	DD6	O1-C20-C19	26.21	133.07	113.38
37	8	318	A86	C24-C1-C2	21.96	152.64	118.94
30	8	305	CLA	C4-C3-C5	-21.81	78.59	115.27
30	2	310	CLA	C4-C3-C5	-20.69	80.47	115.27
30	B	824	CLA	C4-C3-C5	-20.43	80.90	115.27
38	12	313	KC1	C2A-C3A-C4A	-19.93	91.70	106.49
30	2	310	CLA	C5-C3-C2	19.73	161.05	121.12
30	B	824	CLA	C5-C3-C2	19.40	160.37	121.12
39	2	317	DD6	C28-C27-C29	18.64	153.75	116.84
30	8	305	CLA	C5-C3-C2	18.45	158.46	121.12
39	7	314	DD6	C28-C27-C29	18.23	152.94	116.84
39	6	303	DD6	C28-C27-C29	18.21	152.90	116.84
39	7	317	DD6	C28-C27-C29	17.90	152.29	116.84
39	12	317	DD6	C28-C27-C29	17.51	151.51	116.84
39	4	316	DD6	C28-C27-C29	17.33	151.17	116.84
39	3	316	DD6	C28-C27-C29	17.28	151.05	116.84
39	3	313	DD6	C28-C27-C29	17.24	150.98	116.84
39	8	316	DD6	C28-C27-C29	17.21	150.93	116.84
30	B	824	CLA	C4-C3-C2	-17.19	79.57	123.68
39	5	314	DD6	C28-C27-C29	17.14	150.78	116.84
39	11	313	DD6	C28-C27-C29	17.10	150.70	116.84
30	8	305	CLA	C4-C3-C2	-17.06	79.91	123.68
39	6	321	DD6	C28-C27-C29	17.03	150.57	116.84
39	5	313	DD6	C28-C27-C29	17.02	150.54	116.84
39	10	313	DD6	C28-C27-C29	16.91	150.34	116.84
39	1	310	DD6	C28-C27-C29	16.83	150.17	116.84
39	2	316	DD6	C28-C27-C29	16.82	150.15	116.84
30	2	310	CLA	C4-C3-C2	-16.75	80.71	123.68
39	13	314	DD6	C28-C27-C29	16.70	149.92	116.84
39	10	314	DD6	C28-C27-C29	16.66	149.84	116.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	6	319	DD6	C28-C27-C29	16.65	149.82	116.84
39	16	313	DD6	C28-C27-C29	16.58	149.68	116.84
39	6	318	DD6	C28-C27-C29	16.57	149.65	116.84
39	9	314	DD6	C28-C27-C29	16.50	149.51	116.84
39	8	317	DD6	C28-C27-C29	16.49	149.50	116.84
39	15	318	DD6	C28-C27-C29	16.47	149.45	116.84
39	4	313	DD6	C28-C27-C29	16.40	149.33	116.84
39	12	315	DD6	C28-C27-C29	16.30	149.13	116.84
39	7	302	DD6	C28-C27-C29	16.22	148.96	116.84
39	7	318	DD6	C28-C27-C29	16.17	148.87	116.84
39	15	319	DD6	C28-C27-C29	16.15	148.82	116.84
39	3	312	DD6	C29-C30-C31	-16.12	134.61	175.43
39	15	319	DD6	C29-C30-C31	-15.83	135.34	175.43
39	3	312	DD6	C28-C27-C29	15.78	148.09	116.84
39	7	318	DD6	C29-C30-C31	-15.24	136.83	175.43
39	12	317	DD6	C29-C30-C31	-15.16	137.03	175.43
39	11	313	DD6	C29-C30-C31	-14.86	137.79	175.43
39	9	314	DD6	C29-C30-C31	-14.79	137.98	175.43
39	15	318	DD6	C29-C30-C31	-14.59	138.49	175.43
39	8	317	DD6	C29-C30-C31	-14.54	138.61	175.43
39	6	321	DD6	C29-C30-C31	-14.52	138.66	175.43
39	5	314	DD6	C29-C30-C31	-14.48	138.77	175.43
39	7	314	DD6	C29-C30-C31	-14.42	138.92	175.43
39	6	318	DD6	C29-C30-C31	-14.38	139.01	175.43
39	16	313	DD6	C29-C30-C31	-14.36	139.08	175.43
39	1	310	DD6	C29-C30-C31	-14.32	139.17	175.43
39	13	314	DD6	C29-C30-C31	-14.32	139.18	175.43
39	5	313	DD6	C29-C30-C31	-14.27	139.31	175.43
39	10	314	DD6	C29-C30-C31	-14.23	139.41	175.43
38	5	306	KC1	CMA-C3A-C4A	-14.17	103.46	125.04
39	10	313	DD6	C29-C30-C31	-14.16	139.57	175.43
39	12	315	DD6	C29-C30-C31	-14.16	139.58	175.43
39	2	315	DD6	C28-C27-C29	14.04	144.64	116.84
39	2	316	DD6	C29-C30-C31	-14.03	139.89	175.43
37	9	313	A86	C21-C20-C19	-13.80	98.75	114.28
39	4	313	DD6	C29-C30-C31	-13.73	140.68	175.43
39	3	313	DD6	C29-C30-C31	-13.71	140.72	175.43
39	8	316	DD6	C29-C30-C31	-13.68	140.78	175.43
39	10	313	DD6	C12-C11-C10	-13.64	103.81	122.92
39	7	302	DD6	C29-C30-C31	-13.59	141.02	175.43
39	4	316	DD6	C29-C30-C31	-13.57	141.07	175.43
37	6	320	A86	O1-C15-C14	-13.56	86.00	113.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	16	313	DD6	C37-C36-C31	-13.39	106.15	124.35
39	9	314	DD6	C37-C36-C31	-13.36	106.19	124.35
39	6	319	DD6	C29-C30-C31	-13.31	141.73	175.43
39	13	314	DD6	C12-C11-C10	-13.10	104.57	122.92
38	3	311	KC1	CMA-C3A-C4A	-13.07	105.13	125.04
39	6	321	DD6	C37-C36-C31	-13.05	106.62	124.35
37	3	315	A86	C21-C20-C19	-13.03	99.62	114.28
39	10	314	DD6	C37-C36-C31	-12.95	106.76	124.35
39	8	316	DD6	C12-C11-C10	-12.84	104.94	122.92
39	1	310	DD6	C37-C36-C31	-12.77	106.99	124.35
39	2	315	DD6	C9-C10-C11	-12.75	109.12	127.31
39	7	317	DD6	C37-C36-C31	-12.72	107.06	124.35
37	16	314	A86	O1-C20-C21	-12.71	99.83	115.06
39	7	317	DD6	C9-C10-C11	-12.68	109.21	127.31
39	4	313	DD6	C37-C36-C31	-12.67	107.13	124.35
39	3	316	DD6	C29-C30-C31	-12.61	143.49	175.43
39	10	313	DD6	C37-C36-C31	-12.61	107.22	124.35
37	10	316	A86	C21-C20-C19	-12.61	100.10	114.28
39	8	317	DD6	C37-C36-C31	-12.60	107.23	124.35
39	7	317	DD6	C29-C30-C31	-12.59	143.55	175.43
37	15	321	A86	C21-C20-C19	-12.48	100.23	114.28
39	12	315	DD6	C37-C36-C31	-12.45	107.43	124.35
39	8	316	DD6	C37-C36-C31	-12.28	107.66	124.35
37	5	316	A86	C21-C20-C19	-12.28	100.47	114.28
37	5	301	A86	C21-C20-C19	-12.27	100.48	114.28
39	4	316	DD6	C3-C2-C1	-12.21	109.89	127.31
37	15	322	A86	C21-C20-C19	-12.19	100.57	114.28
39	3	313	DD6	C37-C36-C31	-12.13	107.86	124.35
37	11	314	A86	C21-C20-C19	-12.13	100.63	114.28
37	4	312	A86	C21-C20-C19	-12.11	100.66	114.28
39	11	313	DD6	C37-C36-C31	-12.08	107.94	124.35
39	5	313	DD6	C37-C36-C31	-12.07	107.95	124.35
39	12	317	DD6	C37-C36-C31	-12.03	108.00	124.35
39	13	314	DD6	C37-C36-C31	-12.03	108.00	124.35
37	14	315	A86	C21-C20-C19	-11.97	100.81	114.28
37	12	316	A86	C21-C20-C19	-11.97	100.82	114.28
39	7	314	DD6	C13-C11-C10	-11.95	100.61	118.94
37	9	316	A86	O1-C20-C21	-11.94	100.75	115.06
37	14	316	A86	C21-C20-C19	-11.93	100.86	114.28
39	3	312	DD6	C37-C36-C31	-11.91	108.17	124.35
39	3	313	DD6	C9-C10-C11	-11.89	110.34	127.31
38	12	313	KC1	CMA-C3A-C4A	-11.88	106.95	125.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	2	316	DD6	C37-C36-C31	-11.87	108.22	124.35
37	11	316	A86	C21-C20-C19	-11.77	101.04	114.28
37	8	318	A86	O1-C20-C21	-11.76	100.96	115.06
38	12	311	KC1	CMA-C3A-C4A	-11.66	107.28	125.04
38	9	310	KC1	CMA-C3A-C4A	-11.66	107.28	125.04
38	9	311	KC1	CMA-C3A-C4A	-11.63	107.33	125.04
38	10	306	KC1	CMA-C3A-C4A	-11.60	107.37	125.04
37	11	315	A86	C17-C16-C15	11.60	120.99	109.16
37	14	317	A86	C21-C20-C19	-11.59	101.25	114.28
39	7	318	DD6	C37-C36-C31	-11.58	108.61	124.35
38	4	310	KC1	CMA-C3A-C4A	-11.58	107.41	125.04
39	6	303	DD6	C29-C30-C31	-11.56	146.16	175.43
39	5	314	DD6	C37-C36-C31	-11.51	108.70	124.35
37	14	314	A86	C21-C20-C19	-11.47	101.38	114.28
39	7	314	DD6	C37-C36-C31	-11.46	108.78	124.35
37	2	319	A86	C17-C16-C15	11.45	120.85	109.16
38	5	305	KC1	CMA-C3A-C4A	-11.45	107.60	125.04
38	8	307	KC1	CMA-C3A-C4A	-11.45	107.60	125.04
39	4	316	DD6	C4-C5-C6	-11.45	110.97	127.31
39	5	314	DD6	C13-C11-C10	-11.45	101.38	118.94
37	5	315	A86	O1-C20-C21	-11.42	101.37	115.06
39	3	316	DD6	C9-C10-C11	-11.40	111.04	127.31
38	2	314	KC1	CMA-C3A-C4A	-11.40	107.68	125.04
39	6	318	DD6	C37-C36-C31	-11.40	108.86	124.35
37	1	309	A86	C21-C20-C19	-11.40	101.46	114.28
37	15	315	A86	C21-C20-C19	-11.38	101.47	114.28
39	6	321	DD6	C12-C11-C10	-11.37	106.99	122.92
38	11	305	KC1	CMA-C3A-C4A	-11.35	107.76	125.04
37	16	312	A86	C4-C5-C6	-11.34	111.12	127.31
37	14	318	A86	C21-C20-C19	-11.34	101.52	114.28
38	5	310	KC1	CMA-C3A-C4A	-11.34	107.78	125.04
37	2	302	A86	C21-C20-C19	-11.33	101.54	114.28
37	10	315	A86	C21-C20-C19	-11.32	101.54	114.28
39	4	316	DD6	C37-C36-C31	-11.32	108.97	124.35
39	6	319	DD6	C12-C11-C10	-11.31	107.08	122.92
39	2	317	DD6	C3-C2-C1	-11.31	111.17	127.31
37	8	315	A86	C21-C20-C19	-11.27	101.60	114.28
38	16	311	KC1	C2A-C3A-C4A	-11.26	98.13	106.49
39	2	316	DD6	C12-C11-C10	-11.26	107.15	122.92
38	6	308	KC1	CMA-C3A-C4A	-11.26	107.90	125.04
38	6	311	KC1	CMA-C3A-C4A	-11.23	107.94	125.04
38	3	304	KC1	CMA-C3A-C4A	-11.20	107.98	125.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	10	301	A86	C17-C16-C15	11.19	120.58	109.16
37	14	315	A86	O1-C20-C21	-11.16	101.68	115.06
39	8	317	DD6	C13-C11-C10	-11.16	101.81	118.94
38	5	312	KC1	CMA-C3A-C4A	-11.13	108.08	125.04
37	13	315	A86	O1-C20-C21	-11.13	101.72	115.06
38	13	305	KC1	CMA-C3A-C4A	-11.12	108.11	125.04
37	4	315	A86	C21-C20-C19	-11.11	101.78	114.28
39	7	318	DD6	C9-C10-C11	-11.10	111.47	127.31
39	6	319	DD6	C37-C36-C31	-11.10	109.27	124.35
39	7	317	DD6	C3-C2-C1	-11.09	111.49	127.31
37	15	320	A86	C21-C20-C19	-11.08	101.81	114.28
39	15	318	DD6	C37-C36-C31	-11.08	109.29	124.35
37	15	317	A86	O1-C20-C21	-11.07	101.80	115.06
38	8	311	KC1	CMA-C3A-C4A	-11.05	108.21	125.04
38	2	306	KC1	CMA-C3A-C4A	-11.04	108.22	125.04
39	7	302	DD6	C37-C36-C31	-11.03	109.36	124.35
37	14	317	A86	O1-C20-C21	-11.03	101.84	115.06
39	15	319	DD6	C-C1-C2	-11.02	107.49	122.92
39	12	317	DD6	C12-C11-C10	-10.98	107.54	122.92
38	8	313	KC1	CMA-C3A-C4A	-10.93	108.39	125.04
37	13	313	A86	C21-C20-C19	-10.93	101.98	114.28
37	3	314	A86	C17-C16-C15	10.93	120.31	109.16
39	7	317	DD6	C12-C11-C10	-10.92	107.63	122.92
38	10	312	KC1	CMA-C3A-C4A	-10.92	108.41	125.04
37	10	301	A86	C25-C26-C27	-10.92	111.73	127.31
38	1	308	KC1	CMA-C3A-C4A	-10.91	108.42	125.04
39	3	316	DD6	C37-C36-C31	-10.91	109.53	124.35
37	14	319	A86	C21-C20-C19	-10.88	102.03	114.28
37	15	323	A86	O1-C20-C21	-10.88	102.02	115.06
37	13	315	A86	C21-C20-C19	-10.85	102.08	114.28
38	12	305	KC1	CMA-C3A-C4A	-10.85	108.52	125.04
39	11	313	DD6	C9-C10-C11	-10.85	111.83	127.31
37	1	309	A86	O1-C20-C21	-10.85	102.06	115.06
39	16	313	DD6	C12-C11-C10	-10.84	107.73	122.92
39	3	312	DD6	C13-C11-C10	-10.81	102.36	118.94
38	13	308	KC1	CMA-C3A-C4A	-10.81	108.58	125.04
37	14	320	A86	C17-C16-C15	10.80	120.18	109.16
37	15	323	A86	C21-C20-C19	-10.79	102.14	114.28
37	13	313	A86	O1-C20-C21	-10.79	102.12	115.06
39	15	319	DD6	C3-C2-C1	-10.78	111.92	127.31
38	12	309	KC1	C2A-C3A-C4A	-10.77	98.50	106.49
39	10	313	DD6	C9-C10-C11	-10.76	111.96	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	14	318	A86	O1-C20-C21	-10.74	102.19	115.06
38	13	310	KC1	CMA-C3A-C4A	-10.73	108.70	125.04
37	4	317	A86	C21-C20-C19	-10.72	102.22	114.28
38	6	313	KC1	CMA-C3A-C4A	-10.71	108.74	125.04
38	2	312	KC1	CMA-C3A-C4A	-10.70	108.75	125.04
39	8	317	DD6	C12-C11-C10	-10.69	107.95	122.92
38	4	308	KC1	C2A-C3A-C4A	-10.68	98.56	106.49
30	2	303	CLA	C1D-ND-C4D	-10.68	98.75	106.33
39	15	319	DD6	C9-C10-C11	-10.63	112.14	127.31
37	8	318	A86	C21-C20-C19	-10.62	102.33	114.28
39	6	321	DD6	C9-C10-C11	-10.61	112.16	127.31
39	3	313	DD6	C12-C11-C10	-10.61	108.07	122.92
30	L	202	CLA	C1D-ND-C4D	-10.61	98.80	106.33
39	6	318	DD6	C12-C11-C10	-10.60	108.07	122.92
38	8	306	KC1	CMA-C3A-C4A	-10.60	108.89	125.04
37	15	317	A86	C21-C20-C19	-10.60	102.36	114.28
38	8	310	KC1	CMA-C3A-C4A	-10.59	108.91	125.04
37	2u	203	A86	O1-C20-C21	-10.59	102.36	115.06
39	7	314	DD6	C12-C11-C10	-10.59	108.09	122.92
38	11	307	KC1	CMA-C3A-C4A	-10.57	108.94	125.04
37	16	312	A86	C21-C20-C19	-10.57	102.39	114.28
37	2	318	A86	C17-C16-C15	10.53	119.90	109.16
37	14	301	A86	C21-C20-C19	-10.51	102.45	114.28
38	9	304	KC1	CMA-C3A-C4A	-10.51	109.04	125.04
39	10	314	DD6	C13-C11-C10	-10.50	102.82	118.94
37	10	317	A86	O1-C20-C21	-10.50	102.48	115.06
38	11	311	KC1	CMA-C3A-C4A	-10.49	109.06	125.04
37	11	301	A86	C21-C20-C19	-10.49	102.48	114.28
39	6	303	DD6	C32-C31-C36	-10.49	107.82	122.63
38	1	306	KC1	CMA-C3A-C4A	-10.48	109.08	125.04
38	14	311	KC1	CMA-C3A-C4A	-10.47	109.09	125.04
39	11	313	DD6	C4-C5-C6	-10.41	112.45	127.31
39	12	317	DD6	C3-C2-C1	-10.41	112.45	127.31
37	8	315	A86	O1-C20-C21	-10.41	102.59	115.06
39	15	319	DD6	C12-C11-C10	-10.41	108.35	122.92
37	12	314	A86	C21-C20-C19	-10.40	102.58	114.28
37	1	309	A86	C4-C5-C6	-10.39	112.49	127.31
39	15	318	DD6	C4-C5-C6	-10.38	112.50	127.31
37	15	321	A86	O1-C20-C21	-10.38	102.62	115.06
37	7	315	A86	C21-C20-C19	-10.37	102.61	114.28
37	10	302	A86	O1-C20-C21	-10.37	102.63	115.06
37	5	315	A86	C21-C20-C19	-10.37	102.62	114.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	9	314	DD6	C4-C5-C6	-10.37	112.51	127.31
38	10	310	KC1	CMA-C3A-C4A	-10.37	109.25	125.04
37	2	319	A86	C21-C20-C19	-10.36	102.62	114.28
37	14	314	A86	C33-C32-C31	10.36	119.28	109.21
37	7	319	A86	C21-C20-C19	-10.35	102.63	114.28
37	4	314	A86	C21-C20-C19	-10.35	102.63	114.28
37	7	315	A86	C17-C16-C15	10.34	119.71	109.16
39	4	316	DD6	C12-C11-C10	-10.33	108.46	122.92
37	14	319	A86	O1-C20-C21	-10.32	102.69	115.06
39	16	313	DD6	C13-C11-C10	-10.31	103.12	118.94
30	A	806	CLA	C1D-ND-C4D	-10.31	99.01	106.33
37	10	302	A86	C21-C20-C19	-10.30	102.70	114.28
37	7	319	A86	O1-C20-C21	-10.30	102.72	115.06
39	13	314	DD6	C4-C5-C6	-10.29	112.62	127.31
38	13	312	KC1	CMA-C3A-C4A	-10.29	109.36	125.04
37	6	320	A86	C17-C16-C15	10.29	119.66	109.16
39	2	315	DD6	C8-C6-C5	-10.28	103.16	118.94
39	1	310	DD6	C12-C11-C10	-10.28	108.52	122.92
30	B	830	CLA	C1D-ND-C4D	-10.27	99.04	106.33
30	14	307	CLA	C1D-ND-C4D	-10.26	99.05	106.33
39	7	318	DD6	C4-C5-C6	-10.25	112.68	127.31
39	9	314	DD6	C12-C11-C10	-10.25	108.56	122.92
37	14	301	A86	O1-C20-C21	-10.24	102.79	115.06
39	2	315	DD6	C37-C36-C31	-10.23	110.44	124.35
39	2	317	DD6	C37-C36-C31	-10.22	110.46	124.35
39	5	313	DD6	C13-C11-C10	-10.22	103.26	118.94
30	B	820	CLA	C1D-ND-C4D	-10.22	99.08	106.33
37	10	317	A86	C21-C20-C19	-10.22	102.78	114.28
37	9	316	A86	C21-C20-C19	-10.21	102.79	114.28
37	11	314	A86	O1-C20-C21	-10.21	102.82	115.06
37	3	314	A86	C21-C20-C19	-10.19	102.81	114.28
38	3	308	KC1	C2A-C3A-C4A	-10.19	98.93	106.49
30	16	303	CLA	C1D-ND-C4D	-10.18	99.10	106.33
39	7	318	DD6	C12-C11-C10	-10.18	108.67	122.92
38	3	308	KC1	CMA-C3A-C4A	-10.16	109.56	125.04
38	11	311	KC1	C2A-C3A-C4A	-10.16	98.95	106.49
37	4	312	A86	O1-C20-C21	-10.15	102.90	115.06
39	2	317	DD6	C9-C10-C11	-10.13	112.85	127.31
39	10	313	DD6	C8-C6-C5	-10.13	103.40	118.94
39	7	314	DD6	C3-C2-C1	-10.12	112.87	127.31
38	10	310	KC1	C2A-C3A-C4A	-10.11	98.98	106.49
39	2	315	DD6	C7-C6-C5	-10.10	108.78	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	2	318	A86	C33-C32-C31	10.08	119.01	109.21
38	8	313	KC1	C2A-C3A-C4A	-10.07	99.01	106.49
38	9	312	KC1	CMA-C3A-C2A	-10.07	103.64	128.30
38	13	308	KC1	C2A-C3A-C4A	-10.04	99.04	106.49
37	2u	203	A86	C21-C20-C19	-10.04	102.99	114.28
38	7	313	KC1	CMA-C3A-C4A	-10.03	109.76	125.04
39	12	315	DD6	C12-C11-C10	-10.03	108.87	122.92
37	11	301	A86	O1-C20-C21	-10.03	103.04	115.06
38	7	308	KC1	CMA-C3A-C4A	-10.03	109.77	125.04
39	3	316	DD6	C4-C5-C6	-10.01	113.02	127.31
39	12	317	DD6	C9-C10-C11	-10.01	113.03	127.31
37	2u	205	A86	C17-C16-C15	10.01	119.37	109.16
39	7	302	DD6	C9-C10-C11	-10.00	113.04	127.31
38	6	313	KC1	C2A-C3A-C4A	-10.00	99.07	106.49
37	4	314	A86	O1-C20-C21	-10.00	103.08	115.06
38	4	307	KC1	C2A-C3A-C4A	-9.98	99.08	106.49
30	15	302	CLA	C1D-ND-C4D	-9.98	99.25	106.33
38	6	312	KC1	CMA-C3A-C4A	-9.98	109.84	125.04
39	10	313	DD6	C7-C6-C5	-9.95	108.98	122.92
37	7	316	A86	C21-C20-C19	-9.94	103.09	114.28
37	12	314	A86	O1-C20-C21	-9.94	103.15	115.06
39	16	313	DD6	C3-C2-C1	-9.93	113.14	127.31
39	15	319	DD6	C4-C5-C6	-9.92	113.15	127.31
39	5	314	DD6	C4-C5-C6	-9.92	113.15	127.31
38	1	306	KC1	C2A-C3A-C4A	-9.92	99.13	106.49
38	6	311	KC1	C2A-C3A-C4A	-9.91	99.13	106.49
38	7	308	KC1	C2A-C3A-C4A	-9.91	99.13	106.49
39	11	313	DD6	C7-C6-C5	-9.91	109.05	122.92
30	A	827	CLA	C1D-ND-C4D	-9.90	99.30	106.33
38	14	308	KC1	C2A-C3A-C4A	-9.90	99.14	106.49
39	15	318	DD6	C9-C10-C11	-9.89	113.19	127.31
30	B	822	CLA	C1D-ND-C4D	-9.89	99.31	106.33
39	2	316	DD6	C13-C11-C10	-9.88	103.78	118.94
38	2	306	KC1	C2A-C3A-C4A	-9.88	99.16	106.49
38	14	311	KC1	C2A-C3A-C4A	-9.88	99.16	106.49
39	5	313	DD6	C4-C5-C6	-9.87	113.22	127.31
39	6	318	DD6	C9-C10-C11	-9.86	113.25	127.31
30	B	820	CLA	C2D-C1D-ND	9.85	117.36	110.10
37	12	316	A86	O1-C20-C21	-9.85	103.25	115.06
39	5	314	DD6	C12-C11-C10	-9.85	109.12	122.92
39	4	313	DD6	C12-C11-C10	-9.84	109.14	122.92
37	15	320	A86	O1-C20-C21	-9.83	103.27	115.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	15	319	DD6	C37-C36-C31	-9.83	110.99	124.35
39	2	317	DD6	C29-C30-C31	-9.83	150.54	175.43
30	L	202	CLA	C2D-C1D-ND	9.82	117.34	110.10
38	13	306	KC1	CMA-C3A-C4A	-9.81	110.10	125.04
39	10	314	DD6	C12-C11-C10	-9.81	109.19	122.92
37	15	316	A86	C21-C20-C19	-9.80	103.26	114.28
38	9	311	KC1	C2A-C3A-C4A	-9.79	99.22	106.49
30	15	314	CLA	C1D-ND-C4D	-9.79	99.38	106.33
30	B	817	CLA	C1D-ND-C4D	-9.78	99.39	106.33
30	A	818	CLA	C1D-ND-C4D	-9.78	99.39	106.33
39	4	313	DD6	C9-C10-C11	-9.78	113.36	127.31
39	12	315	DD6	C4-C5-C6	-9.76	113.38	127.31
30	B	830	CLA	C2D-C1D-ND	9.75	117.29	110.10
38	13	305	KC1	C2A-C3A-C4A	-9.74	99.26	106.49
39	3	312	DD6	C12-C11-C10	-9.73	109.29	122.92
38	5	310	KC1	C2A-C3A-C4A	-9.73	99.27	106.49
39	6	318	DD6	C4-C5-C6	-9.72	113.44	127.31
39	2	315	DD6	C29-C30-C31	-9.71	150.84	175.43
38	9	304	KC1	C2A-C3A-C4A	-9.71	99.28	106.49
39	2	317	DD6	C12-C11-C10	-9.71	109.33	122.92
38	10	312	KC1	C2A-C3A-C4A	-9.70	99.29	106.49
30	A	817	CLA	C1D-ND-C4D	-9.70	99.45	106.33
37	10	315	A86	O1-C20-C21	-9.69	103.44	115.06
30	B	816	CLA	C1D-ND-C4D	-9.69	99.45	106.33
38	5	312	KC1	C2A-C3A-C4A	-9.68	99.30	106.49
30	13	301	CLA	C1D-ND-C4D	-9.68	99.46	106.33
38	14	308	KC1	CMA-C3A-C4A	-9.67	110.31	125.04
37	2	302	A86	O1-C20-C21	-9.67	103.47	115.06
38	14	306	KC1	C2A-C3A-C4A	-9.67	99.31	106.49
39	3	316	DD6	C12-C11-C10	-9.67	109.38	122.92
38	11	307	KC1	C2A-C3A-C4A	-9.66	99.32	106.49
30	8	305	CLA	C1D-ND-C4D	-9.65	99.48	106.33
38	9	310	KC1	C2A-C3A-C4A	-9.64	99.33	106.49
39	6	303	DD6	C37-C36-C31	-9.63	111.26	124.35
37	15	322	A86	O1-C20-C21	-9.63	103.52	115.06
39	7	318	DD6	C7-C6-C5	-9.63	109.44	122.92
38	4	310	KC1	C2A-C3A-C4A	-9.63	99.35	106.49
39	4	313	DD6	C3-C2-C1	-9.62	113.58	127.31
39	6	303	DD6	C3-C2-C1	-9.62	113.58	127.31
30	16	301	CLA	C1D-ND-C4D	-9.61	99.50	106.33
30	7	305	CLA	C1D-ND-C4D	-9.61	99.51	106.33
39	1	310	DD6	C9-C10-C11	-9.60	113.60	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	11	304	CLA	C1D-ND-C4D	-9.60	99.51	106.33
30	A	823	CLA	C1D-ND-C4D	-9.60	99.52	106.33
39	7	302	DD6	C12-C11-C10	-9.60	109.48	122.92
38	8	310	KC1	C2A-C3A-C4A	-9.58	99.38	106.49
37	14	315	A86	C4-C5-C6	-9.58	113.63	127.31
38	12	305	KC1	C2A-C3A-C4A	-9.58	99.38	106.49
39	6	319	DD6	C9-C10-C11	-9.58	113.64	127.31
39	10	314	DD6	C4-C5-C6	-9.58	113.64	127.31
39	8	316	DD6	C4-C5-C6	-9.57	113.65	127.31
39	16	313	DD6	C-C1-C2	-9.57	109.52	122.92
38	9	312	KC1	CMA-C3A-C4A	-9.56	110.48	125.04
37	11	316	A86	O1-C20-C21	-9.54	103.62	115.06
37	15	316	A86	O1-C20-C21	-9.54	103.63	115.06
30	13	303	CLA	C1D-ND-C4D	-9.54	99.56	106.33
30	2	311	CLA	C1D-ND-C4D	-9.53	99.56	106.33
39	7	318	DD6	C-C1-C2	-9.52	109.59	122.92
38	14	306	KC1	CMA-C3A-C4A	-9.51	110.56	125.04
37	2u	205	A86	C21-C20-C19	-9.51	103.59	114.28
38	13	312	KC1	C2A-C3A-C4A	-9.50	99.44	106.49
30	13	304	CLA	C1D-ND-C4D	-9.50	99.59	106.33
37	2	318	A86	O1-C20-C21	-9.50	103.67	115.06
37	9	315	A86	C17-C16-C15	9.50	118.85	109.16
39	15	319	DD6	C7-C6-C5	-9.49	109.63	122.92
39	16	313	DD6	C7-C6-C5	-9.49	109.63	122.92
38	1	308	KC1	C2A-C3A-C4A	-9.48	99.45	106.49
39	6	318	DD6	C3-C2-C1	-9.47	113.79	127.31
30	1	307	CLA	C1D-ND-C4D	-9.46	99.61	106.33
30	12	310	CLA	C1D-ND-C4D	-9.46	99.61	106.33
38	11	305	KC1	C2A-C3A-C4A	-9.45	99.48	106.49
39	2	315	DD6	C12-C11-C10	-9.45	109.69	122.92
39	11	313	DD6	C3-C2-C1	-9.45	113.83	127.31
39	15	318	DD6	C12-C11-C10	-9.44	109.69	122.92
37	15	315	A86	C3-C2-C1	-9.44	113.83	127.31
30	3	309	CLA	C1D-ND-C4D	-9.44	99.63	106.33
30	14	313	CLA	C1D-ND-C4D	-9.44	99.63	106.33
39	12	317	DD6	C-C1-C2	-9.42	109.73	122.92
37	14	314	A86	C4-C5-C6	-9.42	113.87	127.31
39	6	321	DD6	C3-C2-C1	-9.41	113.88	127.31
39	5	314	DD6	C3-C2-C1	-9.40	113.89	127.31
38	7	313	KC1	C2A-C3A-C4A	-9.40	99.51	106.49
37	3	314	A86	O1-C20-C21	-9.37	103.82	115.06
30	7	307	CLA	C1D-ND-C4D	-9.37	99.68	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	13	310	KC1	C2A-C3A-C4A	-9.37	99.53	106.49
30	B	836	CLA	C1D-ND-C4D	-9.37	99.68	106.33
39	13	314	DD6	C13-C11-C10	-9.37	104.56	118.94
39	3	316	DD6	C3-C2-C1	-9.37	113.94	127.31
30	15	309	CLA	C1D-ND-C4D	-9.36	99.68	106.33
39	15	318	DD6	C7-C6-C5	-9.36	109.82	122.92
30	A	803	CLA	C2D-C1D-ND	9.35	117.00	110.10
30	B	801	CLA	C1D-ND-C4D	-9.35	99.70	106.33
39	2	317	DD6	C-C1-C2	-9.33	109.86	122.92
30	10	311	CLA	C1D-ND-C4D	-9.33	99.71	106.33
37	10	301	A86	C21-C20-C19	-9.33	103.79	114.28
30	14	310	CLA	C1D-ND-C4D	-9.32	99.71	106.33
30	A	812	CLA	C1D-ND-C4D	-9.32	99.71	106.33
30	A	828	CLA	C2D-C1D-ND	9.32	116.97	110.10
30	15	304	CLA	C1D-ND-C4D	-9.32	99.72	106.33
30	B	839	CLA	C1D-ND-C4D	-9.31	99.72	106.33
30	7	303	CLA	C1D-ND-C4D	-9.31	99.72	106.33
30	16	309	CLA	C1D-ND-C4D	-9.30	99.73	106.33
37	16	314	A86	C21-C20-C19	-9.30	103.82	114.28
30	A	828	CLA	C1D-ND-C4D	-9.29	99.73	106.33
30	3	307	CLA	C1D-ND-C4D	-9.29	99.73	106.33
38	16	304	KC1	C2A-C3A-C4A	-9.29	99.59	106.49
39	1	310	DD6	C4-C5-C6	-9.29	114.06	127.31
39	9	314	DD6	C3-C2-C1	-9.29	114.06	127.31
38	13	311	KC1	C2A-C3A-C4A	-9.28	99.60	106.49
30	9	301	CLA	C1D-ND-C4D	-9.28	99.74	106.33
39	4	316	DD6	C-C1-C2	-9.27	109.93	122.92
39	4	313	DD6	C-C1-C2	-9.27	109.94	122.92
37	14	317	A86	C33-C32-C31	9.27	118.22	109.21
37	4	312	A86	C33-C32-C31	9.27	118.22	109.21
30	B	810	CLA	C1D-ND-C4D	-9.25	99.76	106.33
30	4	311	CLA	C1D-ND-C4D	-9.25	99.76	106.33
30	L	203	CLA	C1D-ND-C4D	-9.25	99.76	106.33
39	8	316	DD6	C3-C2-C1	-9.25	114.11	127.31
30	1	303	CLA	C1D-ND-C4D	-9.25	99.76	106.33
30	10	309	CLA	C1D-ND-C4D	-9.25	99.76	106.33
30	A	808	CLA	C1D-ND-C4D	-9.24	99.77	106.33
30	2	313	CLA	C1D-ND-C4D	-9.24	99.77	106.33
39	10	313	DD6	C3-C2-C1	-9.23	114.13	127.31
30	F	201	CLA	C1D-ND-C4D	-9.23	99.78	106.33
30	B	831	CLA	C1D-ND-C4D	-9.23	99.78	106.33
30	B	802	CLA	C2D-C1D-ND	9.23	116.91	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	14	302	CLA	C1D-ND-C4D	-9.23	99.78	106.33
30	A	811	CLA	C1D-ND-C4D	-9.22	99.78	106.33
30	2	309	CLA	C1D-ND-C4D	-9.22	99.78	106.33
30	9	302	CLA	C1D-ND-C4D	-9.22	99.78	106.33
39	2	315	DD6	C3-C2-C1	-9.22	114.15	127.31
30	5	311	CLA	C1D-ND-C4D	-9.21	99.79	106.33
30	10	305	CLA	C1D-ND-C4D	-9.21	99.79	106.33
39	9	314	DD6	C13-C11-C10	-9.21	104.81	118.94
30	15	313	CLA	C1D-ND-C4D	-9.20	99.80	106.33
30	A	842	CLA	C1D-ND-C4D	-9.20	99.80	106.33
38	2	312	KC1	C2A-C3A-C4A	-9.20	99.66	106.49
30	B	803	CLA	C2D-C1D-ND	9.20	116.88	110.10
30	7	310	CLA	C1D-ND-C4D	-9.18	99.81	106.33
30	A	816	CLA	C1D-ND-C4D	-9.18	99.81	106.33
30	2u	202	CLA	C1D-ND-C4D	-9.18	99.81	106.33
39	2	316	DD6	C8-C6-C5	-9.18	104.86	118.94
37	4	315	A86	C33-C32-C31	9.17	118.13	109.21
30	B	837	CLA	C1D-ND-C4D	-9.17	99.82	106.33
30	A	827	CLA	C2D-C1D-ND	9.17	116.86	110.10
30	1	302	CLA	C1D-ND-C4D	-9.17	99.82	106.33
38	8	307	KC1	C2A-C3A-C4A	-9.16	99.69	106.49
30	5	304	CLA	C1D-ND-C4D	-9.15	99.83	106.33
39	3	313	DD6	C7-C6-C5	-9.15	110.11	122.92
30	15	311	CLA	C1D-ND-C4D	-9.15	99.84	106.33
30	2	301	CLA	C1D-ND-C4D	-9.14	99.84	106.33
37	16	312	A86	O1-C20-C21	-9.14	104.10	115.06
37	2	302	A86	C4-C5-C6	-9.14	114.26	127.31
30	12	308	CLA	C1D-ND-C4D	-9.14	99.84	106.33
30	6	317	CLA	C1D-ND-C4D	-9.13	99.85	106.33
39	4	316	DD6	C7-C6-C5	-9.13	110.13	122.92
30	6	314	CLA	C1D-ND-C4D	-9.13	99.85	106.33
39	11	313	DD6	C12-C11-C10	-9.13	110.13	122.92
30	11	309	CLA	C1D-ND-C4D	-9.13	99.85	106.33
30	B	802	CLA	C1D-ND-C4D	-9.13	99.85	106.33
39	2	317	DD6	C32-C31-C36	-9.13	109.74	122.63
37	9	316	A86	C17-C16-C15	9.13	118.47	109.16
39	13	314	DD6	C7-C6-C5	-9.13	110.14	122.92
39	10	314	DD6	C7-C6-C5	-9.12	110.14	122.92
39	3	313	DD6	C3-C2-C1	-9.12	114.30	127.31
30	4	305	CLA	C1D-ND-C4D	-9.11	99.86	106.33
30	B	836	CLA	C2D-C1D-ND	9.11	116.82	110.10
30	15	303	CLA	C1D-ND-C4D	-9.11	99.87	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	5	314	DD6	C7-C6-C5	-9.10	110.17	122.92
30	4	306	CLA	C1D-ND-C4D	-9.10	99.87	106.33
30	8	302	CLA	C1D-ND-C4D	-9.10	99.87	106.33
39	7	302	DD6	C4-C5-C6	-9.10	114.32	127.31
37	11	315	A86	C33-C32-C31	9.10	118.05	109.21
30	14	304	CLA	C1D-ND-C4D	-9.10	99.87	106.33
38	8	306	KC1	C2A-C3A-C4A	-9.09	99.74	106.49
30	11	308	CLA	C1D-ND-C4D	-9.09	99.88	106.33
39	1	310	DD6	C7-C6-C5	-9.08	110.20	122.92
30	A	833	CLA	C1D-ND-C4D	-9.08	99.88	106.33
39	12	315	DD6	C3-C2-C1	-9.08	114.35	127.31
39	6	321	DD6	C13-C11-C10	-9.08	105.01	118.94
30	A	810	CLA	C1D-ND-C4D	-9.07	99.89	106.33
30	A	804	CLA	C1D-ND-C4D	-9.07	99.89	106.33
30	4	301	CLA	C1D-ND-C4D	-9.05	99.90	106.33
38	6	312	KC1	C2A-C3A-C4A	-9.05	99.77	106.49
30	8	301	CLA	C1D-ND-C4D	-9.05	99.91	106.33
39	9	314	DD6	C-C1-C2	-9.05	110.25	122.92
30	3	310	CLA	C1D-ND-C4D	-9.04	99.91	106.33
30	16	308	CLA	C1D-ND-C4D	-9.03	99.92	106.33
39	7	318	DD6	C3-C2-C1	-9.03	114.42	127.31
30	8	305	CLA	C2D-C1D-ND	9.03	116.76	110.10
38	6	308	KC1	C2A-C3A-C4A	-9.03	99.79	106.49
39	3	316	DD6	C7-C6-C5	-9.03	110.27	122.92
39	12	317	DD6	C7-C6-C5	-9.02	110.29	122.92
30	B	803	CLA	C1D-ND-C4D	-9.01	99.93	106.33
30	6	306	CLA	C1D-ND-C4D	-9.01	99.94	106.33
30	16	303	CLA	C2D-C1D-ND	9.00	116.74	110.10
39	3	312	DD6	C3-C2-C1	-9.00	114.46	127.31
30	5	302	CLA	C1D-ND-C4D	-9.00	99.94	106.33
30	3	303	CLA	C1D-ND-C4D	-9.00	99.94	106.33
39	5	314	DD6	C8-C6-C5	-9.00	105.14	118.94
30	14	312	CLA	C1D-ND-C4D	-8.99	99.95	106.33
30	F	202	CLA	C1D-ND-C4D	-8.99	99.95	106.33
39	10	314	DD6	C3-C2-C1	-8.99	114.48	127.31
38	2	314	KC1	C2A-C3A-C4A	-8.98	99.82	106.49
30	9	308	CLA	C1D-ND-C4D	-8.98	99.95	106.33
38	11	312	KC1	C2A-C3A-C4A	-8.98	99.82	106.49
39	4	316	DD6	C13-C11-C10	-8.98	105.16	118.94
30	2	308	CLA	C1D-ND-C4D	-8.97	99.96	106.33
30	3	301	CLA	C1D-ND-C4D	-8.97	99.96	106.33
30	B	851	CLA	C1D-ND-C4D	-8.96	99.97	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	15	310	CLA	C1D-ND-C4D	-8.96	99.97	106.33
39	8	317	DD6	C8-C6-C5	-8.95	105.20	118.94
30	A	829	CLA	C1D-ND-C4D	-8.95	99.98	106.33
38	4	307	KC1	CMA-C3A-C4A	-8.95	111.41	125.04
30	4	303	CLA	C1D-ND-C4D	-8.95	99.98	106.33
30	B	826	CLA	C1D-ND-C4D	-8.95	99.98	106.33
30	12	312	CLA	C1D-ND-C4D	-8.94	99.98	106.33
30	14	307	CLA	C2D-C1D-ND	8.93	116.69	110.10
30	6	315	CLA	C1D-ND-C4D	-8.93	99.99	106.33
30	9	301	CLA	C2D-C1D-ND	8.93	116.69	110.10
38	12	311	KC1	C2A-C3A-C4A	-8.93	99.86	106.49
30	10	308	CLA	C1D-ND-C4D	-8.93	99.99	106.33
30	A	824	CLA	C1D-ND-C4D	-8.93	99.99	106.33
39	7	302	DD6	C7-C6-C5	-8.93	110.42	122.92
30	16	307	CLA	C1D-ND-C4D	-8.92	100.00	106.33
30	1	304	CLA	C1D-ND-C4D	-8.92	100.00	106.33
30	F	203	CLA	C1D-ND-C4D	-8.92	100.00	106.33
30	8	303	CLA	C1D-ND-C4D	-8.92	100.00	106.33
30	5	309	CLA	C1D-ND-C4D	-8.91	100.00	106.33
30	9	303	CLA	C1D-ND-C4D	-8.91	100.00	106.33
38	8	311	KC1	C2A-C3A-C4A	-8.91	99.87	106.49
30	A	819	CLA	C1D-ND-C4D	-8.91	100.01	106.33
30	11	306	CLA	C1D-ND-C4D	-8.90	100.01	106.33
30	16	302	CLA	C1D-ND-C4D	-8.90	100.01	106.33
30	A	839	CLA	C1D-ND-C4D	-8.90	100.01	106.33
30	14	303	CLA	C1D-ND-C4D	-8.90	100.02	106.33
37	11	314	A86	C4-C5-C6	-8.89	114.62	127.31
30	11	310	CLA	C1D-ND-C4D	-8.89	100.02	106.33
39	6	321	DD6	C-C1-C2	-8.89	110.47	122.92
30	B	806	CLA	C1D-ND-C4D	-8.89	100.02	106.33
30	B	835	CLA	C1D-ND-C4D	-8.89	100.02	106.33
30	B	804	CLA	C1D-ND-C4D	-8.89	100.02	106.33
37	14	314	A86	O1-C20-C21	-8.88	104.41	115.06
37	7	316	A86	C17-C16-C15	8.88	118.23	109.16
30	A	806	CLA	C2D-C1D-ND	8.88	116.65	110.10
30	5	308	CLA	C1D-ND-C4D	-8.88	100.03	106.33
37	14	320	A86	C21-C20-C19	-8.88	104.29	114.28
30	A	803	CLA	C1D-ND-C4D	-8.88	100.03	106.33
30	B	808	CLA	C1D-ND-C4D	-8.88	100.03	106.33
30	16	310	CLA	C1D-ND-C4D	-8.88	100.03	106.33
30	A	834	CLA	C1D-ND-C4D	-8.87	100.03	106.33
30	4	304	CLA	C1D-ND-C4D	-8.87	100.03	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	8	308	CLA	C1D-ND-C4D	-8.86	100.04	106.33
30	A	844	CLA	C1D-ND-C4D	-8.86	100.04	106.33
30	13	309	CLA	C1D-ND-C4D	-8.86	100.04	106.33
30	A	840	CLA	C1D-ND-C4D	-8.86	100.04	106.33
30	12	304	CLA	C1D-ND-C4D	-8.86	100.04	106.33
39	7	302	DD6	C-C1-C2	-8.86	110.52	122.92
39	12	315	DD6	C7-C6-C5	-8.86	110.52	122.92
37	4	315	A86	O1-C20-C21	-8.86	104.44	115.06
30	8	309	CLA	C1D-ND-C4D	-8.85	100.05	106.33
39	7	302	DD6	C3-C2-C1	-8.85	114.68	127.31
37	3	315	A86	O1-C20-C21	-8.85	104.45	115.06
37	7	316	A86	O1-C20-C21	-8.85	104.45	115.06
30	16	301	CLA	C2D-C1D-ND	8.85	116.63	110.10
30	15	306	CLA	C1D-ND-C4D	-8.85	100.05	106.33
39	2	316	DD6	C3-C2-C1	-8.85	114.68	127.31
39	12	315	DD6	C-C1-C2	-8.84	110.54	122.92
39	11	313	DD6	C-C1-C2	-8.84	110.54	122.92
30	6	304	CLA	C1D-ND-C4D	-8.84	100.06	106.33
30	13	307	CLA	C1D-ND-C4D	-8.84	100.06	106.33
39	13	314	DD6	C9-C10-C11	-8.84	114.70	127.31
38	9	312	KC1	C2A-C3A-C4A	-8.84	99.93	106.49
38	5	306	KC1	C2A-C3A-C4A	-8.84	99.93	106.49
39	7	317	DD6	C-C1-C2	-8.83	110.55	122.92
30	7	307	CLA	C2D-C1D-ND	8.83	116.61	110.10
38	5	306	KC1	CMA-C3A-C2A	-8.82	106.70	128.30
30	12	321	CLA	C1D-ND-C4D	-8.82	100.07	106.33
30	2	305	CLA	C1D-ND-C4D	-8.82	100.07	106.33
38	6	308	KC1	CMA-C3A-C2A	-8.82	106.71	128.30
30	A	805	CLA	C1D-ND-C4D	-8.81	100.07	106.33
30	4	302	CLA	C1D-ND-C4D	-8.81	100.07	106.33
29	A	801	CL0	C1D-ND-C4D	-8.81	100.08	106.33
30	9	307	CLA	C1D-ND-C4D	-8.81	100.08	106.33
30	12	302	CLA	C1D-ND-C4D	-8.81	100.08	106.33
30	15	305	CLA	C1D-ND-C4D	-8.81	100.08	106.33
39	8	317	DD6	C4-C5-C6	-8.80	114.75	127.31
30	1	301	CLA	C1D-ND-C4D	-8.80	100.08	106.33
30	A	813	CLA	C1D-ND-C4D	-8.80	100.08	106.33
30	B	807	CLA	C1D-ND-C4D	-8.80	100.08	106.33
39	12	315	DD6	C9-C10-C11	-8.80	114.76	127.31
30	B	825	CLA	C1D-ND-C4D	-8.79	100.09	106.33
37	11	314	A86	C17-C16-C15	8.78	118.12	109.16
39	12	317	DD6	C8-C6-C5	-8.77	105.48	118.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	15	315	A86	C25-C26-C27	-8.77	114.79	127.31
30	A	823	CLA	C2D-C1D-ND	8.77	116.57	110.10
30	5	303	CLA	C1D-ND-C4D	-8.77	100.10	106.33
30	15	307	CLA	C1D-ND-C4D	-8.77	100.11	106.33
38	3	304	KC1	C2A-C3A-C4A	-8.77	99.98	106.49
30	10	303	CLA	C1D-ND-C4D	-8.77	100.11	106.33
30	9	305	CLA	C1D-ND-C4D	-8.76	100.11	106.33
37	14	316	A86	O1-C20-C21	-8.75	104.57	115.06
30	B	814	CLA	C1D-ND-C4D	-8.75	100.12	106.33
30	2	310	CLA	C1D-ND-C4D	-8.75	100.12	106.33
39	6	303	DD6	C7-C6-C5	-8.75	110.66	122.92
39	2	315	DD6	C-C1-C2	-8.75	110.67	122.92
30	A	818	CLA	C2D-C1D-ND	8.75	116.55	110.10
30	B	805	CLA	C1D-ND-C4D	-8.74	100.12	106.33
30	12	307	CLA	C1D-ND-C4D	-8.73	100.13	106.33
38	10	306	KC1	CMA-C3A-C2A	-8.73	106.93	128.30
30	13	302	CLA	C1D-ND-C4D	-8.73	100.13	106.33
39	1	310	DD6	C13-C11-C10	-8.73	105.55	118.94
30	7	309	CLA	C1D-ND-C4D	-8.72	100.14	106.33
30	3	302	CLA	C1D-ND-C4D	-8.71	100.15	106.33
30	4	309	CLA	C1D-ND-C4D	-8.71	100.15	106.33
30	B	811	CLA	C1D-ND-C4D	-8.71	100.15	106.33
30	7	311	CLA	C1D-ND-C4D	-8.71	100.15	106.33
30	B	827	CLA	C1D-ND-C4D	-8.71	100.15	106.33
39	4	316	DD6	C9-C10-C11	-8.70	114.89	127.31
39	9	314	DD6	C7-C6-C5	-8.69	110.74	122.92
30	B	832	CLA	C1D-ND-C4D	-8.69	100.16	106.33
37	15	315	A86	C17-C16-C15	8.69	118.03	109.16
30	10	304	CLA	C1D-ND-C4D	-8.69	100.16	106.33
37	11	315	A86	C21-C20-C19	-8.68	104.52	114.28
30	F	201	CLA	C2D-C1D-ND	8.68	116.50	110.10
30	A	830	CLA	C1D-ND-C4D	-8.68	100.17	106.33
37	15	322	A86	C17-C16-C15	8.67	118.01	109.16
30	7	312	CLA	C1D-ND-C4D	-8.67	100.18	106.33
37	14	319	A86	C33-C32-C31	8.67	117.64	109.21
30	16	305	CLA	C1D-ND-C4D	-8.67	100.18	106.33
30	F	202	CLA	C2D-C1D-ND	8.67	116.49	110.10
38	10	306	KC1	C2A-C3A-C4A	-8.67	100.06	106.49
30	3	305	CLA	C1D-ND-C4D	-8.66	100.18	106.33
39	8	317	DD6	C7-C6-C5	-8.66	110.79	122.92
30	A	843	CLA	C1D-ND-C4D	-8.66	100.18	106.33
30	B	838	CLA	C1D-ND-C4D	-8.65	100.19	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	6	305	CLA	C1D-ND-C4D	-8.64	100.20	106.33
38	3	311	KC1	CMA-C3A-C2A	-8.64	107.15	128.30
30	7	304	CLA	C1D-ND-C4D	-8.64	100.20	106.33
39	10	313	DD6	C-C1-C2	-8.63	110.83	122.92
30	16	306	CLA	C1D-ND-C4D	-8.63	100.20	106.33
30	B	833	CLA	C1D-ND-C4D	-8.63	100.21	106.33
30	9	306	CLA	C1D-ND-C4D	-8.63	100.21	106.33
39	12	315	DD6	C13-C11-C10	-8.62	105.71	118.94
37	14	320	A86	C33-C32-C31	8.62	117.59	109.21
30	2	303	CLA	C2D-C1D-ND	8.61	116.45	110.10
38	13	306	KC1	C2A-C3A-C4A	-8.61	100.10	106.49
38	5	305	KC1	C2A-C3A-C4A	-8.61	100.10	106.49
30	B	839	CLA	C2D-C1D-ND	8.60	116.44	110.10
30	A	821	CLA	C1D-ND-C4D	-8.60	100.22	106.33
37	5	301	A86	C17-C16-C15	8.60	117.93	109.16
30	14	305	CLA	C1D-ND-C4D	-8.57	100.25	106.33
38	16	311	KC1	CMA-C3A-C4A	-8.57	111.99	125.04
30	7	303	CLA	C2D-C1D-ND	8.56	116.41	110.10
30	B	804	CLA	C2D-C1D-ND	8.56	116.41	110.10
30	15	308	CLA	C1D-ND-C4D	-8.56	100.25	106.33
38	12	309	KC1	CMA-C3A-C4A	-8.55	112.02	125.04
30	B	829	CLA	C1D-ND-C4D	-8.55	100.26	106.33
30	B	824	CLA	C1D-ND-C4D	-8.55	100.26	106.33
39	3	313	DD6	C4-C5-C6	-8.55	115.11	127.31
30	A	814	CLA	C1D-ND-C4D	-8.54	100.27	106.33
37	2	318	A86	C21-C20-C19	-8.54	104.67	114.28
30	15	312	CLA	C1D-ND-C4D	-8.54	100.27	106.33
30	6	310	CLA	C1D-ND-C4D	-8.53	100.27	106.33
30	1	305	CLA	C1D-ND-C4D	-8.52	100.28	106.33
39	1	310	DD6	C3-C2-C1	-8.52	115.15	127.31
30	A	807	CLA	C1D-ND-C4D	-8.52	100.28	106.33
37	5	316	A86	C17-C16-C15	8.51	117.84	109.16
39	3	316	DD6	C-C1-C2	-8.51	111.01	122.92
37	15	315	A86	O1-C20-C21	-8.50	104.87	115.06
30	A	825	CLA	C1D-ND-C4D	-8.50	100.30	106.33
30	2	304	CLA	C1D-ND-C4D	-8.50	100.30	106.33
30	4	301	CLA	C2D-C1D-ND	8.50	116.37	110.10
30	15	314	CLA	C2D-C1D-ND	8.50	116.37	110.10
37	2	302	A86	C25-C26-C27	-8.50	115.18	127.31
39	3	312	DD6	C-C1-C2	-8.49	111.03	122.92
30	5	307	CLA	C1D-ND-C4D	-8.49	100.30	106.33
38	8	307	KC1	CMA-C3A-C2A	-8.49	107.52	128.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	826	CLA	C2D-C1D-ND	8.48	116.35	110.10
37	5	316	A86	C33-C32-C31	8.48	117.45	109.21
38	5	305	KC1	CMA-C3A-C2A	-8.47	107.55	128.30
39	2	315	DD6	C32-C31-C36	-8.47	110.67	122.63
39	16	313	DD6	C8-C6-C5	-8.47	105.94	118.94
39	10	314	DD6	C-C1-C2	-8.47	111.06	122.92
30	A	837	CLA	C1D-ND-C4D	-8.45	100.33	106.33
30	B	818	CLA	C1D-ND-C4D	-8.45	100.33	106.33
30	13	301	CLA	C2D-C1D-ND	8.45	116.33	110.10
30	12	306	CLA	C1D-ND-C4D	-8.45	100.33	106.33
30	A	826	CLA	C1D-ND-C4D	-8.45	100.33	106.33
30	A	832	CLA	C1D-ND-C4D	-8.44	100.34	106.33
39	15	319	DD6	C32-C31-C36	-8.43	110.73	122.63
39	5	313	DD6	C12-C11-C10	-8.43	111.11	122.92
39	6	319	DD6	C3-C2-C1	-8.43	115.28	127.31
30	A	812	CLA	C2D-C1D-ND	8.42	116.31	110.10
30	10	307	CLA	C1D-ND-C4D	-8.42	100.36	106.33
30	A	809	CLA	C1D-ND-C4D	-8.41	100.36	106.33
30	A	831	CLA	O2D-CGD-CBD	8.41	126.20	111.27
38	8	312	KC1	C1A-C2A-C3A	-8.41	100.44	107.11
38	3	311	KC1	C2A-C3A-C4A	-8.40	100.26	106.49
38	5	306	KC1	C2B-C1B-NB	8.39	116.29	110.10
30	B	816	CLA	C2D-C1D-ND	8.39	116.29	110.10
30	B	809	CLA	C1D-ND-C4D	-8.38	100.38	106.33
39	8	316	DD6	C7-C6-C5	-8.38	111.18	122.92
30	9	309	CLA	C1D-ND-C4D	-8.38	100.38	106.33
30	14	309	CLA	C1D-ND-C4D	-8.37	100.39	106.33
39	13	314	DD6	C-C1-C2	-8.37	111.20	122.92
37	13	313	A86	C4-C5-C6	-8.37	115.37	127.31
38	13	311	KC1	CMA-C3A-C2A	-8.37	107.82	128.30
30	A	842	CLA	C2D-C1D-ND	8.36	116.27	110.10
39	6	321	DD6	C4-C5-C6	-8.36	115.38	127.31
30	A	835	CLA	C1D-ND-C4D	-8.35	100.40	106.33
37	3	314	A86	C4-C5-C6	-8.35	115.39	127.31
38	12	313	KC1	C2B-C1B-NB	8.35	116.26	110.10
30	B	815	CLA	C1D-ND-C4D	-8.34	100.41	106.33
38	8	314	KC1	C2B-C1B-NB	8.34	116.25	110.10
39	7	314	DD6	C4-C5-C6	-8.34	115.41	127.31
30	B	817	CLA	C2D-C1D-ND	8.34	116.25	110.10
30	2	301	CLA	C2D-C1D-ND	8.33	116.24	110.10
37	7	315	A86	O1-C20-C21	-8.32	105.08	115.06
30	8	304	CLA	C1D-ND-C4D	-8.32	100.43	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	807	CLA	C2D-C1D-ND	8.32	116.23	110.10
39	2	316	DD6	C-C1-C2	-8.32	111.27	122.92
30	A	804	CLA	C2D-C1D-ND	8.32	116.23	110.10
39	5	313	DD6	C3-C2-C1	-8.31	115.44	127.31
38	11	312	KC1	CMA-C3A-C4A	-8.31	112.38	125.04
39	5	314	DD6	C-C1-C2	-8.31	111.28	122.92
30	15	302	CLA	C2D-C1D-ND	8.31	116.23	110.10
30	J	101	CLA	C1D-ND-C4D	-8.31	100.43	106.33
38	9	311	KC1	CMA-C3A-C2A	-8.31	107.97	128.30
37	14	315	A86	C33-C32-C31	8.30	117.28	109.21
30	2	307	CLA	C1D-ND-C4D	-8.30	100.44	106.33
30	A	811	CLA	C2D-C1D-ND	8.28	116.20	110.10
30	10	307	CLA	C2D-C1D-ND	8.27	116.20	110.10
30	A	808	CLA	C2D-C1D-ND	8.27	116.20	110.10
30	5	307	CLA	C2D-C1D-ND	8.27	116.20	110.10
30	8	302	CLA	C2D-C1D-ND	8.27	116.19	110.10
30	12	303	CLA	C1D-ND-C4D	-8.25	100.47	106.33
30	B	813	CLA	C1D-ND-C4D	-8.25	100.48	106.33
30	6	309	CLA	C1D-ND-C4D	-8.24	100.48	106.33
30	A	816	CLA	C2D-C1D-ND	8.24	116.18	110.10
30	1	303	CLA	C2D-C1D-ND	8.24	116.17	110.10
30	A	810	CLA	C2D-C1D-ND	8.24	116.17	110.10
37	11	315	A86	O1-C20-C21	-8.24	105.19	115.06
39	6	303	DD6	C-C1-C2	-8.23	111.39	122.92
37	9	315	A86	O1-C20-C21	-8.23	105.19	115.06
37	9	315	A86	C25-C26-C27	-8.23	115.57	127.31
30	8	301	CLA	C2D-C1D-ND	8.23	116.17	110.10
39	6	303	DD6	C9-C10-C11	-8.23	115.57	127.31
30	9	307	CLA	C2D-C1D-ND	8.22	116.17	110.10
39	16	313	DD6	C4-C5-C6	-8.22	115.57	127.31
39	2	317	DD6	C7-C6-C5	-8.22	111.41	122.92
37	14	319	A86	C4-C5-C6	-8.22	115.58	127.31
30	A	817	CLA	C2D-C1D-ND	8.21	116.15	110.10
30	B	828	CLA	C1D-ND-C4D	-8.21	100.51	106.33
39	10	313	DD6	C13-C11-C10	-8.21	106.35	118.94
30	7	306	CLA	C1D-ND-C4D	-8.20	100.51	106.33
30	B	812	CLA	C1D-ND-C4D	-8.19	100.51	106.33
30	9	308	CLA	C2D-C1D-ND	8.19	116.14	110.10
30	11	304	CLA	C2D-C1D-ND	8.19	116.14	110.10
39	7	317	DD6	C4-C5-C6	-8.18	115.63	127.31
30	A	819	CLA	C2D-C1D-ND	8.18	116.14	110.10
39	4	313	DD6	C4-C5-C6	-8.18	115.63	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	813	CLA	C2D-C1D-ND	8.18	116.13	110.10
37	10	302	A86	C33-C32-C31	8.18	117.16	109.21
30	10	311	CLA	C2D-C1D-ND	8.18	116.13	110.10
30	5	308	CLA	C2D-C1D-ND	8.18	116.13	110.10
39	3	313	DD6	C-C1-C2	-8.17	111.47	122.92
30	3	309	CLA	C2D-C1D-ND	8.17	116.13	110.10
30	5	311	CLA	C2D-C1D-ND	8.16	116.12	110.10
30	3	301	CLA	C2D-C1D-ND	8.16	116.11	110.10
30	A	836	CLA	C1D-ND-C4D	-8.15	100.54	106.33
30	2	308	CLA	C2D-C1D-ND	8.15	116.11	110.10
30	A	822	CLA	C1D-ND-C4D	-8.15	100.54	106.33
37	7	315	A86	C33-C32-C31	8.15	117.13	109.21
37	2	319	A86	C33-C32-C31	8.15	117.13	109.21
37	14	318	A86	C4-C5-C6	-8.14	115.69	127.31
30	A	829	CLA	C2D-C1D-ND	8.14	116.10	110.10
30	B	825	CLA	C2D-C1D-ND	8.14	116.10	110.10
37	2	302	A86	C17-C16-C15	8.13	117.46	109.16
39	8	317	DD6	C3-C2-C1	-8.13	115.71	127.31
38	4	310	KC1	C2B-C1B-NB	8.13	116.09	110.10
30	3	305	CLA	C2D-C1D-ND	8.12	116.09	110.10
30	1	304	CLA	C2D-C1D-ND	8.11	116.08	110.10
39	6	321	DD6	C8-C6-C5	-8.11	106.50	118.94
30	2	311	CLA	C2D-C1D-ND	8.10	116.08	110.10
30	4	311	CLA	C2D-C1D-ND	8.10	116.07	110.10
30	B	834	CLA	C1D-ND-C4D	-8.10	100.58	106.33
30	L	203	CLA	C2D-C1D-ND	8.10	116.07	110.10
30	9	302	CLA	C2D-C1D-ND	8.10	116.07	110.10
38	11	305	KC1	CMA-C3A-C2A	-8.10	108.48	128.30
30	B	801	CLA	C2D-C1D-ND	8.09	116.07	110.10
30	A	841	CLA	C1D-ND-C4D	-8.09	100.59	106.33
30	B	821	CLA	C1D-ND-C4D	-8.08	100.59	106.33
30	15	303	CLA	C2D-C1D-ND	8.08	116.06	110.10
38	8	314	KC1	C1A-C2A-C3A	-8.08	100.70	107.11
30	A	809	CLA	C2D-C1D-ND	8.08	116.06	110.10
30	4	305	CLA	C2D-C1D-ND	8.07	116.05	110.10
30	A	831	CLA	C1D-ND-C4D	-8.07	100.60	106.33
30	B	823	CLA	C1D-ND-C4D	-8.07	100.60	106.33
30	B	833	CLA	C2D-C1D-ND	8.07	116.05	110.10
30	3	306	CLA	C1D-ND-C4D	-8.06	100.61	106.33
30	6	316	CLA	C1D-ND-C4D	-8.06	100.61	106.33
30	A	805	CLA	C2D-C1D-ND	8.06	116.05	110.10
30	A	838	CLA	C1D-ND-C4D	-8.06	100.61	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	10	309	CLA	C2D-C1D-ND	8.06	116.04	110.10
30	4	306	CLA	C2D-C1D-ND	8.06	116.04	110.10
37	14	317	A86	C4-C5-C6	-8.06	115.81	127.31
30	4	303	CLA	C2D-C1D-ND	8.05	116.04	110.10
39	15	318	DD6	C3-C2-C1	-8.05	115.82	127.31
39	1	310	DD6	C-C1-C2	-8.05	111.65	122.92
30	A	833	CLA	C2D-C1D-ND	8.04	116.03	110.10
30	2u	202	CLA	C2D-C1D-ND	8.04	116.03	110.10
30	A	826	CLA	C2D-C1D-ND	8.03	116.02	110.10
39	6	303	DD6	C12-C11-C10	-8.03	111.68	122.92
30	7	305	CLA	C2D-C1D-ND	8.03	116.02	110.10
30	6	307	CLA	C1D-ND-C4D	-8.02	100.64	106.33
30	3	302	CLA	C2D-C1D-ND	8.02	116.01	110.10
39	7	317	DD6	C7-C6-C5	-8.02	111.69	122.92
30	B	827	CLA	C2D-C1D-ND	8.01	116.01	110.10
30	9	305	CLA	C2D-C1D-ND	8.01	116.01	110.10
37	15	317	A86	C4-C5-C6	-8.01	115.88	127.31
30	15	308	CLA	C2D-C1D-ND	8.01	116.00	110.10
30	A	815	CLA	C1D-ND-C4D	-8.00	100.65	106.33
37	10	316	A86	O1-C20-C21	-8.00	105.47	115.06
30	15	304	CLA	C2D-C1D-ND	8.00	116.00	110.10
38	8	314	KC1	C2A-C3A-C4A	-8.00	100.55	106.49
30	A	834	CLA	C2D-C1D-ND	8.00	116.00	110.10
30	B	810	CLA	C2D-C1D-ND	8.00	116.00	110.10
30	13	302	CLA	C2D-C1D-ND	7.99	115.99	110.10
30	2	309	CLA	C2D-C1D-ND	7.99	115.99	110.10
38	12	309	KC1	C2B-C1B-NB	7.99	115.99	110.10
39	5	314	DD6	C9-C10-C11	-7.98	115.92	127.31
30	15	309	CLA	C2D-C1D-ND	7.98	115.98	110.10
30	2	305	CLA	C2D-C1D-ND	7.98	115.98	110.10
37	12	314	A86	C33-C32-C31	7.97	116.96	109.21
39	8	316	DD6	C8-C6-C5	-7.96	106.72	118.94
30	B	837	CLA	C2D-C1D-ND	7.96	115.97	110.10
30	5	304	CLA	C2D-C1D-ND	7.96	115.97	110.10
30	16	302	CLA	C2D-C1D-ND	7.96	115.97	110.10
39	5	313	DD6	C-C1-C2	-7.96	111.77	122.92
30	B	831	CLA	C2D-C1D-ND	7.96	115.97	110.10
30	1	307	CLA	C2D-C1D-ND	7.95	115.97	110.10
39	12	317	DD6	C4-C5-C6	-7.95	115.96	127.31
30	12	310	CLA	C2D-C1D-ND	7.95	115.96	110.10
38	2	314	KC1	CMA-C3A-C2A	-7.95	108.84	128.30
30	4	302	CLA	C2D-C1D-ND	7.95	115.96	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	13	315	A86	C33-C32-C31	7.94	116.93	109.21
30	B	806	CLA	C2D-C1D-ND	7.94	115.96	110.10
38	5	312	KC1	CMA-C3A-C2A	-7.94	108.87	128.30
30	F	203	CLA	C2D-C1D-ND	7.93	115.95	110.10
30	5	303	CLA	C2D-C1D-ND	7.93	115.95	110.10
30	15	311	CLA	C2D-C1D-ND	7.93	115.95	110.10
39	6	303	DD6	C8-C6-C5	-7.93	106.78	118.94
37	5	316	A86	O1-C20-C21	-7.93	105.56	115.06
30	6	315	CLA	C2D-C1D-ND	7.92	115.94	110.10
30	B	809	CLA	C2D-C1D-ND	7.92	115.94	110.10
30	6	317	CLA	C2D-C1D-ND	7.92	115.94	110.10
38	10	310	KC1	C2B-C1B-NB	7.91	115.94	110.10
38	4	307	KC1	C2B-C1B-NB	7.91	115.94	110.10
39	6	321	DD6	C7-C6-C5	-7.91	111.84	122.92
38	16	311	KC1	C2B-C1B-NB	7.91	115.93	110.10
38	8	314	KC1	O2D-CGD-CBD	7.91	125.32	111.27
30	8	308	CLA	C2D-C1D-ND	7.90	115.93	110.10
37	9	315	A86	C21-C20-C19	-7.90	105.39	114.28
29	A	801	CL0	C2D-C1D-ND	7.90	115.93	110.10
39	6	318	DD6	C-C1-C2	-7.90	111.86	122.92
30	15	313	CLA	C2D-C1D-ND	7.90	115.92	110.10
30	16	305	CLA	C2D-C1D-ND	7.89	115.92	110.10
30	2	313	CLA	C2D-C1D-ND	7.89	115.92	110.10
30	13	304	CLA	C2D-C1D-ND	7.89	115.92	110.10
30	A	831	CLA	C2D-C1D-ND	7.89	115.92	110.10
39	15	318	DD6	C32-C31-C36	-7.89	111.50	122.63
30	7	304	CLA	C2D-C1D-ND	7.89	115.92	110.10
30	12	312	CLA	C2D-C1D-ND	7.88	115.91	110.10
30	7	309	CLA	C2D-C1D-ND	7.88	115.91	110.10
30	B	822	CLA	C2D-C1D-ND	7.88	115.91	110.10
30	13	303	CLA	C2D-C1D-ND	7.88	115.91	110.10
30	16	309	CLA	C2D-C1D-ND	7.88	115.91	110.10
30	9	303	CLA	C2D-C1D-ND	7.87	115.91	110.10
30	A	807	CLA	C2D-C1D-ND	7.86	115.90	110.10
30	14	310	CLA	C2D-C1D-ND	7.86	115.89	110.10
37	1	309	A86	C17-C16-C15	7.85	117.17	109.16
37	10	302	A86	C25-C26-C27	-7.85	116.11	127.31
30	A	820	CLA	C1D-ND-C4D	-7.85	100.76	106.33
30	A	830	CLA	C2D-C1D-ND	7.85	115.89	110.10
30	5	309	CLA	C2D-C1D-ND	7.85	115.89	110.10
30	15	310	CLA	C2D-C1D-ND	7.84	115.89	110.10
30	7	306	CLA	C2D-C1D-ND	7.84	115.88	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	805	CLA	C2D-C1D-ND	7.84	115.88	110.10
30	12	304	CLA	CAA-C2A-C3A	-7.84	91.32	112.78
30	16	308	CLA	C2D-C1D-ND	7.83	115.88	110.10
38	13	305	KC1	CMA-C3A-C2A	-7.83	109.13	128.30
30	B	815	CLA	C2D-C1D-ND	7.83	115.87	110.10
30	B	838	CLA	C2D-C1D-ND	7.83	115.87	110.10
30	12	307	CLA	C2D-C1D-ND	7.83	115.87	110.10
30	3	310	CLA	C2D-C1D-ND	7.83	115.87	110.10
30	A	839	CLA	C2D-C1D-ND	7.82	115.87	110.10
30	15	306	CLA	C2D-C1D-ND	7.82	115.87	110.10
30	A	814	CLA	C2D-C1D-ND	7.82	115.87	110.10
30	12	302	CLA	C2D-C1D-ND	7.82	115.87	110.10
37	15	321	A86	C33-C32-C31	7.82	116.81	109.21
37	7	316	A86	C33-C32-C31	7.82	116.81	109.21
38	12	311	KC1	C2B-C1B-NB	7.81	115.86	110.10
39	8	317	DD6	C9-C10-C11	-7.81	116.16	127.31
30	13	309	CLA	C2D-C1D-ND	7.81	115.86	110.10
39	5	313	DD6	C9-C10-C11	-7.81	116.17	127.31
38	12	311	KC1	CMA-C3A-C2A	-7.80	109.19	128.30
39	13	314	DD6	C3-C2-C1	-7.80	116.17	127.31
38	13	306	KC1	CMA-C3A-C2A	-7.80	109.20	128.30
30	6	306	CLA	C2D-C1D-ND	7.80	115.85	110.10
37	5	315	A86	C17-C16-C15	7.80	117.12	109.16
39	6	318	DD6	C7-C6-C5	-7.80	112.00	122.92
38	13	305	KC1	C2B-C1B-NB	7.79	115.85	110.10
30	15	312	CLA	CMD-C2D-C1D	7.79	138.44	124.71
38	4	308	KC1	C2B-C1B-NB	7.79	115.84	110.10
37	12	314	A86	C4-C5-C6	-7.79	116.20	127.31
30	10	304	CLA	C2D-C1D-ND	7.79	115.84	110.10
30	12	308	CLA	C2D-C1D-ND	7.78	115.84	110.10
30	15	307	CLA	C2D-C1D-ND	7.78	115.84	110.10
30	8	304	CLA	CAA-C2A-C3A	-7.78	91.48	112.78
30	B	835	CLA	C2D-C1D-ND	7.78	115.83	110.10
39	3	312	DD6	C4-C5-C6	-7.77	116.22	127.31
30	1	302	CLA	C2D-C1D-ND	7.76	115.82	110.10
30	12	321	CLA	C2D-C1D-ND	7.76	115.82	110.10
30	11	306	CLA	C2D-C1D-ND	7.75	115.82	110.10
39	7	314	DD6	C8-C6-C5	-7.75	107.05	118.94
30	6	304	CLA	C2D-C1D-ND	7.75	115.81	110.10
30	3	307	CLA	C2D-C1D-ND	7.75	115.81	110.10
30	B	834	CLA	C2D-C1D-ND	7.75	115.81	110.10
39	6	303	DD6	C13-C11-C10	-7.75	107.06	118.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	840	CLA	C2D-C1D-ND	7.75	115.81	110.10
30	15	305	CLA	C2D-C1D-ND	7.74	115.81	110.10
39	6	319	DD6	C-C1-C2	-7.74	112.08	122.92
30	14	304	CLA	C2D-C1D-ND	7.74	115.81	110.10
30	12	303	CLA	C2D-C1D-ND	7.74	115.81	110.10
30	10	305	CLA	C2D-C1D-ND	7.73	115.80	110.10
38	7	313	KC1	C2B-C1B-NB	7.73	115.80	110.10
30	11	308	CLA	C2D-C1D-ND	7.73	115.80	110.10
39	3	312	DD6	C9-C10-C11	-7.72	116.29	127.31
39	8	316	DD6	C-C1-C2	-7.72	112.11	122.92
30	B	813	CLA	C2D-C1D-ND	7.72	115.79	110.10
30	1	301	CLA	C2D-C1D-ND	7.72	115.79	110.10
30	7	311	CLA	C2D-C1D-ND	7.71	115.79	110.10
39	10	314	DD6	C9-C10-C11	-7.70	116.33	127.31
30	14	313	CLA	C2D-C1D-ND	7.69	115.77	110.10
38	8	313	KC1	CMA-C3A-C2A	-7.69	109.47	128.30
30	B	832	CLA	C2D-C1D-ND	7.69	115.77	110.10
30	A	839	CLA	O2D-CGD-CBD	7.69	124.93	111.27
39	8	317	DD6	C-C1-C2	-7.68	112.16	122.92
38	14	308	KC1	C2B-C1B-NB	7.68	115.77	110.10
30	8	304	CLA	C2D-C1D-ND	7.68	115.76	110.10
37	4	317	A86	O1-C20-C21	-7.68	105.86	115.06
38	8	311	KC1	CMA-C3A-C2A	-7.67	109.52	128.30
38	9	310	KC1	C2B-C1B-NB	7.67	115.75	110.10
30	2	304	CLA	C2D-C1D-ND	7.66	115.75	110.10
37	4	317	A86	C17-C16-C15	7.65	116.97	109.16
38	13	308	KC1	C2B-C1B-NB	7.65	115.74	110.10
37	9	313	A86	C17-C16-C15	7.65	116.97	109.16
37	14	301	A86	C33-C32-C31	7.65	116.65	109.21
37	5	301	A86	O1-C20-C21	-7.65	105.89	115.06
30	A	802	CLA	C1D-ND-C4D	-7.65	100.90	106.33
38	16	304	KC1	C2B-C1B-NB	7.64	115.74	110.10
30	16	310	CLA	C2D-C1D-ND	7.64	115.73	110.10
30	14	312	CLA	C2D-C1D-ND	7.64	115.73	110.10
30	7	310	CLA	C2D-C1D-ND	7.64	115.73	110.10
37	12	316	A86	C4-C5-C6	-7.63	116.42	127.31
37	2u	205	A86	C33-C32-C31	7.63	116.63	109.21
37	14	318	A86	C33-C32-C31	7.63	116.62	109.21
38	3	304	KC1	CMA-C3A-C2A	-7.62	109.63	128.30
30	9	306	CLA	C2D-C1D-ND	7.62	115.72	110.10
38	6	311	KC1	CMA-C3A-C2A	-7.61	109.66	128.30
30	B	829	CLA	C2D-C1D-ND	7.61	115.71	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	2	306	KC1	C2B-C1B-NB	7.61	115.71	110.10
38	3	311	KC1	C2B-C1B-NB	7.61	115.71	110.10
37	14	320	A86	C25-C26-C27	-7.61	116.45	127.31
30	8	303	CLA	C2D-C1D-ND	7.61	115.71	110.10
39	7	314	DD6	C15-C14-C13	7.60	142.06	125.99
39	7	302	DD6	C32-C31-C36	-7.60	111.90	122.63
30	5	302	CLA	C2D-C1D-ND	7.60	115.70	110.10
30	14	303	CLA	C2D-C1D-ND	7.60	115.70	110.10
37	15	320	A86	C17-C16-C15	7.60	116.92	109.16
38	8	310	KC1	CMA-C3A-C2A	-7.60	109.70	128.30
30	A	832	CLA	C2D-C1D-ND	7.59	115.70	110.10
30	10	303	CLA	C2D-C1D-ND	7.59	115.70	110.10
37	12	316	A86	C33-C32-C31	7.59	116.58	109.21
30	3	303	CLA	C2D-C1D-ND	7.59	115.69	110.10
30	B	819	CLA	C1D-ND-C4D	-7.58	100.95	106.33
39	16	313	DD6	C15-C14-C13	7.58	142.01	125.99
30	7	312	CLA	C2D-C1D-ND	7.57	115.69	110.10
38	1	308	KC1	CMA-C3A-C2A	-7.57	109.76	128.30
30	2	310	CLA	C2D-C1D-ND	7.57	115.68	110.10
39	3	312	DD6	C7-C6-C5	-7.57	112.32	122.92
30	A	843	CLA	C2D-C1D-ND	7.56	115.68	110.10
30	4	309	CLA	C2D-C1D-ND	7.56	115.68	110.10
30	14	305	CLA	C2D-C1D-ND	7.56	115.67	110.10
30	6	310	CLA	C2D-C1D-ND	7.55	115.67	110.10
38	7	313	KC1	CMA-C3A-C2A	-7.54	109.83	128.30
30	2	307	CLA	C2D-C1D-ND	7.54	115.66	110.10
38	6	311	KC1	C2B-C1B-NB	7.53	115.65	110.10
38	9	310	KC1	CMA-C3A-C2A	-7.53	109.88	128.30
30	A	821	CLA	C2D-C1D-ND	7.52	115.65	110.10
30	B	828	CLA	CMD-C2D-C1D	7.52	137.97	124.71
37	13	313	A86	C33-C32-C31	7.52	116.52	109.21
30	13	307	CLA	C2D-C1D-ND	7.51	115.64	110.10
39	2	317	DD6	C8-C6-C5	-7.51	107.42	118.94
39	12	315	DD6	C8-C6-C5	-7.50	107.42	118.94
30	B	818	CLA	C2D-C1D-ND	7.50	115.63	110.10
38	2	306	KC1	CMA-C3A-C2A	-7.50	109.93	128.30
38	6	308	KC1	C2B-C1B-NB	7.50	115.63	110.10
37	11	301	A86	C33-C32-C31	7.50	116.50	109.21
37	10	315	A86	C17-C16-C15	7.50	116.81	109.16
30	12	304	CLA	C2D-C1D-ND	7.49	115.62	110.10
37	2	302	A86	C33-C32-C31	7.48	116.48	109.21
38	6	312	KC1	CMA-C3A-C2A	-7.47	110.01	128.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	10	317	A86	C17-C16-C15	7.47	116.78	109.16
37	10	316	A86	C33-C32-C31	7.47	116.47	109.21
37	7	319	A86	C17-C16-C15	7.46	116.77	109.16
30	A	838	CLA	C2D-C1D-ND	7.46	115.60	110.10
39	15	318	DD6	C-C1-C2	-7.46	112.48	122.92
30	6	305	CLA	C2D-C1D-ND	7.45	115.60	110.10
38	12	305	KC1	CMA-C3A-C2A	-7.45	110.06	128.30
30	A	825	CLA	C2D-C1D-ND	7.45	115.60	110.10
30	16	307	CLA	C2D-C1D-ND	7.44	115.59	110.10
37	10	302	A86	C4-C5-C6	-7.43	116.70	127.31
38	12	305	KC1	C2B-C1B-NB	7.43	115.58	110.10
30	A	841	CLA	C2D-C1D-ND	7.43	115.58	110.10
37	5	301	A86	C4-C5-C6	-7.43	116.71	127.31
38	3	304	KC1	C2B-C1B-NB	7.43	115.58	110.10
30	A	840	CLA	CMD-C2D-C1D	7.42	137.80	124.71
30	B	812	CLA	C2D-C1D-ND	7.42	115.57	110.10
30	14	302	CLA	C2D-C1D-ND	7.42	115.57	110.10
38	11	307	KC1	C2B-C1B-NB	7.42	115.57	110.10
39	7	317	DD6	C8-C6-C5	-7.42	107.55	118.94
38	14	306	KC1	C2B-C1B-NB	7.42	115.57	110.10
30	10	308	CLA	C2D-C1D-ND	7.42	115.57	110.10
30	12	306	CLA	C2D-C1D-ND	7.42	115.57	110.10
30	8	309	CLA	C2D-C1D-ND	7.40	115.56	110.10
39	15	318	DD6	C8-C6-C5	-7.40	107.58	118.94
38	11	311	KC1	C2B-C1B-NB	7.40	115.56	110.10
39	15	319	DD6	C8-C6-C5	-7.40	107.59	118.94
38	8	306	KC1	C2B-C1B-NB	7.40	115.56	110.10
38	10	312	KC1	CMA-C3A-C2A	-7.40	110.19	128.30
37	16	312	A86	C17-C16-C15	7.39	116.70	109.16
38	2	314	KC1	C2B-C1B-NB	7.39	115.55	110.10
39	7	314	DD6	C7-C6-C5	-7.38	112.58	122.92
37	2	319	A86	O1-C20-C21	-7.38	106.22	115.06
37	2u	205	A86	O1-C20-C21	-7.38	106.22	115.06
38	4	310	KC1	CMA-C3A-C2A	-7.37	110.25	128.30
30	6	309	CLA	C2D-C1D-ND	7.37	115.54	110.10
30	11	309	CLA	C2D-C1D-ND	7.37	115.54	110.10
39	7	318	DD6	C24-C1-C2	-7.36	107.64	118.94
38	1	306	KC1	CMA-C3A-C2A	-7.36	110.29	128.30
37	14	316	A86	C17-C16-C15	7.35	116.66	109.16
37	16	312	A86	C3-C2-C1	-7.34	116.83	127.31
30	14	302	CLA	CMD-C2D-C1D	7.34	137.65	124.71
39	4	313	DD6	C8-C6-C5	-7.34	107.69	118.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	1	310	DD6	C24-C1-C2	-7.33	107.69	118.94
38	5	312	KC1	C2B-C1B-NB	7.33	115.51	110.10
39	3	312	DD6	C32-C31-C36	-7.33	112.28	122.63
30	7	305	CLA	CMD-C2D-C1D	7.33	137.63	124.71
38	5	310	KC1	C2B-C1B-NB	7.32	115.50	110.10
37	3	314	A86	C3-C2-C1	-7.31	116.87	127.31
39	5	313	DD6	C7-C6-C5	-7.31	112.68	122.92
38	9	304	KC1	C2B-C1B-NB	7.31	115.49	110.10
39	4	313	DD6	C13-C11-C10	-7.30	107.75	118.94
38	6	313	KC1	CMA-C3A-C2A	-7.29	110.44	128.30
38	3	311	KC1	C1A-C2A-C3A	-7.29	101.33	107.11
39	1	310	DD6	C8-C6-C5	-7.28	107.77	118.94
38	13	306	KC1	C1A-C2A-C3A	-7.28	101.34	107.11
30	B	808	CLA	C2D-C1D-ND	7.27	115.46	110.10
38	2	312	KC1	CMA-C3A-C2A	-7.27	110.51	128.30
37	7	319	A86	C33-C32-C31	7.27	116.27	109.21
38	13	312	KC1	CMA-C3A-C2A	-7.27	110.51	128.30
38	10	306	KC1	O2D-CGD-CBD	7.26	124.18	111.27
38	16	311	KC1	C3A-C4A-NA	7.26	118.50	110.57
38	10	310	KC1	CMA-C3A-C2A	-7.26	110.53	128.30
38	13	308	KC1	CMA-C3A-C2A	-7.26	110.53	128.30
38	8	307	KC1	C2B-C1B-NB	7.25	115.45	110.10
30	6	314	CLA	C2D-C1D-ND	7.25	115.44	110.10
38	10	312	KC1	C2B-C1B-NB	7.25	115.44	110.10
30	B	851	CLA	C2D-C1D-ND	7.24	115.44	110.10
30	A	836	CLA	C2D-C1D-ND	7.24	115.44	110.10
38	5	310	KC1	CMA-C3A-C2A	-7.24	110.57	128.30
38	13	312	KC1	C2B-C1B-NB	7.24	115.44	110.10
38	3	308	KC1	CMA-C3A-C2A	-7.23	110.60	128.30
30	A	815	CLA	CMD-C2D-C1D	7.23	137.45	124.71
30	B	814	CLA	C2D-C1D-ND	7.22	115.43	110.10
37	10	302	A86	C17-C16-C15	7.22	116.53	109.16
39	6	319	DD6	C7-C6-C5	-7.22	112.81	122.92
30	3	306	CLA	C2D-C1D-ND	7.21	115.42	110.10
39	3	316	DD6	C32-C31-C36	-7.21	112.45	122.63
39	6	318	DD6	C12-C11-C13	-7.21	106.72	118.08
30	9	309	CLA	C2D-C1D-ND	7.20	115.41	110.10
39	12	317	DD6	C13-C11-C10	-7.20	107.89	118.94
37	6	320	A86	C21-C20-C19	-7.20	106.18	114.28
38	8	311	KC1	C2B-C1B-NB	7.19	115.41	110.10
38	9	304	KC1	CMA-C3A-C2A	-7.19	110.70	128.30
30	14	309	CLA	C2D-C1D-ND	7.19	115.40	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	4	314	A86	C33-C32-C31	7.18	116.19	109.21
38	9	311	KC1	C2B-C1B-NB	7.18	115.40	110.10
30	1	305	CLA	C2D-C1D-ND	7.18	115.40	110.10
38	11	307	KC1	CMA-C3A-C2A	-7.18	110.72	128.30
30	A	824	CLA	C2D-C1D-ND	7.18	115.39	110.10
39	12	317	DD6	C32-C31-C36	-7.18	112.50	122.63
30	4	304	CLA	C2D-C1D-ND	7.17	115.39	110.10
30	6	314	CLA	CMD-C2D-C1D	7.17	137.35	124.71
38	13	310	KC1	C2B-C1B-NB	7.16	115.38	110.10
39	10	314	DD6	C8-C6-C5	-7.16	107.95	118.94
37	14	314	A86	C17-C16-C15	7.16	116.47	109.16
38	10	310	KC1	C3A-C4A-NA	7.16	118.39	110.57
38	8	314	KC1	CMA-C3A-C4A	-7.15	114.15	125.04
38	4	310	KC1	CHB-C4A-C3A	-7.15	113.81	124.98
38	13	310	KC1	CMA-C3A-C2A	-7.15	110.79	128.30
38	1	308	KC1	C2B-C1B-NB	7.15	115.37	110.10
30	11	310	CLA	CMD-C2D-C1D	7.14	137.31	124.71
38	5	306	KC1	C1A-C2A-C3A	-7.14	101.44	107.11
30	B	830	CLA	CMD-C2D-C1D	7.14	137.30	124.71
30	A	802	CLA	C2D-C1D-ND	7.13	115.36	110.10
30	A	844	CLA	C2D-C1D-ND	7.13	115.36	110.10
37	16	312	A86	C33-C32-C31	7.13	116.14	109.21
38	12	309	KC1	CHB-C4A-C3A	-7.13	113.84	124.98
30	A	837	CLA	C2D-C1D-ND	7.13	115.36	110.10
30	14	310	CLA	CMD-C2D-C1D	7.12	137.27	124.71
30	B	823	CLA	C2D-C1D-ND	7.12	115.35	110.10
38	2	312	KC1	C2B-C1B-NB	7.12	115.35	110.10
30	A	835	CLA	C2D-C1D-ND	7.12	115.35	110.10
38	16	311	KC1	CHB-C4A-C3A	-7.12	113.86	124.98
37	4	314	A86	C17-C16-C15	7.11	116.42	109.16
38	8	313	KC1	C2B-C1B-NB	7.10	115.34	110.10
38	8	312	KC1	C2A-C3A-C4A	-7.10	101.22	106.49
38	1	306	KC1	C2B-C1B-NB	7.10	115.33	110.10
37	14	316	A86	C33-C32-C31	7.10	116.11	109.21
38	6	312	KC1	C2B-C1B-NB	7.09	115.33	110.10
30	A	828	CLA	CHD-C4C-C3C	-7.09	114.42	124.84
30	6	304	CLA	CMD-C2D-C1D	7.09	137.21	124.71
38	4	308	KC1	CHB-C4A-C3A	-7.09	113.90	124.98
37	15	315	A86	C33-C32-C31	7.08	116.10	109.21
38	13	306	KC1	C2B-C1B-NB	7.08	115.32	110.10
37	6	320	A86	C33-C32-C31	7.08	116.09	109.21
39	8	317	DD6	C24-C1-C2	-7.08	108.08	118.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	830	CLA	CHD-C1D-ND	-7.08	117.95	124.45
30	A	815	CLA	C2D-C1D-ND	7.06	115.31	110.10
39	8	316	DD6	C9-C10-C11	-7.06	117.23	127.31
39	2	315	DD6	C4-C5-C6	-7.06	117.23	127.31
30	6	316	CLA	C2D-C1D-ND	7.05	115.30	110.10
30	11	310	CLA	C2D-C1D-ND	7.05	115.30	110.10
30	B	835	CLA	CMD-C2D-C1D	7.05	137.13	124.71
39	6	319	DD6	C4-C5-C6	-7.04	117.27	127.31
39	15	319	DD6	C13-C11-C10	-7.03	108.15	118.94
30	B	825	CLA	CMD-C2D-C1D	7.03	137.10	124.71
37	4	317	A86	C33-C32-C31	7.02	116.04	109.21
38	11	311	KC1	CMA-C3A-C2A	-7.02	111.12	128.30
38	5	305	KC1	C2B-C1B-NB	7.02	115.28	110.10
30	B	832	CLA	CMD-C2D-C1D	7.02	137.08	124.71
37	15	315	A86	C24-C1-C2	7.02	129.71	118.94
39	11	313	DD6	C32-C31-C36	-7.01	112.73	122.63
38	13	311	KC1	CMA-C3A-C4A	-7.01	114.37	125.04
30	A	827	CLA	CMD-C2D-C1D	7.01	137.06	124.71
38	14	311	KC1	C2B-C1B-NB	7.01	115.27	110.10
38	7	308	KC1	C2B-C1B-NB	7.00	115.27	110.10
38	10	306	KC1	C2B-C1B-NB	7.00	115.27	110.10
37	10	315	A86	C33-C32-C31	7.00	116.02	109.21
30	B	820	CLA	CHD-C4C-C3C	-7.00	114.55	124.84
38	11	312	KC1	C1A-C2A-C3A	-7.00	101.56	107.11
30	16	308	CLA	CMD-C2D-C1D	7.00	137.05	124.71
38	14	311	KC1	CMA-C3A-C2A	-7.00	111.17	128.30
39	7	302	DD6	C8-C6-C5	-7.00	108.20	118.94
38	6	311	KC1	CHB-C4A-C3A	-7.00	114.05	124.98
37	15	323	A86	C4-C5-C6	-6.99	117.33	127.31
30	15	302	CLA	CHD-C1D-ND	-6.99	118.03	124.45
39	7	314	DD6	C14-C13-C11	6.98	136.37	125.53
38	8	314	KC1	CHB-C4A-C3A	-6.98	114.07	124.98
30	14	307	CLA	CHD-C1D-ND	-6.98	118.04	124.45
30	A	817	CLA	CMD-C2D-C1D	6.98	137.01	124.71
38	6	313	KC1	C2B-C1B-NB	6.98	115.25	110.10
30	B	839	CLA	O2D-CGD-CBD	6.97	123.65	111.27
38	12	311	KC1	C1A-C2A-C3A	-6.97	101.58	107.11
38	6	311	KC1	C3A-C4A-NA	6.97	118.18	110.57
30	15	314	CLA	CMD-C2D-C1D	6.96	136.98	124.71
30	A	826	CLA	O2D-CGD-CBD	6.96	123.64	111.27
30	B	824	CLA	C2D-C1D-ND	6.96	115.23	110.10
38	7	313	KC1	CHB-C4A-C3A	-6.96	114.11	124.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	16	310	CLA	CMD-C2D-C1D	6.95	136.96	124.71
38	3	308	KC1	C2B-C1B-NB	6.95	115.23	110.10
38	12	311	KC1	CHB-C4A-C3A	-6.94	114.14	124.98
39	2	317	DD6	C12-C11-C13	-6.94	107.15	118.08
38	16	304	KC1	C1A-C2A-C3A	-6.93	101.61	107.11
38	4	310	KC1	C3A-C4A-NA	6.93	118.14	110.57
38	6	308	KC1	CHB-C4A-C3A	-6.93	114.15	124.98
37	10	316	A86	C4-C5-C6	-6.93	117.42	127.31
37	11	314	A86	C33-C32-C31	6.93	115.94	109.21
30	16	306	CLA	C2D-C1D-ND	6.91	115.20	110.10
38	2	314	KC1	C1A-C2A-C3A	-6.91	101.63	107.11
38	10	310	KC1	CHB-C4A-C3A	-6.91	114.18	124.98
38	9	312	KC1	C2B-C1B-NB	6.91	115.19	110.10
37	3	314	A86	C33-C32-C31	6.90	115.92	109.21
38	8	306	KC1	C1A-C2A-C3A	-6.90	101.64	107.11
30	3	310	CLA	CMD-C2D-C1D	6.90	136.87	124.71
30	15	306	CLA	O2D-CGD-CBD	6.89	123.52	111.27
38	11	305	KC1	C2B-C1B-NB	6.89	115.18	110.10
39	7	314	DD6	C32-C31-C36	-6.89	112.90	122.63
38	13	305	KC1	CHB-C4A-C3A	-6.89	114.22	124.98
30	15	302	CLA	CMD-C2D-C1D	6.89	136.85	124.71
30	7	312	CLA	CMD-C2D-C1D	6.88	136.84	124.71
37	15	316	A86	C17-C16-C15	6.88	116.18	109.16
30	7	310	CLA	CMD-C2D-C1D	6.88	136.83	124.71
38	12	309	KC1	C3A-C4A-NA	6.87	118.08	110.57
30	B	823	CLA	O2D-CGD-CBD	6.87	123.47	111.27
30	A	835	CLA	O2D-CGD-CBD	6.87	123.47	111.27
30	A	820	CLA	C2D-C1D-ND	6.86	115.16	110.10
30	15	309	CLA	CMD-C2D-C1D	6.86	136.80	124.71
30	A	835	CLA	CMD-C2D-C1D	6.86	136.80	124.71
38	9	310	KC1	CHB-C4A-C3A	-6.85	114.27	124.98
37	15	316	A86	C33-C32-C31	6.85	115.87	109.21
30	B	817	CLA	CMD-C2D-C1D	6.85	136.78	124.71
30	B	831	CLA	O2D-CGD-CBD	6.84	123.42	111.27
37	14	320	A86	O1-C20-C21	-6.84	106.86	115.06
30	13	301	CLA	CMD-C2D-C1D	6.83	136.76	124.71
30	B	824	CLA	CMD-C2D-C1D	6.83	136.75	124.71
30	13	309	CLA	CMD-C2D-C1D	6.83	136.75	124.71
30	15	312	CLA	C2D-C1D-ND	6.83	115.13	110.10
30	J	101	CLA	CMD-C2D-C1D	6.83	136.74	124.71
38	12	313	KC1	CMD-C2D-C1D	6.82	138.94	128.46
38	5	305	KC1	C1A-C2A-C3A	-6.82	101.70	107.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	4	316	DD6	C32-C31-C36	-6.82	113.01	122.63
30	A	827	CLA	CHD-C4C-C3C	-6.82	114.82	124.84
38	14	311	KC1	CHB-C4A-C3A	-6.81	114.34	124.98
30	2	313	CLA	CMD-C2D-C1D	6.80	136.70	124.71
30	14	304	CLA	CMD-C2D-C1D	6.80	136.70	124.71
30	A	822	CLA	C2D-C1D-ND	6.80	115.12	110.10
30	4	304	CLA	CMD-C2D-C1D	6.79	136.69	124.71
38	6	312	KC1	C1A-C2A-C3A	-6.79	101.72	107.11
30	A	837	CLA	CMD-C2D-C1D	6.79	136.69	124.71
30	1	305	CLA	CMD-C2D-C1D	6.79	136.69	124.71
37	5	301	A86	C33-C32-C31	6.79	115.81	109.21
37	4	312	A86	C4-C5-C6	-6.79	117.62	127.31
30	13	304	CLA	CMD-C2D-C1D	6.79	136.67	124.71
38	6	308	KC1	C1A-C2A-C3A	-6.78	101.73	107.11
38	11	312	KC1	C2B-C1B-NB	6.78	115.10	110.10
38	14	311	KC1	C3A-C4A-NA	6.78	117.97	110.57
30	6	317	CLA	CMD-C2D-C1D	6.78	136.66	124.71
30	14	313	CLA	CMD-C2D-C1D	6.78	136.66	124.71
38	2	306	KC1	CHB-C4A-C3A	-6.78	114.39	124.98
38	13	310	KC1	C1A-C2A-C3A	-6.78	101.73	107.11
30	A	806	CLA	CMD-C2D-C1D	6.78	136.66	124.71
30	9	302	CLA	O2D-CGD-CBD	6.78	123.31	111.27
38	13	308	KC1	C3A-C4A-NA	6.78	117.97	110.57
30	B	837	CLA	CMD-C2D-C1D	6.77	136.65	124.71
30	J	101	CLA	C2D-C1D-ND	6.77	115.10	110.10
38	11	311	KC1	CHB-C4A-C3A	-6.77	114.40	124.98
30	9	306	CLA	CMD-C2D-C1D	6.77	136.65	124.71
30	A	829	CLA	CMD-C2D-C1D	6.77	136.64	124.71
30	A	819	CLA	CMD-C2D-C1D	6.77	136.64	124.71
38	3	304	KC1	O2D-CGD-CBD	6.76	123.29	111.27
30	L	203	CLA	CMD-C2D-C1D	6.76	136.62	124.71
30	A	844	CLA	CMD-C2D-C1D	6.75	136.62	124.71
30	13	303	CLA	CMD-C2D-C1D	6.75	136.62	124.71
30	15	304	CLA	CMD-C2D-C1D	6.75	136.62	124.71
30	A	810	CLA	CMD-C2D-C1D	6.75	136.61	124.71
30	12	304	CLA	CMD-C2D-C1D	6.75	136.61	124.71
38	13	308	KC1	CHB-C4A-C3A	-6.75	114.43	124.98
30	3	303	CLA	O2D-CGD-CBD	6.75	123.26	111.27
37	8	315	A86	C17-C16-C15	6.75	116.05	109.16
37	1	309	A86	C33-C32-C31	6.75	115.77	109.21
38	8	307	KC1	CHB-C4A-C3A	-6.75	114.44	124.98
30	2	301	CLA	C2C-C1C-NC	6.75	116.29	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	811	CLA	C2D-C1D-ND	6.74	115.07	110.10
38	11	312	KC1	CHB-C4A-C3A	-6.74	114.44	124.98
39	12	317	DD6	C24-C1-C2	-6.74	108.59	118.94
30	B	823	CLA	CMD-C2D-C1D	6.74	136.59	124.71
30	4	302	CLA	CMD-C2D-C1D	6.74	136.59	124.71
38	5	310	KC1	CHB-C4A-C3A	-6.74	114.45	124.98
38	12	305	KC1	CHB-C4A-C3A	-6.74	114.45	124.98
38	4	308	KC1	C3A-C4A-NA	6.74	117.93	110.57
38	5	310	KC1	C3A-C4A-NA	6.74	117.93	110.57
30	A	824	CLA	CMD-C2D-C1D	6.74	136.59	124.71
30	9	302	CLA	CMD-C2D-C1D	6.73	136.58	124.71
38	1	308	KC1	C1A-C2A-C3A	-6.73	101.77	107.11
38	8	307	KC1	C1A-C2A-C3A	-6.73	101.77	107.11
38	16	304	KC1	CHB-C4A-C3A	-6.73	114.46	124.98
38	8	313	KC1	C3A-C4A-NA	6.73	117.92	110.57
38	3	304	KC1	C1A-C2A-C3A	-6.73	101.77	107.11
30	6	305	CLA	CMD-C2D-C1D	6.73	136.57	124.71
39	6	321	DD6	C12-C11-C13	-6.73	107.48	118.08
38	6	308	KC1	C3A-C4A-NA	6.73	117.92	110.57
38	9	310	KC1	C3A-C4A-NA	6.72	117.91	110.57
30	15	314	CLA	CHD-C1D-ND	-6.72	118.28	124.45
38	5	306	KC1	CHB-C4A-C3A	-6.72	114.48	124.98
38	1	308	KC1	CHB-C4A-C3A	-6.72	114.48	124.98
38	11	311	KC1	C3A-C4A-NA	6.72	117.91	110.57
38	13	312	KC1	CHB-C4A-C3A	-6.72	114.48	124.98
37	15	317	A86	C17-C16-C15	6.71	116.01	109.16
38	14	308	KC1	CHB-C4A-C3A	-6.71	114.50	124.98
30	A	834	CLA	CMD-C2D-C1D	6.71	136.54	124.71
38	14	306	KC1	C3A-C4A-NA	6.71	117.89	110.57
39	15	318	DD6	C13-C11-C10	-6.71	108.65	118.94
30	9	307	CLA	CMD-C2D-C1D	6.70	136.53	124.71
39	7	318	DD6	C32-C31-C36	-6.70	113.17	122.63
38	10	312	KC1	C3A-C4A-NA	6.70	117.89	110.57
38	13	310	KC1	CHB-C4A-C3A	-6.70	114.51	124.98
30	L	202	CLA	CHD-C1D-ND	-6.70	118.30	124.45
30	8	302	CLA	CMD-C2D-C1D	6.70	136.51	124.71
30	B	808	CLA	CMD-C2D-C1D	6.69	136.51	124.71
38	8	306	KC1	CHB-C4A-C3A	-6.69	114.53	124.98
39	13	314	DD6	C7-C6-C8	-6.69	107.54	118.08
38	1	306	KC1	C3A-C4A-NA	6.69	117.87	110.57
38	13	310	KC1	C3A-C4A-NA	6.68	117.87	110.57
30	10	305	CLA	CMD-C2D-C1D	6.68	136.49	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	307	KC1	CHB-C4A-C3A	-6.68	114.54	124.98
39	5	314	DD6	C24-C1-C2	-6.68	108.69	118.94
38	3	308	KC1	CHB-C4A-C3A	-6.68	114.55	124.98
38	16	304	KC1	CMA-C3A-C4A	-6.68	114.87	125.04
30	8	305	CLA	CMD-C2D-C1D	6.67	136.48	124.71
30	B	851	CLA	CMD-C2D-C1D	6.67	136.48	124.71
30	15	311	CLA	CMD-C2D-C1D	6.67	136.48	124.71
37	15	317	A86	C36-C31-C32	-6.67	113.08	119.70
30	4	311	CLA	CMD-C2D-C1D	6.67	136.46	124.71
38	3	311	KC1	CHB-C4A-C3A	-6.67	114.56	124.98
30	15	313	CLA	CMD-C2D-C1D	6.66	136.46	124.71
39	4	313	DD6	C21-C20-C19	-6.66	106.78	114.28
30	14	312	CLA	CMD-C2D-C1D	6.66	136.46	124.71
30	2	305	CLA	O2D-CGD-CBD	6.66	123.11	111.27
30	B	816	CLA	CMD-C2D-C1D	6.66	136.45	124.71
30	B	839	CLA	CHD-C4C-C3C	-6.66	115.06	124.84
30	2	309	CLA	CMD-C2D-C1D	6.65	136.44	124.71
38	14	306	KC1	CMA-C3A-C2A	-6.65	112.02	128.30
38	1	306	KC1	CHB-C4A-C3A	-6.65	114.59	124.98
38	9	310	KC1	C1A-C2A-C3A	-6.64	101.84	107.11
30	A	808	CLA	CMD-C2D-C1D	6.64	136.41	124.71
30	11	304	CLA	CMD-C2D-C1D	6.64	136.41	124.71
30	14	309	CLA	CMD-C2D-C1D	6.64	136.41	124.71
30	3	303	CLA	CMD-C2D-C1D	6.64	136.41	124.71
30	4	301	CLA	CMD-C2D-C1D	6.63	136.40	124.71
30	10	311	CLA	CMD-C2D-C1D	6.63	136.40	124.71
38	14	306	KC1	C1A-C2A-C3A	-6.63	101.85	107.11
38	7	308	KC1	C3A-C4A-NA	6.63	117.81	110.57
38	5	312	KC1	CHB-C4A-C3A	-6.63	114.62	124.98
37	11	316	A86	C33-C32-C31	6.63	115.65	109.21
39	10	313	DD6	C-C1-C24	-6.63	107.64	118.08
30	3	309	CLA	CMD-C2D-C1D	6.62	136.39	124.71
30	9	305	CLA	O2D-CGD-CBD	6.62	123.04	111.27
37	5	315	A86	C33-C32-C31	6.62	115.65	109.21
38	4	310	KC1	C1A-C2A-C3A	-6.62	101.86	107.11
38	10	306	KC1	C1A-C2A-C3A	-6.62	101.86	107.11
37	7	319	A86	C25-C26-C27	-6.62	117.87	127.31
30	B	803	CLA	CHD-C1D-ND	-6.61	118.38	124.45
30	15	303	CLA	CMD-C2D-C1D	6.61	136.36	124.71
30	B	836	CLA	CMD-C2D-C1D	6.61	136.36	124.71
38	8	313	KC1	CHB-C4A-C3A	-6.61	114.66	124.98
30	8	308	CLA	CMD-C2D-C1D	6.61	136.36	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	7	313	KC1	C1A-C2A-C3A	-6.61	101.87	107.11
38	10	312	KC1	C1A-C2A-C3A	-6.60	101.87	107.11
30	9	301	CLA	O2D-CGD-CBD	6.60	123.00	111.27
30	B	821	CLA	CMD-C2D-C1D	6.60	136.35	124.71
38	8	310	KC1	C2B-C1B-NB	6.60	114.97	110.10
30	12	312	CLA	CMD-C2D-C1D	6.60	136.34	124.71
30	B	821	CLA	C2D-C1D-ND	6.60	114.97	110.10
38	1	308	KC1	C3A-C4A-NA	6.59	117.77	110.57
30	A	825	CLA	CMD-C2D-C1D	6.59	136.33	124.71
37	15	322	A86	C25-C26-C27	-6.59	117.91	127.31
39	3	313	DD6	C12-C11-C13	-6.59	107.69	118.08
38	3	304	KC1	CHB-C4A-C3A	-6.59	114.69	124.98
38	2	312	KC1	C1A-C2A-C3A	-6.59	101.88	107.11
39	4	313	DD6	C7-C6-C5	-6.59	113.70	122.92
30	16	309	CLA	CMD-C2D-C1D	6.58	136.32	124.71
30	15	305	CLA	CMD-C2D-C1D	6.58	136.31	124.71
30	B	818	CLA	CMD-C2D-C1D	6.58	136.31	124.71
30	7	309	CLA	CMD-C2D-C1D	6.58	136.31	124.71
30	B	831	CLA	CMD-C2D-C1D	6.58	136.31	124.71
30	B	806	CLA	CMD-C2D-C1D	6.58	136.31	124.71
38	4	308	KC1	CMA-C3A-C4A	-6.58	115.02	125.04
38	8	311	KC1	C1A-C2A-C3A	-6.57	101.89	107.11
38	4	310	KC1	C3B-C2B-C1B	-6.57	100.80	107.08
38	10	312	KC1	CHB-C4A-C3A	-6.57	114.71	124.98
38	6	311	KC1	C1A-C2A-C3A	-6.57	101.90	107.11
30	11	308	CLA	CMD-C2D-C1D	6.57	136.29	124.71
38	3	308	KC1	C3A-C4A-NA	6.57	117.74	110.57
38	7	308	KC1	CHB-C4A-C3A	-6.57	114.72	124.98
37	16	314	A86	C33-C32-C31	6.57	115.59	109.21
30	A	818	CLA	CMD-C2D-C1D	6.56	136.28	124.71
38	13	305	KC1	C3A-C4A-NA	6.56	117.73	110.57
38	5	310	KC1	C1A-C2A-C3A	-6.56	101.91	107.11
30	B	828	CLA	O2D-CGD-CBD	6.56	122.92	111.27
30	1	307	CLA	CMD-C2D-C1D	6.56	136.27	124.71
30	15	310	CLA	CMD-C2D-C1D	6.56	136.27	124.71
30	A	817	CLA	CHD-C1D-ND	-6.56	118.43	124.45
38	2	306	KC1	C3A-C4A-NA	6.55	117.73	110.57
38	14	308	KC1	C3A-C4A-NA	6.55	117.73	110.57
39	11	313	DD6	C12-C11-C13	-6.55	107.76	118.08
30	6	315	CLA	CMD-C2D-C1D	6.55	136.25	124.71
39	7	314	DD6	C-C1-C2	-6.55	113.75	122.92
37	15	323	A86	C33-C32-C31	6.55	115.57	109.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	4	317	A86	C3-C2-C1	-6.54	117.97	127.31
39	3	316	DD6	C24-C1-C2	-6.54	108.90	118.94
37	11	301	A86	C17-C16-C15	6.54	115.84	109.16
37	4	317	A86	C25-C26-C27	-6.54	117.97	127.31
30	14	303	CLA	CMD-C2D-C1D	6.54	136.24	124.71
38	14	306	KC1	CHB-C4A-C3A	-6.54	114.77	124.98
38	13	312	KC1	C3A-C4A-NA	6.53	117.70	110.57
38	4	307	KC1	C3A-C4A-NA	6.53	117.70	110.57
30	B	834	CLA	CHD-C4C-C3C	-6.53	115.24	124.84
30	B	801	CLA	CHD-C4C-C3C	-6.52	115.25	124.84
30	4	309	CLA	CMD-C2D-C1D	6.52	136.21	124.71
30	9	306	CLA	C2C-C1C-NC	6.52	116.08	109.97
39	3	313	DD6	C8-C6-C5	-6.52	108.94	118.94
38	8	310	KC1	CHB-C4A-C3A	-6.52	114.80	124.98
38	2	312	KC1	CHB-C4A-C3A	-6.52	114.80	124.98
30	1	304	CLA	CHD-C4C-C3C	-6.52	115.26	124.84
30	16	301	CLA	CHD-C4C-C3C	-6.52	115.26	124.84
30	A	812	CLA	CMD-C2D-C1D	6.52	136.20	124.71
30	6	306	CLA	CMD-C2D-C1D	6.51	136.19	124.71
30	3	305	CLA	CMD-C2D-C1D	6.51	136.19	124.71
30	5	302	CLA	CMD-C2D-C1D	6.51	136.19	124.71
38	5	312	KC1	C3A-C4A-NA	6.51	117.68	110.57
38	13	312	KC1	C1A-C2A-C3A	-6.50	101.95	107.11
30	5	311	CLA	O2D-CGD-CBD	6.50	122.82	111.27
39	5	313	DD6	C24-C1-C2	-6.50	108.97	118.94
38	13	311	KC1	C1A-C2A-C3A	-6.50	101.96	107.11
30	A	812	CLA	CHD-C1D-ND	-6.50	118.48	124.45
38	12	311	KC1	C3A-C4A-NA	6.49	117.66	110.57
30	4	305	CLA	CHD-C1D-ND	-6.49	118.49	124.45
30	13	307	CLA	CMD-C2D-C1D	6.49	136.16	124.71
39	12	317	DD6	C12-C11-C13	-6.49	107.85	118.08
30	6	316	CLA	CMD-C2D-C1D	6.49	136.16	124.71
30	5	304	CLA	CMD-C2D-C1D	6.49	136.16	124.71
30	B	833	CLA	CMD-C2D-C1D	6.49	136.15	124.71
38	12	305	KC1	C3A-C4A-NA	6.49	117.66	110.57
30	B	838	CLA	C2C-C1C-NC	6.49	116.05	109.97
30	15	312	CLA	CHD-C1D-ND	-6.49	118.49	124.45
30	2	301	CLA	CBC-CAC-C3C	-6.49	94.55	112.43
38	7	313	KC1	C3B-C2B-C1B	-6.49	100.88	107.08
38	10	306	KC1	CHB-C4A-C3A	-6.48	114.85	124.98
39	2	316	DD6	C7-C6-C5	-6.48	113.84	122.92
30	10	304	CLA	CMD-C2D-C1D	6.48	136.13	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	804	CLA	O2D-CGD-CBD	6.48	122.78	111.27
39	6	321	DD6	C24-C1-C2	-6.48	109.00	118.94
38	11	307	KC1	CHB-C4A-C3A	-6.48	114.86	124.98
38	5	306	KC1	C3B-C2B-C1B	-6.47	100.90	107.08
37	9	316	A86	C33-C32-C31	6.47	115.50	109.21
30	10	308	CLA	CMD-C2D-C1D	6.47	136.12	124.71
37	12	314	A86	C17-C16-C15	6.47	115.76	109.16
30	16	302	CLA	CMD-C2D-C1D	6.47	136.11	124.71
30	7	310	CLA	CHD-C1D-ND	-6.47	118.51	124.45
30	A	833	CLA	CMD-C2D-C1D	6.47	136.11	124.71
38	6	313	KC1	CHB-C4A-C3A	-6.46	114.88	124.98
38	13	306	KC1	CHB-C4A-C3A	-6.46	114.89	124.98
30	B	835	CLA	CHD-C1D-ND	-6.46	118.52	124.45
38	2	314	KC1	CHB-C4A-C3A	-6.46	114.89	124.98
38	12	309	KC1	C3B-C2B-C1B	-6.46	100.91	107.08
30	A	827	CLA	CHD-C1D-ND	-6.45	118.53	124.45
38	8	311	KC1	CHB-C4A-C3A	-6.45	114.90	124.98
30	A	820	CLA	CMD-C2D-C1D	6.45	136.07	124.71
30	9	305	CLA	CMD-C2D-C1D	6.45	136.07	124.71
38	5	305	KC1	CHB-C4A-C3A	-6.45	114.91	124.98
37	6	320	A86	O1-C20-C21	-6.45	107.33	115.06
38	9	304	KC1	CHB-C4A-C3A	-6.45	114.91	124.98
30	3	307	CLA	CMD-C2D-C1D	6.44	136.07	124.71
30	14	307	CLA	CMD-C2D-C1D	6.44	136.06	124.71
30	A	839	CLA	CMD-C2D-C1D	6.44	136.06	124.71
38	8	307	KC1	C3A-C4A-NA	6.44	117.60	110.57
37	15	315	A86	C3-C4-C5	-6.44	110.29	123.47
30	F	202	CLA	CMD-C2D-C1D	6.43	136.04	124.71
30	9	301	CLA	CMD-C2D-C1D	6.43	136.04	124.71
30	A	811	CLA	CMD-C2D-C1D	6.42	136.03	124.71
38	11	305	KC1	CHB-C4A-C3A	-6.42	114.95	124.98
30	7	305	CLA	O2D-CGD-CBD	6.42	122.67	111.27
37	10	317	A86	C33-C32-C31	6.42	115.45	109.21
39	7	318	DD6	C8-C6-C5	-6.41	109.10	118.94
30	6	307	CLA	C2D-C1D-ND	6.41	114.83	110.10
30	7	307	CLA	CMD-C2D-C1D	6.41	136.01	124.71
30	12	321	CLA	CMD-C2D-C1D	6.41	136.01	124.71
30	16	303	CLA	CMD-C2D-C1D	6.41	136.01	124.71
30	15	309	CLA	CHD-C1D-ND	-6.41	118.56	124.45
37	2u	203	A86	C17-C16-C15	6.41	115.70	109.16
30	B	815	CLA	CMD-C2D-C1D	6.40	135.99	124.71
30	B	838	CLA	CMD-C2D-C1D	6.40	135.99	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	4	312	A86	C17-C16-C15	6.40	115.69	109.16
30	8	309	CLA	CMD-C2D-C1D	6.40	135.99	124.71
30	1	303	CLA	CMD-C2D-C1D	6.39	135.98	124.71
30	15	306	CLA	CMD-C2D-C1D	6.39	135.98	124.71
30	A	823	CLA	CMD-C2D-C1D	6.39	135.98	124.71
38	7	313	KC1	C3A-C4A-NA	6.39	117.55	110.57
30	12	310	CLA	CMD-C2D-C1D	6.39	135.97	124.71
38	9	304	KC1	C3A-C4A-NA	6.39	117.55	110.57
38	7	308	KC1	CMA-C3A-C2A	-6.39	112.67	128.30
39	2	315	DD6	C-C1-C24	-6.38	108.02	118.08
30	B	839	CLA	C4A-NA-C1A	-6.38	103.84	106.71
39	13	314	DD6	C32-C31-C36	-6.38	113.62	122.63
38	9	312	KC1	C1A-C2A-C3A	-6.38	102.05	107.11
30	8	305	CLA	CHD-C4C-C3C	-6.38	115.46	124.84
38	14	308	KC1	CMA-C3A-C2A	-6.38	112.68	128.30
37	10	301	A86	O1-C20-C21	-6.38	107.41	115.06
30	6	310	CLA	CMD-C2D-C1D	6.38	135.96	124.71
37	6	320	A86	C4-C5-C6	-6.38	118.21	127.31
37	7	315	A86	C3-C2-C1	-6.37	118.21	127.31
30	A	818	CLA	CHD-C4C-C3C	-6.37	115.47	124.84
30	11	306	CLA	CMD-C2D-C1D	6.37	135.94	124.71
39	7	318	DD6	C12-C11-C13	-6.37	108.04	118.08
38	13	311	KC1	C2B-C1B-NB	6.37	114.80	110.10
38	16	311	KC1	C3B-C2B-C1B	-6.37	100.99	107.08
38	10	310	KC1	C1A-C2A-C3A	-6.37	102.06	107.11
30	A	830	CLA	CHD-C4C-C3C	-6.37	115.48	124.84
38	9	311	KC1	CHB-C4A-C3A	-6.36	115.04	124.98
38	14	308	KC1	C3C-C4C-NC	6.36	115.87	109.88
38	5	306	KC1	C3A-C4A-NA	6.36	117.52	110.57
30	14	310	CLA	CHD-C1D-ND	-6.36	118.61	124.45
30	1	302	CLA	CMD-C2D-C1D	6.36	135.92	124.71
30	10	303	CLA	CMD-C2D-C1D	6.36	135.92	124.71
30	16	307	CLA	CMD-C2D-C1D	6.36	135.92	124.71
30	4	303	CLA	CMD-C2D-C1D	6.36	135.92	124.71
38	16	304	KC1	C3A-C4A-NA	6.36	117.51	110.57
39	7	314	DD6	C9-C10-C11	-6.35	118.24	127.31
39	3	313	DD6	C32-C31-C36	-6.35	113.66	122.63
38	9	311	KC1	O2D-CGD-CBD	6.35	122.56	111.27
37	11	315	A86	C4-C5-C6	-6.35	118.25	127.31
30	B	822	CLA	CMD-C2D-C1D	6.35	135.90	124.71
30	10	309	CLA	CMD-C2D-C1D	6.35	135.90	124.71
38	8	314	KC1	C3B-C2B-C1B	-6.35	101.02	107.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	2u	203	A86	C33-C32-C31	6.35	115.38	109.21
30	A	838	CLA	CMD-C2D-C1D	6.34	135.89	124.71
30	9	308	CLA	O2D-CGD-CBD	6.34	122.54	111.27
30	13	309	CLA	CHD-C1D-ND	-6.34	118.63	124.45
38	6	313	KC1	C3A-C4A-NA	6.34	117.50	110.57
30	14	305	CLA	CMD-C2D-C1D	6.34	135.89	124.71
30	A	821	CLA	C2C-C1C-NC	6.34	115.91	109.97
30	B	807	CLA	CMD-C2D-C1D	6.34	135.88	124.71
30	14	304	CLA	CHD-C1D-ND	-6.34	118.63	124.45
39	10	314	DD6	C32-C31-C36	-6.34	113.69	122.63
38	11	305	KC1	C1A-C2A-C3A	-6.34	102.08	107.11
30	16	303	CLA	CHD-C1D-ND	-6.34	118.63	124.45
38	8	310	KC1	C3A-C4A-NA	6.33	117.49	110.57
38	6	312	KC1	CHB-C4A-C3A	-6.33	115.09	124.98
30	6	307	CLA	CMD-C2D-C1D	6.33	135.87	124.71
30	B	805	CLA	CMD-C2D-C1D	6.33	135.86	124.71
30	5	311	CLA	CMD-C2D-C1D	6.32	135.86	124.71
39	10	313	DD6	C32-C31-C36	-6.32	113.71	122.63
38	11	307	KC1	C3A-C4A-NA	6.32	117.47	110.57
30	F	201	CLA	CHD-C4C-C3C	-6.32	115.55	124.84
30	A	832	CLA	O2D-CGD-CBD	6.31	122.49	111.27
39	9	314	DD6	C7-C6-C8	-6.31	108.13	118.08
30	A	806	CLA	O2D-CGD-CBD	6.31	122.48	111.27
39	2	316	DD6	C9-C10-C11	-6.31	118.31	127.31
30	12	304	CLA	CHD-C1D-ND	-6.31	118.66	124.45
30	A	807	CLA	CMD-C2D-C1D	6.31	135.83	124.71
30	15	302	CLA	O2D-CGD-CBD	6.30	122.47	111.27
30	B	810	CLA	CMD-C2D-C1D	6.30	135.82	124.71
30	B	825	CLA	O2D-CGD-CBD	6.30	122.47	111.27
39	5	313	DD6	C32-C31-C36	-6.29	113.75	122.63
30	B	813	CLA	CMD-C2D-C1D	6.29	135.81	124.71
38	9	304	KC1	C1A-C2A-C3A	-6.29	102.12	107.11
39	13	314	DD6	C14-C13-C11	6.29	135.29	125.53
38	8	310	KC1	C1A-C2A-C3A	-6.29	102.12	107.11
39	7	318	DD6	C13-C11-C10	-6.29	109.29	118.94
38	13	306	KC1	C3A-C4A-NA	6.29	117.44	110.57
38	2	306	KC1	C3B-C2B-C1B	-6.28	101.08	107.08
38	11	305	KC1	C3A-C4A-NA	6.28	117.43	110.57
30	11	309	CLA	CMD-C2D-C1D	6.28	135.78	124.71
30	7	306	CLA	C2C-C1C-NC	6.28	115.86	109.97
30	15	304	CLA	CHD-C1D-ND	-6.28	118.68	124.45
38	9	311	KC1	C3A-C4A-NA	6.28	117.43	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	831	CLA	O2D-CGD-O1D	-6.28	111.56	123.84
30	B	816	CLA	CHD-C1D-ND	-6.28	118.69	124.45
38	8	312	KC1	CMA-C3A-C2A	-6.28	112.94	128.30
30	A	814	CLA	CMD-C2D-C1D	6.27	135.77	124.71
30	16	301	CLA	CMD-C2D-C1D	6.27	135.77	124.71
38	12	313	KC1	C3B-C2B-C1B	-6.27	101.09	107.08
39	7	317	DD6	C12-C11-C13	-6.27	108.19	118.08
30	13	304	CLA	CHD-C1D-ND	-6.27	118.69	124.45
30	A	832	CLA	CMD-C2D-C1D	6.27	135.76	124.71
38	6	312	KC1	C3A-C4A-NA	6.27	117.41	110.57
30	B	834	CLA	CMD-C2D-C1D	6.27	135.75	124.71
30	A	835	CLA	CHD-C1D-ND	-6.26	118.70	124.45
30	3	307	CLA	C2C-C1C-NC	6.26	115.84	109.97
30	A	828	CLA	O2D-CGD-CBD	6.26	122.39	111.27
30	14	313	CLA	CHD-C1D-ND	-6.26	118.70	124.45
30	3	306	CLA	CHD-C1D-ND	-6.25	118.71	124.45
38	7	308	KC1	C1A-C2A-C3A	-6.25	102.15	107.11
39	11	313	DD6	C24-C1-C2	-6.25	109.34	118.94
38	13	311	KC1	C3A-C4A-NA	6.25	117.40	110.57
30	F	203	CLA	CMD-C2D-C1D	6.25	135.73	124.71
30	6	304	CLA	CHD-C1D-ND	-6.25	118.71	124.45
30	9	308	CLA	CMD-C2D-C1D	6.25	135.73	124.71
29	A	801	CL0	C2C-C1C-NC	6.25	115.83	109.97
30	4	306	CLA	CMD-C2D-C1D	6.25	135.72	124.71
39	11	313	DD6	C-C1-C24	-6.25	108.23	118.08
39	2	317	DD6	C4-C5-C6	-6.25	118.40	127.31
30	9	307	CLA	CHD-C4C-C3C	-6.24	115.66	124.84
30	4	305	CLA	CMD-C2D-C1D	6.24	135.72	124.71
38	12	305	KC1	C1A-C2A-C3A	-6.24	102.16	107.11
30	5	309	CLA	CMD-C2D-C1D	6.24	135.71	124.71
38	14	306	KC1	CAC-C3C-C4C	6.24	132.91	124.81
30	B	815	CLA	O2D-CGD-CBD	6.23	122.35	111.27
30	A	819	CLA	CHD-C4C-C3C	-6.23	115.68	124.84
30	A	804	CLA	CMD-C2D-C1D	6.23	135.69	124.71
38	8	306	KC1	C3A-C4A-NA	6.22	117.37	110.57
30	5	303	CLA	CMD-C2D-C1D	6.22	135.68	124.71
38	2	306	KC1	O2D-CGD-CBD	6.22	122.33	111.27
30	1	303	CLA	CHD-C1D-ND	-6.22	118.74	124.45
30	12	302	CLA	CMD-C2D-C1D	6.22	135.68	124.71
30	A	809	CLA	CMD-C2D-C1D	6.22	135.68	124.71
38	6	308	KC1	C3B-C2B-C1B	-6.22	101.14	107.08
38	11	312	KC1	C3A-C4A-NA	6.21	117.36	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	15	307	CLA	C2C-C1C-NC	6.21	115.79	109.97
30	A	805	CLA	O2D-CGD-CBD	6.21	122.31	111.27
30	1	301	CLA	CMD-C2D-C1D	6.21	135.66	124.71
38	9	310	KC1	C3B-C2B-C1B	-6.21	101.15	107.08
30	2	304	CLA	CMD-C2D-C1D	6.21	135.66	124.71
30	2	311	CLA	CMD-C2D-C1D	6.21	135.65	124.71
30	B	831	CLA	CHD-C1D-ND	-6.21	118.75	124.45
30	4	311	CLA	CHD-C1D-ND	-6.20	118.75	124.45
38	1	306	KC1	C1A-C2A-C3A	-6.20	102.19	107.11
30	13	303	CLA	CHD-C1D-ND	-6.20	118.75	124.45
39	3	312	DD6	C8-C6-C5	-6.20	109.43	118.94
39	4	316	DD6	C-C1-C24	-6.20	108.31	118.08
38	2	312	KC1	C3A-C4A-NA	6.20	117.34	110.57
29	A	801	CL0	CHD-C4C-C3C	-6.19	115.74	124.84
37	10	301	A86	C4-C5-C6	-6.19	118.48	127.31
38	12	313	KC1	C3A-C4A-NA	6.19	117.33	110.57
37	10	301	A86	C-C1-C24	6.19	127.82	118.08
30	8	301	CLA	CHD-C4C-C3C	-6.18	115.75	124.84
30	13	301	CLA	CHD-C4C-C3C	-6.18	115.75	124.84
30	15	306	CLA	C2C-C1C-NC	6.18	115.76	109.97
30	A	842	CLA	CHD-C4C-C3C	-6.18	115.76	124.84
30	5	307	CLA	CHD-C4C-C3C	-6.18	115.76	124.84
38	9	312	KC1	CHB-C4A-C3A	-6.17	115.34	124.98
30	7	304	CLA	CMD-C2D-C1D	6.17	135.59	124.71
37	15	320	A86	C4-C5-C6	-6.17	118.50	127.31
39	15	319	DD6	C12-C11-C13	-6.17	108.36	118.08
39	7	318	DD6	C7-C6-C8	-6.17	108.36	118.08
38	4	308	KC1	C3B-C2B-C1B	-6.17	101.19	107.08
30	12	307	CLA	CHD-C4C-C3C	-6.16	115.78	124.84
30	B	804	CLA	CMD-C2D-C1D	6.16	135.57	124.71
30	14	302	CLA	CHD-C1D-ND	-6.16	118.80	124.45
30	B	817	CLA	CHD-C1D-ND	-6.16	118.80	124.45
30	B	820	CLA	CMD-C2D-C1D	6.15	135.55	124.71
30	10	308	CLA	CHD-C1D-ND	-6.15	118.80	124.45
38	3	304	KC1	C3A-C4A-NA	6.15	117.28	110.57
38	13	308	KC1	C1A-C2A-C3A	-6.15	102.24	107.11
39	6	319	DD6	C8-C6-C5	-6.14	109.51	118.94
30	3	310	CLA	CHD-C1D-ND	-6.14	118.81	124.45
38	13	310	KC1	C3B-C2B-C1B	-6.14	101.21	107.08
30	5	307	CLA	CMD-C2D-C1D	6.14	135.54	124.71
30	A	841	CLA	CMD-C2D-C1D	6.14	135.54	124.71
37	1	309	A86	C4-C3-C2	-6.14	110.90	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	3	309	CLA	CHD-C1D-ND	-6.14	118.81	124.45
30	15	303	CLA	CHD-C1D-ND	-6.14	118.81	124.45
30	A	816	CLA	CMD-C2D-C1D	6.14	135.53	124.71
30	B	817	CLA	CHD-C4C-C3C	-6.14	115.82	124.84
30	B	832	CLA	CHD-C1D-ND	-6.14	118.81	124.45
30	A	807	CLA	CHD-C4C-C3C	-6.14	115.82	124.84
30	A	805	CLA	CMD-C2D-C1D	6.13	135.52	124.71
30	A	813	CLA	CMD-C2D-C1D	6.13	135.52	124.71
30	A	828	CLA	CMD-C2D-C1D	6.13	135.52	124.71
30	2u	202	CLA	CHD-C4C-C3C	-6.13	115.83	124.84
38	11	307	KC1	C1A-C2A-C3A	-6.13	102.25	107.11
30	3	306	CLA	CMD-C2D-C1D	6.13	135.51	124.71
30	2	310	CLA	CMD-C2D-C1D	6.13	135.51	124.71
30	B	806	CLA	CHD-C4C-C3C	-6.12	115.84	124.84
30	2	304	CLA	O2D-CGD-CBD	6.12	122.15	111.27
38	2	314	KC1	C3A-C4A-NA	6.12	117.25	110.57
30	B	825	CLA	CHD-C4C-C3C	-6.12	115.84	124.84
30	13	309	CLA	C2C-C1C-NC	6.12	115.71	109.97
30	7	307	CLA	CHD-C4C-C3C	-6.12	115.85	124.84
37	2u	205	A86	O4-C38-C39	6.12	122.34	111.09
30	9	306	CLA	CHD-C1D-ND	-6.11	118.83	124.45
39	16	313	DD6	C9-C10-C11	-6.11	118.59	127.31
38	8	313	KC1	C3B-C2B-C1B	-6.11	101.24	107.08
30	14	305	CLA	CHD-C1D-ND	-6.11	118.84	124.45
37	11	301	A86	C3-C2-C1	-6.11	118.59	127.31
30	7	305	CLA	CHD-C1D-ND	-6.10	118.85	124.45
30	A	823	CLA	CHD-C1D-ND	-6.10	118.85	124.45
38	14	311	KC1	C1A-C2A-C3A	-6.10	102.27	107.11
30	15	302	CLA	C4A-NA-C1A	-6.09	103.97	106.71
30	A	815	CLA	CHD-C1D-ND	-6.09	118.86	124.45
37	2u	205	A86	C-C1-C2	-6.09	114.39	122.92
39	7	302	DD6	C13-C11-C10	-6.09	109.60	118.94
30	A	839	CLA	CHD-C1D-ND	-6.09	118.86	124.45
30	L	202	CLA	CMD-C2D-C1D	6.09	135.44	124.71
30	16	309	CLA	O2D-CGD-CBD	6.09	122.08	111.27
30	12	308	CLA	CMD-C2D-C1D	6.09	135.44	124.71
38	10	310	KC1	C1A-NA-C4A	-6.08	103.97	106.71
30	6	317	CLA	CHD-C1D-ND	-6.08	118.86	124.45
30	7	309	CLA	C2C-C1C-NC	6.08	115.67	109.97
38	5	312	KC1	C1A-C2A-C3A	-6.08	102.29	107.11
37	2u	203	A86	O4-C38-C39	6.08	122.27	111.09
38	13	310	KC1	C3C-C4C-NC	6.08	115.60	109.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	840	CLA	CHD-C1D-ND	-6.08	118.87	124.45
38	4	307	KC1	C3B-C2B-C1B	-6.07	101.28	107.08
30	12	303	CLA	CMD-C2D-C1D	6.07	135.42	124.71
30	A	834	CLA	CHD-C1D-ND	-6.07	118.87	124.45
30	A	811	CLA	CHD-C1D-ND	-6.07	118.87	124.45
30	16	308	CLA	CHD-C1D-ND	-6.07	118.88	124.45
30	A	833	CLA	CHD-C1D-ND	-6.07	118.88	124.45
30	A	838	CLA	CHD-C4C-C3C	-6.06	115.93	124.84
30	11	308	CLA	CHD-C1D-ND	-6.06	118.88	124.45
38	10	306	KC1	C3A-C4A-NA	6.06	117.19	110.57
30	A	821	CLA	O2D-CGD-CBD	6.06	122.04	111.27
38	11	311	KC1	C3B-C2B-C1B	-6.06	101.29	107.08
38	8	306	KC1	CMA-C3A-C2A	-6.06	113.47	128.30
30	B	824	CLA	CHD-C1D-ND	-6.06	118.89	124.45
30	A	842	CLA	CMD-C2D-C1D	6.05	135.38	124.71
30	B	829	CLA	CMD-C2D-C1D	6.05	135.38	124.71
38	8	307	KC1	C3B-C2B-C1B	-6.05	101.30	107.08
39	8	316	DD6	C32-C31-C36	-6.05	114.09	122.63
38	8	313	KC1	C3C-C4C-NC	6.05	115.57	109.88
30	A	810	CLA	CHD-C1D-ND	-6.05	118.90	124.45
30	B	802	CLA	O2D-CGD-CBD	6.04	122.00	111.27
30	A	824	CLA	CHD-C4C-C3C	-6.04	115.96	124.84
30	3	302	CLA	CHD-C4C-C3C	-6.04	115.96	124.84
38	2	314	KC1	C3B-C2B-C1B	-6.04	101.31	107.08
30	2u	202	CLA	CMD-C2D-C1D	6.04	135.35	124.71
38	12	305	KC1	C3B-C2B-C1B	-6.04	101.31	107.08
30	B	818	CLA	CHD-C1D-ND	-6.03	118.91	124.45
39	5	313	DD6	C8-C6-C5	-6.03	109.68	118.94
38	16	304	KC1	C3B-C2B-C1B	-6.03	101.32	107.08
39	2	316	DD6	C4-C5-C6	-6.03	118.70	127.31
30	A	837	CLA	O2D-CGD-CBD	6.03	121.98	111.27
30	7	303	CLA	CHD-C4C-C3C	-6.03	115.98	124.84
30	8	303	CLA	O2D-CGD-CBD	6.03	121.98	111.27
30	1	303	CLA	CHD-C4C-C3C	-6.03	115.98	124.84
30	A	836	CLA	C2C-C1C-NC	6.02	115.62	109.97
30	B	826	CLA	CHD-C4C-C3C	-6.02	115.99	124.84
30	2	308	CLA	CMD-C2D-C1D	6.02	135.32	124.71
30	5	302	CLA	CHD-C4C-C3C	-6.02	115.99	124.84
38	4	307	KC1	C1A-C2A-C3A	-6.02	102.34	107.11
38	14	308	KC1	C1A-C2A-C3A	-6.02	102.34	107.11
30	2	313	CLA	CHD-C1D-ND	-6.02	118.92	124.45
30	11	309	CLA	CHD-C1D-ND	-6.02	118.92	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	802	CLA	C4A-NA-C1A	-6.02	104.00	106.71
30	9	301	CLA	CHD-C1D-ND	-6.02	118.92	124.45
30	A	826	CLA	CMD-C2D-C1D	6.01	135.31	124.71
39	16	313	DD6	C32-C31-C36	-6.01	114.14	122.63
30	A	820	CLA	CHD-C1D-ND	-6.01	118.93	124.45
30	A	829	CLA	CHD-C1D-ND	-6.01	118.93	124.45
38	3	311	KC1	C3A-C4A-NA	6.01	117.13	110.57
30	A	804	CLA	O2D-CGD-CBD	6.01	121.94	111.27
30	A	826	CLA	C2C-C1C-NC	6.00	115.60	109.97
39	16	313	DD6	C24-C1-C2	-6.00	109.73	118.94
37	10	315	A86	C3-C2-C1	-6.00	118.74	127.31
30	10	307	CLA	CHD-C4C-C3C	-6.00	116.02	124.84
30	3	303	CLA	CHD-C1D-ND	-5.99	118.95	124.45
30	B	822	CLA	CHD-C1D-ND	-5.99	118.95	124.45
30	5	307	CLA	C2C-C1C-NC	5.99	115.58	109.97
38	12	313	KC1	C3C-C4C-NC	5.99	115.52	109.88
38	11	307	KC1	C3B-C2B-C1B	-5.99	101.36	107.08
30	10	305	CLA	CHD-C1D-ND	-5.98	118.95	124.45
39	1	310	DD6	C12-C11-C13	-5.98	108.65	118.08
38	9	304	KC1	C3B-C2B-C1B	-5.98	101.36	107.08
30	11	304	CLA	CHD-C1D-ND	-5.98	118.96	124.45
38	3	304	KC1	CMD-C2D-C1D	5.98	137.66	128.46
30	9	303	CLA	CMD-C2D-C1D	5.98	135.25	124.71
30	6	306	CLA	CHD-C4C-C3C	-5.98	116.05	124.84
38	6	308	KC1	C3C-C4C-NC	5.98	115.51	109.88
30	7	311	CLA	CMD-C2D-C1D	5.98	135.25	124.71
30	F	202	CLA	CHD-C4C-C3C	-5.98	116.06	124.84
38	8	311	KC1	C3A-C4A-NA	5.97	117.09	110.57
30	2	308	CLA	CHD-C4C-C3C	-5.97	116.06	124.84
30	13	302	CLA	CHD-C4C-C3C	-5.97	116.06	124.84
30	16	303	CLA	CHD-C4C-C3C	-5.97	116.06	124.84
30	3	301	CLA	CMD-C2D-C1D	5.97	135.23	124.71
30	8	308	CLA	CHD-C1D-ND	-5.97	118.97	124.45
30	4	303	CLA	CHD-C1D-ND	-5.97	118.97	124.45
39	9	314	DD6	C24-C1-C2	-5.97	109.79	118.94
30	16	310	CLA	CHD-C1D-ND	-5.97	118.97	124.45
38	11	311	KC1	C1A-C2A-C3A	-5.96	102.38	107.11
30	A	802	CLA	CHD-C1D-ND	-5.96	118.97	124.45
30	B	828	CLA	C2D-C1D-ND	5.96	114.50	110.10
30	A	840	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
30	A	838	CLA	O2D-CGD-CBD	5.96	121.86	111.27
30	B	807	CLA	CHD-C1D-ND	-5.96	118.98	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	814	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
38	8	313	KC1	C1A-C2A-C3A	-5.96	102.39	107.11
37	11	301	A86	C7-C6-C8	5.95	127.46	118.08
38	5	305	KC1	C3A-C4A-NA	5.95	117.07	110.57
39	2	315	DD6	C13-C11-C10	-5.95	109.81	118.94
30	A	838	CLA	CHD-C1D-ND	-5.95	118.99	124.45
30	9	308	CLA	CHD-C1D-ND	-5.95	118.99	124.45
38	2	306	KC1	C1A-C2A-C3A	-5.94	102.39	107.11
30	B	816	CLA	CHD-C4C-C3C	-5.94	116.11	124.84
39	13	314	DD6	C24-C1-C2	-5.94	109.82	118.94
30	4	311	CLA	C2C-C1C-NC	5.94	115.54	109.97
30	6	305	CLA	CHD-C1D-ND	-5.94	119.00	124.45
30	6	314	CLA	CHD-C1D-ND	-5.94	119.00	124.45
30	11	306	CLA	CHD-C1D-ND	-5.94	119.00	124.45
30	A	806	CLA	CHD-C1D-ND	-5.93	119.00	124.45
30	16	309	CLA	CHD-C1D-ND	-5.93	119.00	124.45
30	14	309	CLA	CHD-C1D-ND	-5.93	119.00	124.45
30	3	305	CLA	CHD-C4C-C3C	-5.93	116.12	124.84
38	8	314	KC1	C3A-C4A-NA	5.93	117.04	110.57
30	12	303	CLA	CHD-C4C-C3C	-5.93	116.13	124.84
30	A	829	CLA	CHD-C4C-C3C	-5.92	116.14	124.84
30	9	303	CLA	CHD-C4C-C3C	-5.92	116.14	124.84
38	2	312	KC1	C3C-C4C-NC	5.92	115.45	109.88
38	3	311	KC1	C3B-C2B-C1B	-5.92	101.43	107.08
30	B	809	CLA	C2C-C1C-NC	5.91	115.51	109.97
30	A	818	CLA	CHD-C1D-ND	-5.91	119.02	124.45
30	1	305	CLA	C2C-C1C-NC	5.91	115.51	109.97
30	B	810	CLA	CHD-C4C-C3C	-5.91	116.15	124.84
30	4	302	CLA	CHD-C4C-C3C	-5.91	116.15	124.84
30	15	310	CLA	CHD-C1D-ND	-5.91	119.03	124.45
30	13	302	CLA	CMD-C2D-C1D	5.91	135.12	124.71
30	7	312	CLA	C2C-C1C-NC	5.91	115.50	109.97
30	11	306	CLA	CHD-C4C-C3C	-5.91	116.16	124.84
30	A	813	CLA	CHD-C4C-C3C	-5.90	116.16	124.84
30	9	302	CLA	CHD-C1D-ND	-5.90	119.03	124.45
37	10	315	A86	C25-C26-C27	-5.90	118.89	127.31
30	F	203	CLA	CHD-C4C-C3C	-5.90	116.17	124.84
37	6	320	A86	C20-C19-C18	-5.90	101.08	112.75
39	10	313	DD6	C24-C1-C2	-5.89	109.90	118.94
30	A	834	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
30	7	304	CLA	CHD-C1D-ND	-5.89	119.04	124.45
30	14	313	CLA	CHD-C4C-C3C	-5.89	116.18	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	5	315	A86	C25-C26-C27	-5.89	118.91	127.31
30	A	808	CLA	CHD-C4C-C3C	-5.89	116.19	124.84
30	16	302	CLA	CHD-C4C-C3C	-5.89	116.19	124.84
37	11	301	A86	C4-C5-C6	-5.89	118.91	127.31
38	9	311	KC1	C1A-C2A-C3A	-5.88	102.44	107.11
38	14	311	KC1	C3C-C4C-NC	5.88	115.42	109.88
30	1	305	CLA	CHD-C1D-ND	-5.88	119.05	124.45
39	13	314	DD6	C21-C20-C19	-5.88	107.66	114.28
30	15	313	CLA	CHD-C1D-ND	-5.88	119.05	124.45
30	9	305	CLA	CHD-C4C-C3C	-5.88	116.20	124.84
30	14	312	CLA	CHD-C1D-ND	-5.88	119.05	124.45
30	9	308	CLA	CHD-C4C-C3C	-5.88	116.20	124.84
30	8	302	CLA	CHD-C4C-C3C	-5.88	116.20	124.84
30	A	822	CLA	CMD-C2D-C1D	5.88	135.07	124.71
38	14	306	KC1	O2D-CGD-CBD	5.88	121.71	111.27
39	10	313	DD6	C21-C20-C19	-5.87	107.67	114.28
39	3	316	DD6	C8-C6-C5	-5.87	109.93	118.94
30	9	309	CLA	CMD-C2D-C1D	5.87	135.06	124.71
30	15	303	CLA	CHD-C4C-C3C	-5.87	116.21	124.84
30	A	823	CLA	O2D-CGD-CBD	5.87	121.70	111.27
30	5	311	CLA	CHD-C1D-ND	-5.87	119.06	124.45
39	7	314	DD6	O1-C20-C21	-5.87	108.02	115.06
38	4	307	KC1	CMA-C3A-C2A	-5.87	113.94	128.30
30	10	311	CLA	CHD-C4C-C3C	-5.87	116.22	124.84
30	B	811	CLA	CHD-C4C-C3C	-5.87	116.22	124.84
39	8	316	DD6	C24-C1-C2	-5.86	109.94	118.94
37	14	320	A86	C20-C19-C18	-5.86	101.15	112.75
30	B	807	CLA	C2C-C1C-NC	5.86	115.46	109.97
38	2	312	KC1	C3B-C2B-C1B	-5.86	101.48	107.08
37	8	315	A86	O4-C38-C39	5.86	121.87	111.09
38	5	305	KC1	C3B-C2B-C1B	-5.86	101.48	107.08
30	B	812	CLA	CMD-C2D-C1D	5.86	135.03	124.71
37	14	314	A86	C8-C6-C5	5.86	127.93	118.94
39	6	321	DD6	C7-C6-C8	-5.85	108.85	118.08
30	15	307	CLA	CMD-C2D-C1D	5.85	135.03	124.71
30	14	309	CLA	C2C-C1C-NC	5.85	115.45	109.97
30	15	303	CLA	C2C-C1C-NC	5.85	115.45	109.97
38	8	312	KC1	C3C-C4C-NC	5.85	115.39	109.88
38	6	313	KC1	C3B-C2B-C1B	-5.85	101.49	107.08
30	A	831	CLA	C2C-C1C-NC	5.85	115.45	109.97
30	A	804	CLA	CHD-C4C-C3C	-5.85	116.24	124.84
30	12	310	CLA	CHD-C4C-C3C	-5.85	116.24	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	815	CLA	C2C-C1C-NC	5.85	115.45	109.97
30	B	826	CLA	CMD-C2D-C1D	5.85	135.02	124.71
30	B	836	CLA	C2C-C1C-NC	5.85	115.45	109.97
39	8	317	DD6	C32-C31-C36	-5.85	114.38	122.63
30	3	310	CLA	C2C-C1C-NC	5.84	115.45	109.97
30	F	203	CLA	CHD-C1D-ND	-5.84	119.09	124.45
30	13	304	CLA	C2C-C1C-NC	5.84	115.44	109.97
38	6	313	KC1	C1A-C2A-C3A	-5.84	102.48	107.11
30	8	302	CLA	CHD-C1D-ND	-5.83	119.09	124.45
30	B	802	CLA	CHD-C4C-C3C	-5.83	116.26	124.84
30	8	304	CLA	CHD-C4C-C3C	-5.83	116.26	124.84
37	8	318	A86	C17-C16-C15	5.83	115.11	109.16
30	4	301	CLA	CHD-C4C-C3C	-5.83	116.27	124.84
38	14	311	KC1	C3B-C2B-C1B	-5.83	101.51	107.08
30	2	311	CLA	CHD-C1D-ND	-5.83	119.09	124.45
39	9	314	DD6	C12-C11-C13	-5.83	108.89	118.08
30	12	308	CLA	CHD-C4C-C3C	-5.83	116.27	124.84
30	A	841	CLA	CHD-C1D-ND	-5.83	119.10	124.45
30	A	805	CLA	CHD-C1D-ND	-5.83	119.10	124.45
30	A	815	CLA	C2C-C1C-NC	5.83	115.43	109.97
30	2	308	CLA	CHD-C1D-ND	-5.83	119.10	124.45
30	13	303	CLA	O2D-CGD-CBD	5.83	121.62	111.27
38	8	311	KC1	C3B-C2B-C1B	-5.82	101.52	107.08
30	16	305	CLA	CMD-C2D-C1D	5.82	134.97	124.71
38	13	311	KC1	CHB-C4A-C3A	-5.82	115.89	124.98
30	B	808	CLA	O2D-CGD-CBD	5.82	121.60	111.27
38	8	306	KC1	C3B-C2B-C1B	-5.82	101.52	107.08
30	10	304	CLA	CHD-C4C-C3C	-5.82	116.29	124.84
39	6	303	DD6	C35-C36-C31	-5.82	107.37	120.57
30	B	813	CLA	CHD-C4C-C3C	-5.82	116.29	124.84
30	A	843	CLA	CMD-C2D-C1D	5.81	134.96	124.71
37	2u	205	A86	C24-C1-C2	5.81	127.86	118.94
30	9	302	CLA	C2C-C1C-NC	5.81	115.42	109.97
30	B	805	CLA	CHD-C1D-ND	-5.81	119.12	124.45
30	3	302	CLA	CMD-C2D-C1D	5.81	134.95	124.71
39	4	313	DD6	C12-C11-C13	-5.81	108.93	118.08
30	B	836	CLA	CHD-C1D-ND	-5.81	119.12	124.45
38	3	304	KC1	C3B-C2B-C1B	-5.81	101.53	107.08
30	4	304	CLA	CHD-C4C-C3C	-5.81	116.31	124.84
30	2	301	CLA	CMD-C2D-C1D	5.80	134.94	124.71
38	13	308	KC1	O2D-CGD-CBD	5.80	121.58	111.27
30	B	837	CLA	CHD-C4C-C3C	-5.80	116.31	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	825	CLA	CHD-C1D-ND	-5.80	119.12	124.45
30	B	803	CLA	CHD-C4C-C3C	-5.80	116.32	124.84
30	A	837	CLA	CHD-C1D-ND	-5.80	119.13	124.45
30	16	310	CLA	CHD-C4C-C3C	-5.80	116.32	124.84
30	12	302	CLA	CHD-C4C-C3C	-5.80	116.32	124.84
39	12	315	DD6	C-C1-C24	-5.80	108.95	118.08
30	12	312	CLA	CHD-C1D-ND	-5.79	119.13	124.45
38	6	311	KC1	C3B-C2B-C1B	-5.79	101.55	107.08
30	5	303	CLA	CHD-C4C-C3C	-5.79	116.33	124.84
30	15	314	CLA	C2C-C1C-NC	5.79	115.40	109.97
39	16	313	DD6	C-C1-C24	-5.79	108.95	118.08
30	2	309	CLA	CHD-C1D-ND	-5.79	119.13	124.45
37	14	320	A86	C4-C3-C2	-5.79	111.61	123.47
37	9	313	A86	C33-C32-C31	5.79	114.84	109.21
38	8	310	KC1	C3C-C4C-NC	5.79	115.33	109.88
30	6	310	CLA	C2C-C1C-NC	5.79	115.39	109.97
30	B	823	CLA	CHD-C4C-C3C	-5.78	116.34	124.84
30	4	301	CLA	CHD-C1D-ND	-5.78	119.14	124.45
30	6	306	CLA	CHD-C1D-ND	-5.78	119.14	124.45
37	11	316	A86	C17-C16-C15	5.78	115.06	109.16
30	14	303	CLA	CHD-C1D-ND	-5.78	119.14	124.45
30	6	315	CLA	CHD-C4C-C3C	-5.78	116.35	124.84
30	B	829	CLA	O2D-CGD-CBD	5.78	121.54	111.27
30	12	306	CLA	C2C-C1C-NC	5.78	115.39	109.97
30	8	308	CLA	CHD-C4C-C3C	-5.78	116.35	124.84
30	6	315	CLA	CHD-C1D-ND	-5.78	119.15	124.45
30	A	808	CLA	CHD-C1D-ND	-5.77	119.15	124.45
37	11	316	A86	O4-C38-C39	5.77	121.71	111.09
30	16	306	CLA	CMD-C2D-C1D	5.77	134.88	124.71
38	8	312	KC1	C2B-C1B-NB	5.77	114.35	110.10
39	2	316	DD6	C24-C1-C2	-5.77	110.09	118.94
30	B	831	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
38	13	308	KC1	C3B-C2B-C1B	-5.77	101.57	107.08
37	3	314	A86	C25-C26-C27	-5.77	119.08	127.31
30	B	804	CLA	CHD-C4C-C3C	-5.77	116.37	124.84
30	A	832	CLA	CHD-C4C-C3C	-5.76	116.37	124.84
30	A	812	CLA	C2C-C1C-NC	5.76	115.37	109.97
38	9	311	KC1	C3B-C2B-C1B	-5.76	101.57	107.08
30	B	836	CLA	CHD-C4C-C3C	-5.76	116.37	124.84
30	B	828	CLA	C2C-C1C-NC	5.76	115.37	109.97
30	15	304	CLA	C2C-C1C-NC	5.76	115.37	109.97
30	2	303	CLA	C3D-C4D-ND	5.76	119.56	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	2	310	CLA	CHD-C4C-C3C	-5.76	116.37	124.84
30	14	313	CLA	O2D-CGD-CBD	5.76	121.50	111.27
39	10	314	DD6	C-C1-C24	-5.76	109.01	118.08
30	13	309	CLA	CHD-C4C-C3C	-5.76	116.38	124.84
30	10	307	CLA	CMD-C2D-C1D	5.76	134.86	124.71
30	3	307	CLA	CHD-C1D-ND	-5.76	119.17	124.45
38	9	312	KC1	C3A-C4A-NA	5.75	116.86	110.57
30	11	310	CLA	CHD-C1D-ND	-5.75	119.17	124.45
30	16	305	CLA	C2C-C1C-NC	5.75	115.36	109.97
39	15	318	DD6	C12-C11-C13	-5.75	109.02	118.08
30	16	309	CLA	C2C-C1C-NC	5.75	115.36	109.97
39	3	313	DD6	C7-C6-C8	-5.75	109.02	118.08
30	7	305	CLA	CHD-C4C-C3C	-5.75	116.39	124.84
30	4	309	CLA	CHD-C1D-ND	-5.75	119.17	124.45
30	15	311	CLA	CHD-C1D-ND	-5.75	119.17	124.45
30	5	304	CLA	CHD-C4C-C3C	-5.74	116.40	124.84
37	14	317	A86	C41-C32-C31	-5.74	105.33	110.47
30	A	840	CLA	O2D-CGD-CBD	5.74	121.47	111.27
30	B	807	CLA	CHD-C4C-C3C	-5.74	116.40	124.84
39	4	313	DD6	C-C1-C24	-5.74	109.04	118.08
30	A	805	CLA	CHD-C4C-C3C	-5.74	116.41	124.84
30	12	303	CLA	C2C-C1C-NC	5.74	115.35	109.97
30	6	310	CLA	CHD-C1D-ND	-5.74	119.18	124.45
30	2	304	CLA	CHD-C4C-C3C	-5.73	116.41	124.84
30	A	802	CLA	C2C-C1C-NC	5.73	115.34	109.97
38	13	305	KC1	C1A-C2A-C3A	-5.73	102.56	107.11
37	15	322	A86	C4-C3-C2	-5.73	111.73	123.47
30	5	311	CLA	C2C-C1C-NC	5.73	115.34	109.97
39	4	316	DD6	C7-C6-C8	-5.73	109.05	118.08
30	A	816	CLA	CHD-C4C-C3C	-5.73	116.42	124.84
30	A	807	CLA	CAA-C2A-C3A	-5.73	97.09	112.78
30	B	838	CLA	CHD-C1D-ND	-5.73	119.19	124.45
38	13	312	KC1	C3B-C2B-C1B	-5.73	101.61	107.08
38	3	308	KC1	C3B-C2B-C1B	-5.73	101.61	107.08
30	A	816	CLA	O2D-CGD-CBD	5.72	121.44	111.27
38	12	311	KC1	C3B-C2B-C1B	-5.72	101.61	107.08
30	1	307	CLA	C2C-C1C-NC	5.72	115.33	109.97
37	13	315	A86	C3-C2-C1	-5.72	119.14	127.31
30	9	309	CLA	C2C-C1C-NC	5.72	115.33	109.97
39	6	303	DD6	C-C1-C24	-5.72	109.06	118.08
30	B	839	CLA	CMD-C2D-C1D	5.72	134.79	124.71
30	2u	202	CLA	O2D-CGD-CBD	5.72	121.43	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	15	312	CLA	CBA-CAA-C2A	-5.72	96.99	113.86
39	9	314	DD6	C9-C10-C11	-5.71	119.15	127.31
39	7	317	DD6	C13-C11-C10	-5.71	110.17	118.94
38	13	305	KC1	C3C-C4C-NC	5.71	115.26	109.88
30	10	303	CLA	CHD-C1D-ND	-5.71	119.20	124.45
38	10	312	KC1	C3B-C2B-C1B	-5.71	101.62	107.08
30	1	302	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
30	10	303	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
30	7	312	CLA	CHD-C1D-ND	-5.71	119.21	124.45
30	10	311	CLA	CHD-C1D-ND	-5.71	119.21	124.45
30	B	814	CLA	O2D-CGD-CBD	5.71	121.41	111.27
30	A	811	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
30	A	841	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
39	12	315	DD6	C32-C31-C36	-5.70	114.58	122.63
38	14	308	KC1	C3B-C2B-C1B	-5.70	101.63	107.08
38	10	306	KC1	C3C-C4C-NC	5.70	115.25	109.88
30	B	824	CLA	O2D-CGD-CBD	5.70	121.40	111.27
30	15	313	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
38	14	308	KC1	O2D-CGD-CBD	5.70	121.40	111.27
30	4	306	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
38	11	312	KC1	CMD-C2D-C1D	5.70	137.22	128.46
30	2	304	CLA	CHD-C1D-ND	-5.70	119.22	124.45
30	3	309	CLA	CHD-C4C-C3C	-5.70	116.47	124.84
30	14	302	CLA	O2D-CGD-CBD	5.70	121.39	111.27
39	15	319	DD6	C7-C6-C8	-5.69	109.10	118.08
30	15	311	CLA	C2C-C1C-NC	5.69	115.31	109.97
30	A	803	CLA	CHD-C1D-ND	-5.69	119.22	124.45
30	B	813	CLA	CHD-C1D-ND	-5.69	119.22	124.45
30	L	203	CLA	CHD-C4C-C3C	-5.69	116.47	124.84
30	3	301	CLA	CHD-C1D-ND	-5.69	119.23	124.45
38	14	306	KC1	C3C-C4C-NC	5.69	115.23	109.88
30	13	307	CLA	O2D-CGD-CBD	5.69	121.38	111.27
30	12	310	CLA	CHD-C1D-ND	-5.69	119.23	124.45
39	7	317	DD6	C24-C1-C2	-5.69	110.22	118.94
30	B	827	CLA	CHD-C4C-C3C	-5.68	116.48	124.84
37	2u	205	A86	C4-C3-C2	-5.68	111.83	123.47
30	B	835	CLA	CHD-C4C-C3C	-5.68	116.49	124.84
30	15	312	CLA	O2D-CGD-CBD	5.68	121.36	111.27
37	2u	205	A86	C25-C26-C27	-5.68	119.20	127.31
30	B	818	CLA	C4A-NA-C1A	-5.68	104.15	106.71
37	2	319	A86	C4-C5-C6	-5.68	119.20	127.31
39	10	314	DD6	C24-C1-C2	-5.68	110.22	118.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	833	CLA	CHD-C4C-C3C	-5.68	116.49	124.84
30	10	305	CLA	CHD-C4C-C3C	-5.68	116.49	124.84
37	16	314	A86	C25-C26-C27	-5.68	119.20	127.31
39	6	303	DD6	C4-C5-C6	-5.68	119.21	127.31
30	B	834	CLA	O2D-CGD-CBD	5.68	121.36	111.27
30	B	818	CLA	CHD-C4C-C3C	-5.68	116.50	124.84
30	10	304	CLA	C2C-C1C-NC	5.68	115.29	109.97
30	7	310	CLA	CHD-C4C-C3C	-5.67	116.50	124.84
30	12	302	CLA	C2C-C1C-NC	5.67	115.29	109.97
30	12	306	CLA	CMD-C2D-C1D	5.67	134.71	124.71
30	A	840	CLA	C2C-C1C-NC	5.67	115.29	109.97
39	11	313	DD6	C8-C6-C5	-5.67	110.24	118.94
30	1	301	CLA	CHD-C1D-ND	-5.67	119.24	124.45
30	A	826	CLA	CHD-C4C-C3C	-5.67	116.50	124.84
30	10	304	CLA	CHD-C1D-ND	-5.67	119.25	124.45
30	J	101	CLA	C2C-C1C-NC	5.67	115.28	109.97
30	16	308	CLA	C2C-C1C-NC	5.67	115.28	109.97
30	3	305	CLA	CHD-C1D-ND	-5.67	119.25	124.45
30	B	812	CLA	C2C-C1C-NC	5.67	115.28	109.97
30	12	312	CLA	CHD-C4C-C3C	-5.67	116.51	124.84
30	B	804	CLA	CHD-C1D-ND	-5.66	119.25	124.45
30	B	837	CLA	CHD-C1D-ND	-5.66	119.25	124.45
30	2	301	CLA	O2D-CGD-CBD	5.66	121.33	111.27
30	A	810	CLA	C2C-C1C-NC	5.66	115.28	109.97
39	15	319	DD6	C24-C1-C2	-5.66	110.25	118.94
30	15	302	CLA	CHD-C4C-C3C	-5.66	116.52	124.84
30	6	317	CLA	CHD-C4C-C3C	-5.66	116.52	124.84
30	15	311	CLA	CHD-C4C-C3C	-5.66	116.52	124.84
39	7	302	DD6	C24-C1-C2	-5.65	110.27	118.94
38	9	312	KC1	C3B-C2B-C1B	-5.65	101.68	107.08
30	1	307	CLA	O2D-CGD-CBD	5.65	121.31	111.27
30	15	305	CLA	CHD-C1D-ND	-5.65	119.26	124.45
30	2	310	CLA	CHD-C1D-ND	-5.65	119.26	124.45
38	8	311	KC1	C3C-C4C-NC	5.65	115.19	109.88
30	6	309	CLA	CHD-C4C-C3C	-5.65	116.54	124.84
30	6	314	CLA	C2C-C1C-NC	5.64	115.26	109.97
38	8	314	KC1	C3C-C4C-NC	5.64	115.19	109.88
38	13	305	KC1	O2D-CGD-CBD	5.64	121.29	111.27
30	B	808	CLA	C2C-C1C-NC	5.64	115.26	109.97
30	A	820	CLA	C2C-C1C-NC	5.64	115.26	109.97
30	2	307	CLA	C2C-C1C-NC	5.64	115.26	109.97
38	16	311	KC1	C3C-C4C-NC	5.64	115.19	109.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	819	CLA	C2D-C1D-ND	5.64	114.26	110.10
30	2	313	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
38	3	311	KC1	CMD-C2D-C1D	5.64	137.13	128.46
39	6	318	DD6	C-C1-C24	-5.64	109.20	118.08
39	13	314	DD6	C-C1-C24	-5.64	109.20	118.08
37	11	315	A86	O4-C38-C39	5.64	121.46	111.09
30	10	305	CLA	O2D-CGD-CBD	5.63	121.28	111.27
30	A	825	CLA	C2C-C1C-NC	5.63	115.24	109.97
30	10	309	CLA	CHD-C1D-ND	-5.63	119.28	124.45
30	1	302	CLA	CHD-C1D-ND	-5.63	119.28	124.45
30	A	835	CLA	CHD-C4C-C3C	-5.63	116.57	124.84
30	15	305	CLA	O2D-CGD-CBD	5.62	121.26	111.27
30	A	839	CLA	CHD-C4C-C3C	-5.62	116.58	124.84
37	15	323	A86	C17-C16-C15	5.62	114.90	109.16
30	5	304	CLA	CHD-C1D-ND	-5.62	119.29	124.45
30	16	301	CLA	CHD-C1D-ND	-5.62	119.29	124.45
30	B	801	CLA	CMD-C2D-C1D	5.62	134.62	124.71
30	A	844	CLA	CHD-C1D-ND	-5.62	119.29	124.45
30	B	820	CLA	CHD-C1D-ND	-5.62	119.29	124.45
38	13	305	KC1	C3B-C2B-C1B	-5.62	101.71	107.08
30	13	307	CLA	CHD-C1D-ND	-5.62	119.29	124.45
30	15	306	CLA	CHD-C4C-C3C	-5.62	116.58	124.84
30	16	305	CLA	CHD-C4C-C3C	-5.62	116.58	124.84
30	9	303	CLA	CHD-C1D-ND	-5.61	119.29	124.45
38	8	310	KC1	C3B-C2B-C1B	-5.61	101.72	107.08
30	15	308	CLA	CMD-C2D-C1D	5.61	134.61	124.71
30	7	307	CLA	CHD-C1D-ND	-5.61	119.30	124.45
30	L	203	CLA	CHD-C1D-ND	-5.61	119.30	124.45
39	8	316	DD6	C13-C11-C10	-5.61	110.33	118.94
30	B	805	CLA	C2C-C1C-NC	5.61	115.23	109.97
30	B	829	CLA	CHD-C1D-ND	-5.61	119.30	124.45
39	5	313	DD6	C12-C11-C13	-5.61	109.24	118.08
39	2	315	DD6	C35-C36-C31	-5.61	107.84	120.57
30	8	303	CLA	CHD-C4C-C3C	-5.60	116.60	124.84
30	A	807	CLA	C4A-NA-C1A	-5.60	104.19	106.71
39	12	315	DD6	C12-C11-C13	-5.60	109.25	118.08
30	6	305	CLA	C4A-NA-C1A	-5.60	104.19	106.71
30	9	305	CLA	CHD-C1D-ND	-5.60	119.31	124.45
30	5	308	CLA	CHD-C4C-C3C	-5.60	116.61	124.84
37	14	319	A86	O4-C38-C39	5.60	121.39	111.09
30	2	309	CLA	CHD-C4C-C3C	-5.60	116.61	124.84
30	2	305	CLA	CMD-C2D-C1D	5.60	134.58	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	833	CLA	CHD-C1D-ND	-5.60	119.31	124.45
37	9	313	A86	O4-C38-C39	5.59	121.38	111.09
30	B	810	CLA	O2D-CGD-CBD	5.59	121.21	111.27
37	10	316	A86	C17-C16-C15	5.59	114.87	109.16
30	B	821	CLA	C2C-C1C-NC	5.59	115.21	109.97
38	6	311	KC1	C1A-NA-C4A	-5.59	104.19	106.71
38	3	308	KC1	C1A-C2A-C3A	-5.59	102.68	107.11
39	15	318	DD6	C24-C1-C2	-5.59	110.36	118.94
30	B	802	CLA	C4A-NA-C1A	-5.59	104.19	106.71
30	15	314	CLA	CHD-C4C-C3C	-5.59	116.62	124.84
30	4	306	CLA	CHD-C1D-ND	-5.59	119.32	124.45
30	A	809	CLA	CHD-C4C-C3C	-5.59	116.63	124.84
30	11	310	CLA	C4A-NA-C1A	-5.59	104.19	106.71
38	11	305	KC1	C3B-C2B-C1B	-5.58	101.74	107.08
30	12	307	CLA	CMD-C2D-C1D	5.58	134.56	124.71
30	B	836	CLA	O2D-CGD-CBD	5.58	121.19	111.27
30	B	808	CLA	CHD-C4C-C3C	-5.58	116.63	124.84
30	B	828	CLA	CHD-C1D-ND	-5.58	119.32	124.45
30	B	818	CLA	O2D-CGD-CBD	5.58	121.19	111.27
30	8	309	CLA	C2C-C1C-NC	5.58	115.20	109.97
30	14	304	CLA	CHD-C4C-C3C	-5.58	116.64	124.84
30	A	833	CLA	CHD-C4C-C3C	-5.58	116.64	124.84
30	3	303	CLA	CHD-C4C-C3C	-5.58	116.64	124.84
30	6	314	CLA	O2D-CGD-CBD	5.58	121.18	111.27
30	3	301	CLA	C2C-C1C-NC	5.58	115.20	109.97
30	15	307	CLA	CHD-C4C-C3C	-5.58	116.64	124.84
30	A	842	CLA	CHD-C1D-ND	-5.58	119.33	124.45
30	14	312	CLA	CHD-C4C-C3C	-5.58	116.64	124.84
39	9	314	DD6	C8-C6-C5	-5.58	110.38	118.94
30	A	837	CLA	C2C-C1C-NC	5.58	115.20	109.97
30	A	802	CLA	CMD-C2D-C1D	5.58	134.54	124.71
30	B	815	CLA	CHD-C1D-ND	-5.57	119.33	124.45
30	12	308	CLA	C2C-C1C-NC	5.57	115.19	109.97
37	14	320	A86	O4-C38-C39	5.57	121.34	111.09
30	B	826	CLA	C2C-C1C-NC	5.57	115.19	109.97
30	3	301	CLA	CHD-C4C-C3C	-5.57	116.65	124.84
38	6	311	KC1	C3C-C4C-NC	5.57	115.12	109.88
38	2	314	KC1	C3C-C4C-NC	5.57	115.12	109.88
38	4	308	KC1	C1A-C2A-C3A	-5.57	102.69	107.11
30	B	851	CLA	CHD-C4C-C3C	-5.57	116.66	124.84
38	9	312	KC1	CMD-C2D-C1D	5.57	137.02	128.46
30	7	304	CLA	C2C-C1C-NC	5.56	115.18	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	1	307	CLA	CHD-C1D-ND	-5.56	119.34	124.45
38	16	304	KC1	CMD-C2D-C1D	5.56	137.01	128.46
38	7	308	KC1	C3C-C4C-NC	5.56	115.11	109.88
37	10	302	A86	C7-C6-C8	5.56	126.83	118.08
30	B	838	CLA	CHD-C4C-C3C	-5.56	116.67	124.84
30	5	309	CLA	CHD-C1D-ND	-5.56	119.35	124.45
30	3	309	CLA	O2D-CGD-CBD	5.56	121.14	111.27
39	9	314	DD6	C-C1-C24	-5.55	109.33	118.08
30	A	843	CLA	C2C-C1C-NC	5.55	115.17	109.97
30	4	303	CLA	C4A-NA-C1A	-5.55	104.21	106.71
38	13	306	KC1	C3C-C4C-NC	5.55	115.10	109.88
30	14	310	CLA	C2C-C1C-NC	5.55	115.17	109.97
30	9	307	CLA	CHD-C1D-ND	-5.55	119.36	124.45
30	5	308	CLA	CMD-C2D-C1D	5.55	134.49	124.71
30	10	309	CLA	CHD-C4C-C3C	-5.55	116.69	124.84
30	16	309	CLA	CHD-C4C-C3C	-5.55	116.69	124.84
39	2	317	DD6	C13-C11-C10	-5.55	110.43	118.94
39	5	314	DD6	C12-C11-C13	-5.55	109.34	118.08
30	4	305	CLA	CHD-C4C-C3C	-5.55	116.69	124.84
30	A	835	CLA	C2C-C1C-NC	5.54	115.17	109.97
30	6	304	CLA	CHD-C4C-C3C	-5.54	116.69	124.84
30	5	308	CLA	O2D-CGD-CBD	5.54	121.12	111.27
30	11	304	CLA	CHD-C4C-C3C	-5.54	116.69	124.84
37	2	302	A86	C4-C3-C2	-5.54	112.12	123.47
30	A	838	CLA	C2C-C1C-NC	5.54	115.16	109.97
30	9	309	CLA	CHD-C4C-C3C	-5.54	116.70	124.84
38	3	308	KC1	O2D-CGD-CBD	5.54	121.11	111.27
30	A	824	CLA	C4A-NA-C1A	-5.54	104.22	106.71
30	5	311	CLA	CHD-C4C-C3C	-5.54	116.70	124.84
30	15	304	CLA	CHD-C4C-C3C	-5.54	116.70	124.84
30	B	826	CLA	O2D-CGD-CBD	5.54	121.11	111.27
30	B	851	CLA	CHD-C1D-ND	-5.54	119.37	124.45
30	5	308	CLA	CHD-C1D-ND	-5.54	119.37	124.45
30	11	309	CLA	O2D-CGD-CBD	5.54	121.11	111.27
39	3	316	DD6	C13-C11-C10	-5.53	110.45	118.94
30	B	825	CLA	CHD-C1D-ND	-5.53	119.37	124.45
30	2u	202	CLA	CHD-C1D-ND	-5.53	119.37	124.45
30	15	310	CLA	CHD-C4C-C3C	-5.53	116.71	124.84
30	6	315	CLA	C2C-C1C-NC	5.53	115.15	109.97
39	12	317	DD6	C-C1-C24	-5.53	109.37	118.08
30	14	302	CLA	CHD-C4C-C3C	-5.53	116.72	124.84
30	4	302	CLA	CHD-C1D-ND	-5.53	119.38	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	14	305	CLA	CHD-C4C-C3C	-5.53	116.72	124.84
30	B	839	CLA	CHD-C1D-ND	-5.53	119.38	124.45
30	5	302	CLA	CHD-C1D-ND	-5.53	119.38	124.45
30	J	101	CLA	CHD-C4C-C3C	-5.52	116.72	124.84
30	A	812	CLA	CHD-C4C-C3C	-5.52	116.72	124.84
38	5	310	KC1	O2D-CGD-CBD	5.52	121.08	111.27
30	B	814	CLA	C2C-C1C-NC	5.52	115.15	109.97
30	15	305	CLA	C2C-C1C-NC	5.52	115.15	109.97
30	12	306	CLA	CHD-C4C-C3C	-5.52	116.72	124.84
38	5	312	KC1	C3C-C4C-NC	5.52	115.08	109.88
37	4	315	A86	C17-C16-C15	5.52	114.80	109.16
38	9	310	KC1	O2D-CGD-CBD	5.52	121.07	111.27
30	14	303	CLA	CHD-C4C-C3C	-5.52	116.73	124.84
38	10	306	KC1	C3B-C2B-C1B	-5.52	101.81	107.08
30	A	843	CLA	CHD-C4C-C3C	-5.52	116.73	124.84
30	2	311	CLA	CHD-C4C-C3C	-5.51	116.73	124.84
30	12	307	CLA	C4A-NA-C1A	-5.51	104.23	106.71
37	4	314	A86	C4-C5-C6	-5.51	119.44	127.31
30	9	306	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
30	A	802	CLA	O2D-CGD-CBD	5.51	121.06	111.27
30	B	811	CLA	CMD-C2D-C1D	5.51	134.43	124.71
38	5	312	KC1	C3B-C2B-C1B	-5.51	101.81	107.08
30	B	834	CLA	C4A-NA-C1A	-5.51	104.23	106.71
30	16	307	CLA	C2C-C1C-NC	5.51	115.13	109.97
38	5	310	KC1	C3C-C4C-NC	5.51	115.06	109.88
30	A	822	CLA	CHD-C4C-C3C	-5.51	116.75	124.84
30	7	309	CLA	CHD-C4C-C3C	-5.51	116.75	124.84
37	5	316	A86	C3-C2-C1	-5.51	119.45	127.31
30	A	843	CLA	CHD-C1D-ND	-5.50	119.39	124.45
30	6	305	CLA	CHD-C4C-C3C	-5.50	116.75	124.84
30	A	813	CLA	C2C-C1C-NC	5.50	115.13	109.97
30	12	304	CLA	CHD-C4C-C3C	-5.50	116.75	124.84
30	15	312	CLA	C2C-C1C-NC	5.50	115.13	109.97
38	11	305	KC1	CMD-C2D-C1D	5.50	136.92	128.46
30	B	805	CLA	O2D-CGD-CBD	5.50	121.05	111.27
30	2	301	CLA	CHD-C1D-ND	-5.50	119.40	124.45
39	6	319	DD6	C32-C31-C36	-5.50	114.87	122.63
30	A	832	CLA	CHD-C1D-ND	-5.50	119.40	124.45
30	A	815	CLA	O2D-CGD-CBD	5.50	121.04	111.27
38	6	313	KC1	C3C-C4C-NC	5.50	115.05	109.88
30	15	306	CLA	CHD-C1D-ND	-5.50	119.40	124.45
30	16	310	CLA	C2C-C1C-NC	5.50	115.12	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	806	CLA	CHD-C4C-C3C	-5.49	116.76	124.84
30	14	305	CLA	C2C-C1C-NC	5.49	115.12	109.97
30	14	310	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
30	2	304	CLA	C4A-NA-C1A	-5.49	104.24	106.71
30	2	313	CLA	O2D-CGD-CBD	5.49	121.03	111.27
30	13	301	CLA	CHD-C1D-ND	-5.49	119.41	124.45
38	8	311	KC1	CMD-C2D-C1D	5.49	136.90	128.46
30	B	829	CLA	CHD-C4C-C3C	-5.49	116.78	124.84
39	10	313	DD6	C4-C5-C6	-5.48	119.48	127.31
30	B	830	CLA	C3D-C2D-C1D	-5.48	98.35	105.83
30	14	307	CLA	C2C-C1C-NC	5.48	115.11	109.97
38	13	312	KC1	CMD-C2D-C1D	5.48	136.89	128.46
39	4	316	DD6	C8-C6-C5	-5.48	110.53	118.94
37	10	302	A86	O4-C38-C39	5.48	121.18	111.09
30	1	307	CLA	CHD-C4C-C3C	-5.48	116.78	124.84
30	12	321	CLA	CHD-C1D-ND	-5.48	119.42	124.45
30	12	312	CLA	C2C-C1C-NC	5.48	115.11	109.97
30	A	828	CLA	C3D-C2D-C1D	-5.48	98.35	105.83
30	5	309	CLA	CHD-C4C-C3C	-5.48	116.78	124.84
30	2	310	CLA	C2C-C1C-NC	5.48	115.11	109.97
38	12	311	KC1	CMD-C2D-C1D	5.48	136.89	128.46
39	7	317	DD6	C32-C31-C36	-5.48	114.90	122.63
30	B	820	CLA	O2D-CGD-CBD	5.48	121.00	111.27
37	9	313	A86	C4-C5-C6	-5.48	119.49	127.31
39	4	313	DD6	C32-C31-C36	-5.47	114.91	122.63
39	6	303	DD6	C24-C1-C2	-5.47	110.54	118.94
30	B	806	CLA	CHD-C1D-ND	-5.47	119.42	124.45
30	2	305	CLA	CHD-C1D-ND	-5.47	119.42	124.45
37	3	315	A86	C33-C32-C31	5.47	114.53	109.21
30	B	809	CLA	CHD-C4C-C3C	-5.47	116.80	124.84
30	13	304	CLA	CHD-C4C-C3C	-5.47	116.80	124.84
38	6	312	KC1	C3B-C2B-C1B	-5.47	101.86	107.08
30	16	307	CLA	CHD-C4C-C3C	-5.47	116.80	124.84
38	9	310	KC1	C3C-C4C-NC	5.47	115.02	109.88
30	10	305	CLA	C2C-C1C-NC	5.47	115.09	109.97
38	16	311	KC1	CMD-C2D-C1D	5.46	136.86	128.46
37	15	316	A86	C3-C2-C1	-5.46	119.51	127.31
30	4	309	CLA	C2C-C1C-NC	5.46	115.09	109.97
38	10	310	KC1	C3B-C2B-C1B	-5.46	101.86	107.08
30	4	301	CLA	C2C-C1C-NC	5.46	115.09	109.97
30	12	321	CLA	C2C-C1C-NC	5.46	115.09	109.97
37	4	312	A86	O4-C38-C39	5.46	121.14	111.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	2	303	CLA	CHD-C1D-ND	-5.46	119.44	124.45
30	16	302	CLA	CHD-C1D-ND	-5.46	119.44	124.45
37	4	314	A86	O4-C38-C39	5.46	121.13	111.09
30	A	836	CLA	CMD-C2D-C1D	5.46	134.33	124.71
39	3	312	DD6	C24-C1-C2	-5.46	110.57	118.94
38	1	308	KC1	C3C-C4C-NC	5.46	115.01	109.88
30	15	313	CLA	C2C-C1C-NC	5.45	115.08	109.97
30	11	308	CLA	CHD-C4C-C3C	-5.45	116.82	124.84
30	A	809	CLA	CHD-C1D-ND	-5.45	119.44	124.45
30	A	816	CLA	CHD-C1D-ND	-5.45	119.44	124.45
30	15	310	CLA	C2C-C1C-NC	5.45	115.08	109.97
39	5	313	DD6	C-C1-C24	-5.45	109.49	118.08
39	2	317	DD6	C35-C36-C31	-5.45	108.20	120.57
30	7	306	CLA	CHD-C4C-C3C	-5.45	116.83	124.84
30	15	308	CLA	CHD-C4C-C3C	-5.45	116.83	124.84
39	6	318	DD6	C32-C31-C36	-5.45	114.94	122.63
30	1	301	CLA	CHD-C4C-C3C	-5.45	116.83	124.84
30	8	309	CLA	CHD-C1D-ND	-5.45	119.45	124.45
30	B	823	CLA	C2C-C1C-NC	5.45	115.07	109.97
30	11	306	CLA	C4A-NA-C1A	-5.45	104.26	106.71
30	10	308	CLA	CHD-C4C-C3C	-5.44	116.84	124.84
38	12	309	KC1	CMA-C3A-C2A	-5.44	114.97	128.30
30	B	819	CLA	CMD-C2D-C1D	5.44	134.30	124.71
30	15	308	CLA	C2C-C1C-NC	5.44	115.07	109.97
30	2	305	CLA	CHD-C4C-C3C	-5.44	116.84	124.84
30	A	844	CLA	CHD-C4C-C3C	-5.44	116.84	124.84
30	B	819	CLA	CHD-C4C-C3C	-5.44	116.85	124.84
30	A	807	CLA	CHD-C1D-ND	-5.44	119.46	124.45
30	L	202	CLA	CHD-C4C-C3C	-5.44	116.85	124.84
30	B	834	CLA	C2C-C1C-NC	5.43	115.06	109.97
30	A	819	CLA	CHD-C1D-ND	-5.43	119.46	124.45
38	8	306	KC1	CMD-C2D-C1D	5.43	136.81	128.46
30	9	309	CLA	CHD-C1D-ND	-5.43	119.47	124.45
30	2	305	CLA	C2C-C1C-NC	5.43	115.06	109.97
30	14	304	CLA	C2C-C1C-NC	5.42	115.05	109.97
38	8	312	KC1	CHB-C4A-C3A	-5.42	116.50	124.98
39	6	318	DD6	C8-C6-C5	-5.42	110.62	118.94
39	3	313	DD6	C24-C1-C2	-5.42	110.62	118.94
39	15	318	DD6	C-C1-C24	-5.42	109.53	118.08
39	1	310	DD6	C32-C31-C36	-5.42	114.98	122.63
30	12	310	CLA	C2C-C1C-NC	5.42	115.05	109.97
30	A	827	CLA	C3D-C2D-C1D	-5.42	98.43	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	8	303	CLA	C2C-C1C-NC	5.42	115.05	109.97
30	13	303	CLA	C2C-C1C-NC	5.42	115.05	109.97
30	5	309	CLA	C2C-C1C-NC	5.42	115.05	109.97
37	6	320	A86	C25-C26-C27	-5.41	119.58	127.31
30	B	832	CLA	CHD-C4C-C3C	-5.41	116.88	124.84
30	B	827	CLA	C2C-C1C-NC	5.41	115.04	109.97
37	9	316	A86	C4-C5-C6	-5.41	119.58	127.31
39	1	310	DD6	C-C1-C24	-5.41	109.55	118.08
30	B	820	CLA	C3D-C2D-C1D	-5.41	98.45	105.83
30	4	303	CLA	C2C-C1C-NC	5.41	115.04	109.97
30	15	309	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
30	3	306	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
30	6	314	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
30	13	307	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
30	6	309	CLA	CHD-C1D-ND	-5.40	119.49	124.45
30	16	307	CLA	CHD-C1D-ND	-5.40	119.49	124.45
30	A	824	CLA	CHD-C1D-ND	-5.40	119.49	124.45
30	6	316	CLA	CHD-C1D-ND	-5.40	119.49	124.45
39	9	314	DD6	O1-C20-C21	-5.40	108.59	115.06
37	14	316	A86	C25-C26-C27	-5.40	119.61	127.31
30	B	821	CLA	CHD-C4C-C3C	-5.39	116.91	124.84
30	2	309	CLA	C2C-C1C-NC	5.39	115.03	109.97
30	3	302	CLA	C2C-C1C-NC	5.39	115.03	109.97
30	8	305	CLA	C3D-C2D-C1D	-5.39	98.47	105.83
30	2	310	CLA	C4A-NA-C1A	-5.39	104.28	106.71
30	15	312	CLA	CHD-C4C-C3C	-5.39	116.91	124.84
39	15	318	DD6	C33-C34-C35	5.39	117.69	110.30
30	1	302	CLA	O2D-CGD-CBD	5.39	120.85	111.27
30	12	321	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
30	6	317	CLA	C2C-C1C-NC	5.39	115.02	109.97
30	A	814	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
30	A	817	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
30	4	304	CLA	CHD-C1D-ND	-5.39	119.50	124.45
37	13	315	A86	C17-C16-C15	5.39	114.66	109.16
30	16	306	CLA	C4A-NA-C1A	-5.39	104.28	106.71
30	7	304	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
39	9	314	DD6	C32-C31-C36	-5.39	115.03	122.63
30	B	830	CLA	O2D-CGD-CBD	5.39	120.84	111.27
30	1	301	CLA	C2C-C1C-NC	5.39	115.02	109.97
30	2	307	CLA	CHD-C4C-C3C	-5.38	116.92	124.84
38	7	308	KC1	C3B-C2B-C1B	-5.38	101.93	107.08
37	13	313	A86	C17-C16-C15	5.38	114.66	109.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	13	302	CLA	C2C-C1C-NC	5.38	115.02	109.97
30	1	304	CLA	CMD-C2D-C1D	5.38	134.20	124.71
30	6	307	CLA	C2C-C1C-NC	5.38	115.01	109.97
38	13	311	KC1	CMD-C2D-C1D	5.38	136.73	128.46
38	4	307	KC1	O2D-CGD-CBD	5.38	120.83	111.27
37	8	318	A86	C10-C9-C8	-5.38	106.43	123.22
38	10	310	KC1	C3C-C4C-NC	5.38	114.94	109.88
38	11	311	KC1	C3C-C4C-NC	5.38	114.94	109.88
30	2u	202	CLA	C2C-C1C-NC	5.38	115.01	109.97
30	A	822	CLA	C2C-C1C-NC	5.37	115.01	109.97
30	F	202	CLA	C2C-C1C-NC	5.37	115.01	109.97
30	15	307	CLA	CHD-C1D-ND	-5.37	119.52	124.45
30	3	302	CLA	CHD-C1D-ND	-5.37	119.52	124.45
30	A	809	CLA	O2D-CGD-CBD	5.37	120.81	111.27
30	3	310	CLA	CHD-C4C-C3C	-5.37	116.94	124.84
30	B	836	CLA	C3D-C2D-C1D	-5.37	98.51	105.83
30	B	826	CLA	CHD-C1D-ND	-5.37	119.52	124.45
30	B	809	CLA	CMD-C2D-C1D	5.36	134.16	124.71
30	2	313	CLA	C2C-C1C-NC	5.36	115.00	109.97
30	7	303	CLA	O2D-CGD-CBD	5.36	120.80	111.27
30	3	305	CLA	C2C-C1C-NC	5.36	114.99	109.97
30	5	303	CLA	CHD-C1D-ND	-5.36	119.53	124.45
30	16	308	CLA	CHD-C4C-C3C	-5.36	116.96	124.84
38	13	311	KC1	C3C-C4C-NC	5.36	114.92	109.88
30	12	307	CLA	O2D-CGD-CBD	5.36	120.78	111.27
37	13	315	A86	O4-C38-C39	5.35	120.94	111.09
37	14	316	A86	C4-C5-C6	-5.35	119.67	127.31
30	A	823	CLA	CHD-C4C-C3C	-5.35	116.97	124.84
38	3	311	KC1	C3C-C4C-NC	5.35	114.92	109.88
30	A	834	CLA	C2C-C1C-NC	5.35	114.98	109.97
38	12	309	KC1	O2D-CGD-CBD	5.35	120.77	111.27
30	B	802	CLA	CHD-C1D-ND	-5.35	119.54	124.45
39	12	317	DD6	C21-C20-C19	-5.35	108.27	114.28
30	2	304	CLA	C2C-C1C-NC	5.35	114.98	109.97
30	4	311	CLA	CHD-C4C-C3C	-5.35	116.98	124.84
38	6	312	KC1	C3C-C4C-NC	5.34	114.91	109.88
30	4	309	CLA	CHD-C4C-C3C	-5.34	116.98	124.84
30	L	202	CLA	O2D-CGD-CBD	5.34	120.77	111.27
39	7	317	DD6	C7-C6-C8	-5.34	109.66	118.08
30	7	312	CLA	CHD-C4C-C3C	-5.34	116.98	124.84
30	5	308	CLA	C2C-C1C-NC	5.34	114.98	109.97
37	2	318	A86	C20-C19-C18	-5.34	102.18	112.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	10	312	KC1	CMD-C2D-C1D	5.34	136.68	128.46
30	B	808	CLA	CHD-C1D-ND	-5.34	119.55	124.45
37	10	301	A86	C20-C19-C18	-5.34	102.18	112.75
30	A	821	CLA	CMD-C2D-C1D	5.34	134.13	124.71
37	9	316	A86	C25-C26-C27	-5.34	119.69	127.31
30	B	812	CLA	CHD-C4C-C3C	-5.34	116.99	124.84
30	8	302	CLA	C2C-C1C-NC	5.34	114.97	109.97
30	8	303	CLA	CMD-C2D-C1D	5.34	134.12	124.71
30	12	303	CLA	CHD-C1D-ND	-5.34	119.55	124.45
38	5	306	KC1	CMD-C2D-C1D	5.34	136.67	128.46
30	B	814	CLA	CMD-C2D-C1D	5.34	134.12	124.71
38	6	311	KC1	O2D-CGD-CBD	5.34	120.75	111.27
37	2u	205	A86	C7-C6-C5	-5.34	115.45	122.92
30	A	822	CLA	CHD-C1D-ND	-5.34	119.55	124.45
38	12	313	KC1	CHD-C4C-C3C	-5.34	115.31	125.33
30	B	833	CLA	C2C-C1C-NC	5.34	114.97	109.97
30	11	308	CLA	C2C-C1C-NC	5.33	114.97	109.97
30	6	306	CLA	O2D-CGD-CBD	5.33	120.74	111.27
38	8	312	KC1	C3B-C2B-C1B	-5.33	101.98	107.08
38	13	306	KC1	C3B-C2B-C1B	-5.33	101.98	107.08
30	16	302	CLA	C2C-C1C-NC	5.33	114.97	109.97
30	A	810	CLA	CHD-C4C-C3C	-5.33	117.00	124.84
30	F	203	CLA	O2D-CGD-CBD	5.33	120.74	111.27
30	F	202	CLA	CHD-C1D-ND	-5.33	119.56	124.45
30	J	101	CLA	CHD-C1D-ND	-5.33	119.56	124.45
38	12	311	KC1	O2D-CGD-CBD	5.33	120.73	111.27
30	1	302	CLA	C2C-C1C-NC	5.33	114.96	109.97
30	A	802	CLA	CHD-C4C-C3C	-5.32	117.01	124.84
30	B	810	CLA	CHD-C1D-ND	-5.32	119.56	124.45
30	16	306	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
30	A	816	CLA	C2C-C1C-NC	5.32	114.96	109.97
30	A	820	CLA	C4A-NA-C1A	-5.32	104.31	106.71
38	12	305	KC1	C3C-C4C-NC	5.32	114.89	109.88
30	10	309	CLA	C2C-C1C-NC	5.32	114.95	109.97
39	16	313	DD6	C14-C13-C11	5.32	133.78	125.53
30	4	306	CLA	O2D-CGD-CBD	5.32	120.72	111.27
30	B	824	CLA	C4A-NA-C1A	-5.32	104.31	106.71
30	A	842	CLA	O2D-CGD-CBD	5.32	120.72	111.27
38	12	313	KC1	O2D-CGD-CBD	5.32	120.72	111.27
30	B	811	CLA	C2C-C1C-NC	5.31	114.95	109.97
30	A	837	CLA	CHD-C4C-C3C	-5.31	117.03	124.84
30	B	813	CLA	O2D-CGD-CBD	5.31	120.70	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	8	316	DD6	C-C1-C24	-5.31	109.71	118.08
30	7	309	CLA	CHD-C1D-ND	-5.31	119.57	124.45
30	7	306	CLA	CMD-C2D-C1D	5.31	134.06	124.71
30	A	814	CLA	CHD-C1D-ND	-5.30	119.58	124.45
30	7	311	CLA	CHD-C4C-C3C	-5.30	117.04	124.84
39	3	312	DD6	C-C1-C24	-5.30	109.72	118.08
39	15	319	DD6	C-C1-C24	-5.30	109.72	118.08
30	11	310	CLA	C2C-C1C-NC	5.30	114.94	109.97
30	6	309	CLA	CMD-C2D-C1D	5.30	134.06	124.71
37	14	319	A86	C17-C16-C15	5.30	114.57	109.16
38	8	314	KC1	CMD-C2D-C1D	5.30	136.61	128.46
37	5	315	A86	C4-C5-C6	-5.30	119.75	127.31
37	13	315	A86	C4-C5-C6	-5.30	119.75	127.31
30	B	818	CLA	C2C-C1C-NC	5.30	114.94	109.97
38	4	310	KC1	CMD-C2D-C1D	5.30	136.61	128.46
30	A	808	CLA	O2D-CGD-CBD	5.30	120.68	111.27
39	3	316	DD6	C-C1-C24	-5.30	109.73	118.08
39	7	314	DD6	C24-C1-C2	-5.30	110.81	118.94
30	B	820	CLA	C3C-C4C-NC	5.29	116.51	110.57
30	A	804	CLA	CHD-C1D-ND	-5.29	119.59	124.45
30	F	203	CLA	C2C-C1C-NC	5.29	114.93	109.97
30	A	821	CLA	CHD-C4C-C3C	-5.29	117.06	124.84
39	2	316	DD6	C32-C31-C36	-5.29	115.16	122.63
30	A	809	CLA	C2C-C1C-NC	5.29	114.93	109.97
30	6	305	CLA	C2C-C1C-NC	5.29	114.93	109.97
30	A	811	CLA	C2C-C1C-NC	5.29	114.92	109.97
30	7	311	CLA	C2C-C1C-NC	5.29	114.92	109.97
39	4	316	DD6	O1-C20-C21	-5.29	108.72	115.06
30	14	307	CLA	C4A-NA-C1A	-5.28	104.33	106.71
38	11	312	KC1	CHC-C1C-C2C	-5.28	116.72	124.98
30	6	316	CLA	CHD-C4C-C3C	-5.28	117.07	124.84
38	3	304	KC1	C3C-C4C-NC	5.28	114.85	109.88
30	B	803	CLA	CMD-C2D-C1D	5.28	134.02	124.71
30	3	306	CLA	C4A-NA-C1A	-5.28	104.33	106.71
30	F	201	CLA	C2C-C1C-NC	5.27	114.91	109.97
30	7	303	CLA	CMD-C2D-C1D	5.27	134.01	124.71
30	6	309	CLA	C2C-C1C-NC	5.27	114.91	109.97
30	6	309	CLA	O2D-CGD-CBD	5.27	120.64	111.27
30	A	844	CLA	C2C-C1C-NC	5.27	114.91	109.97
38	10	312	KC1	C1A-NA-C4A	-5.27	104.34	106.71
38	7	313	KC1	CMD-C2D-C1D	5.27	136.56	128.46
30	B	832	CLA	C2C-C1C-NC	5.27	114.91	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	813	CLA	CHD-C1D-ND	-5.27	119.61	124.45
38	5	310	KC1	C3B-C2B-C1B	-5.27	102.05	107.08
37	11	315	A86	C25-C26-C27	-5.27	119.80	127.31
30	2	301	CLA	C1C-C2C-C3C	-5.26	101.42	106.96
30	13	303	CLA	CHD-C4C-C3C	-5.26	117.10	124.84
38	11	312	KC1	C3C-C4C-NC	5.26	114.83	109.88
30	1	305	CLA	CHD-C4C-C3C	-5.26	117.11	124.84
38	8	310	KC1	CHD-C4C-C3C	-5.26	115.45	125.33
30	9	307	CLA	C2C-C1C-NC	5.26	114.90	109.97
30	9	302	CLA	CHD-C4C-C3C	-5.26	117.11	124.84
38	12	305	KC1	CMD-C2D-C1D	5.26	136.54	128.46
38	9	312	KC1	C3C-C4C-NC	5.26	114.83	109.88
38	12	309	KC1	C3C-C4C-NC	5.26	114.83	109.88
30	4	309	CLA	O2D-CGD-CBD	5.25	120.60	111.27
38	3	308	KC1	C3C-C4C-NC	5.25	114.82	109.88
30	A	803	CLA	CHD-C4C-C3C	-5.25	117.12	124.84
37	3	315	A86	C36-C31-C32	-5.25	114.49	119.70
30	6	314	CLA	C4A-NA-C1A	-5.25	104.35	106.71
37	2u	203	A86	C7-C6-C5	-5.25	115.58	122.92
30	14	312	CLA	C2C-C1C-NC	5.25	114.89	109.97
30	12	302	CLA	CHD-C1D-ND	-5.24	119.63	124.45
30	13	302	CLA	CHD-C1D-ND	-5.24	119.64	124.45
30	B	830	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
30	B	816	CLA	O2D-CGD-CBD	5.24	120.58	111.27
30	7	311	CLA	CHD-C1D-ND	-5.24	119.64	124.45
30	8	305	CLA	CHD-C1D-ND	-5.24	119.64	124.45
30	16	302	CLA	C4A-NA-C1A	-5.24	104.35	106.71
38	14	306	KC1	C1A-NA-C4A	-5.24	104.35	106.71
38	2	306	KC1	CMD-C2D-C1D	5.23	136.51	128.46
30	5	303	CLA	C2C-C1C-NC	5.23	114.88	109.97
30	8	303	CLA	CHD-C1D-ND	-5.23	119.64	124.45
30	A	824	CLA	C2C-C1C-NC	5.23	114.87	109.97
30	A	840	CLA	C4A-NA-C1A	-5.23	104.35	106.71
30	15	305	CLA	CHD-C4C-C3C	-5.23	117.15	124.84
30	6	307	CLA	CHD-C1D-ND	-5.23	119.65	124.45
30	B	812	CLA	CHD-C1D-ND	-5.23	119.65	124.45
38	5	305	KC1	C3C-C4C-NC	5.23	114.80	109.88
30	B	824	CLA	CAA-C2A-C3A	-5.23	98.47	112.78
30	8	301	CLA	CMD-C2D-C1D	5.23	133.92	124.71
30	B	805	CLA	CHD-C4C-C3C	-5.23	117.16	124.84
30	13	307	CLA	C2C-C1C-NC	5.23	114.87	109.97
39	7	318	DD6	C-C1-C24	-5.23	109.84	118.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	3	303	CLA	C2C-C1C-NC	5.22	114.87	109.97
38	1	308	KC1	C3B-C2B-C1B	-5.22	102.09	107.08
30	13	301	CLA	C2C-C1C-NC	5.22	114.86	109.97
30	12	304	CLA	O2D-CGD-CBD	5.22	120.55	111.27
30	15	310	CLA	O2D-CGD-CBD	5.22	120.55	111.27
30	12	321	CLA	C4A-NA-C1A	-5.22	104.36	106.71
30	10	307	CLA	CHD-C1D-ND	-5.22	119.66	124.45
30	8	309	CLA	CHD-C4C-C3C	-5.22	117.17	124.84
30	13	301	CLA	O2D-CGD-CBD	5.22	120.54	111.27
39	6	319	DD6	C24-C1-C2	-5.22	110.94	118.94
30	14	309	CLA	CHD-C4C-C3C	-5.22	117.17	124.84
38	4	308	KC1	CMD-C2D-C1D	5.22	136.48	128.46
37	15	323	A86	O4-C38-C39	5.21	120.68	111.09
30	3	306	CLA	O2D-CGD-CBD	5.21	120.53	111.27
30	B	819	CLA	C2C-C1C-NC	5.21	114.86	109.97
30	A	836	CLA	CHD-C4C-C3C	-5.21	117.18	124.84
30	4	303	CLA	O2D-CGD-CBD	5.21	120.53	111.27
30	7	305	CLA	C2C-C1C-NC	5.21	114.85	109.97
38	11	312	KC1	C3B-C2B-C1B	-5.21	102.10	107.08
30	A	823	CLA	C2C-C1C-NC	5.21	114.85	109.97
30	11	309	CLA	C2C-C1C-NC	5.21	114.85	109.97
30	6	310	CLA	CHD-C4C-C3C	-5.21	117.19	124.84
37	4	315	A86	C40-C32-C31	-5.20	105.82	110.47
38	14	311	KC1	CMD-C2D-C1D	5.20	136.46	128.46
30	8	309	CLA	O2D-CGD-CBD	5.20	120.51	111.27
30	A	832	CLA	C2C-C1C-NC	5.20	114.84	109.97
38	9	311	KC1	C3C-C4C-NC	5.20	114.77	109.88
30	15	303	CLA	C4A-NA-C1A	-5.20	104.37	106.71
30	A	831	CLA	CHD-C4C-C3C	-5.19	117.20	124.84
30	14	303	CLA	C2C-C1C-NC	5.19	114.84	109.97
30	16	305	CLA	CHD-C1D-ND	-5.19	119.68	124.45
39	2	316	DD6	C-C1-C24	-5.19	109.90	118.08
37	10	302	A86	C7-C6-C5	-5.19	115.66	122.92
39	6	318	DD6	C13-C11-C10	-5.19	110.98	118.94
38	12	309	KC1	CMD-C2D-C1D	5.19	136.44	128.46
30	5	304	CLA	C2C-C1C-NC	5.19	114.83	109.97
30	9	301	CLA	C2C-C1C-NC	5.18	114.83	109.97
30	4	303	CLA	CHD-C4C-C3C	-5.18	117.22	124.84
30	A	836	CLA	CHD-C1D-ND	-5.18	119.69	124.45
39	6	303	DD6	C21-C20-C19	-5.18	108.45	114.28
30	7	304	CLA	C4A-NA-C1A	-5.18	104.38	106.71
30	A	830	CLA	C2C-C1C-NC	5.18	114.83	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	6	318	DD6	C24-C1-C2	-5.18	110.99	118.94
30	B	835	CLA	O2D-CGD-CBD	5.18	120.47	111.27
30	6	307	CLA	CHD-C4C-C3C	-5.18	117.23	124.84
37	2u	203	A86	C7-C6-C8	5.18	126.23	118.08
30	9	305	CLA	C2C-C1C-NC	5.17	114.82	109.97
37	1	309	A86	C41-C32-C31	-5.17	105.84	110.47
37	5	316	A86	O4-C38-C39	5.17	120.60	111.09
37	10	317	A86	C3-C2-C1	-5.17	119.93	127.31
38	8	313	KC1	CHD-C4C-C3C	-5.17	115.62	125.33
39	2	317	DD6	C-C1-C24	-5.17	109.93	118.08
38	16	304	KC1	C3C-C4C-NC	5.17	114.74	109.88
39	3	316	DD6	C12-C11-C13	-5.17	109.94	118.08
39	5	314	DD6	C21-C20-C19	-5.16	108.47	114.28
30	B	821	CLA	CHD-C1D-ND	-5.16	119.71	124.45
37	15	320	A86	C3-C4-C5	-5.16	112.90	123.47
38	13	308	KC1	CMD-C2D-C1D	5.16	136.39	128.46
38	14	311	KC1	CHD-C4C-C3C	-5.16	115.65	125.33
30	L	202	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
38	3	311	KC1	O2D-CGD-CBD	5.15	120.42	111.27
30	8	308	CLA	C2C-C1C-NC	5.15	114.80	109.97
38	13	306	KC1	CMD-C2D-C1D	5.15	136.38	128.46
30	F	202	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
38	6	308	KC1	CHD-C4C-C3C	-5.15	115.66	125.33
38	8	307	KC1	C3C-C4C-NC	5.15	114.72	109.88
30	15	309	CLA	C2C-C1C-NC	5.15	114.79	109.97
30	12	304	CLA	C4A-NA-C1A	-5.14	104.39	106.71
30	8	305	CLA	O2D-CGD-CBD	5.14	120.41	111.27
39	2	315	DD6	C24-C1-C2	-5.14	111.05	118.94
39	2	317	DD6	C21-C20-C15	-5.14	113.64	122.26
30	15	308	CLA	CHD-C1D-ND	-5.14	119.73	124.45
38	1	306	KC1	C3C-C4C-NC	5.14	114.72	109.88
30	16	301	CLA	C2C-C1C-NC	5.14	114.78	109.97
30	11	310	CLA	CHD-C4C-C3C	-5.14	117.29	124.84
30	A	802	CLA	CAA-C2A-C3A	-5.14	98.71	112.78
38	6	312	KC1	CMD-C2D-C1D	5.14	136.36	128.46
37	10	317	A86	O4-C38-C39	5.13	120.53	111.09
30	12	306	CLA	O2D-CGD-CBD	5.13	120.39	111.27
30	8	304	CLA	CHD-C1D-ND	-5.13	119.74	124.45
38	8	312	KC1	CMD-C2D-C1D	5.13	136.35	128.46
29	A	801	CL0	CMD-C2D-C1D	5.13	133.76	124.71
30	9	305	CLA	CAA-C2A-C3A	-5.13	98.73	112.78
38	11	305	KC1	C3C-C4C-NC	5.13	114.71	109.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	6	316	CLA	C2C-C1C-NC	5.13	114.78	109.97
39	7	302	DD6	C21-C20-C15	-5.13	113.67	122.26
30	8	304	CLA	CMD-C2D-C1D	5.13	133.75	124.71
30	B	815	CLA	CHD-C4C-C3C	-5.13	117.30	124.84
38	4	308	KC1	C3C-C4C-NC	5.12	114.70	109.88
30	A	815	CLA	CHD-C4C-C3C	-5.12	117.31	124.84
38	1	306	KC1	C1A-NA-C4A	-5.12	104.40	106.71
38	12	309	KC1	C1A-C2A-C3A	-5.12	103.05	107.11
38	13	308	KC1	C3C-C4C-NC	5.12	114.70	109.88
30	A	808	CLA	C2C-C1C-NC	5.12	114.77	109.97
30	A	820	CLA	CHD-C4C-C3C	-5.12	117.32	124.84
30	11	306	CLA	CAA-C2A-C3A	-5.12	98.76	112.78
30	A	820	CLA	O2D-CGD-CBD	5.12	120.36	111.27
30	B	825	CLA	C3D-C2D-C1D	-5.12	98.85	105.83
30	B	824	CLA	CHD-C4C-C3C	-5.12	117.32	124.84
37	4	315	A86	C4-C5-C6	-5.12	120.01	127.31
39	1	310	DD6	C7-C6-C8	-5.12	110.02	118.08
30	B	816	CLA	C2C-C1C-NC	5.11	114.76	109.97
37	11	314	A86	C41-C32-C31	-5.11	105.90	110.47
30	L	203	CLA	C2C-C1C-NC	5.11	114.76	109.97
38	10	306	KC1	CMD-C2D-C1D	5.11	136.32	128.46
37	12	316	A86	C17-C16-C15	5.11	114.38	109.16
38	13	306	KC1	O2D-CGD-CBD	5.11	120.35	111.27
30	7	310	CLA	C4A-NA-C1A	-5.11	104.41	106.71
39	12	315	DD6	C24-C1-C2	-5.11	111.10	118.94
37	15	321	A86	O4-C38-C39	5.11	120.49	111.09
39	3	316	DD6	C7-C6-C8	-5.11	110.03	118.08
30	A	839	CLA	C2C-C1C-NC	5.11	114.75	109.97
30	J	101	CLA	C4A-NA-C1A	-5.10	104.41	106.71
30	B	823	CLA	CHD-C1D-ND	-5.10	119.76	124.45
30	A	817	CLA	C2C-C1C-NC	5.10	114.75	109.97
30	8	301	CLA	C2C-C1C-NC	5.10	114.75	109.97
37	10	302	A86	C36-C31-C32	-5.10	114.63	119.70
38	4	310	KC1	C3C-C4C-NC	5.10	114.68	109.88
29	A	801	CL0	O2D-CGD-CBD	5.10	120.33	111.27
38	8	306	KC1	C3C-C4C-NC	5.10	114.68	109.88
30	3	302	CLA	C4A-NA-C1A	-5.10	104.41	106.71
30	2	303	CLA	C2C-C1C-NC	5.10	114.75	109.97
37	9	315	A86	C4-C3-C2	-5.10	113.04	123.47
38	16	311	KC1	C1A-C2A-C3A	-5.09	103.07	107.11
30	A	840	CLA	C3D-C2D-C1D	-5.09	98.88	105.83
38	11	307	KC1	CMD-C2D-C1D	5.09	136.29	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	16	304	KC1	O2D-CGD-CBD	5.09	120.32	111.27
30	11	309	CLA	CHD-C4C-C3C	-5.09	117.35	124.84
30	6	315	CLA	O2D-CGD-CBD	5.09	120.32	111.27
30	B	811	CLA	O2D-CGD-CBD	5.09	120.32	111.27
30	7	303	CLA	CHD-C1D-ND	-5.09	119.78	124.45
37	10	316	A86	C25-C26-C27	-5.09	120.05	127.31
30	A	839	CLA	C4A-NA-C1A	-5.09	104.42	106.71
30	6	307	CLA	C4A-NA-C1A	-5.09	104.42	106.71
30	4	301	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
30	4	305	CLA	O2D-CGD-CBD	5.09	120.30	111.27
30	9	301	CLA	C3D-C2D-C1D	-5.08	98.89	105.83
37	10	301	A86	O4-C38-C39	5.08	120.44	111.09
30	12	303	CLA	C4A-NA-C1A	-5.08	104.42	106.71
30	16	306	CLA	C2C-C1C-NC	5.08	114.73	109.97
38	5	306	KC1	C3C-C4C-NC	5.08	114.66	109.88
30	10	304	CLA	C4A-NA-C1A	-5.08	104.42	106.71
30	9	303	CLA	C2C-C1C-NC	5.08	114.73	109.97
30	2	307	CLA	CMD-C2D-C1D	5.08	133.66	124.71
39	5	314	DD6	C32-C31-C36	-5.08	115.46	122.63
30	A	814	CLA	O2D-CGD-CBD	5.08	120.29	111.27
30	A	833	CLA	C2C-C1C-NC	5.08	114.73	109.97
38	9	310	KC1	C1A-NA-C4A	-5.08	104.42	106.71
38	8	307	KC1	O2D-CGD-CBD	5.08	120.29	111.27
30	5	304	CLA	O2D-CGD-CBD	5.07	120.28	111.27
30	12	308	CLA	CHD-C1D-ND	-5.07	119.80	124.45
30	B	822	CLA	C4A-NA-C1A	-5.07	104.43	106.71
30	B	834	CLA	CHD-C1D-ND	-5.07	119.80	124.45
30	B	803	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
37	15	320	A86	O4-C38-C39	5.07	120.41	111.09
30	6	304	CLA	C2C-C1C-NC	5.07	114.72	109.97
30	16	305	CLA	O2D-CGD-CBD	5.06	120.27	111.27
38	12	311	KC1	C3C-C4C-NC	5.06	114.64	109.88
30	B	829	CLA	C2C-C1C-NC	5.06	114.71	109.97
38	11	312	KC1	C2C-C1C-NC	5.06	116.09	110.57
30	6	304	CLA	C4A-NA-C1A	-5.06	104.43	106.71
38	8	307	KC1	CMD-C2D-C1D	5.06	136.24	128.46
37	14	301	A86	O4-C38-C39	5.05	120.39	111.09
30	16	307	CLA	O2D-CGD-CBD	5.05	120.25	111.27
38	10	310	KC1	O2D-CGD-CBD	5.05	120.25	111.27
39	11	313	DD6	C21-C20-C15	-5.05	113.79	122.26
37	9	315	A86	C20-C19-C18	-5.05	102.75	112.75
39	6	319	DD6	C21-C20-C19	-5.05	108.59	114.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	2u	203	A86	C25-C26-C27	-5.05	120.10	127.31
38	13	312	KC1	C3C-C4C-NC	5.05	114.63	109.88
30	3	309	CLA	C2C-C1C-NC	5.05	114.70	109.97
37	6	320	A86	C4-C3-C2	-5.05	113.13	123.47
30	10	307	CLA	C2C-C1C-NC	5.05	114.70	109.97
39	7	314	DD6	C-C1-C24	-5.05	110.12	118.08
30	A	829	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
30	A	807	CLA	C2C-C1C-NC	5.05	114.70	109.97
39	4	313	DD6	C24-C1-C2	-5.05	111.20	118.94
37	9	316	A86	O4-C38-C39	5.04	120.36	111.09
39	12	315	DD6	C21-C20-C19	-5.04	108.61	114.28
38	8	310	KC1	O2D-CGD-CBD	5.04	120.22	111.27
30	3	301	CLA	O2D-CGD-CBD	5.04	120.22	111.27
37	12	316	A86	C3-C2-C1	-5.04	120.12	127.31
37	16	312	A86	C36-C31-C32	-5.04	114.70	119.70
30	B	837	CLA	C2C-C1C-NC	5.04	114.69	109.97
38	2	314	KC1	CMD-C2D-C1D	5.03	136.20	128.46
30	B	802	CLA	C2C-C1C-NC	5.03	114.69	109.97
30	8	301	CLA	CHD-C1D-ND	-5.03	119.83	124.45
39	5	314	DD6	C-C1-C24	-5.03	110.15	118.08
37	10	316	A86	C4-C3-C2	-5.03	113.17	123.47
38	4	308	KC1	CHC-C1C-C2C	-5.03	117.13	124.98
30	B	822	CLA	CHD-C4C-C3C	-5.03	117.45	124.84
30	2	307	CLA	CHD-C1D-ND	-5.03	119.84	124.45
30	A	823	CLA	C3D-C2D-C1D	-5.02	98.97	105.83
37	16	314	A86	O4-C38-C39	5.02	120.33	111.09
30	A	814	CLA	CAC-C3C-C4C	5.02	131.33	124.81
30	9	301	CLA	CHD-C4C-C3C	-5.02	117.46	124.84
30	B	821	CLA	O2D-CGD-CBD	5.02	120.19	111.27
30	9	308	CLA	C4A-NA-C1A	-5.02	104.45	106.71
39	4	316	DD6	C21-C20-C19	-5.02	108.63	114.28
30	14	307	CLA	CAC-C3C-C4C	5.02	131.32	124.81
30	1	303	CLA	C2C-C1C-NC	5.02	114.67	109.97
30	12	304	CLA	C2C-C1C-NC	5.02	114.67	109.97
37	2	318	A86	C3-C2-C1	-5.02	120.15	127.31
38	1	306	KC1	C3B-C2B-C1B	-5.02	102.28	107.08
37	7	319	A86	O4-C38-C39	5.02	120.32	111.09
30	B	813	CLA	C2C-C1C-NC	5.02	114.67	109.97
30	16	306	CLA	O2D-CGD-CBD	5.02	120.18	111.27
38	5	310	KC1	C1A-NA-C4A	-5.02	104.45	106.71
30	3	307	CLA	CHD-C4C-C3C	-5.01	117.47	124.84
37	3	315	A86	O4-C38-C39	5.01	120.31	111.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	804	CLA	C2C-C1C-NC	5.01	114.67	109.97
30	B	801	CLA	O2D-CGD-CBD	5.01	120.17	111.27
38	8	312	KC1	C3A-C4A-NA	5.01	116.04	110.57
39	3	313	DD6	C-C1-C24	-5.01	110.18	118.08
38	5	305	KC1	CMD-C2D-C1D	5.01	136.17	128.46
39	7	317	DD6	C-C1-C24	-5.01	110.18	118.08
38	5	306	KC1	C1A-NA-C4A	-5.01	104.45	106.71
39	16	313	DD6	C12-C11-C13	-5.01	110.19	118.08
38	9	304	KC1	C3C-C4C-NC	5.00	114.59	109.88
30	A	831	CLA	CMD-C2D-C1D	5.00	133.53	124.71
30	B	831	CLA	C2C-C1C-NC	5.00	114.66	109.97
38	14	306	KC1	C3B-C2B-C1B	-5.00	102.30	107.08
38	11	311	KC1	CMD-C2D-C1D	5.00	136.15	128.46
30	11	306	CLA	O2D-CGD-CBD	5.00	120.15	111.27
30	2	301	CLA	CHD-C4C-C3C	-4.99	117.50	124.84
38	9	304	KC1	CMD-C2D-C1D	4.99	136.14	128.46
37	14	317	A86	O4-C38-C39	4.99	120.28	111.09
30	B	828	CLA	CHD-C4C-C3C	-4.99	117.50	124.84
37	4	317	A86	C41-C32-C31	-4.99	106.01	110.47
30	16	308	CLA	C4A-NA-C1A	-4.99	104.46	106.71
30	A	826	CLA	CHD-C1D-ND	-4.99	119.87	124.45
30	9	308	CLA	CAA-C2A-C3A	-4.99	99.12	112.78
30	16	301	CLA	C3D-C2D-C1D	-4.99	99.03	105.83
30	B	807	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
30	7	307	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
30	14	313	CLA	C2C-C1C-NC	4.98	114.64	109.97
39	6	318	DD6	C21-C20-C15	-4.98	113.92	122.26
30	B	817	CLA	O2D-CGD-CBD	4.98	120.11	111.27
30	10	303	CLA	C2C-C1C-NC	4.98	114.64	109.97
39	10	314	DD6	C7-C6-C8	-4.98	110.24	118.08
37	7	316	A86	C3-C2-C1	-4.97	120.22	127.31
38	13	310	KC1	O2D-CGD-CBD	4.97	120.10	111.27
38	13	311	KC1	C1A-NA-C4A	-4.97	104.47	106.71
30	4	304	CLA	C2C-C1C-NC	4.97	114.63	109.97
38	2	306	KC1	C3C-C4C-NC	4.97	114.56	109.88
37	10	316	A86	O4-C38-C39	4.96	120.22	111.09
30	6	309	CLA	C4A-NA-C1A	-4.96	104.47	106.71
37	14	318	A86	C41-C32-C31	-4.96	106.03	110.47
38	11	307	KC1	O2D-CGD-CBD	4.96	120.09	111.27
38	12	305	KC1	O2D-CGD-CBD	4.96	120.09	111.27
30	4	305	CLA	C2C-C1C-NC	4.96	114.62	109.97
38	5	310	KC1	CMD-C2D-C1D	4.96	136.09	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	8	302	CLA	C4A-NA-C1A	-4.96	104.48	106.71
30	B	807	CLA	O2D-CGD-CBD	4.96	120.08	111.27
30	8	302	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
37	2	318	A86	O4-C38-C39	4.96	120.21	111.09
37	2	319	A86	O4-C38-C39	4.96	120.21	111.09
37	14	315	A86	O4-C38-C39	4.96	120.21	111.09
30	A	804	CLA	C2C-C1C-NC	4.96	114.62	109.97
37	15	322	A86	O4-C38-C39	4.96	120.21	111.09
37	2	318	A86	C4-C5-C6	-4.95	120.24	127.31
38	1	306	KC1	O2D-CGD-CBD	4.95	120.07	111.27
30	B	801	CLA	CHD-C1D-ND	-4.95	119.90	124.45
30	B	824	CLA	C2C-C1C-NC	4.95	114.61	109.97
38	11	311	KC1	O2D-CGD-CBD	4.95	120.06	111.27
37	11	314	A86	O4-C38-C39	4.95	120.19	111.09
30	B	834	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
30	B	802	CLA	C3C-C4C-NC	4.95	116.12	110.57
30	A	804	CLA	C4A-NA-C1A	-4.94	104.48	106.71
30	5	307	CLA	CHD-C1D-ND	-4.94	119.91	124.45
30	12	310	CLA	O2D-CGD-CBD	4.94	120.05	111.27
30	4	304	CLA	O2D-CGD-CBD	4.94	120.05	111.27
30	16	303	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
30	12	306	CLA	CHD-C1D-ND	-4.94	119.92	124.45
37	15	315	A86	C4-C3-C2	4.94	133.59	123.47
38	10	312	KC1	C3C-C4C-NC	4.94	114.53	109.88
30	16	308	CLA	O2D-CGD-CBD	4.94	120.04	111.27
37	4	312	A86	C41-C32-C31	-4.93	106.06	110.47
30	5	307	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
30	A	819	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
38	13	310	KC1	CHD-C4C-C3C	-4.93	116.08	125.33
39	16	313	DD6	C21-C20-C19	-4.93	108.74	114.28
30	B	809	CLA	CHD-C1D-ND	-4.93	119.93	124.45
30	14	303	CLA	O2D-CGD-CBD	4.93	120.02	111.27
38	13	312	KC1	O2D-CGD-CBD	4.92	120.02	111.27
38	8	310	KC1	CMD-C2D-C1D	4.92	136.03	128.46
39	6	321	DD6	C-C1-C24	-4.92	110.32	118.08
37	3	315	A86	C4-C5-C6	-4.92	120.29	127.31
37	14	314	A86	O4-C38-C39	4.92	120.14	111.09
30	4	302	CLA	C2C-C1C-NC	4.92	114.58	109.97
37	15	316	A86	O4-C38-C39	4.92	120.14	111.09
30	2	305	CLA	CAA-C2A-C3A	-4.92	99.31	112.78
30	10	311	CLA	C2C-C1C-NC	4.92	114.58	109.97
30	A	818	CLA	C3D-C2D-C1D	-4.92	99.12	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	2	311	CLA	C2C-C1C-NC	4.92	114.58	109.97
30	A	825	CLA	CHD-C4C-C3C	-4.92	117.61	124.84
37	4	317	A86	O4-C38-C39	4.91	120.13	111.09
30	A	835	CLA	C4A-NA-C1A	-4.91	104.50	106.71
38	5	306	KC1	O2D-CGD-CBD	4.91	119.99	111.27
30	A	838	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
38	6	311	KC1	C2C-C1C-NC	4.90	115.93	110.57
30	L	202	CLA	C2C-C1C-NC	4.90	114.57	109.97
30	A	809	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
30	A	842	CLA	C2C-C1C-NC	4.90	114.56	109.97
37	14	301	A86	C41-C32-C31	-4.90	106.08	110.47
30	12	303	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
38	13	311	KC1	C3B-C2B-C1B	-4.90	102.40	107.08
39	12	317	DD6	C7-C6-C8	-4.90	110.36	118.08
37	5	301	A86	O4-C38-C39	4.90	120.10	111.09
37	4	315	A86	O4-C38-C39	4.89	120.09	111.09
37	6	320	A86	O4-C38-C39	4.89	120.09	111.09
30	B	802	CLA	CAA-C2A-C3A	-4.89	99.39	112.78
38	13	306	KC1	CHD-C4C-C3C	-4.89	116.15	125.33
39	6	319	DD6	C-C1-C24	-4.89	110.37	118.08
37	15	315	A86	O4-C38-C39	4.89	120.08	111.09
38	8	314	KC1	CHD-C4C-C3C	-4.89	116.16	125.33
37	5	315	A86	O4-C38-C39	4.89	120.08	111.09
37	8	315	A86	C10-C9-C8	-4.88	107.97	123.22
30	B	835	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
30	A	828	CLA	C3C-C4C-NC	4.88	116.05	110.57
30	4	306	CLA	C2C-C1C-NC	4.88	114.55	109.97
39	7	314	DD6	C21-C20-C19	-4.88	108.79	114.28
30	A	807	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
30	3	305	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
30	16	306	CLA	CHD-C1D-ND	-4.88	119.97	124.45
30	A	808	CLA	C3D-C2D-C1D	-4.88	99.18	105.83
30	4	301	CLA	O2D-CGD-CBD	4.88	119.93	111.27
37	13	315	A86	C25-C26-C27	-4.87	120.35	127.31
37	13	315	A86	C41-C32-C31	-4.87	106.11	110.47
39	9	314	DD6	C21-C20-C19	-4.87	108.80	114.28
38	16	304	KC1	CMA-C3A-C2A	-4.87	116.37	128.30
30	9	307	CLA	C3D-C2D-C1D	-4.87	99.19	105.83
30	B	839	CLA	C2C-C1C-NC	4.87	114.53	109.97
37	15	322	A86	C36-C31-C32	-4.87	114.87	119.70
37	9	313	A86	C3-C2-C1	-4.87	120.36	127.31
37	14	301	A86	C17-C16-C15	4.87	114.13	109.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	8	316	DD6	C21-C20-C19	-4.86	108.81	114.28
30	14	309	CLA	O2D-CGD-CBD	4.86	119.91	111.27
37	16	314	A86	C17-C16-C15	4.86	114.12	109.16
30	B	802	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
30	6	306	CLA	C2C-C1C-NC	4.86	114.53	109.97
30	14	304	CLA	O2D-CGD-CBD	4.86	119.90	111.27
30	B	829	CLA	C4A-NA-C1A	-4.86	104.52	106.71
30	15	308	CLA	O2D-CGD-CBD	4.86	119.90	111.27
39	10	314	DD6	C12-C11-C13	-4.86	110.42	118.08
30	F	201	CLA	C3C-C4C-NC	4.86	116.02	110.57
38	6	313	KC1	CHD-C4C-C3C	-4.86	116.21	125.33
30	B	804	CLA	C3D-C2D-C1D	-4.86	99.21	105.83
38	1	306	KC1	CMD-C2D-C1D	4.85	135.93	128.46
37	11	301	A86	O4-C38-C39	4.85	120.02	111.09
39	7	317	DD6	C21-C20-C15	-4.85	114.13	122.26
38	12	309	KC1	CBA-CAA-C2A	-4.85	106.78	125.27
30	A	830	CLA	C3C-C4C-NC	4.85	116.01	110.57
30	4	311	CLA	C3D-C2D-C1D	-4.85	99.21	105.83
38	7	308	KC1	CHD-C4C-C3C	-4.85	116.23	125.33
30	A	841	CLA	C4A-NA-C1A	-4.85	104.53	106.71
30	A	827	CLA	C2C-C1C-NC	4.85	114.51	109.97
30	13	301	CLA	C3D-C2D-C1D	-4.85	99.22	105.83
30	5	303	CLA	C4A-NA-C1A	-4.85	104.53	106.71
30	A	810	CLA	C3D-C2D-C1D	-4.85	99.22	105.83
30	8	305	CLA	C2C-C1C-NC	4.85	114.51	109.97
30	B	835	CLA	C2C-C1C-NC	4.84	114.51	109.97
39	2	316	DD6	C7-C6-C8	-4.84	110.45	118.08
38	16	311	KC1	O2D-CGD-CBD	4.84	119.87	111.27
38	13	310	KC1	CMD-C2D-C1D	4.84	135.91	128.46
37	8	318	A86	O4-C38-C39	4.84	120.00	111.09
38	7	313	KC1	C3C-C4C-NC	4.84	114.43	109.88
30	9	305	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
30	B	830	CLA	C2C-C1C-NC	4.84	114.51	109.97
37	2u	205	A86	C20-C19-C18	-4.84	103.17	112.75
37	2u	205	A86	C25-C24-C1	-4.84	112.82	126.42
30	B	816	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
37	2	319	A86	C3-C2-C1	-4.84	120.41	127.31
30	15	313	CLA	C4A-NA-C1A	-4.84	104.53	106.71
30	A	834	CLA	C3D-C2D-C1D	-4.83	99.23	105.83
38	8	313	KC1	C1A-NA-C4A	-4.83	104.53	106.71
38	8	312	KC1	C2A-C1A-NA	4.83	117.15	109.40
30	B	806	CLA	C2C-C1C-NC	4.83	114.50	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	833	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
30	B	825	CLA	C2C-C1C-NC	4.83	114.50	109.97
37	11	301	A86	C25-C26-C27	-4.83	120.42	127.31
37	15	317	A86	O4-C38-C39	4.83	119.97	111.09
38	8	307	KC1	CHD-C4C-C3C	-4.83	116.27	125.33
39	3	312	DD6	C7-C6-C8	-4.83	110.47	118.08
38	12	309	KC1	CHD-C4C-C3C	-4.83	116.27	125.33
38	11	307	KC1	C3C-C4C-NC	4.82	114.42	109.88
30	B	827	CLA	CMD-C2D-C1D	4.82	133.21	124.71
38	13	306	KC1	C1A-NA-C4A	-4.82	104.54	106.71
30	4	311	CLA	CBA-CAA-C2A	-4.82	99.63	113.86
30	A	824	CLA	O2D-CGD-CBD	4.82	119.83	111.27
30	14	312	CLA	C4A-NA-C1A	-4.82	104.54	106.71
30	7	306	CLA	O2D-CGD-CBD	4.82	119.83	111.27
30	A	806	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
30	14	307	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
30	15	314	CLA	C3D-C2D-C1D	-4.82	99.26	105.83
30	B	833	CLA	C3D-C2D-C1D	-4.82	99.26	105.83
37	3	314	A86	C41-C32-C31	-4.82	106.16	110.47
38	8	307	KC1	C1A-NA-C4A	-4.82	104.54	106.71
30	B	833	CLA	O2D-CGD-CBD	4.82	119.83	111.27
37	14	316	A86	C3-C2-C1	-4.81	120.44	127.31
30	7	304	CLA	C3D-C2D-C1D	-4.81	99.26	105.83
30	16	307	CLA	C4A-NA-C1A	-4.81	104.54	106.71
30	A	842	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
30	15	302	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
38	4	308	KC1	O2D-CGD-CBD	4.81	119.81	111.27
30	A	804	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
37	14	318	A86	C17-C16-C15	4.81	114.06	109.16
30	A	814	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
30	B	838	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
30	B	822	CLA	C2C-C1C-NC	4.80	114.47	109.97
39	15	318	DD6	C7-C6-C8	-4.80	110.51	118.08
30	A	812	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
30	B	838	CLA	O2D-CGD-CBD	4.80	119.80	111.27
38	1	308	KC1	O2D-CGD-CBD	4.80	119.79	111.27
38	13	311	KC1	CHD-C4C-C3C	-4.80	116.32	125.33
38	10	306	KC1	CHD-C4C-C3C	-4.80	116.33	125.33
30	10	307	CLA	C3D-C2D-C1D	-4.80	99.29	105.83
30	2	310	CLA	O2D-CGD-CBD	4.79	119.79	111.27
37	8	315	A86	C4-C5-C6	-4.79	120.47	127.31
39	11	313	DD6	C7-C6-C8	-4.79	110.53	118.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	817	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
38	10	310	KC1	CMD-C2D-C1D	4.79	135.83	128.46
30	A	828	CLA	CHD-C1D-ND	-4.79	120.05	124.45
37	2	319	A86	C20-C19-C18	-4.79	103.28	112.75
38	6	308	KC1	O2D-CGD-CBD	4.79	119.77	111.27
30	A	811	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
30	14	313	CLA	C4A-NA-C1A	-4.78	104.56	106.71
39	6	319	DD6	C21-C20-C15	-4.78	114.24	122.26
37	2u	205	A86	C4-C5-C6	-4.78	120.48	127.31
30	15	304	CLA	C4A-NA-C1A	-4.78	104.56	106.71
37	7	315	A86	C23-C16-C22	-4.78	100.32	107.37
37	3	315	A86	C17-C16-C15	4.78	114.04	109.16
37	9	315	A86	O4-C38-C39	4.78	119.88	111.09
30	B	839	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
30	4	311	CLA	C4A-NA-C1A	-4.78	104.56	106.71
30	13	307	CLA	C4A-NA-C1A	-4.78	104.56	106.71
30	B	815	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
30	B	806	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
38	10	312	KC1	CHD-C4C-C3C	-4.78	116.36	125.33
37	14	316	A86	O4-C38-C39	4.77	119.87	111.09
37	4	314	A86	C7-C6-C8	4.77	125.60	118.08
30	15	306	CLA	C4A-NA-C1A	-4.77	104.56	106.71
30	B	832	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
30	9	308	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
30	8	304	CLA	O2D-CGD-CBD	4.77	119.74	111.27
30	B	826	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
30	L	203	CLA	C3D-C2D-C1D	-4.77	99.33	105.83
38	4	310	KC1	C1A-NA-C4A	-4.77	104.56	106.71
38	16	304	KC1	CHC-C1C-C2C	-4.77	117.53	124.98
38	6	312	KC1	CHD-C4C-C3C	-4.77	116.38	125.33
30	7	312	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
30	B	813	CLA	C4A-NA-C1A	-4.76	104.56	106.71
30	3	302	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
30	10	311	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
30	A	813	CLA	C3D-C2D-C1D	-4.76	99.34	105.83
38	3	311	KC1	CHC-C1C-C2C	-4.76	117.54	124.98
37	14	315	A86	C17-C16-C15	4.76	114.02	109.16
30	7	311	CLA	O2D-CGD-CBD	4.75	119.72	111.27
37	14	318	A86	O4-C38-C39	4.75	119.84	111.09
30	7	309	CLA	C3D-C2D-C1D	-4.75	99.34	105.83
30	F	203	CLA	C4A-NA-C1A	-4.75	104.57	106.71
38	13	308	KC1	C1A-NA-C4A	-4.75	104.57	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	14	310	CLA	O2D-CGD-CBD	4.75	119.71	111.27
30	2	308	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
30	B	817	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
30	B	835	CLA	C4A-NA-C1A	-4.75	104.57	106.71
38	8	312	KC1	CHD-C4C-C3C	-4.75	116.42	125.33
30	B	834	CLA	C3C-C4C-NC	4.75	115.89	110.57
38	4	307	KC1	C3C-C4C-NC	4.75	114.35	109.88
37	15	316	A86	C41-C32-C31	-4.74	106.23	110.47
38	9	310	KC1	CHD-C4C-C3C	-4.74	116.42	125.33
30	L	203	CLA	O2D-CGD-CBD	4.74	119.70	111.27
30	16	310	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
30	5	302	CLA	C2C-C1C-NC	4.74	114.42	109.97
30	B	819	CLA	C4A-NA-C1A	-4.74	104.57	106.71
30	A	829	CLA	C2C-C1C-NC	4.74	114.41	109.97
30	3	301	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
38	4	307	KC1	CMD-C2D-C1D	4.74	135.75	128.46
30	B	822	CLA	C3D-C4D-ND	4.74	117.91	110.24
37	14	317	A86	C17-C16-C15	4.74	114.00	109.16
38	4	307	KC1	CHC-C1C-C2C	-4.74	117.58	124.98
37	1	309	A86	O4-C38-C39	4.74	119.81	111.09
38	5	310	KC1	CHD-C4C-C3C	-4.74	116.44	125.33
38	2	312	KC1	CMD-C2D-C1D	4.74	135.74	128.46
30	16	302	CLA	C3D-C2D-C1D	-4.73	99.37	105.83
30	5	303	CLA	C3D-C2D-C1D	-4.73	99.37	105.83
37	16	312	A86	C9-C10-C11	-4.73	112.70	126.61
37	15	322	A86	C33-C32-C31	4.73	113.81	109.21
30	11	308	CLA	O2D-CGD-CBD	4.73	119.67	111.27
30	16	303	CLA	C2C-C1C-NC	4.73	114.40	109.97
30	12	307	CLA	CHD-C1D-ND	-4.73	120.11	124.45
30	A	816	CLA	C3D-C2D-C1D	-4.72	99.38	105.83
30	1	303	CLA	C3D-C2D-C1D	-4.72	99.38	105.83
30	1	304	CLA	CHD-C1D-ND	-4.72	120.11	124.45
30	A	826	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
30	3	309	CLA	C4A-NA-C1A	-4.72	104.58	106.71
30	14	309	CLA	C4A-NA-C1A	-4.72	104.58	106.71
30	8	308	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
30	11	304	CLA	C2C-C1C-NC	4.72	114.39	109.97
38	1	308	KC1	C1A-NA-C4A	-4.72	104.58	106.71
37	10	315	A86	O4-C38-C39	4.72	119.77	111.09
30	B	813	CLA	C3C-C4C-NC	4.72	115.86	110.57
38	14	308	KC1	C2C-C1C-NC	4.72	115.72	110.57
30	4	302	CLA	C3D-C2D-C1D	-4.71	99.40	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	2	312	KC1	CHD-C4C-C3C	-4.71	116.48	125.33
30	3	309	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
30	4	303	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
30	A	817	CLA	O2D-CGD-CBD	4.71	119.64	111.27
30	12	312	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
30	A	803	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
39	3	312	DD6	C12-C11-C13	-4.71	110.66	118.08
37	5	315	A86	C40-C32-C31	-4.71	106.26	110.47
30	A	813	CLA	O2D-CGD-CBD	4.71	119.63	111.27
38	9	304	KC1	C1A-NA-C4A	-4.70	104.59	106.71
38	3	308	KC1	C2C-C1C-NC	4.70	115.70	110.57
30	B	813	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
30	9	306	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
29	A	801	CL0	CAA-C2A-C3A	-4.70	99.91	112.78
30	15	308	CLA	C3C-C4C-NC	4.70	115.84	110.57
37	12	316	A86	O4-C38-C39	4.70	119.73	111.09
30	A	831	CLA	CHD-C1D-ND	-4.70	120.14	124.45
30	13	309	CLA	C3D-C2D-C1D	-4.69	99.42	105.83
38	11	307	KC1	CHC-C1C-C2C	-4.69	117.64	124.98
30	F	201	CLA	C4A-NA-C1A	-4.69	104.60	106.71
30	A	839	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
30	15	309	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
30	A	819	CLA	C4A-NA-C1A	-4.69	104.60	106.71
39	2	315	DD6	C7-C6-C8	-4.69	110.69	118.08
30	10	311	CLA	O2D-CGD-CBD	4.69	119.60	111.27
29	A	801	CL0	CHD-C1D-ND	-4.69	120.14	124.45
39	2	317	DD6	C24-C1-C2	-4.69	111.75	118.94
37	2	302	A86	C41-C32-C31	-4.69	106.28	110.47
30	15	313	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
30	6	304	CLA	C3D-C2D-C1D	-4.69	99.44	105.83
30	9	303	CLA	O2D-CGD-CBD	4.68	119.59	111.27
39	8	317	DD6	C21-C20-C19	-4.68	109.01	114.28
30	5	311	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
30	15	302	CLA	C2C-C1C-NC	4.68	114.36	109.97
37	16	312	A86	O4-C38-C39	4.68	119.70	111.09
38	5	305	KC1	O2D-CGD-CBD	4.68	119.59	111.27
30	15	304	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
30	10	304	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
30	B	811	CLA	CHD-C1D-ND	-4.68	120.15	124.45
30	6	315	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
30	F	203	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
37	8	318	A86	C4-C3-C2	-4.68	113.89	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	815	CLA	C3D-C2D-C1D	-4.68	99.45	105.83
30	2	308	CLA	O2D-CGD-CBD	4.68	119.58	111.27
37	16	314	A86	C3-C2-C1	-4.68	120.63	127.31
30	A	838	CLA	C4A-NA-C1A	-4.68	104.60	106.71
30	B	822	CLA	CAA-C2A-C1A	-4.67	96.65	111.97
30	B	801	CLA	C2C-C1C-NC	4.67	114.35	109.97
30	3	310	CLA	C3D-C2D-C1D	-4.67	99.45	105.83
30	A	842	CLA	C4A-NA-C1A	-4.67	104.61	106.71
30	15	302	CLA	C3D-C4D-ND	4.67	117.79	110.24
38	11	311	KC1	CHD-C4C-C3C	-4.67	116.56	125.33
37	15	320	A86	C33-C32-C31	4.67	113.75	109.21
38	5	312	KC1	CHD-C4C-C3C	-4.67	116.56	125.33
30	5	302	CLA	O2D-CGD-CBD	4.67	119.57	111.27
38	8	306	KC1	CHD-C4C-C3C	-4.67	116.56	125.33
30	15	311	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
30	2	303	CLA	O2D-CGD-CBD	4.67	119.56	111.27
38	9	311	KC1	CMD-C2D-C1D	4.67	135.64	128.46
38	10	310	KC1	C2C-C1C-NC	4.67	115.67	110.57
30	6	317	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
30	7	303	CLA	C2C-C1C-NC	4.66	114.34	109.97
30	15	303	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
38	10	312	KC1	O2D-CGD-CBD	4.66	119.55	111.27
38	6	311	KC1	CMD-C2D-C1D	4.66	135.62	128.46
39	2	317	DD6	C7-C6-C8	-4.66	110.74	118.08
30	A	805	CLA	C2C-C1C-NC	4.66	114.33	109.97
37	10	301	A86	C33-C32-C31	4.65	113.73	109.21
38	2	314	KC1	CHD-C4C-C3C	-4.65	116.59	125.33
38	16	311	KC1	CHD-C4C-C3C	-4.65	116.59	125.33
30	15	311	CLA	O2D-CGD-CBD	4.65	119.53	111.27
38	8	306	KC1	CHC-C1C-C2C	-4.65	117.71	124.98
30	A	818	CLA	C2C-C1C-NC	4.65	114.33	109.97
38	4	308	KC1	C4B-C3B-C2B	-4.65	102.94	106.75
38	8	311	KC1	O2D-CGD-CBD	4.65	119.52	111.27
30	B	831	CLA	C3D-C2D-C1D	-4.64	99.49	105.83
30	6	310	CLA	O2D-CGD-CBD	4.64	119.52	111.27
38	9	311	KC1	CHD-C4C-C3C	-4.64	116.61	125.33
30	6	304	CLA	O2D-CGD-CBD	4.64	119.52	111.27
38	13	305	KC1	CHD-C4C-C3C	-4.64	116.62	125.33
30	2	309	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
30	14	302	CLA	C2C-C1C-NC	4.64	114.32	109.97
30	A	803	CLA	CMB-C2B-C3B	4.64	133.36	124.68
30	15	310	CLA	C3D-C2D-C1D	-4.64	99.50	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	2	317	DD6	C21-C20-C19	-4.64	109.06	114.28
30	B	851	CLA	C2C-C1C-NC	4.64	114.32	109.97
39	8	317	DD6	O1-C20-C21	-4.64	109.50	115.06
30	2	308	CLA	C4A-NA-C1A	-4.64	104.62	106.71
30	15	312	CLA	C4A-NA-C1A	-4.63	104.62	106.71
30	13	302	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
30	2	313	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
30	16	308	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
38	13	308	KC1	CHD-C4C-C3C	-4.63	116.64	125.33
37	2u	205	A86	C7-C6-C8	4.63	125.37	118.08
30	A	830	CLA	C4A-NA-C1A	-4.63	104.62	106.71
30	B	817	CLA	C4A-NA-C1A	-4.63	104.62	106.71
38	4	310	KC1	O2D-CGD-CBD	4.63	119.49	111.27
37	14	316	A86	C41-C32-C31	-4.62	106.33	110.47
30	2	304	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
38	11	305	KC1	C1A-NA-C4A	-4.62	104.63	106.71
37	5	316	A86	C4-C5-C6	-4.62	120.71	127.31
38	5	310	KC1	C4B-C3B-C2B	-4.62	102.96	106.75
38	13	305	KC1	CMD-C2D-C1D	4.62	135.56	128.46
30	13	304	CLA	O2D-CGD-CBD	4.62	119.48	111.27
30	A	805	CLA	C4A-NA-C1A	-4.62	104.63	106.71
30	6	316	CLA	C4A-NA-C1A	-4.62	104.63	106.71
30	5	308	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
30	A	841	CLA	C2C-C1C-NC	4.62	114.30	109.97
38	9	304	KC1	CHD-C4C-C3C	-4.62	116.66	125.33
37	12	314	A86	O4-C38-C39	4.62	119.58	111.09
30	B	830	CLA	C4A-NA-C1A	-4.62	104.63	106.71
30	8	308	CLA	O2D-CGD-CBD	4.61	119.47	111.27
39	3	313	DD6	C21-C20-C15	-4.61	114.53	122.26
30	2	307	CLA	O2D-CGD-CBD	4.61	119.47	111.27
30	2	303	CLA	CHD-C4C-C3C	-4.61	118.06	124.84
30	6	306	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
37	13	313	A86	C41-C32-C31	-4.61	106.34	110.47
30	15	313	CLA	O2D-CGD-CBD	4.61	119.46	111.27
30	A	828	CLA	C1D-CHD-C4C	-4.61	116.11	126.06
30	14	304	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
30	A	818	CLA	O2D-CGD-CBD	4.61	119.46	111.27
30	6	305	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
38	6	311	KC1	CHD-C4C-C3C	-4.61	116.68	125.33
30	9	302	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
30	10	308	CLA	C4A-NA-C1A	-4.61	104.64	106.71
38	10	310	KC1	C4B-C3B-C2B	-4.61	102.97	106.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	12	302	CLA	O2D-CGD-CBD	4.60	119.45	111.27
39	15	318	DD6	C35-C36-C31	-4.60	110.12	120.57
38	7	308	KC1	CMD-C2D-C1D	4.60	135.54	128.46
30	10	309	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
30	B	818	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
30	8	308	CLA	C4A-NA-C1A	-4.60	104.64	106.71
39	8	317	DD6	C7-C6-C8	-4.60	110.83	118.08
38	7	313	KC1	CHD-C4C-C3C	-4.60	116.69	125.33
38	11	305	KC1	CHD-C4C-C3C	-4.60	116.69	125.33
30	2u	202	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
30	B	837	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
30	14	307	CLA	C3D-C4D-ND	4.60	117.68	110.24
30	A	805	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
30	A	825	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
30	3	302	CLA	O2D-CGD-CBD	4.60	119.44	111.27
30	11	304	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
30	A	827	CLA	O2D-CGD-CBD	4.59	119.43	111.27
30	L	202	CLA	C3D-C4D-ND	4.59	117.67	110.24
38	16	311	KC1	CMA-C3A-C2A	-4.59	117.06	128.30
30	A	835	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
37	7	316	A86	C20-C19-C18	-4.59	103.67	112.75
30	3	306	CLA	C2C-C1C-NC	4.59	114.27	109.97
30	4	306	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
37	4	312	A86	C36-C31-C32	-4.59	115.14	119.70
38	12	313	KC1	C2C-C1C-NC	4.59	115.58	110.57
30	7	310	CLA	C2C-C1C-NC	4.59	114.27	109.97
39	10	314	DD6	C21-C20-C19	-4.58	109.12	114.28
30	B	826	CLA	C3C-C4C-NC	4.58	115.71	110.57
39	8	316	DD6	C15-C14-C13	4.58	135.69	125.99
30	A	831	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
38	3	304	KC1	CHD-C4C-C3C	-4.58	116.73	125.33
30	B	810	CLA	C2C-C1C-NC	4.58	114.27	109.97
30	16	303	CLA	O2D-CGD-CBD	4.58	119.41	111.27
30	A	837	CLA	C4A-NA-C1A	-4.58	104.65	106.71
38	13	312	KC1	CHD-C4C-C3C	-4.58	116.73	125.33
30	A	843	CLA	O2D-CGD-CBD	4.58	119.41	111.27
37	7	319	A86	C9-C8-C6	-4.58	113.55	126.42
30	13	304	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
30	4	309	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
30	7	312	CLA	O2D-CGD-CBD	4.58	119.40	111.27
38	14	308	KC1	CHD-C4C-C3C	-4.58	116.74	125.33
38	14	308	KC1	CHC-C1C-C2C	-4.58	117.83	124.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	16	312	A86	C8-C6-C5	4.58	125.96	118.94
38	11	305	KC1	O2D-CGD-CBD	4.58	119.40	111.27
30	4	305	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
38	12	305	KC1	CHC-C1C-C2C	-4.57	117.83	124.98
30	8	304	CLA	C2C-C1C-NC	4.57	114.26	109.97
39	16	313	DD6	C7-C6-C8	-4.57	110.87	118.08
37	7	316	A86	C35-C34-C33	4.57	117.86	109.88
30	B	801	CLA	C1D-CHD-C4C	-4.57	116.20	126.06
30	12	304	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
30	16	303	CLA	C4A-NA-C1A	-4.57	104.65	106.71
30	12	321	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
30	2	305	CLA	C4A-NA-C1A	-4.57	104.65	106.71
30	A	832	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
30	13	303	CLA	C3D-C2D-C1D	-4.56	99.60	105.83
38	4	308	KC1	CHD-C4C-C3C	-4.56	116.77	125.33
38	13	305	KC1	CHC-C1C-C2C	-4.56	117.86	124.98
39	7	302	DD6	C21-C20-C19	-4.56	109.15	114.28
37	3	314	A86	O4-C38-C39	4.56	119.47	111.09
30	9	305	CLA	O2D-CGD-O1D	-4.56	114.93	123.84
30	A	819	CLA	C2C-C1C-NC	4.56	114.24	109.97
38	13	311	KC1	O2D-CGD-CBD	4.56	119.36	111.27
38	1	308	KC1	CHD-C4C-C3C	-4.55	116.78	125.33
30	A	834	CLA	C4A-NA-C1A	-4.55	104.66	106.71
30	B	821	CLA	C4A-NA-C1A	-4.55	104.66	106.71
30	A	841	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
30	1	302	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
38	14	311	KC1	O2D-CGD-CBD	4.55	119.36	111.27
39	6	319	DD6	C13-C11-C10	-4.55	111.96	118.94
30	16	303	CLA	C3D-C4D-ND	4.55	117.60	110.24
37	4	315	A86	C25-C26-C27	-4.55	120.81	127.31
38	2	306	KC1	C1A-NA-C4A	-4.55	104.66	106.71
30	A	803	CLA	CMD-C2D-C1D	4.55	132.73	124.71
30	B	801	CLA	CAA-C2A-C3A	-4.55	100.32	112.78
38	5	305	KC1	CHD-C4C-C3C	-4.55	116.79	125.33
30	4	304	CLA	O2A-CGA-CBA	4.55	126.18	111.91
29	A	801	CL0	C3C-C4C-NC	4.55	115.67	110.57
30	14	313	CLA	C3D-C4D-ND	4.55	117.59	110.24
30	15	305	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
30	5	309	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
30	14	312	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
37	15	321	A86	C3-C2-C1	-4.54	120.83	127.31
38	2	312	KC1	C2C-C1C-NC	4.54	115.53	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	1	306	KC1	C4B-C3B-C2B	-4.54	103.02	106.75
30	B	828	CLA	CMB-C2B-C3B	4.54	133.17	124.68
30	A	822	CLA	O2D-CGD-CBD	4.54	119.33	111.27
30	1	304	CLA	C3C-C4C-NC	4.54	115.66	110.57
30	16	309	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
30	7	306	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
38	13	308	KC1	CHC-C1C-C2C	-4.53	117.89	124.98
30	B	805	CLA	C3D-C2D-C1D	-4.53	99.64	105.83
30	B	806	CLA	C4A-NA-C1A	-4.53	104.67	106.71
38	12	305	KC1	CHD-C4C-C3C	-4.53	116.82	125.33
30	F	202	CLA	O2D-CGD-CBD	4.53	119.32	111.27
38	11	312	KC1	C4B-C3B-C2B	-4.53	103.03	106.75
30	6	316	CLA	O2D-CGD-CBD	4.53	119.32	111.27
30	B	827	CLA	C4A-NA-C1A	-4.53	104.67	106.71
38	13	310	KC1	C2C-C1C-NC	4.53	115.52	110.57
38	6	313	KC1	CMD-C2D-C1D	4.53	135.42	128.46
30	9	306	CLA	O2D-CGD-CBD	4.53	119.31	111.27
30	10	305	CLA	CAA-C2A-C3A	-4.53	100.38	112.78
30	2	301	CLA	C1-O2A-CGA	4.53	128.32	116.44
30	B	801	CLA	C3C-C4C-NC	4.53	115.65	110.57
30	2	310	CLA	C1D-CHD-C4C	-4.53	116.30	126.06
30	9	308	CLA	C2C-C1C-NC	4.52	114.21	109.97
30	1	301	CLA	O2D-CGD-CBD	4.52	119.31	111.27
30	3	310	CLA	O2D-CGD-CBD	4.52	119.31	111.27
30	12	302	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
30	8	301	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
37	16	314	A86	C4-C5-C6	-4.52	120.86	127.31
30	1	305	CLA	C4A-NA-C1A	-4.52	104.67	106.71
30	11	306	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
38	3	308	KC1	CHC-C1C-C2C	-4.52	117.92	124.98
30	15	306	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
38	8	311	KC1	CHD-C4C-C3C	-4.52	116.84	125.33
30	B	812	CLA	C3D-C2D-C1D	-4.52	99.67	105.83
30	15	314	CLA	O2D-CGD-CBD	4.52	119.29	111.27
38	3	308	KC1	CBA-CAA-C2A	-4.51	108.07	125.27
30	16	305	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
30	7	306	CLA	CHD-C1D-ND	-4.51	120.31	124.45
30	10	305	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
38	9	312	KC1	CHC-C1C-C2C	-4.51	117.93	124.98
30	7	309	CLA	O2D-CGD-CBD	4.51	119.28	111.27
30	B	838	CLA	C1C-C2C-C3C	-4.51	102.22	106.96
30	B	810	CLA	C4A-NA-C1A	-4.51	104.68	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	5	306	KC1	CHD-C4C-C3C	-4.51	116.87	125.33
30	A	820	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
39	4	316	DD6	C24-C1-C2	-4.50	112.03	118.94
30	A	829	CLA	O2D-CGD-CBD	4.50	119.27	111.27
38	4	310	KC1	CHD-C4C-C3C	-4.50	116.88	125.33
30	A	825	CLA	O2D-CGD-CBD	4.50	119.27	111.27
30	5	302	CLA	C4A-NA-C1A	-4.50	104.68	106.71
37	11	316	A86	C4-C5-C6	-4.50	120.89	127.31
30	7	303	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
30	15	308	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
38	11	312	KC1	O2D-CGD-CBD	4.50	119.27	111.27
30	14	305	CLA	O2D-CGD-CBD	4.50	119.26	111.27
30	7	303	CLA	C4A-NA-C1A	-4.50	104.68	106.71
30	14	305	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
30	9	303	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
30	13	303	CLA	C3D-C4D-ND	4.50	117.52	110.24
30	A	811	CLA	O2D-CGD-CBD	4.50	119.26	111.27
30	14	310	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
30	B	831	CLA	C4A-NA-C1A	-4.50	104.68	106.71
30	2	301	CLA	C3D-C2D-C1D	-4.50	99.70	105.83
38	10	310	KC1	CHC-C1C-C2C	-4.49	117.96	124.98
30	11	310	CLA	O2D-CGD-CBD	4.49	119.25	111.27
39	12	317	DD6	C35-C36-C31	-4.49	110.38	120.57
30	6	310	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
38	10	312	KC1	C2A-C1A-NA	4.49	116.60	109.40
38	3	304	KC1	CHC-C1C-C2C	-4.49	117.97	124.98
30	1	304	CLA	C2C-C1C-NC	4.49	114.17	109.97
38	13	306	KC1	C2A-C1A-NA	4.48	116.59	109.40
30	1	301	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
38	8	312	KC1	CMA-C3A-C4A	-4.48	118.21	125.04
38	14	306	KC1	C2A-C1A-NA	4.48	116.59	109.40
30	11	309	CLA	C4A-NA-C1A	-4.48	104.69	106.71
30	10	308	CLA	C2C-C1C-NC	4.48	114.17	109.97
30	11	304	CLA	O2D-CGD-CBD	4.48	119.23	111.27
30	14	313	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
38	10	310	KC1	C2A-C1A-NA	4.48	116.58	109.40
39	10	314	DD6	C21-C20-C15	-4.48	114.75	122.26
38	6	311	KC1	CHC-C1C-C2C	-4.48	117.98	124.98
38	8	310	KC1	CHC-C1C-C2C	-4.48	117.98	124.98
38	3	308	KC1	CHD-C4C-C3C	-4.48	116.92	125.33
30	12	310	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
38	3	311	KC1	CHD-C4C-C3C	-4.48	116.93	125.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	828	CLA	C4A-NA-C1A	-4.48	104.69	106.71
30	A	806	CLA	C3D-C4D-ND	4.47	117.48	110.24
30	12	307	CLA	C2C-C1C-NC	4.47	114.16	109.97
30	B	829	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
39	15	319	DD6	C35-C36-C31	-4.47	110.42	120.57
37	10	317	A86	C4-C5-C6	-4.47	120.93	127.31
37	7	319	A86	C25-C24-C1	-4.47	113.85	126.42
38	12	311	KC1	CHD-C4C-C3C	-4.47	116.93	125.33
38	13	305	KC1	C2C-C1C-NC	4.47	115.45	110.57
30	F	201	CLA	CHD-C1D-ND	-4.47	120.34	124.45
39	11	313	DD6	C21-C20-C19	-4.47	109.25	114.28
30	10	303	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
30	7	305	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
38	2	312	KC1	CHC-C1C-C2C	-4.47	118.00	124.98
39	8	317	DD6	C-C1-C24	-4.47	111.04	118.08
37	7	315	A86	O4-C38-C39	4.47	119.31	111.09
30	A	814	CLA	C2C-C1C-NC	4.47	114.16	109.97
30	B	827	CLA	CHD-C1D-ND	-4.46	120.35	124.45
38	8	314	KC1	CHC-C1C-C2C	-4.46	118.01	124.98
30	8	304	CLA	C4A-NA-C1A	-4.46	104.70	106.71
38	10	306	KC1	C2C-C1C-NC	4.46	115.44	110.57
38	11	307	KC1	C2C-C1C-NC	4.46	115.44	110.57
30	2	305	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
38	6	313	KC1	O2D-CGD-CBD	4.46	119.19	111.27
38	2	306	KC1	CHD-C4C-C3C	-4.46	116.96	125.33
39	10	314	DD6	C15-C14-C13	-4.46	116.57	125.99
38	6	311	KC1	C2A-C1A-NA	4.46	116.55	109.40
30	12	307	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
30	7	311	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
30	14	307	CLA	CHD-C4C-C3C	-4.46	118.29	124.84
38	13	308	KC1	CBA-CAA-C2A	-4.46	108.28	125.27
30	8	304	CLA	C3D-C2D-C1D	-4.45	99.75	105.83
30	3	306	CLA	C3D-C2D-C1D	-4.45	99.75	105.83
30	11	309	CLA	C3D-C4D-ND	4.45	117.44	110.24
30	11	306	CLA	C2C-C1C-NC	4.45	114.14	109.97
37	11	314	A86	C25-C26-C27	-4.45	120.96	127.31
30	B	803	CLA	C1D-CHD-C4C	-4.45	116.46	126.06
30	F	202	CLA	C3C-C4C-NC	4.45	115.56	110.57
30	1	305	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
38	12	313	KC1	CHC-C1C-C2C	-4.45	118.03	124.98
38	9	310	KC1	CMD-C2D-C1D	4.45	135.30	128.46
30	9	301	CLA	CAC-C3C-C4C	4.44	130.58	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	5	312	KC1	CHC-C1C-C2C	-4.44	118.04	124.98
38	12	305	KC1	C2C-C1C-NC	4.44	115.42	110.57
37	11	315	A86	C41-C32-C31	-4.44	106.50	110.47
39	6	303	DD6	C7-C6-C8	-4.44	111.08	118.08
30	2	311	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
30	11	308	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
39	13	314	DD6	O1-C20-C21	-4.44	109.74	115.06
30	B	851	CLA	C4A-NA-C1A	-4.44	104.71	106.71
39	6	319	DD6	C12-C11-C13	-4.44	111.08	118.08
30	A	802	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
38	13	310	KC1	C1A-NA-C4A	-4.44	104.71	106.71
39	7	314	DD6	C35-C36-C31	-4.44	110.50	120.57
30	8	301	CLA	C3C-C4C-NC	4.44	115.55	110.57
30	B	812	CLA	O2D-CGD-CBD	4.44	119.15	111.27
39	1	310	DD6	C21-C20-C15	-4.44	114.83	122.26
30	A	837	CLA	C3D-C2D-C1D	-4.44	99.78	105.83
37	12	316	A86	C40-C32-C31	-4.43	106.50	110.47
30	8	304	CLA	C1D-CHD-C4C	-4.43	116.49	126.06
38	6	308	KC1	C1A-NA-C4A	-4.43	104.71	106.71
30	12	312	CLA	O2D-CGD-CBD	4.43	119.14	111.27
30	1	304	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
30	B	820	CLA	C2C-C1C-NC	4.43	114.12	109.97
38	10	310	KC1	CHD-C4C-C3C	-4.43	117.02	125.33
30	7	310	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
38	13	311	KC1	C2A-C1A-NA	4.43	116.50	109.40
38	8	311	KC1	CHC-C1C-C2C	-4.43	118.06	124.98
39	5	314	DD6	C7-C6-C8	-4.43	111.10	118.08
38	12	313	KC1	CMA-C3A-C2A	-4.43	117.46	128.30
38	12	311	KC1	CHC-C1C-C2C	-4.43	118.06	124.98
30	14	304	CLA	C4A-NA-C1A	-4.43	104.72	106.71
30	B	825	CLA	C3C-C4C-NC	4.43	115.53	110.57
30	B	809	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
37	10	315	A86	C40-C32-C31	-4.43	106.51	110.47
30	B	810	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
30	B	839	CLA	C3C-C4C-NC	4.42	115.53	110.57
38	9	312	KC1	CHD-C4C-C3C	-4.42	117.02	125.33
38	13	312	KC1	C1A-NA-C4A	-4.42	104.72	106.71
39	2	315	DD6	C21-C20-C19	-4.42	109.30	114.28
38	11	312	KC1	CHD-C4C-C3C	-4.42	117.03	125.33
30	15	307	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
38	5	306	KC1	C2A-C1A-NA	4.42	116.49	109.40
37	4	317	A86	C20-C19-C18	-4.42	104.00	112.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	817	CLA	C3D-C4D-ND	4.42	117.39	110.24
38	16	304	KC1	C1A-NA-C4A	-4.42	104.72	106.71
39	3	316	DD6	C21-C20-C19	-4.42	109.31	114.28
38	11	311	KC1	C1A-NA-C4A	-4.42	104.72	106.71
30	1	307	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
30	14	309	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
30	2	311	CLA	C3D-C4D-ND	4.41	117.38	110.24
39	12	315	DD6	C7-C6-C8	-4.41	111.13	118.08
30	B	824	CLA	C1-C2-C3	-4.41	118.42	126.04
38	3	308	KC1	CMD-C2D-C1D	4.41	135.24	128.46
37	11	301	A86	C7-C6-C5	-4.41	116.75	122.92
30	A	827	CLA	CAA-C2A-C3A	-4.41	100.72	112.78
30	14	302	CLA	C4A-NA-C1A	-4.40	104.73	106.71
30	2	310	CLA	C3D-C2D-C1D	-4.40	99.82	105.83
30	A	803	CLA	C2C-C1C-NC	4.40	114.10	109.97
38	16	304	KC1	C2A-C1A-NA	4.40	116.46	109.40
30	14	302	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
38	1	306	KC1	CHC-C1C-C2C	-4.40	118.11	124.98
30	16	309	CLA	C4A-NA-C1A	-4.40	104.73	106.71
38	9	312	KC1	C2C-C1C-NC	4.40	115.37	110.57
38	12	309	KC1	CHC-C1C-C2C	-4.40	118.11	124.98
37	15	321	A86	C17-C16-C15	4.40	113.65	109.16
30	15	310	CLA	C4A-NA-C1A	-4.40	104.73	106.71
38	9	304	KC1	C2A-C1A-NA	4.39	116.45	109.40
30	B	817	CLA	C3D-C4D-ND	4.39	117.35	110.24
38	16	304	KC1	C2C-C1C-NC	4.39	115.37	110.57
30	A	830	CLA	O2D-CGD-CBD	4.39	119.08	111.27
38	1	308	KC1	C4B-C3B-C2B	-4.39	103.14	106.75
38	9	310	KC1	C2A-C1A-NA	4.39	116.44	109.40
30	B	811	CLA	C3D-C4D-ND	4.39	117.34	110.24
30	13	304	CLA	C3D-C4D-ND	4.39	117.34	110.24
30	7	307	CLA	C2C-C1C-NC	4.39	114.08	109.97
38	5	310	KC1	CHC-C1C-C2C	-4.39	118.12	124.98
38	2	314	KC1	CHC-C1C-C2C	-4.39	118.12	124.98
30	B	837	CLA	O2D-CGD-CBD	4.39	119.06	111.27
30	A	831	CLA	C3C-C4C-NC	4.39	115.49	110.57
30	15	314	CLA	C3D-C4D-ND	4.38	117.33	110.24
37	10	316	A86	C10-C9-C8	-4.38	109.54	123.22
30	B	816	CLA	C3D-C4D-ND	4.38	117.33	110.24
38	6	312	KC1	C1A-NA-C4A	-4.38	104.74	106.71
30	2	308	CLA	C2C-C1C-NC	4.38	114.08	109.97
30	5	309	CLA	O2D-CGD-CBD	4.38	119.05	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	809	CLA	O2D-CGD-CBD	4.38	119.05	111.27
30	14	303	CLA	C3D-C2D-C1D	-4.38	99.86	105.83
30	11	304	CLA	C3D-C4D-ND	4.38	117.32	110.24
30	15	303	CLA	O2D-CGD-CBD	4.38	119.04	111.27
37	2	302	A86	O4-C38-C39	4.37	119.14	111.09
30	B	814	CLA	CHD-C1D-ND	-4.37	120.44	124.45
37	10	301	A86	C4-C3-C2	-4.37	114.52	123.47
30	8	309	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
30	3	310	CLA	C1C-C2C-C3C	-4.37	102.36	106.96
37	10	316	A86	C40-C32-C31	-4.37	106.56	110.47
30	13	302	CLA	O2D-CGD-CBD	4.37	119.03	111.27
30	13	307	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
39	10	313	DD6	C12-C11-C13	-4.37	111.20	118.08
30	3	307	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
38	9	304	KC1	CHC-C1C-C2C	-4.37	118.16	124.98
38	7	313	KC1	O2D-CGD-CBD	4.36	119.02	111.27
39	3	316	DD6	C37-C36-C35	-4.36	106.27	114.36
30	15	303	CLA	C3C-C4C-NC	4.36	115.46	110.57
30	B	802	CLA	CMD-C2D-C1D	4.36	132.40	124.71
30	10	308	CLA	C3D-C4D-ND	4.36	117.29	110.24
38	1	306	KC1	C2A-C1A-NA	4.36	116.39	109.40
37	14	301	A86	C3-C2-C1	-4.36	121.09	127.31
30	7	311	CLA	C4A-NA-C1A	-4.36	104.75	106.71
39	13	314	DD6	C15-C14-C13	4.36	135.21	125.99
38	4	308	KC1	C2C-C1C-NC	4.36	115.33	110.57
38	7	308	KC1	C2C-C1C-NC	4.35	115.33	110.57
37	15	320	A86	C41-C32-C31	-4.35	106.58	110.47
38	3	311	KC1	C2C-C1C-NC	4.35	115.32	110.57
30	2	311	CLA	O2D-CGD-CBD	4.35	119.00	111.27
38	11	305	KC1	C2C-C1C-NC	4.35	115.32	110.57
37	8	315	A86	C12-C11-C13	4.35	123.33	116.02
30	10	308	CLA	C3D-C2D-C1D	-4.35	99.89	105.83
38	5	312	KC1	C4B-C3B-C2B	-4.35	103.18	106.75
30	B	823	CLA	C3D-C2D-C1D	-4.35	99.90	105.83
37	10	316	A86	C12-C11-C13	4.35	123.33	116.02
38	2	314	KC1	C2A-C1A-NA	4.35	116.38	109.40
30	14	302	CLA	C3D-C4D-ND	4.35	117.27	110.24
29	A	801	CL0	C1C-C2C-C3C	-4.35	102.39	106.96
30	6	317	CLA	O2D-CGD-CBD	4.35	118.99	111.27
30	A	819	CLA	C3C-C4C-NC	4.35	115.45	110.57
30	3	303	CLA	CAA-C2A-C3A	-4.35	100.88	112.78
38	12	311	KC1	C1A-NA-C4A	-4.35	104.75	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	5	310	KC1	C2A-C1A-NA	4.35	116.37	109.40
38	13	312	KC1	CHC-C1C-C2C	-4.34	118.19	124.98
30	8	305	CLA	C3C-C4C-NC	4.34	115.44	110.57
30	13	302	CLA	C4A-NA-C1A	-4.34	104.75	106.71
30	8	303	CLA	C3D-C4D-ND	4.34	117.27	110.24
38	5	305	KC1	CHC-C1C-C2C	-4.34	118.19	124.98
30	B	807	CLA	C3C-C4C-NC	4.34	115.44	110.57
38	3	304	KC1	C2C-C1C-NC	4.34	115.31	110.57
30	8	301	CLA	O2D-CGD-CBD	4.34	118.98	111.27
38	14	306	KC1	CHC-C1C-C2C	-4.34	118.20	124.98
38	11	305	KC1	CHC-C1C-C2C	-4.34	118.20	124.98
37	7	316	A86	C4-C5-C6	-4.34	121.12	127.31
38	4	307	KC1	C2C-C1C-NC	4.34	115.31	110.57
38	8	306	KC1	C2C-C1C-NC	4.33	115.30	110.57
30	B	833	CLA	C4A-NA-C1A	-4.33	104.76	106.71
30	12	310	CLA	C4A-NA-C1A	-4.33	104.76	106.71
30	6	314	CLA	C3D-C4D-ND	4.33	117.24	110.24
37	9	315	A86	C33-C32-C31	4.33	113.42	109.21
38	10	306	KC1	CHC-C1C-C2C	-4.33	118.22	124.98
30	1	303	CLA	O2D-CGD-CBD	4.33	118.96	111.27
38	1	308	KC1	C2A-C1A-NA	4.33	116.34	109.40
38	14	306	KC1	C4B-C3B-C2B	-4.33	103.20	106.75
30	F	201	CLA	C3D-C2D-C1D	-4.33	99.93	105.83
38	6	312	KC1	C2A-C1A-NA	4.33	116.34	109.40
38	8	307	KC1	C2A-C1A-NA	4.33	116.34	109.40
38	11	311	KC1	CHC-C1C-C2C	-4.33	118.22	124.98
30	6	309	CLA	C3D-C2D-C1D	-4.32	99.93	105.83
30	16	301	CLA	C3C-C4C-NC	4.32	115.42	110.57
30	16	306	CLA	C3D-C4D-ND	4.32	117.23	110.24
38	11	305	KC1	C2A-C1A-NA	4.32	116.34	109.40
30	12	310	CLA	C3D-C4D-ND	4.32	117.23	110.24
30	3	301	CLA	C4A-NA-C1A	-4.32	104.76	106.71
30	6	316	CLA	C3D-C2D-C1D	-4.32	99.93	105.83
30	10	307	CLA	C3C-C4C-NC	4.32	115.42	110.57
37	4	314	A86	C7-C6-C5	-4.32	116.87	122.92
30	B	827	CLA	C3C-C4C-NC	4.32	115.41	110.57
30	B	830	CLA	C3C-C4C-NC	4.32	115.41	110.57
30	15	312	CLA	C3D-C2D-C1D	-4.32	99.94	105.83
38	8	314	KC1	O2D-CGD-O1D	-4.32	115.40	123.84
38	1	306	KC1	CHD-C4C-C3C	-4.32	117.23	125.33
37	14	320	A86	C9-C8-C6	-4.31	114.30	126.42
30	9	309	CLA	C3D-C2D-C1D	-4.31	99.95	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	4	311	CLA	O2D-CGD-CBD	4.31	118.93	111.27
38	9	311	KC1	C1A-NA-C4A	-4.31	104.77	106.71
30	7	306	CLA	C3C-C4C-NC	4.31	115.40	110.57
30	10	305	CLA	C3D-C4D-ND	4.31	117.21	110.24
30	1	303	CLA	C4A-NA-C1A	-4.31	104.77	106.71
30	B	801	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
30	5	302	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
30	1	307	CLA	C3D-C4D-ND	4.30	117.20	110.24
38	13	306	KC1	C4B-C3B-C2B	-4.30	103.22	106.75
30	5	304	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
30	5	307	CLA	C3C-C4C-NC	4.30	115.40	110.57
30	12	308	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
30	F	202	CLA	C4A-NA-C1A	-4.30	104.77	106.71
30	B	822	CLA	CAA-C2A-C3A	-4.30	101.00	112.78
35	B	852	LMT	O1B-C4'-C3'	4.30	118.72	107.28
38	13	311	KC1	C4B-C3B-C2B	-4.30	103.22	106.75
30	3	303	CLA	C3D-C2D-C1D	-4.30	99.97	105.83
38	7	308	KC1	C4B-C3B-C2B	-4.30	103.22	106.75
38	7	308	KC1	CHC-C1C-C2C	-4.30	118.27	124.98
30	7	305	CLA	C3D-C4D-ND	4.30	117.19	110.24
30	5	307	CLA	C3B-C4B-NB	4.29	114.76	109.21
30	A	826	CLA	C3C-C4C-NC	4.29	115.39	110.57
38	14	306	KC1	CMD-C2D-C1D	4.29	135.06	128.46
30	2	313	CLA	C4A-NA-C1A	-4.29	104.78	106.71
30	1	302	CLA	C3D-C4D-ND	4.29	117.18	110.24
38	10	306	KC1	C1A-NA-C4A	-4.29	104.78	106.71
30	16	307	CLA	C3D-C2D-C1D	-4.29	99.98	105.83
30	B	801	CLA	CMA-C3A-C2A	-4.29	96.53	113.83
30	3	309	CLA	C3D-C4D-ND	4.29	117.17	110.24
38	1	306	KC1	C2C-C1C-NC	4.29	115.25	110.57
30	7	310	CLA	C3D-C4D-ND	4.29	117.17	110.24
30	9	307	CLA	C3C-C4C-NC	4.28	115.38	110.57
39	7	317	DD6	C15-C14-C13	4.28	135.05	125.99
30	12	304	CLA	C3D-C4D-ND	4.28	117.17	110.24
30	A	828	CLA	C4C-C3C-C2C	-4.28	100.65	106.90
30	15	312	CLA	C1C-C2C-C3C	-4.28	102.45	106.96
38	6	311	KC1	C4B-C3B-C2B	-4.28	103.23	106.75
30	J	101	CLA	O2D-CGD-CBD	4.28	118.88	111.27
30	A	821	CLA	CHD-C1D-ND	-4.28	120.52	124.45
30	5	311	CLA	C4A-NA-C1A	-4.28	104.78	106.71
30	A	838	CLA	CMB-C2B-C3B	4.28	132.69	124.68
38	8	312	KC1	O2D-CGD-CBD	4.28	118.87	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	310	KC1	CHC-C1C-C2C	-4.28	118.29	124.98
30	14	312	CLA	O2D-CGD-CBD	4.28	118.87	111.27
38	9	312	KC1	C2A-C1A-NA	4.28	116.26	109.40
38	16	311	KC1	CBA-CAA-C2A	-4.28	108.97	125.27
30	4	301	CLA	C3C-C4C-NC	4.27	115.36	110.57
37	14	314	A86	C4-C3-C2	-4.27	114.72	123.47
30	A	842	CLA	C3C-C4C-NC	4.27	115.36	110.57
30	7	303	CLA	C3C-C4C-NC	4.27	115.36	110.57
30	B	831	CLA	C3D-C4D-ND	4.27	117.14	110.24
30	15	304	CLA	C3C-C4C-NC	4.27	115.36	110.57
30	10	303	CLA	C4A-NA-C1A	-4.27	104.79	106.71
39	5	313	DD6	O1-C20-C21	-4.27	109.94	115.06
30	A	838	CLA	C1D-CHD-C4C	-4.27	116.85	126.06
38	1	308	KC1	CHC-C1C-C2C	-4.27	118.31	124.98
30	10	305	CLA	C4A-NA-C1A	-4.27	104.79	106.71
38	11	312	KC1	CMA-C3A-C2A	-4.27	117.86	128.30
30	7	303	CLA	C3D-C4D-ND	4.27	117.14	110.24
30	B	851	CLA	C3D-C4D-ND	4.26	117.14	110.24
30	A	844	CLA	O2D-CGD-CBD	4.26	118.84	111.27
30	10	307	CLA	O2D-CGD-CBD	4.26	118.84	111.27
30	10	309	CLA	C4A-NA-C1A	-4.26	104.79	106.71
30	10	311	CLA	C4A-NA-C1A	-4.26	104.79	106.71
30	A	824	CLA	C3D-C4D-ND	4.26	117.13	110.24
30	A	833	CLA	O2D-CGD-CBD	4.26	118.84	111.27
30	15	304	CLA	C3D-C4D-ND	4.26	117.13	110.24
30	A	812	CLA	C3C-C4C-NC	4.26	115.35	110.57
39	8	316	DD6	C23-C16-C17	-4.26	101.59	108.98
30	15	309	CLA	C3D-C4D-ND	4.26	117.12	110.24
38	2	314	KC1	C2C-C1C-NC	4.26	115.22	110.57
30	11	308	CLA	C3D-C4D-ND	4.26	117.12	110.24
38	2	306	KC1	CHC-C1C-C2C	-4.26	118.33	124.98
37	14	319	A86	C36-C31-C32	-4.25	115.47	119.70
38	7	313	KC1	C1A-NA-C4A	-4.25	104.79	106.71
37	14	320	A86	C25-C24-C1	-4.25	114.47	126.42
30	2	307	CLA	C3D-C2D-C1D	-4.25	100.03	105.83
38	16	304	KC1	CHD-C4C-C3C	-4.25	117.35	125.33
30	3	303	CLA	C3D-C4D-ND	4.25	117.11	110.24
30	3	307	CLA	C3D-C4D-ND	4.25	117.11	110.24
38	13	308	KC1	C2C-C1C-NC	4.25	115.21	110.57
38	3	311	KC1	C2A-C1A-NA	4.25	116.21	109.40
39	7	318	DD6	C15-C14-C13	4.25	134.97	125.99
30	A	827	CLA	C3C-C4C-NC	4.25	115.33	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	836	CLA	C3C-C4C-NC	4.25	115.33	110.57
30	15	314	CLA	C4A-NA-C1A	-4.24	104.80	106.71
30	6	305	CLA	O2D-CGD-CBD	4.24	118.81	111.27
39	11	313	DD6	C13-C11-C10	-4.24	112.43	118.94
30	A	836	CLA	C3D-C2D-C1D	-4.24	100.04	105.83
30	B	810	CLA	C3C-C4C-NC	4.24	115.33	110.57
38	4	308	KC1	CBA-CAA-C2A	-4.24	109.10	125.27
37	11	301	A86	C36-C31-C32	-4.24	115.49	119.70
30	A	834	CLA	O2D-CGD-CBD	4.24	118.81	111.27
30	14	310	CLA	C3D-C4D-ND	4.24	117.10	110.24
29	A	801	CL0	C3D-C2D-C1D	-4.24	100.04	105.83
30	6	314	CLA	C3D-C2D-C1D	-4.24	100.05	105.83
30	10	303	CLA	O2D-CGD-CBD	4.24	118.80	111.27
37	10	317	A86	C25-C26-C27	-4.24	121.26	127.31
38	6	313	KC1	C2C-C1C-NC	4.24	115.20	110.57
30	A	843	CLA	C3D-C2D-C1D	-4.24	100.05	105.83
30	B	807	CLA	C4A-NA-C1A	-4.24	104.80	106.71
38	5	310	KC1	C2C-C1C-NC	4.24	115.20	110.57
39	6	318	DD6	C15-C14-C13	-4.24	117.04	125.99
38	5	305	KC1	C2A-C1A-NA	4.24	116.19	109.40
39	2	315	DD6	C25-C24-C1	-4.24	114.52	126.42
30	15	309	CLA	C4A-NA-C1A	-4.24	104.80	106.71
38	6	313	KC1	CHC-C1C-C2C	-4.23	118.36	124.98
39	4	313	DD6	C7-C6-C8	-4.23	111.41	118.08
30	B	814	CLA	C3D-C4D-ND	4.23	117.09	110.24
34	6	322	LHG	O4-P-O5	4.23	133.17	112.24
39	2	317	DD6	C15-C14-C13	4.23	134.94	125.99
30	16	301	CLA	O2D-CGD-CBD	4.23	118.79	111.27
30	B	814	CLA	C3C-C4C-NC	4.23	115.32	110.57
30	9	302	CLA	C3D-C4D-ND	4.23	117.08	110.24
30	B	827	CLA	O2D-CGD-CBD	4.23	118.78	111.27
30	8	302	CLA	O2D-CGD-CBD	4.23	118.78	111.27
38	5	312	KC1	C2C-C1C-NC	4.23	115.19	110.57
30	15	313	CLA	C3D-C4D-ND	4.23	117.08	110.24
34	9	318	LHG	O4-P-O5	4.23	133.15	112.24
30	A	844	CLA	C3D-C4D-ND	4.23	117.08	110.24
30	2u	202	CLA	C3D-C4D-ND	4.23	117.08	110.24
30	B	814	CLA	C1D-CHD-C4C	-4.23	116.94	126.06
30	9	306	CLA	C3C-C4C-NC	4.23	115.31	110.57
30	B	827	CLA	C3D-C2D-C1D	-4.23	100.06	105.83
37	4	314	A86	C25-C26-C27	-4.23	121.28	127.31
30	2	309	CLA	C3D-C4D-ND	4.23	117.08	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	13	312	KC1	C2A-C1A-NA	4.23	116.18	109.40
30	7	309	CLA	C1D-CHD-C4C	-4.23	116.94	126.06
30	7	310	CLA	O2D-CGD-CBD	4.22	118.78	111.27
38	16	311	KC1	C2C-C1C-NC	4.22	115.18	110.57
38	14	308	KC1	CBA-CAA-C2A	-4.22	109.17	125.27
30	A	802	CLA	C3C-C4C-NC	4.22	115.31	110.57
30	B	809	CLA	C1C-C2C-C3C	-4.22	102.52	106.96
30	A	821	CLA	C1C-C2C-C3C	-4.22	102.52	106.96
37	8	318	A86	C33-C32-C31	4.22	113.31	109.21
39	15	318	DD6	C23-C16-C15	4.22	121.44	110.05
38	5	305	KC1	C2C-C1C-NC	4.22	115.18	110.57
38	9	311	KC1	CHC-C1C-C2C	-4.22	118.39	124.98
30	14	304	CLA	C3D-C4D-ND	4.22	117.06	110.24
30	B	825	CLA	C4A-NA-C1A	-4.22	104.81	106.71
30	A	819	CLA	O2D-CGD-CBD	4.22	118.76	111.27
38	4	307	KC1	CHD-C4C-C3C	-4.22	117.41	125.33
37	14	319	A86	C41-C32-C31	-4.22	106.70	110.47
30	A	812	CLA	C3D-C4D-ND	4.22	117.06	110.24
37	12	314	A86	C4-C3-C2	-4.22	114.84	123.47
30	15	307	CLA	C1C-C2C-C3C	-4.22	102.53	106.96
37	10	301	A86	C24-C1-C2	-4.22	112.47	118.94
30	B	810	CLA	C1D-CHD-C4C	-4.21	116.97	126.06
37	1	309	A86	C25-C26-C27	-4.21	121.30	127.31
37	9	313	A86	C25-C24-C1	-4.21	114.58	126.42
30	A	844	CLA	C4A-NA-C1A	-4.21	104.81	106.71
30	B	824	CLA	C3D-C2D-C1D	-4.21	100.08	105.83
30	11	310	CLA	C3D-C2D-C1D	-4.21	100.08	105.83
38	13	308	KC1	C2A-C1A-NA	4.21	116.16	109.40
30	15	307	CLA	C4A-NA-C1A	-4.21	104.81	106.71
38	6	311	KC1	C1C-C2C-C3C	-4.21	102.53	106.96
37	10	301	A86	C36-C31-C32	-4.21	115.52	119.70
30	13	301	CLA	C3D-C4D-ND	4.21	117.05	110.24
30	B	811	CLA	C3C-C4C-NC	4.21	115.29	110.57
38	13	305	KC1	C4B-C3B-C2B	-4.21	103.30	106.75
30	11	310	CLA	C3D-C4D-ND	4.21	117.05	110.24
30	6	317	CLA	C3D-C4D-ND	4.21	117.04	110.24
30	8	301	CLA	C3D-C4D-ND	4.21	117.04	110.24
30	A	838	CLA	C3C-C4C-NC	4.21	115.29	110.57
34	5	317	LHG	O4-P-O5	4.21	133.03	112.24
30	12	303	CLA	C3C-C4C-NC	4.21	115.29	110.57
30	13	309	CLA	C3C-C4C-NC	4.21	115.29	110.57
30	A	812	CLA	O2D-CGD-CBD	4.20	118.74	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	14	317	A86	C12-C11-C13	4.20	123.08	116.02
38	9	312	KC1	O2D-CGD-CBD	4.20	118.74	111.27
30	12	308	CLA	C3D-C4D-ND	4.20	117.04	110.24
39	4	313	DD6	C15-C14-C13	4.20	134.88	125.99
38	13	311	KC1	C2C-C1C-NC	4.20	115.16	110.57
30	10	311	CLA	C3D-C4D-ND	4.20	117.03	110.24
38	5	312	KC1	O2D-CGD-CBD	4.20	118.73	111.27
30	15	306	CLA	C3C-C4C-NC	4.20	115.28	110.57
30	13	301	CLA	C4A-NA-C1A	-4.20	104.82	106.71
30	B	815	CLA	C1D-CHD-C4C	-4.20	117.00	126.06
30	12	302	CLA	C4A-NA-C1A	-4.20	104.82	106.71
38	7	313	KC1	C2A-C1A-NA	4.20	116.13	109.40
30	13	309	CLA	O2D-CGD-CBD	4.20	118.73	111.27
30	B	822	CLA	CAA-CBA-CGA	-4.20	100.99	113.25
37	15	315	A86	C41-C32-C31	-4.20	106.72	110.47
37	15	316	A86	C9-C8-C6	-4.20	114.63	126.42
30	8	302	CLA	CMB-C2B-C3B	4.20	132.53	124.68
30	2	313	CLA	C3D-C4D-ND	4.19	117.02	110.24
30	14	312	CLA	C3D-C4D-ND	4.19	117.02	110.24
30	A	839	CLA	O2D-CGD-O1D	-4.19	115.64	123.84
38	2	312	KC1	O2D-CGD-CBD	4.19	118.72	111.27
38	7	308	KC1	O2D-CGD-CBD	4.19	118.72	111.27
34	A	852	LHG	O4-P-O5	4.19	132.96	112.24
30	1	303	CLA	C3D-C4D-ND	4.19	117.02	110.24
30	A	823	CLA	C3D-C4D-ND	4.19	117.02	110.24
30	B	828	CLA	C3D-C4D-ND	4.19	117.02	110.24
30	13	309	CLA	C4A-NA-C1A	-4.19	104.82	106.71
30	A	832	CLA	C3C-C4C-NC	4.19	115.27	110.57
38	13	310	KC1	C2A-C1A-NA	4.19	116.12	109.40
38	12	311	KC1	C2A-C1A-NA	4.19	116.12	109.40
30	L	203	CLA	C4A-NA-C1A	-4.19	104.82	106.71
30	15	304	CLA	C1D-CHD-C4C	-4.19	117.03	126.06
30	J	101	CLA	C3D-C2D-C1D	-4.19	100.12	105.83
39	7	318	DD6	C35-C36-C31	-4.19	111.07	120.57
30	9	303	CLA	C3D-C4D-ND	4.18	117.01	110.24
30	B	835	CLA	C3D-C4D-ND	4.18	117.00	110.24
30	4	305	CLA	C3D-C4D-ND	4.18	117.00	110.24
30	A	818	CLA	C3C-C4C-NC	4.18	115.26	110.57
30	16	307	CLA	C3D-C4D-ND	4.18	117.00	110.24
37	3	315	A86	C4-C3-C2	-4.18	114.91	123.47
37	7	316	A86	C41-C32-C31	-4.18	106.73	110.47
30	5	304	CLA	C3D-C4D-ND	4.18	117.00	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	10	309	CLA	C3D-C4D-ND	4.18	117.00	110.24
30	9	303	CLA	C4A-NA-C1A	-4.18	104.83	106.71
30	B	820	CLA	CBC-CAC-C3C	-4.18	100.91	112.43
30	7	307	CLA	O2D-CGD-CBD	4.18	118.69	111.27
38	9	304	KC1	O2D-CGD-CBD	4.18	118.69	111.27
30	10	308	CLA	O2D-CGD-CBD	4.18	118.69	111.27
38	11	307	KC1	CHD-C4C-C3C	-4.18	117.49	125.33
38	12	311	KC1	C2C-C1C-NC	4.18	115.13	110.57
30	11	306	CLA	C3D-C4D-ND	4.18	117.00	110.24
30	13	301	CLA	C3C-C4C-NC	4.18	115.26	110.57
37	14	315	A86	C36-C31-C32	-4.18	115.55	119.70
30	A	806	CLA	C2C-C1C-NC	4.18	113.89	109.97
30	A	818	CLA	C3D-C4D-ND	4.18	116.99	110.24
30	14	310	CLA	C1D-CHD-C4C	-4.18	117.05	126.06
30	1	305	CLA	O2D-CGD-CBD	4.18	118.69	111.27
30	9	309	CLA	C4A-NA-C1A	-4.18	104.83	106.71
38	8	313	KC1	C2A-C1A-NA	4.17	116.10	109.40
30	8	309	CLA	C3D-C4D-ND	4.17	116.99	110.24
38	9	312	KC1	C1A-NA-C4A	-4.17	104.83	106.71
38	10	306	KC1	C2A-C1A-NA	4.17	116.09	109.40
30	14	307	CLA	C3C-C4C-NC	4.17	115.25	110.57
30	L	203	CLA	C3D-C4D-ND	4.17	116.98	110.24
39	6	303	DD6	C21-C20-C15	-4.17	115.28	122.26
30	15	314	CLA	C3C-C4C-NC	4.17	115.25	110.57
37	15	322	A86	C9-C8-C6	-4.17	114.71	126.42
30	A	816	CLA	C3D-C4D-ND	4.17	116.98	110.24
30	B	851	CLA	C3D-C2D-C1D	-4.17	100.14	105.83
38	4	310	KC1	C2A-C1A-NA	4.17	116.08	109.40
30	6	310	CLA	C1C-C2C-C3C	-4.17	102.58	106.96
30	12	306	CLA	C3D-C2D-C1D	-4.17	100.15	105.83
30	4	311	CLA	C1C-C2C-C3C	-4.16	102.58	106.96
30	B	834	CLA	C1D-CHD-C4C	-4.16	117.08	126.06
37	4	315	A86	C36-C31-C32	-4.16	115.57	119.70
30	B	824	CLA	C3D-C4D-ND	4.16	116.97	110.24
30	15	306	CLA	C1D-CHD-C4C	-4.16	117.08	126.06
30	3	310	CLA	C3D-C4D-ND	4.16	116.97	110.24
30	A	808	CLA	C3C-C4C-NC	4.16	115.23	110.57
30	B	829	CLA	C3D-C4D-ND	4.16	116.96	110.24
37	14	318	A86	C3-C2-C1	-4.16	121.38	127.31
30	A	843	CLA	C3D-C4D-ND	4.16	116.96	110.24
30	2u	202	CLA	C4A-NA-C1A	-4.16	104.84	106.71
30	2	307	CLA	C4A-NA-C1A	-4.16	104.84	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	9	311	KC1	C2A-C1A-NA	4.16	116.07	109.40
37	7	315	A86	C25-C26-C27	-4.16	121.38	127.31
30	16	309	CLA	C3D-C4D-ND	4.15	116.96	110.24
38	8	306	KC1	C2A-C1A-NA	4.15	116.06	109.40
39	7	302	DD6	C-C1-C24	-4.15	111.53	118.08
30	14	303	CLA	C3D-C4D-ND	4.15	116.96	110.24
30	B	819	CLA	C3C-C4C-NC	4.15	115.23	110.57
39	7	302	DD6	C7-C6-C8	-4.15	111.53	118.08
30	6	306	CLA	C3D-C4D-ND	4.15	116.95	110.24
30	2	305	CLA	C3D-C4D-ND	4.15	116.95	110.24
30	4	304	CLA	C3D-C4D-ND	4.15	116.95	110.24
38	12	309	KC1	C2C-C1C-NC	4.15	115.10	110.57
30	F	201	CLA	C3D-C4D-ND	4.15	116.95	110.24
39	13	314	DD6	C8-C6-C5	-4.15	112.58	118.94
30	B	817	CLA	C3C-C4C-NC	4.15	115.22	110.57
30	B	808	CLA	C3D-C2D-C1D	-4.15	100.17	105.83
38	1	308	KC1	C2C-C1C-NC	4.15	115.10	110.57
30	4	309	CLA	C4A-NA-C1A	-4.15	104.84	106.71
30	15	303	CLA	C1D-CHD-C4C	-4.15	117.11	126.06
30	A	824	CLA	C3C-C4C-NC	4.15	115.22	110.57
38	12	313	KC1	C1C-C2C-C3C	-4.14	102.60	106.96
38	6	308	KC1	CMD-C2D-C1D	4.14	134.83	128.46
38	13	308	KC1	C4B-C3B-C2B	-4.14	103.35	106.75
30	12	312	CLA	C3D-C4D-ND	4.14	116.94	110.24
38	11	312	KC1	C1C-C2C-C3C	-4.14	102.60	106.96
38	2	306	KC1	C2A-C1A-NA	4.14	116.04	109.40
30	5	307	CLA	C1D-CHD-C4C	-4.14	117.13	126.06
30	10	304	CLA	O2D-CGD-CBD	4.14	118.62	111.27
30	2u	202	CLA	C3C-C4C-NC	4.14	115.21	110.57
30	5	308	CLA	C3D-C4D-ND	4.14	116.93	110.24
30	16	301	CLA	C3D-C4D-ND	4.14	116.93	110.24
38	6	313	KC1	C2A-C1A-NA	4.14	116.04	109.40
37	2	318	A86	C25-C24-C1	-4.14	114.79	126.42
30	2	310	CLA	C3D-C4D-ND	4.14	116.93	110.24
39	1	310	DD6	C21-C20-C19	-4.14	109.63	114.28
38	13	311	KC1	CBA-CAA-C2A	-4.13	109.51	125.27
30	B	839	CLA	C3D-C4D-ND	4.13	116.93	110.24
30	A	830	CLA	C3D-C4D-ND	4.13	116.92	110.24
37	15	317	A86	C33-C32-C31	4.13	113.23	109.21
37	15	320	A86	C9-C10-C11	-4.13	114.46	126.61
30	A	844	CLA	C3D-C2D-C1D	-4.13	100.19	105.83
30	B	805	CLA	C4A-NA-C1A	-4.13	104.85	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	13	303	CLA	C4A-NA-C1A	-4.13	104.85	106.71
30	B	819	CLA	O2D-CGD-CBD	4.13	118.61	111.27
38	8	306	KC1	C1C-C2C-C3C	-4.13	102.62	106.96
30	12	307	CLA	C3C-C4C-NC	4.13	115.20	110.57
30	15	307	CLA	CAA-C2A-C3A	-4.13	101.48	112.78
38	13	306	KC1	CHC-C1C-C2C	-4.13	118.53	124.98
30	A	813	CLA	C3C-C4C-NC	4.13	115.20	110.57
30	10	304	CLA	C3C-C4C-NC	4.13	115.20	110.57
38	11	311	KC1	C2C-C1C-NC	4.13	115.08	110.57
37	16	314	A86	C40-C32-C31	-4.13	106.78	110.47
37	15	321	A86	C4-C5-C6	-4.12	121.42	127.31
30	15	310	CLA	C3D-C4D-ND	4.12	116.91	110.24
30	15	311	CLA	C3D-C4D-ND	4.12	116.91	110.24
30	8	301	CLA	C4A-NA-C1A	-4.12	104.85	106.71
30	A	828	CLA	C2C-C1C-NC	4.12	113.83	109.97
39	5	314	DD6	C35-C36-C31	-4.12	111.21	120.57
30	B	837	CLA	C4A-NA-C1A	-4.12	104.85	106.71
34	A	853	LHG	O4-P-O5	4.12	132.61	112.24
38	2	312	KC1	C2A-C1A-NA	4.12	116.01	109.40
38	9	310	KC1	CBA-CAA-C2A	-4.12	109.56	125.27
30	3	307	CLA	C3C-C4C-NC	4.12	115.19	110.57
38	10	306	KC1	C4B-C3B-C2B	-4.12	103.37	106.75
39	15	319	DD6	C15-C14-C13	4.12	134.70	125.99
30	A	808	CLA	C3D-C4D-ND	4.12	116.90	110.24
30	A	811	CLA	C3D-C4D-ND	4.12	116.90	110.24
30	A	833	CLA	C3D-C4D-ND	4.12	116.90	110.24
30	3	301	CLA	C3D-C4D-ND	4.12	116.90	110.24
30	7	312	CLA	C4A-NA-C1A	-4.12	104.85	106.71
30	9	306	CLA	C1C-C2C-C3C	-4.12	102.63	106.96
39	9	314	DD6	C37-C36-C35	-4.12	106.72	114.36
30	B	831	CLA	C1D-CHD-C4C	-4.12	117.17	126.06
30	B	820	CLA	C3D-C4D-ND	4.12	116.90	110.24
30	12	307	CLA	C1D-CHD-C4C	-4.12	117.17	126.06
38	6	312	KC1	O2D-CGD-CBD	4.12	118.58	111.27
37	15	323	A86	C41-C32-C31	-4.12	106.79	110.47
30	4	311	CLA	C3D-C4D-ND	4.12	116.90	110.24
30	A	840	CLA	C1C-C2C-C3C	-4.12	102.63	106.96
30	9	301	CLA	C3B-C4B-NB	4.12	114.53	109.21
38	3	308	KC1	C1A-NA-C4A	-4.11	104.86	106.71
38	8	307	KC1	CHC-C1C-C2C	-4.11	118.55	124.98
38	8	314	KC1	C2C-C1C-NC	4.11	115.06	110.57
37	11	314	A86	C36-C31-C32	-4.11	115.62	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	15	322	A86	C25-C24-C1	-4.11	114.87	126.42
38	7	313	KC1	CHC-C1C-C2C	-4.11	118.56	124.98
30	11	309	CLA	C3D-C2D-C1D	-4.11	100.23	105.83
38	13	312	KC1	C2C-C1C-NC	4.11	115.06	110.57
30	4	306	CLA	C3D-C4D-ND	4.11	116.88	110.24
30	10	303	CLA	C3D-C4D-ND	4.11	116.88	110.24
30	8	303	CLA	C3D-C2D-C1D	-4.11	100.23	105.83
30	B	803	CLA	C3C-C4C-NC	4.11	115.18	110.57
30	5	308	CLA	C4A-NA-C1A	-4.11	104.86	106.71
37	13	313	A86	C9-C10-C11	-4.11	114.54	126.61
30	A	812	CLA	CAA-C2A-C3A	-4.11	101.54	112.78
30	A	836	CLA	C1C-C2C-C3C	-4.10	102.64	106.96
38	12	311	KC1	C4B-C3B-C2B	-4.10	103.38	106.75
30	6	304	CLA	C3D-C4D-ND	4.10	116.88	110.24
39	7	314	DD6	C37-C36-C35	-4.10	106.75	114.36
38	8	306	KC1	O2D-CGD-CBD	4.10	118.56	111.27
38	11	311	KC1	C2A-C1A-NA	4.10	115.98	109.40
38	3	304	KC1	C2A-C1A-NA	4.10	115.98	109.40
30	B	808	CLA	C1D-CHD-C4C	-4.10	117.21	126.06
30	16	308	CLA	C3D-C4D-ND	4.10	116.87	110.24
38	8	306	KC1	CBA-CAA-C2A	-4.10	109.64	125.27
30	F	201	CLA	C1D-CHD-C4C	-4.10	117.22	126.06
38	8	311	KC1	C2C-C1C-NC	4.10	115.05	110.57
30	B	818	CLA	CBA-CAA-C2A	4.10	125.96	113.86
30	A	812	CLA	C4A-NA-C1A	-4.10	104.86	106.71
30	1	305	CLA	C3D-C4D-ND	4.10	116.86	110.24
39	3	316	DD6	C21-C20-C15	-4.10	115.40	122.26
30	A	827	CLA	C1C-C2C-C3C	-4.10	102.65	106.96
30	16	303	CLA	CAA-C2A-C3A	-4.09	101.57	112.78
30	A	824	CLA	C3D-C2D-C1D	-4.09	100.25	105.83
30	2	308	CLA	C3D-C4D-ND	4.09	116.86	110.24
30	A	826	CLA	C3B-C4B-NB	4.09	114.50	109.21
30	4	305	CLA	C4A-NA-C1A	-4.09	104.87	106.71
30	12	302	CLA	C3C-C4C-NC	4.09	115.16	110.57
39	2	316	DD6	C21-C20-C19	-4.09	109.68	114.28
30	1	301	CLA	C3D-C4D-ND	4.09	116.85	110.24
38	10	312	KC1	CHC-C1C-C2C	-4.09	118.59	124.98
30	5	302	CLA	C3D-C4D-ND	4.09	116.85	110.24
30	6	314	CLA	CBC-CAC-C3C	-4.09	101.17	112.43
30	A	803	CLA	O2D-CGD-CBD	4.09	118.53	111.27
38	6	313	KC1	CAA-CBA-CGA	-4.09	106.26	127.26
30	9	309	CLA	C3D-C4D-ND	4.09	116.85	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	5	316	A86	C36-C31-C32	-4.09	115.64	119.70
38	9	304	KC1	C2C-C1C-NC	4.09	115.03	110.57
30	B	830	CLA	C3D-C4D-ND	4.08	116.85	110.24
38	7	308	KC1	C2A-C1A-NA	4.08	115.95	109.40
30	8	301	CLA	C1D-CHD-C4C	-4.08	117.25	126.06
30	A	842	CLA	C3D-C4D-ND	4.08	116.84	110.24
30	5	307	CLA	C1C-C2C-C3C	-4.08	102.66	106.96
30	A	829	CLA	C1D-CHD-C4C	-4.08	117.25	126.06
38	14	311	KC1	C1A-NA-C4A	-4.08	104.87	106.71
30	12	306	CLA	C1D-CHD-C4C	-4.08	117.25	126.06
30	B	837	CLA	C3D-C4D-ND	4.08	116.84	110.24
38	13	311	KC1	CHC-C1C-C2C	-4.08	118.61	124.98
30	B	819	CLA	C1D-CHD-C4C	-4.08	117.26	126.06
30	4	309	CLA	C1D-CHD-C4C	-4.08	117.26	126.06
30	F	203	CLA	C3D-C4D-ND	4.08	116.84	110.24
38	14	311	KC1	CBA-CAA-C2A	-4.08	109.72	125.27
30	A	807	CLA	C1D-CHD-C4C	-4.08	117.26	126.06
39	5	313	DD6	C37-C36-C35	-4.08	106.80	114.36
38	14	311	KC1	C2C-C1C-NC	4.08	115.02	110.57
30	A	804	CLA	C3D-C4D-ND	4.08	116.83	110.24
30	A	839	CLA	C3D-C4D-ND	4.07	116.83	110.24
30	8	305	CLA	C1D-CHD-C4C	-4.07	117.27	126.06
30	12	310	CLA	C3C-C4C-NC	4.07	115.14	110.57
30	13	302	CLA	C3C-C4C-NC	4.07	115.14	110.57
37	14	317	A86	C36-C31-C32	-4.07	115.66	119.70
30	A	827	CLA	C3D-C4D-ND	4.07	116.83	110.24
37	14	315	A86	C10-C9-C8	-4.07	110.51	123.22
37	15	323	A86	C25-C24-C1	-4.07	114.98	126.42
39	6	321	DD6	C21-C20-C15	-4.07	115.44	122.26
30	7	309	CLA	C1C-C2C-C3C	-4.07	102.68	106.96
30	A	822	CLA	C3D-C4D-ND	4.07	116.82	110.24
30	15	312	CLA	C3D-C4D-ND	4.07	116.82	110.24
30	A	802	CLA	CMB-C2B-C3B	4.07	132.29	124.68
30	16	305	CLA	C1D-CHD-C4C	-4.07	117.28	126.06
30	B	823	CLA	C3C-C4C-NC	4.07	115.14	110.57
30	1	304	CLA	C1D-CHD-C4C	-4.07	117.28	126.06
30	B	805	CLA	C3D-C4D-ND	4.07	116.82	110.24
30	F	203	CLA	C1D-CHD-C4C	-4.07	117.28	126.06
37	13	313	A86	C36-C35-C34	4.07	116.56	111.75
38	14	306	KC1	CHD-C4C-C3C	-4.07	117.69	125.33
38	8	314	KC1	C2A-C1A-NA	4.07	115.93	109.40
30	16	306	CLA	C3C-C4C-NC	4.07	115.13	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	6	307	CLA	O2D-CGD-CBD	4.07	118.50	111.27
30	6	315	CLA	C3D-C4D-ND	4.07	116.82	110.24
30	12	302	CLA	C3D-C4D-ND	4.07	116.82	110.24
30	15	307	CLA	C3C-C4C-NC	4.07	115.13	110.57
39	7	318	DD6	C21-C20-C15	-4.07	115.44	122.26
30	14	305	CLA	C3D-C4D-ND	4.07	116.82	110.24
38	2	306	KC1	C2C-C1C-NC	4.07	115.01	110.57
30	10	311	CLA	C1D-CHD-C4C	-4.07	117.29	126.06
30	A	823	CLA	C1C-C2C-C3C	-4.07	102.68	106.96
30	3	301	CLA	C1C-C2C-C3C	-4.07	102.68	106.96
30	F	201	CLA	CMD-C2D-C1D	4.06	131.88	124.71
37	2	318	A86	C36-C31-C32	-4.06	115.66	119.70
30	3	310	CLA	CBC-CAC-C3C	-4.06	101.23	112.43
38	3	308	KC1	C1C-C2C-C3C	-4.06	102.68	106.96
30	10	307	CLA	C4A-NA-C1A	-4.06	104.88	106.71
30	14	303	CLA	C4A-NA-C1A	-4.06	104.88	106.71
30	B	810	CLA	C3D-C4D-ND	4.06	116.81	110.24
30	15	307	CLA	C3D-C4D-ND	4.06	116.81	110.24
30	13	301	CLA	C1D-CHD-C4C	-4.06	117.29	126.06
30	16	301	CLA	C1D-CHD-C4C	-4.06	117.30	126.06
30	12	308	CLA	C3C-C4C-NC	4.06	115.13	110.57
30	15	303	CLA	C3D-C4D-ND	4.06	116.81	110.24
30	9	308	CLA	C3D-C4D-ND	4.06	116.81	110.24
30	4	304	CLA	C3D-C2D-C1D	-4.06	100.29	105.83
30	1	301	CLA	C4A-NA-C1A	-4.06	104.88	106.71
30	1	303	CLA	C3C-C4C-NC	4.06	115.12	110.57
38	8	312	KC1	C2C-C1C-NC	4.06	115.00	110.57
30	B	808	CLA	C3D-C4D-ND	4.06	116.80	110.24
30	12	302	CLA	C1D-CHD-C4C	-4.06	117.31	126.06
30	13	304	CLA	C1C-C2C-C3C	-4.06	102.69	106.96
30	4	304	CLA	C4A-NA-C1A	-4.05	104.88	106.71
30	8	304	CLA	C3C-C4C-NC	4.05	115.12	110.57
30	2	305	CLA	CBA-CAA-C2A	4.05	125.83	113.86
30	5	311	CLA	C3D-C4D-ND	4.05	116.80	110.24
30	B	836	CLA	C1C-C2C-C3C	-4.05	102.69	106.96
38	3	304	KC1	C4B-C3B-C2B	-4.05	103.42	106.75
39	3	313	DD6	C21-C20-C19	-4.05	109.72	114.28
30	8	302	CLA	C3D-C4D-ND	4.05	116.79	110.24
38	11	307	KC1	C1C-C2C-C3C	-4.05	102.70	106.96
30	B	807	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
30	3	305	CLA	C4A-NA-C1A	-4.05	104.89	106.71
37	4	317	A86	C3-C4-C5	-4.05	115.18	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	7	306	CLA	C1D-CHD-C4C	-4.05	117.32	126.06
30	A	830	CLA	CMD-C2D-C1D	4.05	131.85	124.71
30	12	310	CLA	C1D-CHD-C4C	-4.05	117.33	126.06
37	16	314	A86	C36-C31-C32	-4.05	115.68	119.70
30	B	818	CLA	C3D-C4D-ND	4.05	116.79	110.24
37	2	319	A86	C26-C25-C24	-4.05	110.58	123.22
30	6	305	CLA	C3D-C4D-ND	4.05	116.78	110.24
39	15	318	DD6	C15-C14-C13	4.05	134.55	125.99
30	16	310	CLA	C3D-C4D-ND	4.05	116.78	110.24
37	13	315	A86	C36-C31-C32	-4.05	115.68	119.70
30	11	308	CLA	C1D-CHD-C4C	-4.04	117.33	126.06
38	16	311	KC1	CHC-C1C-C2C	-4.04	118.66	124.98
30	7	304	CLA	O2D-CGD-CBD	4.04	118.45	111.27
30	4	303	CLA	C3D-C4D-ND	4.04	116.78	110.24
30	10	305	CLA	CBA-CAA-C2A	4.04	125.79	113.86
30	7	311	CLA	C3D-C4D-ND	4.04	116.78	110.24
39	15	318	DD6	C21-C20-C19	-4.04	109.73	114.28
30	12	306	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
38	5	305	KC1	C1A-NA-C4A	-4.04	104.89	106.71
30	6	307	CLA	C3D-C4D-ND	4.04	116.77	110.24
38	6	312	KC1	CHC-C1C-C2C	-4.04	118.67	124.98
38	12	313	KC1	CHB-C4A-C3A	-4.04	118.67	124.98
39	12	317	DD6	O1-C20-C21	-4.04	110.22	115.06
30	B	802	CLA	C3D-C4D-ND	4.04	116.77	110.24
30	5	309	CLA	C3D-C4D-ND	4.04	116.77	110.24
30	13	307	CLA	C3D-C4D-ND	4.03	116.77	110.24
30	8	305	CLA	CMB-C2B-C3B	4.03	132.22	124.68
30	15	305	CLA	C3D-C4D-ND	4.03	116.76	110.24
30	7	304	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
30	1	302	CLA	C4A-NA-C1A	-4.03	104.89	106.71
30	11	304	CLA	C4A-NA-C1A	-4.03	104.89	106.71
30	6	314	CLA	C1D-CHD-C4C	-4.03	117.36	126.06
37	15	322	A86	C-C1-C2	-4.03	117.28	122.92
30	B	818	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
30	A	836	CLA	C4A-NA-C1A	-4.03	104.89	106.71
30	B	819	CLA	C3D-C4D-ND	4.03	116.76	110.24
38	6	313	KC1	C1A-NA-C4A	-4.03	104.89	106.71
30	2	307	CLA	CAA-C2A-C3A	-4.03	101.75	112.78
30	13	309	CLA	C3D-C4D-ND	4.03	116.75	110.24
30	B	832	CLA	C4A-NA-C1A	-4.03	104.90	106.71
38	8	313	KC1	CMD-C2D-C1D	4.03	134.65	128.46
30	6	309	CLA	C3D-C4D-ND	4.02	116.75	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	806	CLA	CAA-C2A-C3A	-4.02	101.76	112.78
30	A	834	CLA	C3C-C4C-NC	4.02	115.08	110.57
30	6	314	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
30	16	305	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
39	15	318	DD6	O1-C20-C21	-4.02	110.24	115.06
37	7	319	A86	C36-C31-C32	-4.02	115.71	119.70
30	16	302	CLA	O2D-CGD-CBD	4.02	118.41	111.27
30	J	101	CLA	C1D-CHD-C4C	-4.02	117.39	126.06
30	15	306	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
30	B	822	CLA	C3D-C2D-C1D	-4.02	100.35	105.83
30	3	310	CLA	C4A-NA-C1A	-4.02	104.90	106.71
30	8	303	CLA	C4A-NA-C1A	-4.02	104.90	106.71
30	12	307	CLA	C3D-C4D-ND	4.02	116.73	110.24
34	B	848	LHG	O4-P-O5	4.02	132.09	112.24
30	9	307	CLA	C1D-CHD-C4C	-4.02	117.39	126.06
39	7	317	DD6	C22-C16-C15	4.02	120.89	110.05
38	6	312	KC1	C2C-C1C-NC	4.01	114.95	110.57
37	15	317	A86	C3-C2-C1	-4.01	121.58	127.31
30	A	811	CLA	C1D-CHD-C4C	-4.01	117.40	126.06
30	9	306	CLA	C3D-C4D-ND	4.01	116.73	110.24
30	A	804	CLA	C1D-CHD-C4C	-4.01	117.40	126.06
30	B	837	CLA	C3C-C4C-NC	4.01	115.07	110.57
38	11	307	KC1	C2A-C1A-NA	4.01	115.83	109.40
30	B	801	CLA	C3D-C4D-ND	4.01	116.73	110.24
38	8	311	KC1	C2A-C1A-NA	4.01	115.83	109.40
30	16	310	CLA	C3C-C4C-NC	4.01	115.07	110.57
30	A	838	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
38	11	305	KC1	C4B-C3B-C2B	-4.01	103.46	106.75
30	8	302	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
30	B	832	CLA	O2D-CGD-CBD	4.01	118.39	111.27
38	14	308	KC1	C4B-C3B-C2B	-4.01	103.46	106.75
30	12	321	CLA	C3D-C4D-ND	4.01	116.72	110.24
30	7	304	CLA	C3D-C4D-ND	4.01	116.72	110.24
30	B	803	CLA	C2C-C1C-NC	4.01	113.72	109.97
30	5	307	CLA	O2D-CGD-CBD	4.00	118.38	111.27
30	7	312	CLA	C3D-C4D-ND	4.00	116.71	110.24
30	A	836	CLA	C3D-C4D-ND	4.00	116.71	110.24
38	8	310	KC1	C2A-C1A-NA	4.00	115.82	109.40
30	A	807	CLA	C3C-C4C-NC	4.00	115.06	110.57
38	6	308	KC1	C2A-C1A-NA	4.00	115.82	109.40
30	7	306	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
39	6	318	DD6	C7-C6-C8	-4.00	111.78	118.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	10	306	KC1	C1C-C2C-C3C	-4.00	102.75	106.96
30	A	815	CLA	C4A-NA-C1A	-4.00	104.91	106.71
30	6	317	CLA	C4A-NA-C1A	-4.00	104.91	106.71
30	8	309	CLA	C4A-NA-C1A	-4.00	104.91	106.71
30	2	301	CLA	C3D-C4D-ND	4.00	116.70	110.24
30	12	308	CLA	C1D-CHD-C4C	-4.00	117.44	126.06
30	1	302	CLA	C1D-CHD-C4C	-3.99	117.44	126.06
30	B	838	CLA	C3D-C4D-ND	3.99	116.70	110.24
30	9	301	CLA	CAA-C2A-C3A	-3.99	101.84	112.78
30	1	304	CLA	C3D-C4D-ND	3.99	116.70	110.24
38	16	311	KC1	C1C-C2C-C3C	-3.99	102.76	106.96
30	A	837	CLA	C3D-C4D-ND	3.99	116.70	110.24
30	16	310	CLA	C4A-NA-C1A	-3.99	104.91	106.71
30	3	302	CLA	C3C-C4C-NC	3.99	115.05	110.57
30	B	811	CLA	C4A-NA-C1A	-3.99	104.91	106.71
38	2	314	KC1	C1A-NA-C4A	-3.99	104.91	106.71
29	A	801	CL0	C3D-C4D-ND	3.99	116.69	110.24
30	9	305	CLA	C3C-C4C-NC	3.99	115.05	110.57
30	B	851	CLA	C1D-CHD-C4C	-3.99	117.45	126.06
30	B	820	CLA	C4C-C3C-C2C	-3.99	101.08	106.90
30	4	309	CLA	C3D-C4D-ND	3.99	116.69	110.24
38	4	307	KC1	C1C-C2C-C3C	-3.99	102.77	106.96
30	12	304	CLA	O2A-CGA-CBA	3.99	124.42	111.91
30	A	830	CLA	C1D-CHD-C4C	-3.99	117.46	126.06
30	A	836	CLA	O2D-CGD-CBD	3.98	118.35	111.27
38	13	310	KC1	CHC-C1C-C2C	-3.98	118.75	124.98
37	15	323	A86	C3-C4-C5	-3.98	115.31	123.47
30	A	831	CLA	CMB-C2B-C3B	3.98	132.13	124.68
30	2	304	CLA	C1D-CHD-C4C	-3.98	117.46	126.06
30	6	306	CLA	C3C-C4C-NC	3.98	115.04	110.57
38	12	305	KC1	C2A-C1A-NA	3.98	115.79	109.40
37	2	318	A86	C40-C32-C31	-3.98	106.91	110.47
37	12	316	A86	C10-C9-C8	-3.98	110.79	123.22
30	12	321	CLA	C1D-CHD-C4C	-3.98	117.47	126.06
30	1	304	CLA	O2D-CGD-CBD	3.98	118.34	111.27
37	14	315	A86	C12-C11-C13	3.98	122.71	116.02
30	2	307	CLA	C3D-C4D-ND	3.98	116.67	110.24
37	7	319	A86	C24-C1-C2	3.98	125.05	118.94
30	16	302	CLA	C3D-C4D-ND	3.98	116.67	110.24
30	13	304	CLA	C1D-CHD-C4C	-3.98	117.48	126.06
30	15	314	CLA	C1D-CHD-C4C	-3.98	117.48	126.06
30	A	821	CLA	C3C-C4C-NC	3.97	115.03	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	835	CLA	C3D-C4D-ND	3.97	116.67	110.24
37	15	316	A86	C12-C11-C13	3.97	122.69	116.02
30	A	810	CLA	C3D-C4D-ND	3.97	116.66	110.24
30	A	821	CLA	C3D-C2D-C1D	-3.97	100.41	105.83
30	J	101	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
30	A	821	CLA	C3D-C4D-ND	3.97	116.66	110.24
30	9	306	CLA	C1D-CHD-C4C	-3.97	117.49	126.06
30	16	306	CLA	C1D-CHD-C4C	-3.97	117.49	126.06
38	5	312	KC1	C2A-C1A-NA	3.97	115.77	109.40
30	A	821	CLA	C1-C2-C3	-3.97	119.18	126.04
37	9	316	A86	C36-C31-C32	-3.97	115.76	119.70
30	15	306	CLA	C3D-C4D-ND	3.97	116.66	110.24
38	4	307	KC1	C2A-C1A-NA	3.97	115.77	109.40
39	10	314	DD6	C37-C36-C35	-3.97	107.00	114.36
30	A	834	CLA	C3D-C4D-ND	3.97	116.66	110.24
30	4	303	CLA	CAC-C3C-C4C	3.97	129.96	124.81
30	A	815	CLA	C3B-C4B-NB	3.97	114.34	109.21
30	14	309	CLA	C3D-C4D-ND	3.97	116.65	110.24
30	3	306	CLA	C3D-C4D-ND	3.97	116.65	110.24
38	11	311	KC1	CBA-CAA-C2A	-3.96	110.16	125.27
30	A	814	CLA	C1D-CHD-C4C	-3.96	117.51	126.06
30	2	310	CLA	C3C-C4C-NC	3.96	115.02	110.57
30	15	307	CLA	O2D-CGD-CBD	3.96	118.31	111.27
30	15	304	CLA	O2D-CGD-CBD	3.96	118.31	111.27
30	A	812	CLA	C1C-C2C-C3C	-3.96	102.79	106.96
30	A	843	CLA	C1C-C2C-C3C	-3.96	102.79	106.96
30	4	303	CLA	C3C-C4C-NC	3.96	115.01	110.57
30	3	307	CLA	O2D-CGD-CBD	3.96	118.30	111.27
37	4	317	A86	C12-C11-C13	3.96	122.67	116.02
30	A	813	CLA	C1D-CHD-C4C	-3.96	117.52	126.06
38	16	304	KC1	CBA-CAA-C2A	-3.96	110.18	125.27
33	L	204	BCR	C24-C23-C22	-3.96	120.26	126.23
39	2	315	DD6	C12-C11-C13	-3.96	111.84	118.08
30	9	305	CLA	C4A-NA-C1A	-3.95	104.93	106.71
30	9	308	CLA	C3C-C4C-NC	3.95	115.01	110.57
30	13	302	CLA	C3D-C4D-ND	3.95	116.64	110.24
38	14	308	KC1	C2A-C1A-NA	3.95	115.74	109.40
30	3	302	CLA	C1D-CHD-C4C	-3.95	117.53	126.06
30	3	305	CLA	C3C-C4C-NC	3.95	115.00	110.57
30	7	312	CLA	C1D-CHD-C4C	-3.95	117.53	126.06
30	16	308	CLA	C1D-CHD-C4C	-3.95	117.53	126.06
30	6	317	CLA	C1C-C2C-C3C	-3.95	102.80	106.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	4	301	CLA	C3D-C4D-ND	3.95	116.63	110.24
37	2	318	A86	C41-C32-C31	-3.95	106.94	110.47
30	B	817	CLA	C2C-C1C-NC	3.95	113.67	109.97
30	B	813	CLA	C4C-C3C-C2C	-3.95	101.14	106.90
30	A	822	CLA	C3D-C2D-C1D	-3.95	100.44	105.83
37	7	316	A86	C26-C25-C24	-3.95	110.90	123.22
30	B	851	CLA	O2D-CGD-CBD	3.95	118.28	111.27
30	12	303	CLA	O2D-CGD-CBD	3.95	118.28	111.27
30	7	307	CLA	C1D-CHD-C4C	-3.94	117.55	126.06
30	B	808	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
30	13	309	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
30	A	825	CLA	C4A-NA-C1A	-3.94	104.93	106.71
30	13	304	CLA	C4A-NA-C1A	-3.94	104.93	106.71
30	3	305	CLA	C1D-CHD-C4C	-3.94	117.55	126.06
30	A	831	CLA	C1D-CHD-C4C	-3.94	117.56	126.06
30	16	302	CLA	C3C-C4C-NC	3.94	114.99	110.57
30	B	832	CLA	C3D-C4D-ND	3.94	116.61	110.24
30	8	308	CLA	C3D-C4D-ND	3.94	116.61	110.24
30	J	101	CLA	C3D-C4D-ND	3.94	116.61	110.24
37	15	321	A86	C12-C11-C13	3.94	122.64	116.02
30	B	821	CLA	C3D-C4D-ND	3.94	116.61	110.24
38	6	311	KC1	CBA-CAA-C2A	-3.94	110.26	125.27
30	F	203	CLA	C1C-C2C-C3C	-3.94	102.82	106.96
30	3	302	CLA	C3D-C4D-ND	3.94	116.61	110.24
30	2u	202	CLA	C1D-CHD-C4C	-3.94	117.56	126.06
30	A	827	CLA	C1D-CHD-C4C	-3.94	117.57	126.06
38	1	308	KC1	CAA-CBA-CGA	-3.93	107.04	127.26
38	10	310	KC1	CBA-CAA-C2A	-3.93	110.27	125.27
30	B	802	CLA	C1D-CHD-C4C	-3.93	117.57	126.06
30	B	828	CLA	C3C-C4C-NC	3.93	114.98	110.57
30	10	304	CLA	C3D-C4D-ND	3.93	116.60	110.24
30	15	308	CLA	C4A-NA-C1A	-3.93	104.94	106.71
30	10	309	CLA	C3C-C4C-NC	3.93	114.98	110.57
30	B	839	CLA	C1D-CHD-C4C	-3.93	117.58	126.06
37	15	321	A86	C36-C31-C32	-3.93	115.80	119.70
30	A	804	CLA	C3C-C4C-NC	3.93	114.98	110.57
30	14	310	CLA	C1C-C2C-C3C	-3.93	102.83	106.96
30	A	835	CLA	C1D-CHD-C4C	-3.93	117.58	126.06
30	10	307	CLA	C1D-CHD-C4C	-3.93	117.58	126.06
38	9	311	KC1	C2C-C1C-NC	3.93	114.86	110.57
38	1	308	KC1	CMD-C2D-C1D	3.93	134.50	128.46
30	B	827	CLA	C3D-C4D-ND	3.93	116.59	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	817	CLA	C1D-CHD-C4C	-3.93	117.58	126.06
39	16	313	DD6	C37-C36-C35	-3.93	107.08	114.36
30	5	311	CLA	O2D-CGD-O1D	-3.93	116.16	123.84
30	B	833	CLA	C3C-C4C-NC	3.93	114.97	110.57
30	B	834	CLA	CMB-C2B-C3B	3.93	132.03	124.68
30	A	842	CLA	C1D-CHD-C4C	-3.93	117.59	126.06
38	11	311	KC1	C4B-C3B-C2B	-3.93	103.53	106.75
30	B	821	CLA	C3D-C2D-C1D	-3.93	100.47	105.83
30	A	840	CLA	C3C-C4C-NC	3.93	114.97	110.57
30	9	309	CLA	C1C-C2C-C3C	-3.92	102.83	106.96
38	11	307	KC1	CBA-CAA-C2A	-3.92	110.31	125.27
30	A	806	CLA	C1D-CHD-C4C	-3.92	117.59	126.06
30	B	819	CLA	CHD-C1D-ND	-3.92	120.85	124.45
30	6	316	CLA	C3D-C4D-ND	3.92	116.58	110.24
30	B	807	CLA	C3D-C4D-ND	3.92	116.58	110.24
30	A	819	CLA	C1D-CHD-C4C	-3.92	117.60	126.06
30	A	816	CLA	C3C-C4C-NC	3.92	114.97	110.57
30	5	311	CLA	C3C-C4C-NC	3.92	114.97	110.57
38	8	312	KC1	CHC-C1C-C2C	-3.92	118.86	124.98
30	9	307	CLA	O2D-CGD-CBD	3.92	118.23	111.27
38	9	310	KC1	CHC-C1C-C2C	-3.92	118.86	124.98
38	10	312	KC1	C4B-C3B-C2B	-3.92	103.53	106.75
30	16	310	CLA	O2D-CGD-O1D	-3.92	116.18	123.84
38	11	312	KC1	C2A-C1A-NA	3.92	115.68	109.40
38	12	305	KC1	C1C-C2C-C3C	-3.92	102.84	106.96
30	2	304	CLA	C3D-C4D-ND	3.92	116.57	110.24
38	14	308	KC1	CMD-C2D-C1D	3.91	134.48	128.46
38	2	314	KC1	O2D-CGD-CBD	3.91	118.22	111.27
30	5	304	CLA	C3C-C4C-NC	3.91	114.96	110.57
30	B	806	CLA	C1D-CHD-C4C	-3.91	117.61	126.06
38	5	306	KC1	CHC-C1C-C2C	-3.91	118.86	124.98
30	12	306	CLA	C3D-C4D-ND	3.91	116.57	110.24
39	3	316	DD6	C35-C36-C31	-3.91	111.69	120.57
30	4	304	CLA	C1D-CHD-C4C	-3.91	117.62	126.06
30	2	307	CLA	C3C-C4C-NC	3.91	114.96	110.57
30	16	303	CLA	C3C-C4C-NC	3.91	114.96	110.57
38	3	304	KC1	C1C-C2C-C3C	-3.91	102.84	106.96
30	5	311	CLA	C1D-CHD-C4C	-3.91	117.62	126.06
38	4	307	KC1	C4B-C3B-C2B	-3.91	103.54	106.75
30	16	309	CLA	C1C-C2C-C3C	-3.91	102.84	106.96
38	7	308	KC1	C1A-NA-C4A	-3.91	104.95	106.71
30	A	818	CLA	C1D-CHD-C4C	-3.91	117.62	126.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	14	308	KC1	C1A-NA-C4A	-3.91	104.95	106.71
37	2u	205	A86	C36-C31-C32	-3.91	115.82	119.70
30	3	307	CLA	C1C-C2C-C3C	-3.91	102.85	106.96
30	7	312	CLA	C1C-C2C-C3C	-3.91	102.85	106.96
37	16	312	A86	C26-C25-C24	-3.91	111.02	123.22
38	13	310	KC1	C1C-C2C-C3C	-3.91	102.85	106.96
30	16	306	CLA	CAA-C2A-C3A	-3.91	102.08	112.78
30	12	304	CLA	CBA-CAA-C2A	3.91	125.39	113.86
30	5	303	CLA	C3C-C4C-NC	3.91	114.95	110.57
30	A	802	CLA	C1D-CHD-C4C	-3.91	117.63	126.06
37	5	301	A86	C41-C32-C31	-3.91	106.98	110.47
30	5	303	CLA	C3D-C4D-ND	3.91	116.56	110.24
30	2	303	CLA	C1C-C2C-C3C	-3.90	102.85	106.96
39	7	302	DD6	C35-C36-C31	-3.90	111.71	120.57
30	12	308	CLA	O2D-CGD-CBD	3.90	118.20	111.27
30	6	310	CLA	C3D-C4D-ND	3.90	116.55	110.24
38	13	311	KC1	C1C-C2C-C3C	-3.90	102.86	106.96
30	A	822	CLA	C3C-C4C-NC	3.90	114.95	110.57
30	8	305	CLA	C3D-C4D-ND	3.90	116.55	110.24
30	9	301	CLA	C3D-C4D-ND	3.90	116.55	110.24
30	A	806	CLA	CMB-C2B-C3B	3.90	131.98	124.68
30	9	302	CLA	C1C-C2C-C3C	-3.90	102.86	106.96
37	15	315	A86	C-C1-C24	-3.90	111.93	118.08
38	11	305	KC1	C1C-C2C-C3C	-3.90	102.86	106.96
30	14	305	CLA	C4A-NA-C1A	-3.90	104.95	106.71
30	A	805	CLA	C3D-C4D-ND	3.90	116.55	110.24
30	5	302	CLA	C1D-CHD-C4C	-3.90	117.65	126.06
30	16	309	CLA	C1D-CHD-C4C	-3.90	117.65	126.06
30	1	305	CLA	C1C-C2C-C3C	-3.90	102.86	106.96
30	14	304	CLA	C1D-CHD-C4C	-3.90	117.65	126.06
30	15	311	CLA	C1C-C2C-C3C	-3.90	102.86	106.96
35	A	854	LMT	C1B-O5B-C5B	3.90	121.34	113.69
30	2	313	CLA	C3C-C4C-NC	3.90	114.94	110.57
30	7	307	CLA	C3D-C4D-ND	3.90	116.54	110.24
30	A	807	CLA	O2A-CGA-CBA	3.90	124.14	111.91
30	B	804	CLA	C3C-C4C-NC	3.90	114.94	110.57
30	9	303	CLA	C1D-CHD-C4C	-3.90	117.66	126.06
37	14	301	A86	C4-C5-C6	-3.90	121.75	127.31
38	4	310	KC1	C2C-C1C-NC	3.89	114.82	110.57
30	A	814	CLA	C3D-C4D-ND	3.89	116.54	110.24
30	15	302	CLA	C1D-CHD-C4C	-3.89	117.66	126.06
30	A	841	CLA	C3C-C4C-NC	3.89	114.94	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	6	305	CLA	C1D-CHD-C4C	-3.89	117.66	126.06
39	7	318	DD6	C22-C16-C15	3.89	120.56	110.05
30	B	838	CLA	C4A-NA-C1A	-3.89	104.96	106.71
30	16	302	CLA	C1D-CHD-C4C	-3.89	117.66	126.06
30	13	309	CLA	C1D-CHD-C4C	-3.89	117.66	126.06
30	B	812	CLA	C3D-C4D-ND	3.89	116.53	110.24
30	6	306	CLA	O2A-CGA-CBA	3.89	124.12	111.91
30	8	308	CLA	C1C-C2C-C3C	-3.89	102.87	106.96
30	12	302	CLA	C1C-C2C-C3C	-3.89	102.87	106.96
38	10	310	KC1	C1C-C2C-C3C	-3.89	102.87	106.96
30	A	829	CLA	C3C-C4C-NC	3.89	114.93	110.57
30	14	307	CLA	O2D-CGD-CBD	3.89	118.18	111.27
30	2	309	CLA	C4A-NA-C1A	-3.89	104.96	106.71
30	16	307	CLA	C1D-CHD-C4C	-3.89	117.67	126.06
30	J	101	CLA	CAA-C2A-C3A	-3.89	102.13	112.78
30	F	202	CLA	C1D-CHD-C4C	-3.89	117.67	126.06
38	3	308	KC1	C2A-C1A-NA	3.89	115.64	109.40
30	5	302	CLA	C3C-C4C-NC	3.89	114.93	110.57
30	1	307	CLA	C1D-CHD-C4C	-3.89	117.67	126.06
30	1	304	CLA	C4A-NA-C1A	-3.89	104.96	106.71
38	5	312	KC1	C1A-NA-C4A	-3.89	104.96	106.71
30	6	315	CLA	C1C-C2C-C3C	-3.89	102.87	106.96
30	15	314	CLA	C1C-C2C-C3C	-3.89	102.87	106.96
30	11	306	CLA	C3C-C4C-NC	3.89	114.93	110.57
37	15	316	A86	C4-C5-C6	-3.89	121.76	127.31
30	7	309	CLA	C3D-C4D-ND	3.89	116.53	110.24
30	9	309	CLA	C3C-C4C-NC	3.89	114.93	110.57
30	4	302	CLA	C1D-CHD-C4C	-3.89	117.67	126.06
30	14	305	CLA	CAA-C2A-C3A	-3.89	102.14	112.78
30	8	304	CLA	CAA-CBA-CGA	-3.88	101.90	113.25
39	8	316	DD6	C7-C6-C8	-3.88	111.96	118.08
30	6	304	CLA	C1C-C2C-C3C	-3.88	102.87	106.96
30	A	829	CLA	C4A-NA-C1A	-3.88	104.96	106.71
30	B	806	CLA	C3D-C4D-ND	3.88	116.52	110.24
30	15	308	CLA	CAC-C3C-C4C	3.88	129.85	124.81
30	4	302	CLA	C3D-C4D-ND	3.88	116.52	110.24
30	15	312	CLA	C1D-CHD-C4C	-3.88	117.68	126.06
37	7	316	A86	C4-C3-C2	-3.88	115.52	123.47
37	15	317	A86	C25-C26-C27	-3.88	121.77	127.31
30	A	818	CLA	C4A-NA-C1A	-3.88	104.96	106.71
30	11	308	CLA	C4A-NA-C1A	-3.88	104.96	106.71
30	15	311	CLA	C1D-CHD-C4C	-3.88	117.69	126.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	14	309	CLA	C1D-CHD-C4C	-3.88	117.69	126.06
30	A	810	CLA	C3C-C4C-NC	3.88	114.92	110.57
30	F	203	CLA	C3C-C4C-NC	3.88	114.92	110.57
30	6	315	CLA	C1D-CHD-C4C	-3.88	117.69	126.06
30	15	305	CLA	C4A-NA-C1A	-3.88	104.96	106.71
38	14	311	KC1	CHC-C1C-C2C	-3.88	118.92	124.98
30	3	302	CLA	C1C-C2C-C3C	-3.88	102.88	106.96
30	7	307	CLA	C3C-C4C-NC	3.88	114.92	110.57
38	5	310	KC1	CBA-CAA-C2A	-3.88	110.49	125.27
30	A	803	CLA	C3C-C4C-NC	3.88	114.92	110.57
38	9	312	KC1	C4B-C3B-C2B	-3.88	103.57	106.75
30	A	813	CLA	C3D-C4D-ND	3.87	116.51	110.24
30	A	820	CLA	C3D-C4D-ND	3.87	116.51	110.24
30	A	813	CLA	C4A-NA-C1A	-3.87	104.96	106.71
30	5	311	CLA	C1C-C2C-C3C	-3.87	102.88	106.96
30	A	841	CLA	O2D-CGD-CBD	3.87	118.15	111.27
30	16	305	CLA	C3D-C4D-ND	3.87	116.50	110.24
30	10	303	CLA	C1D-CHD-C4C	-3.87	117.70	126.06
30	1	307	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
30	14	309	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
30	2	310	CLA	C1-C2-C3	-3.87	119.35	126.04
30	A	806	CLA	CAC-C3C-C4C	3.87	129.83	124.81
38	8	310	KC1	CAA-CBA-CGA	-3.87	107.37	127.26
30	B	815	CLA	C3C-C4C-NC	3.87	114.91	110.57
37	5	301	A86	C36-C31-C32	-3.87	115.86	119.70
37	7	316	A86	C8-C6-C5	-3.87	113.00	118.94
30	8	303	CLA	C3C-C4C-NC	3.87	114.91	110.57
30	A	820	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
39	5	314	DD6	O1-C20-C21	-3.87	110.42	115.06
30	B	837	CLA	C1D-CHD-C4C	-3.87	117.72	126.06
38	6	312	KC1	C4B-C3B-C2B	-3.87	103.58	106.75
30	6	316	CLA	C1D-CHD-C4C	-3.87	117.72	126.06
30	6	316	CLA	C3C-C4C-NC	3.87	114.91	110.57
30	A	825	CLA	C1C-C2C-C3C	-3.86	102.89	106.96
38	2	306	KC1	C1C-C2C-C3C	-3.86	102.89	106.96
30	B	809	CLA	C3D-C4D-ND	3.86	116.49	110.24
37	7	319	A86	C9-C10-C11	-3.86	115.25	126.61
30	16	309	CLA	C3C-C4C-NC	3.86	114.90	110.57
30	12	303	CLA	C1D-CHD-C4C	-3.86	117.72	126.06
30	10	311	CLA	C3C-C4C-NC	3.86	114.90	110.57
30	15	311	CLA	C3C-C4C-NC	3.86	114.90	110.57
30	A	832	CLA	C3D-C4D-ND	3.86	116.48	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	8	309	CLA	C1D-CHD-C4C	-3.86	117.73	126.06
37	7	316	A86	O4-C38-C39	3.86	118.19	111.09
30	B	814	CLA	C3D-C2D-C1D	-3.86	100.56	105.83
30	14	304	CLA	C3C-C4C-NC	3.86	114.90	110.57
30	2	304	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
39	5	313	DD6	C7-C6-C8	-3.86	112.00	118.08
30	B	823	CLA	C1D-CHD-C4C	-3.86	117.74	126.06
30	13	302	CLA	C1D-CHD-C4C	-3.86	117.74	126.06
30	15	313	CLA	C1D-CHD-C4C	-3.86	117.74	126.06
30	A	822	CLA	C4A-NA-C1A	-3.86	104.97	106.71
30	B	823	CLA	C4A-NA-C1A	-3.86	104.97	106.71
30	B	836	CLA	C4A-NA-C1A	-3.86	104.97	106.71
30	B	805	CLA	C3B-C4B-NB	3.86	114.20	109.21
30	A	841	CLA	C3D-C4D-ND	3.86	116.47	110.24
30	B	809	CLA	C3C-C4C-NC	3.86	114.89	110.57
38	6	313	KC1	C1C-C2C-C3C	-3.86	102.90	106.96
30	1	307	CLA	C3C-C4C-NC	3.85	114.89	110.57
30	B	821	CLA	C1C-C2C-C3C	-3.85	102.90	106.96
39	15	319	DD6	C21-C20-C15	-3.85	115.80	122.26
30	3	307	CLA	C1D-CHD-C4C	-3.85	117.74	126.06
30	B	804	CLA	C3D-C4D-ND	3.85	116.47	110.24
37	11	315	A86	C20-C19-C18	-3.85	105.13	112.75
30	14	305	CLA	C3C-C4C-NC	3.85	114.89	110.57
30	16	305	CLA	C3C-C4C-NC	3.85	114.89	110.57
30	A	827	CLA	C4A-NA-C1A	-3.85	104.97	106.71
38	3	311	KC1	C4B-C3B-C2B	-3.85	103.59	106.75
38	11	307	KC1	CAC-C3C-C4C	3.85	129.81	124.81
30	15	308	CLA	C3D-C4D-ND	3.85	116.47	110.24
30	12	310	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
30	B	817	CLA	CAA-C2A-C3A	-3.85	102.23	112.78
37	2u	203	A86	C3-C2-C1	-3.85	121.81	127.31
30	A	819	CLA	C3D-C4D-ND	3.85	116.47	110.24
38	8	313	KC1	O2D-CGD-CBD	3.85	118.11	111.27
30	2	305	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
38	7	308	KC1	C1C-C2C-C3C	-3.85	102.91	106.96
30	A	802	CLA	C3D-C4D-ND	3.85	116.46	110.24
30	10	305	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
30	A	839	CLA	C1D-CHD-C4C	-3.85	117.75	126.06
30	9	309	CLA	C1D-CHD-C4C	-3.85	117.75	126.06
30	B	826	CLA	C3D-C4D-ND	3.85	116.46	110.24
37	12	316	A86	C25-C26-C27	-3.85	121.82	127.31
38	3	304	KC1	C1A-NA-C4A	-3.85	104.98	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	7	305	CLA	C3C-C4C-NC	3.85	114.89	110.57
30	14	310	CLA	C3C-C4C-NC	3.85	114.89	110.57
30	12	312	CLA	C1D-CHD-C4C	-3.85	117.76	126.06
30	B	838	CLA	C3B-C4B-NB	3.85	114.18	109.21
30	B	833	CLA	C1D-CHD-C4C	-3.84	117.77	126.06
37	11	316	A86	C36-C31-C32	-3.84	115.88	119.70
38	2	312	KC1	C4B-C3B-C2B	-3.84	103.60	106.75
30	8	302	CLA	C1D-CHD-C4C	-3.84	117.77	126.06
30	A	826	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
38	5	305	KC1	C1C-C2C-C3C	-3.84	102.92	106.96
30	B	822	CLA	O2D-CGD-CBD	3.84	118.09	111.27
30	8	303	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
30	12	312	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
30	4	309	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
39	2	316	DD6	O1-C20-C21	-3.84	110.46	115.06
30	A	840	CLA	C3D-C4D-ND	3.84	116.44	110.24
30	A	816	CLA	C1D-CHD-C4C	-3.84	117.78	126.06
30	A	840	CLA	C1D-CHD-C4C	-3.84	117.78	126.06
30	12	304	CLA	C1D-CHD-C4C	-3.84	117.78	126.06
30	B	811	CLA	C1D-CHD-C4C	-3.84	117.78	126.06
37	2u	203	A86	C25-C24-C1	-3.84	115.64	126.42
30	16	306	CLA	CAC-C3C-C4C	3.84	129.79	124.81
39	7	318	DD6	C21-C20-C19	-3.83	109.97	114.28
37	14	301	A86	C12-C11-C13	3.83	122.46	116.02
30	A	835	CLA	O2D-CGD-O1D	-3.83	116.34	123.84
30	A	824	CLA	C1D-CHD-C4C	-3.83	117.79	126.06
39	7	302	DD6	C12-C11-C13	-3.83	112.04	118.08
30	11	309	CLA	C1D-CHD-C4C	-3.83	117.79	126.06
30	8	301	CLA	C1-C2-C3	-3.83	119.42	126.04
37	3	314	A86	C9-C10-C11	-3.83	115.34	126.61
30	A	830	CLA	C3D-C2D-C1D	-3.83	100.60	105.83
30	A	807	CLA	C3D-C4D-ND	3.83	116.44	110.24
30	2	309	CLA	C3C-C4C-NC	3.83	114.87	110.57
30	6	309	CLA	O2A-CGA-CBA	3.83	123.93	111.91
30	9	305	CLA	C3D-C4D-ND	3.83	116.44	110.24
39	16	313	DD6	C21-C20-C15	-3.83	115.84	122.26
30	9	303	CLA	CMC-C2C-C1C	3.83	130.87	125.04
37	4	315	A86	C12-C11-C13	3.83	122.45	116.02
38	2	312	KC1	CAA-CBA-CGA	-3.83	107.59	127.26
30	2	308	CLA	C3C-C4C-NC	3.83	114.86	110.57
30	14	312	CLA	C3C-C4C-NC	3.83	114.86	110.57
30	A	810	CLA	C1C-C2C-C3C	-3.83	102.93	106.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	812	CLA	CMB-C2B-C3B	3.83	131.84	124.68
30	A	815	CLA	C3D-C4D-ND	3.83	116.43	110.24
30	B	813	CLA	C3D-C4D-ND	3.83	116.43	110.24
39	6	303	DD6	C12-C11-C13	-3.83	112.05	118.08
30	6	306	CLA	C1D-CHD-C4C	-3.83	117.81	126.06
38	14	311	KC1	C2A-C1A-NA	3.83	115.54	109.40
38	3	308	KC1	CMB-C2B-C1B	3.82	131.45	124.71
38	13	308	KC1	C1C-C2C-C3C	-3.82	102.94	106.96
30	B	829	CLA	C3C-C4C-NC	3.82	114.86	110.57
30	16	306	CLA	C3D-C2D-C1D	-3.82	100.62	105.83
30	16	310	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
37	15	322	A86	C9-C10-C11	-3.82	115.38	126.61
30	L	203	CLA	C1D-CHD-C4C	-3.82	117.82	126.06
38	12	309	KC1	C1C-C2C-C3C	-3.82	102.94	106.96
30	B	812	CLA	C3C-C4C-NC	3.82	114.85	110.57
30	8	302	CLA	C3C-C4C-NC	3.82	114.85	110.57
37	9	313	A86	C12-C11-C13	3.82	122.43	116.02
30	B	803	CLA	C3D-C4D-ND	3.82	116.41	110.24
30	A	809	CLA	C1D-CHD-C4C	-3.82	117.82	126.06
38	13	312	KC1	C1C-C2C-C3C	-3.82	102.94	106.96
30	6	315	CLA	C3C-C4C-NC	3.82	114.85	110.57
30	B	814	CLA	C4A-NA-C1A	-3.81	104.99	106.71
30	A	814	CLA	C3C-C4C-NC	3.81	114.85	110.57
30	15	310	CLA	C3C-C4C-NC	3.81	114.85	110.57
30	8	304	CLA	C3D-C4D-ND	3.81	116.41	110.24
39	12	315	DD6	C37-C36-C35	-3.81	107.29	114.36
30	12	306	CLA	C3C-C4C-NC	3.81	114.85	110.57
30	12	303	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
30	B	815	CLA	C4A-NA-C1A	-3.81	104.99	106.71
38	3	308	KC1	C4B-C3B-C2B	-3.81	103.62	106.75
30	A	841	CLA	CMB-C2B-C3B	3.81	131.81	124.68
30	B	836	CLA	C3D-C4D-ND	3.81	116.40	110.24
30	13	307	CLA	C1D-CHD-C4C	-3.81	117.84	126.06
30	16	303	CLA	C1D-CHD-C4C	-3.81	117.84	126.06
30	B	803	CLA	C4C-C3C-C2C	-3.81	101.34	106.90
30	2	307	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
39	6	319	DD6	C35-C36-C31	-3.81	111.92	120.57
30	4	304	CLA	C3C-C4C-NC	3.81	114.84	110.57
37	14	320	A86	C-C1-C2	-3.81	117.59	122.92
30	3	310	CLA	C1D-CHD-C4C	-3.81	117.84	126.06
30	15	307	CLA	C1D-CHD-C4C	-3.81	117.84	126.06
30	A	825	CLA	C3D-C4D-ND	3.81	116.40	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	2	304	CLA	C3C-C4C-NC	3.81	114.84	110.57
30	6	305	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
30	B	828	CLA	O2D-CGD-O1D	-3.81	116.39	123.84
30	9	305	CLA	C1D-CHD-C4C	-3.81	117.84	126.06
30	10	305	CLA	C3C-C4C-NC	3.81	114.84	110.57
30	4	302	CLA	O2D-CGD-CBD	3.81	118.03	111.27
39	6	318	DD6	C21-C20-C19	-3.81	110.00	114.28
30	15	310	CLA	C1D-CHD-C4C	-3.81	117.85	126.06
30	B	811	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
37	12	314	A86	C40-C32-C31	-3.81	107.07	110.47
30	B	809	CLA	C1D-CHD-C4C	-3.81	117.85	126.06
39	5	313	DD6	C21-C20-C19	-3.81	110.00	114.28
37	11	315	A86	C3-C2-C1	-3.81	121.88	127.31
30	2	307	CLA	C1D-CHD-C4C	-3.81	117.85	126.06
30	B	833	CLA	C3D-C4D-ND	3.80	116.39	110.24
30	6	304	CLA	CBC-CAC-C3C	-3.80	101.94	112.43
30	A	809	CLA	C1C-C2C-C3C	-3.80	102.96	106.96
39	8	317	DD6	C37-C36-C35	-3.80	107.31	114.36
38	12	305	KC1	C1A-NA-C4A	-3.80	105.00	106.71
30	A	803	CLA	C3D-C4D-ND	3.80	116.39	110.24
30	15	309	CLA	C1D-CHD-C4C	-3.80	117.86	126.06
38	11	305	KC1	CBA-CAA-C2A	-3.80	110.79	125.27
34	2	320	LHG	O4-P-O5	3.80	131.02	112.24
30	5	308	CLA	C1D-CHD-C4C	-3.80	117.86	126.06
30	A	836	CLA	C3C-C4C-NC	3.80	114.83	110.57
39	6	319	DD6	C7-C6-C8	-3.80	112.09	118.08
30	A	815	CLA	C1D-CHD-C4C	-3.80	117.87	126.06
30	B	839	CLA	C1C-C2C-C3C	-3.80	102.97	106.96
38	8	313	KC1	CHC-C1C-C2C	-3.80	119.05	124.98
38	9	310	KC1	C2C-C1C-NC	3.80	114.72	110.57
38	2	314	KC1	C1C-C2C-C3C	-3.80	102.97	106.96
30	A	816	CLA	C3B-C4B-NB	3.79	114.12	109.21
30	B	816	CLA	C1D-CHD-C4C	-3.79	117.87	126.06
30	14	313	CLA	C1D-CHD-C4C	-3.79	117.87	126.06
30	3	301	CLA	C1D-CHD-C4C	-3.79	117.87	126.06
38	13	312	KC1	C4B-C3B-C2B	-3.79	103.64	106.75
30	A	831	CLA	C4A-NA-C1A	-3.79	105.00	106.71
30	A	826	CLA	C1D-CHD-C4C	-3.79	117.88	126.06
30	B	821	CLA	C1D-CHD-C4C	-3.79	117.88	126.06
30	B	832	CLA	C1D-CHD-C4C	-3.79	117.88	126.06
30	A	822	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
38	8	311	KC1	C4B-C3B-C2B	-3.79	103.64	106.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	15	310	CLA	C3B-C4B-NB	3.79	114.11	109.21
30	A	806	CLA	C3C-C4C-NC	3.79	114.82	110.57
30	8	309	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
30	B	851	CLA	CAA-C2A-C3A	-3.78	102.42	112.78
30	A	825	CLA	CAC-C3C-C4C	3.78	129.72	124.81
30	15	313	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
30	9	301	CLA	CMB-C2B-C3B	3.78	131.75	124.68
30	5	309	CLA	C4A-NA-C1A	-3.78	105.01	106.71
38	3	311	KC1	C1A-NA-C4A	-3.78	105.01	106.71
30	A	833	CLA	C3C-C4C-NC	3.78	114.81	110.57
30	A	839	CLA	C3C-C4C-NC	3.78	114.81	110.57
30	7	310	CLA	C3C-C4C-NC	3.78	114.81	110.57
33	L	204	BCR	C31-C1-C6	3.78	116.43	110.30
30	F	202	CLA	C3D-C4D-ND	3.78	116.35	110.24
30	12	312	CLA	C4A-NA-C1A	-3.78	105.01	106.71
30	B	804	CLA	C1D-CHD-C4C	-3.78	117.91	126.06
39	3	312	DD6	C21-C20-C19	-3.78	110.03	114.28
30	B	822	CLA	CMA-C3A-C2A	-3.78	98.59	113.83
30	F	201	CLA	O2D-CGD-CBD	3.78	117.98	111.27
37	10	301	A86	C12-C11-C13	3.78	122.37	116.02
37	14	314	A86	C41-C32-C31	-3.78	107.09	110.47
37	14	317	A86	C3-C2-C1	-3.78	121.92	127.31
38	5	306	KC1	C2C-C1C-NC	3.78	114.69	110.57
30	B	828	CLA	C3B-C4B-NB	3.78	114.09	109.21
30	8	308	CLA	C1D-CHD-C4C	-3.78	117.91	126.06
30	5	309	CLA	C1D-CHD-C4C	-3.77	117.92	126.06
30	10	304	CLA	C1D-CHD-C4C	-3.77	117.92	126.06
37	7	315	A86	C40-C32-C31	-3.77	107.09	110.47
30	L	203	CLA	C3C-C4C-NC	3.77	114.80	110.57
38	16	304	KC1	C4B-C3B-C2B	-3.77	103.65	106.75
30	9	308	CLA	C1D-CHD-C4C	-3.77	117.92	126.06
30	B	808	CLA	CAA-C2A-C3A	-3.77	102.45	112.78
30	A	805	CLA	CMB-C2B-C3B	3.77	131.73	124.68
30	7	309	CLA	C3C-C4C-NC	3.77	114.80	110.57
37	6	320	A86	C9-C8-C6	-3.77	115.83	126.42
37	12	314	A86	C36-C31-C32	-3.77	115.96	119.70
30	15	310	CLA	CMB-C2B-C3B	3.77	131.73	124.68
37	4	314	A86	C3-C2-C1	-3.77	121.93	127.31
30	6	317	CLA	C1D-CHD-C4C	-3.77	117.93	126.06
30	B	805	CLA	C1C-C2C-C3C	-3.77	103.00	106.96
30	B	827	CLA	C1D-CHD-C4C	-3.77	117.93	126.06
30	1	301	CLA	C1-C2-C3	-3.77	119.53	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	808	CLA	C3C-C4C-NC	3.77	114.80	110.57
30	3	303	CLA	C1D-CHD-C4C	-3.77	117.93	126.06
30	14	312	CLA	C1D-CHD-C4C	-3.77	117.93	126.06
30	A	834	CLA	C1C-C2C-C3C	-3.77	103.00	106.96
38	5	312	KC1	CAC-C3C-C4C	3.77	129.70	124.81
30	16	307	CLA	C3C-C4C-NC	3.76	114.79	110.57
30	A	817	CLA	C1D-CHD-C4C	-3.76	117.94	126.06
30	6	309	CLA	C1D-CHD-C4C	-3.76	117.94	126.06
38	14	306	KC1	CBA-CAA-C2A	-3.76	110.92	125.27
30	B	815	CLA	C3B-C4B-NB	3.76	114.07	109.21
30	5	309	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
30	A	835	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
39	15	318	DD6	C21-C20-C15	-3.76	115.96	122.26
39	15	318	DD6	C37-C36-C35	-3.76	107.39	114.36
30	B	815	CLA	C3D-C4D-ND	3.76	116.32	110.24
30	15	303	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
30	6	307	CLA	C3D-C2D-C1D	-3.76	100.70	105.83
30	A	844	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
30	14	305	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
38	4	308	KC1	C1C-C2C-C3C	-3.76	103.00	106.96
30	B	809	CLA	CAA-C2A-C3A	-3.76	102.48	112.78
30	16	307	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
30	A	837	CLA	C3C-C4C-NC	3.76	114.79	110.57
30	B	816	CLA	C3C-C4C-NC	3.76	114.78	110.57
30	A	830	CLA	CHD-C1D-ND	-3.76	121.00	124.45
37	5	315	A86	C12-C11-C13	3.76	122.33	116.02
30	A	803	CLA	CHB-C4A-NA	3.76	129.71	124.51
38	9	304	KC1	C1C-C2C-C3C	-3.76	103.01	106.96
30	11	306	CLA	C1D-CHD-C4C	-3.76	117.96	126.06
38	1	308	KC1	C1C-C2C-C3C	-3.75	103.01	106.96
30	9	301	CLA	C3C-C4C-NC	3.75	114.78	110.57
38	9	312	KC1	C1C-C2C-C3C	-3.75	103.01	106.96
39	3	312	DD6	C35-C36-C31	-3.75	112.05	120.57
30	12	308	CLA	C4A-NA-C1A	-3.75	105.02	106.71
30	5	308	CLA	C1C-C2C-C3C	-3.75	103.01	106.96
30	13	304	CLA	C3C-C4C-NC	3.75	114.78	110.57
38	6	308	KC1	CHC-C1C-C2C	-3.75	119.12	124.98
30	12	308	CLA	C1C-C2C-C3C	-3.75	103.01	106.96
30	6	309	CLA	C3C-C4C-NC	3.75	114.78	110.57
30	3	305	CLA	C3D-C4D-ND	3.75	116.30	110.24
30	15	305	CLA	C1C-C2C-C3C	-3.75	103.02	106.96
30	A	821	CLA	C1D-CHD-C4C	-3.75	117.97	126.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	7	319	A86	C-C1-C2	-3.75	117.67	122.92
30	9	302	CLA	C3C-C4C-NC	3.75	114.77	110.57
30	A	811	CLA	C3C-C4C-NC	3.75	114.77	110.57
30	7	311	CLA	C3C-C4C-NC	3.75	114.77	110.57
30	A	829	CLA	C3D-C4D-ND	3.75	116.30	110.24
34	B	848	LHG	O8-C23-C24	3.75	121.20	111.38
30	2	311	CLA	C3C-C4C-NC	3.75	114.77	110.57
30	A	812	CLA	C1D-CHD-C4C	-3.74	117.98	126.06
30	A	832	CLA	C4A-NA-C1A	-3.74	105.02	106.71
37	14	301	A86	C25-C26-C27	-3.74	121.97	127.31
30	2	313	CLA	C1D-CHD-C4C	-3.74	117.99	126.06
30	15	313	CLA	C3C-C4C-NC	3.74	114.77	110.57
30	4	305	CLA	C1C-C2C-C3C	-3.74	103.02	106.96
30	14	303	CLA	C1C-C2C-C3C	-3.74	103.02	106.96
30	B	826	CLA	C4A-NA-C1A	-3.74	105.02	106.71
30	A	810	CLA	C3B-C4B-NB	3.74	114.05	109.21
30	B	824	CLA	C3C-C4C-NC	3.74	114.77	110.57
30	1	305	CLA	C3C-C4C-NC	3.74	114.77	110.57
30	A	802	CLA	C3B-C4B-NB	3.74	114.04	109.21
30	9	307	CLA	C3D-C4D-ND	3.74	116.28	110.24
30	B	806	CLA	C1C-C2C-C3C	-3.74	103.03	106.96
30	11	308	CLA	C1C-C2C-C3C	-3.74	103.03	106.96
38	1	306	KC1	C1C-C2C-C3C	-3.74	103.03	106.96
30	5	303	CLA	C1D-CHD-C4C	-3.74	118.00	126.06
30	7	305	CLA	C3B-C4B-NB	3.74	114.04	109.21
30	12	303	CLA	C3D-C4D-ND	3.74	116.28	110.24
30	B	812	CLA	C1D-CHD-C4C	-3.74	118.00	126.06
30	A	829	CLA	CAA-C2A-C3A	-3.74	102.55	112.78
29	A	801	CL0	C1D-CHD-C4C	-3.73	118.00	126.06
30	B	826	CLA	C1D-CHD-C4C	-3.73	118.00	126.06
33	B	844	BCR	C15-C16-C17	-3.73	115.82	123.47
30	2	310	CLA	C3B-C4B-NB	3.73	114.04	109.21
30	A	809	CLA	C3C-C4C-NC	3.73	114.76	110.57
30	B	838	CLA	C3C-C4C-NC	3.73	114.76	110.57
38	8	313	KC1	CAA-CBA-CGA	-3.73	108.07	127.26
30	A	831	CLA	C3B-C4B-NB	3.73	114.04	109.21
30	15	305	CLA	C3C-C4C-NC	3.73	114.76	110.57
30	1	302	CLA	C1C-C2C-C3C	-3.73	103.03	106.96
30	6	307	CLA	C1C-C2C-C3C	-3.73	103.03	106.96
30	8	303	CLA	C1D-CHD-C4C	-3.73	118.01	126.06
30	B	825	CLA	C1D-CHD-C4C	-3.73	118.01	126.06
30	A	805	CLA	C3C-C4C-NC	3.73	114.75	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	4	311	CLA	C1D-CHD-C4C	-3.73	118.02	126.06
30	4	302	CLA	C3C-C4C-NC	3.73	114.75	110.57
30	A	837	CLA	C1C-C2C-C3C	-3.73	103.04	106.96
38	6	312	KC1	C1C-C2C-C3C	-3.73	103.04	106.96
30	10	309	CLA	C1D-CHD-C4C	-3.73	118.02	126.06
30	13	303	CLA	C1D-CHD-C4C	-3.73	118.02	126.06
37	1	309	A86	C10-C9-C8	-3.73	111.59	123.22
37	15	320	A86	C35-C34-C33	3.73	116.38	109.88
30	B	805	CLA	C3C-C4C-NC	3.73	114.75	110.57
30	7	307	CLA	C4A-NA-C1A	-3.73	105.03	106.71
30	11	306	CLA	CBA-CAA-C2A	3.72	124.86	113.86
30	3	309	CLA	C3C-C4C-NC	3.72	114.75	110.57
30	8	308	CLA	C3C-C4C-NC	3.72	114.75	110.57
39	11	313	DD6	C35-C36-C31	-3.72	112.12	120.57
30	10	305	CLA	C1D-CHD-C4C	-3.72	118.03	126.06
30	4	305	CLA	C3C-C4C-NC	3.72	114.75	110.57
30	A	802	CLA	C1C-C2C-C3C	-3.72	103.04	106.96
38	8	306	KC1	C4B-C3B-C2B	-3.72	103.70	106.75
30	13	303	CLA	C1C-C2C-C3C	-3.72	103.05	106.96
37	14	314	A86	C10-C9-C8	-3.72	111.61	123.22
30	3	307	CLA	C4A-NA-C1A	-3.72	105.03	106.71
30	4	301	CLA	C4A-NA-C1A	-3.72	105.03	106.71
30	16	310	CLA	C1D-CHD-C4C	-3.72	118.04	126.06
30	10	304	CLA	C1C-C2C-C3C	-3.72	103.05	106.96
30	13	302	CLA	C1C-C2C-C3C	-3.72	103.05	106.96
38	1	308	KC1	CAA-C2A-C1A	-3.72	107.65	124.75
30	1	305	CLA	C1D-CHD-C4C	-3.72	118.04	126.06
30	3	309	CLA	C1D-CHD-C4C	-3.72	118.04	126.06
30	A	833	CLA	C1C-C2C-C3C	-3.72	103.05	106.96
30	B	831	CLA	C3C-C4C-NC	3.72	114.74	110.57
30	16	308	CLA	C3C-C4C-NC	3.72	114.74	110.57
30	A	814	CLA	C4C-C3C-C2C	-3.72	101.48	106.90
30	6	304	CLA	C1D-CHD-C4C	-3.72	118.04	126.06
30	16	308	CLA	C1C-C2C-C3C	-3.72	103.05	106.96
30	F	201	CLA	C1C-C2C-C3C	-3.71	103.05	106.96
30	7	306	CLA	C3D-C4D-ND	3.71	116.25	110.24
30	2	311	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
37	9	313	A86	C41-C32-C31	-3.71	107.15	110.47
30	12	307	CLA	CAC-C3C-C4C	3.71	129.63	124.81
30	B	809	CLA	C4A-NA-C1A	-3.71	105.04	106.71
30	A	843	CLA	C3C-C4C-NC	3.71	114.73	110.57
38	13	305	KC1	C1C-C2C-C3C	-3.71	103.06	106.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	14	303	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
30	A	813	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
38	2	312	KC1	C1C-C2C-C3C	-3.71	103.06	106.96
30	B	828	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
30	3	305	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
30	13	307	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
30	15	311	CLA	C4A-NA-C1A	-3.71	105.04	106.71
38	8	307	KC1	C2C-C1C-NC	3.71	114.62	110.57
37	9	313	A86	C3-C4-C5	-3.71	115.88	123.47
30	7	305	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
30	3	301	CLA	C4-C3-C5	3.71	121.50	115.27
30	L	202	CLA	C3C-C4C-NC	3.71	114.73	110.57
30	A	814	CLA	C4A-NA-C1A	-3.71	105.04	106.71
37	14	320	A86	C3-C4-C5	3.71	131.06	123.47
38	11	307	KC1	C4B-C3B-C2B	-3.71	103.71	106.75
30	B	806	CLA	C3C-C4C-NC	3.70	114.73	110.57
30	A	837	CLA	C1D-CHD-C4C	-3.70	118.07	126.06
37	13	313	A86	C8-C6-C5	3.70	124.62	118.94
38	6	313	KC1	C4B-C3B-C2B	-3.70	103.71	106.75
39	10	313	DD6	C21-C20-C15	-3.70	116.05	122.26
30	6	309	CLA	C1C-C2C-C3C	-3.70	103.06	106.96
30	A	835	CLA	C3C-C4C-NC	3.70	114.72	110.57
30	B	803	CLA	O2D-CGD-CBD	3.70	117.85	111.27
30	9	306	CLA	C4A-NA-C1A	-3.70	105.04	106.71
38	8	312	KC1	C1A-NA-C4A	-3.70	105.04	106.71
30	8	303	CLA	C3B-C4B-NB	3.70	113.99	109.21
39	4	316	DD6	C37-C36-C35	-3.70	107.50	114.36
30	10	309	CLA	O2D-CGD-CBD	3.70	117.84	111.27
30	2	309	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
30	15	310	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
30	1	303	CLA	C1D-CHD-C4C	-3.70	118.08	126.06
30	5	311	CLA	C3B-C4B-NB	3.69	113.99	109.21
30	12	303	CLA	CMB-C2B-C3B	3.69	131.59	124.68
30	16	310	CLA	CED-O2D-CGD	3.69	124.29	115.94
38	12	305	KC1	C4B-C3B-C2B	-3.69	103.72	106.75
35	15	301	LMT	C1B-O5B-C5B	3.69	120.94	113.69
30	3	303	CLA	C1C-C2C-C3C	-3.69	103.07	106.96
30	L	203	CLA	C3B-C4B-NB	3.69	113.98	109.21
30	1	301	CLA	C3C-C4C-NC	3.69	114.71	110.57
38	9	311	KC1	CAA-CBA-CGA	-3.69	108.28	127.26
38	10	306	KC1	O2D-CGD-O1D	-3.69	116.62	123.84
30	4	301	CLA	C1C-C2C-C3C	-3.69	103.08	106.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	2	302	A86	C3-C2-C1	-3.69	122.04	127.31
30	14	302	CLA	C1D-CHD-C4C	-3.69	118.10	126.06
30	7	305	CLA	C1D-CHD-C4C	-3.69	118.10	126.06
38	9	311	KC1	C1C-C2C-C3C	-3.69	103.08	106.96
37	9	313	A86	C23-C16-C22	-3.69	101.93	107.37
37	14	314	A86	C40-C32-C31	-3.69	107.17	110.47
30	2u	202	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
37	7	315	A86	C9-C10-C11	-3.69	115.77	126.61
30	5	304	CLA	C1C-C2C-C3C	-3.68	103.08	106.96
38	13	306	KC1	C2C-C1C-NC	3.68	114.59	110.57
30	B	838	CLA	C1D-CHD-C4C	-3.68	118.11	126.06
30	4	306	CLA	C1D-CHD-C4C	-3.68	118.12	126.06
30	A	805	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
30	3	309	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
38	8	313	KC1	C4C-C3C-C2C	-3.68	101.53	106.90
30	A	844	CLA	C1D-CHD-C4C	-3.68	118.12	126.06
30	B	820	CLA	C1D-CHD-C4C	-3.68	118.12	126.06
30	5	303	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
38	8	312	KC1	C4B-C3B-C2B	-3.68	103.73	106.75
30	9	303	CLA	C3C-C4C-NC	3.68	114.70	110.57
37	14	320	A86	C41-C32-C31	-3.68	107.18	110.47
30	4	302	CLA	C4A-NA-C1A	-3.68	105.05	106.71
30	9	303	CLA	C1C-C2C-C3C	-3.67	103.09	106.96
39	15	319	DD6	C37-C36-C35	-3.67	107.55	114.36
30	A	838	CLA	C3D-C4D-ND	3.67	116.18	110.24
38	14	306	KC1	C2C-C1C-NC	3.67	114.58	110.57
30	A	828	CLA	C3D-C4D-ND	3.67	116.18	110.24
37	10	315	A86	C4-C3-C2	-3.67	115.95	123.47
38	7	313	KC1	CAA-C2A-C1A	-3.67	107.87	124.75
30	3	306	CLA	C3C-C4C-NC	3.67	114.69	110.57
30	2	308	CLA	C1D-CHD-C4C	-3.67	118.14	126.06
38	2	306	KC1	CAA-CBA-CGA	-3.67	108.39	127.26
30	L	202	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
30	A	823	CLA	C3B-C4B-NB	3.67	113.95	109.21
30	B	818	CLA	C1D-CHD-C4C	-3.67	118.14	126.06
38	10	312	KC1	C2C-C1C-NC	3.67	114.58	110.57
30	3	301	CLA	C3C-C4C-NC	3.67	114.69	110.57
30	A	833	CLA	C4A-NA-C1A	-3.67	105.06	106.71
30	11	310	CLA	C1D-CHD-C4C	-3.67	118.15	126.06
30	A	824	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
30	9	303	CLA	CAC-C3C-C4C	3.67	129.57	124.81
30	5	308	CLA	C3C-C4C-NC	3.66	114.68	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	14	309	CLA	C3C-C4C-NC	3.66	114.68	110.57
38	6	308	KC1	C2C-C1C-NC	3.66	114.57	110.57
30	1	303	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
30	B	835	CLA	C3C-C4C-NC	3.66	114.68	110.57
30	2	305	CLA	C3C-C4C-NC	3.66	114.68	110.57
38	7	313	KC1	C2C-C1C-NC	3.66	114.57	110.57
30	B	831	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
30	A	817	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
30	14	310	CLA	C4A-NA-C1A	-3.66	105.06	106.71
30	7	311	CLA	C1D-CHD-C4C	-3.66	118.16	126.06
37	8	315	A86	C36-C31-C32	-3.66	116.06	119.70
30	L	202	CLA	CBC-CAC-C3C	-3.66	102.34	112.43
30	A	831	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
30	12	303	CLA	C3B-C4B-NB	3.66	113.94	109.21
30	7	304	CLA	CAA-C2A-C3A	-3.66	102.76	112.78
30	A	809	CLA	C3D-C4D-ND	3.66	116.16	110.24
30	A	808	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
30	A	807	CLA	O2D-CGD-CBD	3.66	117.77	111.27
30	5	309	CLA	C3C-C4C-NC	3.66	114.67	110.57
30	14	313	CLA	C3C-C4C-NC	3.66	114.67	110.57
30	B	825	CLA	C3D-C4D-ND	3.65	116.15	110.24
38	13	305	KC1	C2A-C1A-NA	3.65	115.26	109.40
30	A	808	CLA	C1D-CHD-C4C	-3.65	118.18	126.06
33	L	201	BCR	C2-C1-C6	3.65	116.11	110.48
39	2	315	DD6	O1-C20-C21	-3.65	110.68	115.06
37	11	316	A86	C3-C4-C5	-3.65	115.99	123.47
38	5	312	KC1	C1C-C2C-C3C	-3.65	103.12	106.96
30	1	301	CLA	C1D-CHD-C4C	-3.65	118.18	126.06
30	A	811	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
30	B	833	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
38	14	311	KC1	C1C-C2C-C3C	-3.65	103.12	106.96
30	2	309	CLA	C1D-CHD-C4C	-3.65	118.18	126.06
30	6	315	CLA	C4A-NA-C1A	-3.65	105.06	106.71
30	A	813	CLA	CMB-C2B-C3B	3.65	131.51	124.68
30	B	828	CLA	CAC-C3C-C4C	3.65	129.54	124.81
30	2	305	CLA	C1D-CHD-C4C	-3.64	118.20	126.06
30	A	834	CLA	C1D-CHD-C4C	-3.64	118.20	126.06
30	7	309	CLA	C4A-NA-C1A	-3.64	105.07	106.71
38	11	311	KC1	C1C-C2C-C3C	-3.64	103.13	106.96
30	6	317	CLA	C3C-C4C-NC	3.64	114.66	110.57
38	14	306	KC1	CAB-C3B-C4B	3.64	133.69	124.90
38	8	314	KC1	CBA-CAA-C2A	-3.64	111.40	125.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	12	312	CLA	C3C-C4C-NC	3.64	114.65	110.57
30	B	828	CLA	C1D-CHD-C4C	-3.64	118.21	126.06
30	6	310	CLA	C1D-CHD-C4C	-3.64	118.21	126.06
30	A	843	CLA	C1-C2-C3	-3.64	119.75	126.04
30	11	304	CLA	C3C-C4C-NC	3.64	114.65	110.57
30	15	309	CLA	C3C-C4C-NC	3.64	114.65	110.57
30	7	304	CLA	C3B-C4B-NB	3.64	113.91	109.21
38	4	310	KC1	CAA-CBA-CGA	-3.64	108.57	127.26
38	10	312	KC1	C1C-C2C-C3C	-3.64	103.13	106.96
30	8	309	CLA	C3C-C4C-NC	3.64	114.65	110.57
30	A	802	CLA	CAC-C3C-C4C	3.64	129.53	124.81
37	7	316	A86	C36-C31-C32	-3.63	116.09	119.70
30	4	311	CLA	CAA-C2A-C3A	-3.63	102.83	112.78
30	A	831	CLA	C3D-C4D-ND	3.63	116.12	110.24
30	11	304	CLA	C1D-CHD-C4C	-3.63	118.22	126.06
37	15	322	A86	C24-C1-C2	3.63	124.52	118.94
37	8	318	A86	C35-C34-C33	3.63	116.21	109.88
30	9	309	CLA	O2D-CGD-CBD	3.63	117.72	111.27
39	6	321	DD6	C32-C31-C36	-3.63	117.51	122.63
37	14	320	A86	C8-C6-C5	-3.63	113.37	118.94
30	B	815	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
30	B	834	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
38	12	313	KC1	CAA-CBA-CGA	-3.63	108.61	127.26
38	16	304	KC1	C1C-C2C-C3C	-3.63	103.14	106.96
30	A	843	CLA	C3B-C4B-NB	3.63	113.90	109.21
30	A	823	CLA	C1D-CHD-C4C	-3.63	118.23	126.06
30	B	826	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
30	3	303	CLA	C3C-C4C-NC	3.63	114.64	110.57
30	15	305	CLA	C1D-CHD-C4C	-3.63	118.24	126.06
30	7	303	CLA	C1D-CHD-C4C	-3.62	118.24	126.06
39	3	312	DD6	C25-C24-C1	-3.62	116.24	126.42
38	3	311	KC1	C1C-C2C-C3C	-3.62	103.15	106.96
30	6	314	CLA	C3B-C4B-NB	3.62	113.89	109.21
30	4	306	CLA	C3C-C4C-NC	3.62	114.63	110.57
30	9	302	CLA	C1-O2A-CGA	3.62	125.95	116.44
30	A	812	CLA	C4-C3-C5	3.62	121.36	115.27
30	A	836	CLA	C1D-CHD-C4C	-3.62	118.25	126.06
30	6	307	CLA	C1D-CHD-C4C	-3.62	118.25	126.06
30	15	302	CLA	C3C-C4C-NC	3.62	114.63	110.57
30	6	310	CLA	C4A-NA-C1A	-3.62	105.08	106.71
38	8	307	KC1	C1C-C2C-C3C	-3.62	103.15	106.96
30	A	841	CLA	C1D-CHD-C4C	-3.62	118.25	126.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	16	302	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
38	14	306	KC1	C4C-C3C-C2C	-3.62	101.63	106.90
30	B	829	CLA	C1D-CHD-C4C	-3.62	118.26	126.06
30	2	313	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
38	2	312	KC1	C1A-NA-C4A	-3.61	105.08	106.71
30	A	832	CLA	C1D-CHD-C4C	-3.61	118.26	126.06
30	2	301	CLA	C1D-CHD-C4C	-3.61	118.26	126.06
37	5	301	A86	C4-C3-C2	-3.61	116.07	123.47
30	A	826	CLA	C3D-C4D-ND	3.61	116.08	110.24
30	B	823	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
30	B	823	CLA	C3D-C4D-ND	3.61	116.08	110.24
30	B	821	CLA	C3B-C4B-NB	3.61	113.88	109.21
39	8	316	DD6	C35-C36-C31	-3.61	112.37	120.57
30	9	307	CLA	C4A-NA-C1A	-3.61	105.08	106.71
29	A	801	CL0	CMA-C3A-C2A	-3.61	99.27	113.83
30	14	313	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
38	12	311	KC1	C1C-C2C-C3C	-3.61	103.16	106.96
37	3	314	A86	C23-C16-C17	-3.61	102.71	108.98
30	11	310	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
30	15	308	CLA	C1D-CHD-C4C	-3.61	118.28	126.06
30	J	101	CLA	C3C-C4C-NC	3.61	114.62	110.57
30	7	304	CLA	C1D-CHD-C4C	-3.61	118.28	126.06
39	7	302	DD6	C15-C14-C13	-3.61	118.37	125.99
30	1	301	CLA	C1C-C2C-C3C	-3.61	103.17	106.96
30	11	308	CLA	C3C-C4C-NC	3.61	114.61	110.57
39	16	313	DD6	O1-C20-C21	-3.60	110.74	115.06
30	10	308	CLA	C1D-CHD-C4C	-3.60	118.28	126.06
30	11	309	CLA	CMB-C2B-C3B	3.60	131.42	124.68
30	10	307	CLA	C3D-C4D-ND	3.60	116.06	110.24
30	F	201	CLA	CAA-C2A-C3A	-3.60	102.92	112.78
37	2u	203	A86	C4-C3-C2	-3.60	116.10	123.47
30	B	836	CLA	C1D-CHD-C4C	-3.60	118.29	126.06
30	A	809	CLA	CAC-C3C-C4C	3.60	129.48	124.81
30	7	311	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
30	B	851	CLA	C3C-C4C-NC	3.60	114.61	110.57
38	13	305	KC1	C1A-NA-C4A	-3.60	105.09	106.71
30	9	305	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
37	6	320	A86	C40-C32-C31	-3.60	107.25	110.47
30	A	809	CLA	C4A-NA-C1A	-3.60	105.09	106.71
30	6	316	CLA	CMB-C2B-C3B	3.59	131.40	124.68
30	A	844	CLA	C3C-C4C-NC	3.59	114.60	110.57
30	B	822	CLA	C1C-C2C-C3C	-3.59	103.18	106.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	812	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
38	4	310	KC1	C1C-C2C-C3C	-3.59	103.18	106.96
30	9	302	CLA	C4A-NA-C1A	-3.59	105.09	106.71
30	12	304	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
38	12	309	KC1	C4B-C3B-C2B	-3.59	103.80	106.75
30	9	301	CLA	C1D-CHD-C4C	-3.59	118.31	126.06
30	A	839	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
30	B	832	CLA	C3C-C4C-NC	3.59	114.60	110.57
37	9	313	A86	O1-C20-C21	-3.59	110.75	115.06
37	2	302	A86	C9-C8-C6	-3.59	116.33	126.42
30	9	307	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
30	A	803	CLA	C4A-NA-C1A	-3.59	105.09	106.71
38	4	307	KC1	C1A-NA-C4A	-3.59	105.09	106.71
30	15	306	CLA	C3B-C4B-NB	3.59	113.85	109.21
37	14	320	A86	C9-C10-C11	-3.59	116.06	126.61
30	6	305	CLA	C3C-C4C-NC	3.59	114.59	110.57
30	A	815	CLA	C1C-C2C-C3C	-3.59	103.19	106.96
30	B	832	CLA	C1C-C2C-C3C	-3.59	103.19	106.96
38	8	310	KC1	C4C-C3C-C2C	-3.59	101.67	106.90
30	9	303	CLA	CMB-C2B-C3B	3.59	131.39	124.68
37	11	316	A86	C25-C24-C1	-3.59	116.34	126.42
30	B	821	CLA	C3C-C4C-NC	3.59	114.59	110.57
38	4	307	KC1	CBA-CAA-C2A	-3.58	111.60	125.27
38	14	308	KC1	C4C-C3C-C2C	-3.58	101.67	106.90
30	12	321	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
29	A	801	CL0	C3B-C4B-NB	3.58	113.84	109.21
39	10	313	DD6	C14-C13-C11	3.58	131.09	125.53
30	6	307	CLA	C3C-C4C-NC	3.58	114.59	110.57
39	4	316	DD6	C12-C11-C13	-3.58	112.44	118.08
30	B	802	CLA	CAC-C3C-C4C	3.58	129.46	124.81
30	12	307	CLA	CMB-C2B-C3B	3.58	131.38	124.68
30	A	827	CLA	CHD-C4C-NC	3.58	129.84	124.20
30	L	203	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
30	14	305	CLA	C1D-CHD-C4C	-3.58	118.34	126.06
30	1	304	CLA	CMC-C2C-C1C	3.58	130.49	125.04
30	B	804	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
30	A	820	CLA	C3C-C4C-NC	3.58	114.58	110.57
34	5	317	LHG	O8-C23-C24	3.58	120.76	111.38
30	8	301	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
30	A	825	CLA	C1D-CHD-C4C	-3.58	118.34	126.06
38	13	311	KC1	CAA-CBA-CGA	-3.58	108.88	127.26
30	F	202	CLA	C3B-C4B-NB	3.57	113.83	109.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	806	CLA	C3B-C4B-NB	3.57	113.83	109.21
30	A	815	CLA	C3C-C4C-NC	3.57	114.58	110.57
30	B	830	CLA	CAC-C3C-C4C	3.57	129.44	124.81
30	1	302	CLA	C3C-C4C-NC	3.57	114.58	110.57
30	5	304	CLA	C1D-CHD-C4C	-3.57	118.36	126.06
30	B	834	CLA	C3D-C4D-ND	3.57	116.01	110.24
30	16	301	CLA	C4A-NA-C1A	-3.57	105.10	106.71
30	12	302	CLA	O2A-CGA-CBA	3.57	123.11	111.91
30	15	304	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
38	8	310	KC1	C4B-C3B-C2B	-3.57	103.82	106.75
30	2	309	CLA	O2D-CGD-CBD	3.57	117.61	111.27
30	14	304	CLA	C1C-C2C-C3C	-3.57	103.21	106.96
30	B	805	CLA	C1D-CHD-C4C	-3.57	118.36	126.06
30	14	303	CLA	C3C-C4C-NC	3.57	114.57	110.57
30	B	806	CLA	O2D-CGD-CBD	3.56	117.60	111.27
38	2	314	KC1	C4B-C3B-C2B	-3.56	103.83	106.75
30	1	307	CLA	C4A-NA-C1A	-3.56	105.10	106.71
38	10	312	KC1	CBA-CAA-C2A	-3.56	111.69	125.27
30	B	829	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
30	B	816	CLA	C4A-NA-C1A	-3.56	105.11	106.71
30	4	301	CLA	C1D-CHD-C4C	-3.56	118.38	126.06
30	B	851	CLA	CAC-C3C-C4C	3.56	129.43	124.81
38	12	313	KC1	C1A-C2A-C3A	3.56	109.94	107.11
30	15	309	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
37	10	302	A86	C12-C11-C13	3.56	122.00	116.02
30	A	805	CLA	C1D-CHD-C4C	-3.56	118.38	126.06
39	8	316	DD6	C12-C11-C13	-3.56	112.47	118.08
39	15	319	DD6	C23-C16-C15	3.56	119.65	110.05
38	8	314	KC1	C4B-C3B-C2B	-3.56	103.83	106.75
38	12	313	KC1	C4B-C3B-C2B	-3.56	103.83	106.75
30	9	309	CLA	C3B-C4B-NB	3.56	113.81	109.21
30	B	807	CLA	C1D-CHD-C4C	-3.56	118.39	126.06
38	9	310	KC1	C1C-C2C-C3C	-3.56	103.22	106.96
30	7	312	CLA	C3C-C4C-NC	3.56	114.56	110.57
30	10	303	CLA	C3C-C4C-NC	3.56	114.56	110.57
38	3	304	KC1	CBA-CAA-C2A	-3.55	111.72	125.27
30	A	843	CLA	C4A-NA-C1A	-3.55	105.11	106.71
30	13	307	CLA	C3C-C4C-NC	3.55	114.56	110.57
30	6	310	CLA	C3C-C4C-NC	3.55	114.56	110.57
30	A	843	CLA	C1D-CHD-C4C	-3.55	118.40	126.06
37	4	314	A86	C35-C34-C33	3.55	116.07	109.88
30	15	308	CLA	C4C-C3C-C2C	-3.55	101.72	106.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	13	306	KC1	CAC-C3C-C4C	3.55	129.42	124.81
30	15	306	CLA	O2D-CGD-O1D	-3.55	116.90	123.84
30	13	304	CLA	C3B-C4B-NB	3.55	113.80	109.21
39	5	314	DD6	C15-C14-C13	-3.55	118.49	125.99
30	2	310	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
38	7	313	KC1	C1C-C2C-C3C	-3.55	103.22	106.96
39	16	313	DD6	C23-C16-C17	-3.55	102.82	108.98
39	12	315	DD6	C21-C20-C15	-3.55	116.31	122.26
38	1	306	KC1	CAC-C3C-C4C	3.55	129.41	124.81
30	A	817	CLA	C4A-NA-C1A	-3.55	105.11	106.71
30	B	822	CLA	O2A-CGA-CBA	3.54	123.03	111.91
30	A	830	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
30	10	309	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
30	4	304	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
30	B	812	CLA	CAC-C3C-C4C	3.54	129.41	124.81
30	A	822	CLA	C1D-CHD-C4C	-3.54	118.42	126.06
30	14	312	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
30	B	805	CLA	CHB-C4A-NA	3.54	129.40	124.51
30	B	803	CLA	CAA-C2A-C3A	-3.54	103.09	112.78
30	B	811	CLA	C3D-C2D-C1D	-3.54	101.00	105.83
30	16	305	CLA	CAA-C2A-C3A	-3.54	103.09	112.78
30	11	309	CLA	C3C-C4C-NC	3.54	114.54	110.57
30	A	815	CLA	CHC-C1C-C2C	-3.54	116.94	126.72
38	7	308	KC1	CBA-CAA-C2A	-3.53	111.79	125.27
38	9	304	KC1	C4B-C3B-C2B	-3.53	103.85	106.75
30	B	814	CLA	C3B-C4B-NB	3.53	113.78	109.21
38	9	311	KC1	C4B-C3B-C2B	-3.53	103.85	106.75
38	11	307	KC1	C1A-NA-C4A	-3.53	105.12	106.71
30	9	302	CLA	C1D-CHD-C4C	-3.53	118.44	126.06
30	B	827	CLA	C1C-C2C-C3C	-3.53	103.24	106.96
30	7	311	CLA	CAC-C3C-C4C	3.53	129.39	124.81
30	B	822	CLA	C1D-CHD-C4C	-3.53	118.44	126.06
39	12	317	DD6	C21-C20-C15	-3.53	116.34	122.26
38	5	305	KC1	C4B-C3B-C2B	-3.53	103.85	106.75
30	B	835	CLA	C1D-CHD-C4C	-3.53	118.45	126.06
39	6	303	DD6	C33-C34-C35	3.53	115.13	110.30
30	B	814	CLA	C1C-C2C-C3C	-3.53	103.25	106.96
38	9	311	KC1	CAA-C2A-C1A	-3.53	108.53	124.75
38	5	310	KC1	C1C-C2C-C3C	-3.53	103.25	106.96
38	14	311	KC1	CMB-C2B-C1B	3.53	130.93	124.71
30	A	804	CLA	CAA-C2A-C3A	-3.53	103.12	112.78
30	A	829	CLA	CMB-C2B-C3B	3.52	131.27	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	802	CLA	C4C-C3C-C2C	-3.52	101.76	106.90
30	8	301	CLA	CMC-C2C-C1C	3.52	130.40	125.04
37	7	319	A86	C7-C6-C5	-3.52	117.99	122.92
30	A	838	CLA	C3B-C4B-NB	3.52	113.76	109.21
30	7	303	CLA	O2A-CGA-CBA	3.52	122.95	111.91
30	B	808	CLA	C3B-C4B-NB	3.52	113.76	109.21
30	2	301	CLA	CHC-C1C-C2C	-3.52	116.99	126.72
33	A	850	BCR	C2-C1-C6	3.52	115.89	110.48
30	4	309	CLA	C3C-C4C-NC	3.52	114.52	110.57
37	10	317	A86	C36-C31-C32	-3.52	116.21	119.70
37	10	301	A86	C22-C16-C17	-3.52	102.87	108.98
37	1	309	A86	C35-C34-C33	3.51	116.01	109.88
30	15	309	CLA	O2D-CGD-CBD	3.51	117.51	111.27
30	5	307	CLA	C3D-C4D-ND	3.51	115.92	110.24
30	A	810	CLA	C1D-CHD-C4C	-3.51	118.48	126.06
30	4	306	CLA	C1C-C2C-C3C	-3.51	103.26	106.96
33	2u	201	BCR	C15-C16-C17	-3.51	116.28	123.47
30	A	824	CLA	C1-C2-C3	-3.51	119.97	126.04
30	B	815	CLA	CAC-C3C-C4C	3.51	129.37	124.81
30	B	830	CLA	C4C-C3C-C2C	-3.51	101.78	106.90
38	8	314	KC1	C1C-C2C-C3C	-3.51	103.27	106.96
38	11	305	KC1	CAA-CBA-CGA	-3.51	109.22	127.26
38	10	306	KC1	CAA-CBA-CGA	-3.51	109.22	127.26
30	4	311	CLA	C3C-C4C-NC	3.51	114.51	110.57
30	15	302	CLA	O2D-CGD-O1D	-3.51	116.98	123.84
30	7	310	CLA	C1C-C2C-C3C	-3.50	103.27	106.96
30	8	301	CLA	CMB-C2B-C3B	3.50	131.23	124.68
36	F	205	LMG	O6-C1-O1	-3.50	101.68	109.97
30	9	305	CLA	CBA-CAA-C2A	3.50	124.20	113.86
38	9	304	KC1	CBA-CAA-C2A	-3.50	111.92	125.27
30	16	301	CLA	C1C-C2C-C3C	-3.50	103.28	106.96
30	2	304	CLA	CMB-C2B-C3B	3.50	131.23	124.68
30	B	813	CLA	C1D-CHD-C4C	-3.50	118.51	126.06
30	4	309	CLA	CAA-C2A-C3A	-3.50	103.20	112.78
30	2	303	CLA	CHB-C4A-NA	3.50	129.35	124.51
34	2	320	LHG	O8-C23-C24	3.50	120.56	111.38
30	B	828	CLA	C3D-C2D-C1D	-3.50	101.06	105.83
30	B	835	CLA	C1C-C2C-C3C	-3.50	103.28	106.96
38	8	307	KC1	CBA-CAA-C2A	-3.50	111.94	125.27
30	7	304	CLA	C3C-C4C-NC	3.50	114.49	110.57
37	10	302	A86	C3-C2-C1	-3.50	122.32	127.31
30	B	811	CLA	CMA-C3A-C2A	-3.50	99.73	113.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	7	314	DD6	C22-C16-C15	3.49	119.48	110.05
38	5	312	KC1	CAA-CBA-CGA	-3.49	109.30	127.26
37	9	313	A86	C35-C34-C33	3.49	115.97	109.88
30	A	820	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
38	14	308	KC1	C1C-C2C-C3C	-3.49	103.29	106.96
37	15	323	A86	C9-C10-C11	-3.49	116.35	126.61
30	2	310	CLA	CMB-C2B-C3B	3.49	131.21	124.68
39	7	314	DD6	C7-C6-C8	-3.49	112.58	118.08
30	13	301	CLA	C1-C2-C3	-3.49	120.01	126.04
39	8	316	DD6	O1-C20-C21	-3.49	110.88	115.06
30	16	306	CLA	CMB-C2B-C3B	3.49	131.21	124.68
37	8	315	A86	C24-C1-C2	-3.49	113.59	118.94
30	A	820	CLA	CBA-CAA-C2A	3.49	124.16	113.86
30	B	823	CLA	CAC-C3C-C4C	3.49	129.34	124.81
30	A	832	CLA	C1C-C2C-C3C	-3.49	103.29	106.96
30	13	301	CLA	C1C-C2C-C3C	-3.49	103.29	106.96
38	2	306	KC1	CBA-CAA-C2A	-3.48	111.99	125.27
30	7	310	CLA	C1D-CHD-C4C	-3.48	118.55	126.06
30	F	202	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
37	4	315	A86	C4-C3-C2	-3.48	116.34	123.47
30	14	303	CLA	CAA-C2A-C3A	-3.48	103.25	112.78
30	2	311	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
30	7	306	CLA	CAC-C3C-C4C	3.48	129.32	124.81
30	A	810	CLA	O2A-CGA-CBA	3.48	122.83	111.91
38	5	306	KC1	C1C-C2C-C3C	-3.48	103.30	106.96
38	8	312	KC1	C1C-C2C-C3C	-3.48	103.30	106.96
30	11	310	CLA	C3C-C4C-NC	3.48	114.47	110.57
38	11	312	KC1	CAC-C3C-C4C	3.48	129.32	124.81
30	2	304	CLA	C3B-C4B-NB	3.47	113.70	109.21
30	9	306	CLA	C3B-C4B-NB	3.47	113.70	109.21
37	11	301	A86	C40-C32-C31	-3.47	107.36	110.47
30	10	303	CLA	C1-C2-C3	-3.47	120.04	126.04
30	B	816	CLA	C3B-C4B-NB	3.47	113.70	109.21
30	1	307	CLA	C3B-C4B-NB	3.47	113.70	109.21
38	14	311	KC1	C4B-C3B-C2B	-3.47	103.90	106.75
39	3	313	DD6	C13-C11-C10	-3.47	113.62	118.94
30	B	838	CLA	C4-C3-C5	3.47	121.11	115.27
30	B	808	CLA	O2A-CGA-CBA	3.47	122.79	111.91
38	5	305	KC1	CAA-CBA-CGA	-3.47	109.44	127.26
30	A	809	CLA	C3B-C4B-NB	3.47	113.69	109.21
30	A	807	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
30	16	303	CLA	C1C-C2C-C3C	-3.47	103.31	106.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	8	310	KC1	C2C-C1C-NC	3.47	114.36	110.57
37	12	314	A86	C41-C32-C31	-3.46	107.37	110.47
37	7	316	A86	C25-C26-C27	-3.46	122.36	127.31
30	6	307	CLA	CAA-C2A-C3A	-3.46	103.29	112.78
30	16	309	CLA	C3B-C4B-NB	3.46	113.69	109.21
38	5	306	KC1	CAA-CBA-CGA	-3.46	109.47	127.26
30	8	305	CLA	C1-C2-C3	-3.46	120.06	126.04
37	14	315	A86	C25-C26-C27	-3.46	122.37	127.31
30	A	815	CLA	CMB-C2B-C3B	3.46	131.15	124.68
30	4	302	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
30	10	308	CLA	CAC-C3C-C4C	3.46	129.30	124.81
37	14	317	A86	C4-C3-C2	-3.46	116.39	123.47
30	B	838	CLA	CHC-C1C-C2C	-3.46	117.16	126.72
30	13	303	CLA	C3C-C4C-NC	3.46	114.45	110.57
37	10	301	A86	C3-C2-C1	-3.46	122.38	127.31
38	7	313	KC1	CAA-CBA-CGA	-3.45	109.51	127.26
30	2	301	CLA	C3C-C4C-NC	3.45	114.44	110.57
30	15	305	CLA	C3B-C4B-NB	3.45	113.67	109.21
30	12	304	CLA	C3C-C4C-NC	3.45	114.44	110.57
30	A	825	CLA	C3C-C4C-NC	3.45	114.44	110.57
30	11	309	CLA	O2A-CGA-CBA	3.45	122.74	111.91
30	B	816	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
30	14	307	CLA	C1D-CHD-C4C	-3.45	118.62	126.06
37	15	321	A86	C41-C32-C31	-3.45	107.39	110.47
30	7	312	CLA	C3B-C4B-NB	3.45	113.67	109.21
30	B	812	CLA	C4A-NA-C1A	-3.45	105.16	106.71
30	12	321	CLA	C3C-C4C-NC	3.45	114.44	110.57
37	14	314	A86	C7-C6-C5	-3.45	118.10	122.92
30	B	830	CLA	C1-O2A-CGA	3.44	125.48	116.44
30	6	305	CLA	CMB-C2B-C3B	3.44	131.12	124.68
30	3	301	CLA	C3B-C4B-NB	3.44	113.66	109.21
30	A	819	CLA	C4C-C3C-C2C	-3.44	101.88	106.90
30	A	811	CLA	C4A-NA-C1A	-3.44	105.16	106.71
37	2	319	A86	C41-C32-C31	-3.44	107.40	110.47
30	B	818	CLA	C3C-C4C-NC	3.44	114.42	110.57
30	5	304	CLA	O2A-CGA-CBA	3.43	122.68	111.91
30	A	809	CLA	CMB-C2B-C3B	3.43	131.10	124.68
30	2	308	CLA	CMC-C2C-C1C	3.43	130.26	125.04
30	3	306	CLA	CAA-C2A-C3A	-3.43	103.39	112.78
38	8	306	KC1	C1A-NA-C4A	-3.43	105.16	106.71
34	6	322	LHG	O8-C23-C24	3.43	120.37	111.38
30	11	304	CLA	C1C-C2C-C3C	-3.43	103.35	106.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	7	303	CLA	C1C-C2C-C3C	-3.43	103.35	106.96
30	2	301	CLA	C3B-C4B-NB	3.43	113.64	109.21
37	8	315	A86	C26-C25-C24	-3.42	112.53	123.22
30	B	822	CLA	C3C-C4C-NC	3.42	114.41	110.57
30	A	835	CLA	CAA-C2A-C3A	-3.42	103.40	112.78
30	B	801	CLA	C4C-C3C-C2C	-3.42	101.91	106.90
30	5	302	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
30	B	826	CLA	C3B-C4B-NB	3.42	113.63	109.21
30	A	842	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
37	2	302	A86	C12-C11-C13	3.42	121.77	116.02
30	6	317	CLA	CAA-C2A-C3A	-3.42	103.41	112.78
30	8	305	CLA	C3B-C4B-NB	3.42	113.63	109.21
30	A	806	CLA	C4C-C3C-C2C	-3.42	101.91	106.90
38	13	312	KC1	CAA-CBA-CGA	-3.42	109.69	127.26
38	11	307	KC1	CAA-CBA-CGA	-3.42	109.69	127.26
39	3	313	DD6	C35-C36-C31	-3.42	112.81	120.57
30	A	806	CLA	CAA-CBA-CGA	-3.42	103.27	113.25
30	6	309	CLA	CMB-C2B-C3B	3.42	131.07	124.68
37	11	316	A86	C3-C2-C1	-3.42	122.43	127.31
30	B	824	CLA	C1D-CHD-C4C	-3.42	118.69	126.06
30	11	309	CLA	C3B-C4B-NB	3.42	113.63	109.21
30	3	306	CLA	C1D-CHD-C4C	-3.42	118.69	126.06
30	A	825	CLA	C3B-C4B-NB	3.41	113.62	109.21
30	A	832	CLA	O2D-CGD-O1D	-3.41	117.16	123.84
30	B	819	CLA	C1C-C2C-C3C	-3.41	103.37	106.96
30	7	309	CLA	C3B-C4B-NB	3.41	113.62	109.21
31	B	840	PQN	C11-C12-C13	-3.41	121.11	126.79
30	6	314	CLA	C3C-C4C-NC	3.41	114.40	110.57
30	A	820	CLA	CAC-C3C-C4C	3.41	129.24	124.81
30	B	837	CLA	C1C-C2C-C3C	-3.41	103.37	106.96
30	14	302	CLA	C1C-C2C-C3C	-3.41	103.37	106.96
37	7	319	A86	C4-C5-C6	-3.41	122.44	127.31
39	7	318	DD6	O1-C20-C21	-3.41	110.97	115.06
38	6	313	KC1	CAA-C2A-C1A	-3.41	109.08	124.75
30	A	821	CLA	C4A-NA-C1A	-3.41	105.17	106.71
39	12	315	DD6	C25-C24-C1	-3.41	116.84	126.42
38	12	305	KC1	CBA-CAA-C2A	-3.41	112.28	125.27
30	A	821	CLA	C3B-C4B-NB	3.41	113.61	109.21
30	15	308	CLA	O2A-CGA-CBA	3.41	124.97	114.03
30	12	321	CLA	C3B-C4B-NB	3.41	113.61	109.21
30	A	826	CLA	O2D-CGD-O1D	-3.41	117.18	123.84
30	15	302	CLA	CMB-C2B-C3B	3.40	131.05	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	11	309	CLA	C1C-C2C-C3C	-3.40	103.38	106.96
30	L	202	CLA	C3B-C4B-NB	3.40	113.61	109.21
30	A	830	CLA	CMC-C2C-C1C	3.40	130.22	125.04
30	2	311	CLA	C4A-NA-C1A	-3.40	105.18	106.71
30	A	816	CLA	C1C-C2C-C3C	-3.40	103.38	106.96
30	A	833	CLA	C1D-CHD-C4C	-3.40	118.72	126.06
37	14	319	A86	C34-O4-C38	-3.40	111.56	117.90
30	A	814	CLA	C3B-C4B-NB	3.40	113.61	109.21
30	A	808	CLA	C4A-NA-C1A	-3.40	105.18	106.71
30	6	305	CLA	C3B-C4B-NB	3.40	113.60	109.21
30	10	303	CLA	C1C-C2C-C3C	-3.40	103.38	106.96
39	5	313	DD6	C15-C14-C13	-3.40	118.81	125.99
30	A	818	CLA	CMC-C2C-C1C	3.40	130.21	125.04
38	3	308	KC1	CAC-C3C-C4C	3.40	129.22	124.81
30	3	310	CLA	C3B-C4B-NB	3.40	113.60	109.21
30	B	826	CLA	CAA-C2A-C3A	-3.40	103.48	112.78
30	12	307	CLA	CAA-C2A-C3A	-3.40	103.48	112.78
30	16	310	CLA	CAA-C2A-C3A	-3.39	103.49	112.78
30	1	305	CLA	C3B-C4B-NB	3.39	113.60	109.21
30	8	304	CLA	CAA-C2A-C1A	-3.39	100.86	111.97
30	2	303	CLA	CAC-C3C-C4C	3.39	129.21	124.81
39	3	312	DD6	C15-C14-C13	-3.39	118.83	125.99
30	15	302	CLA	C1C-C2C-C3C	-3.39	103.39	106.96
30	B	829	CLA	CAA-C2A-C3A	-3.39	103.50	112.78
37	8	315	A86	C3-C4-C5	-3.39	116.53	123.47
37	1	309	A86	C36-C31-C32	-3.39	116.33	119.70
30	9	303	CLA	C3B-C4B-NB	3.39	113.59	109.21
30	A	828	CLA	CHD-C4C-NC	3.39	129.54	124.20
30	A	811	CLA	C3B-C4B-NB	3.39	113.59	109.21
38	8	311	KC1	C1C-C2C-C3C	-3.38	103.40	106.96
39	6	321	DD6	C33-C32-C31	3.38	116.47	109.62
38	9	304	KC1	CAA-CBA-CGA	-3.38	109.88	127.26
30	B	817	CLA	C4C-C3C-C2C	-3.38	101.97	106.90
30	8	302	CLA	C3B-C4B-NB	3.38	113.58	109.21
38	4	308	KC1	CMA-C3A-C2A	-3.38	120.03	128.30
38	16	311	KC1	C4B-C3B-C2B	-3.38	103.98	106.75
30	5	304	CLA	C3B-C4B-NB	3.38	113.58	109.21
30	14	307	CLA	C4C-C3C-C2C	-3.38	101.98	106.90
37	8	315	A86	C4-C3-C2	-3.38	116.56	123.47
30	15	311	CLA	C3B-C4B-NB	3.38	113.57	109.21
29	A	801	CL0	C4A-NA-C1A	-3.37	105.19	106.71
39	10	313	DD6	C3-C4-C5	-3.37	116.56	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	L	202	CLA	C1D-CHD-C4C	-3.37	118.78	126.06
30	B	825	CLA	C4C-C3C-C2C	-3.37	101.98	106.90
30	B	825	CLA	CMB-C2B-C3B	3.37	130.99	124.68
30	B	809	CLA	C3B-C4B-NB	3.37	113.57	109.21
38	10	312	KC1	CAA-CBA-CGA	-3.37	109.93	127.26
30	A	820	CLA	CMB-C2B-C3B	3.37	130.99	124.68
37	5	301	A86	C35-C34-C33	3.37	115.76	109.88
30	6	306	CLA	C1C-C2C-C3C	-3.37	103.41	106.96
30	B	807	CLA	C3B-C4B-NB	3.37	113.57	109.21
30	B	827	CLA	C3B-C4B-NB	3.37	113.57	109.21
39	12	315	DD6	C35-C36-C31	-3.37	112.92	120.57
30	8	304	CLA	C4C-C3C-C2C	-3.37	101.98	106.90
30	A	806	CLA	C4A-NA-C1A	-3.37	105.19	106.71
30	3	303	CLA	C4A-NA-C1A	-3.37	105.19	106.71
30	B	812	CLA	C3B-C4B-NB	3.37	113.57	109.21
30	16	305	CLA	C3B-C4B-NB	3.37	113.57	109.21
30	3	309	CLA	CAA-C2A-C3A	-3.37	103.55	112.78
30	12	302	CLA	CAA-C2A-C1A	-3.37	100.94	111.97
30	A	826	CLA	CAC-C3C-C4C	3.37	129.18	124.81
30	14	302	CLA	C3C-C4C-NC	3.37	114.35	110.57
30	2	305	CLA	O2D-CGD-O1D	-3.37	117.26	123.84
30	9	305	CLA	C3B-C4B-NB	3.37	113.56	109.21
30	6	304	CLA	C3C-C4C-NC	3.37	114.35	110.57
30	6	316	CLA	C1C-C2C-C3C	-3.37	103.42	106.96
30	A	817	CLA	C3C-C4C-NC	3.36	114.34	110.57
30	15	303	CLA	C4-C3-C5	3.36	120.93	115.27
30	6	310	CLA	C3B-C4B-NB	3.36	113.56	109.21
30	B	813	CLA	CAC-C3C-C4C	3.36	129.17	124.81
30	A	813	CLA	C3B-C4B-NB	3.36	113.56	109.21
30	2	308	CLA	C1-C2-C3	-3.36	120.23	126.04
30	10	308	CLA	C3C-C4C-NC	3.36	114.34	110.57
30	4	306	CLA	C4A-NA-C1A	-3.36	105.20	106.71
30	B	801	CLA	C3B-C4B-NB	3.36	113.55	109.21
30	B	821	CLA	CMB-C2B-C3B	3.36	130.96	124.68
30	13	309	CLA	C3B-C4B-NB	3.36	113.55	109.21
30	A	819	CLA	CMB-C2B-C3B	3.36	130.96	124.68
39	4	313	DD6	C35-C36-C31	-3.36	112.95	120.57
30	15	305	CLA	CAC-C3C-C4C	3.36	129.16	124.81
38	5	306	KC1	C4B-C3B-C2B	-3.36	104.00	106.75
30	13	301	CLA	CAC-C3C-C4C	3.35	129.16	124.81
30	A	828	CLA	C3B-C4B-NB	3.35	113.55	109.21
30	B	801	CLA	CMA-C3A-C4A	-3.35	102.76	111.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	10	307	CLA	C1C-C2C-C3C	-3.35	103.43	106.96
38	1	306	KC1	CBA-CAA-C2A	-3.35	112.49	125.27
38	8	310	KC1	C1A-NA-C4A	-3.35	105.20	106.71
37	6	320	A86	C36-C31-C32	-3.35	116.37	119.70
30	A	824	CLA	CMA-C3A-C2A	-3.35	100.31	113.83
38	1	306	KC1	CAA-CBA-CGA	-3.35	110.04	127.26
30	A	817	CLA	C3B-C4B-NB	3.35	113.54	109.21
30	A	836	CLA	CAC-C3C-C4C	3.35	129.16	124.81
30	12	321	CLA	O2D-CGD-CBD	3.35	117.22	111.27
38	9	304	KC1	CAC-C3C-C4C	3.35	129.15	124.81
30	A	820	CLA	C3B-C4B-NB	3.35	113.54	109.21
30	9	302	CLA	CAC-C3C-C4C	3.35	129.15	124.81
30	6	314	CLA	CAA-C2A-C3A	-3.35	103.61	112.78
31	A	845	PQN	C14-C13-C15	3.35	120.90	115.27
30	A	805	CLA	CMC-C2C-C1C	3.34	130.13	125.04
30	A	831	CLA	C4C-C3C-C2C	-3.34	102.03	106.90
30	B	802	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
30	3	307	CLA	C3B-C4B-NB	3.34	113.53	109.21
30	13	303	CLA	C3B-C4B-NB	3.34	113.53	109.21
30	6	306	CLA	C1-O2A-CGA	3.34	125.20	116.44
38	12	309	KC1	C2A-C1A-NA	3.34	114.75	109.40
38	8	314	KC1	CGD-CBD-CAD	-3.34	99.92	110.73
30	B	824	CLA	C1C-C2C-C3C	-3.34	103.45	106.96
39	4	313	DD6	C25-C24-C1	-3.34	117.04	126.42
30	B	831	CLA	C3B-C4B-NB	3.34	113.52	109.21
30	12	304	CLA	C3B-C4B-NB	3.34	113.52	109.21
30	B	819	CLA	C4C-C3C-C2C	-3.33	102.04	106.90
30	B	818	CLA	CMC-C2C-C1C	3.33	130.12	125.04
30	8	309	CLA	C3B-C4B-NB	3.33	113.52	109.21
30	14	309	CLA	C3B-C4B-NB	3.33	113.52	109.21
30	15	303	CLA	O2A-CGA-CBA	3.33	122.36	111.91
30	13	301	CLA	CMC-C2C-C1C	3.33	130.11	125.04
30	B	811	CLA	C3B-C4B-NB	3.33	113.52	109.21
30	15	312	CLA	C3B-C4B-NB	3.33	113.52	109.21
30	13	309	CLA	CAA-C2A-C3A	-3.33	103.66	112.78
38	6	312	KC1	CAA-CBA-CGA	-3.33	110.15	127.26
37	14	316	A86	C12-C11-C13	3.33	121.61	116.02
30	4	303	CLA	C1C-C2C-C3C	-3.33	103.46	106.96
30	1	304	CLA	CAC-C3C-C4C	3.33	129.13	124.81
38	9	311	KC1	CBA-CAA-C2A	-3.33	112.58	125.27
38	8	307	KC1	CMB-C2B-C1B	3.33	130.58	124.71
39	7	317	DD6	C37-C36-C35	-3.33	108.19	114.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	818	CLA	C3B-C4B-NB	3.33	113.51	109.21
30	12	302	CLA	C3B-C4B-NB	3.33	113.51	109.21
37	1	309	A86	C8-C6-C5	3.33	124.05	118.94
30	A	837	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
30	7	306	CLA	C3B-C4B-NB	3.33	113.51	109.21
30	7	306	CLA	C4A-NA-C1A	-3.33	105.21	106.71
30	4	309	CLA	C3B-C4B-NB	3.33	113.51	109.21
30	B	814	CLA	CMB-C2B-C3B	3.32	130.90	124.68
37	16	312	A86	C40-C32-C31	-3.32	107.50	110.47
30	B	834	CLA	C4C-C3C-C2C	-3.32	102.05	106.90
30	B	805	CLA	CAC-C3C-C4C	3.32	129.12	124.81
38	13	308	KC1	CAA-CBA-CGA	-3.32	110.18	127.26
30	A	836	CLA	C3B-C4B-NB	3.32	113.51	109.21
39	6	321	DD6	C21-C20-C19	-3.32	110.54	114.28
30	B	806	CLA	CHD-C4C-NC	3.32	129.44	124.20
30	4	303	CLA	C1D-CHD-C4C	-3.32	118.89	126.06
39	2	317	DD6	C33-C34-C35	3.32	114.85	110.30
30	F	201	CLA	C4C-C3C-C2C	-3.32	102.06	106.90
30	15	304	CLA	C4C-C3C-C2C	-3.32	102.06	106.90
30	5	303	CLA	C4-C3-C5	3.32	120.85	115.27
38	5	306	KC1	CBA-CAA-C2A	-3.32	112.62	125.27
30	B	839	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
30	3	307	CLA	C4C-C3C-C2C	-3.32	102.06	106.90
30	16	308	CLA	C3B-C4B-NB	3.32	113.50	109.21
30	9	306	CLA	CHC-C1C-C2C	-3.32	117.54	126.72
30	12	306	CLA	C3B-C4B-NB	3.32	113.50	109.21
35	9	317	LMT	C1'-C2'-C3'	3.32	116.90	110.00
30	3	303	CLA	CBA-CAA-C2A	3.31	123.65	113.86
39	4	313	DD6	C37-C36-C35	-3.31	108.22	114.36
39	3	312	DD6	O1-C20-C21	-3.31	111.09	115.06
39	4	316	DD6	C35-C36-C31	-3.31	113.05	120.57
30	A	831	CLA	CAC-C3C-C4C	3.31	129.11	124.81
39	10	314	DD6	C19-C18-C17	3.31	117.17	110.77
30	5	309	CLA	C3B-C4B-NB	3.31	113.49	109.21
30	2	301	CLA	C4A-NA-C1A	-3.31	105.22	106.71
38	14	311	KC1	CAA-CBA-CGA	-3.31	110.25	127.26
30	4	302	CLA	C1-C2-C3	-3.31	120.32	126.04
33	I	101	BCR	C31-C1-C6	3.31	115.67	110.30
30	16	308	CLA	CAC-C3C-C4C	3.31	129.10	124.81
30	9	301	CLA	C4C-C3C-C2C	-3.31	102.07	106.90
38	8	306	KC1	CAA-CBA-CGA	-3.31	110.25	127.26
30	14	309	CLA	CHC-C1C-C2C	-3.31	117.57	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	826	CLA	C4C-C3C-C2C	-3.31	102.08	106.90
30	15	309	CLA	C3B-C4B-NB	3.31	113.48	109.21
39	1	310	DD6	C37-C36-C35	-3.31	108.23	114.36
38	12	311	KC1	CAC-C3C-C4C	3.31	129.10	124.81
38	8	310	KC1	CHD-C4C-NC	3.31	129.22	124.20
38	3	311	KC1	CAA-CBA-CGA	-3.30	110.28	127.26
30	B	827	CLA	CAC-C3C-C4C	3.30	129.10	124.81
30	8	305	CLA	C1C-C2C-C3C	-3.30	103.48	106.96
38	6	308	KC1	CAA-CBA-CGA	-3.30	110.28	127.26
30	14	313	CLA	CAA-C2A-C3A	-3.30	103.73	112.78
30	B	809	CLA	CAC-C3C-C4C	3.30	129.09	124.81
39	10	313	DD6	C7-C6-C8	-3.30	112.88	118.08
38	2	306	KC1	C4B-C3B-C2B	-3.30	104.04	106.75
37	9	313	A86	O1-C15-C14	-3.30	106.59	113.21
30	16	306	CLA	C4C-C3C-C2C	-3.30	102.09	106.90
30	B	802	CLA	CMB-C2B-C3B	3.30	130.85	124.68
30	9	301	CLA	C4A-NA-C1A	-3.30	105.22	106.71
30	B	810	CLA	C1C-C2C-C3C	-3.30	103.49	106.96
39	3	312	DD6	C21-C20-C15	-3.30	116.74	122.26
38	2	314	KC1	CAA-CBA-CGA	-3.30	110.33	127.26
30	A	829	CLA	C3B-C4B-NB	3.30	113.47	109.21
30	6	315	CLA	C3B-C4B-NB	3.30	113.47	109.21
30	9	307	CLA	C4-C3-C5	3.30	120.81	115.27
38	13	310	KC1	CHB-C1B-NB	-3.29	121.43	124.45
30	F	202	CLA	C4C-C3C-C2C	-3.29	102.10	106.90
38	13	305	KC1	CAC-C3C-C4C	3.29	129.08	124.81
30	3	310	CLA	C3C-C4C-NC	3.29	114.27	110.57
30	15	307	CLA	C3B-C4B-NB	3.29	113.47	109.21
39	12	317	DD6	C15-C14-C13	3.29	132.96	125.99
38	12	309	KC1	C1A-NA-C4A	-3.29	105.23	106.71
30	B	809	CLA	CHC-C1C-C2C	-3.29	117.62	126.72
30	9	309	CLA	CHC-C1C-C2C	-3.29	117.62	126.72
30	4	311	CLA	C3B-C4B-NB	3.29	113.46	109.21
30	A	841	CLA	C1C-C2C-C3C	-3.29	103.50	106.96
38	13	306	KC1	C4C-C3C-C2C	-3.29	102.11	106.90
30	B	839	CLA	CHD-C4C-NC	3.29	129.38	124.20
30	5	311	CLA	C1-O2A-CGA	3.29	125.07	116.44
30	A	804	CLA	C4C-C3C-C2C	-3.29	102.11	106.90
30	8	303	CLA	CAA-C2A-C3A	-3.29	103.78	112.78
30	B	806	CLA	C4-C3-C5	3.29	120.80	115.27
30	2	305	CLA	C3B-C4B-NB	3.29	113.46	109.21
30	B	823	CLA	O2D-CGD-O1D	-3.28	117.42	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	834	CLA	C3B-C4B-NB	3.28	113.46	109.21
30	2	308	CLA	C1C-C2C-C3C	-3.28	103.50	106.96
30	9	302	CLA	C3B-C4B-NB	3.28	113.45	109.21
39	6	318	DD6	C25-C24-C1	-3.28	117.19	126.42
37	13	313	A86	C25-C26-C27	3.28	131.99	127.31
30	14	302	CLA	C4-C3-C5	3.28	120.79	115.27
30	4	311	CLA	CBC-CAC-C3C	-3.28	103.39	112.43
30	B	815	CLA	CHC-C1C-C2C	-3.28	117.65	126.72
30	8	308	CLA	C1-C2-C3	-3.28	120.37	126.04
30	14	310	CLA	C3B-C4B-NB	3.28	113.45	109.21
30	B	807	CLA	CMC-C2C-C1C	3.28	130.03	125.04
30	A	809	CLA	CMC-C2C-C1C	3.28	130.03	125.04
30	3	305	CLA	C3B-C4B-NB	3.28	113.45	109.21
38	8	313	KC1	C4B-C3B-C2B	-3.28	104.06	106.75
39	15	319	DD6	C33-C34-C35	3.28	114.79	110.30
37	10	317	A86	C40-C32-C31	-3.28	107.54	110.47
37	15	315	A86	C8-C6-C5	-3.28	113.91	118.94
30	10	308	CLA	C1C-C2C-C3C	-3.28	103.51	106.96
38	8	311	KC1	CAA-CBA-CGA	-3.27	110.43	127.26
30	5	308	CLA	C3B-C4B-NB	3.27	113.44	109.21
30	A	818	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
38	10	310	KC1	CAA-CBA-CGA	-3.27	110.44	127.26
37	4	314	A86	C-C1-C2	-3.27	118.34	122.92
37	11	315	A86	C36-C31-C32	-3.27	116.45	119.70
30	7	312	CLA	CHC-C1C-C2C	-3.27	117.67	126.72
30	15	303	CLA	C3B-C4B-NB	3.27	113.44	109.21
30	A	803	CLA	CAA-C2A-C3A	-3.27	103.82	112.78
30	A	803	CLA	C1D-CHD-C4C	-3.27	119.00	126.06
30	15	312	CLA	CBC-CAC-C3C	-3.27	103.42	112.43
37	16	312	A86	C24-C1-C2	3.27	123.96	118.94
39	10	313	DD6	C15-C14-C13	3.27	132.90	125.99
30	8	308	CLA	O2A-CGA-CBA	3.27	122.17	111.91
30	B	825	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
30	3	306	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
30	14	307	CLA	C1C-C2C-C3C	-3.26	103.52	106.96
38	14	306	KC1	CHC-C4B-NB	-3.26	121.45	124.45
37	14	320	A86	C24-C1-C2	3.26	123.95	118.94
30	16	302	CLA	C3B-C4B-NB	3.26	113.43	109.21
30	9	308	CLA	CAC-C3C-C4C	3.26	129.04	124.81
37	9	315	A86	C41-C32-C31	-3.26	107.55	110.47
38	12	313	KC1	CHD-C4C-NC	3.26	129.15	124.20
37	7	315	A86	C26-C25-C24	-3.26	113.04	123.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	13	303	CLA	CAC-C3C-C4C	3.26	129.04	124.81
30	B	814	CLA	C4C-C3C-C2C	-3.26	102.14	106.90
30	B	823	CLA	C3B-C4B-NB	3.26	113.42	109.21
30	8	305	CLA	C4C-C3C-C2C	-3.26	102.15	106.90
39	13	314	DD6	C37-C36-C35	-3.26	108.32	114.36
30	6	316	CLA	CAC-C3C-C4C	3.26	129.04	124.81
30	B	801	CLA	C1-C2-C3	-3.26	120.41	126.04
30	15	306	CLA	CHC-C1C-C2C	-3.26	117.71	126.72
30	12	308	CLA	C3B-C4B-NB	3.26	113.42	109.21
37	15	315	A86	C-C1-C2	-3.26	118.36	122.92
30	5	307	CLA	CMB-C2B-C3B	3.26	130.77	124.68
30	1	301	CLA	C3B-C4B-NB	3.26	113.42	109.21
38	7	308	KC1	CAA-CBA-CGA	-3.26	110.53	127.26
34	A	853	LHG	O8-C23-C24	3.25	119.92	111.38
39	7	317	DD6	C35-C36-C31	-3.25	113.18	120.57
37	2u	203	A86	C4-C5-C6	-3.25	122.67	127.31
30	B	806	CLA	CAA-C2A-C3A	-3.25	103.87	112.78
30	6	307	CLA	CHC-C1C-C2C	-3.25	117.72	126.72
30	B	802	CLA	C4-C3-C5	3.25	120.74	115.27
38	13	310	KC1	C4B-C3B-C2B	-3.25	104.08	106.75
38	8	306	KC1	CMB-C2B-C1B	3.25	130.44	124.71
30	1	305	CLA	CHC-C1C-C2C	-3.25	117.73	126.72
30	16	308	CLA	CHC-C1C-C2C	-3.25	117.73	126.72
30	8	309	CLA	CHC-C1C-C2C	-3.25	117.73	126.72
38	6	308	KC1	C1C-C2C-C3C	-3.25	103.54	106.96
30	4	305	CLA	C1D-CHD-C4C	-3.25	119.05	126.06
30	5	309	CLA	CAC-C3C-C4C	3.25	129.02	124.81
38	3	308	KC1	CAA-CBA-CGA	-3.25	110.57	127.26
30	A	829	CLA	C1C-C2C-C3C	-3.25	103.54	106.96
30	A	830	CLA	C1-C2-C3	-3.25	120.43	126.04
30	B	804	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
38	6	311	KC1	CAA-CBA-CGA	-3.25	110.58	127.26
30	4	311	CLA	CHC-C1C-C2C	-3.25	117.74	126.72
30	A	826	CLA	C4A-NA-C1A	-3.25	105.25	106.71
30	5	307	CLA	C4A-NA-C1A	-3.25	105.25	106.71
30	F	202	CLA	CMB-C2B-C3B	3.24	130.75	124.68
30	6	317	CLA	C3B-C4B-NB	3.24	113.41	109.21
30	10	305	CLA	C3B-C4B-NB	3.24	113.40	109.21
30	13	302	CLA	C3B-C4B-NB	3.24	113.40	109.21
30	4	302	CLA	C3B-C4B-NB	3.24	113.40	109.21
30	B	801	CLA	C4A-NA-C1A	-3.24	105.25	106.71
30	9	308	CLA	C1C-C2C-C3C	-3.24	103.55	106.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	16	301	CLA	CHD-C4C-NC	3.24	129.31	124.20
30	B	807	CLA	CAC-C3C-C4C	3.24	129.02	124.81
30	10	311	CLA	C3B-C4B-NB	3.24	113.40	109.21
30	A	835	CLA	C3B-C4B-NB	3.24	113.40	109.21
30	B	813	CLA	C3B-C4B-NB	3.24	113.40	109.21
30	4	303	CLA	C4C-C3C-C2C	-3.24	102.17	106.90
38	7	313	KC1	CMB-C2B-C1B	3.24	130.42	124.71
37	11	315	A86	C9-C10-C11	-3.24	117.08	126.61
30	B	808	CLA	CBA-CAA-C2A	3.24	123.42	113.86
30	3	306	CLA	CMB-C2B-C3B	3.24	130.73	124.68
38	16	311	KC1	CAA-CBA-CGA	-3.24	110.63	127.26
37	9	315	A86	C-C1-C24	3.24	123.17	118.08
30	3	303	CLA	C3B-C4B-NB	3.23	113.39	109.21
30	A	821	CLA	CHC-C1C-C2C	-3.23	117.77	126.72
30	8	304	CLA	O2A-CGA-CBA	3.23	122.06	111.91
38	10	312	KC1	CHD-C4C-NC	3.23	129.11	124.20
38	6	313	KC1	CBA-CAA-C2A	-3.23	112.95	125.27
37	14	315	A86	C41-C32-C31	-3.23	107.58	110.47
30	B	804	CLA	C3B-C4B-NB	3.23	113.39	109.21
30	16	310	CLA	CGD-CBD-CAD	-3.23	100.26	110.73
38	6	308	KC1	C4C-C3C-C2C	-3.23	102.19	106.90
30	A	816	CLA	CHC-C1C-C2C	-3.23	117.78	126.72
30	7	309	CLA	CHC-C1C-C2C	-3.23	117.79	126.72
30	10	304	CLA	C3B-C4B-NB	3.23	113.39	109.21
37	15	321	A86	C40-C32-C31	-3.23	107.58	110.47
30	B	825	CLA	C1C-C2C-C3C	-3.23	103.56	106.96
38	8	311	KC1	C4C-C3C-C2C	-3.23	102.19	106.90
30	A	821	CLA	O2A-CGA-CBA	3.23	122.04	111.91
30	B	839	CLA	CMC-C2C-C1C	3.23	129.96	125.04
39	6	318	DD6	C19-C18-C17	3.23	117.01	110.77
30	A	831	CLA	C4-C3-C5	3.23	120.70	115.27
30	A	830	CLA	C4C-C3C-C2C	-3.23	102.19	106.90
37	5	316	A86	C12-C11-C13	3.23	121.44	116.02
30	A	823	CLA	C3C-C4C-NC	3.22	114.19	110.57
30	A	826	CLA	CMB-C2B-C3B	3.22	130.71	124.68
30	12	312	CLA	C3B-C4B-NB	3.22	113.38	109.21
37	5	316	A86	C40-C32-C31	-3.22	107.59	110.47
30	1	304	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
37	16	312	A86	C4-C3-C2	-3.22	116.88	123.47
30	10	309	CLA	C3B-C4B-NB	3.22	113.37	109.21
30	A	814	CLA	CHC-C1C-C2C	-3.22	117.82	126.72
37	7	319	A86	C8-C6-C5	3.22	123.88	118.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	8	313	KC1	C2C-C1C-NC	3.22	114.08	110.57
39	11	313	DD6	C37-C36-C35	-3.22	108.39	114.36
30	1	302	CLA	CAA-C2A-C3A	-3.22	103.97	112.78
30	B	802	CLA	O2A-CGA-CBA	3.22	122.00	111.91
37	15	321	A86	C4-C3-C2	-3.21	116.89	123.47
30	2	303	CLA	C3C-C4C-NC	3.21	114.18	110.57
30	L	203	CLA	CMB-C2B-C3B	3.21	130.69	124.68
39	6	321	DD6	C37-C36-C35	-3.21	108.40	114.36
30	7	303	CLA	CMC-C2C-C1C	3.21	129.93	125.04
30	12	312	CLA	CAA-C2A-C3A	-3.21	103.98	112.78
30	B	827	CLA	C4C-C3C-C2C	-3.21	102.22	106.90
37	14	316	A86	C22-C16-C17	-3.21	103.41	108.98
30	4	301	CLA	C4C-C3C-C2C	-3.21	102.22	106.90
38	2	312	KC1	CAC-C3C-C4C	3.21	128.97	124.81
39	2	317	DD6	C3-C4-C5	-3.21	116.90	123.47
30	A	818	CLA	CHD-C4C-NC	3.21	129.26	124.20
30	15	304	CLA	C1-O2A-CGA	3.21	124.86	116.44
38	3	304	KC1	O2D-CGD-O1D	-3.21	117.56	123.84
30	16	305	CLA	C1-C2-C3	-3.21	121.56	126.75
30	15	307	CLA	CHC-C1C-C2C	-3.21	117.85	126.72
30	A	840	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
30	2	307	CLA	CMA-C3A-C4A	-3.21	103.16	111.77
37	9	315	A86	C35-C34-C33	3.21	115.47	109.88
30	B	831	CLA	C4-C3-C5	3.21	120.66	115.27
30	9	308	CLA	C1-C2-C3	-3.20	120.50	126.04
39	5	313	DD6	C35-C36-C31	-3.20	113.30	120.57
38	8	313	KC1	CBA-CAA-C2A	-3.20	113.06	125.27
30	B	820	CLA	CAC-C3C-C2C	3.20	133.01	127.53
30	A	842	CLA	CAA-C2A-C3A	-3.20	104.01	112.78
30	B	824	CLA	C4C-C3C-C2C	-3.20	102.23	106.90
30	15	312	CLA	C3C-C4C-NC	3.20	114.16	110.57
30	A	806	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
30	3	303	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
37	14	315	A86	C24-C1-C2	-3.20	114.03	118.94
30	6	314	CLA	CAC-C3C-C4C	3.20	128.96	124.81
38	8	312	KC1	C4C-C3C-C2C	-3.20	102.24	106.90
30	B	814	CLA	CAA-C2A-C3A	-3.20	104.03	112.78
37	15	315	A86	C25-C24-C1	3.20	135.39	126.42
30	A	836	CLA	C4-C3-C5	3.20	120.65	115.27
30	A	803	CLA	C1C-C2C-C3C	-3.19	103.60	106.96
30	3	305	CLA	O2D-CGD-CBD	3.19	116.94	111.27
30	A	836	CLA	CHC-C1C-C2C	-3.19	117.89	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	837	CLA	CAC-C3C-C4C	3.19	128.95	124.81
30	A	812	CLA	C3B-C4B-NB	3.19	113.34	109.21
30	A	844	CLA	C3B-C4B-NB	3.19	113.34	109.21
30	F	203	CLA	C3B-C4B-NB	3.19	113.34	109.21
30	13	301	CLA	C3B-C4B-NB	3.19	113.34	109.21
30	5	303	CLA	O2D-CGD-CBD	3.19	116.94	111.27
30	A	820	CLA	CHC-C1C-C2C	-3.19	117.89	126.72
30	7	307	CLA	CHD-C4C-NC	3.19	129.23	124.20
30	B	810	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
38	8	314	KC1	CAA-CBA-CGA	-3.19	110.87	127.26
30	A	816	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
30	10	309	CLA	CAC-C3C-C4C	3.19	128.95	124.81
30	15	304	CLA	C3B-C4B-NB	3.19	113.33	109.21
30	16	307	CLA	C3B-C4B-NB	3.19	113.33	109.21
30	B	808	CLA	CHC-C1C-C2C	-3.19	117.91	126.72
30	9	301	CLA	CHC-C1C-C2C	-3.19	117.91	126.72
30	16	310	CLA	C3B-C4B-NB	3.19	113.33	109.21
30	B	813	CLA	O2A-CGA-CBA	3.19	121.90	111.91
30	6	310	CLA	CHC-C1C-C2C	-3.18	117.91	126.72
38	8	314	KC1	CAC-C3C-C4C	3.18	128.94	124.81
30	10	307	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
30	2	309	CLA	CAC-C3C-C4C	3.18	128.94	124.81
39	12	317	DD6	C37-C36-C35	-3.18	108.46	114.36
30	10	311	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
38	8	311	KC1	CBA-CAA-C2A	-3.18	113.14	125.27
30	14	302	CLA	CAC-C3C-C4C	3.18	128.94	124.81
39	10	313	DD6	O1-C20-C21	-3.18	111.24	115.06
37	4	312	A86	C25-C26-C27	-3.18	122.77	127.31
30	B	815	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
30	A	831	CLA	CHC-C1C-C2C	-3.18	117.92	126.72
30	B	833	CLA	C4-C3-C5	3.18	120.62	115.27
30	B	830	CLA	C1D-CHD-C4C	-3.18	119.20	126.06
30	A	811	CLA	CHC-C1C-C2C	-3.18	117.93	126.72
30	8	304	CLA	C4-C3-C5	3.18	120.62	115.27
30	14	303	CLA	C3B-C4B-NB	3.18	113.32	109.21
30	A	815	CLA	O2A-CGA-CBA	3.18	121.88	111.91
30	2	311	CLA	C1-C2-C3	-3.18	120.55	126.04
39	3	313	DD6	C37-C36-C35	-3.18	108.47	114.36
37	15	321	A86	C34-O4-C38	-3.18	111.98	117.90
30	A	842	CLA	C4C-C3C-C2C	-3.18	102.27	106.90
30	15	312	CLA	CHC-C1C-C2C	-3.18	117.94	126.72
30	12	306	CLA	CHC-C1C-C2C	-3.17	117.94	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	16	311	KC1	C1A-NA-C4A	-3.17	105.28	106.71
30	B	818	CLA	C1-C2-C3	-3.17	120.55	126.04
30	11	309	CLA	CAC-C3C-C4C	3.17	128.93	124.81
30	14	305	CLA	CHB-C4A-NA	3.17	128.90	124.51
38	9	312	KC1	CAA-CBA-CGA	-3.17	110.96	127.26
30	2	303	CLA	C1D-CHD-C4C	-3.17	119.22	126.06
30	B	804	CLA	CMC-C2C-C1C	3.17	129.87	125.04
30	1	301	CLA	CHC-C1C-C2C	-3.17	117.95	126.72
30	14	313	CLA	C3B-C4B-NB	3.17	113.31	109.21
30	11	310	CLA	C3B-C4B-NB	3.17	113.31	109.21
39	16	313	DD6	C22-C16-C15	3.17	118.60	110.05
30	B	817	CLA	CMB-C2B-C3B	3.17	130.61	124.68
30	A	803	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
30	11	309	CLA	CHC-C1C-C2C	-3.17	117.96	126.72
37	16	312	A86	C10-C9-C8	3.17	133.10	123.22
30	15	313	CLA	C3B-C4B-NB	3.17	113.30	109.21
30	15	302	CLA	CAA-C2A-C3A	-3.17	104.11	112.78
30	7	309	CLA	CAC-C3C-C4C	3.17	128.92	124.81
30	16	305	CLA	CHC-C1C-C2C	-3.16	117.97	126.72
30	12	307	CLA	C4C-C3C-C2C	-3.16	102.29	106.90
30	A	840	CLA	O2A-CGA-CBA	3.16	121.83	111.91
39	2	317	DD6	C23-C16-C15	3.16	118.58	110.05
30	B	835	CLA	CAA-C2A-C3A	-3.16	104.12	112.78
38	8	307	KC1	CHD-C4C-NC	3.16	129.00	124.20
30	14	310	CLA	C1-C2-C3	-3.16	121.64	126.75
30	A	810	CLA	CAC-C3C-C4C	3.16	128.91	124.81
30	15	314	CLA	CAC-C3C-C4C	3.16	128.91	124.81
30	16	306	CLA	C1C-C2C-C3C	-3.16	103.64	106.96
38	11	312	KC1	CBA-CAA-C2A	-3.16	113.23	125.27
30	2	303	CLA	C3B-C4B-NB	3.16	113.29	109.21
38	16	311	KC1	C2A-C1A-NA	3.15	114.46	109.40
30	A	810	CLA	CHC-C1C-C2C	-3.15	118.00	126.72
38	8	307	KC1	C4B-C3B-C2B	-3.15	104.16	106.75
30	1	302	CLA	C3B-C4B-NB	3.15	113.29	109.21
30	B	802	CLA	C3B-C4B-NB	3.15	113.28	109.21
38	4	307	KC1	CHB-C1B-NB	-3.15	121.56	124.45
30	11	306	CLA	C1C-C2C-C3C	-3.15	103.64	106.96
38	8	313	KC1	CAA-C2A-C1A	-3.15	110.26	124.75
38	8	311	KC1	C1A-NA-C4A	-3.15	105.29	106.71
38	5	312	KC1	CMD-C2D-C1D	3.15	133.30	128.46
30	15	302	CLA	O2A-CGA-CBA	3.15	121.79	111.91
30	A	826	CLA	CHC-C1C-C2C	-3.15	118.01	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	3	310	CLA	CHC-C1C-C2C	-3.15	118.01	126.72
30	7	304	CLA	CHC-C1C-C2C	-3.15	118.01	126.72
30	12	307	CLA	CMC-C2C-C1C	3.15	129.83	125.04
38	14	311	KC1	CMC-C2C-C1C	3.15	129.83	125.04
30	A	808	CLA	C3B-C4B-NB	3.15	113.28	109.21
38	5	310	KC1	C4C-C3C-C2C	-3.15	102.31	106.90
30	9	308	CLA	CMC-C2C-C1C	3.15	129.83	125.04
30	7	305	CLA	CMB-C2B-C3B	3.14	130.56	124.68
38	4	307	KC1	CAC-C3C-C4C	3.14	128.89	124.81
30	A	810	CLA	O2D-CGD-CBD	3.14	116.85	111.27
38	10	310	KC1	CHC-C4B-NB	-3.14	121.57	124.45
30	9	303	CLA	CHD-C4C-NC	3.14	129.15	124.20
30	14	304	CLA	C3B-C4B-NB	3.14	113.27	109.21
30	B	812	CLA	CHC-C1C-C2C	-3.14	118.03	126.72
30	A	815	CLA	CAC-C3C-C4C	3.14	128.88	124.81
30	14	303	CLA	CAC-C3C-C4C	3.14	128.88	124.81
30	14	313	CLA	CHD-C4C-NC	3.14	129.15	124.20
30	6	316	CLA	C1-C2-C3	-3.14	120.61	126.04
30	A	825	CLA	CHC-C1C-C2C	-3.14	118.04	126.72
38	6	312	KC1	CBA-CAA-C2A	-3.14	113.31	125.27
30	7	304	CLA	C4-C3-C5	3.14	120.55	115.27
30	10	311	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
30	A	843	CLA	CHC-C1C-C2C	-3.14	118.04	126.72
37	4	315	A86	C3-C2-C1	-3.14	122.83	127.31
38	13	310	KC1	CBA-CAA-C2A	-3.14	113.31	125.27
30	16	307	CLA	CAA-C2A-C3A	-3.14	104.19	112.78
30	5	308	CLA	CMB-C2B-C3B	3.14	130.54	124.68
30	9	308	CLA	CMB-C2B-C3B	3.14	130.54	124.68
30	A	804	CLA	C1C-C2C-C3C	-3.13	103.66	106.96
30	B	830	CLA	C1C-C2C-C3C	-3.13	103.66	106.96
30	B	832	CLA	C3B-C4B-NB	3.13	113.26	109.21
30	14	305	CLA	C3B-C4B-NB	3.13	113.26	109.21
38	8	310	KC1	CMB-C2B-C1B	3.13	130.24	124.71
39	15	319	DD6	C25-C24-C1	-3.13	117.61	126.42
30	B	803	CLA	C1-C2-C3	-3.13	120.62	126.04
39	10	313	DD6	C37-C36-C35	-3.13	108.55	114.36
30	15	314	CLA	C3B-C4B-NB	3.13	113.26	109.21
30	16	303	CLA	C3B-C4B-NB	3.13	113.26	109.21
30	11	310	CLA	CAC-C3C-C4C	3.13	128.87	124.81
30	7	306	CLA	CHC-C1C-C2C	-3.13	118.06	126.72
30	12	321	CLA	CHC-C1C-C2C	-3.13	118.06	126.72
30	A	833	CLA	C3B-C4B-NB	3.13	113.26	109.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	838	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
38	9	310	KC1	C4B-C3B-C2B	-3.13	104.18	106.75
30	B	805	CLA	CHC-C1C-C2C	-3.13	118.07	126.72
30	6	306	CLA	C3B-C4B-NB	3.13	113.25	109.21
30	5	308	CLA	CAC-C3C-C4C	3.13	128.87	124.81
30	2	307	CLA	C3B-C4B-NB	3.13	113.25	109.21
30	10	303	CLA	C3B-C4B-NB	3.13	113.25	109.21
37	8	315	A86	C33-C32-C31	3.13	112.25	109.21
37	1	309	A86	C26-C25-C24	-3.13	113.46	123.22
38	16	311	KC1	CHB-C1B-NB	-3.13	121.58	124.45
37	15	321	A86	C10-C9-C8	-3.13	113.46	123.22
37	2	318	A86	C12-C11-C13	3.12	121.27	116.02
30	15	311	CLA	CHC-C1C-C2C	-3.12	118.08	126.72
38	4	307	KC1	O2D-CGD-O1D	-3.12	117.73	123.84
30	2	310	CLA	CAC-C3C-C4C	3.12	128.86	124.81
38	2	314	KC1	CED-O2D-CGD	3.12	123.00	115.94
30	5	303	CLA	C3B-C4B-NB	3.12	113.25	109.21
30	A	807	CLA	CHD-C4C-NC	3.12	129.12	124.20
39	8	316	DD6	C37-C36-C35	-3.12	108.57	114.36
30	A	813	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
30	B	821	CLA	CHC-C1C-C2C	-3.12	118.09	126.72
30	2	307	CLA	CHC-C1C-C2C	-3.12	118.09	126.72
30	14	305	CLA	CHC-C1C-C2C	-3.12	118.09	126.72
30	8	301	CLA	C3B-C4B-NB	3.12	113.24	109.21
30	2	308	CLA	CAC-C3C-C4C	3.12	128.86	124.81
39	7	302	DD6	C19-C18-C17	3.12	116.80	110.77
38	3	304	KC1	CAA-CBA-CGA	-3.12	111.24	127.26
30	B	819	CLA	CHC-C1C-C2C	-3.12	118.10	126.72
30	16	306	CLA	C3B-C4B-NB	3.11	113.24	109.21
30	A	802	CLA	CHC-C1C-C2C	-3.11	118.11	126.72
30	13	309	CLA	CHC-C1C-C2C	-3.11	118.11	126.72
30	15	313	CLA	CHC-C1C-C2C	-3.11	118.11	126.72
38	4	308	KC1	CAC-C3C-C4C	3.11	128.85	124.81
30	6	304	CLA	CMC-C2C-C1C	3.11	129.78	125.04
30	A	837	CLA	CHC-C1C-C2C	-3.11	118.11	126.72
39	2	316	DD6	C35-C36-C31	-3.11	113.50	120.57
30	7	303	CLA	C4C-C3C-C2C	-3.11	102.36	106.90
30	2	311	CLA	CAC-C3C-C4C	3.11	128.85	124.81
38	10	306	KC1	CBA-CAA-C2A	-3.11	113.41	125.27
30	12	302	CLA	C4-C3-C5	3.11	120.50	115.27
30	6	316	CLA	C4C-C3C-C2C	-3.11	102.36	106.90
30	B	816	CLA	CHD-C4C-NC	3.11	129.10	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	14	311	KC1	CHD-C4C-NC	3.11	128.92	124.20
30	A	829	CLA	C4C-C3C-C2C	-3.11	102.36	106.90
37	7	316	A86	C9-C8-C6	-3.11	117.68	126.42
30	11	310	CLA	CHC-C1C-C2C	-3.11	118.12	126.72
37	14	319	A86	C3-C4-C5	-3.11	117.11	123.47
30	A	834	CLA	C3B-C4B-NB	3.11	113.23	109.21
30	3	302	CLA	C3B-C4B-NB	3.11	113.23	109.21
39	11	313	DD6	C15-C14-C13	-3.11	119.42	125.99
39	3	312	DD6	C37-C36-C35	-3.11	108.60	114.36
30	2	309	CLA	C3B-C4B-NB	3.11	113.23	109.21
30	A	837	CLA	C3B-C4B-NB	3.11	113.23	109.21
30	A	832	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
30	A	815	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
30	16	305	CLA	O2D-CGD-O1D	-3.11	117.77	123.84
30	B	804	CLA	C4A-NA-C1A	-3.11	105.31	106.71
30	B	808	CLA	C4A-NA-C1A	-3.11	105.31	106.71
30	B	801	CLA	CHD-C4C-NC	3.11	129.10	124.20
30	4	302	CLA	CHD-C4C-NC	3.11	129.10	124.20
30	8	305	CLA	CHD-C4C-NC	3.11	129.10	124.20
30	A	831	CLA	CMA-C3A-C2A	-3.10	101.31	113.83
30	3	303	CLA	CHC-C1C-C2C	-3.10	118.13	126.72
37	2	319	A86	C40-C32-C31	-3.10	107.69	110.47
30	A	829	CLA	CAC-C3C-C4C	3.10	128.84	124.81
30	B	803	CLA	CHC-C1C-C2C	-3.10	118.14	126.72
37	15	315	A86	C7-C6-C8	3.10	122.97	118.08
30	11	308	CLA	CAA-C2A-C3A	-3.10	104.28	112.78
30	7	306	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
38	5	306	KC1	CAC-C3C-C4C	3.10	128.83	124.81
30	4	303	CLA	C3B-C4B-NB	3.10	113.22	109.21
37	9	313	A86	C9-C8-C6	-3.10	117.71	126.42
38	12	309	KC1	CHD-C4C-NC	3.10	128.90	124.20
30	8	305	CLA	C4A-NA-C1A	-3.10	105.31	106.71
37	13	313	A86	C7-C6-C5	-3.10	118.59	122.92
37	11	316	A86	C12-C11-C13	3.10	121.22	116.02
30	B	828	CLA	CHC-C1C-C2C	-3.10	118.16	126.72
30	15	303	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
37	4	314	A86	C25-C24-C1	-3.09	117.72	126.42
38	2	312	KC1	CBA-CAA-C2A	-3.09	113.47	125.27
30	B	818	CLA	CHD-C4C-NC	3.09	129.08	124.20
30	1	304	CLA	CHD-C4C-NC	3.09	129.08	124.20
30	B	803	CLA	CHB-C4A-NA	3.09	128.79	124.51
30	5	302	CLA	CHD-C4C-NC	3.09	129.07	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	822	CLA	CMA-C3A-C4A	-3.09	103.46	111.77
30	B	816	CLA	CAC-C3C-C4C	3.09	128.82	124.81
30	A	826	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
30	2	308	CLA	CHD-C4C-NC	3.09	129.07	124.20
30	B	828	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
38	3	311	KC1	C4C-C3C-C2C	-3.09	102.39	106.90
38	9	310	KC1	CAA-CBA-CGA	-3.09	111.39	127.26
30	11	308	CLA	CHC-C1C-C2C	-3.09	118.18	126.72
30	B	823	CLA	CHC-C1C-C2C	-3.09	118.18	126.72
30	1	305	CLA	CAC-C3C-C4C	3.09	128.82	124.81
30	B	821	CLA	O2A-C1-C2	3.09	116.75	108.64
30	2u	202	CLA	C3B-C4B-NB	3.09	113.20	109.21
30	7	311	CLA	C3B-C4B-NB	3.09	113.20	109.21
30	14	303	CLA	CHC-C1C-C2C	-3.09	118.18	126.72
30	B	808	CLA	O2A-CGA-O1A	-3.09	115.80	123.59
30	5	304	CLA	C1-O2A-CGA	3.09	124.54	116.44
39	7	318	DD6	C19-C18-C17	3.09	116.73	110.77
30	14	307	CLA	CMB-C2B-C3B	3.09	130.45	124.68
37	14	319	A86	C12-C11-C10	-3.09	115.96	123.42
30	12	306	CLA	C4A-NA-C1A	-3.09	105.32	106.71
30	8	301	CLA	C4C-C3C-C2C	-3.08	102.40	106.90
30	3	301	CLA	O2A-CGA-CBA	3.08	121.59	111.91
30	9	302	CLA	CHC-C1C-C2C	-3.08	118.19	126.72
37	15	322	A86	C3-C4-C5	3.08	129.79	123.47
30	10	303	CLA	CHC-C1C-C2C	-3.08	118.19	126.72
38	9	312	KC1	CAC-C3C-C4C	3.08	128.81	124.81
30	1	307	CLA	CHC-C1C-C2C	-3.08	118.19	126.72
38	8	314	KC1	C4C-C3C-C2C	-3.08	102.40	106.90
30	15	306	CLA	CAA-C2A-C3A	-3.08	104.34	112.78
30	9	307	CLA	C3B-C4B-NB	3.08	113.19	109.21
30	1	302	CLA	CHC-C1C-C2C	-3.08	118.19	126.72
33	B	841	BCR	C20-C21-C22	-3.08	122.91	127.31
30	A	822	CLA	CHC-C1C-C2C	-3.08	118.20	126.72
30	12	312	CLA	CHC-C1C-C2C	-3.08	118.20	126.72
30	B	851	CLA	C1C-C2C-C3C	-3.08	103.72	106.96
30	B	802	CLA	CMC-C2C-C1C	3.08	129.73	125.04
30	14	304	CLA	CHC-C1C-C2C	-3.08	118.20	126.72
39	9	314	DD6	C25-C24-C1	-3.08	117.76	126.42
30	2	303	CLA	O2A-CGA-CBA	3.08	121.57	111.91
38	16	304	KC1	C4C-C3C-C2C	-3.08	102.41	106.90
38	7	313	KC1	CHD-C4C-NC	3.08	128.88	124.20
30	2	310	CLA	CHC-C1C-C2C	-3.08	118.20	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	3	307	CLA	CHC-C1C-C2C	-3.08	118.20	126.72
30	13	307	CLA	CHC-C1C-C2C	-3.08	118.20	126.72
30	B	803	CLA	O2A-CGA-CBA	3.08	121.57	111.91
30	B	831	CLA	CAA-C2A-C3A	-3.08	104.35	112.78
30	A	804	CLA	C3B-C4B-NB	3.08	113.19	109.21
38	11	311	KC1	CAC-C3C-C4C	3.08	128.80	124.81
37	10	316	A86	C-C1-C24	3.08	122.92	118.08
37	11	314	A86	C10-C9-C8	-3.08	113.62	123.22
30	B	830	CLA	C6-C7-C8	-3.08	105.98	115.92
30	11	306	CLA	CAC-C3C-C4C	3.08	128.80	124.81
30	B	833	CLA	CHC-C1C-C2C	-3.08	118.22	126.72
30	13	303	CLA	CHC-C1C-C2C	-3.07	118.22	126.72
37	9	313	A86	C36-C31-C32	-3.07	116.65	119.70
39	7	302	DD6	C14-C13-C11	3.07	130.30	125.53
30	A	813	CLA	O2A-CGA-CBA	3.07	121.55	111.91
38	2	312	KC1	C4C-C3C-C2C	-3.07	102.42	106.90
30	16	309	CLA	CAA-C2A-C3A	-3.07	104.37	112.78
30	B	819	CLA	C3D-C2D-C1D	-3.07	101.64	105.83
30	12	304	CLA	CMB-C2B-C3B	3.07	130.42	124.68
37	14	320	A86	C4-C5-C6	3.07	131.69	127.31
37	16	314	A86	C35-C34-C33	3.07	115.23	109.88
30	6	309	CLA	CAA-C2A-C3A	-3.07	104.38	112.78
38	8	311	KC1	CAC-C3C-C4C	3.07	128.79	124.81
30	B	834	CLA	O2A-CGA-CBA	3.07	121.53	111.91
30	4	309	CLA	O2A-CGA-CBA	3.07	121.53	111.91
30	9	302	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
30	6	314	CLA	C4-C3-C5	3.07	120.43	115.27
30	8	304	CLA	C3B-C4B-NB	3.07	113.17	109.21
30	B	832	CLA	CHC-C1C-C2C	-3.07	118.24	126.72
30	B	818	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
30	6	309	CLA	CAC-C3C-C4C	3.07	128.79	124.81
38	13	305	KC1	C4C-C3C-C2C	-3.07	102.43	106.90
30	15	310	CLA	CAC-C3C-C4C	3.06	128.79	124.81
30	12	303	CLA	C4C-C3C-C2C	-3.06	102.43	106.90
30	15	304	CLA	CHC-C1C-C2C	-3.06	118.25	126.72
30	5	303	CLA	CAA-C2A-C3A	-3.06	104.39	112.78
30	16	307	CLA	CHC-C1C-C2C	-3.06	118.25	126.72
30	A	824	CLA	C3B-C4B-NB	3.06	113.17	109.21
38	16	304	KC1	CAA-CBA-CGA	-3.06	111.52	127.26
30	15	310	CLA	CHC-C1C-C2C	-3.06	118.25	126.72
30	5	307	CLA	CMC-C2C-C1C	3.06	129.70	125.04
30	6	306	CLA	C4A-NA-C1A	-3.06	105.33	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	10	315	A86	C12-C11-C13	3.06	121.16	116.02
30	7	307	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
30	B	839	CLA	O2A-CGA-CBA	3.06	121.51	111.91
30	5	309	CLA	CHC-C1C-C2C	-3.06	118.26	126.72
30	B	831	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
30	4	304	CLA	C3B-C4B-NB	3.06	113.17	109.21
30	16	309	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
30	10	304	CLA	CHC-C1C-C2C	-3.06	118.26	126.72
38	5	305	KC1	CMB-C2B-C1B	3.06	130.10	124.71
38	5	310	KC1	CAA-CBA-CGA	-3.06	111.54	127.26
30	10	304	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
30	B	814	CLA	CHC-C1C-C2C	-3.06	118.26	126.72
37	7	316	A86	C12-C11-C13	3.06	121.16	116.02
30	B	851	CLA	O2A-CGA-CBA	3.06	121.50	111.91
30	B	804	CLA	CAC-C3C-C4C	3.06	128.78	124.81
30	12	307	CLA	CHD-C4C-NC	3.05	129.02	124.20
30	4	305	CLA	CAA-C2A-C3A	-3.05	104.41	112.78
30	A	841	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
30	9	307	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
30	1	302	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
30	A	840	CLA	C3B-C4B-NB	3.05	113.16	109.21
30	2	311	CLA	C3B-C4B-NB	3.05	113.16	109.21
30	A	820	CLA	C1-C2-C3	-3.05	120.76	126.04
30	4	302	CLA	CAC-C3C-C4C	3.05	128.77	124.81
30	12	303	CLA	CHC-C1C-C2C	-3.05	118.28	126.72
30	A	807	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
30	A	824	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
39	13	314	DD6	C35-C36-C31	-3.05	113.64	120.57
38	6	308	KC1	CHD-C4C-NC	3.05	128.83	124.20
30	B	825	CLA	O2A-CGA-CBA	3.05	121.48	111.91
38	2	306	KC1	CAC-C3C-C4C	3.05	128.77	124.81
30	2	313	CLA	C3B-C4B-NB	3.05	113.15	109.21
37	3	314	A86	C36-C31-C32	-3.05	116.67	119.70
30	13	307	CLA	C3B-C4B-NB	3.05	113.15	109.21
30	15	309	CLA	CHC-C1C-C2C	-3.05	118.29	126.72
38	8	306	KC1	CBC-CAC-C3C	-3.05	104.03	112.43
30	15	308	CLA	C1C-C2C-C3C	-3.05	103.75	106.96
30	16	301	CLA	C3B-C4B-NB	3.05	113.15	109.21
30	6	315	CLA	CHC-C1C-C2C	-3.05	118.29	126.72
39	8	316	DD6	C25-C24-C1	-3.05	117.86	126.42
30	7	307	CLA	C1C-C2C-C3C	-3.05	103.75	106.96
30	2	303	CLA	CHC-C1C-C2C	-3.05	118.30	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	838	CLA	O2A-CGA-CBA	3.05	121.46	111.91
37	4	315	A86	C10-C9-C8	-3.04	113.72	123.22
30	8	302	CLA	CBC-CAC-C3C	-3.04	104.04	112.43
30	B	804	CLA	CMB-C2B-C3B	3.04	130.37	124.68
39	2	316	DD6	C10-C9-C8	-3.04	113.72	123.22
30	B	805	CLA	CMB-C2B-C3B	3.04	130.37	124.68
30	A	817	CLA	CHC-C1C-C2C	-3.04	118.31	126.72
35	9	317	LMT	C2'-C3'-C4'	3.04	116.63	109.68
39	10	313	DD6	C35-C36-C31	-3.04	113.67	120.57
30	B	801	CLA	CAC-C3C-C4C	3.04	128.76	124.81
30	8	301	CLA	CAC-C3C-C4C	3.04	128.76	124.81
30	14	304	CLA	CAC-C3C-C4C	3.04	128.75	124.81
30	16	309	CLA	CHC-C1C-C2C	-3.04	118.31	126.72
30	B	832	CLA	CHB-C4A-NA	3.04	128.72	124.51
30	3	305	CLA	CHC-C1C-C2C	-3.04	118.31	126.72
30	B	837	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
30	10	309	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
30	12	310	CLA	C3B-C4B-NB	3.04	113.14	109.21
30	13	301	CLA	CHD-C4C-NC	3.04	128.99	124.20
39	7	318	DD6	C37-C36-C35	-3.04	108.73	114.36
30	3	302	CLA	CHD-C4C-NC	3.04	128.99	124.20
30	2	308	CLA	CMB-C2B-C3B	3.04	130.36	124.68
30	A	809	CLA	O2A-CGA-CBA	3.04	121.44	111.91
30	8	303	CLA	CHC-C1C-C2C	-3.04	118.32	126.72
38	9	304	KC1	CAA-C2A-C1A	-3.04	110.79	124.75
38	5	305	KC1	CBA-CAA-C2A	-3.04	113.70	125.27
30	A	832	CLA	C3B-C4B-NB	3.04	113.13	109.21
38	8	313	KC1	CHD-C4C-NC	3.03	128.81	124.20
30	10	303	CLA	CHD-C4C-NC	3.03	128.99	124.20
39	7	302	DD6	C37-C36-C35	-3.03	108.73	114.36
30	4	309	CLA	CHC-C1C-C2C	-3.03	118.33	126.72
30	6	307	CLA	C3B-C4B-NB	3.03	113.13	109.21
30	16	302	CLA	CAA-C2A-C3A	-3.03	104.47	112.78
30	9	302	CLA	O2A-CGA-CBA	3.03	121.43	111.91
37	4	314	A86	C4-C3-C2	-3.03	117.26	123.47
30	5	308	CLA	CHC-C1C-C2C	-3.03	118.33	126.72
30	A	808	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
38	10	310	KC1	CAC-C3C-C4C	3.03	128.74	124.81
38	12	313	KC1	CBD-CHA-C1A	3.03	134.53	128.88
30	5	302	CLA	C1-C2-C3	-3.03	120.80	126.04
30	B	836	CLA	C3B-C4B-NB	3.03	113.13	109.21
30	7	307	CLA	CAC-C3C-C4C	3.03	128.74	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	844	CLA	CHC-C1C-C2C	-3.03	118.34	126.72
30	12	302	CLA	CMC-C2C-C1C	3.03	129.65	125.04
39	15	319	DD6	O1-C20-C21	-3.03	111.42	115.06
30	2	305	CLA	CHC-C1C-C2C	-3.03	118.34	126.72
30	14	305	CLA	C1-C2-C3	-3.03	121.85	126.75
30	A	812	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
30	7	305	CLA	CHC-C1C-C2C	-3.03	118.34	126.72
38	8	312	KC1	CBA-CAA-C2A	-3.03	113.72	125.27
30	A	835	CLA	CHC-C1C-C2C	-3.03	118.34	126.72
38	12	313	KC1	CHB-C1B-NB	-3.03	121.67	124.45
30	B	832	CLA	CMB-C2B-C3B	3.03	130.34	124.68
30	16	303	CLA	CHD-C4C-NC	3.03	128.97	124.20
30	A	802	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
30	9	301	CLA	C1C-C2C-C3C	-3.03	103.77	106.96
30	B	820	CLA	C3B-C4B-NB	3.03	113.12	109.21
38	1	306	KC1	CAB-C3B-C4B	3.03	132.21	124.90
30	6	306	CLA	C4C-C3C-C2C	-3.03	102.49	106.90
30	10	308	CLA	O2A-CGA-CBA	3.03	121.41	111.91
39	6	321	DD6	C15-C14-C13	-3.03	119.59	125.99
30	16	303	CLA	CBA-CAA-C2A	3.03	122.80	113.86
37	14	316	A86	C10-C9-C8	-3.02	113.78	123.22
38	14	306	KC1	CAA-CBA-CGA	-3.02	111.72	127.26
29	A	801	CL0	CMA-C3A-C4A	-3.02	103.64	111.77
30	A	841	CLA	O2A-CGA-CBA	3.02	121.40	111.91
30	1	303	CLA	C4C-C3C-C2C	-3.02	102.49	106.90
30	A	808	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
30	15	305	CLA	CHC-C1C-C2C	-3.02	118.36	126.72
39	3	313	DD6	C25-C24-C1	-3.02	117.93	126.42
30	A	839	CLA	CHC-C1C-C2C	-3.02	118.36	126.72
30	14	312	CLA	CHC-C1C-C2C	-3.02	118.36	126.72
30	1	302	CLA	CHD-C4C-NC	3.02	128.96	124.20
30	A	823	CLA	CHC-C1C-C2C	-3.02	118.36	126.72
30	B	817	CLA	CHD-C4C-NC	3.02	128.96	124.20
37	4	317	A86	C4-C5-C6	-3.02	123.00	127.31
37	4	317	A86	C25-C24-C1	-3.02	117.93	126.42
37	1	309	A86	C12-C11-C10	-3.02	116.12	123.42
30	6	304	CLA	CHD-C4C-NC	3.02	128.96	124.20
30	13	307	CLA	CAC-C3C-C4C	3.02	128.73	124.81
30	2u	202	CLA	CHD-C4C-NC	3.02	128.96	124.20
38	9	312	KC1	C4C-C3C-C2C	-3.02	102.50	106.90
30	12	306	CLA	CHB-C4A-NA	3.02	128.69	124.51
38	9	312	KC1	CMB-C2B-C1B	3.02	130.03	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	9	307	CLA	CHD-C4C-NC	3.02	128.96	124.20
38	5	306	KC1	CAA-C2A-C1A	-3.02	110.88	124.75
39	6	319	DD6	C19-C18-C17	3.02	116.60	110.77
30	A	818	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
30	15	306	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
30	7	307	CLA	CMC-C2C-C1C	3.02	129.63	125.04
30	A	839	CLA	C4C-C3C-C2C	-3.01	102.50	106.90
30	9	308	CLA	C4C-C3C-C2C	-3.01	102.50	106.90
30	3	309	CLA	C3B-C4B-NB	3.01	113.11	109.21
30	15	302	CLA	CAC-C3C-C4C	3.01	128.72	124.81
39	2	315	DD6	C10-C9-C8	3.01	132.62	123.22
30	B	810	CLA	C1-C2-C3	-3.01	120.83	126.04
37	7	316	A86	C7-C6-C8	3.01	122.82	118.08
30	14	310	CLA	CHC-C1C-C2C	-3.01	118.39	126.72
30	B	826	CLA	CHC-C1C-C2C	-3.01	118.39	126.72
30	A	830	CLA	O2A-CGA-CBA	3.01	121.36	111.91
30	6	316	CLA	CHC-C1C-C2C	-3.01	118.39	126.72
30	A	820	CLA	C2A-C3A-C4A	-3.01	97.01	101.87
30	3	301	CLA	CHC-C1C-C2C	-3.01	118.40	126.72
30	A	840	CLA	CHD-C4C-NC	3.01	128.94	124.20
30	B	835	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
30	B	820	CLA	CHD-C4C-NC	3.01	128.94	124.20
30	9	301	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
30	4	306	CLA	C3B-C4B-NB	3.01	113.10	109.21
30	15	307	CLA	C1-C2-C3	-3.01	121.89	126.75
30	A	833	CLA	C4-C3-C5	3.01	120.33	115.27
29	A	801	CL0	O2D-CGD-O1D	-3.01	117.96	123.84
30	8	302	CLA	CHD-C4C-NC	3.01	128.94	124.20
38	8	312	KC1	CMB-C2B-C1B	3.01	130.01	124.71
30	14	302	CLA	CHD-C4C-NC	3.01	128.94	124.20
30	11	309	CLA	C4C-C3C-C2C	-3.01	102.52	106.90
30	10	311	CLA	CAA-C2A-C3A	-3.01	104.55	112.78
30	7	307	CLA	C3B-C4B-NB	3.01	113.09	109.21
30	B	822	CLA	C3B-C4B-NB	3.00	113.09	109.21
30	6	317	CLA	CHC-C1C-C2C	-3.00	118.41	126.72
30	B	833	CLA	C4C-C3C-C2C	-3.00	102.52	106.90
30	11	306	CLA	C4C-C3C-C2C	-3.00	102.52	106.90
30	16	307	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
30	B	812	CLA	C4C-C3C-C2C	-3.00	102.52	106.90
30	4	301	CLA	CHC-C1C-C2C	-3.00	118.42	126.72
38	5	305	KC1	CAC-C3C-C4C	3.00	128.70	124.81
38	13	311	KC1	CHD-C4C-NC	3.00	128.75	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	16	310	CLA	CHC-C1C-C2C	-3.00	118.42	126.72
39	8	317	DD6	C35-C36-C31	-3.00	113.76	120.57
38	1	308	KC1	C4C-C3C-C2C	-3.00	102.53	106.90
30	16	301	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
38	11	312	KC1	CMB-C2B-C1B	3.00	130.00	124.71
30	12	308	CLA	CHC-C1C-C2C	-3.00	118.43	126.72
30	A	822	CLA	C3B-C4B-NB	3.00	113.08	109.21
30	B	816	CLA	C4-C3-C5	3.00	120.31	115.27
30	A	822	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
30	15	312	CLA	CHD-C4C-NC	3.00	128.93	124.20
38	2	306	KC1	CAA-C2A-C1A	-3.00	110.97	124.75
30	16	303	CLA	C1-C2-C3	-3.00	120.86	126.04
30	13	303	CLA	CAA-C2A-C3A	-3.00	104.57	112.78
29	A	801	CL0	C4C-C3C-C2C	-3.00	102.53	106.90
30	2u	202	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
38	8	306	KC1	CHD-C4C-NC	3.00	128.75	124.20
38	13	306	KC1	CHD-C4C-NC	3.00	128.75	124.20
30	8	302	CLA	CAA-C2A-C3A	-3.00	104.58	112.78
30	A	814	CLA	CHB-C4A-NA	3.00	128.65	124.51
30	A	829	CLA	CHD-C4C-NC	3.00	128.92	124.20
38	9	304	KC1	CHD-C4C-NC	3.00	128.75	124.20
30	B	823	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
30	A	819	CLA	C1C-C2C-C3C	-2.99	103.81	106.96
30	2	301	CLA	CAA-C2A-C3A	-2.99	104.58	112.78
38	4	310	KC1	C4B-C3B-C2B	-2.99	104.29	106.75
30	A	828	CLA	C4-C3-C5	2.99	120.31	115.27
30	4	303	CLA	CHC-C1C-C2C	-2.99	118.44	126.72
30	B	835	CLA	C3B-C4B-NB	2.99	113.08	109.21
30	9	309	CLA	CAA-C2A-C3A	-2.99	104.58	112.78
36	7	320	LMG	C1-C2-C3	-2.99	103.76	110.00
30	13	304	CLA	CHC-C1C-C2C	-2.99	118.44	126.72
30	A	821	CLA	CAC-C3C-C4C	2.99	128.69	124.81
30	14	312	CLA	C3B-C4B-NB	2.99	113.08	109.21
39	6	321	DD6	C40-C32-C31	-2.99	105.71	110.47
37	7	316	A86	C3-C4-C5	-2.99	117.35	123.47
38	2	314	KC1	C4C-C3C-C2C	-2.99	102.54	106.90
37	7	319	A86	C3-C4-C5	-2.99	117.35	123.47
30	14	304	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
30	B	832	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
30	A	828	CLA	C4A-NA-C1A	-2.99	105.36	106.71
30	A	838	CLA	C1-C2-C3	-2.99	120.88	126.04
30	11	306	CLA	CHD-C4C-NC	2.99	128.91	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	J	101	CLA	CHC-C1C-C2C	-2.99	118.46	126.72
30	F	203	CLA	CHD-C4C-NC	2.98	128.91	124.20
38	6	313	KC1	CHD-C4C-NC	2.98	128.73	124.20
30	8	308	CLA	CHD-C4C-NC	2.98	128.91	124.20
30	B	815	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
37	2u	205	A86	C40-C32-C31	-2.98	107.80	110.47
30	13	301	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
30	5	304	CLA	CHC-C1C-C2C	-2.98	118.47	126.72
30	4	306	CLA	CHD-C4C-NC	2.98	128.90	124.20
30	8	303	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
30	6	306	CLA	CHD-C4C-NC	2.98	128.90	124.20
37	4	312	A86	C12-C11-C13	2.98	121.03	116.02
30	1	301	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
37	4	312	A86	C3-C2-C1	-2.98	123.06	127.31
30	B	820	CLA	C4A-NA-C1A	-2.98	105.37	106.71
30	B	838	CLA	O2A-CGA-CBA	2.98	121.26	111.91
30	L	203	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
39	1	310	DD6	C35-C36-C31	-2.98	113.81	120.57
30	B	804	CLA	O2A-CGA-CBA	2.98	121.26	111.91
37	5	315	A86	C3-C2-C1	-2.98	123.06	127.31
30	2	307	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
38	7	308	KC1	C4C-C3C-C2C	-2.98	102.56	106.90
30	B	831	CLA	CHD-C4C-NC	2.98	128.90	124.20
30	B	801	CLA	CMB-C2B-C1B	2.98	133.04	128.46
30	10	311	CLA	CAC-C3C-C4C	2.98	128.67	124.81
30	12	308	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
38	14	311	KC1	C4C-C3C-C2C	-2.98	102.56	106.90
30	2	310	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
30	10	305	CLA	CHC-C1C-C2C	-2.98	118.49	126.72
33	A	849	BCR	C15-C14-C13	-2.98	123.06	127.31
30	B	824	CLA	C3B-C4B-NB	2.98	113.06	109.21
30	16	303	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
30	1	303	CLA	CHD-C4C-NC	2.97	128.89	124.20
30	A	842	CLA	O2A-CGA-CBA	2.97	121.24	111.91
30	12	302	CLA	CAC-C3C-C4C	2.97	128.67	124.81
30	A	828	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
30	B	816	CLA	CHC-C1C-C2C	-2.97	118.50	126.72
30	B	829	CLA	CHC-C1C-C2C	-2.97	118.50	126.72
37	2u	203	A86	C12-C11-C10	-2.97	116.23	123.42
30	9	302	CLA	C4C-C3C-C2C	-2.97	102.56	106.90
38	16	311	KC1	C4C-C3C-C2C	-2.97	102.56	106.90
37	11	316	A86	C10-C9-C8	-2.97	113.94	123.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	3	306	CLA	C4-C3-C5	2.97	120.27	115.27
30	6	314	CLA	CHC-C1C-C2C	-2.97	118.50	126.72
30	A	804	CLA	CHC-C1C-C2C	-2.97	118.50	126.72
30	5	311	CLA	CAA-C2A-C3A	-2.97	104.64	112.78
30	A	813	CLA	CHC-C1C-C2C	-2.97	118.50	126.72
30	B	802	CLA	C1C-C2C-C3C	-2.97	103.83	106.96
30	A	842	CLA	CHD-C4C-NC	2.97	128.88	124.20
37	16	312	A86	C7-C6-C5	-2.97	118.76	122.92
30	B	837	CLA	CMB-C2B-C3B	2.97	130.23	124.68
30	16	305	CLA	C4A-NA-C1A	-2.97	105.37	106.71
30	10	311	CLA	CHD-C4C-NC	2.97	128.88	124.20
38	6	312	KC1	CHD-C4C-NC	2.97	128.71	124.20
30	B	836	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
30	B	820	CLA	C1C-C2C-C3C	-2.97	103.84	106.96
30	14	309	CLA	CAC-C3C-C4C	2.97	128.66	124.81
30	16	307	CLA	CAC-C3C-C4C	2.97	128.66	124.81
37	11	301	A86	C12-C11-C10	-2.97	116.24	123.42
30	15	302	CLA	CMC-C2C-C1C	2.97	129.56	125.04
30	10	309	CLA	CHC-C1C-C2C	-2.97	118.52	126.72
30	10	308	CLA	C3B-C4B-NB	2.97	113.04	109.21
38	13	306	KC1	C1C-C2C-C3C	-2.97	103.84	106.96
38	7	313	KC1	C4B-C3B-C2B	-2.96	104.32	106.75
30	A	839	CLA	C3B-C4B-NB	2.96	113.04	109.21
38	4	307	KC1	CAA-CBA-CGA	-2.96	112.03	127.26
37	14	318	A86	C25-C24-C1	-2.96	118.09	126.42
30	2	313	CLA	CHC-C1C-C2C	-2.96	118.52	126.72
37	11	315	A86	C4-C3-C2	-2.96	117.40	123.47
30	B	851	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
30	14	312	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
30	3	305	CLA	CHD-C4C-NC	2.96	128.87	124.20
30	B	836	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
30	A	819	CLA	CHD-C4C-NC	2.96	128.87	124.20
30	15	308	CLA	CHC-C1C-C2C	-2.96	118.53	126.72
30	A	807	CLA	C1-C2-C3	-2.96	120.92	126.04
30	J	101	CLA	CAC-C3C-C4C	2.96	128.65	124.81
30	A	832	CLA	CAC-C3C-C4C	2.96	128.65	124.81
30	B	805	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
30	L	203	CLA	CHC-C1C-C2C	-2.96	118.54	126.72
39	2	315	DD6	C3-C4-C5	-2.96	117.41	123.47
30	9	306	CLA	CAC-C3C-C4C	2.96	128.65	124.81
30	9	305	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
30	7	303	CLA	CAA-C2A-C3A	-2.96	104.68	112.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	11	310	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
38	9	310	KC1	C4C-C3C-C2C	-2.96	102.59	106.90
30	4	302	CLA	CHC-C1C-C2C	-2.96	118.54	126.72
38	2	306	KC1	O2D-CGD-O1D	-2.96	118.06	123.84
30	B	835	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
38	10	310	KC1	C4C-C3C-C2C	-2.96	102.59	106.90
30	5	311	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
30	8	304	CLA	CHC-C1C-C2C	-2.96	118.55	126.72
30	B	834	CLA	CHD-C4C-NC	2.96	128.86	124.20
30	8	304	CLA	CAC-C3C-C4C	2.96	128.65	124.81
38	11	311	KC1	C4C-C3C-C2C	-2.96	102.59	106.90
30	12	302	CLA	CAA-C2A-C3A	-2.95	104.69	112.78
38	12	305	KC1	CAC-C3C-C4C	2.95	128.64	124.81
30	B	818	CLA	CHC-C1C-C2C	-2.95	118.55	126.72
30	7	306	CLA	C1-C2-C3	-2.95	120.94	126.04
30	2	304	CLA	CHC-C1C-C2C	-2.95	118.55	126.72
30	B	811	CLA	CMB-C2B-C3B	2.95	130.20	124.68
38	5	306	KC1	C4C-C3C-C2C	-2.95	102.59	106.90
30	6	307	CLA	CAC-C3C-C4C	2.95	128.64	124.81
37	2u	203	A86	C36-C31-C32	-2.95	116.77	119.70
30	12	321	CLA	CAC-C3C-C4C	2.95	128.64	124.81
38	3	311	KC1	CAC-C3C-C4C	2.95	128.64	124.81
30	B	806	CLA	CMC-C2C-C1C	2.95	129.53	125.04
30	A	817	CLA	CBC-CAC-C3C	-2.95	104.30	112.43
30	A	816	CLA	C4-C3-C5	2.95	120.23	115.27
30	B	825	CLA	C3B-C4B-NB	2.95	113.02	109.21
30	11	308	CLA	C3B-C4B-NB	2.95	113.02	109.21
30	A	802	CLA	CMC-C2C-C1C	2.95	129.53	125.04
30	15	302	CLA	CHD-C4C-NC	2.95	128.85	124.20
37	2	302	A86	C22-C16-C17	-2.95	103.86	108.98
30	4	304	CLA	CHD-C4C-NC	2.95	128.85	124.20
30	2	313	CLA	CAC-C3C-C4C	2.95	128.63	124.81
30	A	805	CLA	C3B-C4B-NB	2.95	113.02	109.21
30	10	307	CLA	CAC-C3C-C4C	2.95	128.63	124.81
30	A	834	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
30	B	810	CLA	C3B-C4B-NB	2.95	113.02	109.21
38	4	308	KC1	C2A-C1A-NA	2.95	114.13	109.40
30	A	808	CLA	CAC-C3C-C4C	2.95	128.63	124.81
30	12	306	CLA	CBC-CAC-C3C	-2.95	104.31	112.43
30	2	309	CLA	CHC-C1C-C2C	-2.94	118.58	126.72
30	A	823	CLA	CHD-C4C-NC	2.94	128.84	124.20
38	8	314	KC1	CHB-C4A-NA	2.94	128.84	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	8	315	A86	C-C1-C24	2.94	122.72	118.08
30	10	311	CLA	CHC-C1C-C2C	-2.94	118.58	126.72
30	B	801	CLA	C1C-C2C-C3C	-2.94	103.86	106.96
30	3	305	CLA	C4-C3-C5	2.94	120.22	115.27
37	12	316	A86	C9-C10-C11	-2.94	117.96	126.61
38	13	310	KC1	CMC-C2C-C1C	2.94	129.52	125.04
30	3	306	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
30	8	309	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
30	A	805	CLA	CHD-C4C-NC	2.94	128.84	124.20
30	7	305	CLA	CAA-C2A-C3A	-2.94	104.72	112.78
30	16	301	CLA	CMC-C2C-C1C	2.94	129.52	125.04
38	5	310	KC1	CAC-C3C-C4C	2.94	128.63	124.81
38	13	308	KC1	CHD-C4C-NC	2.94	128.66	124.20
30	6	307	CLA	C4-C3-C5	2.94	120.22	115.27
30	B	808	CLA	CBC-CAC-C3C	-2.94	104.32	112.43
30	5	307	CLA	CHD-C4C-NC	2.94	128.84	124.20
37	15	320	A86	C36-C31-C32	-2.94	116.78	119.70
38	6	308	KC1	C4B-C3B-C2B	-2.94	104.34	106.75
39	9	314	DD6	C35-C36-C31	-2.94	113.90	120.57
30	B	835	CLA	CHD-C4C-NC	2.94	128.84	124.20
30	12	312	CLA	CHD-C4C-NC	2.94	128.84	124.20
30	6	309	CLA	CHC-C1C-C2C	-2.94	118.59	126.72
39	13	314	DD6	C21-C20-C15	-2.94	117.33	122.26
38	7	308	KC1	CHD-C4C-NC	2.94	128.66	124.20
33	F	204	BCR	C2-C1-C6	2.94	115.00	110.48
38	12	313	KC1	CMB-C2B-C1B	2.94	129.89	124.71
30	A	812	CLA	CHC-C1C-C2C	-2.94	118.59	126.72
30	B	831	CLA	C4C-C3C-C2C	-2.94	102.62	106.90
30	9	309	CLA	CMB-C2B-C3B	2.94	130.17	124.68
30	7	311	CLA	CHC-C1C-C2C	-2.94	118.60	126.72
38	13	310	KC1	CMB-C2B-C1B	2.94	129.89	124.71
39	15	318	DD6	C14-C13-C11	-2.94	120.97	125.53
30	A	807	CLA	CHC-C1C-C2C	-2.94	118.60	126.72
30	A	834	CLA	CHC-C1C-C2C	-2.93	118.60	126.72
30	A	805	CLA	CBC-CAC-C3C	-2.93	104.34	112.43
30	16	302	CLA	C4C-C3C-C2C	-2.93	102.62	106.90
30	8	305	CLA	OBD-CAD-C3D	-2.93	121.46	128.52
30	13	309	CLA	C4C-C3C-C2C	-2.93	102.62	106.90
30	13	307	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
30	16	308	CLA	C4C-C3C-C2C	-2.93	102.62	106.90
38	8	314	KC1	CHD-C4C-NC	2.93	128.65	124.20
30	A	833	CLA	C4C-C3C-C2C	-2.93	102.62	106.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	13	310	KC1	C4C-C3C-C2C	-2.93	102.62	106.90
38	8	314	KC1	CHB-C1B-NB	-2.93	121.76	124.45
38	12	311	KC1	C4C-C3C-C2C	-2.93	102.62	106.90
30	B	822	CLA	CAC-C3C-C4C	2.93	128.61	124.81
30	16	302	CLA	CAC-C3C-C4C	2.93	128.61	124.81
30	6	310	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
30	6	317	CLA	CHD-C4C-NC	2.93	128.82	124.20
30	A	810	CLA	C4A-NA-C1A	-2.93	105.39	106.71
30	6	316	CLA	C3B-C4B-NB	2.93	113.00	109.21
38	5	312	KC1	CMC-C2C-C1C	2.93	129.50	125.04
30	16	310	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
37	2u	205	A86	C12-C11-C10	-2.93	116.33	123.42
30	11	308	CLA	CHB-C4A-NA	2.93	128.56	124.51
30	2	311	CLA	O2A-CGA-CBA	2.93	121.10	111.91
30	B	851	CLA	C3B-C4B-NB	2.93	113.00	109.21
30	12	304	CLA	CHC-C1C-C2C	-2.93	118.62	126.72
30	16	302	CLA	CHD-C4C-NC	2.93	128.82	124.20
30	4	311	CLA	CAC-C3C-C4C	2.93	128.61	124.81
30	10	308	CLA	CHD-C4C-NC	2.93	128.82	124.20
30	B	824	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
30	5	303	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
39	2	315	DD6	C21-C20-C15	-2.93	117.35	122.26
30	A	824	CLA	CHD-C4C-NC	2.93	128.82	124.20
29	A	801	CL0	CHC-C1C-C2C	-2.93	118.62	126.72
38	1	306	KC1	CAA-C2A-C1A	-2.93	111.28	124.75
30	A	832	CLA	O2A-CGA-CBA	2.93	121.10	111.91
30	9	307	CLA	CHC-C1C-C2C	-2.93	118.62	126.72
30	B	811	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
30	13	302	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
30	5	308	CLA	C4-C3-C5	2.93	120.19	115.27
38	12	313	KC1	CMC-C2C-C1C	2.93	129.50	125.04
30	12	302	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
30	A	842	CLA	C4-C3-C5	2.93	120.19	115.27
30	16	302	CLA	CHC-C1C-C2C	-2.93	118.63	126.72
30	6	304	CLA	C1-C2-C3	-2.93	120.98	126.04
30	1	301	CLA	CAC-C3C-C4C	2.93	128.61	124.81
30	B	818	CLA	O2A-CGA-CBA	2.93	121.09	111.91
30	B	829	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
30	A	833	CLA	CAA-C2A-C3A	-2.92	104.77	112.78
39	5	314	DD6	C33-C32-C31	2.92	115.54	109.62
37	7	315	A86	C41-C32-C31	-2.92	107.86	110.47
38	13	312	KC1	CHD-C4C-NC	2.92	128.63	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	1	304	CLA	C1C-C2C-C3C	-2.92	103.89	106.96
37	10	316	A86	C24-C1-C2	-2.92	114.46	118.94
30	6	315	CLA	CHD-C4C-NC	2.92	128.80	124.20
30	12	304	CLA	CHD-C4C-NC	2.92	128.80	124.20
30	7	305	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
30	A	824	CLA	C4-C3-C5	2.92	119.32	115.98
30	15	312	CLA	CMB-C2B-C3B	2.92	130.14	124.68
30	A	811	CLA	CAA-C2A-C3A	-2.92	104.79	112.78
39	16	313	DD6	C35-C36-C31	-2.92	113.95	120.57
30	A	832	CLA	CHC-C1C-C2C	-2.92	118.65	126.72
30	5	309	CLA	CAA-C2A-C3A	-2.92	104.79	112.78
30	A	817	CLA	CMB-C2B-C3B	2.92	130.14	124.68
30	6	310	CLA	CMB-C2B-C3B	2.92	130.14	124.68
30	4	311	CLA	O2A-CGA-CBA	2.92	121.06	111.91
30	3	305	CLA	C4C-C3C-C2C	-2.92	102.65	106.90
30	A	811	CLA	C4C-C3C-C2C	-2.92	102.65	106.90
30	4	304	CLA	C4C-C3C-C2C	-2.92	102.65	106.90
30	12	321	CLA	C4C-C3C-C2C	-2.92	102.65	106.90
30	2u	202	CLA	CAC-C3C-C4C	2.92	128.59	124.81
38	4	308	KC1	CAA-CBA-CGA	-2.92	112.28	127.26
33	M	101	BCR	C15-C16-C17	-2.91	117.50	123.47
30	2	313	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
30	B	813	CLA	CHC-C1C-C2C	-2.91	118.66	126.72
30	11	304	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
30	B	827	CLA	CHC-C1C-C2C	-2.91	118.66	126.72
30	9	308	CLA	CHD-C4C-NC	2.91	128.79	124.20
30	13	302	CLA	CHD-C4C-NC	2.91	128.79	124.20
38	1	306	KC1	C4C-C3C-C2C	-2.91	102.65	106.90
30	3	310	CLA	CHD-C4C-NC	2.91	128.79	124.20
30	9	306	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
30	11	306	CLA	C1-C2-C3	-2.91	121.01	126.04
30	5	308	CLA	O2A-CGA-CBA	2.91	121.04	111.91
30	A	810	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
30	A	835	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
38	6	313	KC1	C4C-C3C-C2C	-2.91	102.66	106.90
38	11	305	KC1	CAA-C2A-C1A	-2.91	111.37	124.75
30	12	307	CLA	C1C-C2C-C3C	-2.91	103.90	106.96
39	5	314	DD6	C21-C20-C15	-2.91	117.39	122.26
30	A	840	CLA	CMC-C2C-C1C	2.91	129.47	125.04
30	A	815	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
37	13	315	A86	C35-C34-C33	2.91	114.95	109.88
30	B	806	CLA	C3B-C4B-NB	2.91	112.97	109.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	9	311	KC1	CHD-C4C-NC	2.91	128.61	124.20
30	16	302	CLA	C1-C2-C3	-2.91	121.02	126.04
30	B	824	CLA	CHC-C1C-C2C	-2.91	118.68	126.72
30	15	314	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
30	3	309	CLA	CHD-C4C-NC	2.91	128.78	124.20
37	4	314	A86	C23-C16-C17	-2.91	103.93	108.98
38	16	304	KC1	CAC-C3C-C4C	2.91	128.58	124.81
30	8	309	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
39	15	319	DD6	C21-C20-C19	-2.90	111.01	114.28
30	A	806	CLA	CHC-C1C-C2C	-2.90	118.69	126.72
30	2u	202	CLA	CHC-C1C-C2C	-2.90	118.69	126.72
30	15	305	CLA	C4C-C3C-C2C	-2.90	102.66	106.90
30	5	311	CLA	C4-C3-C5	2.90	120.16	115.27
30	A	838	CLA	CHD-C4C-NC	2.90	128.78	124.20
30	7	310	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
30	10	303	CLA	CBC-CAC-C3C	-2.90	104.43	112.43
30	A	821	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
37	4	314	A86	C40-C32-C31	-2.90	107.87	110.47
30	14	302	CLA	C3B-C4B-NB	2.90	112.96	109.21
30	14	313	CLA	CHC-C1C-C2C	-2.90	118.69	126.72
30	A	802	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
30	B	816	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
30	6	309	CLA	C3B-C4B-NB	2.90	112.96	109.21
30	A	804	CLA	CHD-C4C-NC	2.90	128.78	124.20
30	B	838	CLA	CAA-C2A-C3A	-2.90	104.83	112.78
30	13	302	CLA	CHC-C1C-C2C	-2.90	118.70	126.72
30	5	304	CLA	CHB-C4A-NA	2.90	128.52	124.51
30	9	309	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
30	15	310	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
30	1	303	CLA	C3B-C4B-NB	2.90	112.96	109.21
30	1	305	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
30	A	811	CLA	C1-C2-C3	-2.90	121.03	126.04
30	15	313	CLA	CHD-C4C-NC	2.90	128.77	124.20
38	11	305	KC1	CHD-C4C-NC	2.90	128.60	124.20
30	12	312	CLA	CBC-CAC-C3C	-2.90	104.44	112.43
30	4	305	CLA	C4-C3-C5	2.90	120.15	115.27
30	A	821	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
30	A	811	CLA	CHD-C4C-NC	2.90	128.77	124.20
37	15	315	A86	C4-C5-C6	2.90	131.45	127.31
30	3	301	CLA	CMB-C2B-C3B	2.90	130.10	124.68
30	A	838	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
30	A	825	CLA	O2A-CGA-CBA	2.90	121.00	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	15	314	CLA	CMC-C2C-C1C	2.90	129.45	125.04
38	5	312	KC1	CBA-CAA-C2A	-2.90	114.23	125.27
37	11	314	A86	C35-C34-C33	2.90	114.93	109.88
37	15	315	A86	C36-C31-C32	-2.90	116.82	119.70
30	6	305	CLA	CHC-C1C-C2C	-2.90	118.71	126.72
30	A	823	CLA	CMB-C2B-C3B	2.90	130.10	124.68
38	8	312	KC1	CAC-C3C-C4C	2.89	128.57	124.81
30	B	831	CLA	CHC-C1C-C2C	-2.89	118.72	126.72
30	9	309	CLA	O2A-CGA-CBA	2.89	120.99	111.91
30	2	309	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
30	5	307	CLA	CHC-C1C-C2C	-2.89	118.72	126.72
36	8	320	LMG	O6-C1-O1	-2.89	103.12	109.97
30	1	307	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
30	A	844	CLA	CHB-C4A-NA	2.89	128.51	124.51
30	B	804	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
30	8	303	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
30	11	306	CLA	CMC-C2C-C1C	2.89	129.44	125.04
30	10	308	CLA	CAA-C2A-C3A	-2.89	104.86	112.78
30	12	304	CLA	CAC-C3C-C4C	2.89	128.56	124.81
30	15	305	CLA	CAA-C2A-C3A	-2.89	104.86	112.78
30	A	819	CLA	CAC-C3C-C4C	2.89	128.56	124.81
30	2	303	CLA	CMD-C2D-C1D	2.89	129.81	124.71
30	6	305	CLA	CAC-C3C-C4C	2.89	128.56	124.81
38	10	306	KC1	C4C-C3C-C2C	-2.89	102.69	106.90
30	6	306	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
30	12	308	CLA	CAA-C2A-C3A	-2.89	104.87	112.78
30	7	311	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
30	9	305	CLA	CHD-C4C-NC	2.89	128.75	124.20
30	8	302	CLA	C4-C3-C5	2.89	120.13	115.27
38	4	310	KC1	CAC-C3C-C4C	2.89	128.56	124.81
38	12	313	KC1	O2D-CGD-O1D	-2.89	118.19	123.84
36	3	317	LMG	O6-C5-C4	2.89	114.94	109.69
39	15	318	DD6	C25-C24-C1	-2.89	118.31	126.42
30	B	805	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
30	A	842	CLA	C3B-C4B-NB	2.89	112.94	109.21
30	B	828	CLA	CMD-C2D-C3D	-2.89	120.98	127.61
30	B	832	CLA	CMA-C3A-C2A	-2.89	102.19	113.83
30	4	306	CLA	CHC-C1C-C2C	-2.88	118.74	126.72
37	7	319	A86	C40-C32-C31	-2.88	107.89	110.47
38	9	310	KC1	O2D-CGD-O1D	-2.88	118.20	123.84
30	B	803	CLA	C3B-C4B-NB	2.88	112.94	109.21
30	5	311	CLA	CHC-C1C-C2C	-2.88	118.75	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	A	850	BCR	C24-C23-C22	-2.88	121.88	126.23
30	A	818	CLA	C3B-C4B-NB	2.88	112.94	109.21
30	A	844	CLA	CAC-C3C-C4C	2.88	128.55	124.81
38	14	308	KC1	CMB-C2B-C1B	2.88	129.79	124.71
30	B	836	CLA	CHC-C1C-C2C	-2.88	118.75	126.72
30	B	835	CLA	O2A-CGA-CBA	2.88	120.95	111.91
38	13	305	KC1	O2D-CGD-O1D	-2.88	118.20	123.84
30	10	305	CLA	CAC-C3C-C4C	2.88	128.55	124.81
37	8	318	A86	C12-C11-C13	2.88	120.86	116.02
30	A	828	CLA	C1-C2-C3	-2.88	121.06	126.04
38	6	312	KC1	C4C-C3C-C2C	-2.88	102.70	106.90
37	11	315	A86	C26-C25-C24	-2.88	114.23	123.22
30	B	802	CLA	CHA-C1A-NA	-2.88	119.80	126.40
30	14	312	CLA	CAA-C2A-C3A	-2.88	104.89	112.78
30	A	838	CLA	CHC-C1C-C2C	-2.88	118.75	126.72
30	10	303	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
30	14	305	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
30	A	834	CLA	CHD-C4C-NC	2.88	128.74	124.20
30	6	315	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
38	1	306	KC1	CHC-C4B-NB	-2.88	121.81	124.45
30	11	306	CLA	C1-O2A-CGA	2.88	124.00	116.44
30	B	808	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
30	9	305	CLA	CHC-C1C-C2C	-2.88	118.76	126.72
38	13	308	KC1	O2D-CGD-O1D	-2.88	118.21	123.84
30	B	825	CLA	CAA-C2A-C3A	-2.88	104.90	112.78
37	8	318	A86	C3-C4-C5	2.88	129.37	123.47
30	F	202	CLA	CAC-C3C-C4C	2.88	128.54	124.81
30	14	302	CLA	CHC-C1C-C2C	-2.88	118.76	126.72
30	B	807	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
30	15	303	CLA	CHC-C1C-C2C	-2.88	118.76	126.72
30	8	304	CLA	C1C-C2C-C3C	-2.88	103.93	106.96
30	9	308	CLA	CBA-CAA-C2A	2.88	122.35	113.86
30	A	817	CLA	CHD-C4C-NC	2.88	128.74	124.20
30	2	304	CLA	CHD-C4C-NC	2.88	128.74	124.20
30	6	305	CLA	O2A-CGA-CBA	2.88	120.93	111.91
38	3	304	KC1	C4C-C3C-C2C	-2.88	102.71	106.90
30	12	312	CLA	CAC-C3C-C4C	2.88	128.54	124.81
38	14	306	KC1	CMC-C2C-C1C	2.88	129.42	125.04
30	B	851	CLA	CHD-C4C-NC	2.88	128.73	124.20
30	11	304	CLA	C3B-C4B-NB	2.88	112.93	109.21
30	2	309	CLA	CAA-C2A-C3A	-2.88	104.91	112.78
30	B	808	CLA	O2D-CGD-O1D	-2.87	118.22	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	9	316	A86	C4-C3-C2	-2.87	117.58	123.47
30	12	312	CLA	C1-C2-C3	-2.87	121.07	126.04
30	1	302	CLA	CBC-CAC-C3C	-2.87	104.51	112.43
30	A	814	CLA	C1-O2A-CGA	2.87	123.98	116.44
30	B	813	CLA	CMB-C2B-C3B	2.87	130.06	124.68
30	B	826	CLA	C1-C2-C3	-2.87	121.07	126.04
30	10	305	CLA	C4-C3-C5	2.87	120.11	115.27
30	5	303	CLA	CHC-C1C-C2C	-2.87	118.77	126.72
30	4	302	CLA	CBC-CAC-C3C	-2.87	104.51	112.43
35	15	301	LMT	O1B-C4'-C3'	2.87	114.92	107.28
30	B	851	CLA	C4-C3-C5	2.87	120.10	115.27
30	13	307	CLA	CMB-C2B-C3B	2.87	130.05	124.68
30	B	829	CLA	C4-C3-C5	2.87	120.10	115.27
38	12	309	KC1	CAA-CBA-CGA	-2.87	112.50	127.26
30	4	301	CLA	C3B-C4B-NB	2.87	112.92	109.21
30	15	304	CLA	CED-O2D-CGD	2.87	122.43	115.94
30	6	304	CLA	CBA-CAA-C2A	2.87	122.33	113.86
30	A	834	CLA	CAA-C2A-C3A	-2.87	104.92	112.78
30	A	803	CLA	C3B-C4B-NB	2.87	112.92	109.21
35	9	317	LMT	O5'-C1'-C2'	2.87	116.42	110.35
30	15	307	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
30	2	308	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
30	8	301	CLA	CHB-C4A-NA	2.87	128.48	124.51
30	12	306	CLA	CAC-C3C-C4C	2.87	128.53	124.81
30	3	303	CLA	CHD-C4C-NC	2.87	128.72	124.20
30	B	835	CLA	CHC-C1C-C2C	-2.87	118.79	126.72
30	L	203	CLA	CHD-C4C-NC	2.87	128.72	124.20
30	5	303	CLA	CHD-C4C-NC	2.87	128.72	124.20
30	7	305	CLA	CHD-C4C-NC	2.87	128.72	124.20
30	B	811	CLA	CHC-C1C-C2C	-2.87	118.79	126.72
33	A	849	BCR	C40-C30-C25	2.87	114.95	110.30
33	J	103	BCR	C27-C26-C25	2.87	126.89	122.73
30	J	101	CLA	C3B-C4B-NB	2.87	112.92	109.21
30	A	841	CLA	CAC-C3C-C4C	2.87	128.53	124.81
30	B	832	CLA	CMA-C3A-C4A	-2.87	104.07	111.77
30	5	308	CLA	CMC-C2C-C1C	2.87	129.40	125.04
30	3	306	CLA	CAC-C3C-C4C	2.87	128.53	124.81
30	B	822	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
30	B	807	CLA	CAA-C2A-C3A	-2.87	104.93	112.78
37	16	312	A86	C35-C34-C33	2.86	114.88	109.88
30	7	305	CLA	CHB-C4A-NA	2.86	128.47	124.51
30	A	843	CLA	CAC-C3C-C4C	2.86	128.53	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	811	CLA	CMB-C2B-C3B	2.86	130.03	124.68
30	14	307	CLA	C3B-C4B-NB	2.86	112.91	109.21
30	A	836	CLA	C4C-C3C-C2C	-2.86	102.72	106.90
30	16	307	CLA	C4C-C3C-C2C	-2.86	102.72	106.90
30	5	302	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
30	A	808	CLA	CMC-C2C-C1C	2.86	129.40	125.04
39	12	317	DD6	C22-C16-C15	2.86	117.77	110.05
38	9	310	KC1	CHD-C4C-NC	2.86	128.54	124.20
33	L	204	BCR	C15-C16-C17	-2.86	117.61	123.47
38	11	312	KC1	C1A-NA-C4A	-2.86	105.42	106.71
30	B	833	CLA	C3B-C4B-NB	2.86	112.91	109.21
30	4	301	CLA	CAA-C2A-C3A	-2.86	104.95	112.78
30	15	309	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
38	4	308	KC1	CBC-CAC-C3C	-2.86	104.55	112.43
30	16	306	CLA	CHC-C1C-C2C	-2.86	118.81	126.72
37	12	316	A86	C3-C4-C5	-2.86	117.62	123.47
37	14	319	A86	C25-C24-C1	-2.86	118.38	126.42
37	10	316	A86	C20-C19-C18	-2.86	107.09	112.75
30	14	310	CLA	CAC-C3C-C4C	2.86	128.52	124.81
30	6	314	CLA	CHD-C4C-NC	2.86	128.71	124.20
30	5	308	CLA	CHD-C4C-NC	2.86	128.71	124.20
30	F	201	CLA	O2A-CGA-CBA	2.86	120.88	111.91
30	16	309	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
37	14	315	A86	C4-C3-C2	-2.86	117.62	123.47
37	14	314	A86	C12-C11-C10	-2.86	116.51	123.42
30	5	304	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
30	B	839	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
38	4	310	KC1	C4C-C3C-C2C	-2.86	102.73	106.90
39	15	319	DD6	C14-C13-C11	-2.86	121.10	125.53
30	3	309	CLA	CHC-C1C-C2C	-2.86	118.82	126.72
30	8	301	CLA	CHD-C4C-NC	2.85	128.70	124.20
37	8	318	A86	C36-C31-C32	-2.85	116.86	119.70
30	A	816	CLA	CAC-C3C-C4C	2.85	128.51	124.81
30	A	809	CLA	CHC-C1C-C2C	-2.85	118.83	126.72
30	12	306	CLA	CAA-C2A-C3A	-2.85	104.96	112.78
30	12	310	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
30	5	302	CLA	C3B-C4B-NB	2.85	112.90	109.21
38	5	312	KC1	C4C-C3C-C2C	-2.85	102.74	106.90
30	14	303	CLA	CHD-C4C-NC	2.85	128.70	124.20
30	A	836	CLA	O2A-CGA-CBA	2.85	120.86	111.91
30	B	822	CLA	CHC-C1C-C2C	-2.85	118.83	126.72
30	10	308	CLA	CMB-C2B-C3B	2.85	130.02	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	835	CLA	CHD-C4C-NC	2.85	128.70	124.20
39	6	321	DD6	C33-C34-C35	2.85	114.21	110.30
30	12	308	CLA	CAC-C3C-C4C	2.85	128.51	124.81
30	15	313	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
30	12	310	CLA	CHC-C1C-C2C	-2.85	118.83	126.72
38	9	304	KC1	CMB-C2B-C1B	2.85	129.74	124.71
30	B	801	CLA	CMC-C2C-C1C	2.85	129.38	125.04
30	6	304	CLA	C3B-C4B-NB	2.85	112.89	109.21
33	A	849	BCR	C27-C26-C25	2.85	126.87	122.73
30	3	302	CLA	CHC-C1C-C2C	-2.85	118.84	126.72
30	11	308	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
37	3	314	A86	C25-C24-C1	-2.85	118.41	126.42
38	4	308	KC1	CHD-C4C-NC	2.85	128.53	124.20
30	B	831	CLA	O1D-CGD-CBD	-2.85	118.65	124.48
30	7	307	CLA	O2A-CGA-CBA	2.85	120.85	111.91
30	11	304	CLA	C4-C3-C5	2.85	120.06	115.27
38	11	305	KC1	CAC-C3C-C4C	2.85	128.51	124.81
37	11	314	A86	C4-C3-C2	-2.85	117.64	123.47
30	A	805	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
30	15	313	CLA	C4-C3-C5	2.85	120.06	115.27
30	B	804	CLA	CHD-C4C-NC	2.85	128.69	124.20
30	A	824	CLA	O2A-CGA-CBA	2.85	120.84	111.91
30	2	307	CLA	CHB-C4A-NA	2.85	128.45	124.51
30	15	311	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
30	7	310	CLA	CHD-C4C-NC	2.85	128.69	124.20
38	9	311	KC1	O2D-CGD-O1D	-2.85	118.27	123.84
30	5	307	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
30	14	310	CLA	CHB-C4A-NA	2.85	128.45	124.51
30	B	817	CLA	CAC-C3C-C4C	2.85	128.50	124.81
30	2	311	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
30	A	820	CLA	C4C-C3C-C2C	-2.84	102.75	106.90
38	12	313	KC1	C4C-C3C-C2C	-2.84	102.75	106.90
38	5	305	KC1	C4C-C3C-C2C	-2.84	102.75	106.90
38	10	312	KC1	CAA-C2A-C1A	-2.84	111.67	124.75
30	A	824	CLA	CHC-C1C-C2C	-2.84	118.86	126.72
30	L	202	CLA	C4C-C3C-C2C	-2.84	102.75	106.90
30	6	309	CLA	CHD-C4C-NC	2.84	128.68	124.20
39	6	319	DD6	C33-C32-C31	2.84	115.38	109.62
30	10	308	CLA	CHC-C1C-C2C	-2.84	118.86	126.72
30	A	840	CLA	CHC-C1C-C2C	-2.84	118.86	126.72
38	8	307	KC1	C4C-C3C-C2C	-2.84	102.76	106.90
36	B	847	LMG	O1-C7-C8	-2.84	104.04	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	11	304	CLA	CAC-C3C-C4C	2.84	128.50	124.81
30	10	305	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
37	16	312	A86	C-C1-C2	-2.84	118.94	122.92
30	14	302	CLA	O2A-CGA-CBA	2.84	120.82	111.91
39	6	319	DD6	C37-C36-C35	-2.84	109.09	114.36
30	12	306	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
30	2	304	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
30	4	301	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
30	A	818	CLA	O2A-CGA-CBA	2.84	120.82	111.91
30	A	835	CLA	O2A-CGA-CBA	2.84	120.82	111.91
30	6	316	CLA	CAA-C2A-C3A	-2.84	105.00	112.78
30	L	203	CLA	CAA-C2A-C3A	-2.84	105.00	112.78
30	13	309	CLA	CAC-C3C-C4C	2.84	128.49	124.81
37	8	315	A86	C25-C26-C27	-2.84	123.26	127.31
30	A	829	CLA	C1-C2-C3	-2.84	121.13	126.04
30	B	806	CLA	CHC-C1C-C2C	-2.84	118.87	126.72
39	5	313	DD6	C21-C20-C15	-2.84	117.50	122.26
30	10	303	CLA	CAC-C3C-C4C	2.84	128.49	124.81
37	15	316	A86	C3-C4-C5	-2.84	117.66	123.47
30	3	302	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
30	2	304	CLA	CAC-C3C-C4C	2.84	128.49	124.81
30	7	312	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
30	A	837	CLA	C4C-C3C-C2C	-2.84	102.77	106.90
30	B	821	CLA	CAC-C3C-C4C	2.83	128.49	124.81
30	7	305	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
30	14	313	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
38	6	311	KC1	C4C-C3C-C2C	-2.83	102.77	106.90
39	8	317	DD6	C15-C14-C13	-2.83	120.00	125.99
30	10	305	CLA	CHD-C4C-NC	2.83	128.67	124.20
33	L	204	BCR	C15-C14-C13	-2.83	123.27	127.31
30	2	301	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
30	A	836	CLA	CAA-C2A-C3A	-2.83	105.03	112.78
30	9	303	CLA	CHC-C1C-C2C	-2.83	118.89	126.72
30	J	101	CLA	CHD-C4C-NC	2.83	128.66	124.20
36	8	320	LMG	O7-C10-O9	-2.83	116.86	123.70
38	12	305	KC1	C4C-C3C-C2C	-2.83	102.77	106.90
30	3	301	CLA	CHD-C4C-NC	2.83	128.66	124.20
30	15	303	CLA	CAA-C2A-C3A	-2.83	105.03	112.78
30	7	303	CLA	CHD-C4C-NC	2.83	128.66	124.20
38	5	310	KC1	CHD-C4C-NC	2.83	128.49	124.20
30	3	309	CLA	C4C-C3C-C2C	-2.83	102.78	106.90
30	16	305	CLA	CHB-C4A-NA	2.83	128.42	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	14	309	CLA	C4C-C3C-C2C	-2.83	102.78	106.90
30	B	807	CLA	CHC-C1C-C2C	-2.83	118.90	126.72
30	15	314	CLA	CHC-C1C-C2C	-2.83	118.90	126.72
39	6	319	DD6	C25-C24-C1	-2.83	118.48	126.42
30	B	806	CLA	CBC-CAC-C3C	-2.83	104.64	112.43
30	11	304	CLA	CHD-C4C-NC	2.83	128.66	124.20
30	4	302	CLA	C4C-C3C-C2C	-2.82	102.78	106.90
39	15	318	DD6	C33-C32-C31	2.82	115.34	109.62
30	8	302	CLA	CHC-C1C-C2C	-2.82	118.91	126.72
30	B	832	CLA	CAA-C2A-C3A	-2.82	105.05	112.78
38	13	312	KC1	CAC-C3C-C4C	2.82	128.47	124.81
30	16	301	CLA	CHC-C1C-C2C	-2.82	118.91	126.72
30	3	305	CLA	CAA-C2A-C3A	-2.82	105.05	112.78
38	11	305	KC1	C4C-C3C-C2C	-2.82	102.78	106.90
30	A	833	CLA	CHC-C1C-C2C	-2.82	118.91	126.72
30	A	818	CLA	CAC-C3C-C4C	2.82	128.47	124.81
30	13	302	CLA	CAC-C3C-C4C	2.82	128.47	124.81
38	2	306	KC1	CHD-C4C-NC	2.82	128.49	124.20
30	13	307	CLA	C4C-C3C-C2C	-2.82	102.78	106.90
33	B	841	BCR	C15-C16-C17	-2.82	117.69	123.47
38	11	311	KC1	CHD-C4C-NC	2.82	128.49	124.20
30	4	304	CLA	CHC-C1C-C2C	-2.82	118.92	126.72
30	3	306	CLA	CHC-C1C-C2C	-2.82	118.92	126.72
30	A	807	CLA	C3B-C4B-NB	2.82	112.86	109.21
30	12	302	CLA	CBC-CAC-C3C	-2.82	104.65	112.43
37	4	312	A86	C26-C25-C24	-2.82	114.41	123.22
30	4	305	CLA	C4C-C3C-C2C	-2.82	102.78	106.90
30	6	305	CLA	CHD-C4C-NC	2.82	128.65	124.20
30	A	828	CLA	CHC-C1C-C2C	-2.82	118.92	126.72
37	16	314	A86	C3-C4-C5	-2.82	117.70	123.47
30	15	309	CLA	CMB-C2B-C3B	2.82	129.95	124.68
30	12	321	CLA	CHD-C4C-NC	2.82	128.65	124.20
30	B	836	CLA	O2A-CGA-CBA	2.82	120.75	111.91
30	B	816	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
30	11	309	CLA	C1-C2-C3	-2.82	121.17	126.04
30	4	306	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
37	9	315	A86	C36-C31-C32	-2.82	116.90	119.70
38	13	308	KC1	C4C-C3C-C2C	-2.82	102.79	106.90
30	2	311	CLA	CHC-C1C-C2C	-2.82	118.93	126.72
30	5	302	CLA	CAC-C3C-C4C	2.82	128.47	124.81
38	9	310	KC1	CAC-C3C-C4C	2.82	128.47	124.81
30	A	830	CLA	CAC-C3C-C4C	2.82	128.47	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	824	CLA	CAC-C3C-C4C	2.82	128.47	124.81
30	4	306	CLA	CAC-C3C-C4C	2.82	128.47	124.81
30	15	308	CLA	O2A-CGA-O1A	-2.82	116.28	123.30
37	14	319	A86	C10-C9-C8	-2.82	114.43	123.22
30	A	813	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
30	5	304	CLA	CHD-C4C-NC	2.82	128.64	124.20
30	A	839	CLA	CAC-C3C-C4C	2.82	128.46	124.81
30	6	307	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
30	16	306	CLA	C1-C2-C3	-2.82	121.17	126.04
38	5	306	KC1	CHD-C4C-NC	2.82	128.47	124.20
30	4	309	CLA	CAC-C3C-C4C	2.81	128.46	124.81
38	8	313	KC1	CAC-C3C-C4C	2.81	128.46	124.81
30	1	302	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
30	6	306	CLA	CHC-C1C-C2C	-2.81	118.94	126.72
30	A	813	CLA	CHD-C4C-NC	2.81	128.64	124.20
39	13	314	DD6	C25-C24-C1	-2.81	118.51	126.42
30	F	203	CLA	CHC-C1C-C2C	-2.81	118.94	126.72
37	12	314	A86	C10-C9-C8	-2.81	114.44	123.22
30	B	838	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
30	3	303	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
30	16	301	CLA	CAC-C3C-C4C	2.81	128.46	124.81
39	8	317	DD6	C10-C9-C8	-2.81	114.44	123.22
30	5	309	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
30	2	303	CLA	C3D-C2D-C1D	-2.81	101.99	105.83
30	2	305	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
38	9	311	KC1	C4C-C3C-C2C	-2.81	102.80	106.90
38	8	314	KC1	CMB-C2B-C1B	2.81	129.67	124.71
38	11	311	KC1	CAA-CBA-CGA	-2.81	112.81	127.26
30	4	306	CLA	CAA-C2A-C3A	-2.81	105.09	112.78
37	4	317	A86	C19-C18-C17	-2.81	105.35	110.77
39	3	316	DD6	O1-C20-C21	-2.81	111.69	115.06
30	A	841	CLA	CAA-C2A-C3A	-2.81	105.09	112.78
37	2u	203	A86	C40-C32-C31	-2.81	107.96	110.47
30	B	851	CLA	CMC-C2C-C1C	2.81	129.31	125.04
30	12	306	CLA	C4C-C3C-C2C	-2.81	102.81	106.90
38	13	308	KC1	CAC-C3C-C4C	2.81	128.45	124.81
37	14	315	A86	C26-C25-C24	-2.81	114.46	123.22
37	15	316	A86	C25-C24-C1	-2.81	118.53	126.42
30	12	307	CLA	C3B-C4B-NB	2.80	112.84	109.21
39	6	318	DD6	C35-C36-C31	-2.80	114.20	120.57
37	4	315	A86	C34-O4-C38	-2.80	112.67	117.90
30	B	837	CLA	CHC-C1C-C2C	-2.80	118.97	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	14	310	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
37	7	319	A86	C23-C16-C17	-2.80	104.11	108.98
30	A	844	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
30	15	302	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
30	12	321	CLA	CAA-C2A-C3A	-2.80	105.11	112.78
30	B	825	CLA	CHD-C4C-NC	2.80	128.62	124.20
30	B	837	CLA	CHD-C4C-NC	2.80	128.62	124.20
30	12	303	CLA	CAA-C2A-C3A	-2.80	105.11	112.78
30	B	810	CLA	CMC-C2C-C1C	2.80	129.30	125.04
30	B	827	CLA	C1-C2-C3	-2.80	121.20	126.04
30	16	303	CLA	O2A-CGA-CBA	2.80	120.69	111.91
30	12	310	CLA	CHD-C4C-NC	2.80	128.62	124.20
30	16	305	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
30	6	304	CLA	CHC-C1C-C2C	-2.80	118.98	126.72
30	A	809	CLA	CHD-C4C-NC	2.80	128.61	124.20
30	16	310	CLA	CHD-C4C-NC	2.80	128.61	124.20
30	L	202	CLA	CHC-C1C-C2C	-2.80	118.98	126.72
30	1	303	CLA	CMB-C2B-C3B	2.80	129.91	124.68
30	A	816	CLA	CHD-C4C-NC	2.80	128.61	124.20
30	A	839	CLA	CHD-C4C-NC	2.80	128.61	124.20
30	2	307	CLA	O2A-CGA-CBA	2.80	120.69	111.91
30	F	203	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
30	3	301	CLA	CBC-CAC-C3C	-2.80	104.72	112.43
30	8	304	CLA	CHD-C4C-NC	2.80	128.61	124.20
37	15	320	A86	C25-C24-C1	-2.80	118.56	126.42
30	A	841	CLA	C3B-C4B-NB	2.80	112.83	109.21
30	11	304	CLA	C1-C2-C3	-2.80	121.21	126.04
30	B	816	CLA	O2A-CGA-CBA	2.80	120.68	111.91
37	13	313	A86	C25-C24-C1	-2.80	118.56	126.42
38	4	310	KC1	CHD-C4C-NC	2.80	128.44	124.20
30	4	301	CLA	CMB-C2B-C3B	2.80	129.91	124.68
30	9	308	CLA	C4-C3-C5	2.80	119.97	115.27
30	6	307	CLA	O2A-CGA-CBA	2.80	120.68	111.91
29	A	801	CL0	CMC-C2C-C1C	2.79	129.29	125.04
39	6	318	DD6	C9-C8-C6	-2.79	118.57	126.42
38	8	310	KC1	CAC-C3C-C4C	2.79	128.44	124.81
30	12	308	CLA	CHD-C4C-NC	2.79	128.60	124.20
30	3	305	CLA	CAC-C3C-C4C	2.79	128.43	124.81
38	6	313	KC1	CMB-C2B-C1B	2.79	129.63	124.71
30	15	309	CLA	CAC-C3C-C4C	2.79	128.43	124.81
38	9	310	KC1	CMB-C2B-C1B	2.79	129.63	124.71
38	13	310	KC1	CAC-C3C-C4C	2.79	128.43	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	13	314	DD6	C23-C16-C17	-2.79	104.13	108.98
37	2	319	A86	C10-C9-C8	-2.79	114.51	123.22
30	3	307	CLA	CAA-C2A-C3A	-2.79	105.14	112.78
30	A	842	CLA	CHC-C1C-C2C	-2.79	119.00	126.72
30	B	818	CLA	CAC-C3C-C4C	2.79	128.43	124.81
30	11	304	CLA	CHC-C1C-C2C	-2.79	119.00	126.72
30	14	313	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
30	15	307	CLA	CAC-C3C-C4C	2.79	128.43	124.81
30	13	303	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
38	12	313	KC1	CBA-CAA-C2A	-2.79	114.64	125.27
30	12	303	CLA	C4-C3-C5	2.79	119.96	115.27
30	B	801	CLA	CHB-C4A-NA	2.79	128.37	124.51
38	8	307	KC1	CAA-CBA-CGA	-2.79	112.93	127.26
38	14	311	KC1	CAC-C3C-C4C	2.79	128.43	124.81
33	B	844	BCR	C15-C14-C13	-2.79	123.33	127.31
30	8	308	CLA	CHC-C1C-C2C	-2.79	119.01	126.72
30	B	814	CLA	CHD-C4C-NC	2.79	128.59	124.20
37	5	301	A86	C26-C25-C24	-2.79	114.52	123.22
30	4	305	CLA	CHC-C1C-C2C	-2.79	119.02	126.72
30	2	310	CLA	CHD-C4C-NC	2.79	128.59	124.20
38	13	311	KC1	C4C-C3C-C2C	-2.78	102.84	106.90
39	2	316	DD6	C37-C36-C35	-2.78	109.20	114.36
38	10	306	KC1	CHD-C4C-NC	2.78	128.43	124.20
30	14	312	CLA	CAC-C3C-C4C	2.78	128.42	124.81
38	3	304	KC1	CHD-C4C-NC	2.78	128.43	124.20
39	10	314	DD6	C35-C36-C31	-2.78	114.26	120.57
38	12	311	KC1	CHD-C4C-NC	2.78	128.42	124.20
37	4	317	A86	C10-C9-C8	-2.78	114.54	123.22
30	6	315	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
39	16	313	DD6	C23-C16-C15	-2.78	102.54	110.05
37	2u	205	A86	C19-C18-C17	-2.78	105.41	110.77
38	2	314	KC1	CBA-CAA-C2A	-2.78	114.67	125.27
30	J	101	CLA	CMB-C2B-C3B	2.78	129.88	124.68
30	10	307	CLA	CHC-C1C-C2C	-2.78	119.03	126.72
30	5	307	CLA	CAC-C3C-C4C	2.78	128.41	124.81
39	5	314	DD6	C25-C24-C1	-2.78	118.61	126.42
30	4	302	CLA	CMC-C2C-C1C	2.78	129.27	125.04
30	7	304	CLA	CHD-C4C-NC	2.78	128.58	124.20
30	12	303	CLA	CHD-C4C-NC	2.78	128.58	124.20
30	12	304	CLA	C4C-C3C-C2C	-2.78	102.85	106.90
30	7	310	CLA	C4-C3-C5	2.78	119.94	115.27
30	10	309	CLA	C4-C3-C5	2.78	119.94	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	807	CLA	CMA-C3A-C2A	-2.78	102.63	113.83
29	A	801	CL0	CHD-C4C-NC	2.78	128.58	124.20
38	14	308	KC1	CAA-CBA-CGA	-2.78	113.00	127.26
30	B	809	CLA	CMC-C2C-C1C	2.78	129.27	125.04
30	15	311	CLA	CHD-C4C-NC	2.78	128.58	124.20
38	4	308	KC1	C4C-C3C-C2C	-2.78	102.85	106.90
30	6	309	CLA	C4C-C3C-C2C	-2.77	102.85	106.90
30	9	305	CLA	CAC-C3C-C4C	2.77	128.41	124.81
30	10	307	CLA	CMC-C2C-C1C	2.77	129.26	125.04
38	5	305	KC1	CHD-C4C-NC	2.77	128.41	124.20
37	14	301	A86	C10-C9-C8	-2.77	114.56	123.22
30	L	202	CLA	CHB-C4A-NA	2.77	128.35	124.51
30	B	834	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
30	14	302	CLA	CMC-C2C-C1C	2.77	129.26	125.04
30	B	817	CLA	O2A-CGA-CBA	2.77	120.61	111.91
37	11	314	A86	C12-C11-C13	2.77	120.68	116.02
30	3	305	CLA	CHB-C4A-NA	2.77	128.35	124.51
30	15	302	CLA	C3B-C4B-NB	2.77	112.79	109.21
30	A	827	CLA	C4-C3-C5	2.77	119.93	115.27
30	B	804	CLA	CHB-C4A-NA	2.77	128.34	124.51
39	8	317	DD6	C12-C11-C13	-2.77	113.71	118.08
30	B	826	CLA	CAC-C3C-C4C	2.77	128.41	124.81
30	A	839	CLA	O2A-CGA-CBA	2.77	120.60	111.91
30	A	808	CLA	CHD-C4C-NC	2.77	128.57	124.20
30	B	838	CLA	CHD-C4C-NC	2.77	128.57	124.20
30	1	303	CLA	CHC-C1C-C2C	-2.77	119.06	126.72
30	A	833	CLA	C1-C2-C3	-2.77	121.25	126.04
38	3	308	KC1	C4C-C3C-C2C	-2.77	102.86	106.90
30	B	808	CLA	CHD-C4C-NC	2.77	128.57	124.20
39	2	316	DD6	C3-C4-C5	-2.77	117.80	123.47
30	A	841	CLA	CHD-C4C-NC	2.77	128.57	124.20
30	4	305	CLA	CHB-C4A-NA	2.77	128.34	124.51
30	A	832	CLA	C1-C2-C3	-2.77	122.27	126.75
30	L	202	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
30	8	308	CLA	C3B-C4B-NB	2.77	112.79	109.21
30	4	303	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
33	A	851	BCR	C15-C16-C17	-2.77	117.81	123.47
30	4	305	CLA	CHD-C4C-NC	2.77	128.56	124.20
30	A	802	CLA	C1B-CHB-C4A	-2.77	124.64	130.12
30	B	814	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
30	9	308	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
37	15	315	A86	C22-C16-C17	-2.77	104.18	108.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	827	CLA	C4C-C3C-C2C	-2.77	102.87	106.90
30	7	310	CLA	C3B-C4B-NB	2.77	112.78	109.21
30	B	821	CLA	C4C-C3C-C2C	-2.77	102.87	106.90
37	6	320	A86	C12-C11-C13	2.77	120.67	116.02
30	B	810	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
30	10	307	CLA	CHD-C4C-NC	2.76	128.56	124.20
30	10	304	CLA	CAA-C2A-C3A	-2.76	105.21	112.78
39	8	317	DD6	C25-C24-C1	-2.76	118.65	126.42
30	7	312	CLA	CAC-C3C-C4C	2.76	128.40	124.81
30	B	824	CLA	O2A-CGA-CBA	2.76	120.58	111.91
30	A	812	CLA	CAC-C3C-C4C	2.76	128.39	124.81
30	11	308	CLA	CHD-C4C-NC	2.76	128.56	124.20
30	1	303	CLA	C1-C2-C3	-2.76	121.27	126.04
30	F	202	CLA	CHC-C1C-C2C	-2.76	119.08	126.72
33	B	845	BCR	C27-C26-C25	2.76	126.74	122.73
30	8	308	CLA	CMC-C2C-C1C	2.76	129.24	125.04
30	7	309	CLA	C4C-C3C-C2C	-2.76	102.87	106.90
38	7	313	KC1	C4C-C3C-C2C	-2.76	102.87	106.90
30	2	307	CLA	CBC-CAC-C3C	-2.76	104.82	112.43
30	5	302	CLA	CBC-CAC-C3C	-2.76	104.82	112.43
30	A	844	CLA	CHD-C4C-NC	2.76	128.55	124.20
33	B	843	BCR	C15-C16-C17	-2.76	117.82	123.47
30	4	304	CLA	CAC-C3C-C4C	2.76	128.39	124.81
30	A	833	CLA	CHD-C4C-NC	2.76	128.55	124.20
30	2	305	CLA	CMB-C2B-C3B	2.76	129.84	124.68
30	4	309	CLA	CMB-C2B-C3B	2.76	129.84	124.68
30	12	310	CLA	O2A-CGA-CBA	2.76	120.56	111.91
30	A	825	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
30	4	305	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
38	9	304	KC1	C4C-C3C-C2C	-2.76	102.88	106.90
30	A	839	CLA	CAA-C2A-C3A	-2.76	105.22	112.78
37	12	314	A86	C26-C25-C24	-2.76	114.61	123.22
30	13	307	CLA	CHD-C4C-NC	2.76	128.55	124.20
30	1	307	CLA	CAC-C3C-C4C	2.76	128.39	124.81
30	A	842	CLA	C1-C2-C3	-2.76	121.28	126.04
30	A	829	CLA	CHC-C1C-C2C	-2.76	119.10	126.72
30	10	308	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
37	7	316	A86	C40-C32-C31	-2.76	108.01	110.47
30	5	309	CLA	CHD-C4C-NC	2.75	128.54	124.20
38	9	311	KC1	CAC-C3C-C4C	2.75	128.38	124.81
30	9	302	CLA	O1D-CGD-CBD	-2.75	118.85	124.48
30	13	307	CLA	CAA-C2A-C3A	-2.75	105.24	112.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	12	312	CLA	O2A-CGA-CBA	2.75	120.55	111.91
38	8	306	KC1	CHB-C1B-NB	-2.75	121.92	124.45
30	5	304	CLA	CAC-C3C-C4C	2.75	128.38	124.81
30	4	311	CLA	C1-C2-C3	-2.75	122.30	126.75
30	A	806	CLA	C4-C3-C5	2.75	119.90	115.27
39	2	317	DD6	C19-C18-C17	2.75	116.09	110.77
30	A	802	CLA	CHA-C1A-NA	-2.75	120.10	126.40
37	12	314	A86	C9-C10-C11	-2.75	118.52	126.61
30	A	832	CLA	CMC-C2C-C1C	2.75	129.23	125.04
30	A	802	CLA	C4-C3-C5	2.75	119.90	115.27
39	4	316	DD6	C23-C16-C17	-2.75	104.20	108.98
30	B	804	CLA	CHC-C1C-C2C	-2.75	119.12	126.72
30	3	306	CLA	O2A-CGA-CBA	2.75	120.54	111.91
30	3	302	CLA	CAA-C2A-C3A	-2.75	105.25	112.78
39	6	303	DD6	O1-C20-C21	-2.75	111.76	115.06
30	2	308	CLA	O2A-CGA-CBA	2.75	120.53	111.91
39	5	313	DD6	C25-C24-C1	-2.75	118.69	126.42
37	6	320	A86	C35-C34-C33	2.75	114.67	109.88
30	14	307	CLA	CHC-C1C-C2C	-2.75	119.12	126.72
30	A	843	CLA	CHD-C4C-NC	2.75	128.53	124.20
38	3	304	KC1	CAC-C3C-C4C	2.75	128.38	124.81
37	14	318	A86	C4-C3-C2	-2.75	117.85	123.47
39	13	314	DD6	C9-C8-C6	-2.75	118.70	126.42
30	B	833	CLA	CHD-C4C-NC	2.75	128.53	124.20
30	7	311	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
30	B	832	CLA	CAC-C3C-C4C	2.75	128.37	124.81
30	6	309	CLA	O2A-C1-C2	2.75	115.85	108.64
30	8	302	CLA	C4C-C3C-C2C	-2.75	102.90	106.90
38	12	309	KC1	C4C-C3C-C2C	-2.75	102.90	106.90
30	14	303	CLA	CHB-C4A-NA	2.75	128.31	124.51
30	A	804	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
30	13	304	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
30	A	836	CLA	CHB-C4A-NA	2.74	128.31	124.51
30	B	823	CLA	CHD-C4C-NC	2.74	128.53	124.20
30	B	851	CLA	CHC-C1C-C2C	-2.74	119.13	126.72
30	6	309	CLA	CBC-CAC-C3C	-2.74	104.87	112.43
30	B	837	CLA	O2A-CGA-CBA	2.74	120.52	111.91
30	3	303	CLA	C1-C2-C3	-2.74	121.30	126.04
30	13	302	CLA	C4-C3-C5	2.74	119.88	115.27
30	4	305	CLA	CAC-C3C-C4C	2.74	128.37	124.81
30	5	303	CLA	CAC-C3C-C4C	2.74	128.37	124.81
38	5	312	KC1	CHD-C4C-NC	2.74	128.36	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	12	314	A86	C-C1-C24	2.74	122.40	118.08
29	A	801	CL0	O2A-CGA-CBA	2.74	120.51	111.91
30	12	302	CLA	CHC-C1C-C2C	-2.74	119.14	126.72
30	A	828	CLA	CMB-C2B-C3B	2.74	129.81	124.68
30	B	810	CLA	CHD-C4C-NC	2.74	128.52	124.20
30	B	801	CLA	C4-C3-C5	2.74	119.88	115.27
38	8	310	KC1	CBA-CAA-C2A	-2.74	114.82	125.27
30	A	843	CLA	CBC-CAC-C3C	-2.74	104.88	112.43
30	12	302	CLA	O2A-CGA-O1A	-2.74	116.67	123.59
30	12	306	CLA	C1-C2-C3	-2.74	121.30	126.04
37	13	315	A86	C12-C11-C10	-2.74	116.79	123.42
30	B	835	CLA	O2A-CGA-O1A	-2.74	116.68	123.59
30	6	304	CLA	O2A-CGA-CBA	2.74	120.51	111.91
30	9	305	CLA	CMB-C2B-C3B	2.74	129.80	124.68
30	5	308	CLA	CBC-CAC-C3C	-2.74	104.88	112.43
29	A	801	CL0	CGD-CBD-CAD	-2.74	101.86	110.73
30	16	305	CLA	CHD-C4C-NC	2.74	128.52	124.20
30	B	808	CLA	CHB-C4A-NA	2.74	128.30	124.51
38	7	313	KC1	CAC-C3C-C4C	2.74	128.36	124.81
30	15	308	CLA	C3B-C4B-NB	2.74	112.75	109.21
30	2	309	CLA	CHD-C4C-NC	2.74	128.52	124.20
30	2u	202	CLA	CMC-C2C-C1C	2.74	129.21	125.04
30	A	840	CLA	CAA-C2A-C3A	-2.74	105.28	112.78
30	B	832	CLA	CHD-C4C-NC	2.74	128.52	124.20
30	A	819	CLA	C1-C2-C3	-2.74	121.31	126.04
30	F	201	CLA	C1-C2-C3	-2.74	121.31	126.04
30	1	305	CLA	O2A-CGA-CBA	2.74	120.50	111.91
30	2	305	CLA	C1-C2-C3	-2.74	121.31	126.04
30	1	305	CLA	C4-C3-C5	2.74	119.87	115.27
30	5	302	CLA	CHC-C1C-C2C	-2.74	119.15	126.72
30	15	313	CLA	CAC-C3C-C4C	2.74	128.36	124.81
38	11	312	KC1	C4C-C3C-C2C	-2.74	102.91	106.90
30	A	810	CLA	CAA-CBA-CGA	-2.74	105.26	113.25
30	6	305	CLA	C1-C2-C3	-2.74	121.31	126.04
30	12	302	CLA	CHD-C4C-NC	2.73	128.51	124.20
39	5	314	DD6	C10-C9-C8	-2.73	114.68	123.22
30	B	816	CLA	CMC-C2C-C1C	2.73	129.20	125.04
37	9	313	A86	C7-C6-C8	2.73	122.39	118.08
30	B	810	CLA	CAC-C3C-C4C	2.73	128.36	124.81
30	A	830	CLA	CHD-C4C-NC	2.73	128.51	124.20
30	B	815	CLA	CAA-C2A-C3A	-2.73	105.29	112.78
38	10	306	KC1	CAC-C3C-C4C	2.73	128.36	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	7	312	CLA	CMB-C2B-C3B	2.73	129.79	124.68
30	B	803	CLA	CHD-C4C-NC	2.73	128.51	124.20
30	4	311	CLA	CHD-C4C-NC	2.73	128.51	124.20
36	2u	204	LMG	O6-C1-O1	-2.73	103.50	109.97
38	14	308	KC1	O2D-CGD-O1D	-2.73	118.50	123.84
30	2	313	CLA	CHD-C4C-NC	2.73	128.51	124.20
37	9	315	A86	C9-C8-C6	-2.73	118.74	126.42
30	13	301	CLA	CHC-C1C-C2C	-2.73	119.17	126.72
30	A	814	CLA	CMB-C2B-C3B	2.73	129.79	124.68
30	10	304	CLA	CHD-C4C-NC	2.73	128.51	124.20
30	B	817	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
30	B	818	CLA	CAA-C2A-C3A	-2.73	105.30	112.78
30	B	833	CLA	CAC-C3C-C4C	2.73	128.35	124.81
30	A	840	CLA	CAC-C3C-C4C	2.73	128.35	124.81
37	10	301	A86	O-C13-C11	-2.73	115.12	121.15
30	4	309	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
37	9	316	A86	C41-C32-C31	-2.73	108.03	110.47
30	2	311	CLA	CMC-C2C-C1C	2.73	129.19	125.04
30	A	825	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
30	B	839	CLA	O1D-CGD-CBD	-2.73	118.90	124.48
30	14	303	CLA	C1-C2-C3	-2.73	121.33	126.04
36	3	317	LMG	C4-C3-C2	-2.73	106.06	110.82
30	A	805	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
38	13	312	KC1	C4C-C3C-C2C	-2.73	102.92	106.90
30	2	303	CLA	CMC-C2C-C1C	2.73	129.19	125.04
39	6	318	DD6	C37-C36-C35	-2.73	109.30	114.36
37	3	314	A86	C7-C6-C5	-2.73	119.10	122.92
30	F	202	CLA	CAA-C2A-C3A	-2.73	105.31	112.78
30	3	301	CLA	CAA-C2A-C3A	-2.73	105.31	112.78
30	B	805	CLA	C4-C3-C5	2.73	119.86	115.27
30	4	309	CLA	CHD-C4C-NC	2.73	128.50	124.20
30	A	816	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
30	2	301	CLA	CMC-C2C-C1C	2.72	129.19	125.04
39	5	314	DD6	C41-C32-C31	-2.72	106.14	110.47
30	A	841	CLA	CHC-C1C-C2C	-2.72	119.19	126.72
30	A	818	CLA	C1-C2-C3	-2.72	121.33	126.04
30	A	805	CLA	CAC-C3C-C4C	2.72	128.34	124.81
30	A	811	CLA	CAC-C3C-C4C	2.72	128.34	124.81
39	11	313	DD6	C19-C18-C17	2.72	116.03	110.77
33	A	847	BCR	C15-C14-C13	-2.72	123.42	127.31
30	B	821	CLA	CHD-C4C-NC	2.72	128.50	124.20
30	14	312	CLA	CHD-C4C-NC	2.72	128.50	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	6	305	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
30	9	308	CLA	CHC-C1C-C2C	-2.72	119.19	126.72
39	2	317	DD6	C37-C36-C35	-2.72	109.31	114.36
38	8	311	KC1	CMB-C2B-C1B	2.72	129.51	124.71
30	13	301	CLA	CHB-C4A-NA	2.72	128.28	124.51
30	B	803	CLA	CMB-C2B-C3B	2.72	129.77	124.68
30	12	302	CLA	CMB-C2B-C3B	2.72	129.77	124.68
30	2	311	CLA	CHD-C4C-NC	2.72	128.49	124.20
30	1	302	CLA	CAC-C3C-C4C	2.72	128.34	124.81
30	6	304	CLA	CAC-C3C-C4C	2.72	128.34	124.81
30	15	312	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
30	8	305	CLA	CAC-C3C-C4C	2.72	128.34	124.81
38	2	306	KC1	C4C-C3C-C2C	-2.72	102.93	106.90
38	3	308	KC1	CHB-C1B-NB	-2.72	121.95	124.45
30	B	811	CLA	CHD-C4C-NC	2.72	128.49	124.20
38	8	307	KC1	CBC-CAC-C3C	-2.72	104.93	112.43
30	15	313	CLA	O2A-CGA-CBA	2.72	120.44	111.91
30	A	804	CLA	CAC-C3C-C4C	2.72	128.34	124.81
30	15	311	CLA	CAC-C3C-C4C	2.72	128.34	124.81
30	7	310	CLA	CHC-C1C-C2C	-2.72	119.20	126.72
30	9	308	CLA	C3B-C4B-NB	2.72	112.72	109.21
36	8	319	LMG	O6-C1-O1	-2.72	103.54	109.97
38	10	312	KC1	C4C-C3C-C2C	-2.72	102.94	106.90
30	A	817	CLA	CAC-C3C-C4C	2.72	128.34	124.81
30	8	303	CLA	CHD-C4C-NC	2.72	128.49	124.20
30	A	817	CLA	C4C-C3C-C2C	-2.72	102.94	106.90
30	10	309	CLA	O2A-CGA-CBA	2.72	120.43	111.91
30	16	305	CLA	CAC-C3C-C4C	2.72	128.34	124.81
37	9	313	A86	C25-C26-C27	-2.72	123.43	127.31
30	A	841	CLA	CMC-C2C-C1C	2.72	129.18	125.04
39	12	317	DD6	C23-C16-C17	-2.72	104.26	108.98
30	12	312	CLA	C4C-C3C-C2C	-2.72	102.94	106.90
30	14	302	CLA	C4C-C3C-C2C	-2.72	102.94	106.90
30	12	302	CLA	C1-C2-C3	-2.72	121.34	126.04
30	B	829	CLA	CHB-C4A-NA	2.72	128.27	124.51
30	A	830	CLA	C4-C3-C5	2.72	119.84	115.27
30	7	303	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
38	10	312	KC1	CMC-C2C-C1C	2.72	129.18	125.04
30	A	810	CLA	C1-C2-C3	-2.72	121.35	126.04
30	9	303	CLA	O2A-CGA-CBA	2.72	120.43	111.91
39	2	316	DD6	C25-C24-C1	-2.72	118.79	126.42
38	6	308	KC1	CMC-C2C-C1C	2.72	129.17	125.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	13	307	CLA	O2A-CGA-CBA	2.71	120.43	111.91
30	5	302	CLA	CMC-C2C-C1C	2.71	129.17	125.04
30	5	308	CLA	C4C-C3C-C2C	-2.71	102.94	106.90
30	14	303	CLA	C4C-C3C-C2C	-2.71	102.94	106.90
30	J	101	CLA	C4C-C3C-C2C	-2.71	102.94	106.90
29	A	801	CL0	CBC-CAC-C3C	-2.71	104.95	112.43
30	13	303	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
30	7	304	CLA	CMB-C2B-C3B	2.71	129.75	124.68
30	2	307	CLA	CMA-C3A-C2A	-2.71	102.89	113.83
30	3	303	CLA	CHB-C4A-NA	2.71	128.26	124.51
33	A	851	BCR	C24-C23-C22	-2.71	122.14	126.23
30	A	803	CLA	CHC-C1C-C2C	-2.71	119.22	126.72
38	13	310	KC1	CAA-CBA-CGA	-2.71	113.33	127.26
30	12	321	CLA	O2A-CGA-CBA	2.71	120.41	111.91
30	3	303	CLA	CAC-C3C-C4C	2.71	128.33	124.81
30	A	819	CLA	C3B-C4B-NB	2.71	112.71	109.21
38	11	307	KC1	CHB-C1B-NB	-2.71	121.96	124.45
30	A	841	CLA	CED-O2D-CGD	2.71	122.06	115.94
30	2	304	CLA	C4C-C3C-C2C	-2.71	102.95	106.90
34	A	852	LHG	O8-C23-C24	2.71	120.41	111.91
30	4	309	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
30	2	304	CLA	O2A-CGA-CBA	2.71	120.41	111.91
30	2	307	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
30	5	304	CLA	O2A-C1-C2	2.71	115.75	108.64
38	13	306	KC1	CAA-CBA-CGA	-2.71	113.35	127.26
30	12	308	CLA	O2A-CGA-CBA	2.71	120.40	111.91
38	10	312	KC1	CAC-C3C-C4C	2.71	128.32	124.81
30	B	837	CLA	C1-C2-C3	-2.71	121.36	126.04
30	B	801	CLA	CHC-C1C-C2C	-2.71	119.24	126.72
30	2	304	CLA	CMC-C2C-C1C	2.71	129.16	125.04
30	B	826	CLA	O1D-CGD-CBD	-2.71	118.95	124.48
30	10	307	CLA	CHB-C4A-NA	2.71	128.25	124.51
30	10	307	CLA	C3B-C4B-NB	2.70	112.71	109.21
30	A	835	CLA	C1-C2-C3	-2.70	121.36	126.04
30	A	812	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
38	4	308	KC1	CHB-C1B-NB	-2.70	121.97	124.45
30	2	305	CLA	CHD-C4C-NC	2.70	128.46	124.20
30	4	306	CLA	CMC-C2C-C1C	2.70	129.16	125.04
30	6	309	CLA	CMC-C2C-C1C	2.70	129.16	125.04
30	14	304	CLA	CHD-C4C-NC	2.70	128.46	124.20
38	13	310	KC1	CHD-C4C-NC	2.70	128.30	124.20
30	B	834	CLA	C1-C2-C3	-2.70	121.37	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	10	306	KC1	CMB-C2B-C1B	2.70	129.47	124.71
30	A	840	CLA	C4C-C3C-C2C	-2.70	102.96	106.90
30	16	303	CLA	CHC-C1C-C2C	-2.70	119.25	126.72
39	15	318	DD6	C19-C18-C17	2.70	115.99	110.77
30	B	823	CLA	CMC-C2C-C1C	2.70	129.15	125.04
37	14	319	A86	C40-C32-C31	-2.70	108.06	110.47
30	9	302	CLA	CAA-C2A-C3A	-2.70	105.38	112.78
37	11	314	A86	C26-C25-C24	-2.70	114.79	123.22
30	12	304	CLA	C1-C2-C3	-2.70	121.37	126.04
30	11	310	CLA	O2A-CGA-CBA	2.70	120.38	111.91
30	9	307	CLA	CHB-C4A-NA	2.70	128.24	124.51
30	7	312	CLA	CHD-C4C-NC	2.70	128.46	124.20
30	A	808	CLA	O2A-CGA-CBA	2.70	120.38	111.91
30	15	309	CLA	CHD-C4C-NC	2.70	128.46	124.20
30	7	304	CLA	CBC-CAC-C3C	-2.70	104.99	112.43
37	15	316	A86	C34-O4-C38	-2.70	112.87	117.90
30	B	811	CLA	C1-C2-C3	-2.70	121.38	126.04
30	1	301	CLA	CHD-C4C-NC	2.70	128.45	124.20
30	3	310	CLA	CAC-C3C-C4C	2.70	128.31	124.81
30	B	819	CLA	CHB-C4A-NA	2.70	128.24	124.51
30	15	313	CLA	CAA-C2A-C3A	-2.70	105.40	112.78
37	10	316	A86	C26-C25-C24	-2.70	114.81	123.22
30	B	827	CLA	O2A-CGA-CBA	2.70	120.37	111.91
38	12	305	KC1	CHD-C4C-NC	2.70	128.29	124.20
30	B	821	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
39	2	315	DD6	C33-C34-C35	2.69	113.99	110.30
39	4	313	DD6	C9-C8-C6	-2.69	118.85	126.42
30	B	839	CLA	C1-C2-C3	-2.69	121.38	126.04
30	13	303	CLA	CHD-C4C-NC	2.69	128.45	124.20
30	B	830	CLA	C3B-C4B-NB	2.69	112.69	109.21
30	3	306	CLA	C1-C2-C3	-2.69	121.39	126.04
30	A	843	CLA	C4C-C3C-C2C	-2.69	102.97	106.90
30	12	307	CLA	CHC-C1C-C2C	-2.69	119.27	126.72
30	F	201	CLA	CHC-C1C-C2C	-2.69	119.28	126.72
30	3	302	CLA	CMB-C2B-C3B	2.69	129.71	124.68
38	11	307	KC1	CMC-C2C-C1C	2.69	129.14	125.04
38	2	314	KC1	CHD-C4C-NC	2.69	128.28	124.20
30	6	306	CLA	CMB-C2B-C3B	2.69	129.71	124.68
37	15	315	A86	C10-C9-C8	2.69	131.61	123.22
30	9	308	CLA	O1D-CGD-CBD	-2.69	118.98	124.48
30	6	309	CLA	O2A-CGA-O1A	-2.69	116.81	123.59
30	11	310	CLA	CMB-C2B-C3B	2.69	129.71	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	1	304	CLA	C3B-C4B-NB	2.69	112.69	109.21
30	16	305	CLA	CBC-CAC-C3C	-2.69	105.02	112.43
30	14	305	CLA	CAC-C3C-C4C	2.69	128.30	124.81
38	7	313	KC1	CBC-CAC-C3C	-2.69	105.02	112.43
30	10	305	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
30	15	310	CLA	CHD-C4C-NC	2.69	128.44	124.20
30	8	305	CLA	CBC-CAC-C3C	-2.69	105.03	112.43
36	3	317	LMG	C1-O6-C5	2.69	118.96	113.69
30	12	304	CLA	O2A-CGA-O1A	-2.69	116.81	123.59
30	B	835	CLA	CBA-CAA-C2A	2.69	121.79	113.86
33	J	102	BCR	C11-C10-C9	-2.69	123.48	127.31
30	A	842	CLA	CMC-C2C-C1C	2.69	129.13	125.04
30	A	843	CLA	CMA-C3A-C2A	-2.69	103.00	113.83
30	13	304	CLA	CAC-C3C-C4C	2.69	128.29	124.81
39	15	318	DD6	C32-C33-C34	2.68	119.71	113.64
30	A	809	CLA	C4C-C3C-C2C	-2.68	102.98	106.90
39	6	303	DD6	C19-C18-C17	2.68	115.95	110.77
30	10	308	CLA	CMC-C2C-C1C	2.68	129.12	125.04
37	12	314	A86	C24-C1-C2	-2.68	114.82	118.94
38	13	312	KC1	CBA-CAA-C2A	-2.68	115.04	125.27
33	L	205	BCR	C15-C16-C17	-2.68	117.98	123.47
38	9	310	KC1	CMC-C2C-C1C	2.68	129.12	125.04
30	8	308	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
38	2	306	KC1	CMB-C2B-C1B	2.68	129.44	124.71
30	B	811	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
36	5	318	LMG	O6-C1-O1	-2.68	103.63	109.97
36	8	321	LMG	O2-C2-C1	-2.68	103.54	110.05
30	7	303	CLA	O2A-C1-C2	2.68	115.68	108.64
30	15	309	CLA	C4-C3-C5	2.68	119.78	115.27
30	F	201	CLA	CHD-C4C-NC	2.68	128.43	124.20
30	12	306	CLA	CHD-C4C-NC	2.68	128.43	124.20
30	F	203	CLA	CAA-C2A-C3A	-2.68	105.44	112.78
30	3	306	CLA	C3B-C4B-NB	2.68	112.67	109.21
38	4	310	KC1	CMB-C2B-C1B	2.68	129.43	124.71
30	15	308	CLA	CAA-CBA-CGA	2.68	119.61	112.51
30	L	202	CLA	CHD-C4C-NC	2.68	128.42	124.20
30	14	302	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
30	12	307	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
38	9	311	KC1	CBC-CAC-C3C	-2.68	105.05	112.43
30	7	305	CLA	O1D-CGD-CBD	-2.68	119.01	124.48
39	12	317	DD6	C3-C4-C5	-2.68	117.99	123.47
37	11	314	A86	C7-C6-C5	-2.68	119.17	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	13	304	CLA	CHD-C4C-NC	2.68	128.42	124.20
37	10	301	A86	C10-C9-C8	-2.67	114.87	123.22
30	B	818	CLA	CMB-C2B-C3B	2.67	129.68	124.68
38	8	312	KC1	CAA-CBA-CGA	-2.67	113.52	127.26
30	4	309	CLA	C1-C2-C3	-2.67	121.42	126.04
37	5	316	A86	C26-C25-C24	-2.67	114.87	123.22
30	A	805	CLA	CMA-C3A-C4A	-2.67	104.59	111.77
30	A	806	CLA	CHD-C4C-NC	2.67	128.42	124.20
38	4	307	KC1	C4C-C3C-C2C	-2.67	103.00	106.90
38	9	312	KC1	CHB-C1B-NB	-2.67	122.00	124.45
30	B	807	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
30	B	829	CLA	C3B-C4B-NB	2.67	112.67	109.21
30	16	310	CLA	CAC-C3C-C4C	2.67	128.28	124.81
30	16	306	CLA	CMA-C3A-C2A	-2.67	103.05	113.83
38	8	306	KC1	C4C-C3C-C2C	-2.67	103.00	106.90
30	5	302	CLA	CMB-C2B-C3B	2.67	129.68	124.68
30	A	835	CLA	CAC-C3C-C4C	2.67	128.28	124.81
30	9	302	CLA	CMB-C2B-C3B	2.67	129.68	124.68
30	2	307	CLA	C1-C2-C3	-2.67	121.42	126.04
30	3	306	CLA	CHD-C4C-NC	2.67	128.41	124.20
30	A	837	CLA	CMB-C2B-C3B	2.67	129.68	124.68
30	A	834	CLA	CBC-CAC-C3C	-2.67	105.07	112.43
30	A	823	CLA	CMC-C2C-C1C	2.67	129.10	125.04
30	B	837	CLA	CAC-C3C-C4C	2.67	128.27	124.81
30	7	304	CLA	C4C-C3C-C2C	-2.67	103.01	106.90
30	6	314	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
38	3	308	KC1	CHD-C4C-NC	2.67	128.25	124.20
30	A	828	CLA	O2A-CGA-CBA	2.67	120.28	111.91
30	11	306	CLA	CMB-C2B-C3B	2.67	129.67	124.68
30	A	827	CLA	C3B-C4B-NB	2.67	112.66	109.21
30	B	837	CLA	C3B-C4B-NB	2.67	112.66	109.21
30	8	304	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
30	16	309	CLA	CHD-C4C-NC	2.67	128.41	124.20
30	A	811	CLA	CHB-C4A-NA	2.67	128.20	124.51
30	16	307	CLA	CHD-C4C-NC	2.67	128.40	124.20
38	8	314	KC1	C1A-NA-C4A	-2.66	105.51	106.71
30	A	832	CLA	CBC-CAC-C3C	-2.66	105.09	112.43
30	9	301	CLA	O1D-CGD-CBD	-2.66	119.03	124.48
30	B	801	CLA	CBC-CAC-C3C	-2.66	105.09	112.43
30	A	805	CLA	CHC-C1C-C2C	-2.66	119.35	126.72
33	B	845	BCR	C20-C21-C22	-2.66	123.51	127.31
30	3	301	CLA	C4C-C3C-C2C	-2.66	103.02	106.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	6	311	KC1	CHB-C1B-NB	-2.66	122.01	124.45
37	6	320	A86	C-C1-C24	2.66	122.27	118.08
38	4	307	KC1	CHD-C4C-NC	2.66	128.24	124.20
37	7	316	A86	C-C1-C24	2.66	122.27	118.08
30	7	311	CLA	O2A-CGA-CBA	2.66	120.25	111.91
30	11	306	CLA	CHC-C1C-C2C	-2.66	119.36	126.72
30	4	305	CLA	O2A-CGA-CBA	2.66	120.25	111.91
39	6	303	DD6	C20-C19-C18	2.66	118.01	112.75
30	2u	202	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
30	7	311	CLA	C1-C2-C3	-2.66	121.44	126.04
30	A	809	CLA	CBA-CAA-C2A	2.66	121.71	113.86
30	A	825	CLA	CHB-C4A-NA	2.66	128.19	124.51
30	9	302	CLA	CHB-C4A-NA	2.66	128.19	124.51
30	7	309	CLA	CHD-C4C-NC	2.66	128.39	124.20
30	9	305	CLA	C1-C2-C3	-2.66	121.45	126.04
30	14	305	CLA	CHD-C4C-NC	2.66	128.39	124.20
30	12	310	CLA	CMC-C2C-C1C	2.66	129.09	125.04
30	14	305	CLA	CMB-C2B-C3B	2.66	129.65	124.68
30	6	317	CLA	C4C-C3C-C2C	-2.66	103.03	106.90
37	15	323	A86	C4-C3-C2	2.66	128.91	123.47
37	4	312	A86	C35-C34-C33	2.66	114.51	109.88
30	B	804	CLA	C4-C3-C5	2.65	119.74	115.27
30	B	839	CLA	CBC-CAC-C3C	-2.65	105.11	112.43
30	A	803	CLA	C1-C2-C3	-2.65	121.45	126.04
30	A	808	CLA	CHB-C4A-NA	2.65	128.18	124.51
30	5	309	CLA	CHB-C4A-NA	2.65	128.18	124.51
30	B	804	CLA	CBC-CAC-C3C	-2.65	105.12	112.43
36	B	847	LMG	O6-C1-O1	-2.65	103.69	109.97
30	F	202	CLA	CHD-C4C-NC	2.65	128.38	124.20
37	9	315	A86	C8-C6-C5	-2.65	114.87	118.94
30	8	305	CLA	CMC-C2C-C1C	2.65	129.08	125.04
30	12	302	CLA	CHB-C4A-NA	2.65	128.18	124.51
30	B	807	CLA	C1-C2-C3	-2.65	121.46	126.04
38	9	304	KC1	CBC-CAC-C3C	-2.65	105.12	112.43
33	A	848	BCR	C27-C26-C25	2.65	126.58	122.73
30	A	823	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
30	5	304	CLA	CMC-C2C-C1C	2.65	129.08	125.04
30	6	314	CLA	CMC-C2C-C1C	2.65	129.08	125.04
30	B	807	CLA	CBC-CAC-C3C	-2.65	105.12	112.43
30	A	830	CLA	C3B-C4B-NB	2.65	112.64	109.21
30	9	301	CLA	C1-C2-C3	-2.65	121.46	126.04
39	5	314	DD6	C37-C36-C35	-2.65	109.44	114.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	16	312	A86	C9-C8-C6	2.65	133.86	126.42
30	A	803	CLA	CAC-C3C-C4C	2.65	128.25	124.81
30	15	307	CLA	CBC-CAC-C3C	-2.65	105.13	112.43
37	15	322	A86	C4-C5-C6	-2.65	123.53	127.31
30	6	310	CLA	C4C-C3C-C2C	-2.65	103.04	106.90
39	11	313	DD6	C9-C8-C6	-2.65	118.97	126.42
30	15	303	CLA	CAC-C3C-C4C	2.65	128.25	124.81
30	2u	202	CLA	CBC-CAC-C3C	-2.65	105.13	112.43
30	16	309	CLA	CAC-C3C-C4C	2.65	128.25	124.81
37	7	315	A86	C36-C31-C32	-2.65	117.07	119.70
30	15	304	CLA	C4-C3-C5	2.65	119.72	115.27
30	4	301	CLA	CHD-C4C-NC	2.65	128.37	124.20
30	L	203	CLA	CAC-C3C-C4C	2.65	128.24	124.81
30	A	829	CLA	CMC-C2C-C1C	2.65	129.07	125.04
33	B	841	BCR	C27-C26-C25	2.64	126.57	122.73
35	B	850	LMT	C1'-C2'-C3'	2.64	115.50	110.00
30	2	305	CLA	CAC-C3C-C4C	2.64	128.24	124.81
30	15	306	CLA	CAC-C3C-C4C	2.64	128.24	124.81
30	9	309	CLA	CHD-C4C-NC	2.64	128.37	124.20
37	14	317	A86	C35-C34-C33	2.64	114.49	109.88
30	A	823	CLA	C4A-NA-C1A	-2.64	105.52	106.71
30	B	829	CLA	CHD-C4C-NC	2.64	128.37	124.20
37	13	315	A86	C25-C24-C1	-2.64	118.99	126.42
38	16	311	KC1	CHD-C4C-NC	2.64	128.21	124.20
38	13	306	KC1	CBA-CAA-C2A	-2.64	115.20	125.27
30	A	832	CLA	CHD-C4C-NC	2.64	128.37	124.20
39	7	317	DD6	C19-C18-C17	2.64	115.87	110.77
38	4	307	KC1	CMB-C2B-C1B	2.64	129.37	124.71
37	5	315	A86	C4-C3-C2	-2.64	118.07	123.47
36	3	317	LMG	O6-C1-O1	-2.64	103.72	109.97
30	11	310	CLA	CAA-C2A-C3A	-2.64	105.55	112.78
30	15	308	CLA	CAA-C2A-C3A	-2.64	105.55	112.78
30	8	308	CLA	CMB-C2B-C3B	2.64	129.61	124.68
38	1	308	KC1	CHD-C4C-NC	2.64	128.20	124.20
30	5	308	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
30	A	808	CLA	CHC-C1C-C2C	-2.64	119.43	126.72
30	4	305	CLA	CMC-C2C-C1C	2.64	129.05	125.04
30	3	305	CLA	O2A-CGA-CBA	2.64	120.18	111.91
30	1	307	CLA	O2D-CGD-O1D	-2.64	118.69	123.84
30	A	825	CLA	CAA-C2A-C3A	-2.63	105.56	112.78
37	14	318	A86	C12-C11-C13	2.63	120.45	116.02
30	2	308	CLA	C3B-C4B-NB	2.63	112.62	109.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	828	CLA	CMB-C2B-C1B	-2.63	124.42	128.46
30	7	307	CLA	CHC-C1C-C2C	-2.63	119.44	126.72
30	8	301	CLA	O2A-CGA-CBA	2.63	120.17	111.91
30	A	829	CLA	CHB-C4A-NA	2.63	128.15	124.51
33	A	849	BCR	C30-C25-C26	-2.63	118.91	122.61
30	1	301	CLA	O2A-C1-C2	2.63	115.55	108.64
38	8	312	KC1	CHD-C4C-NC	2.63	128.19	124.20
37	3	315	A86	C9-C10-C11	-2.63	118.87	126.61
30	9	305	CLA	CMC-C2C-C1C	2.63	129.04	125.04
30	6	310	CLA	CHB-C4A-NA	2.63	128.15	124.51
30	B	809	CLA	C4C-C3C-C2C	-2.63	103.06	106.90
33	A	850	BCR	C3-C4-C5	-2.63	109.38	114.08
30	B	823	CLA	O1D-CGD-CBD	-2.63	119.10	124.48
30	B	817	CLA	CMC-C2C-C1C	2.63	129.04	125.04
30	4	303	CLA	C1-C2-C3	-2.63	121.50	126.04
30	8	303	CLA	CAC-C3C-C4C	2.63	128.22	124.81
30	B	830	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
30	15	308	CLA	CHB-C4A-NA	2.63	128.15	124.51
30	B	819	CLA	C1-C2-C3	-2.63	121.50	126.04
30	A	822	CLA	CAC-C3C-C4C	2.63	128.22	124.81
30	A	829	CLA	O2A-CGA-CBA	2.63	120.15	111.91
30	A	803	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
30	6	317	CLA	CHB-C4A-NA	2.63	128.14	124.51
30	9	305	CLA	O2A-CGA-CBA	2.63	120.15	111.91
30	10	304	CLA	CAC-C3C-C4C	2.63	128.22	124.81
37	15	321	A86	C7-C6-C8	2.62	122.21	118.08
30	2	313	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
30	3	307	CLA	C1-C2-C3	-2.62	121.50	126.04
38	7	313	KC1	CHB-C4A-NA	2.62	128.34	124.20
30	14	310	CLA	CMB-C2B-C3B	2.62	129.59	124.68
30	6	315	CLA	CAC-C3C-C4C	2.62	128.21	124.81
30	3	310	CLA	CMC-C2C-C1C	2.62	129.03	125.04
30	B	806	CLA	C4C-C3C-C2C	-2.62	103.07	106.90
30	9	303	CLA	C4C-C3C-C2C	-2.62	103.07	106.90
39	3	316	DD6	C41-C32-C31	-2.62	106.30	110.47
30	A	814	CLA	C4-C3-C5	2.62	119.68	115.27
30	14	310	CLA	CHD-C4C-NC	2.62	128.34	124.20
30	10	309	CLA	CHD-C4C-NC	2.62	128.33	124.20
30	B	829	CLA	CAC-C3C-C4C	2.62	128.21	124.81
39	4	316	DD6	C21-C20-C15	-2.62	117.87	122.26
30	B	817	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
30	14	307	CLA	C1-C2-C3	-2.62	121.51	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	10	309	CLA	CAA-C2A-C3A	-2.62	105.60	112.78
30	A	806	CLA	O2A-CGA-CBA	2.62	120.13	111.91
30	7	310	CLA	CHB-C4A-NA	2.62	128.13	124.51
30	8	308	CLA	CHB-C4A-NA	2.62	128.13	124.51
30	2	307	CLA	CAC-C3C-C4C	2.62	128.21	124.81
30	B	821	CLA	C4-C3-C2	-2.62	116.96	123.68
30	A	843	CLA	CMC-C2C-C1C	2.62	129.03	125.04
39	8	317	DD6	C21-C20-C15	-2.62	117.87	122.26
30	B	826	CLA	CMB-C2B-C3B	2.62	129.58	124.68
30	16	302	CLA	C4-C3-C5	2.62	119.67	115.27
30	2	303	CLA	CAA-C2A-C1A	-2.62	103.40	111.97
30	11	304	CLA	O2A-CGA-CBA	2.62	120.12	111.91
37	5	315	A86	C10-C9-C8	-2.62	115.05	123.22
30	13	309	CLA	CHD-C4C-NC	2.62	128.33	124.20
30	11	308	CLA	CMB-C2B-C3B	2.62	129.57	124.68
30	B	830	CLA	CHC-C1C-C2C	-2.62	119.48	126.72
30	B	826	CLA	O2A-CGA-CBA	2.62	120.12	111.91
30	1	307	CLA	CHD-C4C-NC	2.62	128.33	124.20
30	5	311	CLA	CHD-C4C-NC	2.62	128.33	124.20
38	9	311	KC1	O1D-CGD-CBD	-2.62	119.13	124.48
38	12	305	KC1	CAA-CBA-CGA	-2.62	113.82	127.26
38	11	312	KC1	CHB-C1B-NB	-2.62	122.05	124.45
33	F	204	BCR	C27-C26-C25	2.62	126.53	122.73
30	B	810	CLA	CHC-C1C-C2C	-2.62	119.49	126.72
30	5	308	CLA	CHB-C4A-NA	2.62	128.13	124.51
30	B	804	CLA	CAA-C2A-C3A	-2.62	105.62	112.78
30	B	825	CLA	C1-C2-C3	-2.61	121.52	126.04
30	A	844	CLA	CMA-C3A-C2A	-2.61	103.29	113.83
30	7	307	CLA	CHB-C4A-NA	2.61	128.12	124.51
30	8	305	CLA	CHC-C1C-C2C	-2.61	119.50	126.72
37	14	315	A86	O1-C15-C14	2.61	118.45	113.21
30	B	811	CLA	C4-C3-C5	2.61	119.66	115.27
30	A	842	CLA	CAC-C3C-C4C	2.61	128.20	124.81
30	15	305	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
30	B	837	CLA	C4-C3-C5	2.61	119.66	115.27
30	15	309	CLA	O2A-CGA-CBA	2.61	120.10	111.91
30	1	301	CLA	CHB-C4A-NA	2.61	128.12	124.51
30	16	305	CLA	O2A-CGA-CBA	2.61	120.10	111.91
30	11	304	CLA	CMB-C2B-C3B	2.61	129.56	124.68
30	15	303	CLA	CHD-C4C-NC	2.61	128.31	124.20
35	A	854	LMT	C1B-C2B-C3B	2.61	115.43	110.00
30	5	309	CLA	C4-C3-C5	2.61	119.66	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	3	304	KC1	O1D-CGD-CBD	-2.61	119.15	124.48
30	15	312	CLA	CMD-C2D-C3D	-2.61	121.62	127.61
30	6	305	CLA	CAA-C2A-C3A	-2.61	105.64	112.78
38	6	313	KC1	CHB-C1B-NB	-2.61	122.06	124.45
30	B	825	CLA	CHC-C1C-C2C	-2.61	119.51	126.72
30	4	306	CLA	CMB-C2B-C3B	2.61	129.56	124.68
39	12	315	DD6	O1-C20-C21	-2.61	111.93	115.06
38	3	311	KC1	CHD-C4C-NC	2.61	128.16	124.20
30	6	307	CLA	C1-C2-C3	-2.61	121.54	126.04
30	3	303	CLA	O1D-CGD-CBD	-2.61	119.15	124.48
37	14	314	A86	C3-C4-C5	2.61	128.81	123.47
30	A	822	CLA	CHD-C4C-NC	2.60	128.31	124.20
39	3	316	DD6	C9-C8-C6	-2.60	119.10	126.42
30	1	307	CLA	O2A-CGA-CBA	2.60	120.08	111.91
30	12	312	CLA	CMC-C2C-C1C	2.60	129.00	125.04
39	13	314	DD6	C20-C19-C18	2.60	117.90	112.75
38	6	311	KC1	CHD-C4C-NC	2.60	128.15	124.20
30	13	301	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
30	15	312	CLA	C2A-C3A-C4A	-2.60	97.67	101.87
38	9	312	KC1	CHD-C4C-NC	2.60	128.15	124.20
30	B	809	CLA	CHD-C4C-NC	2.60	128.30	124.20
37	14	314	A86	C7-C6-C8	-2.60	113.98	118.08
30	9	307	CLA	CAC-C3C-C4C	2.60	128.19	124.81
30	5	302	CLA	CBA-CAA-C2A	2.60	121.54	113.86
30	A	826	CLA	O1D-CGD-CBD	-2.60	119.16	124.48
38	6	311	KC1	CAC-C3C-C4C	2.60	128.19	124.81
30	4	311	CLA	C4C-C3C-C2C	-2.60	103.11	106.90
30	6	305	CLA	CMC-C2C-C1C	2.60	129.00	125.04
30	15	302	CLA	CHC-C1C-C2C	-2.60	119.53	126.72
30	A	834	CLA	O2A-CGA-O1A	-2.60	117.03	123.59
30	15	304	CLA	O2A-C1-C2	2.60	115.47	108.64
38	11	307	KC1	CMB-C2B-C1B	2.60	129.29	124.71
30	B	836	CLA	CHD-C4C-NC	2.60	128.30	124.20
30	8	309	CLA	CAC-C3C-C4C	2.60	128.18	124.81
38	13	311	KC1	CAC-C3C-C4C	2.60	128.18	124.81
30	B	826	CLA	CHD-C4C-NC	2.60	128.30	124.20
38	3	311	KC1	CHB-C4A-NA	2.60	128.30	124.20
30	A	816	CLA	CHB-C4A-NA	2.60	128.11	124.51
30	9	306	CLA	CHB-C4A-NA	2.60	128.11	124.51
30	L	202	CLA	C4A-NA-C1A	-2.60	105.54	106.71
39	2	316	DD6	C33-C32-C31	2.60	114.89	109.62
30	B	827	CLA	CMC-C2C-C1C	2.60	129.00	125.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	807	CLA	O2A-CGA-O1A	-2.60	117.04	123.59
38	11	312	KC1	CHD-C4C-NC	2.60	128.14	124.20
37	4	314	A86	C24-C1-C2	2.60	122.93	118.94
30	4	301	CLA	CHB-C4A-NA	2.60	128.10	124.51
30	6	310	CLA	O2A-CGA-CBA	2.60	120.06	111.91
30	16	308	CLA	CHD-C4C-NC	2.60	128.29	124.20
30	B	815	CLA	CHB-C4A-NA	2.60	128.10	124.51
30	10	309	CLA	CMB-C2B-C3B	2.60	129.53	124.68
38	13	311	KC1	CMB-C2B-C1B	2.60	129.29	124.71
37	2u	203	A86	C-C1-C2	-2.60	119.29	122.92
38	10	306	KC1	O1D-CGD-CBD	-2.60	119.17	124.48
30	B	814	CLA	CHB-C4A-NA	2.60	128.10	124.51
30	16	301	CLA	CHB-C4A-NA	2.60	128.10	124.51
30	12	304	CLA	CBC-CAC-C3C	-2.60	105.28	112.43
37	10	302	A86	C23-C16-C17	-2.60	104.47	108.98
39	13	314	DD6	C22-C16-C15	2.59	117.05	110.05
30	J	101	CLA	CMC-C2C-C1C	2.59	128.99	125.04
30	10	303	CLA	CHB-C4A-NA	2.59	128.10	124.51
30	A	830	CLA	CAA-C2A-C3A	-2.59	105.67	112.78
30	5	311	CLA	CMB-C2B-C3B	2.59	129.53	124.68
38	3	311	KC1	CMB-C2B-C1B	2.59	129.28	124.71
30	A	824	CLA	CMB-C2B-C3B	2.59	129.53	124.68
30	15	304	CLA	CHB-C4A-NA	2.59	128.10	124.51
30	A	820	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
30	1	307	CLA	C4-C3-C5	2.59	119.63	115.27
30	2	308	CLA	CHC-C1C-C2C	-2.59	119.55	126.72
39	2	316	DD6	C21-C20-C15	-2.59	117.92	122.26
30	A	818	CLA	CHC-C1C-C2C	-2.59	119.55	126.72
38	6	308	KC1	CAC-C3C-C4C	2.59	128.17	124.81
37	7	315	A86	C4-C5-C6	-2.59	123.61	127.31
37	4	312	A86	C4-C3-C2	-2.59	118.17	123.47
38	5	310	KC1	CHC-C4B-NB	-2.59	122.07	124.45
30	A	805	CLA	CAA-C2A-C3A	-2.59	105.69	112.78
37	5	301	A86	C12-C11-C13	2.59	120.37	116.02
38	9	304	KC1	CHB-C1B-NB	-2.59	122.08	124.45
30	A	827	CLA	CHC-C1C-C2C	-2.59	119.56	126.72
30	13	304	CLA	CAA-C2A-C3A	-2.59	105.69	112.78
30	8	301	CLA	CBA-CAA-C2A	2.59	121.50	113.86
38	14	306	KC1	O2D-CGD-O1D	-2.59	118.78	123.84
39	15	319	DD6	C19-C18-C17	2.59	115.77	110.77
39	7	302	DD6	C25-C24-C1	-2.59	119.15	126.42
37	5	301	A86	C3-C2-C1	-2.59	123.62	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	3	306	CLA	CHB-C4A-NA	2.59	128.09	124.51
38	2	314	KC1	CAC-C3C-C4C	2.59	128.16	124.81
30	A	815	CLA	CAA-C2A-C3A	-2.59	105.70	112.78
30	3	303	CLA	C4-C3-C5	2.59	119.62	115.27
30	7	306	CLA	CAA-C2A-C3A	-2.59	105.70	112.78
33	B	841	BCR	C7-C8-C9	-2.58	122.33	126.23
30	B	834	CLA	CHC-C1C-C2C	-2.58	119.57	126.72
38	13	305	KC1	CHD-C4C-NC	2.58	128.12	124.20
30	7	311	CLA	CMC-C2C-C1C	2.58	128.97	125.04
30	A	828	CLA	CHB-C4A-NA	2.58	128.09	124.51
37	15	317	A86	C3-C4-C5	-2.58	118.18	123.47
30	6	310	CLA	CAC-C3C-C4C	2.58	128.16	124.81
30	16	310	CLA	CBC-CAC-C3C	-2.58	105.31	112.43
30	5	303	CLA	CMC-C2C-C1C	2.58	128.97	125.04
38	6	308	KC1	CMB-C2B-C1B	2.58	129.26	124.71
39	6	318	DD6	C33-C32-C31	2.58	114.85	109.62
34	B	848	LHG	C11-C10-C9	-2.58	101.32	114.42
30	12	308	CLA	C4-C3-C5	2.58	119.61	115.27
30	8	303	CLA	CMB-C2B-C3B	2.58	129.51	124.68
33	F	204	BCR	C40-C30-C25	2.58	114.48	110.30
38	6	311	KC1	CMB-C2B-C1B	2.58	129.26	124.71
30	A	828	CLA	OBD-CAD-C3D	-2.58	122.31	128.52
30	1	305	CLA	CMB-C2B-C3B	2.58	129.50	124.68
30	2	309	CLA	CHB-C4A-NA	2.58	128.08	124.51
30	14	312	CLA	CMB-C2B-C3B	2.58	129.50	124.68
30	B	803	CLA	CED-O2D-CGD	2.58	121.77	115.94
30	13	302	CLA	CMC-C2C-C1C	2.58	128.97	125.04
38	6	312	KC1	CMB-C2B-C1B	2.58	129.26	124.71
30	B	828	CLA	CAA-C2A-C3A	-2.58	105.72	112.78
30	8	309	CLA	CMB-C2B-C3B	2.58	129.50	124.68
38	11	307	KC1	O2D-CGD-O1D	-2.58	118.80	123.84
30	2	308	CLA	CED-O2D-CGD	2.58	121.77	115.94
33	A	848	BCR	C40-C30-C25	2.58	114.48	110.30
30	1	304	CLA	CHC-C1C-C2C	-2.58	119.59	126.72
30	3	302	CLA	CMC-C2C-C1C	2.58	128.96	125.04
37	12	314	A86	C12-C11-C13	2.58	120.35	116.02
39	7	317	DD6	C21-C20-C19	-2.58	111.38	114.28
30	8	309	CLA	CHB-C4A-NA	2.58	128.07	124.51
35	11	318	LMT	O1B-C4'-C3'	2.58	114.13	107.28
30	B	817	CLA	CHC-C1C-C2C	-2.58	119.60	126.72
30	3	309	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
30	6	306	CLA	CAC-C3C-C4C	2.57	128.15	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	824	CLA	CAC-C3C-C4C	2.57	128.15	124.81
30	A	808	CLA	C4-C3-C5	2.57	118.93	115.98
30	A	836	CLA	CBC-CAC-C3C	-2.57	105.33	112.43
38	6	311	KC1	O2D-CGD-O1D	-2.57	118.81	123.84
30	A	815	CLA	C1-C2-C3	-2.57	121.59	126.04
30	B	812	CLA	C1-O2A-CGA	2.57	123.20	116.44
30	4	305	CLA	C3B-C4B-NB	2.57	112.54	109.21
38	13	312	KC1	CMB-C2B-C1B	2.57	129.25	124.71
30	A	833	CLA	CHB-C4A-NA	2.57	128.07	124.51
30	11	306	CLA	C3B-C4B-NB	2.57	112.54	109.21
30	6	310	CLA	CHD-C4C-NC	2.57	128.26	124.20
30	11	310	CLA	C1-C2-C3	-2.57	121.59	126.04
30	A	818	CLA	CHB-C4A-NA	2.57	128.07	124.51
30	6	310	CLA	C4-C3-C5	2.57	119.60	115.27
30	A	805	CLA	CHB-C4A-NA	2.57	128.07	124.51
30	14	303	CLA	CMC-C2C-C1C	2.57	128.96	125.04
30	B	803	CLA	CHC-C1C-NC	2.57	128.10	124.20
30	9	306	CLA	CMB-C2B-C3B	2.57	129.49	124.68
29	A	801	CL0	CHB-C4A-NA	2.57	128.07	124.51
30	14	313	CLA	CAC-C3C-C4C	2.57	128.15	124.81
30	10	303	CLA	CMB-C2B-C3B	2.57	129.49	124.68
37	11	301	A86	C25-C24-C1	-2.57	119.20	126.42
30	A	836	CLA	CMA-C3A-C4A	-2.57	104.87	111.77
30	6	316	CLA	O2A-CGA-CBA	2.57	119.97	111.91
35	11	317	LMT	C1-O1'-C1'	-2.57	109.58	113.84
30	1	307	CLA	CHB-C4A-NA	2.57	128.06	124.51
30	8	305	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
30	B	813	CLA	CAA-C2A-C3A	-2.57	105.75	112.78
39	11	313	DD6	C25-C24-C1	-2.57	119.21	126.42
30	A	832	CLA	CMB-C2B-C3B	2.57	129.48	124.68
30	14	303	CLA	CMB-C2B-C3B	2.57	129.48	124.68
38	12	309	KC1	CBC-CAC-C3C	-2.57	105.36	112.43
30	15	309	CLA	CAA-C2A-C3A	-2.57	105.75	112.78
30	B	837	CLA	CMC-C2C-C1C	2.57	128.95	125.04
30	A	830	CLA	CHC-C1C-C2C	-2.57	119.63	126.72
33	A	847	BCR	C27-C26-C25	2.56	126.45	122.73
38	11	307	KC1	CHD-C4C-NC	2.56	128.09	124.20
30	A	816	CLA	C4A-NA-C1A	-2.56	105.55	106.71
30	1	303	CLA	C4-C3-C5	2.56	119.58	115.27
38	9	311	KC1	CMB-C2B-C1B	2.56	129.23	124.71
30	A	824	CLA	CAA-C2A-C3A	-2.56	105.76	112.78
33	L	201	BCR	C16-C15-C14	-2.56	118.22	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	11	310	CLA	CHD-C4C-NC	2.56	128.24	124.20
37	8	318	A86	C26-C25-C24	-2.56	115.22	123.22
30	10	307	CLA	C1-C2-C3	-2.56	121.61	126.04
37	15	322	A86	C23-C16-C17	-2.56	104.53	108.98
30	A	819	CLA	CHC-C1C-C2C	-2.56	119.64	126.72
30	2	310	CLA	CBC-CAC-C3C	-2.56	105.37	112.43
30	B	824	CLA	CHB-C4A-NA	2.56	128.05	124.51
30	A	843	CLA	C4-C3-C5	2.56	119.58	115.27
33	A	849	BCR	C38-C26-C27	-2.56	108.70	113.62
38	11	307	KC1	C4C-C3C-C2C	-2.56	103.17	106.90
30	A	841	CLA	CHB-C4A-NA	2.56	128.05	124.51
30	15	314	CLA	CAA-C2A-C3A	-2.56	105.77	112.78
38	6	312	KC1	CAC-C3C-C4C	2.56	128.13	124.81
30	2	309	CLA	C4-C3-C5	2.56	119.57	115.27
30	A	814	CLA	CHD-C4C-NC	2.56	128.23	124.20
30	A	841	CLA	O2A-CGA-O1A	-2.56	117.14	123.59
30	B	851	CLA	CED-O2D-CGD	2.56	121.72	115.94
30	B	836	CLA	CAA-C2A-C3A	-2.56	105.78	112.78
30	A	826	CLA	CMC-C2C-C1C	2.56	128.93	125.04
30	2u	202	CLA	C1-C2-C3	-2.56	121.62	126.04
30	B	808	CLA	C4-C3-C5	2.56	119.57	115.27
34	9	318	LHG	O8-C23-C24	2.56	119.93	111.91
30	B	839	CLA	CHA-C1A-NA	-2.56	120.55	126.40
30	15	304	CLA	CMB-C2B-C3B	2.56	129.46	124.68
38	6	308	KC1	O2D-CGD-O1D	-2.56	118.84	123.84
38	12	311	KC1	CAA-CBA-CGA	-2.56	114.13	127.26
38	13	311	KC1	CBC-CAC-C3C	-2.55	105.39	112.43
30	B	829	CLA	O1D-CGD-CBD	-2.55	119.26	124.48
30	A	819	CLA	CMC-C2C-C1C	2.55	128.93	125.04
30	2	309	CLA	CMC-C2C-C1C	2.55	128.93	125.04
37	14	317	A86	C34-O4-C38	-2.55	113.14	117.90
38	3	311	KC1	O2D-CGD-O1D	-2.55	118.85	123.84
33	I	101	BCR	C29-C30-C25	2.55	114.41	110.48
30	15	307	CLA	CHD-C4C-NC	2.55	128.23	124.20
30	A	828	CLA	CAC-C3C-C2C	2.55	131.90	127.53
38	2	312	KC1	CHD-C4C-NC	2.55	128.07	124.20
30	A	832	CLA	CHB-C4A-NA	2.55	128.04	124.51
38	2	312	KC1	CHB-C1B-NB	-2.55	122.11	124.45
37	14	314	A86	C34-O4-C38	-2.55	113.14	117.90
30	1	304	CLA	C4-C3-C5	2.55	119.56	115.27
33	A	847	BCR	C11-C10-C9	-2.55	123.67	127.31
30	16	301	CLA	C4-C3-C5	2.55	119.56	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	813	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
38	9	304	KC1	CMC-C2C-C1C	2.55	128.92	125.04
39	2	315	DD6	C37-C36-C35	-2.55	109.63	114.36
30	7	306	CLA	CMC-C2C-C1C	2.55	128.92	125.04
30	A	842	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
30	5	311	CLA	CAC-C3C-C4C	2.55	128.12	124.81
36	A	856	LMG	O6-C1-O1	-2.55	103.94	109.97
30	B	802	CLA	CHC-C1C-C2C	-2.55	119.67	126.72
30	4	306	CLA	CAA-CBA-CGA	-2.55	105.81	113.25
30	2	301	CLA	CHB-C4A-NA	2.55	128.04	124.51
30	4	311	CLA	CHB-C4A-NA	2.55	128.04	124.51
30	9	305	CLA	CHB-C4A-NA	2.55	128.04	124.51
30	A	823	CLA	CAC-C3C-C4C	2.55	128.12	124.81
30	A	821	CLA	CAA-C2A-C3A	-2.55	105.81	112.78
30	7	307	CLA	CMB-C2B-C3B	2.55	129.44	124.68
37	14	317	A86	C9-C10-C11	-2.55	119.12	126.61
30	B	836	CLA	CAC-C3C-C4C	2.55	128.11	124.81
38	16	311	KC1	O2D-CGD-O1D	-2.55	118.86	123.84
30	B	804	CLA	C1-C2-C3	-2.54	121.64	126.04
30	A	844	CLA	C4-C3-C5	2.54	119.55	115.27
30	A	815	CLA	CHB-C4A-NA	2.54	128.03	124.51
30	A	827	CLA	CAC-C3C-C2C	2.54	131.88	127.53
37	2	318	A86	C-C1-C24	2.54	122.08	118.08
38	8	314	KC1	O1D-CGD-CBD	-2.54	119.28	124.48
30	12	308	CLA	C1-C2-C3	-2.54	121.65	126.04
30	6	315	CLA	CBC-CAC-C3C	-2.54	105.43	112.43
30	A	808	CLA	CAA-C2A-C3A	-2.54	105.82	112.78
30	B	830	CLA	CHB-C4A-NA	2.54	128.03	124.51
39	13	314	DD6	C19-C18-C17	2.54	115.68	110.77
37	1	309	A86	C34-O4-C38	-2.54	113.16	117.90
30	4	306	CLA	O2A-CGA-CBA	2.54	119.88	111.91
37	12	316	A86	C7-C6-C5	-2.54	119.36	122.92
30	B	827	CLA	CMA-C3A-C2A	-2.54	103.58	113.83
38	1	306	KC1	CHD-C4C-NC	2.54	128.06	124.20
30	5	304	CLA	C4-C3-C5	2.54	119.54	115.27
37	4	315	A86	C-C1-C24	2.54	122.08	118.08
30	16	302	CLA	CMC-C2C-C1C	2.54	128.91	125.04
29	A	801	CL0	C4-C3-C5	2.54	119.54	115.27
30	7	306	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
30	5	307	CLA	C1-C2-C3	-2.54	121.66	126.04
37	3	314	A86	C20-C19-C18	-2.54	107.73	112.75
38	12	305	KC1	CMB-C2B-C1B	2.54	129.18	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	827	CLA	C1-C2-C3	-2.53	121.66	126.04
30	8	305	CLA	O2A-CGA-CBA	2.53	119.86	111.91
39	10	314	DD6	C25-C24-C1	-2.53	119.30	126.42
38	12	311	KC1	CHB-C4A-NA	2.53	128.20	124.20
30	B	810	CLA	CAA-C2A-C3A	-2.53	105.84	112.78
30	B	803	CLA	CAA-CBA-CGA	-2.53	105.85	113.25
30	9	309	CLA	CBC-CAC-C3C	-2.53	105.45	112.43
36	8	319	LMG	O3-C3-C2	-2.53	104.49	110.35
37	15	317	A86	C12-C11-C13	2.53	120.28	116.02
38	8	313	KC1	CED-O2D-CGD	2.53	121.66	115.94
38	13	308	KC1	CMB-C2B-C1B	2.53	129.18	124.71
30	11	304	CLA	CHB-C4A-NA	2.53	128.01	124.51
30	14	304	CLA	CAA-C2A-C3A	-2.53	105.85	112.78
37	14	320	A86	C40-C32-C31	-2.53	108.21	110.47
30	8	304	CLA	C1-C2-C3	-2.53	121.67	126.04
30	B	835	CLA	CMB-C2B-C3B	2.53	129.41	124.68
38	8	307	KC1	O2D-CGD-O1D	-2.53	118.89	123.84
39	1	310	DD6	C4-C3-C2	-2.53	118.29	123.47
38	16	304	KC1	CMB-C2B-C1B	2.53	129.17	124.71
37	4	317	A86	C7-C6-C8	2.53	122.06	118.08
37	5	316	A86	C20-C19-C18	-2.53	107.74	112.75
30	4	306	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
39	6	319	DD6	O1-C20-C21	-2.53	112.03	115.06
30	15	309	CLA	CHB-C4A-NA	2.53	128.01	124.51
30	9	309	CLA	CAC-C3C-C4C	2.53	128.09	124.81
30	A	804	CLA	O2A-CGA-CBA	2.53	119.84	111.91
38	8	313	KC1	C1C-C2C-C3C	-2.53	104.30	106.96
30	A	804	CLA	CMA-C3A-C4A	-2.53	104.98	111.77
37	14	314	A86	C23-C16-C17	-2.53	104.59	108.98
30	9	308	CLA	O2A-CGA-CBA	2.53	119.84	111.91
38	2	312	KC1	CMB-C2B-C1B	2.53	129.16	124.71
30	7	311	CLA	CHD-C4C-NC	2.53	128.18	124.20
30	4	306	CLA	CHB-C4A-NA	2.53	128.00	124.51
38	10	310	KC1	CHD-C4C-NC	2.53	128.03	124.20
30	A	824	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
38	3	311	KC1	CBA-CAA-C2A	-2.53	115.64	125.27
30	B	822	CLA	CBC-CAC-C3C	-2.52	105.47	112.43
30	7	305	CLA	C1-C2-C3	-2.52	121.68	126.04
30	8	309	CLA	CHD-C4C-NC	2.52	128.18	124.20
30	5	303	CLA	CBC-CAC-C3C	-2.52	105.47	112.43
37	8	318	A86	C12-C11-C10	-2.52	117.31	123.42
36	6	301	LMG	O7-C10-O9	-2.52	117.60	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	805	CLA	O2A-CGA-CBA	2.52	119.83	111.91
30	A	841	CLA	C4-C3-C5	2.52	119.52	115.27
35	7	301	LMT	O1B-C4'-C3'	2.52	114.00	107.28
39	1	310	DD6	C25-C24-C1	-2.52	119.33	126.42
37	2	302	A86	C28-C27-C26	-2.52	119.39	122.92
30	A	837	CLA	CHD-C4C-NC	2.52	128.18	124.20
30	F	201	CLA	CMC-C2C-C1C	2.52	128.88	125.04
30	F	203	CLA	CMB-C2B-C3B	2.52	129.40	124.68
37	15	315	A86	C20-C19-C18	-2.52	107.76	112.75
38	12	311	KC1	CBA-CAA-C2A	-2.52	115.65	125.27
30	13	302	CLA	CAA-C2A-C3A	-2.52	105.87	112.78
30	6	307	CLA	CHD-C4C-NC	2.52	128.18	124.20
39	7	314	DD6	C3-C4-C5	-2.52	118.31	123.47
39	9	314	DD6	C21-C20-C15	-2.52	118.03	122.26
30	6	306	CLA	CHB-C4A-NA	2.52	128.00	124.51
36	B	847	LMG	C40-C39-C38	-2.52	101.63	114.42
39	6	303	DD6	C25-C24-C1	-2.52	119.33	126.42
30	6	317	CLA	CAC-C3C-C4C	2.52	128.08	124.81
33	2u	201	BCR	C28-C27-C26	-2.52	109.58	114.08
30	2	309	CLA	CMB-C2B-C3B	2.52	129.39	124.68
30	14	307	CLA	C1-O2A-CGA	2.52	123.05	116.44
30	A	841	CLA	C1-C2-C3	-2.52	121.69	126.04
30	6	310	CLA	C1-C2-C3	-2.52	121.69	126.04
30	15	305	CLA	CMB-C2B-C3B	2.52	129.39	124.68
30	B	826	CLA	C4-C3-C5	2.52	119.51	115.27
30	B	811	CLA	CAA-C2A-C3A	-2.52	105.88	112.78
39	4	316	DD6	C26-C25-C24	-2.52	115.36	123.22
30	A	814	CLA	CHC-C1C-NC	2.52	128.02	124.20
30	7	303	CLA	CHC-C1C-C2C	-2.52	119.76	126.72
30	A	802	CLA	O2A-CGA-CBA	2.52	119.81	111.91
38	16	304	KC1	O2D-CGD-O1D	-2.52	118.92	123.84
30	A	803	CLA	C4-C3-C5	2.52	119.50	115.27
30	15	303	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
37	2u	205	A86	C41-C32-C31	-2.52	108.22	110.47
30	16	301	CLA	CMB-C2B-C3B	2.51	129.38	124.68
30	B	801	CLA	O2A-CGA-CBA	2.51	119.80	111.91
30	F	202	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
30	F	201	CLA	C3B-C4B-NB	2.51	112.46	109.21
30	14	313	CLA	CBC-CAC-C3C	-2.51	105.50	112.43
30	5	309	CLA	CMC-C2C-C1C	2.51	128.87	125.04
39	7	317	DD6	O1-C20-C21	-2.51	112.05	115.06
38	11	312	KC1	CHB-C4A-NA	2.51	128.16	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	13	305	KC1	CMB-C2B-C1B	2.51	129.14	124.71
30	14	302	CLA	CHB-C4A-NA	2.51	127.99	124.51
34	2	320	LHG	C11-C10-C9	-2.51	101.67	114.42
30	14	302	CLA	CMB-C2B-C3B	2.51	129.38	124.68
30	B	820	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
30	3	306	CLA	CMC-C2C-C1C	2.51	128.86	125.04
30	10	307	CLA	C4-C3-C5	2.51	119.50	115.27
30	B	813	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
37	12	316	A86	C36-C31-C32	-2.51	117.21	119.70
30	A	804	CLA	C4-C3-C5	2.51	119.49	115.27
38	4	308	KC1	CHB-C4A-NA	2.51	128.16	124.20
30	10	305	CLA	C1-O2A-CGA	2.51	123.03	116.44
30	B	812	CLA	CHD-C4C-NC	2.51	128.16	124.20
30	B	825	CLA	OBD-CAD-C3D	-2.51	122.48	128.52
38	4	310	KC1	CBA-CAA-C2A	-2.51	115.71	125.27
39	7	314	DD6	C10-C9-C8	-2.51	115.39	123.22
38	3	311	KC1	CHB-C1B-NB	-2.51	122.15	124.45
30	3	302	CLA	C1-C2-C3	-2.51	121.71	126.04
30	13	307	CLA	C1-C2-C3	-2.51	121.71	126.04
30	A	834	CLA	C4-C3-C5	2.51	119.49	115.27
30	2	309	CLA	C1-O2A-CGA	2.51	123.02	116.44
30	3	309	CLA	CMB-C2B-C3B	2.51	129.37	124.68
30	14	303	CLA	CBA-CAA-C2A	2.51	121.26	113.86
30	B	820	CLA	CMB-C2B-C3B	2.51	129.37	124.68
30	12	310	CLA	CAA-C2A-C3A	-2.50	105.92	112.78
30	B	802	CLA	O2A-CGA-O1A	-2.50	117.27	123.59
30	B	807	CLA	CHD-C4C-NC	2.50	128.15	124.20
30	6	317	CLA	CBC-CAC-C3C	-2.50	105.53	112.43
30	B	823	CLA	CMB-C2B-C3B	2.50	129.36	124.68
30	6	304	CLA	C4C-C3C-C2C	-2.50	103.25	106.90
38	12	309	KC1	CAC-C3C-C4C	2.50	128.06	124.81
30	5	307	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
30	14	309	CLA	CHD-C4C-NC	2.50	128.15	124.20
30	1	303	CLA	CHB-C4A-NA	2.50	127.97	124.51
30	11	310	CLA	C4-C3-C5	2.50	119.48	115.27
30	5	309	CLA	O2A-CGA-CBA	2.50	119.76	111.91
30	F	203	CLA	CMC-C2C-C1C	2.50	128.85	125.04
30	F	203	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
30	12	310	CLA	C4-C3-C5	2.50	119.48	115.27
30	4	304	CLA	CMB-C2B-C3B	2.50	129.36	124.68
31	B	840	PQN	C2M-C2-C3	-2.50	120.32	124.40
38	5	310	KC1	O2D-CGD-O1D	-2.50	118.95	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	3	306	CLA	CBC-CAC-C3C	-2.50	105.55	112.43
38	4	307	KC1	CBC-CAC-C3C	-2.50	105.55	112.43
30	11	304	CLA	CMC-C2C-C1C	2.50	128.84	125.04
39	10	313	DD6	C20-C19-C18	2.50	117.69	112.75
30	6	307	CLA	CMA-C3A-C4A	-2.50	105.06	111.77
39	7	317	DD6	C3-C4-C5	-2.50	118.36	123.47
30	6	316	CLA	CHB-C4A-NA	2.50	127.96	124.51
30	B	822	CLA	CHD-C4C-NC	2.50	128.14	124.20
30	10	304	CLA	C1-C2-C3	-2.50	121.73	126.04
30	3	306	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
38	1	308	KC1	O2D-CGD-O1D	-2.50	118.96	123.84
30	B	811	CLA	CMC-C2C-C1C	2.50	128.84	125.04
38	8	310	KC1	C1C-C2C-C3C	-2.50	104.33	106.96
30	B	810	CLA	C4-C3-C5	2.49	119.47	115.27
30	A	839	CLA	O2A-CGA-O1A	-2.49	117.30	123.59
30	4	304	CLA	O2A-CGA-O1A	-2.49	117.30	123.59
30	B	817	CLA	CHB-C4A-NA	2.49	127.96	124.51
37	15	315	A86	C9-C8-C6	2.49	133.42	126.42
30	6	314	CLA	C1-C2-C3	-2.49	121.73	126.04
38	7	313	KC1	CHB-C1B-NB	-2.49	122.16	124.45
30	13	302	CLA	C1-O2A-CGA	2.49	122.98	116.44
30	A	813	CLA	CAC-C3C-C4C	2.49	128.04	124.81
30	11	308	CLA	CAC-C3C-C4C	2.49	128.04	124.81
30	12	310	CLA	CAC-C3C-C4C	2.49	128.04	124.81
30	9	303	CLA	CBC-CAC-C3C	-2.49	105.56	112.43
30	14	303	CLA	CBC-CAC-C3C	-2.49	105.56	112.43
30	14	307	CLA	O2A-CGA-CBA	2.49	119.73	111.91
37	16	314	A86	C7-C6-C8	2.49	122.00	118.08
30	A	834	CLA	O2A-CGA-CBA	2.49	119.72	111.91
33	M	101	BCR	C15-C14-C13	-2.49	123.75	127.31
38	12	305	KC1	CHB-C1B-NB	-2.49	122.17	124.45
30	2u	202	CLA	O2A-CGA-CBA	2.49	119.72	111.91
30	6	317	CLA	CMB-C2B-C3B	2.49	129.34	124.68
37	14	318	A86	C7-C6-C5	-2.49	119.44	122.92
30	9	307	CLA	CMC-C2C-C1C	2.49	128.83	125.04
37	10	317	A86	C23-C16-C17	-2.49	104.66	108.98
30	B	825	CLA	C4-C3-C5	2.49	119.46	115.27
39	6	319	DD6	C20-C19-C18	2.49	117.67	112.75
30	8	305	CLA	CAA-C2A-C3A	-2.49	105.96	112.78
38	13	305	KC1	CAA-CBA-CGA	-2.49	114.47	127.26
37	4	315	A86	C20-C19-C18	-2.49	107.83	112.75
37	12	314	A86	C25-C26-C27	-2.49	123.76	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	1	305	CLA	CHD-C4C-NC	2.49	128.12	124.20
30	A	809	CLA	CHB-C4A-NA	2.49	127.95	124.51
30	15	306	CLA	CHD-C4C-NC	2.49	128.12	124.20
30	15	313	CLA	CBC-CAC-C3C	-2.49	105.57	112.43
30	7	303	CLA	C3B-C4B-NB	2.49	112.43	109.21
30	15	314	CLA	CHD-C4C-NC	2.49	128.12	124.20
37	14	319	A86	C7-C6-C5	-2.49	119.44	122.92
33	A	850	BCR	C27-C26-C25	2.49	126.34	122.73
38	12	311	KC1	CBC-CAC-C3C	-2.49	105.58	112.43
39	8	316	DD6	C40-C32-C31	-2.49	106.52	110.47
30	6	314	CLA	C4C-C3C-C2C	-2.49	103.27	106.90
30	A	833	CLA	CAC-C3C-C4C	2.49	128.04	124.81
33	B	846	BCR	C27-C26-C25	2.49	126.34	122.73
37	1	309	A86	C7-C6-C5	-2.49	119.44	122.92
38	1	308	KC1	CAC-C3C-C4C	2.48	128.03	124.81
30	13	304	CLA	CMB-C2B-C3B	2.48	129.33	124.68
30	3	307	CLA	O2A-CGA-CBA	2.48	119.70	111.91
30	6	309	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
37	4	314	A86	C12-C11-C13	2.48	120.19	116.02
30	B	828	CLA	C1-O2A-CGA	2.48	122.96	116.44
30	A	839	CLA	C1-C2-C3	-2.48	121.75	126.04
38	3	308	KC1	O2D-CGD-O1D	-2.48	118.98	123.84
30	9	306	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
38	4	308	KC1	CHC-C4B-C3B	-2.48	121.01	125.26
30	2	307	CLA	CHD-C4C-NC	2.48	128.12	124.20
37	10	302	A86	C28-C27-C26	-2.48	119.45	122.92
30	A	822	CLA	CHB-C4A-NA	2.48	127.94	124.51
30	7	306	CLA	CHB-C4A-NA	2.48	127.94	124.51
38	11	305	KC1	CMB-C2B-C1B	2.48	129.09	124.71
30	A	838	CLA	C4-C3-C5	2.48	118.82	115.98
30	9	302	CLA	CHD-C4C-NC	2.48	128.11	124.20
33	J	102	BCR	C27-C26-C25	2.48	126.33	122.73
30	5	304	CLA	C4A-NA-C1A	-2.48	105.59	106.71
38	6	311	KC1	CHC-C4B-NB	-2.48	122.17	124.45
30	6	309	CLA	C4-C3-C5	2.48	119.44	115.27
30	A	805	CLA	O1D-CGD-CBD	-2.48	119.41	124.48
30	8	304	CLA	CBA-CAA-C2A	2.48	121.18	113.86
30	5	304	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
30	B	836	CLA	CMC-C2C-C1C	2.48	128.81	125.04
38	13	311	KC1	CMC-C2C-C1C	2.48	128.81	125.04
30	B	851	CLA	CAA-CBA-CGA	-2.48	106.01	113.25
38	8	311	KC1	CHD-C4C-NC	2.48	127.96	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	10	308	CLA	CHB-C4A-NA	2.48	127.94	124.51
30	3	310	CLA	CAA-C2A-C3A	-2.48	105.99	112.78
30	3	305	CLA	CMB-C2B-C3B	2.48	129.31	124.68
30	15	313	CLA	CMB-C2B-C3B	2.48	129.31	124.68
37	3	315	A86	C9-C8-C6	-2.48	119.46	126.42
30	11	309	CLA	CHD-C4C-NC	2.48	128.11	124.20
30	B	814	CLA	C1-C2-C3	-2.48	121.76	126.04
30	2	304	CLA	C1-C2-C3	-2.48	121.76	126.04
30	1	305	CLA	CAA-C2A-C3A	-2.48	106.00	112.78
30	11	309	CLA	O1D-CGD-CBD	-2.48	119.42	124.48
37	9	315	A86	O1-C15-C14	-2.48	108.24	113.21
30	15	313	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
30	12	308	CLA	CMC-C2C-C1C	2.47	128.81	125.04
37	8	318	A86	C7-C6-C5	2.47	126.39	122.92
38	13	312	KC1	CBC-CAC-C3C	-2.47	105.61	112.43
30	A	843	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
30	A	826	CLA	CHD-C4C-NC	2.47	128.10	124.20
30	A	819	CLA	O2A-CGA-CBA	2.47	119.67	111.91
30	B	827	CLA	CHD-C4C-NC	2.47	128.10	124.20
30	6	315	CLA	CAA-C2A-C3A	-2.47	106.01	112.78
30	A	832	CLA	CAA-C2A-C3A	-2.47	106.01	112.78
30	8	302	CLA	O2A-CGA-CBA	2.47	119.66	111.91
30	A	820	CLA	CHD-C4C-NC	2.47	128.10	124.20
30	4	302	CLA	CBA-CAA-C2A	2.47	121.16	113.86
38	4	308	KC1	C1A-NA-C4A	-2.47	105.59	106.71
30	A	813	CLA	C4-C3-C5	2.47	119.43	115.27
30	A	819	CLA	CHB-C4A-NA	2.47	127.93	124.51
30	15	307	CLA	CHB-C4A-NA	2.47	127.93	124.51
39	3	316	DD6	C14-C13-C11	-2.47	121.70	125.53
30	4	304	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
30	3	307	CLA	CHB-C4A-NA	2.47	127.93	124.51
38	8	306	KC1	CHB-C4A-NA	2.47	128.09	124.20
30	15	310	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
30	10	311	CLA	CMB-C2B-C3B	2.47	129.30	124.68
30	A	830	CLA	CMA-C3A-C2A	-2.47	103.87	113.83
30	A	827	CLA	CMC-C2C-C1C	2.47	128.80	125.04
30	A	839	CLA	O1D-CGD-CBD	-2.47	119.43	124.48
36	B	847	LMG	C38-C37-C36	-2.47	101.90	114.42
37	5	316	A86	C3-C4-C5	-2.47	118.42	123.47
39	3	313	DD6	C15-C14-C13	-2.47	120.78	125.99
30	2	304	CLA	CBC-CAC-C3C	-2.47	105.63	112.43
30	B	805	CLA	CHD-C4C-NC	2.47	128.09	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	808	CLA	CMB-C2B-C3B	2.47	129.29	124.68
30	B	821	CLA	O2A-CGA-CBA	2.47	119.65	111.91
30	11	308	CLA	C4-C3-C5	2.47	119.42	115.27
30	15	305	CLA	CHD-C4C-NC	2.47	128.09	124.20
33	L	204	BCR	C1-C6-C5	-2.46	119.14	122.61
30	A	833	CLA	CMB-C2B-C3B	2.46	129.29	124.68
30	B	819	CLA	C3B-C4B-NB	2.46	112.39	109.21
30	B	832	CLA	C4-C3-C5	2.46	119.42	115.27
33	L	204	BCR	C27-C26-C25	2.46	126.31	122.73
39	6	318	DD6	O1-C20-C21	-2.46	112.11	115.06
38	12	305	KC1	O2D-CGD-O1D	-2.46	119.02	123.84
30	2	303	CLA	C4C-C3C-C2C	-2.46	103.31	106.90
33	M	101	BCR	C27-C26-C25	2.46	126.31	122.73
30	A	816	CLA	CAA-C2A-C3A	-2.46	106.04	112.78
38	12	309	KC1	CHB-C4A-NA	2.46	128.08	124.20
30	B	806	CLA	CAC-C3C-C4C	2.46	128.00	124.81
37	15	317	A86	C10-C9-C8	-2.46	115.53	123.22
30	A	818	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
30	14	310	CLA	CMC-C2C-C1C	2.46	128.79	125.04
30	2	309	CLA	O2A-CGA-CBA	2.46	119.63	111.91
30	9	308	CLA	CAA-C2A-C1A	2.46	120.04	111.97
30	A	815	CLA	CHD-C4C-NC	2.46	128.08	124.20
30	6	315	CLA	CMC-C2C-C1C	2.46	128.79	125.04
30	7	304	CLA	CAC-C3C-C4C	2.46	128.00	124.81
37	8	315	A86	C7-C6-C8	2.46	121.95	118.08
30	B	821	CLA	CAA-C2A-C3A	-2.46	106.04	112.78
37	1	309	A86	C24-C1-C2	-2.46	115.17	118.94
30	3	305	CLA	CBC-CAC-C3C	-2.46	105.65	112.43
30	4	309	CLA	C4-C3-C5	2.46	119.41	115.27
36	8	320	LMG	O3-C3-C2	-2.46	104.67	110.35
30	A	807	CLA	CMB-C2B-C3B	2.46	129.28	124.68
30	B	807	CLA	CHB-C4A-NA	2.46	127.91	124.51
30	B	838	CLA	CHB-C4A-NA	2.46	127.91	124.51
37	5	301	A86	C25-C26-C27	-2.46	123.81	127.31
30	B	835	CLA	CHB-C4A-NA	2.46	127.91	124.51
30	A	828	CLA	CAA-C2A-C3A	-2.46	106.05	112.78
30	A	819	CLA	O2D-CGD-O1D	-2.46	119.04	123.84
30	4	306	CLA	C4-C3-C5	2.46	119.40	115.27
34	6	322	LHG	C11-C10-C9	-2.45	101.96	114.42
30	13	303	CLA	C1-C2-C3	-2.45	121.80	126.04
30	A	810	CLA	CHD-C4C-NC	2.45	128.07	124.20
30	A	820	CLA	CAA-C2A-C3A	-2.45	106.06	112.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	7	311	CLA	CMB-C2B-C3B	2.45	129.27	124.68
37	15	320	A86	C7-C6-C5	-2.45	119.49	122.92
37	7	316	A86	C19-C18-C17	-2.45	106.03	110.77
33	A	847	BCR	C7-C8-C9	-2.45	122.53	126.23
30	4	304	CLA	CAA-C2A-C3A	-2.45	106.06	112.78
30	B	825	CLA	CAC-C3C-C4C	2.45	127.99	124.81
30	L	203	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
37	10	301	A86	C7-C6-C8	2.45	121.94	118.08
39	5	314	DD6	C4-C3-C2	-2.45	118.45	123.47
30	J	101	CLA	CHB-C4A-NA	2.45	127.90	124.51
33	B	844	BCR	C40-C30-C25	2.45	114.28	110.30
30	B	830	CLA	O2A-CGA-CBA	2.45	119.60	111.91
30	2	313	CLA	CAA-C2A-C3A	-2.45	106.07	112.78
30	A	806	CLA	CBC-CAC-C3C	-2.45	105.68	112.43
30	2	313	CLA	CMB-C2B-C3B	2.45	129.26	124.68
30	A	835	CLA	CHB-C4A-NA	2.45	127.90	124.51
30	L	202	CLA	C1-C2-C3	-2.45	121.81	126.04
30	4	311	CLA	CMB-C2B-C3B	2.45	129.26	124.68
37	14	314	A86	C25-C24-C1	-2.45	119.54	126.42
30	A	823	CLA	CHB-C4A-NA	2.45	127.90	124.51
30	A	834	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
30	4	304	CLA	CBC-CAC-C3C	-2.45	105.68	112.43
30	6	317	CLA	CMC-C2C-C1C	2.45	128.77	125.04
33	A	851	BCR	C27-C26-C25	2.45	126.28	122.73
30	1	307	CLA	CBC-CAC-C3C	-2.45	105.69	112.43
30	3	303	CLA	CMB-C2B-C3B	2.45	129.25	124.68
33	2u	201	BCR	C29-C30-C25	2.45	114.25	110.48
39	2	317	DD6	C14-C13-C11	-2.45	121.74	125.53
38	4	310	KC1	CHB-C4A-NA	2.44	128.06	124.20
37	4	315	A86	C35-C34-C33	2.44	114.14	109.88
30	14	310	CLA	CBC-CAC-C3C	-2.44	105.69	112.43
30	A	831	CLA	O2A-CGA-CBA	2.44	119.58	111.91
37	2u	205	A86	C23-C16-C17	-2.44	104.74	108.98
38	10	312	KC1	CBC-CAC-C3C	-2.44	105.69	112.43
30	A	814	CLA	CAA-C2A-C3A	-2.44	106.09	112.78
30	14	310	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
30	3	305	CLA	CMC-C2C-C1C	2.44	128.76	125.04
38	7	308	KC1	CAA-C2A-C1A	-2.44	113.52	124.75
33	A	849	BCR	C15-C16-C17	-2.44	118.47	123.47
30	2	301	CLA	CHD-C4C-NC	2.44	128.05	124.20
38	16	304	KC1	CHD-C4C-NC	2.44	127.91	124.20
38	3	304	KC1	CHB-C1B-NB	-2.44	122.21	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	16	309	CLA	CMB-C2B-C3B	2.44	129.24	124.68
39	11	313	DD6	C20-C19-C18	2.44	117.58	112.75
36	8	319	LMG	C38-C37-C36	-2.44	102.04	114.42
30	5	307	CLA	O2A-CGA-CBA	2.44	119.56	111.91
38	2	306	KC1	CHB-C1B-NB	-2.44	122.21	124.45
30	11	306	CLA	CHB-C4A-NA	2.44	127.89	124.51
30	5	302	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
38	13	305	KC1	CHB-C4A-NA	2.44	128.05	124.20
38	14	306	KC1	CAA-C2A-C1A	-2.44	113.53	124.75
37	13	313	A86	C4-C3-C2	-2.44	118.48	123.47
30	16	308	CLA	CMB-C2B-C3B	2.44	129.24	124.68
30	7	311	CLA	CAA-C2A-C3A	-2.44	106.10	112.78
36	8	321	LMG	O3-C3-C2	-2.44	104.71	110.35
30	7	303	CLA	C4-C3-C2	-2.44	117.42	123.68
37	14	316	A86	C4-C3-C2	-2.44	118.48	123.47
38	12	311	KC1	CHC-C4B-NB	-2.44	122.21	124.45
30	2	313	CLA	CHB-C4A-NA	2.44	127.88	124.51
36	B	849	LMG	C38-C37-C36	-2.44	102.05	114.42
30	B	809	CLA	O2A-CGA-CBA	2.44	119.55	111.91
30	14	302	CLA	CBC-CAC-C3C	-2.44	105.72	112.43
30	15	310	CLA	CAA-C2A-C3A	-2.44	106.11	112.78
30	6	315	CLA	CHB-C4A-NA	2.44	127.88	124.51
30	15	314	CLA	CHB-C4A-NA	2.44	127.88	124.51
38	3	304	KC1	CBD-CHA-C1A	2.44	133.42	128.88
37	5	301	A86	C9-C10-C11	-2.43	119.45	126.61
30	13	307	CLA	C4-C3-C5	2.43	119.37	115.27
33	B	844	BCR	C3-C4-C5	-2.43	109.73	114.08
30	B	812	CLA	CMC-C2C-C1C	2.43	128.75	125.04
30	4	304	CLA	CHB-C4A-NA	2.43	127.88	124.51
30	14	305	CLA	CBC-CAC-C3C	-2.43	105.72	112.43
38	14	306	KC1	O1D-CGD-CBD	-2.43	119.50	124.48
29	A	801	CL0	C1-C2-C3	-2.43	121.83	126.04
30	8	303	CLA	C1-C2-C3	-2.43	121.83	126.04
30	15	308	CLA	CAA-C2A-C1A	2.43	119.95	111.97
30	5	307	CLA	CBC-CAC-C3C	-2.43	105.72	112.43
37	11	301	A86	C3-C4-C5	-2.43	118.49	123.47
30	16	307	CLA	CMB-C2B-C3B	2.43	129.23	124.68
30	5	303	CLA	O2A-CGA-CBA	2.43	119.54	111.91
30	A	823	CLA	C4C-C3C-C2C	-2.43	103.35	106.90
38	2	306	KC1	CMC-C2C-C1C	2.43	128.74	125.04
37	11	316	A86	C-C1-C24	2.43	121.91	118.08
30	B	831	CLA	C1-C2-C3	-2.43	121.84	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	10	308	CLA	CBC-CAC-C3C	-2.43	105.73	112.43
30	B	823	CLA	CHA-C1A-NA	-2.43	120.83	126.40
37	10	315	A86	C22-C16-C17	-2.43	104.76	108.98
30	13	304	CLA	CBC-CAC-C3C	-2.43	105.73	112.43
30	A	837	CLA	CBC-CAC-C3C	-2.43	105.73	112.43
30	B	831	CLA	O2A-CGA-CBA	2.43	119.53	111.91
37	15	321	A86	C-C1-C24	2.43	121.91	118.08
30	A	803	CLA	C1-O2A-CGA	2.43	122.82	116.44
30	4	303	CLA	O2A-CGA-CBA	2.43	119.53	111.91
30	8	303	CLA	O2A-CGA-CBA	2.43	119.53	111.91
30	6	304	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
30	B	819	CLA	CAC-C3C-C4C	2.43	127.96	124.81
30	15	304	CLA	CAA-C2A-C3A	-2.43	106.13	112.78
30	16	310	CLA	O1D-CGD-CBD	2.43	129.45	124.48
30	7	303	CLA	CAC-C3C-C4C	2.43	127.96	124.81
37	1	309	A86	C3-C4-C5	2.43	128.44	123.47
38	3	304	KC1	CHB-C4A-NA	2.43	128.03	124.20
37	16	314	A86	C12-C11-C13	2.43	120.10	116.02
30	11	309	CLA	CAA-C2A-C3A	-2.43	106.13	112.78
38	8	313	KC1	CMB-C2B-C1B	2.43	128.99	124.71
30	B	851	CLA	CMB-C2B-C3B	2.43	129.22	124.68
30	3	310	CLA	CHB-C4A-NA	2.43	127.87	124.51
33	B	846	BCR	C16-C15-C14	-2.43	118.51	123.47
39	10	313	DD6	C25-C24-C1	-2.42	119.61	126.42
37	10	316	A86	O-C13-C11	-2.42	115.79	121.15
38	13	305	KC1	CHC-C4B-NB	-2.42	122.23	124.45
39	10	314	DD6	C23-C16-C22	-2.42	103.79	107.37
30	4	309	CLA	CBC-CAC-C3C	-2.42	105.75	112.43
30	B	819	CLA	CED-O2D-CGD	2.42	121.42	115.94
30	10	307	CLA	O2A-CGA-CBA	2.42	119.51	111.91
30	A	825	CLA	CMC-C2C-C1C	2.42	128.73	125.04
30	A	813	CLA	CHB-C4A-NA	2.42	127.86	124.51
30	3	309	CLA	CAC-C3C-C4C	2.42	127.95	124.81
39	10	313	DD6	C19-C18-C17	2.42	115.45	110.77
30	B	806	CLA	O2A-CGA-CBA	2.42	119.51	111.91
30	B	838	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
30	16	303	CLA	CHB-C4A-NA	2.42	127.86	124.51
30	A	817	CLA	CAA-C2A-C3A	-2.42	106.14	112.78
30	B	837	CLA	CAA-C2A-C3A	-2.42	106.14	112.78
30	6	316	CLA	CHD-C4C-NC	2.42	128.02	124.20
38	5	305	KC1	CHB-C4A-NA	2.42	128.02	124.20
30	3	301	CLA	CHB-C4A-NA	2.42	127.86	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	12	313	KC1	CAC-C3C-C4C	2.42	127.95	124.81
30	12	310	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
30	A	817	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
38	10	306	KC1	CMC-C2C-C1C	2.42	128.72	125.04
37	7	316	A86	C24-C1-C2	-2.42	115.23	118.94
39	6	319	DD6	C9-C8-C6	-2.42	119.62	126.42
30	A	802	CLA	CBC-CAC-C3C	-2.42	105.76	112.43
30	12	321	CLA	C4-C3-C5	2.42	119.34	115.27
30	13	309	CLA	CHB-C4A-NA	2.42	127.86	124.51
30	B	811	CLA	O2A-CGA-CBA	2.42	119.50	111.91
39	12	317	DD6	C19-C18-C17	2.42	115.44	110.77
33	B	844	BCR	C27-C26-C25	2.42	126.24	122.73
38	11	305	KC1	CHB-C1B-NB	-2.42	122.23	124.45
30	4	301	CLA	CAC-C3C-C4C	2.42	127.94	124.81
30	5	303	CLA	CHB-C4A-NA	2.42	127.85	124.51
30	4	304	CLA	CMC-C2C-C1C	2.42	128.72	125.04
30	A	824	CLA	CMC-C2C-C1C	2.41	128.72	125.04
30	A	836	CLA	CMA-C3A-C2A	-2.41	104.09	113.83
30	1	307	CLA	CMB-C2B-C3B	2.41	129.19	124.68
30	9	306	CLA	CBC-CAC-C3C	-2.41	105.78	112.43
30	4	311	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
30	L	202	CLA	CAC-C3C-C4C	2.41	127.94	124.81
36	F	205	LMG	O7-C10-O9	-2.41	117.88	123.70
30	2	304	CLA	O1D-CGD-CBD	-2.41	119.55	124.48
38	11	305	KC1	CBC-CAC-C3C	-2.41	105.79	112.43
30	8	303	CLA	CBC-CAC-C3C	-2.41	105.79	112.43
30	A	806	CLA	CHB-C4A-NA	2.41	127.84	124.51
30	1	305	CLA	CHB-C4A-NA	2.41	127.84	124.51
30	B	806	CLA	CED-O2D-CGD	2.41	121.39	115.94
38	8	311	KC1	CHB-C4A-NA	2.41	128.00	124.20
39	2	316	DD6	C34-C35-C36	-2.41	107.06	111.85
38	7	308	KC1	CAC-C3C-C4C	2.41	127.94	124.81
30	9	309	CLA	CED-O2D-CGD	2.41	121.38	115.94
30	5	304	CLA	CMB-C2B-C3B	2.41	129.18	124.68
30	2	310	CLA	CMC-C2C-C1C	2.41	128.71	125.04
30	7	305	CLA	O2A-CGA-CBA	2.41	119.46	111.91
30	B	827	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
30	2	305	CLA	C1-O2A-CGA	2.41	122.76	116.44
38	16	304	KC1	CHB-C4A-NA	2.41	128.00	124.20
30	3	301	CLA	CMC-C2C-C1C	2.41	128.70	125.04
30	15	305	CLA	CMC-C2C-C1C	2.41	128.70	125.04
30	8	309	CLA	CAA-C2A-C3A	-2.41	106.19	112.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	840	PQN	C17-C16-C15	-2.40	106.83	113.36
30	16	306	CLA	CMC-C2C-C1C	2.40	128.70	125.04
30	B	812	CLA	CHB-C4A-NA	2.40	127.84	124.51
30	A	837	CLA	CMC-C2C-C1C	2.40	128.70	125.04
38	5	306	KC1	O2D-CGD-O1D	-2.40	119.14	123.84
30	A	825	CLA	C1-C2-C3	-2.40	121.89	126.04
37	7	315	A86	C20-C19-C18	-2.40	108.00	112.75
30	A	836	CLA	CHD-C4C-NC	2.40	127.99	124.20
37	15	321	A86	O1-C15-C14	2.40	118.03	113.21
30	A	822	CLA	CMB-C2B-C3B	2.40	129.17	124.68
30	A	842	CLA	CMB-C2B-C3B	2.40	129.17	124.68
30	B	819	CLA	CMB-C2B-C3B	2.40	129.17	124.68
30	6	315	CLA	CMB-C2B-C3B	2.40	129.17	124.68
35	A	854	LMT	O1B-C4'-C3'	2.40	113.67	107.28
30	15	306	CLA	O1D-CGD-CBD	-2.40	119.57	124.48
39	12	317	DD6	C20-C19-C18	2.40	117.50	112.75
30	A	805	CLA	C1-C2-C3	-2.40	121.89	126.04
37	3	315	A86	C35-C34-C33	2.40	114.07	109.88
39	11	313	DD6	O1-C20-C21	-2.40	112.18	115.06
30	7	304	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
30	B	809	CLA	C4-C3-C5	2.40	119.31	115.27
30	2	311	CLA	CHB-C4A-NA	2.40	127.83	124.51
30	8	302	CLA	CMC-C2C-C1C	2.40	128.69	125.04
30	2	304	CLA	CHB-C4A-NA	2.40	127.83	124.51
37	15	320	A86	C23-C16-C17	-2.40	104.81	108.98
30	6	306	CLA	O2A-C1-C2	2.40	114.94	108.64
31	A	845	PQN	C11-C12-C13	-2.40	122.80	126.79
30	B	824	CLA	CMB-C2B-C3B	2.40	129.16	124.68
30	6	307	CLA	CMB-C2B-C3B	2.40	129.16	124.68
37	8	318	A86	C22-C16-C17	-2.40	104.82	108.98
30	A	806	CLA	C1C-C2C-C3C	-2.40	104.44	106.96
30	10	303	CLA	CBA-CAA-C2A	2.40	120.94	113.86
38	3	308	KC1	CMC-C2C-C1C	2.40	128.69	125.04
30	A	810	CLA	CBC-CAC-C3C	-2.40	105.82	112.43
30	B	814	CLA	CAC-C3C-C4C	2.40	127.92	124.81
30	15	304	CLA	CAC-C3C-C4C	2.40	127.92	124.81
30	13	303	CLA	CHB-C4A-NA	2.40	127.83	124.51
30	A	823	CLA	O2A-CGA-CBA	2.40	119.43	111.91
30	B	811	CLA	CAC-C3C-C4C	2.40	127.92	124.81
30	10	304	CLA	O2A-CGA-CBA	2.40	119.42	111.91
30	B	811	CLA	CHB-C4A-NA	2.40	127.82	124.51
33	A	850	BCR	C15-C14-C13	-2.39	123.89	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	828	CLA	C1-C2-C3	-2.39	121.90	126.04
38	9	311	KC1	CMC-C2C-C1C	2.39	128.69	125.04
30	5	309	CLA	CMB-C2B-C3B	2.39	129.16	124.68
35	15	301	LMT	C4B-C3B-C2B	2.39	115.00	110.82
30	A	804	CLA	O1D-CGD-CBD	-2.39	119.59	124.48
30	8	304	CLA	C1-O2A-CGA	2.39	122.72	116.44
33	F	204	BCR	C38-C26-C27	-2.39	109.02	113.62
38	5	306	KC1	CHB-C4A-NA	2.39	127.97	124.20
30	A	815	CLA	CBC-CAC-C3C	-2.39	105.83	112.43
30	B	822	CLA	CHB-C4A-NA	2.39	127.82	124.51
30	12	321	CLA	CMB-C2B-C3B	2.39	129.16	124.68
30	3	309	CLA	CMC-C2C-C1C	2.39	128.68	125.04
30	3	302	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
30	A	839	CLA	CBC-CAC-C3C	-2.39	105.83	112.43
39	16	313	DD6	C10-C9-C8	-2.39	115.75	123.22
30	15	304	CLA	O2A-CGA-CBA	2.39	119.42	111.91
30	A	828	CLA	O1D-CGD-CBD	-2.39	119.59	124.48
38	12	311	KC1	O2D-CGD-O1D	-2.39	119.16	123.84
30	15	306	CLA	CMB-C2B-C3B	2.39	129.15	124.68
30	B	819	CLA	CAA-C2A-C3A	-2.39	106.23	112.78
30	B	814	CLA	CBC-CAC-C3C	-2.39	105.84	112.43
30	1	301	CLA	O2A-CGA-CBA	2.39	119.41	111.91
38	1	306	KC1	CMB-C2B-C1B	2.39	128.93	124.71
37	13	313	A86	C36-C31-C32	-2.39	117.32	119.70
37	2	319	A86	C23-C16-C17	-2.39	104.83	108.98
37	11	316	A86	C40-C32-C31	-2.39	108.33	110.47
30	4	305	CLA	CBC-CAC-C3C	-2.39	105.84	112.43
39	7	318	DD6	C9-C8-C6	-2.39	119.70	126.42
38	2	314	KC1	CAA-C2A-C1A	-2.39	113.76	124.75
30	15	309	CLA	C1-C2-C3	-2.39	121.91	126.04
30	3	303	CLA	CBC-CAC-C3C	-2.39	105.84	112.43
30	12	303	CLA	O2A-CGA-CBA	2.39	119.40	111.91
30	B	832	CLA	CBC-CAC-C3C	-2.39	105.85	112.43
38	12	311	KC1	CMB-C2B-C1B	2.39	128.92	124.71
30	9	303	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
30	7	309	CLA	CHB-C4A-NA	2.39	127.81	124.51
30	A	822	CLA	CED-O2D-CGD	2.39	121.34	115.94
30	B	831	CLA	CMB-C2B-C3B	2.39	129.14	124.68
30	13	307	CLA	CBC-CAC-C3C	-2.39	105.85	112.43
39	16	313	DD6	C25-C24-C1	-2.39	119.71	126.42
30	A	812	CLA	CMC-C2C-C1C	2.39	128.67	125.04
30	15	314	CLA	O2D-CGD-O1D	-2.39	119.17	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	9	306	CLA	CAA-C2A-C3A	-2.39	106.25	112.78
37	4	315	A86	C7-C6-C8	2.39	121.83	118.08
38	12	309	KC1	O2D-CGD-O1D	-2.38	119.17	123.84
30	B	813	CLA	CHB-C4A-NA	2.38	127.81	124.51
39	10	313	DD6	C22-C16-C17	-2.38	104.84	108.98
30	11	309	CLA	CHB-C4A-NA	2.38	127.81	124.51
37	10	302	A86	C40-C32-C31	-2.38	108.34	110.47
38	10	306	KC1	CHB-C4A-NA	2.38	127.96	124.20
30	3	301	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
30	2	301	CLA	CAA-CBA-CGA	-2.38	106.29	113.25
30	A	823	CLA	CBC-CAC-C3C	-2.38	105.86	112.43
30	B	818	CLA	C4C-C3C-C2C	-2.38	103.42	106.90
37	9	316	A86	C9-C10-C11	-2.38	119.60	126.61
30	A	803	CLA	CHD-C4C-NC	2.38	127.96	124.20
30	7	310	CLA	O2A-CGA-CBA	2.38	119.38	111.91
38	12	309	KC1	CMC-C2C-C1C	2.38	128.67	125.04
30	12	312	CLA	CMB-C2B-C3B	2.38	129.13	124.68
30	15	302	CLA	CGD-CBD-CAD	-2.38	103.02	110.73
30	5	309	CLA	C1-C2-C3	-2.38	121.92	126.04
38	12	309	KC1	CMB-C2B-C1B	2.38	128.91	124.71
30	B	812	CLA	O2A-CGA-CBA	2.38	119.38	111.91
30	3	301	CLA	CAC-C3C-C4C	2.38	127.90	124.81
36	B	847	LMG	O3-C3-C2	-2.38	104.85	110.35
38	14	306	KC1	C1C-C2C-C3C	-2.38	104.45	106.96
37	14	315	A86	C40-C32-C31	-2.38	108.34	110.47
30	2	308	CLA	CHB-C4A-NA	2.38	127.80	124.51
30	B	829	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
38	2	306	KC1	O1D-CGD-CBD	-2.38	119.61	124.48
38	8	307	KC1	CHB-C4A-NA	2.38	127.95	124.20
39	9	314	DD6	C4-C3-C2	-2.38	118.60	123.47
30	12	304	CLA	CHB-C4A-NA	2.38	127.80	124.51
30	A	823	CLA	O1D-CGD-CBD	-2.38	119.62	124.48
38	5	312	KC1	O2D-CGD-O1D	-2.38	119.19	123.84
39	7	302	DD6	O1-C20-C21	-2.38	112.21	115.06
30	8	301	CLA	CMA-C3A-C2A	-2.38	104.24	113.83
30	14	303	CLA	O1D-CGD-CBD	-2.38	119.62	124.48
30	3	305	CLA	C1-C2-C3	-2.38	121.93	126.04
30	3	307	CLA	CMB-C2B-C3B	2.38	129.12	124.68
30	8	309	CLA	O2A-CGA-CBA	2.37	119.36	111.91
39	6	319	DD6	C34-C35-C36	-2.37	107.12	111.85
30	B	802	CLA	C1B-CHB-C4A	-2.37	125.41	130.12
37	10	302	A86	C3-C4-C5	-2.37	118.61	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	4	311	CLA	CMC-C2C-C1C	2.37	128.66	125.04
30	11	308	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
30	12	304	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
30	2	301	CLA	C4-C3-C5	2.37	119.26	115.27
30	12	306	CLA	CMC-C2C-C1C	2.37	128.65	125.04
30	15	312	CLA	CAC-C3C-C4C	2.37	127.89	124.81
30	9	306	CLA	CHD-C4C-NC	2.37	127.94	124.20
30	2u	202	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
30	A	830	CLA	CMB-C2B-C3B	2.37	129.11	124.68
30	2	305	CLA	O1D-CGD-CBD	-2.37	119.63	124.48
30	B	803	CLA	CBC-CAC-C3C	-2.37	105.90	112.43
30	9	303	CLA	C4-C3-C5	2.37	119.26	115.27
30	A	825	CLA	CHD-C4C-NC	2.37	127.94	124.20
30	7	306	CLA	O2A-CGA-CBA	2.37	119.34	111.91
30	B	813	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
30	4	311	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
33	B	846	BCR	C10-C11-C12	-2.37	115.82	123.22
30	L	202	CLA	O2A-CGA-CBA	2.37	119.34	111.91
37	3	314	A86	C28-C27-C26	-2.37	119.61	122.92
30	6	305	CLA	CBC-CAC-C3C	-2.37	105.90	112.43
30	10	305	CLA	CMC-C2C-C1C	2.37	128.65	125.04
30	B	815	CLA	O1D-CGD-CBD	-2.37	119.64	124.48
30	B	812	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
30	16	302	CLA	CBC-CAC-C3C	-2.37	105.90	112.43
30	2	304	CLA	CAA-C2A-C3A	-2.37	106.29	112.78
38	9	312	KC1	CBA-CAA-C2A	-2.37	116.25	125.27
38	12	311	KC1	CAA-C2A-C1A	-2.37	113.87	124.75
30	15	303	CLA	CMC-C2C-C1C	2.37	128.64	125.04
39	7	318	DD6	C14-C13-C11	-2.37	121.86	125.53
30	3	302	CLA	CAC-C3C-C4C	2.37	127.88	124.81
30	15	304	CLA	CHD-C4C-NC	2.37	127.93	124.20
37	15	322	A86	O1-C15-C14	2.37	117.96	113.21
38	4	310	KC1	O2D-CGD-O1D	-2.37	119.21	123.84
30	B	833	CLA	O2A-CGA-CBA	2.37	119.33	111.91
39	4	316	DD6	C23-C16-C15	2.36	116.43	110.05
37	2	319	A86	C9-C10-C11	-2.36	119.66	126.61
30	A	812	CLA	CHD-C4C-NC	2.36	127.93	124.20
30	9	309	CLA	C4-C3-C5	2.36	119.25	115.27
30	16	309	CLA	CHB-C4A-NA	2.36	127.78	124.51
33	F	204	BCR	C30-C25-C26	-2.36	119.28	122.61
36	14	321	LMG	O6-C1-O1	-2.36	104.38	109.97
33	B	846	BCR	C15-C16-C17	-2.36	118.63	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	6	308	KC1	CHB-C4A-NA	2.36	127.93	124.20
38	6	313	KC1	CAC-C3C-C4C	2.36	127.88	124.81
30	2	311	CLA	CMB-C2B-C3B	2.36	129.10	124.68
38	10	310	KC1	O2D-CGD-O1D	-2.36	119.22	123.84
38	5	306	KC1	CHB-C1B-NB	-2.36	122.28	124.45
37	5	315	A86	C7-C6-C8	2.36	121.80	118.08
37	7	315	A86	C4-C3-C2	-2.36	118.64	123.47
37	15	323	A86	C7-C6-C5	-2.36	119.61	122.92
30	F	202	CLA	CMC-C2C-C1C	2.36	128.64	125.04
30	A	831	CLA	CHB-C4A-NA	2.36	127.78	124.51
30	15	305	CLA	CHB-C4A-NA	2.36	127.78	124.51
30	15	310	CLA	CHB-C4A-NA	2.36	127.78	124.51
30	9	302	CLA	O2A-C1-C2	2.36	114.84	108.64
30	6	314	CLA	O2A-CGA-CBA	2.36	119.32	111.91
30	8	301	CLA	CBC-CAC-C3C	-2.36	105.92	112.43
38	11	311	KC1	CHB-C1B-NB	-2.36	122.28	124.45
30	1	307	CLA	CMC-C2C-C1C	2.36	128.63	125.04
30	5	302	CLA	CMA-C3A-C2A	-2.36	104.31	113.83
30	A	803	CLA	CMC-C2C-C1C	2.36	128.63	125.04
33	A	850	BCR	C11-C10-C9	-2.36	123.94	127.31
30	7	303	CLA	C6-C7-C8	-2.36	108.29	115.92
30	9	307	CLA	C1-C2-C3	-2.36	121.96	126.04
30	12	310	CLA	CBC-CAC-C3C	-2.36	105.93	112.43
30	15	302	CLA	C4-C3-C5	2.36	119.24	115.27
33	L	205	BCR	C15-C14-C13	-2.36	123.94	127.31
38	13	305	KC1	CAA-C2A-C1A	-2.36	113.90	124.75
30	B	817	CLA	C3B-C4B-NB	2.36	112.26	109.21
30	B	819	CLA	CHD-C4C-NC	2.36	127.92	124.20
33	L	201	BCR	C3-C4-C5	-2.36	109.86	114.08
30	B	802	CLA	C1-C2-C3	-2.36	121.96	126.04
30	B	832	CLA	C1-C2-C3	-2.36	121.96	126.04
30	8	304	CLA	CMB-C2B-C3B	2.36	129.09	124.68
38	7	313	KC1	CMC-C2C-C1C	2.36	128.63	125.04
30	B	827	CLA	O2A-C1-C2	2.36	114.83	108.64
30	9	307	CLA	CMB-C2B-C3B	2.36	129.09	124.68
38	3	304	KC1	CMB-C2B-C1B	2.36	128.87	124.71
37	15	323	A86	C3-C2-C1	2.36	130.67	127.31
30	A	814	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
30	8	308	CLA	CAC-C3C-C4C	2.36	127.87	124.81
36	5	318	LMG	O1-C7-C8	-2.36	105.21	110.90
30	B	834	CLA	CHA-C1A-NA	-2.36	121.00	126.40
36	2u	204	LMG	O3-C3-C2	-2.36	104.90	110.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	9	315	A86	C28-C27-C26	-2.36	119.62	122.92
30	5	302	CLA	O2A-CGA-CBA	2.35	119.30	111.91
33	B	841	BCR	C37-C22-C21	-2.35	119.62	122.92
30	B	835	CLA	C1-C2-C3	-2.35	121.97	126.04
30	B	833	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
38	2	312	KC1	CMC-C2C-C1C	2.35	128.62	125.04
30	13	309	CLA	CMC-C2C-C1C	2.35	128.62	125.04
38	6	312	KC1	CMC-C2C-C1C	2.35	128.62	125.04
38	8	312	KC1	CHB-C1B-NB	-2.35	122.29	124.45
37	11	315	A86	C35-C34-C33	2.35	113.98	109.88
30	A	844	CLA	CMB-C2B-C3B	2.35	129.08	124.68
37	5	301	A86	C-C1-C24	2.35	121.78	118.08
30	A	803	CLA	O2A-CGA-CBA	2.35	119.29	111.91
30	A	813	CLA	C1-C2-C3	-2.35	121.98	126.04
37	15	320	A86	C3-C2-C1	-2.35	123.95	127.31
30	A	821	CLA	CHD-C4C-NC	2.35	127.91	124.20
30	B	824	CLA	CHD-C4C-NC	2.35	127.91	124.20
30	16	305	CLA	CMC-C2C-C1C	2.35	128.62	125.04
30	7	306	CLA	C4-C3-C5	2.35	119.23	115.27
30	A	822	CLA	C1-C2-C3	-2.35	121.98	126.04
30	1	302	CLA	CMC-C2C-C1C	2.35	128.62	125.04
30	16	303	CLA	CMC-C2C-C1C	2.35	128.62	125.04
38	2	306	KC1	CBC-CAC-C3C	-2.35	105.95	112.43
33	A	850	BCR	C15-C16-C17	-2.35	118.66	123.47
39	7	317	DD6	C23-C16-C17	-2.35	104.90	108.98
30	16	308	CLA	CAA-C2A-C3A	-2.35	106.34	112.78
36	8	321	LMG	O1-C1-C2	-2.35	104.64	108.30
30	A	835	CLA	CMB-C2B-C3B	2.35	129.07	124.68
30	15	306	CLA	CHB-C4A-NA	2.35	127.76	124.51
33	B	844	BCR	C11-C10-C9	-2.35	123.96	127.31
30	3	310	CLA	C4C-C3C-C2C	-2.35	103.48	106.90
30	14	307	CLA	CMC-C2C-C1C	2.35	128.61	125.04
30	1	301	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
30	13	301	CLA	CBA-CAA-C2A	2.35	120.79	113.86
30	A	826	CLA	CHB-C4A-NA	2.35	127.75	124.51
30	12	310	CLA	C1-C2-C3	-2.35	121.99	126.04
30	4	306	CLA	CBC-CAC-C3C	-2.35	105.97	112.43
37	12	316	A86	O-C13-C11	-2.34	115.97	121.15
37	6	320	A86	C9-C10-C11	-2.34	119.71	126.61
38	13	310	KC1	CBC-CAC-C3C	-2.34	105.97	112.43
30	A	839	CLA	CMB-C2B-C3B	2.34	129.06	124.68
30	13	307	CLA	CHB-C4A-NA	2.34	127.75	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	5	301	A86	C20-C19-C18	-2.34	108.11	112.75
37	7	319	A86	C4-C3-C2	-2.34	118.67	123.47
30	12	303	CLA	CAC-C3C-C4C	2.34	127.85	124.81
30	14	309	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
38	11	305	KC1	CMC-C2C-C1C	2.34	128.61	125.04
30	13	309	CLA	CBC-CAC-C3C	-2.34	105.97	112.43
30	B	804	CLA	O1D-CGD-CBD	-2.34	119.69	124.48
38	16	311	KC1	CMB-C2B-C1B	2.34	128.84	124.71
30	5	311	CLA	CHB-C4A-NA	2.34	127.75	124.51
30	13	303	CLA	CMB-C2B-C3B	2.34	129.06	124.68
37	10	316	A86	C7-C6-C8	2.34	121.77	118.08
30	7	306	CLA	CMB-C2B-C3B	2.34	129.06	124.68
30	A	809	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
33	2u	201	BCR	C15-C14-C13	-2.34	123.97	127.31
30	14	304	CLA	CMC-C2C-C1C	2.34	128.60	125.04
38	11	312	KC1	CAA-CBA-CGA	-2.34	115.23	127.26
38	13	312	KC1	CMC-C2C-C1C	2.34	128.60	125.04
30	A	837	CLA	CHB-C4A-NA	2.34	127.75	124.51
30	14	312	CLA	CHB-C4A-NA	2.34	127.75	124.51
30	15	313	CLA	CHB-C4A-NA	2.34	127.75	124.51
33	B	842	BCR	C29-C30-C25	2.34	114.08	110.48
38	8	307	KC1	CHB-C1B-NB	-2.34	122.31	124.45
30	A	834	CLA	CAC-C3C-C4C	2.34	127.84	124.81
30	L	202	CLA	CMB-C2B-C3B	2.34	129.05	124.68
30	A	821	CLA	CHB-C4A-NA	2.34	127.75	124.51
30	4	302	CLA	CHB-C4A-NA	2.34	127.75	124.51
30	A	833	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
30	8	308	CLA	CAA-C2A-C3A	-2.34	106.38	112.78
38	8	314	KC1	CMC-C2C-C1C	2.34	128.60	125.04
36	B	847	LMG	C42-C41-C40	-2.34	102.56	114.42
30	B	807	CLA	C4-C3-C5	2.34	119.20	115.27
30	B	839	CLA	C4-C3-C5	2.34	119.20	115.27
30	B	806	CLA	CHB-C4A-NA	2.34	127.74	124.51
38	12	305	KC1	CHB-C4A-NA	2.34	127.89	124.20
30	3	301	CLA	O2A-CGA-O1A	-2.34	117.70	123.59
30	F	201	CLA	CMB-C2B-C3B	2.34	129.05	124.68
30	A	807	CLA	CHB-C4A-NA	2.34	127.74	124.51
36	A	856	LMG	O2-C2-C1	-2.33	104.38	110.05
38	5	305	KC1	CMC-C2C-C1C	2.33	128.59	125.04
30	B	808	CLA	CAC-C3C-C4C	2.33	127.84	124.81
38	2	306	KC1	CHB-C4A-NA	2.33	127.88	124.20
38	7	308	KC1	CMB-C2B-C1B	2.33	128.82	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	14	309	CLA	CMB-C2B-C3B	2.33	129.04	124.68
30	B	823	CLA	CHB-C4A-NA	2.33	127.74	124.51
30	4	309	CLA	CHB-C4A-NA	2.33	127.74	124.51
30	2	309	CLA	C1-C2-C3	-2.33	122.01	126.04
30	4	303	CLA	CMC-C2C-C1C	2.33	128.59	125.04
30	B	822	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
30	10	307	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
30	B	816	CLA	CHB-C4A-NA	2.33	127.74	124.51
30	7	312	CLA	CHB-C4A-NA	2.33	127.74	124.51
30	16	301	CLA	CBC-CAC-C3C	-2.33	106.00	112.43
30	4	301	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
30	6	305	CLA	CHB-C4A-NA	2.33	127.73	124.51
36	14	321	LMG	O3-C3-C2	-2.33	104.96	110.35
37	8	318	A86	C4-C5-C6	2.33	130.64	127.31
30	A	834	CLA	CHB-C4A-NA	2.33	127.73	124.51
30	A	834	CLA	CMA-C3A-C2A	-2.33	104.43	113.83
30	6	307	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
30	F	203	CLA	CBC-CAC-C3C	-2.33	106.01	112.43
30	A	804	CLA	C1-C2-C3	-2.33	122.02	126.04
37	10	317	A86	C-C1-C2	-2.33	119.66	122.92
38	1	308	KC1	CED-O2D-CGD	2.33	121.20	115.94
30	14	310	CLA	O2A-CGA-CBA	2.33	119.21	111.91
30	5	308	CLA	CAA-C2A-C3A	-2.33	106.40	112.78
30	A	809	CLA	C4-C3-C5	2.33	119.19	115.27
30	A	822	CLA	CBC-CAC-C3C	-2.33	106.02	112.43
38	5	310	KC1	CAB-C3B-C4B	2.33	130.52	124.90
30	5	304	CLA	CBC-CAC-C3C	-2.33	106.02	112.43
30	5	303	CLA	CED-O2D-CGD	2.33	121.20	115.94
34	A	853	LHG	C11-C10-C9	-2.33	102.62	114.42
30	3	302	CLA	CBC-CAC-C3C	-2.33	106.02	112.43
33	I	101	BCR	C1-C6-C5	-2.32	119.34	122.61
30	3	310	CLA	O2D-CGD-O1D	-2.32	119.29	123.84
38	8	307	KC1	CAC-C3C-C4C	2.32	127.83	124.81
30	15	314	CLA	CBC-CAC-C3C	-2.32	106.02	112.43
33	M	101	BCR	C40-C30-C25	2.32	114.07	110.30
30	B	823	CLA	O2A-CGA-CBA	2.32	119.20	111.91
30	5	309	CLA	CBC-CAC-C3C	-2.32	106.03	112.43
38	2	312	KC1	CHB-C4A-NA	2.32	127.86	124.20
36	7	320	LMG	O1-C7-C8	-2.32	105.29	110.90
38	7	313	KC1	CBA-CAA-C2A	-2.32	116.41	125.27
30	2	303	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
30	13	309	CLA	CED-O2D-CGD	2.32	121.19	115.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	J	103	BCR	C15-C14-C13	-2.32	124.00	127.31
30	A	822	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
38	4	308	KC1	O2D-CGD-O1D	-2.32	119.30	123.84
38	13	310	KC1	O2D-CGD-O1D	-2.32	119.30	123.84
30	A	836	CLA	CED-O2D-CGD	2.32	121.19	115.94
30	A	815	CLA	C4-C3-C5	2.32	119.18	115.27
37	2	319	A86	C3-C4-C5	-2.32	118.72	123.47
30	2	303	CLA	C1-O2A-CGA	2.32	122.53	116.44
37	7	315	A86	C19-C18-C17	2.32	115.26	110.77
38	11	311	KC1	CMC-C2C-C1C	2.32	128.57	125.04
33	L	201	BCR	C27-C26-C25	2.32	126.10	122.73
30	16	310	CLA	CMC-C2C-C1C	2.32	128.57	125.04
30	15	302	CLA	C11-C12-C13	-2.32	108.42	115.92
30	A	821	CLA	O2A-C1-C2	2.32	114.73	108.64
30	5	309	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
30	12	308	CLA	CMB-C2B-C3B	2.32	129.02	124.68
30	7	310	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
30	13	303	CLA	CMC-C2C-C1C	2.32	128.57	125.04
30	F	201	CLA	C4-C3-C5	2.32	119.17	115.27
30	16	303	CLA	CAC-C3C-C4C	2.32	127.82	124.81
37	14	315	A86	C7-C6-C5	-2.32	119.68	122.92
34	5	317	LHG	C11-C10-C9	-2.32	102.66	114.42
30	A	844	CLA	CED-O2D-CGD	2.32	121.18	115.94
30	15	311	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
30	7	310	CLA	C1-C2-C3	-2.32	122.03	126.04
30	10	303	CLA	O2A-CGA-CBA	2.32	119.18	111.91
30	11	308	CLA	CBC-CAC-C3C	-2.32	106.05	112.43
30	16	307	CLA	CMC-C2C-C1C	2.32	128.57	125.04
30	2u	202	CLA	CHB-C4A-NA	2.32	127.71	124.51
39	2	316	DD6	C20-C19-C18	-2.32	108.17	112.75
38	13	311	KC1	O2D-CGD-O1D	-2.32	119.31	123.84
30	8	301	CLA	CHC-C1C-C2C	-2.32	120.32	126.72
30	9	302	CLA	CMC-C2C-C1C	2.32	128.56	125.04
39	1	310	DD6	C15-C14-C13	-2.32	121.10	125.99
30	13	303	CLA	C4-C3-C5	2.31	119.17	115.27
38	8	307	KC1	CAA-C2A-C1A	-2.31	114.11	124.75
38	8	312	KC1	CMC-C2C-C1C	2.31	128.56	125.04
30	B	839	CLA	CHC-C1C-C2C	-2.31	120.32	126.72
37	4	312	A86	C10-C9-C8	-2.31	116.00	123.22
33	I	101	BCR	C15-C16-C17	-2.31	118.73	123.47
39	15	319	DD6	C33-C32-C31	2.31	114.31	109.62
38	2	314	KC1	CHB-C4A-NA	2.31	127.85	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	13	309	CLA	CMB-C2B-C3B	2.31	129.01	124.68
37	2	302	A86	C7-C6-C5	-2.31	119.68	122.92
30	B	833	CLA	CMB-C2B-C3B	2.31	129.00	124.68
30	16	306	CLA	CHD-C4C-NC	2.31	127.85	124.20
37	14	318	A86	C9-C10-C11	-2.31	119.81	126.61
30	14	302	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
39	5	314	DD6	C34-C35-C36	-2.31	107.25	111.85
30	15	312	CLA	C4C-C3C-C2C	-2.31	103.53	106.90
30	2	308	CLA	CBA-CAA-C2A	2.31	120.68	113.86
37	15	323	A86	C36-C31-C32	-2.31	117.40	119.70
30	7	310	CLA	CMC-C2C-C1C	2.31	128.56	125.04
38	5	312	KC1	CAA-C2A-C1A	-2.31	114.13	124.75
30	B	822	CLA	CED-O2D-CGD	2.31	121.16	115.94
33	2u	201	BCR	C33-C5-C6	-2.31	121.94	124.53
30	12	321	CLA	C1-C2-C3	-2.31	122.05	126.04
30	J	101	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
38	1	306	KC1	O2D-CGD-O1D	-2.31	119.33	123.84
30	A	819	CLA	CBA-CAA-C2A	2.31	120.67	113.86
30	B	813	CLA	CHD-C4C-NC	2.31	127.84	124.20
38	11	305	KC1	O2D-CGD-O1D	-2.31	119.33	123.84
38	10	306	KC1	CBD-CHA-C1A	2.31	133.18	128.88
38	13	305	KC1	CBD-CHA-C1A	2.31	133.18	128.88
30	14	309	CLA	CHB-C4A-NA	2.30	127.70	124.51
30	A	807	CLA	O2D-CGD-O1D	-2.30	119.33	123.84
36	8	321	LMG	O6-C1-O1	-2.30	104.52	109.97
38	5	306	KC1	CMB-C2B-C1B	2.30	128.77	124.71
30	A	826	CLA	O2A-CGA-CBA	2.30	119.14	111.91
38	13	308	KC1	CBC-CAC-C3C	-2.30	106.08	112.43
38	10	310	KC1	CAB-C3B-C4B	2.30	130.46	124.90
30	10	304	CLA	O2D-CGD-O1D	-2.30	119.33	123.84
37	11	301	A86	C4-C3-C2	-2.30	118.76	123.47
38	10	310	KC1	CAA-C2A-C1A	-2.30	114.16	124.75
30	5	311	CLA	O2A-CGA-CBA	2.30	119.13	111.91
30	16	303	CLA	C4-C3-C5	2.30	119.14	115.27
33	B	844	BCR	C2-C1-C6	2.30	114.02	110.48
38	14	308	KC1	CAC-C3C-C4C	2.30	127.80	124.81
37	14	317	A86	O1-C15-C14	2.30	117.83	113.21
30	A	821	CLA	O1D-CGD-CBD	-2.30	119.78	124.48
30	14	309	CLA	CBC-CAC-C3C	-2.30	106.09	112.43
37	8	318	A86	O1-C15-C14	2.30	117.83	113.21
30	B	839	CLA	C3B-C4B-NB	2.30	112.18	109.21
37	10	301	A86	C-C1-C2	-2.30	119.70	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	4	303	CLA	C4-C3-C5	2.30	119.14	115.27
30	A	827	CLA	CMB-C2B-C3B	2.30	128.98	124.68
30	12	308	CLA	CHB-C4A-NA	2.30	127.69	124.51
37	14	320	A86	C28-C27-C26	-2.30	119.70	122.92
30	6	306	CLA	CMC-C2C-C1C	2.30	128.54	125.04
37	15	317	A86	C7-C6-C5	-2.30	119.70	122.92
37	15	322	A86	O-C13-C14	-2.30	116.99	121.66
39	13	314	DD6	C4-C3-C2	-2.30	118.77	123.47
37	16	314	A86	C10-C9-C8	-2.30	116.05	123.22
30	A	813	CLA	CAA-C2A-C3A	-2.30	106.49	112.78
30	B	837	CLA	CHB-C4A-NA	2.30	127.69	124.51
30	15	313	CLA	C1-C2-C3	-2.30	122.07	126.04
30	F	202	CLA	C4-C3-C5	2.30	119.13	115.27
30	15	302	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
34	9	318	LHG	C11-C10-C9	-2.29	102.78	114.42
30	2	305	CLA	CHB-C4A-NA	2.29	127.69	124.51
37	14	314	A86	C35-C34-C33	2.29	113.88	109.88
30	15	311	CLA	CBC-CAC-C3C	-2.29	106.11	112.43
30	14	303	CLA	C4-C3-C5	2.29	119.13	115.27
30	4	311	CLA	C5-C3-C4	2.29	119.67	114.60
39	7	314	DD6	C26-C25-C24	-2.29	116.06	123.22
30	2	313	CLA	CMC-C2C-C1C	2.29	128.53	125.04
30	15	308	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
30	7	305	CLA	CAC-C3C-C4C	2.29	127.78	124.81
37	4	312	A86	C9-C10-C11	-2.29	119.87	126.61
33	L	201	BCR	C16-C17-C18	-2.29	124.04	127.31
39	8	317	DD6	C4-C3-C2	-2.29	118.78	123.47
38	13	312	KC1	CHB-C4A-NA	2.29	127.82	124.20
30	8	302	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
30	L	202	CLA	CMC-C2C-C1C	2.29	128.53	125.04
38	13	306	KC1	CMC-C2C-C1C	2.29	128.53	125.04
30	B	834	CLA	CMC-C2C-C1C	2.29	128.53	125.04
30	11	310	CLA	CHB-C4A-NA	2.29	127.68	124.51
30	12	302	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
37	11	314	A86	C8-C6-C5	2.29	122.46	118.94
37	14	316	A86	C3-C4-C5	-2.29	118.78	123.47
30	6	304	CLA	CHB-C4A-NA	2.29	127.68	124.51
36	6	301	LMG	O6-C1-O1	-2.29	104.55	109.97
30	B	806	CLA	CMB-C2B-C3B	2.29	128.96	124.68
38	13	312	KC1	CHB-C1B-NB	-2.29	122.35	124.45
30	A	830	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
38	9	310	KC1	CHB-C4A-NA	2.29	127.81	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	5	305	KC1	O2D-CGD-O1D	-2.29	119.36	123.84
30	B	806	CLA	C1-C2-C3	-2.29	122.09	126.04
30	A	826	CLA	CHA-C1A-NA	-2.29	121.16	126.40
37	6	320	A86	C3-C2-C1	-2.29	124.05	127.31
36	A	856	LMG	O3-C3-C2	-2.29	105.06	110.35
38	14	311	KC1	CHB-C1B-NB	-2.29	122.35	124.45
30	15	311	CLA	CMB-C2B-C3B	2.29	128.96	124.68
33	B	841	BCR	C15-C14-C13	-2.28	124.05	127.31
30	A	820	CLA	O2A-CGA-CBA	2.28	119.08	111.91
38	9	304	KC1	O2D-CGD-O1D	-2.28	119.37	123.84
30	B	816	CLA	CBC-CAC-C3C	-2.28	106.14	112.43
30	2	310	CLA	O2A-CGA-CBA	2.28	119.07	111.91
33	A	849	BCR	C16-C17-C18	-2.28	124.05	127.31
30	B	814	CLA	C4-C3-C5	2.28	119.11	115.27
30	B	809	CLA	O2D-CGD-O1D	-2.28	119.37	123.84
30	B	818	CLA	CBC-CAC-C3C	-2.28	106.14	112.43
30	A	818	CLA	CBC-CAC-C3C	-2.28	106.14	112.43
30	B	828	CLA	C4-C3-C5	2.28	119.11	115.27
30	B	817	CLA	C4-C3-C5	2.28	119.11	115.27
39	6	321	DD6	C23-C16-C17	-2.28	105.02	108.98
30	A	812	CLA	CHB-C4A-NA	2.28	127.67	124.51
30	B	814	CLA	O2A-CGA-CBA	2.28	119.06	111.91
30	A	836	CLA	CMC-C2C-C1C	2.28	128.51	125.04
30	14	304	CLA	CMB-C2B-C3B	2.28	128.94	124.68
30	1	303	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
35	A	855	LMT	C1B-O1B-C4'	-2.28	112.33	117.96
30	7	309	CLA	CMC-C2C-C1C	2.28	128.51	125.04
30	13	307	CLA	CMC-C2C-C1C	2.28	128.51	125.04
30	2	310	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
30	9	303	CLA	C1-C2-C3	-2.28	122.10	126.04
33	A	848	BCR	C30-C25-C26	-2.28	119.41	122.61
30	F	201	CLA	C11-C10-C8	-2.28	108.56	115.92
30	B	817	CLA	C1-C2-C3	-2.28	122.11	126.04
30	16	310	CLA	CHB-C4A-NA	2.28	127.66	124.51
30	B	805	CLA	CBA-CAA-C2A	2.28	120.58	113.86
39	7	317	DD6	C14-C13-C11	-2.28	122.00	125.53
30	12	312	CLA	CHB-C4A-NA	2.28	127.66	124.51
35	6	302	LMT	O5'-C5'-C4'	2.27	114.55	109.75
37	2u	203	A86	C3-C4-C5	-2.27	118.81	123.47
30	A	843	CLA	O2A-CGA-CBA	2.27	119.05	111.91
30	A	804	CLA	CMB-C2B-C3B	2.27	128.93	124.68
30	15	312	CLA	CMC-C2C-C1C	2.27	128.50	125.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	834	CLA	C1-C2-C3	-2.27	122.11	126.04
38	8	311	KC1	CHB-C1B-NB	-2.27	122.36	124.45
30	10	309	CLA	CHB-C4A-NA	2.27	127.66	124.51
39	13	314	DD6	C12-C11-C13	-2.27	114.50	118.08
30	B	815	CLA	CHD-C4C-NC	2.27	127.78	124.20
38	9	312	KC1	CHB-C4A-NA	2.27	127.78	124.20
30	6	306	CLA	CAA-C2A-C3A	-2.27	106.56	112.78
30	A	838	CLA	CMC-C2C-C1C	2.27	128.50	125.04
37	9	313	A86	C-C1-C24	2.27	121.66	118.08
38	5	306	KC1	CMC-C2C-C1C	2.27	128.50	125.04
38	11	307	KC1	CAA-C2A-C1A	-2.27	114.31	124.75
30	6	316	CLA	CED-O2D-CGD	2.27	121.07	115.94
39	6	303	DD6	C4-C3-C2	-2.27	118.82	123.47
30	F	203	CLA	CHB-C4A-NA	2.27	127.65	124.51
33	L	205	BCR	C7-C8-C9	-2.27	122.81	126.23
30	7	303	CLA	CMB-C2B-C3B	2.27	128.93	124.68
37	5	301	A86	C10-C9-C8	-2.27	116.14	123.22
33	B	842	BCR	C28-C27-C26	-2.27	110.03	114.08
30	13	303	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
30	15	311	CLA	CHB-C4A-NA	2.27	127.65	124.51
36	B	847	LMG	O2-C2-C1	-2.27	104.54	110.05
30	8	301	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
38	14	308	KC1	CHB-C1B-NB	-2.27	122.37	124.45
38	11	311	KC1	O2D-CGD-O1D	-2.27	119.41	123.84
30	1	303	CLA	CAA-C2A-C3A	-2.27	106.57	112.78
30	B	851	CLA	CBC-CAC-C3C	-2.27	106.18	112.43
39	16	313	DD6	C3-C4-C5	-2.27	118.83	123.47
33	F	204	BCR	C35-C13-C14	-2.27	119.75	122.92
38	14	308	KC1	CHB-C4A-NA	2.27	127.78	124.20
30	13	303	CLA	CBA-CAA-C2A	2.27	120.55	113.86
38	8	311	KC1	O1D-CGD-CBD	-2.27	119.85	124.48
30	7	310	CLA	CMB-C2B-C3B	2.27	128.92	124.68
30	A	823	CLA	CAA-C2A-C3A	-2.27	106.57	112.78
30	14	303	CLA	CMA-C3A-C4A	-2.27	105.68	111.77
30	16	302	CLA	CMB-C2B-C3B	2.27	128.92	124.68
37	5	301	A86	C34-O4-C38	-2.27	113.67	117.90
33	B	843	BCR	C11-C10-C9	-2.26	124.08	127.31
30	A	827	CLA	CBC-CAC-C3C	-2.26	106.19	112.43
30	12	312	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
37	5	315	A86	C28-C27-C26	-2.26	119.75	122.92
37	2	319	A86	C12-C11-C13	2.26	119.83	116.02
30	12	307	CLA	CHB-C4A-NA	2.26	127.64	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	827	CLA	OBD-CAD-C3D	-2.26	123.07	128.52
37	14	315	A86	C8-C6-C5	2.26	122.41	118.94
38	6	311	KC1	CHB-C4A-NA	2.26	127.77	124.20
37	2	318	A86	C3-C4-C5	-2.26	118.84	123.47
38	5	312	KC1	CBC-CAC-C3C	-2.26	106.19	112.43
30	12	306	CLA	CMB-C2B-C3B	2.26	128.91	124.68
30	A	833	CLA	CED-O2D-CGD	2.26	121.05	115.94
30	3	302	CLA	C4-C3-C5	2.26	119.08	115.27
30	F	202	CLA	CHA-C1A-NA	-2.26	121.22	126.40
30	16	305	CLA	C5-C3-C4	2.26	119.60	114.60
37	14	301	A86	C25-C24-C1	-2.26	120.06	126.42
30	B	803	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
30	14	312	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
33	A	850	BCR	C16-C15-C14	-2.26	118.84	123.47
30	12	304	CLA	CMC-C2C-C1C	2.26	128.48	125.04
30	12	310	CLA	CHB-C4A-NA	2.26	127.64	124.51
30	14	313	CLA	CMB-C2B-C3B	2.26	128.91	124.68
33	B	845	BCR	C30-C25-C26	-2.26	119.43	122.61
30	2	303	CLA	CHD-C4C-NC	2.26	127.77	124.20
30	16	308	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
30	B	807	CLA	O2A-CGA-CBA	2.26	119.00	111.91
39	4	313	DD6	C33-C32-C31	2.26	114.20	109.62
30	9	301	CLA	CHD-C4C-NC	2.26	127.76	124.20
30	14	305	CLA	O2A-CGA-CBA	2.26	119.00	111.91
30	7	307	CLA	C1-O2A-CGA	2.26	122.37	116.44
30	A	805	CLA	O2A-CGA-CBA	2.26	118.99	111.91
30	B	833	CLA	CHA-C1A-NA	-2.26	121.23	126.40
30	13	302	CLA	CBC-CAC-C3C	-2.26	106.21	112.43
30	7	306	CLA	CHD-C4C-NC	2.26	127.76	124.20
30	10	309	CLA	CMC-C2C-C1C	2.26	128.48	125.04
30	A	815	CLA	CHC-C1C-NC	2.26	127.63	124.20
30	7	305	CLA	OBD-CAD-C3D	-2.26	123.09	128.52
37	15	316	A86	O-C13-C11	-2.26	116.16	121.15
30	9	305	CLA	CBC-CAC-C3C	-2.26	106.21	112.43
30	15	307	CLA	CMB-C2B-C3B	2.26	128.90	124.68
30	1	303	CLA	CMC-C2C-C1C	2.26	128.47	125.04
37	11	301	A86	C20-C19-C18	-2.26	108.29	112.75
30	15	307	CLA	C5-C3-C4	2.26	119.58	114.60
37	3	315	A86	C-C1-C24	2.26	121.63	118.08
30	15	302	CLA	C1-C2-C3	-2.25	122.14	126.04
30	4	309	CLA	CMC-C2C-C1C	2.25	128.47	125.04
30	A	838	CLA	CHA-C1A-NA	-2.25	121.23	126.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	4	303	CLA	CHD-C4C-NC	2.25	127.76	124.20
30	16	308	CLA	CHB-C4A-NA	2.25	127.63	124.51
39	6	303	DD6	C15-C14-C13	-2.25	121.23	125.99
30	8	305	CLA	C11-C10-C8	-2.25	108.64	115.92
37	15	323	A86	C24-C1-C2	-2.25	115.48	118.94
30	14	302	CLA	C4-C3-C2	-2.25	117.90	123.68
38	4	307	KC1	CHB-C4A-NA	2.25	127.75	124.20
30	L	203	CLA	CHB-C4A-NA	2.25	127.63	124.51
30	A	840	CLA	CBC-CAC-C3C	-2.25	106.22	112.43
37	2u	203	A86	C41-C32-C31	-2.25	108.46	110.47
30	11	309	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
33	2u	201	BCR	C7-C8-C9	-2.25	122.83	126.23
30	4	302	CLA	CMB-C2B-C3B	2.25	128.89	124.68
30	3	307	CLA	C4-C3-C5	2.25	119.06	115.27
37	14	316	A86	C25-C24-C1	-2.25	120.09	126.42
30	6	314	CLA	CMB-C2B-C3B	2.25	128.89	124.68
38	1	308	KC1	CHB-C4A-NA	2.25	127.75	124.20
30	A	831	CLA	CAA-C2A-C3A	-2.25	106.61	112.78
30	B	822	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
30	A	844	CLA	CMC-C2C-C1C	2.25	128.47	125.04
30	14	313	CLA	CMC-C2C-C1C	2.25	128.47	125.04
30	16	302	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
38	6	313	KC1	O2D-CGD-O1D	-2.25	119.44	123.84
30	A	839	CLA	CBA-CAA-C2A	2.25	120.50	113.86
38	5	305	KC1	CHB-C1B-NB	-2.25	122.39	124.45
36	3	317	LMG	O3-C3-C2	-2.25	105.15	110.35
30	A	809	CLA	O1D-CGD-CBD	-2.25	119.88	124.48
38	8	310	KC1	O2D-CGD-O1D	-2.25	119.44	123.84
36	8	320	LMG	O2-C2-C1	-2.25	104.59	110.05
35	A	854	LMT	O3'-C3'-C2'	-2.25	105.15	110.35
30	12	321	CLA	CHB-C4A-NA	2.25	127.62	124.51
30	10	311	CLA	O2D-CGD-O1D	-2.25	119.45	123.84
39	4	316	DD6	C10-C9-C8	-2.25	116.21	123.22
37	16	314	A86	C34-O4-C38	-2.25	113.71	117.90
30	3	307	CLA	CHA-C1A-NA	-2.25	121.25	126.40
30	7	311	CLA	CHB-C4A-NA	2.25	127.62	124.51
30	A	840	CLA	O2A-CGA-O1A	-2.25	117.93	123.59
38	14	308	KC1	O2A-CGA-O1A	-2.24	118.01	122.67
30	7	312	CLA	CAA-C2A-C3A	-2.24	106.63	112.78
30	7	309	CLA	CBC-CAC-C3C	-2.24	106.24	112.43
30	A	807	CLA	CHA-C1A-NA	-2.24	121.26	126.40
39	6	321	DD6	O1-C20-C21	-2.24	112.37	115.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	819	CLA	C11-C10-C8	-2.24	108.67	115.92
30	B	810	CLA	CMB-C2B-C3B	2.24	128.88	124.68
30	A	822	CLA	CAA-C2A-C3A	-2.24	106.64	112.78
30	A	809	CLA	CBC-CAC-C3C	-2.24	106.25	112.43
37	7	316	A86	C10-C9-C8	-2.24	116.22	123.22
30	A	810	CLA	CED-O2D-CGD	2.24	121.01	115.94
37	9	316	A86	C7-C6-C5	-2.24	119.78	122.92
37	11	315	A86	C22-C16-C17	-2.24	105.09	108.98
30	13	303	CLA	CBC-CAC-C3C	-2.24	106.25	112.43
30	B	821	CLA	C4-C3-C5	2.24	119.04	115.27
38	10	306	KC1	CBC-CAC-C3C	-2.24	106.25	112.43
30	A	824	CLA	O2A-C1-C2	2.24	114.53	108.64
38	3	308	KC1	O1D-CGD-CBD	-2.24	119.90	124.48
33	J	103	BCR	C15-C16-C17	-2.24	118.88	123.47
39	3	312	DD6	C3-C4-C5	-2.24	118.88	123.47
37	15	320	A86	C4-C3-C2	2.24	128.06	123.47
30	1	302	CLA	C1-C2-C3	-2.24	122.17	126.04
30	1	307	CLA	C1-C2-C3	-2.24	122.17	126.04
33	F	204	BCR	C31-C1-C6	2.24	113.93	110.30
30	11	309	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
37	2u	203	A86	O4-C38-O5	-2.24	118.51	122.96
30	2u	202	CLA	C1-O2A-CGA	2.24	122.32	116.44
30	B	825	CLA	CHB-C4A-NA	2.24	127.61	124.51
30	15	312	CLA	CHB-C4A-NA	2.24	127.61	124.51
37	15	317	A86	C-C1-C24	2.24	121.61	118.08
36	B	849	LMG	C1-C2-C3	-2.24	105.33	110.00
29	A	801	CL0	CAC-C3C-C4C	2.24	127.71	124.81
30	9	302	CLA	CBC-CAC-C3C	-2.24	106.26	112.43
30	12	307	CLA	CMA-C3A-C2A	-2.24	104.80	113.83
30	15	303	CLA	CBC-CAC-C3C	-2.24	106.26	112.43
30	9	301	CLA	CHB-C4A-NA	2.24	127.61	124.51
33	B	841	BCR	C30-C25-C26	-2.24	119.46	122.61
30	A	834	CLA	CMC-C2C-C1C	2.24	128.44	125.04
30	B	839	CLA	CMB-C2B-C3B	2.24	128.86	124.68
33	L	204	BCR	C20-C21-C22	-2.23	124.12	127.31
37	14	317	A86	C7-C6-C5	-2.23	119.79	122.92
39	8	317	DD6	C3-C4-C5	-2.23	118.90	123.47
38	5	310	KC1	CBC-CAC-C3C	-2.23	106.27	112.43
37	11	315	A86	C-C1-C24	2.23	121.60	118.08
30	9	305	CLA	C4-C3-C5	2.23	119.03	115.27
37	8	315	A86	C8-C6-C5	-2.23	115.51	118.94
30	B	851	CLA	O2A-CGA-O1A	-2.23	117.95	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	10	305	CLA	O2A-CGA-CBA	2.23	118.92	111.91
30	7	312	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
38	7	308	KC1	CHB-C1B-NB	-2.23	122.40	124.45
30	9	303	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
30	A	811	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
30	14	304	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
37	14	315	A86	C-C1-C24	2.23	121.59	118.08
30	B	810	CLA	CHB-C4A-NA	2.23	127.60	124.51
30	6	307	CLA	CHB-C4A-NA	2.23	127.60	124.51
30	B	829	CLA	CBC-CAC-C3C	-2.23	106.28	112.43
30	16	302	CLA	CED-O2D-CGD	2.23	120.98	115.94
30	15	307	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
37	9	315	A86	C7-C6-C8	2.23	121.59	118.08
37	16	312	A86	C22-C16-C17	-2.23	105.11	108.98
38	8	310	KC1	CHB-C4A-NA	2.23	127.72	124.20
37	7	315	A86	C-C1-C2	-2.23	119.80	122.92
30	6	304	CLA	CMB-C2B-C3B	2.23	128.85	124.68
37	15	322	A86	C12-C11-C13	2.23	119.77	116.02
37	4	314	A86	C36-C31-C32	-2.23	117.48	119.70
38	1	308	KC1	CBC-CAC-C3C	-2.23	106.29	112.43
30	A	818	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
30	9	307	CLA	O2A-CGA-CBA	2.23	118.90	111.91
30	1	304	CLA	CMB-C2B-C3B	2.23	128.85	124.68
30	9	308	CLA	CBC-CAC-C3C	-2.23	106.29	112.43
37	10	315	A86	C7-C6-C8	2.23	121.59	118.08
30	2u	202	CLA	O1D-CGD-CBD	-2.23	119.93	124.48
36	14	321	LMG	O2-C2-C1	-2.23	104.64	110.05
37	3	315	A86	C34-O4-C38	-2.23	113.75	117.90
38	4	307	KC1	CAA-C2A-C1A	-2.23	114.51	124.75
30	A	819	CLA	C4-C3-C5	2.23	119.02	115.27
39	8	317	DD6	C23-C16-C17	-2.23	105.11	108.98
30	16	309	CLA	CMC-C2C-C1C	2.23	128.43	125.04
30	A	816	CLA	C1-O2A-CGA	2.23	122.29	116.44
30	4	303	CLA	CMB-C2B-C3B	2.23	128.84	124.68
30	10	311	CLA	CMC-C2C-C1C	2.23	128.43	125.04
30	B	835	CLA	C4-C3-C5	2.23	119.02	115.27
30	7	306	CLA	CBC-CAC-C3C	-2.23	106.30	112.43
38	11	312	KC1	CBC-CAC-C3C	-2.23	106.30	112.43
38	14	311	KC1	CBC-CAC-C3C	-2.23	106.30	112.43
37	3	315	A86	C3-C2-C1	-2.22	124.14	127.31
30	14	313	CLA	CMA-C3A-C2A	-2.22	104.85	113.83
30	A	806	CLA	O1D-CGD-CBD	-2.22	119.93	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	10	301	A86	C25-C24-C1	2.22	132.66	126.42
30	12	312	CLA	C4-C3-C5	2.22	119.01	115.27
33	A	847	BCR	C15-C16-C17	-2.22	118.92	123.47
38	3	308	KC1	CHB-C4A-NA	2.22	127.71	124.20
35	8	322	LMT	C2'-C3'-C4'	2.22	114.76	109.68
33	J	102	BCR	C38-C26-C27	-2.22	109.35	113.62
30	12	306	CLA	O2A-CGA-CBA	2.22	118.88	111.91
30	A	810	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
30	16	301	CLA	CBA-CAA-C2A	2.22	120.42	113.86
36	7	320	LMG	O3-C3-C2	-2.22	105.21	110.35
30	2	303	CLA	CBC-CAC-C3C	-2.22	106.31	112.43
30	A	832	CLA	C5-C3-C4	2.22	119.51	114.60
30	B	822	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
35	9	317	LMT	C1B-O1B-C4'	-2.22	112.47	117.96
30	B	809	CLA	CBC-CAC-C3C	-2.22	106.31	112.43
30	16	307	CLA	CBC-CAC-C3C	-2.22	106.31	112.43
30	15	311	CLA	CAA-C2A-C3A	-2.22	106.70	112.78
37	2	318	A86	C10-C9-C8	-2.22	116.29	123.22
30	A	830	CLA	CED-O2D-CGD	2.22	120.96	115.94
30	B	816	CLA	C1-C2-C3	-2.22	122.20	126.04
30	B	826	CLA	CMC-C2C-C1C	2.22	128.42	125.04
30	B	830	CLA	CMB-C2B-C3B	2.22	128.83	124.68
30	15	313	CLA	CMC-C2C-C1C	2.22	128.42	125.04
37	3	314	A86	C9-C8-C6	-2.22	120.18	126.42
30	A	827	CLA	O2A-CGA-CBA	2.22	118.87	111.91
30	5	304	CLA	CAA-C2A-C3A	-2.22	106.70	112.78
30	14	305	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
30	11	309	CLA	CMA-C3A-C2A	-2.22	104.88	113.83
30	B	833	CLA	CMC-C2C-C1C	2.22	128.41	125.04
38	13	312	KC1	O2D-CGD-O1D	-2.22	119.50	123.84
38	4	310	KC1	CHB-C1B-NB	-2.22	122.42	124.45
33	A	849	BCR	C11-C10-C9	-2.22	124.15	127.31
30	A	831	CLA	OBD-CAD-C3D	-2.22	123.19	128.52
37	10	317	A86	C12-C11-C10	-2.22	118.06	123.42
30	4	304	CLA	C1-C2-C3	-2.22	122.21	126.04
38	8	311	KC1	CAA-C2A-C1A	-2.21	114.56	124.75
30	7	309	CLA	O2A-CGA-CBA	2.21	118.86	111.91
30	B	811	CLA	CMA-C3A-C4A	-2.21	105.82	111.77
37	8	318	A86	O-C13-C11	-2.21	116.26	121.15
30	B	821	CLA	CHB-C4A-NA	2.21	127.57	124.51
38	1	306	KC1	CMC-C2C-C1C	2.21	128.41	125.04
30	A	820	CLA	CBC-CAC-C3C	-2.21	106.33	112.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	819	CLA	CHA-C1A-NA	-2.21	121.33	126.40
30	10	307	CLA	CMB-C2B-C3B	2.21	128.82	124.68
36	F	205	LMG	O3-C3-C2	-2.21	105.23	110.35
30	1	305	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
37	13	313	A86	C3-C2-C1	-2.21	124.15	127.31
30	2	303	CLA	O2A-C1-C2	2.21	114.45	108.64
30	16	301	CLA	C4-C3-C2	-2.21	118.00	123.68
30	A	815	CLA	CHA-C1A-NA	-2.21	121.33	126.40
30	13	302	CLA	CHB-C4A-NA	2.21	127.57	124.51
38	5	312	KC1	CHB-C4A-NA	2.21	127.69	124.20
30	14	302	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
30	7	304	CLA	C1-C2-C3	-2.21	122.22	126.04
30	B	823	CLA	C4-C3-C5	2.21	118.99	115.27
30	5	302	CLA	CHB-C4A-NA	2.21	127.57	124.51
37	3	314	A86	C8-C6-C5	2.21	122.33	118.94
30	15	311	CLA	CMC-C2C-C1C	2.21	128.41	125.04
30	B	812	CLA	C4-C3-C5	2.21	118.99	115.27
38	12	309	KC1	CHB-C1B-NB	-2.21	122.42	124.45
38	14	306	KC1	CHB-C1B-C2B	-2.21	120.84	125.48
30	A	811	CLA	CMC-C2C-C1C	2.21	128.40	125.04
39	5	314	DD6	C23-C16-C15	2.21	116.01	110.05
30	B	820	CLA	CHC-C1C-C2C	-2.21	120.61	126.72
38	5	310	KC1	O1D-CGD-CBD	-2.21	119.96	124.48
30	13	304	CLA	CMC-C2C-C1C	2.21	128.40	125.04
30	7	307	CLA	C6-C7-C8	-2.21	108.78	115.92
30	10	307	CLA	CAA-C2A-C3A	-2.21	106.73	112.78
30	B	835	CLA	CAC-C3C-C4C	2.21	127.68	124.81
30	12	307	CLA	CMA-C3A-C4A	-2.21	105.84	111.77
38	8	306	KC1	CAC-C3C-C4C	2.21	127.67	124.81
30	3	302	CLA	O2A-CGA-CBA	2.21	118.84	111.91
30	A	827	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
38	13	305	KC1	CMC-C2C-C1C	2.21	128.40	125.04
30	10	305	CLA	CBC-CAC-C3C	-2.21	106.34	112.43
38	11	311	KC1	CHB-C4A-NA	2.21	127.68	124.20
38	11	311	KC1	CBC-CAC-C3C	-2.21	106.35	112.43
30	A	802	CLA	CHD-C4C-NC	2.21	127.68	124.20
30	12	303	CLA	C1-C2-C3	-2.21	122.23	126.04
30	10	309	CLA	CED-O2D-CGD	2.21	120.93	115.94
35	7	321	LMT	C1B-O1B-C4'	-2.21	112.51	117.96
38	13	306	KC1	CHB-C4A-NA	2.20	127.68	124.20
37	7	316	A86	C34-O4-C38	-2.20	113.79	117.90
30	12	321	CLA	CBC-CAC-C3C	-2.20	106.36	112.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	803	CLA	CMA-C3A-C2A	-2.20	104.94	113.83
38	14	311	KC1	CHB-C4A-NA	2.20	127.68	124.20
30	12	308	CLA	CBC-CAC-C3C	-2.20	106.36	112.43
33	B	845	BCR	C16-C15-C14	-2.20	118.96	123.47
30	A	839	CLA	C4-C3-C5	2.20	118.98	115.27
37	14	320	A86	C7-C6-C8	2.20	121.55	118.08
30	B	851	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
38	10	312	KC1	O2D-CGD-O1D	-2.20	119.53	123.84
30	B	803	CLA	C1C-C2C-C3C	-2.20	104.64	106.96
30	B	813	CLA	CHA-C1A-NA	-2.20	121.36	126.40
30	A	844	CLA	CBC-CAC-C3C	-2.20	106.37	112.43
39	9	314	DD6	C10-C9-C8	-2.20	116.35	123.22
30	4	305	CLA	C1-C2-C3	-2.20	122.24	126.04
30	1	301	CLA	CMB-C2B-C3B	2.20	128.79	124.68
30	8	308	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
39	6	321	DD6	C3-C4-C5	-2.20	118.97	123.47
38	16	304	KC1	CHB-C1B-NB	-2.20	122.43	124.45
30	6	309	CLA	CBA-CAA-C2A	2.20	120.35	113.86
30	7	309	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
30	A	807	CLA	CMC-C2C-C1C	2.20	128.39	125.04
30	6	305	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
30	10	305	CLA	CHB-C4A-NA	2.20	127.55	124.51
30	B	830	CLA	CAA-C2A-C3A	-2.20	106.76	112.78
38	14	306	KC1	CMB-C2B-C1B	2.20	128.59	124.71
30	14	309	CLA	CAA-C2A-C3A	-2.20	106.76	112.78
36	5	318	LMG	O3-C3-C2	-2.20	105.27	110.35
39	15	319	DD6	C9-C8-C6	-2.20	120.25	126.42
38	11	307	KC1	CHB-C4A-NA	2.20	127.66	124.20
30	A	842	CLA	CHB-C4A-NA	2.20	127.55	124.51
30	7	310	CLA	CBA-CAA-C2A	2.19	120.34	113.86
30	B	818	CLA	C2A-C3A-C4A	-2.19	98.32	101.87
30	1	307	CLA	O1D-CGD-CBD	-2.19	119.99	124.48
38	11	311	KC1	CMB-C2B-C1B	2.19	128.58	124.71
33	A	847	BCR	C38-C26-C27	-2.19	109.40	113.62
30	A	810	CLA	CHB-C4A-NA	2.19	127.55	124.51
30	B	827	CLA	CBC-CAC-C3C	-2.19	106.38	112.43
38	8	310	KC1	CHC-C1C-NC	2.19	127.66	124.20
30	16	307	CLA	CHB-C4A-NA	2.19	127.55	124.51
37	15	320	A86	C10-C9-C8	2.19	130.06	123.22
37	5	316	A86	C7-C6-C5	-2.19	119.85	122.92
30	L	202	CLA	CAA-C2A-C3A	-2.19	106.77	112.78
37	14	317	A86	C10-C9-C8	-2.19	116.38	123.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	1	304	CLA	C1-C2-C3	-2.19	122.25	126.04
30	A	836	CLA	CMB-C2B-C3B	2.19	128.78	124.68
30	8	304	CLA	CBC-CAC-C3C	-2.19	106.39	112.43
38	13	306	KC1	OBD-CAD-C3D	-2.19	124.34	127.98
30	15	305	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
33	B	845	BCR	C38-C26-C27	-2.19	109.41	113.62
30	14	302	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
30	1	304	CLA	CHB-C4A-NA	2.19	127.54	124.51
37	10	316	A86	C19-C18-C17	-2.19	106.55	110.77
39	7	314	DD6	C23-C16-C22	-2.19	104.14	107.37
37	15	322	A86	C28-C27-C26	-2.19	119.86	122.92
30	B	832	CLA	O2A-CGA-CBA	2.19	118.77	111.91
30	9	308	CLA	CHA-C1A-NA	-2.19	121.39	126.40
37	9	316	A86	C19-C18-C17	2.19	115.00	110.77
33	B	843	BCR	C15-C14-C13	-2.19	124.19	127.31
30	14	302	CLA	CAA-C2A-C3A	-2.19	106.79	112.78
30	6	317	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
30	B	828	CLA	CBC-CAC-C3C	-2.19	106.41	112.43
30	13	301	CLA	O2A-CGA-CBA	2.19	118.77	111.91
30	A	840	CLA	CHA-C1A-NA	-2.19	121.39	126.40
30	B	826	CLA	CHB-C4A-NA	2.18	127.53	124.51
30	3	305	CLA	CHA-C1A-NA	-2.18	121.40	126.40
30	8	303	CLA	O1D-CGD-CBD	-2.18	120.02	124.48
33	F	204	BCR	C16-C15-C14	-2.18	119.00	123.47
30	B	825	CLA	CMC-C2C-C1C	2.18	128.36	125.04
30	14	309	CLA	CHA-C1A-NA	-2.18	121.40	126.40
37	6	320	A86	C28-C27-C26	-2.18	119.86	122.92
30	15	307	CLA	CMC-C2C-C1C	2.18	128.36	125.04
30	B	803	CLA	CAC-C3C-C4C	2.18	127.64	124.81
30	B	830	CLA	CHA-C1A-NA	-2.18	121.40	126.40
39	3	316	DD6	C3-C4-C5	-2.18	119.00	123.47
30	3	306	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
38	13	306	KC1	O2D-CGD-O1D	-2.18	119.57	123.84
37	4	317	A86	C28-C27-C26	-2.18	119.87	122.92
37	15	315	A86	C28-C27-C26	-2.18	119.87	122.92
34	A	852	LHG	C20-C19-C18	-2.18	103.35	114.42
30	A	844	CLA	CAA-C2A-C3A	-2.18	106.81	112.78
39	10	314	DD6	O1-C20-C21	-2.18	112.44	115.06
37	13	315	A86	C3-C4-C5	-2.18	119.01	123.47
38	16	311	KC1	CHB-C4A-NA	2.18	127.64	124.20
30	15	308	CLA	CMC-C2C-C1C	2.18	128.36	125.04
38	12	313	KC1	CBC-CAC-C3C	-2.18	106.42	112.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	802	CLA	C1-C2-C3	-2.18	122.27	126.04
37	16	314	A86	C9-C10-C11	-2.18	120.20	126.61
30	2	309	CLA	CED-O2D-CGD	2.18	120.86	115.94
36	6	301	LMG	O3-C3-C2	-2.18	105.31	110.35
30	1	302	CLA	CHB-C4A-NA	2.18	127.52	124.51
38	10	306	KC1	CHB-C1B-NB	-2.18	122.45	124.45
34	A	852	LHG	C27-C26-C25	-2.18	103.37	114.42
30	B	838	CLA	CMB-C2B-C3B	2.18	128.75	124.68
30	B	851	CLA	C1-C2-C3	-2.18	122.28	126.04
30	A	829	CLA	C4-C3-C5	2.18	118.93	115.27
30	3	306	CLA	C2A-C3A-C4A	-2.18	98.35	101.87
37	7	316	A86	C23-C16-C22	-2.18	104.16	107.37
30	6	314	CLA	CMD-C2D-C3D	-2.18	122.61	127.61
30	A	829	CLA	C1B-CHB-C4A	-2.18	125.81	130.12
30	A	838	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
30	6	316	CLA	O1D-CGD-CBD	-2.18	120.03	124.48
33	B	843	BCR	C24-C23-C22	-2.17	122.95	126.23
35	11	302	LMT	C1-O1'-C1'	-2.17	110.23	113.84
30	11	310	CLA	CMD-C2D-C3D	-2.17	122.61	127.61
36	2u	204	LMG	O2-C2-C1	-2.17	104.76	110.05
30	7	303	CLA	C6-C5-C3	-2.17	107.75	113.45
39	2	316	DD6	C22-C16-C17	-2.17	105.21	108.98
30	B	811	CLA	CBC-CAC-C3C	-2.17	106.44	112.43
38	6	313	KC1	CMC-C2C-C1C	2.17	128.35	125.04
37	14	301	A86	C34-O4-C38	-2.17	113.85	117.90
35	1	311	LMT	O3'-C3'-C2'	-2.17	105.33	110.35
38	13	306	KC1	O1D-CGD-CBD	-2.17	120.04	124.48
30	B	830	CLA	CMC-C2C-C1C	2.17	128.34	125.04
33	J	102	BCR	C30-C25-C26	-2.17	119.56	122.61
38	6	313	KC1	CHB-C4A-NA	2.17	127.62	124.20
33	A	851	BCR	C10-C11-C12	-2.17	116.44	123.22
38	8	310	KC1	CHB-C1B-NB	-2.17	122.46	124.45
30	7	305	CLA	C4-C3-C5	2.17	118.92	115.27
30	5	307	CLA	CBA-CAA-C2A	2.17	120.27	113.86
39	6	319	DD6	C23-C16-C22	-2.17	104.17	107.37
30	B	801	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
37	10	301	A86	C26-C25-C24	2.17	129.99	123.22
38	4	310	KC1	CMC-C2C-C1C	2.17	128.34	125.04
30	2	308	CLA	CBC-CAC-C3C	-2.17	106.45	112.43
30	A	844	CLA	C1-C2-C3	-2.17	122.29	126.04
30	A	816	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
36	7	320	LMG	O8-C28-O10	-2.17	118.12	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	831	CLA	CBC-CAC-C3C	-2.17	106.45	112.43
30	2	311	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
30	11	306	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
39	6	318	DD6	C20-C19-C18	2.17	117.04	112.75
30	8	302	CLA	CHB-C4A-NA	2.17	127.51	124.51
38	5	310	KC1	CHB-C4A-NA	2.17	127.62	124.20
30	A	807	CLA	C4-C3-C5	2.17	118.92	115.27
37	10	301	A86	O3-C36-C37	-2.17	105.54	109.39
38	12	309	KC1	O1D-CGD-CBD	-2.17	120.05	124.48
30	3	309	CLA	CHB-C4A-NA	2.17	127.51	124.51
37	8	315	A86	C3-C2-C1	-2.17	124.22	127.31
33	J	103	BCR	C33-C5-C6	-2.17	122.10	124.53
30	15	303	CLA	CMB-C2B-C3B	2.17	128.73	124.68
39	6	318	DD6	C41-C32-C31	-2.17	107.03	110.47
38	11	305	KC1	CHB-C4A-NA	2.17	127.62	124.20
38	13	306	KC1	CHC-C4B-NB	-2.17	122.46	124.45
30	8	301	CLA	O2A-C1-C2	2.17	114.33	108.64
30	1	302	CLA	CMB-C2B-C3B	2.17	128.73	124.68
30	13	303	CLA	O2A-CGA-CBA	2.17	118.70	111.91
30	3	309	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
38	7	313	KC1	O2D-CGD-O1D	-2.17	119.61	123.84
30	B	826	CLA	CHA-C1A-NA	-2.16	121.44	126.40
30	B	802	CLA	CHD-C4C-NC	2.16	127.61	124.20
37	11	315	A86	C12-C11-C13	2.16	119.66	116.02
30	B	819	CLA	O2A-CGA-CBA	2.16	118.70	111.91
30	16	310	CLA	CMB-C2B-C3B	2.16	128.73	124.68
38	11	312	KC1	CED-O2D-CGD	2.16	120.83	115.94
30	A	818	CLA	C4-C3-C5	2.16	118.91	115.27
30	7	305	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
37	14	315	A86	C3-C4-C5	-2.16	119.04	123.47
38	12	313	KC1	CGD-CBD-CAD	-2.16	103.73	110.73
30	16	309	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
39	7	318	DD6	C4-C3-C2	-2.16	119.04	123.47
30	7	310	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
38	5	305	KC1	CAA-C2A-C1A	-2.16	114.81	124.75
30	B	835	CLA	CMC-C2C-C1C	2.16	128.33	125.04
37	2	318	A86	C26-C25-C24	2.16	129.96	123.22
30	B	820	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
38	13	310	KC1	CHB-C4A-NA	2.16	127.61	124.20
30	16	306	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
30	10	308	CLA	C1-C2-C3	-2.16	122.31	126.04
30	2	313	CLA	CBC-CAC-C3C	-2.16	106.48	112.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	10	304	CLA	CMB-C2B-C3B	2.16	128.72	124.68
30	8	301	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
37	15	321	A86	C8-C6-C5	-2.16	115.63	118.94
30	B	831	CLA	CHB-C4A-NA	2.16	127.50	124.51
38	8	313	KC1	OBD-CAD-C3D	-2.16	124.40	127.98
30	10	308	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
30	12	303	CLA	CED-O2D-CGD	2.16	120.82	115.94
30	15	302	CLA	CBC-CAC-C3C	-2.16	106.48	112.43
30	A	842	CLA	CMA-C3A-C2A	-2.16	105.12	113.83
30	8	302	CLA	C1-C2-C3	-2.16	122.31	126.04
30	B	833	CLA	CHB-C4A-NA	2.16	127.50	124.51
38	9	310	KC1	CAA-C2A-C1A	-2.16	114.83	124.75
30	A	803	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
38	5	310	KC1	CMB-C2B-C1B	2.16	128.51	124.71
30	B	828	CLA	CHB-C4A-NA	2.16	127.49	124.51
30	1	305	CLA	C1-C2-C3	-2.16	122.31	126.04
30	A	810	CLA	CAA-C2A-C1A	2.15	119.04	111.97
30	14	303	CLA	O2A-CGA-CBA	2.15	118.67	111.91
30	B	811	CLA	C16-C15-C13	-2.15	108.96	115.92
30	3	302	CLA	CHB-C4A-NA	2.15	127.49	124.51
37	16	314	A86	C26-C25-C24	-2.15	116.50	123.22
30	B	825	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
37	2	318	A86	C4-C3-C2	-2.15	119.06	123.47
30	4	301	CLA	O2A-CGA-CBA	2.15	118.66	111.91
37	5	301	A86	C7-C6-C5	-2.15	119.91	122.92
38	13	308	KC1	CHB-C4A-NA	2.15	127.59	124.20
30	A	843	CLA	CHB-C4A-NA	2.15	127.49	124.51
30	13	304	CLA	CHB-C4A-NA	2.15	127.49	124.51
30	7	307	CLA	C4-C3-C5	2.15	118.89	115.27
39	7	302	DD6	C23-C16-C22	-2.15	104.20	107.37
35	1	311	LMT	O1B-C4'-C3'	2.15	113.00	107.28
37	4	317	A86	C8-C6-C5	-2.15	115.64	118.94
38	13	305	KC1	CAB-C3B-C4B	2.15	130.09	124.90
30	13	302	CLA	CED-O2D-CGD	2.15	120.80	115.94
30	B	823	CLA	C1-O2A-CGA	2.15	122.08	116.44
30	9	303	CLA	CHB-C4A-NA	2.15	127.48	124.51
38	13	311	KC1	CHB-C1B-NB	-2.15	122.48	124.45
30	14	310	CLA	C5-C3-C4	2.15	119.35	114.60
33	A	850	BCR	C20-C21-C22	-2.15	124.24	127.31
30	8	308	CLA	CBC-CAC-C3C	-2.15	106.51	112.43
37	14	318	A86	O1-C15-C14	2.15	117.52	113.21
30	15	310	CLA	CMC-C2C-C1C	2.15	128.31	125.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	14	308	KC1	O1D-CGD-CBD	-2.15	120.09	124.48
30	6	310	CLA	CBC-CAC-C3C	-2.15	106.51	112.43
38	12	311	KC1	O1D-CGD-CBD	-2.15	120.09	124.48
30	B	810	CLA	O2A-CGA-CBA	2.15	118.64	111.91
38	12	305	KC1	CMC-C2C-C1C	2.15	128.31	125.04
30	16	306	CLA	CHB-C4A-NA	2.15	127.48	124.51
30	9	301	CLA	O2A-CGA-CBA	2.15	118.64	111.91
37	10	316	A86	C28-C27-C26	-2.15	119.92	122.92
30	10	305	CLA	CMB-C2B-C1B	2.15	131.76	128.46
33	A	848	BCR	C38-C26-C27	-2.15	109.49	113.62
30	5	307	CLA	CAA-C2A-C3A	-2.15	106.90	112.78
39	8	316	DD6	C33-C32-C31	2.15	113.97	109.62
33	B	843	BCR	C27-C26-C25	2.14	125.84	122.73
30	8	303	CLA	C4-C3-C5	2.14	118.88	115.27
38	3	304	KC1	CMC-C2C-C1C	2.14	128.31	125.04
37	5	316	A86	C7-C6-C8	2.14	121.46	118.08
34	B	848	LHG	O8-C23-O10	-2.14	118.18	123.59
30	2	308	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
30	A	830	CLA	CHB-C4A-NA	2.14	127.48	124.51
30	8	303	CLA	CHB-C4A-NA	2.14	127.48	124.51
30	13	301	CLA	CBC-CAC-C3C	-2.14	106.52	112.43
38	4	310	KC1	CBC-CAC-C3C	-2.14	106.52	112.43
38	12	311	KC1	CMC-C2C-C1C	2.14	128.30	125.04
39	6	319	DD6	C15-C14-C13	-2.14	121.46	125.99
30	11	310	CLA	CED-O2D-CGD	2.14	120.78	115.94
30	12	303	CLA	CHA-C1A-NA	-2.14	121.49	126.40
30	A	836	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
30	B	818	CLA	CHA-C1A-NA	-2.14	121.49	126.40
37	5	315	A86	C22-C16-C17	-2.14	105.26	108.98
30	B	836	CLA	CHB-C4A-NA	2.14	127.47	124.51
30	3	305	CLA	CED-O2D-CGD	2.14	120.78	115.94
30	A	822	CLA	C1-O2A-CGA	2.14	122.06	116.44
30	B	834	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
30	7	309	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
37	15	315	A86	O-C13-C14	-2.14	117.31	121.66
30	A	825	CLA	CBC-CAC-C3C	-2.14	106.53	112.43
37	14	318	A86	C10-C9-C8	-2.14	116.54	123.22
36	2u	204	LMG	C6-C5-C4	-2.14	107.99	113.00
33	I	101	BCR	C38-C26-C27	-2.14	109.51	113.62
38	12	311	KC1	CAB-C3B-C4B	2.14	130.06	124.90
30	A	804	CLA	CHB-C4A-NA	2.14	127.47	124.51
30	6	310	CLA	CAA-C2A-C3A	-2.14	106.92	112.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	7	318	DD6	C23-C16-C17	-2.14	105.27	108.98
30	6	317	CLA	C4-C3-C5	2.14	118.87	115.27
30	B	808	CLA	C1-C2-C3	-2.14	122.35	126.04
30	5	303	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
30	1	302	CLA	O2A-CGA-CBA	2.14	118.61	111.91
30	14	313	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
37	11	314	A86	C-C1-C24	2.14	121.44	118.08
37	8	315	A86	O4-C38-O5	-2.14	118.72	122.96
30	7	304	CLA	O2A-CGA-CBA	2.14	118.61	111.91
30	2	310	CLA	CHB-C4A-NA	2.13	127.46	124.51
30	15	309	CLA	CBC-CAC-C3C	-2.13	106.55	112.43
37	14	301	A86	C4-C3-C2	-2.13	119.10	123.47
30	15	312	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
38	8	307	KC1	CMC-C2C-C1C	2.13	128.29	125.04
30	B	811	CLA	C2A-C1A-CHA	-2.13	120.13	123.86
30	11	309	CLA	C4-C3-C5	2.13	118.86	115.27
38	11	312	KC1	CMC-C2C-C1C	2.13	128.29	125.04
30	10	311	CLA	CHB-C4A-NA	2.13	127.46	124.51
36	5	318	LMG	O2-C2-C1	-2.13	104.87	110.05
37	4	312	A86	C23-C16-C17	-2.13	105.28	108.98
30	F	201	CLA	CAC-C3C-C4C	2.13	127.58	124.81
33	B	842	BCR	C30-C25-C26	-2.13	119.61	122.61
37	4	312	A86	C7-C6-C5	-2.13	119.94	122.92
34	9	318	LHG	C27-C26-C25	-2.13	103.60	114.42
30	3	307	CLA	C1-O2A-CGA	2.13	122.04	116.44
37	10	315	A86	C36-C31-C32	-2.13	117.58	119.70
30	7	303	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
30	A	840	CLA	CHB-C4A-NA	2.13	127.46	124.51
30	2	310	CLA	CHA-C1A-NA	-2.13	121.52	126.40
30	B	818	CLA	CAA-C2A-C1A	-2.13	105.00	111.97
34	A	852	LHG	C11-C10-C9	-2.13	103.62	114.42
39	10	314	DD6	C14-C13-C11	2.13	128.83	125.53
30	B	805	CLA	C11-C10-C8	-2.13	109.04	115.92
38	12	311	KC1	CHB-C1B-NB	-2.13	122.50	124.45
39	15	318	DD6	C3-C4-C5	-2.13	119.11	123.47
30	15	308	CLA	CHA-C1A-NA	-2.13	121.53	126.40
36	F	205	LMG	C9-C8-C7	-2.13	106.76	111.79
37	1	309	A86	C-C1-C24	2.13	121.43	118.08
36	3	317	LMG	C9-C8-C7	-2.13	106.76	111.79
39	3	312	DD6	C33-C34-C35	2.13	113.22	110.30
30	5	307	CLA	CHA-C1A-NA	-2.13	121.53	126.40
30	J	101	CLA	CBC-CAC-C3C	-2.13	106.57	112.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	6	308	KC1	CHB-C1B-NB	-2.13	122.50	124.45
30	B	804	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
30	A	830	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
30	A	806	CLA	CHC-C1C-NC	2.13	127.43	124.20
30	B	815	CLA	CMB-C2B-C3B	2.13	128.66	124.68
30	A	807	CLA	CAC-C3C-C4C	2.12	127.57	124.81
33	J	102	BCR	C33-C5-C6	-2.12	122.14	124.53
30	3	302	CLA	CMA-C3A-C2A	-2.12	105.26	113.83
36	F	205	LMG	C3-C4-C5	-2.12	106.45	110.24
30	5	303	CLA	CMB-C2B-C3B	2.12	128.65	124.68
30	11	308	CLA	C1-O2A-CGA	2.12	122.02	116.44
38	6	311	KC1	CMC-C2C-C1C	2.12	128.27	125.04
37	2	319	A86	C4-C3-C2	-2.12	119.12	123.47
30	6	307	CLA	CBC-CAC-C3C	-2.12	106.58	112.43
39	7	302	DD6	C20-C19-C18	2.12	116.95	112.75
36	5	318	LMG	O1-C1-C2	-2.12	104.99	108.30
30	2	303	CLA	CED-O2D-CGD	2.12	120.74	115.94
30	10	305	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
30	2	305	CLA	CBC-CAC-C3C	-2.12	106.58	112.43
36	8	319	LMG	O1-C1-C2	-2.12	104.99	108.30
38	9	304	KC1	CHB-C4A-NA	2.12	127.55	124.20
37	13	315	A86	C-C1-C2	-2.12	119.95	122.92
30	A	826	CLA	C4-C3-C5	2.12	118.84	115.27
30	B	814	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
30	13	302	CLA	CMB-C2B-C3B	2.12	128.65	124.68
30	13	304	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
30	B	825	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
30	2	303	CLA	C2A-C3A-C4A	-2.12	98.44	101.87
38	4	308	KC1	CHC-C1C-NC	2.12	127.55	124.20
30	9	309	CLA	CHB-C4A-NA	2.12	127.44	124.51
38	6	312	KC1	CAB-C3B-C4B	2.12	130.02	124.90
33	J	102	BCR	C35-C13-C14	-2.12	119.95	122.92
30	B	813	CLA	C7-C6-C5	-2.12	107.60	113.36
36	8	320	LMG	O1-C1-C2	-2.12	104.99	108.30
30	B	831	CLA	C1-O2A-CGA	2.12	122.00	116.44
30	7	312	CLA	CBC-CAC-C3C	-2.12	106.59	112.43
30	B	829	CLA	C1-C2-C3	-2.12	122.38	126.04
30	12	321	CLA	CHA-C1A-NA	-2.12	121.55	126.40
30	A	839	CLA	CMC-C2C-C1C	2.12	128.26	125.04
38	5	306	KC1	CBC-CAC-C3C	-2.12	106.59	112.43
30	11	308	CLA	O2A-CGA-CBA	2.12	118.55	111.91
33	A	851	BCR	C15-C14-C13	-2.12	124.29	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	12	315	DD6	C33-C32-C31	2.12	113.91	109.62
30	A	835	CLA	CBC-CAC-C3C	-2.12	106.59	112.43
36	8	321	LMG	O1-C7-C8	-2.12	105.79	110.90
37	5	316	A86	C10-C9-C8	-2.12	116.61	123.22
37	5	315	A86	C34-O4-C38	-2.12	113.95	117.90
30	B	819	CLA	C4-C3-C5	2.12	118.83	115.27
33	L	205	BCR	C27-C26-C25	2.12	125.80	122.73
30	B	808	CLA	O1D-CGD-CBD	-2.12	120.15	124.48
30	A	810	CLA	CMC-C2C-C1C	2.12	128.26	125.04
30	16	303	CLA	CMB-C2B-C3B	2.12	128.64	124.68
30	F	201	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
30	2	309	CLA	CBC-CAC-C3C	-2.12	106.60	112.43
38	1	306	KC1	CHB-C4A-NA	2.12	127.54	124.20
38	2	312	KC1	CAA-C2A-C1A	-2.12	115.02	124.75
37	4	317	A86	O1-C15-C14	-2.12	108.97	113.21
38	14	308	KC1	CBD-CHA-C1A	2.11	132.82	128.88
30	5	311	CLA	CBC-CAC-C3C	-2.11	106.60	112.43
30	16	306	CLA	C4-C3-C5	2.11	118.83	115.27
30	B	834	CLA	CAC-C3C-C2C	2.11	131.14	127.53
37	14	316	A86	C7-C6-C8	2.11	121.41	118.08
39	6	321	DD6	C25-C24-C1	-2.11	120.48	126.42
30	14	307	CLA	CED-O2D-CGD	2.11	120.72	115.94
30	16	305	CLA	CMB-C2B-C3B	2.11	128.63	124.68
30	10	304	CLA	C4-C3-C5	2.11	118.83	115.27
30	5	308	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
37	11	301	A86	C22-C16-C17	-2.11	105.31	108.98
30	14	304	CLA	CHB-C4A-NA	2.11	127.43	124.51
38	11	307	KC1	CBC-CAC-C3C	-2.11	106.61	112.43
37	14	315	A86	C22-C16-C17	-2.11	105.31	108.98
35	11	302	LMT	C1B-O1B-C4'	-2.11	112.74	117.96
30	B	851	CLA	CHB-C4A-NA	2.11	127.43	124.51
30	A	825	CLA	C4-C3-C5	2.11	118.82	115.27
38	14	311	KC1	CBD-CHA-C1A	2.11	132.82	128.88
33	B	843	BCR	C40-C30-C25	2.11	113.72	110.30
38	9	311	KC1	CHB-C4A-NA	2.11	127.53	124.20
30	10	307	CLA	CHA-C1A-NA	-2.11	121.56	126.40
30	B	802	CLA	CGD-CBD-CAD	-2.11	103.90	110.73
30	15	305	CLA	O2A-CGA-CBA	2.11	120.81	114.03
30	10	303	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
30	6	309	CLA	C2A-C3A-C4A	-2.11	98.46	101.87
30	4	303	CLA	CAA-C2A-C3A	-2.11	107.00	112.78
37	2	318	A86	C-C1-C2	-2.11	119.97	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	841	CLA	O2D-CGD-O1D	-2.11	119.72	123.84
30	1	303	CLA	O2A-CGA-CBA	2.11	118.52	111.91
30	B	819	CLA	CMA-C3A-C4A	-2.11	106.11	111.77
30	A	818	CLA	CMB-C2B-C3B	2.11	128.62	124.68
30	B	838	CLA	CHA-C1A-NA	-2.11	121.57	126.40
30	B	832	CLA	O2D-CGD-O1D	-2.11	119.72	123.84
30	2	307	CLA	C4-C3-C5	2.11	118.81	115.27
38	2	314	KC1	CHB-C1B-NB	-2.11	122.52	124.45
38	13	308	KC1	CHB-C1B-NB	-2.11	122.52	124.45
30	10	304	CLA	CMC-C2C-C1C	2.11	128.25	125.04
30	A	814	CLA	CHA-C1A-NA	-2.11	121.58	126.40
30	A	813	CLA	C6-C7-C8	-2.10	109.12	115.92
30	A	833	CLA	CMC-C2C-C1C	2.10	128.24	125.04
38	13	305	KC1	CBC-CAC-C3C	-2.10	106.63	112.43
30	B	801	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
30	A	803	CLA	CGD-CBD-CAD	2.10	117.55	110.73
30	9	309	CLA	C1-C2-C3	-2.10	122.41	126.04
30	L	202	CLA	C4-C3-C5	2.10	118.81	115.27
30	3	303	CLA	CMC-C2C-C1C	2.10	128.24	125.04
30	12	302	CLA	C11-C12-C13	-2.10	109.12	115.92
30	12	303	CLA	CHB-C4A-NA	2.10	127.42	124.51
30	B	824	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
38	12	311	KC1	O2A-CGA-O1A	-2.10	118.30	122.67
30	A	807	CLA	CBC-CAC-C3C	-2.10	106.64	112.43
30	14	305	CLA	CMC-C2C-C1C	2.10	128.24	125.04
39	8	316	DD6	C4-C3-C2	-2.10	119.17	123.47
30	A	811	CLA	O2A-CGA-CBA	2.10	118.50	111.91
30	11	306	CLA	O2A-CGA-CBA	2.10	118.50	111.91
30	A	835	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
30	7	312	CLA	CHA-C1A-NA	-2.10	121.59	126.40
30	5	303	CLA	C1-O2A-CGA	2.10	121.95	116.44
37	11	301	A86	C-C1-C2	-2.10	119.98	122.92
30	A	804	CLA	CBC-CAC-C3C	-2.10	106.64	112.43
37	15	316	A86	C19-C18-C17	2.10	114.83	110.77
33	B	844	BCR	C24-C23-C22	-2.10	123.06	126.23
30	B	816	CLA	CBA-CAA-C2A	2.10	120.06	113.86
30	5	307	CLA	CHB-C4A-NA	2.10	127.41	124.51
30	B	831	CLA	CBC-CAC-C3C	-2.10	106.65	112.43
38	10	310	KC1	CHB-C1B-C2B	-2.10	121.08	125.48
37	7	319	A86	O-C13-C11	-2.10	116.52	121.15
30	6	307	CLA	CBA-CAA-C2A	-2.10	107.67	113.86
30	12	321	CLA	CED-O2D-CGD	2.10	120.68	115.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	828	CLA	CHD-C4C-NC	2.10	127.51	124.20
30	B	824	CLA	CAA-C2A-C1A	-2.10	105.10	111.97
30	F	202	CLA	C1-O2A-CGA	2.10	121.94	116.44
30	14	307	CLA	CHA-C1A-NA	-2.10	121.60	126.40
37	16	312	A86	C41-C32-C31	-2.10	108.60	110.47
38	9	312	KC1	CAA-C2A-C1A	-2.10	115.11	124.75
30	16	306	CLA	O1D-CGD-CBD	-2.10	120.20	124.48
30	6	314	CLA	O1D-CGD-CBD	-2.10	120.20	124.48
35	7	321	LMT	C1-O1'-C1'	-2.09	110.37	113.84
38	3	304	KC1	CAA-C2A-C1A	-2.09	115.12	124.75
38	2	314	KC1	CMB-C2B-C1B	2.09	128.40	124.71
30	2	301	CLA	CMB-C2B-C3B	2.09	128.60	124.68
37	10	317	A86	C34-O4-C38	-2.09	113.99	117.90
37	9	315	A86	C12-C11-C13	2.09	119.54	116.02
30	B	812	CLA	CAA-C2A-C3A	-2.09	107.05	112.78
30	B	827	CLA	CMB-C2B-C3B	2.09	128.59	124.68
37	2	318	A86	C7-C6-C8	2.09	121.37	118.08
30	4	309	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
30	16	308	CLA	CHA-C1A-NA	-2.09	121.61	126.40
37	4	312	A86	C40-C32-C31	-2.09	108.60	110.47
37	16	312	A86	C20-C19-C18	-2.09	108.61	112.75
38	13	308	KC1	O1D-CGD-CBD	-2.09	120.21	124.48
37	15	315	A86	C9-C10-C11	-2.09	120.46	126.61
30	8	305	CLA	CHB-C4A-NA	2.09	127.40	124.51
37	2	302	A86	C36-C31-C32	-2.09	117.62	119.70
38	10	310	KC1	CMB-C2B-C1B	2.09	128.39	124.71
39	11	313	DD6	C23-C16-C17	-2.09	105.35	108.98
38	6	312	KC1	O2D-CGD-O1D	-2.09	119.75	123.84
31	A	845	PQN	C17-C16-C15	-2.09	107.69	113.36
30	B	834	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
30	15	312	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
38	6	312	KC1	CHB-C4A-NA	2.09	127.49	124.20
37	7	319	A86	C3-C2-C1	-2.09	124.33	127.31
30	9	305	CLA	CGD-CBD-CAD	-2.09	103.98	110.73
30	3	305	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
30	16	303	CLA	O2D-CGD-O1D	-2.09	119.76	123.84
39	8	316	DD6	C9-C8-C6	-2.08	120.56	126.42
33	L	204	BCR	C37-C22-C21	-2.08	120.00	122.92
37	15	315	A86	C12-C11-C10	-2.08	118.38	123.42
30	A	814	CLA	C1-C2-C3	-2.08	122.44	126.04
37	14	301	A86	C7-C6-C8	2.08	121.36	118.08
39	8	316	DD6	C20-C19-C18	-2.08	108.63	112.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	6	304	CLA	CAA-C2A-C3A	-2.08	107.07	112.78
30	9	308	CLA	CHB-C4A-NA	2.08	127.39	124.51
39	4	313	DD6	C23-C16-C17	-2.08	105.36	108.98
37	5	315	A86	C36-C31-C32	-2.08	117.63	119.70
30	15	303	CLA	CHB-C4A-NA	2.08	127.39	124.51
30	A	844	CLA	O2A-CGA-CBA	2.08	118.44	111.91
38	14	308	KC1	CHD-C4C-NC	2.08	127.36	124.20
30	5	308	CLA	C1-C2-C3	-2.08	122.44	126.04
35	B	850	LMT	C2'-C3'-C4'	2.08	114.43	109.68
39	5	313	DD6	C10-C9-C8	-2.08	116.72	123.22
30	11	306	CLA	CGD-CBD-CAD	-2.08	103.99	110.73
30	A	817	CLA	CHB-C4A-NA	2.08	127.39	124.51
37	2	318	A86	C34-O4-C38	-2.08	114.02	117.90
38	6	311	KC1	CBC-CAC-C3C	-2.08	106.70	112.43
30	4	304	CLA	CAA-CBA-CGA	2.08	119.33	113.25
30	15	303	CLA	CHA-C1A-NA	-2.08	121.64	126.40
30	A	829	CLA	CMA-C3A-C2A	-2.08	105.44	113.83
30	B	805	CLA	CMC-C2C-C1C	2.08	128.21	125.04
30	9	307	CLA	CHA-C1A-NA	-2.08	121.64	126.40
35	B	850	LMT	O3'-C3'-C2'	-2.08	105.54	110.35
30	7	306	CLA	CHA-C1A-NA	-2.08	121.64	126.40
36	B	849	LMG	O3-C3-C2	-2.08	105.55	110.35
30	B	835	CLA	CBC-CAC-C3C	-2.08	106.70	112.43
30	1	303	CLA	CBC-CAC-C3C	-2.08	106.70	112.43
30	6	304	CLA	CMA-C3A-C2A	-2.08	105.45	113.83
30	A	839	CLA	CHB-C4A-NA	2.08	127.39	124.51
39	8	317	DD6	C33-C32-C31	2.08	113.83	109.62
37	12	316	A86	C25-C24-C1	-2.08	120.58	126.42
30	9	306	CLA	CGD-CBD-CAD	-2.08	104.01	110.73
30	L	203	CLA	CMC-C2C-C1C	2.08	128.20	125.04
30	A	844	CLA	O2D-CGD-O1D	-2.08	119.78	123.84
30	1	304	CLA	CBC-CAC-C3C	-2.08	106.71	112.43
30	11	306	CLA	O2D-CGD-O1D	-2.07	119.78	123.84
37	14	316	A86	C20-C19-C18	-2.07	108.64	112.75
30	10	303	CLA	CMC-C2C-C1C	2.07	128.20	125.04
33	B	841	BCR	C11-C10-C9	-2.07	124.35	127.31
30	8	303	CLA	CMC-C2C-C1C	2.07	128.20	125.04
37	9	316	A86	C40-C32-C31	-2.07	108.62	110.47
30	7	304	CLA	CMC-C2C-C1C	2.07	128.19	125.04
38	12	305	KC1	O2A-CGA-O1A	-2.07	118.36	122.67
38	7	308	KC1	CHB-C4A-NA	2.07	127.47	124.20
30	B	805	CLA	CHA-C1A-NA	-2.07	121.66	126.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	11	310	CLA	O2D-CGD-O1D	-2.07	119.79	123.84
30	7	304	CLA	C6-C7-C8	-2.07	109.23	115.92
30	3	305	CLA	CBA-CAA-C2A	2.07	119.97	113.86
30	B	836	CLA	CHA-C1A-NA	-2.07	121.66	126.40
35	B	852	LMT	C1'-C2'-C3'	2.07	114.31	110.00
36	B	847	LMG	O7-C10-O9	-2.07	118.70	123.70
30	8	304	CLA	C2A-C3A-C4A	-2.07	98.53	101.87
37	13	315	A86	C28-C27-C26	-2.07	120.03	122.92
30	A	822	CLA	O2A-CGA-CBA	2.07	118.40	111.91
36	7	320	LMG	O7-C10-O9	-2.07	118.70	123.70
30	12	304	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
30	A	837	CLA	CAA-C2A-C3A	-2.07	107.12	112.78
30	2u	202	CLA	CAA-C2A-C3A	-2.07	107.12	112.78
38	9	312	KC1	CED-O2D-CGD	2.07	120.61	115.94
30	7	311	CLA	CBC-CAC-C3C	-2.07	106.74	112.43
30	A	810	CLA	CMB-C2B-C3B	2.06	128.54	124.68
37	14	319	A86	C8-C6-C5	2.06	122.11	118.94
30	A	827	CLA	CHB-C4A-NA	2.06	127.37	124.51
30	A	820	CLA	O2A-C1-C2	2.06	114.06	108.64
37	7	315	A86	O-C13-C11	-2.06	116.59	121.15
30	15	313	CLA	CGD-CBD-CAD	-2.06	104.05	110.73
30	6	305	CLA	CMA-C3A-C4A	-2.06	106.23	111.77
30	2	313	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
37	10	316	A86	C34-O4-C38	-2.06	114.06	117.90
37	11	315	A86	C9-C8-C6	-2.06	120.63	126.42
35	9	317	LMT	C1'-O5'-C5'	2.06	117.73	113.69
39	8	316	DD6	C22-C16-C15	2.06	115.61	110.05
30	9	305	CLA	CAA-C2A-C1A	2.06	118.72	111.97
31	B	840	PQN	C11-C3-C4	2.06	120.70	118.50
30	9	306	CLA	CMC-C2C-C1C	2.06	128.17	125.04
30	B	838	CLA	C1-C2-C3	-2.06	122.48	126.04
38	2	314	KC1	CMC-C2C-C1C	2.06	128.17	125.04
30	11	308	CLA	C1-C2-C3	-2.06	122.48	126.04
30	12	308	CLA	CED-O2D-CGD	2.06	120.59	115.94
30	B	819	CLA	O2D-CGD-O1D	-2.06	119.82	123.84
37	10	315	A86	C28-C27-C26	-2.06	120.04	122.92
30	5	307	CLA	C2A-C3A-C4A	-2.06	98.55	101.87
30	12	306	CLA	C4-C3-C5	2.06	118.73	115.27
38	8	311	KC1	CED-O2D-CGD	2.06	120.59	115.94
39	4	313	DD6	C4-C3-C2	-2.06	119.26	123.47
38	6	308	KC1	CBC-CAC-C3C	-2.06	106.76	112.43
30	1	303	CLA	CAC-C3C-C4C	2.06	127.48	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	7	305	CLA	C4A-NA-C1A	-2.06	105.78	106.71
30	A	812	CLA	CMB-C2B-C3B	2.06	128.52	124.68
37	2u	205	A86	O4-C38-O5	-2.05	118.88	122.96
36	8	319	LMG	O2-C2-C1	-2.05	105.06	110.05
30	F	201	CLA	O2D-CGD-O1D	-2.05	119.82	123.84
30	3	302	CLA	CHA-C1A-NA	-2.05	121.69	126.40
35	A	855	LMT	C1'-C2'-C3'	2.05	114.27	110.00
30	7	305	CLA	CMC-C2C-C1C	2.05	128.17	125.04
30	B	801	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
30	B	833	CLA	CBC-CAC-C3C	-2.05	106.77	112.43
38	8	313	KC1	CHB-C1B-NB	-2.05	122.57	124.45
30	1	304	CLA	O2A-CGA-CBA	2.05	118.35	111.91
30	2	303	CLA	CMA-C3A-C4A	-2.05	106.25	111.77
30	A	821	CLA	CMC-C2C-C1C	2.05	128.16	125.04
30	4	302	CLA	O2A-CGA-CBA	2.05	118.35	111.91
38	7	308	KC1	O2D-CGD-O1D	-2.05	119.83	123.84
37	15	323	A86	C35-C34-C33	2.05	113.46	109.88
38	13	311	KC1	CAB-C3B-C4B	2.05	129.85	124.90
30	16	308	CLA	O2A-CGA-O1A	-2.05	118.19	123.30
30	16	306	CLA	CAA-C2A-C1A	2.05	118.69	111.97
37	11	301	A86	C8-C6-C5	-2.05	115.80	118.94
30	1	304	CLA	O2D-CGD-O1D	-2.05	119.83	123.84
30	B	830	CLA	CHD-C4C-NC	2.05	127.43	124.20
30	A	806	CLA	C1-C2-C3	-2.05	122.50	126.04
30	9	307	CLA	O2D-CGD-O1D	-2.05	119.83	123.84
38	8	312	KC1	O2A-CGA-O1A	-2.05	118.41	122.67
33	A	847	BCR	C33-C5-C6	-2.05	122.23	124.53
38	10	310	KC1	CHB-C4A-NA	2.05	127.43	124.20
30	B	821	CLA	CMC-C2C-C1C	2.05	128.16	125.04
30	5	304	CLA	C2A-C3A-C4A	-2.05	98.56	101.87
30	F	203	CLA	O1D-CGD-CBD	-2.05	120.30	124.48
30	10	311	CLA	CBC-CAC-C3C	-2.05	106.79	112.43
39	3	313	DD6	O1-C20-C21	-2.05	112.61	115.06
33	M	101	BCR	C33-C5-C6	-2.05	122.23	124.53
30	B	837	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
30	9	309	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
37	4	312	A86	C3-C4-C5	-2.04	119.29	123.47
30	A	831	CLA	CMA-C3A-C4A	-2.04	106.28	111.77
33	B	842	BCR	C7-C8-C9	-2.04	123.15	126.23
39	10	314	DD6	C10-C9-C8	-2.04	116.84	123.22
35	A	854	LMT	C4B-C3B-C2B	2.04	114.39	110.82
30	11	306	CLA	CHA-C1A-NA	-2.04	121.72	126.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	8	313	KC1	CHB-C4A-NA	2.04	127.42	124.20
30	F	202	CLA	C1-C2-C3	-2.04	122.51	126.04
39	6	319	DD6	C33-C34-C35	-2.04	107.51	110.30
30	8	309	CLA	CBC-CAC-C3C	-2.04	106.80	112.43
30	15	314	CLA	CMB-C2B-C3B	2.04	128.50	124.68
30	7	303	CLA	CBC-CAC-C3C	-2.04	106.80	112.43
38	2	314	KC1	CBC-CAC-C3C	-2.04	106.80	112.43
37	4	314	A86	C41-C32-C31	-2.04	108.64	110.47
30	9	301	CLA	C4-C3-C5	2.04	118.70	115.27
30	11	304	CLA	CAA-C2A-C3A	-2.04	107.19	112.78
30	3	302	CLA	C6-C7-C8	-2.04	109.33	115.92
30	14	312	CLA	CED-O2D-CGD	2.04	120.55	115.94
38	2	312	KC1	CED-O2D-CGD	2.04	120.55	115.94
30	16	303	CLA	CBC-CAC-C3C	-2.04	106.81	112.43
30	3	307	CLA	O2D-CGD-O1D	-2.04	119.85	123.84
33	L	205	BCR	C33-C5-C6	-2.04	122.24	124.53
30	3	310	CLA	CED-O2D-CGD	2.04	120.55	115.94
30	A	808	CLA	C1-C2-C3	-2.04	122.52	126.04
30	6	317	CLA	CHA-C1A-NA	-2.04	121.73	126.40
30	3	307	CLA	CAC-C3C-C4C	2.04	127.45	124.81
30	16	301	CLA	C6-C7-C8	-2.04	109.33	115.92
30	A	831	CLA	C1-C2-C3	-2.04	122.52	126.04
30	1	305	CLA	CBC-CAC-C3C	-2.04	106.82	112.43
30	B	803	CLA	CAC-C3C-C2C	2.04	131.01	127.53
39	11	313	DD6	C22-C16-C17	2.04	112.52	108.98
30	B	827	CLA	CHB-C4A-NA	2.04	127.33	124.51
35	A	855	LMT	O3'-C3'-C2'	-2.04	105.64	110.35
30	6	306	CLA	CBC-CAC-C3C	-2.04	106.82	112.43
30	5	307	CLA	O2D-CGD-O1D	-2.04	119.86	123.84
37	2	318	A86	C23-C16-C17	-2.04	105.45	108.98
30	2u	202	CLA	C4-C3-C5	2.03	118.69	115.27
30	10	304	CLA	CHB-C4A-NA	2.03	127.32	124.51
30	6	307	CLA	CMC-C2C-C1C	2.03	128.13	125.04
37	9	316	A86	C3-C2-C1	-2.03	124.41	127.31
30	2	304	CLA	CHA-C1A-NA	-2.03	121.74	126.40
30	7	304	CLA	CHB-C4A-NA	2.03	127.32	124.51
30	16	301	CLA	C11-C10-C8	-2.03	109.35	115.92
33	B	845	BCR	C24-C23-C22	-2.03	123.17	126.23
30	B	838	CLA	C6-C7-C8	-2.03	109.35	115.92
30	10	305	CLA	CAA-C2A-C1A	2.03	118.63	111.97
36	3	317	LMG	C3-C4-C5	-2.03	106.62	110.24
30	B	827	CLA	CBA-CAA-C2A	2.03	119.86	113.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	A	851	BCR	C8-C7-C6	-2.03	121.50	127.20
30	A	828	CLA	CAC-C3C-C4C	2.03	127.44	124.81
30	4	311	CLA	CHA-C1A-NA	-2.03	121.75	126.40
30	A	813	CLA	CMC-C2C-C1C	2.03	128.13	125.04
38	8	310	KC1	O1D-CGD-CBD	-2.03	120.33	124.48
38	10	312	KC1	CHB-C4A-NA	2.03	127.40	124.20
33	J	103	BCR	C10-C11-C12	-2.03	116.89	123.22
30	A	802	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
30	B	834	CLA	C4-C3-C5	2.03	118.68	115.27
37	8	318	A86	C40-C32-C31	-2.03	108.66	110.47
33	2u	201	BCR	C10-C11-C12	-2.03	116.89	123.22
39	10	313	DD6	C41-C32-C31	-2.03	107.25	110.47
39	12	315	DD6	C3-C4-C5	-2.03	119.32	123.47
30	14	313	CLA	CGD-CBD-CAD	-2.03	104.17	110.73
37	11	316	A86	O4-C38-O5	-2.03	118.94	122.96
30	4	306	CLA	O1D-CGD-CBD	-2.03	120.34	124.48
30	16	308	CLA	CMC-C2C-C1C	2.03	128.12	125.04
38	9	311	KC1	CHB-C1B-NB	-2.03	122.59	124.45
30	F	203	CLA	CAC-C3C-C4C	2.02	127.44	124.81
30	11	310	CLA	CBC-CAC-C3C	-2.02	106.85	112.43
30	A	832	CLA	O1D-CGD-CBD	-2.02	120.34	124.48
38	1	308	KC1	CBA-CAA-C2A	-2.02	117.56	125.27
30	8	304	CLA	CMC-C2C-C1C	2.02	128.12	125.04
30	A	812	CLA	C11-C12-C13	-2.02	109.38	115.92
30	A	820	CLA	C1-O2A-CGA	2.02	121.75	116.44
30	14	302	CLA	C1-O2A-CGA	2.02	121.75	116.44
30	13	304	CLA	CED-O2D-CGD	2.02	120.51	115.94
39	9	314	DD6	C19-C18-C17	2.02	114.67	110.77
30	A	810	CLA	CHA-C1A-NA	-2.02	121.77	126.40
30	8	308	CLA	CHA-C1A-NA	-2.02	121.77	126.40
30	16	301	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
39	7	317	DD6	C25-C24-C1	-2.02	120.74	126.42
30	A	821	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
37	13	315	A86	O1-C15-C14	2.02	117.26	113.21
30	A	827	CLA	CAA-C2A-C1A	-2.02	105.36	111.97
30	1	304	CLA	CED-O2D-CGD	2.02	120.50	115.94
30	6	309	CLA	CHB-C4A-NA	2.02	127.30	124.51
30	6	307	CLA	CHC-C1C-NC	2.02	127.27	124.20
30	9	306	CLA	CAA-C2A-C1A	2.02	118.59	111.97
38	8	312	KC1	CHB-C4A-NA	2.02	127.39	124.20
30	B	839	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
33	M	101	BCR	C38-C26-C27	-2.02	109.74	113.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	6	312	KC1	CHB-C1B-NB	-2.02	122.60	124.45
39	6	303	DD6	C37-C36-C35	-2.02	110.62	114.36
30	A	821	CLA	CBC-CAC-C3C	-2.02	106.87	112.43
30	B	826	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
30	A	805	CLA	CHA-C1A-NA	-2.02	121.78	126.40
30	4	305	CLA	CMA-C3A-C4A	-2.02	106.35	111.77
30	2	305	CLA	CMC-C2C-C1C	2.02	128.11	125.04
30	6	314	CLA	CHA-C1A-NA	-2.02	121.78	126.40
30	B	810	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
37	15	316	A86	C35-C34-C33	2.02	113.39	109.88
33	A	849	BCR	C35-C13-C14	-2.01	120.10	122.92
30	6	309	CLA	O1D-CGD-CBD	-2.01	120.36	124.48
37	15	320	A86	C9-C8-C6	2.01	132.07	126.42
30	A	820	CLA	CMC-C2C-C1C	2.01	128.11	125.04
30	A	842	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
30	2	301	CLA	O1D-CGD-CBD	-2.01	120.36	124.48
30	B	836	CLA	CMB-C2B-C3B	2.01	128.44	124.68
30	9	301	CLA	CHC-C1C-NC	2.01	127.26	124.20
30	14	305	CLA	C5-C3-C4	2.01	119.05	114.60
38	12	305	KC1	CBC-CAC-C3C	-2.01	106.88	112.43
37	3	315	A86	C40-C32-C31	-2.01	108.67	110.47
37	15	315	A86	C26-C25-C24	2.01	129.50	123.22
37	2u	203	A86	C20-C19-C18	-2.01	108.77	112.75
39	12	315	DD6	C20-C19-C18	-2.01	108.77	112.75
30	3	303	CLA	CAA-C2A-C1A	2.01	118.57	111.97
30	A	816	CLA	O2A-CGA-CBA	2.01	118.22	111.91
37	10	315	A86	C8-C6-C5	-2.01	115.86	118.94
30	A	816	CLA	CHC-C1C-NC	2.01	127.25	124.20
37	14	314	A86	C3-C2-C1	-2.01	124.44	127.31
39	2	317	DD6	C25-C24-C1	-2.01	120.77	126.42
36	6	301	LMG	O2-C2-C1	-2.01	105.16	110.05
30	F	202	CLA	O2A-CGA-CBA	2.01	118.22	111.91
38	6	312	KC1	CAA-C2A-C1A	-2.01	115.50	124.75
39	7	314	DD6	C33-C34-C35	2.01	113.06	110.30
37	13	313	A86	C-C1-C24	2.01	121.24	118.08
30	13	302	CLA	O2A-CGA-CBA	2.01	118.21	111.91
30	4	303	CLA	CHA-C1A-NA	-2.01	121.80	126.40
33	B	846	BCR	C8-C9-C10	-2.01	115.86	118.94
38	3	304	KC1	CBC-CAC-C3C	-2.01	106.89	112.43
35	11	318	LMT	C1-O1'-C1'	-2.01	110.51	113.84
37	2	302	A86	C8-C6-C5	2.01	122.02	118.94
30	A	838	CLA	CAC-C3C-C4C	2.01	127.41	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	2	315	DD6	C9-C8-C6	2.01	132.05	126.42
30	A	809	CLA	C1-O2A-CGA	2.01	121.71	116.44
37	11	315	A86	C7-C6-C8	2.01	121.24	118.08
30	B	815	CLA	CHA-C1A-NA	-2.01	121.81	126.40
30	12	302	CLA	CBA-CAA-C2A	2.01	119.78	113.86
30	13	301	CLA	O2A-C1-C2	2.00	113.90	108.64
30	F	203	CLA	O2A-CGA-CBA	2.00	120.47	114.03
33	B	842	BCR	C15-C16-C17	-2.00	119.37	123.47
30	A	810	CLA	C4-C3-C5	2.00	118.64	115.27
30	8	304	CLA	CHB-C4A-NA	2.00	127.28	124.51
30	A	828	CLA	CHC-C1C-NC	2.00	127.24	124.20
30	15	305	CLA	CHA-C1A-NA	-2.00	121.81	126.40
30	6	314	CLA	CHB-C4A-NA	2.00	127.28	124.51
37	4	314	A86	C3-C4-C5	-2.00	119.37	123.47
30	A	834	CLA	CHA-C1A-NA	-2.00	121.81	126.40
30	15	309	CLA	CMC-C2C-C1C	2.00	128.09	125.04
30	1	305	CLA	CHA-C1A-NA	-2.00	121.81	126.40
30	B	807	CLA	C6-C7-C8	-2.00	109.45	115.92
30	A	812	CLA	CBC-CAC-C3C	-2.00	106.92	112.43
37	14	301	A86	C3-C4-C5	-2.00	119.38	123.47
37	11	315	A86	C10-C9-C8	-2.00	116.97	123.22
30	A	843	CLA	CMB-C2B-C1B	2.00	131.54	128.46

All (185) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
29	A	801	CL0	NA
29	A	801	CL0	ND
29	A	801	CL0	NC
30	A	802	CLA	ND
30	A	803	CLA	ND
30	A	804	CLA	ND
30	A	805	CLA	ND
30	A	806	CLA	ND
30	A	807	CLA	ND
30	A	808	CLA	ND
30	A	809	CLA	ND
30	A	810	CLA	ND
30	A	811	CLA	ND
30	A	812	CLA	ND
30	A	813	CLA	ND
30	A	814	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
30	A	815	CLA	ND
30	A	816	CLA	ND
30	A	820	CLA	ND
30	A	821	CLA	ND
30	A	822	CLA	ND
30	A	824	CLA	ND
30	A	825	CLA	ND
30	A	826	CLA	ND
30	A	827	CLA	ND
30	A	828	CLA	ND
30	A	829	CLA	ND
30	A	830	CLA	ND
30	A	831	CLA	ND
30	A	833	CLA	ND
30	A	834	CLA	ND
30	A	835	CLA	ND
30	A	836	CLA	ND
30	A	837	CLA	ND
30	A	838	CLA	ND
30	A	839	CLA	ND
30	A	840	CLA	ND
30	A	841	CLA	ND
30	A	842	CLA	ND
30	A	843	CLA	ND
30	A	844	CLA	ND
30	B	801	CLA	ND
30	B	802	CLA	ND
30	B	803	CLA	ND
30	B	804	CLA	ND
30	B	805	CLA	ND
30	B	806	CLA	ND
30	B	807	CLA	ND
30	B	808	CLA	ND
30	B	809	CLA	ND
30	B	810	CLA	ND
30	B	811	CLA	ND
30	B	812	CLA	ND
30	B	813	CLA	ND
30	B	814	CLA	ND
30	B	815	CLA	ND
30	B	817	CLA	ND
30	B	818	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
30	B	819	CLA	ND
30	B	821	CLA	ND
30	B	823	CLA	ND
30	B	824	CLA	ND
30	B	825	CLA	ND
30	B	826	CLA	ND
30	B	827	CLA	ND
30	B	828	CLA	ND
30	B	829	CLA	ND
30	B	830	CLA	ND
30	B	832	CLA	ND
30	B	833	CLA	ND
30	B	834	CLA	ND
30	B	835	CLA	ND
30	B	836	CLA	ND
30	B	837	CLA	ND
30	B	838	CLA	ND
30	B	839	CLA	ND
30	F	201	CLA	ND
30	F	202	CLA	ND
30	F	203	CLA	ND
30	J	101	CLA	ND
30	L	202	CLA	ND
30	L	203	CLA	ND
30	2u	202	CLA	ND
30	1	301	CLA	ND
30	1	302	CLA	ND
30	1	303	CLA	ND
30	1	304	CLA	ND
30	1	305	CLA	ND
30	2	301	CLA	ND
30	2	304	CLA	ND
30	2	305	CLA	ND
30	2	307	CLA	ND
30	2	309	CLA	ND
30	2	310	CLA	ND
30	3	301	CLA	ND
30	3	302	CLA	ND
30	3	303	CLA	ND
30	3	305	CLA	ND
30	3	306	CLA	ND
30	3	307	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
30	4	301	CLA	ND
30	4	302	CLA	ND
30	4	303	CLA	ND
30	4	304	CLA	ND
30	4	305	CLA	ND
30	4	306	CLA	ND
30	4	309	CLA	ND
30	4	311	CLA	ND
30	5	302	CLA	ND
30	5	303	CLA	ND
30	5	304	CLA	ND
30	5	307	CLA	ND
30	5	309	CLA	ND
30	5	311	CLA	ND
30	6	304	CLA	ND
30	6	305	CLA	ND
30	6	306	CLA	ND
30	6	307	CLA	ND
30	6	309	CLA	ND
30	6	310	CLA	ND
30	6	315	CLA	ND
30	6	316	CLA	ND
30	6	317	CLA	ND
30	7	303	CLA	ND
30	7	304	CLA	ND
30	7	305	CLA	ND
30	7	306	CLA	ND
30	7	309	CLA	ND
30	7	311	CLA	ND
30	7	312	CLA	ND
30	8	301	CLA	ND
30	8	302	CLA	ND
30	8	304	CLA	ND
30	8	308	CLA	ND
30	9	301	CLA	ND
30	9	302	CLA	ND
30	9	305	CLA	ND
30	9	306	CLA	ND
30	9	307	CLA	ND
30	9	308	CLA	ND
30	9	309	CLA	ND
30	10	303	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
30	10	304	CLA	ND
30	10	305	CLA	ND
30	10	307	CLA	ND
30	10	308	CLA	ND
30	10	309	CLA	ND
30	11	304	CLA	ND
30	11	306	CLA	ND
30	11	308	CLA	ND
30	11	310	CLA	ND
30	12	303	CLA	ND
30	12	304	CLA	ND
30	12	306	CLA	ND
30	12	307	CLA	ND
30	12	308	CLA	ND
30	12	312	CLA	ND
30	12	321	CLA	ND
30	13	301	CLA	ND
30	13	302	CLA	ND
30	13	307	CLA	ND
30	13	309	CLA	ND
30	14	302	CLA	ND
30	14	303	CLA	ND
30	14	304	CLA	ND
30	14	305	CLA	ND
30	14	309	CLA	ND
30	14	310	CLA	ND
30	14	313	CLA	ND
30	15	303	CLA	ND
30	15	304	CLA	ND
30	15	305	CLA	ND
30	15	306	CLA	ND
30	15	307	CLA	ND
30	15	308	CLA	ND
30	15	310	CLA	ND
30	15	311	CLA	ND
30	15	312	CLA	ND
30	16	302	CLA	ND
30	16	303	CLA	ND
30	16	305	CLA	ND
30	16	306	CLA	ND
30	16	307	CLA	ND
30	16	308	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
30	16	310	CLA	ND

All (3979) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	A	804	CLA	C3A-C2A-CAA-CBA
30	A	806	CLA	C1A-C2A-CAA-CBA
30	A	806	CLA	C3A-C2A-CAA-CBA
30	A	807	CLA	C1A-C2A-CAA-CBA
30	A	807	CLA	CBD-CGD-O2D-CED
30	A	809	CLA	C1A-C2A-CAA-CBA
30	A	809	CLA	C3A-C2A-CAA-CBA
30	A	809	CLA	C6-C7-C8-C9
30	A	812	CLA	C1A-C2A-CAA-CBA
30	A	819	CLA	C3A-C2A-CAA-CBA
30	A	820	CLA	C1A-C2A-CAA-CBA
30	A	820	CLA	C3A-C2A-CAA-CBA
30	A	821	CLA	C2-C3-C5-C6
30	A	821	CLA	C4-C3-C5-C6
30	A	824	CLA	C2A-CAA-CBA-CGA
30	A	825	CLA	CHA-CBD-CGD-O1D
30	A	825	CLA	CHA-CBD-CGD-O2D
30	A	831	CLA	C4-C3-C5-C6
30	A	833	CLA	C2-C3-C5-C6
30	A	833	CLA	C4-C3-C5-C6
30	A	835	CLA	CHA-CBD-CGD-O1D
30	A	835	CLA	CHA-CBD-CGD-O2D
30	A	836	CLA	C2-C3-C5-C6
30	A	836	CLA	C4-C3-C5-C6
30	A	837	CLA	CHA-CBD-CGD-O1D
30	A	837	CLA	CHA-CBD-CGD-O2D
30	A	838	CLA	C1A-C2A-CAA-CBA
30	A	840	CLA	CHA-CBD-CGD-O1D
30	A	840	CLA	CHA-CBD-CGD-O2D
30	A	841	CLA	CHA-CBD-CGD-O1D
30	A	842	CLA	C2A-CAA-CBA-CGA
30	A	842	CLA	C2-C3-C5-C6
30	A	842	CLA	C4-C3-C5-C6
30	A	844	CLA	CBA-CGA-O2A-C1
30	A	844	CLA	O1A-CGA-O2A-C1
30	A	844	CLA	C11-C12-C13-C14
30	B	801	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	B	801	CLA	CHA-CBD-CGD-O2D
30	B	801	CLA	CBD-CGD-O2D-CED
30	B	802	CLA	C2-C3-C5-C6
30	B	802	CLA	C4-C3-C5-C6
30	B	805	CLA	C3A-C2A-CAA-CBA
30	B	806	CLA	C2-C3-C5-C6
30	B	806	CLA	C4-C3-C5-C6
30	B	807	CLA	CHA-CBD-CGD-O1D
30	B	808	CLA	CHA-CBD-CGD-O2D
30	B	810	CLA	C2A-CAA-CBA-CGA
30	B	816	CLA	C1A-C2A-CAA-CBA
30	B	816	CLA	C3A-C2A-CAA-CBA
30	B	818	CLA	C3A-C2A-CAA-CBA
30	B	821	CLA	C2-C3-C5-C6
30	B	821	CLA	C4-C3-C5-C6
30	B	824	CLA	CHA-CBD-CGD-O2D
30	B	827	CLA	C1A-C2A-CAA-CBA
30	B	827	CLA	C3A-C2A-CAA-CBA
30	B	828	CLA	CHA-CBD-CGD-O1D
30	B	828	CLA	CHA-CBD-CGD-O2D
30	B	831	CLA	C2-C3-C5-C6
30	B	831	CLA	C4-C3-C5-C6
30	B	833	CLA	C1A-C2A-CAA-CBA
30	B	833	CLA	C3A-C2A-CAA-CBA
30	B	833	CLA	C2-C3-C5-C6
30	B	833	CLA	C4-C3-C5-C6
30	F	203	CLA	C1A-C2A-CAA-CBA
30	F	203	CLA	C3A-C2A-CAA-CBA
30	1	301	CLA	C1A-C2A-CAA-CBA
30	1	301	CLA	C3A-C2A-CAA-CBA
30	1	304	CLA	C1A-C2A-CAA-CBA
30	1	307	CLA	C1A-C2A-CAA-CBA
30	1	307	CLA	C3A-C2A-CAA-CBA
30	2	303	CLA	C3A-C2A-CAA-CBA
30	2	303	CLA	CBD-CGD-O2D-CED
30	2	305	CLA	C1A-C2A-CAA-CBA
30	2	308	CLA	C3A-C2A-CAA-CBA
30	2	309	CLA	CBD-CGD-O2D-CED
30	3	303	CLA	C1A-C2A-CAA-CBA
30	3	303	CLA	C3A-C2A-CAA-CBA
30	3	303	CLA	CHA-CBD-CGD-O1D
30	3	303	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	3	305	CLA	C1A-C2A-CAA-CBA
30	3	305	CLA	C3A-C2A-CAA-CBA
30	3	305	CLA	C4-C3-C5-C6
30	3	309	CLA	CHA-CBD-CGD-O1D
30	3	309	CLA	CHA-CBD-CGD-O2D
30	4	301	CLA	C2A-CAA-CBA-CGA
30	4	301	CLA	C2-C1-O2A-CGA
30	4	302	CLA	C1A-C2A-CAA-CBA
30	4	302	CLA	C3A-C2A-CAA-CBA
30	4	305	CLA	C2-C3-C5-C6
30	4	305	CLA	C4-C3-C5-C6
30	5	302	CLA	C1A-C2A-CAA-CBA
30	5	302	CLA	C3A-C2A-CAA-CBA
30	5	304	CLA	C1A-C2A-CAA-CBA
30	5	304	CLA	C3A-C2A-CAA-CBA
30	5	307	CLA	C1A-C2A-CAA-CBA
30	5	307	CLA	C3A-C2A-CAA-CBA
30	5	308	CLA	C2-C3-C5-C6
30	5	308	CLA	C4-C3-C5-C6
30	5	311	CLA	CHA-CBD-CGD-O1D
30	5	311	CLA	CHA-CBD-CGD-O2D
30	5	311	CLA	CAD-CBD-CGD-O1D
30	6	304	CLA	C1A-C2A-CAA-CBA
30	6	304	CLA	C3A-C2A-CAA-CBA
30	6	307	CLA	C2-C3-C5-C6
30	6	307	CLA	C4-C3-C5-C6
30	6	309	CLA	C1A-C2A-CAA-CBA
30	6	314	CLA	CHA-CBD-CGD-O2D
30	7	304	CLA	C2-C3-C5-C6
30	7	304	CLA	C4-C3-C5-C6
30	7	307	CLA	C1A-C2A-CAA-CBA
30	7	307	CLA	C3A-C2A-CAA-CBA
30	7	307	CLA	CHA-CBD-CGD-O1D
30	7	307	CLA	CHA-CBD-CGD-O2D
30	7	307	CLA	CBD-CGD-O2D-CED
30	7	310	CLA	C1A-C2A-CAA-CBA
30	7	310	CLA	C3A-C2A-CAA-CBA
30	8	301	CLA	C3A-C2A-CAA-CBA
30	8	302	CLA	C2-C3-C5-C6
30	8	302	CLA	C4-C3-C5-C6
30	8	304	CLA	C2-C3-C5-C6
30	8	304	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	8	305	CLA	C1A-C2A-CAA-CBA
30	9	305	CLA	C1A-C2A-CAA-CBA
30	9	305	CLA	CAD-CBD-CGD-O2D
30	9	305	CLA	CBD-CGD-O2D-CED
30	9	307	CLA	C1A-C2A-CAA-CBA
30	9	307	CLA	C3A-C2A-CAA-CBA
30	9	308	CLA	C1A-C2A-CAA-CBA
30	10	303	CLA	C3A-C2A-CAA-CBA
30	10	305	CLA	C1A-C2A-CAA-CBA
30	10	307	CLA	C1A-C2A-CAA-CBA
30	10	307	CLA	C3A-C2A-CAA-CBA
30	10	309	CLA	C2-C3-C5-C6
30	10	309	CLA	C4-C3-C5-C6
30	10	311	CLA	C1A-C2A-CAA-CBA
30	11	304	CLA	C4-C3-C5-C6
30	11	306	CLA	C1A-C2A-CAA-CBA
30	12	307	CLA	CHA-CBD-CGD-O1D
30	12	307	CLA	CHA-CBD-CGD-O2D
30	12	312	CLA	C1A-C2A-CAA-CBA
30	13	301	CLA	C3A-C2A-CAA-CBA
30	13	303	CLA	C1A-C2A-CAA-CBA
30	13	309	CLA	C1A-C2A-CAA-CBA
30	13	309	CLA	C3A-C2A-CAA-CBA
30	14	303	CLA	C1A-C2A-CAA-CBA
30	14	312	CLA	CHA-CBD-CGD-O1D
30	14	312	CLA	CHA-CBD-CGD-O2D
30	14	313	CLA	C1A-C2A-CAA-CBA
30	14	313	CLA	CHA-CBD-CGD-O1D
30	14	313	CLA	CHA-CBD-CGD-O2D
30	15	302	CLA	C2-C3-C5-C6
30	15	302	CLA	C4-C3-C5-C6
30	15	303	CLA	C3A-C2A-CAA-CBA
30	15	303	CLA	C2-C3-C5-C6
30	15	303	CLA	C4-C3-C5-C6
30	15	305	CLA	CHA-CBD-CGD-O2D
30	15	306	CLA	CHA-CBD-CGD-O1D
30	15	306	CLA	CHA-CBD-CGD-O2D
30	15	308	CLA	C1A-C2A-CAA-CBA
30	15	309	CLA	CBD-CGD-O2D-CED
30	15	310	CLA	CHA-CBD-CGD-O2D
30	15	311	CLA	C1A-C2A-CAA-CBA
30	15	313	CLA	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	15	313	CLA	C2-C3-C5-C6
30	15	313	CLA	C4-C3-C5-C6
30	16	301	CLA	C3A-C2A-CAA-CBA
30	16	303	CLA	C1A-C2A-CAA-CBA
30	16	303	CLA	C3A-C2A-CAA-CBA
30	16	303	CLA	C2-C3-C5-C6
30	16	303	CLA	C4-C3-C5-C6
30	16	306	CLA	C1A-C2A-CAA-CBA
30	16	307	CLA	C1A-C2A-CAA-CBA
30	16	307	CLA	CHA-CBD-CGD-O1D
30	16	307	CLA	CHA-CBD-CGD-O2D
30	16	308	CLA	C1A-C2A-CAA-CBA
30	16	309	CLA	CHA-CBD-CGD-O1D
30	16	309	CLA	CHA-CBD-CGD-O2D
30	16	310	CLA	CBD-CGD-O2D-CED
33	A	847	BCR	C1-C6-C7-C8
33	A	847	BCR	C7-C8-C9-C34
33	A	847	BCR	C21-C22-C23-C24
33	A	847	BCR	C37-C22-C23-C24
33	A	848	BCR	C1-C6-C7-C8
33	A	848	BCR	C11-C12-C13-C35
33	A	848	BCR	C20-C21-C22-C37
33	A	849	BCR	C1-C6-C7-C8
33	A	849	BCR	C7-C8-C9-C10
33	A	849	BCR	C7-C8-C9-C34
33	A	849	BCR	C16-C17-C18-C36
33	A	849	BCR	C37-C22-C23-C24
33	A	850	BCR	C1-C6-C7-C8
33	A	850	BCR	C7-C8-C9-C34
33	A	850	BCR	C20-C21-C22-C37
33	A	850	BCR	C37-C22-C23-C24
33	A	851	BCR	C1-C6-C7-C8
33	A	851	BCR	C20-C21-C22-C37
33	A	851	BCR	C37-C22-C23-C24
33	B	841	BCR	C7-C8-C9-C10
33	B	841	BCR	C23-C24-C25-C30
33	B	842	BCR	C1-C6-C7-C8
33	B	842	BCR	C21-C22-C23-C24
33	B	842	BCR	C37-C22-C23-C24
33	B	843	BCR	C1-C6-C7-C8
33	B	843	BCR	C7-C8-C9-C34
33	B	844	BCR	C7-C8-C9-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	B	844	BCR	C23-C24-C25-C30
33	B	845	BCR	C7-C8-C9-C10
33	B	845	BCR	C7-C8-C9-C34
33	B	845	BCR	C11-C12-C13-C35
33	B	845	BCR	C21-C22-C23-C24
33	B	845	BCR	C37-C22-C23-C24
33	B	846	BCR	C1-C6-C7-C8
33	F	204	BCR	C7-C8-C9-C34
33	F	204	BCR	C37-C22-C23-C24
33	I	101	BCR	C7-C8-C9-C34
33	J	102	BCR	C11-C12-C13-C35
33	J	102	BCR	C20-C21-C22-C37
33	J	102	BCR	C21-C22-C23-C24
33	J	102	BCR	C37-C22-C23-C24
33	J	103	BCR	C6-C7-C8-C9
33	J	103	BCR	C20-C21-C22-C37
33	J	103	BCR	C21-C22-C23-C24
33	L	201	BCR	C7-C8-C9-C34
33	L	201	BCR	C11-C10-C9-C8
33	L	201	BCR	C20-C21-C22-C23
33	L	204	BCR	C6-C7-C8-C9
33	L	204	BCR	C37-C22-C23-C24
33	L	204	BCR	C23-C24-C25-C26
33	L	205	BCR	C1-C6-C7-C8
33	M	101	BCR	C1-C6-C7-C8
33	M	101	BCR	C7-C8-C9-C10
33	M	101	BCR	C21-C22-C23-C24
33	2u	201	BCR	C6-C7-C8-C9
33	2u	201	BCR	C10-C11-C12-C13
33	2u	201	BCR	C11-C12-C13-C14
33	2u	201	BCR	C11-C12-C13-C35
33	2u	201	BCR	C37-C22-C23-C24
34	B	848	LHG	O1-C1-C2-C3
34	B	848	LHG	O10-C23-O8-C6
34	B	848	LHG	C24-C23-O8-C6
34	2	320	LHG	O1-C1-C2-O2
34	2	320	LHG	O1-C1-C2-C3
34	2	320	LHG	C1-C2-C3-O3
34	2	320	LHG	C3-O3-P-O4
34	2	320	LHG	C3-O3-P-O6
34	2	320	LHG	C4-O6-P-O5
34	6	322	LHG	C4-O6-P-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	9	318	LHG	O1-C1-C2-O2
34	9	318	LHG	O1-C1-C2-C3
34	9	318	LHG	C3-O3-P-O5
34	9	318	LHG	C4-O6-P-O5
34	9	318	LHG	C8-C7-O7-C5
35	A	854	LMT	C2'-C1'-O1'-C1
35	A	854	LMT	O5'-C1'-O1'-C1
35	A	855	LMT	C2'-C1'-O1'-C1
35	A	855	LMT	O5'-C1'-O1'-C1
35	A	855	LMT	C2-C1-O1'-C1'
35	11	303	LMT	C2'-C1'-O1'-C1
35	11	303	LMT	O5'-C1'-O1'-C1
35	12	301	LMT	O5'-C1'-O1'-C1
36	A	856	LMG	C11-C10-O7-C8
36	B	847	LMG	C2-C1-O1-C7
36	B	847	LMG	O6-C1-O1-C7
36	B	849	LMG	O6-C1-O1-C7
36	F	205	LMG	C2-C1-O1-C7
36	F	205	LMG	O6-C1-O1-C7
36	2u	204	LMG	C2-C1-O1-C7
36	2u	204	LMG	O6-C1-O1-C7
36	2u	204	LMG	C11-C10-O7-C8
36	3	317	LMG	O6-C1-O1-C7
36	6	301	LMG	O1-C7-C8-O7
36	6	301	LMG	C11-C10-O7-C8
36	8	320	LMG	O1-C7-C8-O7
37	2u	203	A86	C10-C11-C13-O
37	2u	203	A86	C12-C11-C13-O
37	2u	203	A86	C7-C6-C8-C9
37	2u	205	A86	C10-C11-C13-O
37	2u	205	A86	C12-C11-C13-O
37	2u	205	A86	C13-C14-C15-O1
37	1	309	A86	C10-C11-C13-O
37	1	309	A86	C12-C11-C13-O
37	1	309	A86	C5-C6-C8-C9
37	2	302	A86	C11-C10-C9-C8
37	2	302	A86	C10-C11-C13-O
37	2	302	A86	C12-C11-C13-O
37	2	302	A86	C1-C2-C3-C4
37	2	318	A86	C39-C38-O4-C34
37	2	319	A86	C39-C38-O4-C34
37	2	319	A86	C5-C6-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	2	319	A86	C7-C6-C8-C9
37	3	314	A86	C11-C10-C9-C8
37	3	315	A86	C-C1-C24-C25
37	3	315	A86	C2-C1-C24-C25
37	3	315	A86	C10-C11-C13-O
37	3	315	A86	C13-C14-C15-C16
37	3	315	A86	C24-C25-C26-C27
37	3	315	A86	C39-C38-O4-C34
37	3	315	A86	O5-C38-O4-C34
37	3	315	A86	C5-C6-C8-C9
37	3	315	A86	C7-C6-C8-C9
37	4	312	A86	C11-C13-C14-C15
37	4	312	A86	C13-C14-C15-O1
37	4	312	A86	C39-C38-O4-C34
37	4	312	A86	O5-C38-O4-C34
37	4	314	A86	C39-C38-O4-C34
37	4	314	A86	O5-C38-O4-C34
37	4	315	A86	C-C1-C24-C25
37	4	315	A86	C2-C1-C24-C25
37	4	315	A86	C39-C38-O4-C34
37	4	317	A86	C39-C38-O4-C34
37	4	317	A86	O5-C38-O4-C34
37	5	301	A86	C13-C14-C15-C16
37	5	301	A86	C39-C38-O4-C34
37	5	301	A86	O5-C38-O4-C34
37	5	301	A86	C5-C6-C8-C9
37	5	301	A86	C7-C6-C8-C9
37	5	315	A86	C26-C27-C29-C30
37	5	315	A86	C39-C38-O4-C34
37	5	315	A86	O5-C38-O4-C34
37	5	316	A86	C26-C27-C29-C30
37	5	316	A86	C28-C27-C29-C30
37	5	316	A86	C39-C38-O4-C34
37	6	320	A86	C-C1-C24-C25
37	6	320	A86	C2-C1-C24-C25
37	6	320	A86	C26-C27-C29-C30
37	6	320	A86	C28-C27-C29-C30
37	7	315	A86	C-C1-C24-C25
37	7	315	A86	C13-C14-C15-O1
37	7	315	A86	C39-C38-O4-C34
37	7	315	A86	O5-C38-O4-C34
37	7	315	A86	C5-C6-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	7	315	A86	C7-C6-C8-C9
37	7	316	A86	C11-C10-C9-C8
37	7	316	A86	C10-C11-C13-O
37	7	316	A86	C12-C11-C13-O
37	7	316	A86	C5-C6-C8-C9
37	7	316	A86	C7-C6-C8-C9
37	7	319	A86	C13-C14-C15-O1
37	7	319	A86	C39-C38-O4-C34
37	7	319	A86	O5-C38-O4-C34
37	8	315	A86	C-C1-C24-C25
37	8	318	A86	C-C1-C24-C25
37	8	318	A86	C3-C4-C5-C6
37	9	313	A86	C2-C1-C24-C25
37	9	313	A86	O5-C38-O4-C34
37	9	313	A86	C5-C6-C8-C9
37	9	313	A86	C7-C6-C8-C9
37	9	315	A86	C-C1-C24-C25
37	9	315	A86	C2-C1-C24-C25
37	9	315	A86	C11-C10-C9-C8
37	9	316	A86	C26-C27-C29-C30
37	9	316	A86	C28-C27-C29-C30
37	9	316	A86	C39-C38-O4-C34
37	10	301	A86	C39-C38-O4-C34
37	10	302	A86	C12-C11-C13-C14
37	10	315	A86	C-C1-C24-C25
37	10	315	A86	C2-C1-C24-C25
37	10	315	A86	C11-C13-C14-C15
37	10	315	A86	C35-C34-O4-C38
37	10	315	A86	C3-C4-C5-C6
37	10	316	A86	C13-C14-C15-C16
37	10	316	A86	C39-C38-O4-C34
37	10	316	A86	O5-C38-O4-C34
37	10	316	A86	C5-C6-C8-C9
37	10	316	A86	C7-C6-C8-C9
37	10	317	A86	C12-C11-C13-C14
37	11	301	A86	C12-C11-C13-C14
37	11	301	A86	C39-C38-O4-C34
37	11	301	A86	O5-C38-O4-C34
37	11	314	A86	O-C13-C14-C15
37	11	314	A86	C11-C13-C14-C15
37	11	314	A86	C13-C14-C15-C16
37	11	314	A86	C39-C38-O4-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	11	315	A86	C-C1-C24-C25
37	11	315	A86	C2-C1-C24-C25
37	11	315	A86	C26-C27-C29-C30
37	11	315	A86	C28-C27-C29-C30
37	11	315	A86	C33-C34-O4-C38
37	11	315	A86	C39-C38-O4-C34
37	11	315	A86	O5-C38-O4-C34
37	11	315	A86	C5-C6-C8-C9
37	11	315	A86	C7-C6-C8-C9
37	11	316	A86	C13-C14-C15-C16
37	11	316	A86	C1-C2-C3-C4
37	11	316	A86	C24-C25-C26-C27
37	11	316	A86	O5-C38-O4-C34
37	11	316	A86	C5-C6-C8-C9
37	11	316	A86	C7-C6-C8-C9
37	12	314	A86	C-C1-C24-C25
37	12	314	A86	C2-C1-C24-C25
37	12	314	A86	C13-C14-C15-C16
37	12	314	A86	C5-C6-C8-C9
37	12	314	A86	C7-C6-C8-C9
37	12	316	A86	C13-C14-C15-C16
37	12	316	A86	C13-C14-C15-O1
37	12	316	A86	C39-C38-O4-C34
37	12	316	A86	C3-C4-C5-C6
37	12	316	A86	C5-C6-C8-C9
37	12	316	A86	C7-C6-C8-C9
37	13	313	A86	C-C1-C24-C25
37	13	313	A86	C2-C1-C24-C25
37	13	313	A86	C12-C11-C13-C14
37	13	315	A86	C13-C14-C15-C16
37	13	315	A86	C26-C27-C29-C30
37	13	315	A86	C28-C27-C29-C30
37	13	315	A86	C39-C38-O4-C34
37	13	315	A86	O5-C38-O4-C34
37	14	301	A86	C-C1-C24-C25
37	14	301	A86	C2-C1-C24-C25
37	14	301	A86	C39-C38-O4-C34
37	14	301	A86	O5-C38-O4-C34
37	14	314	A86	C-C1-C24-C25
37	14	314	A86	C2-C1-C24-C25
37	14	314	A86	C10-C11-C13-O
37	14	314	A86	C10-C11-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	14	314	A86	C12-C11-C13-O
37	14	315	A86	C-C1-C24-C25
37	14	315	A86	C2-C1-C24-C25
37	14	315	A86	C11-C10-C9-C8
37	14	315	A86	O-C13-C14-C15
37	14	315	A86	C11-C13-C14-C15
37	14	315	A86	C24-C25-C26-C27
37	14	316	A86	C-C1-C24-C25
37	14	316	A86	C13-C14-C15-C16
37	14	317	A86	C-C1-C24-C25
37	14	317	A86	C2-C1-C24-C25
37	14	317	A86	C11-C13-C14-C15
37	14	317	A86	C13-C14-C15-C16
37	14	317	A86	C26-C27-C29-C30
37	14	317	A86	C3-C4-C5-C6
37	14	318	A86	C-C1-C24-C25
37	14	318	A86	C2-C1-C24-C25
37	14	318	A86	O-C13-C14-C15
37	14	318	A86	C11-C13-C14-C15
37	14	318	A86	C13-C14-C15-C16
37	14	318	A86	C24-C25-C26-C27
37	14	319	A86	C10-C11-C13-O
37	14	319	A86	C10-C11-C13-C14
37	14	319	A86	C12-C11-C13-O
37	14	319	A86	C1-C2-C3-C4
37	14	319	A86	C24-C25-C26-C27
37	14	320	A86	C13-C14-C15-O1
37	14	320	A86	O5-C38-O4-C34
37	14	320	A86	C3-C4-C5-C6
37	15	316	A86	C11-C10-C9-C8
37	15	316	A86	C10-C11-C13-O
37	15	316	A86	C10-C11-C13-C14
37	15	316	A86	C12-C11-C13-O
37	15	316	A86	C13-C14-C15-O1
37	15	316	A86	C24-C25-C26-C27
37	15	316	A86	C39-C38-O4-C34
37	15	317	A86	C11-C13-C14-C15
37	15	317	A86	C13-C14-C15-O1
37	15	320	A86	C-C1-C24-C25
37	15	320	A86	C2-C1-C24-C25
37	15	320	A86	C10-C11-C13-O
37	15	320	A86	C12-C11-C13-O

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	15	320	A86	C13-C14-C15-O1
37	15	320	A86	C24-C25-C26-C27
37	15	320	A86	C39-C38-O4-C34
37	15	320	A86	C5-C6-C8-C9
37	15	320	A86	C7-C6-C8-C9
37	15	321	A86	C-C1-C24-C25
37	15	321	A86	C2-C1-C24-C25
37	15	321	A86	C13-C14-C15-C16
37	15	321	A86	C24-C25-C26-C27
37	15	322	A86	O-C13-C14-C15
37	15	322	A86	C11-C13-C14-C15
37	15	322	A86	C13-C14-C15-O1
37	15	322	A86	C26-C27-C29-C30
37	15	322	A86	C28-C27-C29-C30
37	15	322	A86	C3-C4-C5-C6
37	15	322	A86	C7-C6-C8-C9
37	15	323	A86	C-C1-C24-C25
37	15	323	A86	C2-C1-C24-C25
37	15	323	A86	C13-C14-C15-O1
37	15	323	A86	C24-C25-C26-C27
37	15	323	A86	C39-C38-O4-C34
37	15	323	A86	O5-C38-O4-C34
37	16	312	A86	C13-C14-C15-O1
37	16	312	A86	C28-C27-C29-C30
37	16	314	A86	C-C1-C24-C25
37	16	314	A86	C2-C1-C24-C25
37	16	314	A86	C24-C25-C26-C27
37	16	314	A86	C5-C6-C8-C9
37	16	314	A86	C7-C6-C8-C9
38	1	306	KC1	C2A-CAA-CBA-CGA
38	2	306	KC1	C2B-C3B-CAB-CBB
38	2	306	KC1	C4B-C3B-CAB-CBB
38	2	314	KC1	C2A-CAA-CBA-CGA
38	3	308	KC1	C3A-C2A-CAA-CBA
38	3	308	KC1	C2A-CAA-CBA-CGA
38	3	308	KC1	CHA-CBD-CGD-O2D
38	3	311	KC1	C2A-CAA-CBA-CGA
38	4	307	KC1	C3A-C2A-CAA-CBA
38	4	307	KC1	C2A-CAA-CBA-CGA
38	4	308	KC1	C3A-C2A-CAA-CBA
38	4	310	KC1	C2B-C3B-CAB-CBB
38	4	310	KC1	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
38	5	305	KC1	C3A-C2A-CAA-CBA
38	5	305	KC1	C2B-C3B-CAB-CBB
38	5	305	KC1	C4B-C3B-CAB-CBB
38	5	310	KC1	C3A-C2A-CAA-CBA
38	5	310	KC1	C2A-CAA-CBA-CGA
38	5	310	KC1	CHA-CBD-CGD-O1D
38	5	310	KC1	CHA-CBD-CGD-O2D
38	6	308	KC1	C1A-C2A-CAA-CBA
38	6	308	KC1	C2A-CAA-CBA-CGA
38	6	311	KC1	C3A-C2A-CAA-CBA
38	6	311	KC1	C2A-CAA-CBA-CGA
38	6	311	KC1	CHA-CBD-CGD-O1D
38	6	311	KC1	CHA-CBD-CGD-O2D
38	6	312	KC1	C3A-C2A-CAA-CBA
38	7	308	KC1	C2A-CAA-CBA-CGA
38	7	313	KC1	C2B-C3B-CAB-CBB
38	7	313	KC1	C4B-C3B-CAB-CBB
38	8	306	KC1	C3A-C2A-CAA-CBA
38	8	306	KC1	C2A-CAA-CBA-CGA
38	8	307	KC1	C3A-C2A-CAA-CBA
38	8	307	KC1	C2B-C3B-CAB-CBB
38	8	307	KC1	C4B-C3B-CAB-CBB
38	8	307	KC1	C2A-CAA-CBA-CGA
38	8	310	KC1	C2B-C3B-CAB-CBB
38	8	310	KC1	C4B-C3B-CAB-CBB
38	8	312	KC1	C1A-C2A-CAA-CBA
38	8	312	KC1	C2B-C3B-CAB-CBB
38	8	312	KC1	C4B-C3B-CAB-CBB
38	8	312	KC1	C2A-CAA-CBA-CGA
38	8	313	KC1	C3A-C2A-CAA-CBA
38	8	313	KC1	C2B-C3B-CAB-CBB
38	8	314	KC1	C3A-C2A-CAA-CBA
38	8	314	KC1	CHA-CBD-CGD-O1D
38	8	314	KC1	CHA-CBD-CGD-O2D
38	9	304	KC1	C3A-C2A-CAA-CBA
38	9	304	KC1	C2A-CAA-CBA-CGA
38	9	310	KC1	C3A-C2A-CAA-CBA
38	9	310	KC1	C2A-CAA-CBA-CGA
38	9	311	KC1	C2B-C3B-CAB-CBB
38	9	311	KC1	C4B-C3B-CAB-CBB
38	9	311	KC1	C2A-CAA-CBA-CGA
38	9	312	KC1	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
38	10	306	KC1	C2A-CAA-CBA-CGA
38	10	306	KC1	CHA-CBD-CGD-O1D
38	10	306	KC1	CHA-CBD-CGD-O2D
38	10	310	KC1	C3A-C2A-CAA-CBA
38	10	310	KC1	C2A-CAA-CBA-CGA
38	10	312	KC1	C2A-CAA-CBA-CGA
38	11	305	KC1	C3A-C2A-CAA-CBA
38	11	305	KC1	C2A-CAA-CBA-CGA
38	11	307	KC1	C3A-C2A-CAA-CBA
38	11	307	KC1	C2A-CAA-CBA-CGA
38	11	307	KC1	CHA-CBD-CGD-O2D
38	11	311	KC1	C3A-C2A-CAA-CBA
38	11	311	KC1	C2A-CAA-CBA-CGA
38	11	312	KC1	C1A-C2A-CAA-CBA
38	11	312	KC1	C2A-CAA-CBA-CGA
38	12	305	KC1	C1A-C2A-CAA-CBA
38	12	305	KC1	C2A-CAA-CBA-CGA
38	12	309	KC1	C3A-C2A-CAA-CBA
38	12	309	KC1	C2A-CAA-CBA-CGA
38	12	311	KC1	C2A-CAA-CBA-CGA
38	12	313	KC1	C1A-C2A-CAA-CBA
38	12	313	KC1	C3A-C2A-CAA-CBA
38	12	313	KC1	C2A-CAA-CBA-CGA
38	13	305	KC1	C1A-C2A-CAA-CBA
38	13	305	KC1	C2A-CAA-CBA-CGA
38	13	305	KC1	CHA-CBD-CGD-O1D
38	13	305	KC1	CHA-CBD-CGD-O2D
38	13	306	KC1	C1A-C2A-CAA-CBA
38	13	306	KC1	C2A-CAA-CBA-CGA
38	13	308	KC1	C3A-C2A-CAA-CBA
38	13	308	KC1	C2A-CAA-CBA-CGA
38	13	308	KC1	CHA-CBD-CGD-O1D
38	13	308	KC1	CHA-CBD-CGD-O2D
38	13	310	KC1	C1A-C2A-CAA-CBA
38	13	310	KC1	C2B-C3B-CAB-CBB
38	13	310	KC1	C4B-C3B-CAB-CBB
38	13	310	KC1	C2A-CAA-CBA-CGA
38	13	311	KC1	C3A-C2A-CAA-CBA
38	13	312	KC1	C1A-C2A-CAA-CBA
38	13	312	KC1	CAA-CBA-CGA-O1A
38	13	312	KC1	CAA-CBA-CGA-O2A
38	14	306	KC1	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
38	14	308	KC1	C3A-C2A-CAA-CBA
38	14	308	KC1	C2A-CAA-CBA-CGA
38	14	308	KC1	CHA-CBD-CGD-O1D
38	14	308	KC1	CHA-CBD-CGD-O2D
38	14	311	KC1	C3A-C2A-CAA-CBA
38	16	304	KC1	C3A-C2A-CAA-CBA
38	16	304	KC1	C2A-CAA-CBA-CGA
38	16	304	KC1	CAA-CBA-CGA-O1A
38	16	304	KC1	CAA-CBA-CGA-O2A
38	16	311	KC1	C3A-C2A-CAA-CBA
38	16	311	KC1	C2B-C3B-CAB-CBB
38	16	311	KC1	C4B-C3B-CAB-CBB
38	16	311	KC1	C2A-CAA-CBA-CGA
39	1	310	DD6	C-C1-C2-C3
39	1	310	DD6	C-C1-C24-C25
39	1	310	DD6	C9-C10-C11-C12
39	1	310	DD6	C10-C11-C13-C14
39	1	310	DD6	C12-C11-C13-C14
39	1	310	DD6	C4-C5-C6-C7
39	1	310	DD6	C7-C6-C8-C9
39	2	315	DD6	C-C1-C2-C3
39	2	315	DD6	C9-C10-C11-C12
39	2	315	DD6	C9-C10-C11-C13
39	2	315	DD6	C12-C11-C13-C14
39	2	315	DD6	C4-C5-C6-C7
39	2	315	DD6	C5-C6-C8-C9
39	2	315	DD6	C7-C6-C8-C9
39	2	316	DD6	C-C1-C2-C3
39	2	316	DD6	C-C1-C24-C25
39	2	316	DD6	C9-C10-C11-C13
39	2	316	DD6	C12-C11-C13-C14
39	2	316	DD6	C13-C14-C15-O1
39	2	316	DD6	C4-C5-C6-C8
39	2	316	DD6	C7-C6-C8-C9
39	2	317	DD6	C-C1-C2-C3
39	2	317	DD6	C-C1-C24-C25
39	2	317	DD6	C9-C10-C11-C13
39	2	317	DD6	C13-C14-C15-C16
39	2	317	DD6	C5-C6-C8-C9
39	2	317	DD6	C7-C6-C8-C9
39	3	312	DD6	C-C1-C2-C3
39	3	312	DD6	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
39	3	312	DD6	C12-C11-C13-C14
39	3	312	DD6	C4-C5-C6-C7
39	3	313	DD6	C-C1-C2-C3
39	3	313	DD6	C9-C10-C11-C12
39	3	313	DD6	C4-C5-C6-C7
39	3	316	DD6	C-C1-C2-C3
39	3	316	DD6	C9-C10-C11-C12
39	3	316	DD6	C4-C5-C6-C7
39	3	316	DD6	C7-C6-C8-C9
39	4	313	DD6	C-C1-C2-C3
39	4	313	DD6	C-C1-C24-C25
39	4	313	DD6	C9-C10-C11-C12
39	4	313	DD6	C13-C14-C15-C20
39	4	313	DD6	C13-C14-C15-O1
39	4	313	DD6	C4-C5-C6-C8
39	4	313	DD6	C7-C6-C8-C9
39	4	316	DD6	C-C1-C2-C3
39	4	316	DD6	C-C1-C24-C25
39	4	316	DD6	C9-C10-C11-C12
39	4	316	DD6	C9-C10-C11-C13
39	4	316	DD6	C12-C11-C13-C14
39	4	316	DD6	C13-C14-C15-O1
39	4	316	DD6	C4-C5-C6-C7
39	4	316	DD6	C5-C6-C8-C9
39	4	316	DD6	C7-C6-C8-C9
39	5	313	DD6	C-C1-C2-C3
39	5	313	DD6	C-C1-C24-C25
39	5	313	DD6	C9-C10-C11-C12
39	5	313	DD6	C4-C5-C6-C7
39	5	313	DD6	C5-C6-C8-C9
39	5	314	DD6	C-C1-C2-C3
39	5	314	DD6	C-C1-C24-C25
39	5	314	DD6	C9-C10-C11-C12
39	5	314	DD6	C13-C14-C15-O1
39	5	314	DD6	C4-C5-C6-C7
39	5	314	DD6	C5-C6-C8-C9
39	6	303	DD6	C-C1-C2-C3
39	6	303	DD6	C-C1-C24-C25
39	6	303	DD6	C9-C10-C11-C13
39	6	303	DD6	C4-C5-C6-C8
39	6	303	DD6	C7-C6-C8-C9
39	6	318	DD6	C-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
39	6	318	DD6	C-C1-C24-C25
39	6	318	DD6	C9-C10-C11-C12
39	6	318	DD6	C11-C10-C9-C8
39	6	318	DD6	C4-C5-C6-C7
39	6	319	DD6	C-C1-C2-C3
39	6	319	DD6	C-C1-C24-C25
39	6	319	DD6	C4-C5-C6-C8
39	6	319	DD6	C7-C6-C8-C9
39	6	321	DD6	C-C1-C2-C3
39	6	321	DD6	C2-C1-C24-C25
39	6	321	DD6	C9-C10-C11-C12
39	6	321	DD6	C4-C5-C6-C8
39	6	321	DD6	C5-C6-C8-C9
39	6	321	DD6	C7-C6-C8-C9
39	7	302	DD6	C-C1-C2-C3
39	7	302	DD6	C-C1-C24-C25
39	7	302	DD6	C2-C1-C24-C25
39	7	302	DD6	C9-C10-C11-C12
39	7	302	DD6	C24-C25-C26-C27
39	7	302	DD6	C4-C5-C6-C7
39	7	302	DD6	C5-C6-C8-C9
39	7	314	DD6	C-C1-C2-C3
39	7	314	DD6	C-C1-C24-C25
39	7	314	DD6	C9-C10-C11-C12
39	7	314	DD6	C10-C11-C13-C14
39	7	314	DD6	C12-C11-C13-C14
39	7	314	DD6	C4-C5-C6-C7
39	7	314	DD6	C7-C6-C8-C9
39	7	317	DD6	C-C1-C2-C3
39	7	317	DD6	C2-C1-C24-C25
39	7	317	DD6	C9-C10-C11-C12
39	7	317	DD6	C13-C14-C15-C16
39	7	317	DD6	C4-C5-C6-C8
39	7	318	DD6	C-C1-C2-C3
39	7	318	DD6	C-C1-C24-C25
39	7	318	DD6	C2-C1-C24-C25
39	7	318	DD6	C9-C10-C11-C13
39	7	318	DD6	C12-C11-C13-C14
39	7	318	DD6	C4-C5-C6-C7
39	7	318	DD6	C7-C6-C8-C9
39	8	316	DD6	C-C1-C2-C3
39	8	316	DD6	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
39	8	316	DD6	C11-C10-C9-C8
39	8	316	DD6	C12-C11-C13-C14
39	8	316	DD6	C13-C14-C15-C20
39	8	316	DD6	C13-C14-C15-O1
39	8	316	DD6	C4-C5-C6-C7
39	8	316	DD6	C5-C6-C8-C9
39	8	316	DD6	C7-C6-C8-C9
39	8	317	DD6	C-C1-C2-C3
39	8	317	DD6	C9-C10-C11-C13
39	8	317	DD6	C10-C11-C13-C14
39	8	317	DD6	C12-C11-C13-C14
39	8	317	DD6	C4-C5-C6-C7
39	8	317	DD6	C5-C6-C8-C9
39	9	314	DD6	C-C1-C2-C3
39	9	314	DD6	C-C1-C24-C25
39	9	314	DD6	C9-C10-C11-C13
39	9	314	DD6	C10-C11-C13-C14
39	9	314	DD6	C12-C11-C13-C14
39	9	314	DD6	C4-C5-C6-C7
39	10	313	DD6	C-C1-C2-C3
39	10	313	DD6	C-C1-C24-C25
39	10	313	DD6	C9-C10-C11-C13
39	10	313	DD6	C13-C14-C15-O1
39	10	313	DD6	C4-C5-C6-C7
39	10	314	DD6	C-C1-C2-C3
39	10	314	DD6	C9-C10-C11-C12
39	10	314	DD6	C4-C5-C6-C7
39	10	314	DD6	C5-C6-C8-C9
39	10	314	DD6	C7-C6-C8-C9
39	11	313	DD6	C-C1-C2-C3
39	11	313	DD6	C-C1-C24-C25
39	11	313	DD6	C9-C10-C11-C13
39	11	313	DD6	C4-C5-C6-C7
39	11	313	DD6	C7-C6-C8-C9
39	12	315	DD6	C-C1-C2-C3
39	12	315	DD6	C9-C10-C11-C12
39	12	315	DD6	C10-C11-C13-C14
39	12	315	DD6	C12-C11-C13-C14
39	12	315	DD6	C4-C5-C6-C7
39	12	317	DD6	C-C1-C2-C3
39	12	317	DD6	C-C1-C24-C25
39	12	317	DD6	C2-C1-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
39	12	317	DD6	C9-C10-C11-C12
39	12	317	DD6	C9-C10-C11-C13
39	12	317	DD6	C12-C11-C13-C14
39	12	317	DD6	C4-C5-C6-C7
39	12	317	DD6	C5-C6-C8-C9
39	12	317	DD6	C7-C6-C8-C9
39	13	314	DD6	C-C1-C2-C3
39	13	314	DD6	C-C1-C24-C25
39	13	314	DD6	C9-C10-C11-C12
39	13	314	DD6	C12-C11-C13-C14
39	13	314	DD6	C13-C14-C15-O1
39	13	314	DD6	C3-C4-C5-C6
39	13	314	DD6	C4-C5-C6-C7
39	13	314	DD6	C7-C6-C8-C9
39	15	318	DD6	C24-C1-C2-C3
39	15	318	DD6	C-C1-C24-C25
39	15	318	DD6	C9-C10-C11-C13
39	15	318	DD6	C13-C14-C15-C16
39	15	318	DD6	C1-C2-C3-C4
39	15	318	DD6	C4-C5-C6-C7
39	15	318	DD6	C7-C6-C8-C9
39	15	319	DD6	C-C1-C2-C3
39	15	319	DD6	C2-C1-C24-C25
39	15	319	DD6	C9-C10-C11-C12
39	15	319	DD6	C13-C14-C15-C16
39	15	319	DD6	C1-C2-C3-C4
39	15	319	DD6	C4-C5-C6-C7
39	15	319	DD6	C5-C6-C8-C9
39	16	313	DD6	C-C1-C2-C3
39	16	313	DD6	C9-C10-C11-C13
39	16	313	DD6	C13-C14-C15-C20
39	16	313	DD6	C13-C14-C15-O1
39	16	313	DD6	C4-C5-C6-C7
39	16	313	DD6	C5-C6-C8-C9
39	16	313	DD6	C7-C6-C8-C9
37	2u	203	A86	C39-C38-O4-C34
37	2	319	A86	O5-C38-O4-C34
37	10	315	A86	C39-C38-O4-C34
37	10	317	A86	C39-C38-O4-C34
37	14	320	A86	C39-C38-O4-C34
37	15	315	A86	C39-C38-O4-C34
37	15	317	A86	C39-C38-O4-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	15	321	A86	C39-C38-O4-C34
37	15	322	A86	C39-C38-O4-C34
37	16	314	A86	C39-C38-O4-C34
30	A	807	CLA	O1D-CGD-O2D-CED
30	2	303	CLA	O1D-CGD-O2D-CED
35	A	854	LMT	O5B-C1B-O1B-C4'
35	B	852	LMT	C3'-C4'-O1B-C1B
37	2	318	A86	O5-C38-O4-C34
37	5	316	A86	O5-C38-O4-C34
37	9	313	A86	C39-C38-O4-C34
37	9	316	A86	O5-C38-O4-C34
37	10	301	A86	O5-C38-O4-C34
37	11	314	A86	O5-C38-O4-C34
37	11	316	A86	C39-C38-O4-C34
37	14	316	A86	C39-C38-O4-C34
37	14	317	A86	C39-C38-O4-C34
37	15	320	A86	O5-C38-O4-C34
37	15	321	A86	O5-C38-O4-C34
37	15	322	A86	O5-C38-O4-C34
30	F	201	CLA	O1D-CGD-O2D-CED
30	7	307	CLA	O1D-CGD-O2D-CED
30	15	304	CLA	O1D-CGD-O2D-CED
30	15	314	CLA	O1D-CGD-O2D-CED
30	16	310	CLA	O1D-CGD-O2D-CED
30	A	811	CLA	CBD-CGD-O2D-CED
30	A	829	CLA	CBD-CGD-O2D-CED
30	B	822	CLA	CBD-CGD-O2D-CED
30	F	201	CLA	CBD-CGD-O2D-CED
30	6	317	CLA	CBD-CGD-O2D-CED
30	9	309	CLA	CBD-CGD-O2D-CED
30	12	308	CLA	CBD-CGD-O2D-CED
30	14	310	CLA	CBD-CGD-O2D-CED
30	15	304	CLA	CBD-CGD-O2D-CED
30	15	314	CLA	CBD-CGD-O2D-CED
38	2	314	KC1	CBD-CGD-O2D-CED
38	5	312	KC1	CBD-CGD-O2D-CED
30	A	804	CLA	O1A-CGA-O2A-C1
30	B	810	CLA	O1A-CGA-O2A-C1
30	1	304	CLA	O1A-CGA-O2A-C1
30	2	303	CLA	O1A-CGA-O2A-C1
30	7	307	CLA	O1A-CGA-O2A-C1
35	15	301	LMT	O5B-C1B-O1B-C4'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	15	315	A86	O5-C38-O4-C34
38	2	314	KC1	O1D-CGD-O2D-CED
37	2u	203	A86	O5-C38-O4-C34
30	9	305	CLA	O1D-CGD-O2D-CED
30	15	309	CLA	O1D-CGD-O2D-CED
30	A	804	CLA	CBA-CGA-O2A-C1
30	1	304	CLA	CBA-CGA-O2A-C1
30	2	303	CLA	CBA-CGA-O2A-C1
30	7	307	CLA	CBA-CGA-O2A-C1
36	8	319	LMG	C29-C28-O8-C9
30	A	820	CLA	CBD-CGD-O2D-CED
30	A	835	CLA	CBD-CGD-O2D-CED
30	1	302	CLA	CBD-CGD-O2D-CED
30	3	307	CLA	CBD-CGD-O2D-CED
30	8	301	CLA	CBD-CGD-O2D-CED
30	11	310	CLA	CBD-CGD-O2D-CED
38	5	306	KC1	CBD-CGD-O2D-CED
38	8	311	KC1	CBD-CGD-O2D-CED
38	10	306	KC1	CBD-CGD-O2D-CED
38	11	307	KC1	CBD-CGD-O2D-CED
38	13	305	KC1	CBD-CGD-O2D-CED
38	13	306	KC1	CBD-CGD-O2D-CED
37	2u	205	A86	C39-C38-O4-C34
37	2u	205	A86	O5-C38-O4-C34
37	10	302	A86	C39-C38-O4-C34
30	A	806	CLA	O1A-CGA-O2A-C1
30	A	809	CLA	O1A-CGA-O2A-C1
30	A	821	CLA	O1A-CGA-O2A-C1
30	A	843	CLA	O1A-CGA-O2A-C1
30	4	301	CLA	O1A-CGA-O2A-C1
30	7	306	CLA	O1A-CGA-O2A-C1
30	11	304	CLA	O1A-CGA-O2A-C1
30	12	306	CLA	O1A-CGA-O2A-C1
34	9	318	LHG	O10-C23-O8-C6
36	6	301	LMG	O10-C28-O8-C9
36	8	319	LMG	O10-C28-O8-C9
30	B	801	CLA	O1D-CGD-O2D-CED
30	2	309	CLA	O1D-CGD-O2D-CED
37	10	315	A86	O5-C38-O4-C34
37	15	317	A86	O5-C38-O4-C34
30	15	306	CLA	CBD-CGD-O2D-CED
38	7	308	KC1	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	9	318	LHG	O9-C7-O7-C5
36	A	856	LMG	O9-C10-O7-C8
36	B	849	LMG	O9-C10-O7-C8
36	2u	204	LMG	O9-C10-O7-C8
37	14	318	A86	C39-C38-O4-C34
30	A	809	CLA	C3-C5-C6-C7
30	A	810	CLA	C3-C5-C6-C7
30	A	816	CLA	C3-C5-C6-C7
30	A	821	CLA	C3-C5-C6-C7
30	A	822	CLA	C3-C5-C6-C7
30	A	844	CLA	C3-C5-C6-C7
30	B	806	CLA	C3-C5-C6-C7
30	B	808	CLA	C3-C5-C6-C7
30	B	813	CLA	C3-C5-C6-C7
30	B	834	CLA	C3-C5-C6-C7
30	F	202	CLA	C3-C5-C6-C7
30	1	301	CLA	C3-C5-C6-C7
30	2	307	CLA	C3-C5-C6-C7
30	2	310	CLA	C3-C5-C6-C7
30	3	303	CLA	C3-C5-C6-C7
30	3	306	CLA	C3-C5-C6-C7
30	3	307	CLA	C3-C5-C6-C7
30	4	309	CLA	C3-C5-C6-C7
30	5	302	CLA	C3-C5-C6-C7
30	5	303	CLA	C3-C5-C6-C7
30	5	304	CLA	C3-C5-C6-C7
30	6	305	CLA	C3-C5-C6-C7
30	6	307	CLA	C3-C5-C6-C7
30	6	309	CLA	C3-C5-C6-C7
30	6	317	CLA	C3-C5-C6-C7
30	7	303	CLA	C3-C5-C6-C7
30	7	306	CLA	C3-C5-C6-C7
30	7	310	CLA	C3-C5-C6-C7
30	7	311	CLA	C3-C5-C6-C7
30	8	304	CLA	C3-C5-C6-C7
30	9	308	CLA	C3-C5-C6-C7
30	10	304	CLA	C3-C5-C6-C7
30	10	309	CLA	C3-C5-C6-C7
30	11	309	CLA	C3-C5-C6-C7
30	14	303	CLA	C3-C5-C6-C7
30	16	302	CLA	C3-C5-C6-C7
31	B	840	PQN	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	A	806	CLA	CBA-CGA-O2A-C1
30	A	809	CLA	CBA-CGA-O2A-C1
30	A	821	CLA	CBA-CGA-O2A-C1
30	A	843	CLA	CBA-CGA-O2A-C1
30	B	810	CLA	CBA-CGA-O2A-C1
30	4	301	CLA	CBA-CGA-O2A-C1
30	5	309	CLA	CBA-CGA-O2A-C1
30	11	304	CLA	CBA-CGA-O2A-C1
36	6	301	LMG	C29-C28-O8-C9
36	7	320	LMG	C29-C28-O8-C9
37	4	315	A86	O5-C38-O4-C34
37	10	302	A86	O5-C38-O4-C34
30	3	303	CLA	CBD-CGD-O2D-CED
37	12	316	A86	O5-C38-O4-C34
30	14	310	CLA	O1A-CGA-O2A-C1
37	15	316	A86	O5-C38-O4-C34
37	16	314	A86	O5-C38-O4-C34
30	B	811	CLA	C4-C3-C5-C6
30	1	305	CLA	C4-C3-C5-C6
30	2	309	CLA	C4-C3-C5-C6
30	3	301	CLA	C4-C3-C5-C6
30	5	303	CLA	C4-C3-C5-C6
30	A	831	CLA	C2-C3-C5-C6
30	3	301	CLA	C2-C3-C5-C6
30	3	305	CLA	C2-C3-C5-C6
30	11	304	CLA	C2-C3-C5-C6
30	A	823	CLA	CBD-CGD-O2D-CED
30	A	825	CLA	CBD-CGD-O2D-CED
30	A	841	CLA	CBD-CGD-O2D-CED
30	13	302	CLA	CBD-CGD-O2D-CED
38	13	308	KC1	CBD-CGD-O2D-CED
30	A	802	CLA	C2A-CAA-CBA-CGA
30	A	817	CLA	C2A-CAA-CBA-CGA
30	A	825	CLA	C2A-CAA-CBA-CGA
30	A	830	CLA	C2A-CAA-CBA-CGA
30	A	832	CLA	C2A-CAA-CBA-CGA
30	B	823	CLA	C2A-CAA-CBA-CGA
30	1	307	CLA	C2A-CAA-CBA-CGA
30	2	303	CLA	C2A-CAA-CBA-CGA
30	4	306	CLA	C2A-CAA-CBA-CGA
30	6	317	CLA	C2A-CAA-CBA-CGA
30	7	305	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	7	312	CLA	C2A-CAA-CBA-CGA
30	16	310	CLA	C2A-CAA-CBA-CGA
36	3	317	LMG	O10-C28-O8-C9
37	2	302	A86	C39-C38-O4-C34
37	10	317	A86	O5-C38-O4-C34
30	A	811	CLA	C3-C5-C6-C7
30	B	810	CLA	C3-C5-C6-C7
30	1	307	CLA	C3-C5-C6-C7
30	6	314	CLA	C3-C5-C6-C7
30	9	301	CLA	C3-C5-C6-C7
30	9	305	CLA	C3-C5-C6-C7
30	10	308	CLA	C3-C5-C6-C7
30	12	303	CLA	C3-C5-C6-C7
30	14	302	CLA	C3-C5-C6-C7
30	A	815	CLA	CBA-CGA-O2A-C1
30	A	820	CLA	CBA-CGA-O2A-C1
30	B	821	CLA	CBA-CGA-O2A-C1
30	7	306	CLA	CBA-CGA-O2A-C1
30	10	309	CLA	CBA-CGA-O2A-C1
30	12	306	CLA	CBA-CGA-O2A-C1
30	14	302	CLA	CBA-CGA-O2A-C1
36	2u	204	LMG	C29-C28-O8-C9
36	F	205	LMG	C29-C28-O8-C9
37	14	317	A86	O5-C38-O4-C34
30	5	302	CLA	CBD-CGD-O2D-CED
30	9	303	CLA	CBD-CGD-O2D-CED
30	A	829	CLA	O1D-CGD-O2D-CED
30	9	309	CLA	O1D-CGD-O2D-CED
30	14	310	CLA	O1D-CGD-O2D-CED
36	F	205	LMG	O9-C10-O7-C8
30	A	815	CLA	O1A-CGA-O2A-C1
30	B	821	CLA	O1A-CGA-O2A-C1
30	14	302	CLA	O1A-CGA-O2A-C1
30	15	307	CLA	O1A-CGA-O2A-C1
30	16	306	CLA	O1A-CGA-O2A-C1
37	14	316	A86	O5-C38-O4-C34
37	9	315	A86	C3-C4-C5-C6
37	10	302	A86	C3-C4-C5-C6
37	10	316	A86	C24-C25-C26-C27
37	11	314	A86	C11-C10-C9-C8
37	12	316	A86	C24-C25-C26-C27
37	14	315	A86	C3-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	14	317	A86	C24-C25-C26-C27
37	14	318	A86	C3-C4-C5-C6
37	15	322	A86	C11-C10-C9-C8
37	15	323	A86	C1-C2-C3-C4
37	16	314	A86	C11-C10-C9-C8
39	2	317	DD6	C11-C10-C9-C8
39	4	313	DD6	C11-C10-C9-C8
39	6	321	DD6	C1-C2-C3-C4
39	9	314	DD6	C3-C4-C5-C6
39	12	317	DD6	C11-C10-C9-C8
39	13	314	DD6	C11-C10-C9-C8
39	15	318	DD6	C24-C25-C26-C27
39	15	319	DD6	C11-C10-C9-C8
36	8	320	LMG	O6-C5-C6-O5
30	A	810	CLA	CBD-CGD-O2D-CED
30	A	822	CLA	CBD-CGD-O2D-CED
30	B	804	CLA	CBD-CGD-O2D-CED
30	B	809	CLA	CBD-CGD-O2D-CED
30	B	831	CLA	CBD-CGD-O2D-CED
30	3	306	CLA	CBD-CGD-O2D-CED
30	5	303	CLA	CBD-CGD-O2D-CED
30	11	309	CLA	CBD-CGD-O2D-CED
30	12	321	CLA	CBD-CGD-O2D-CED
30	15	303	CLA	CBD-CGD-O2D-CED
38	8	306	KC1	CBD-CGD-O2D-CED
30	6	317	CLA	O1D-CGD-O2D-CED
34	B	848	LHG	O2-C2-C3-O3
34	2	320	LHG	O2-C2-C3-O3
30	B	812	CLA	C3-C5-C6-C7
30	B	821	CLA	C3-C5-C6-C7
30	B	822	CLA	C3-C5-C6-C7
30	B	823	CLA	C3-C5-C6-C7
30	B	824	CLA	C3-C5-C6-C7
30	B	832	CLA	C3-C5-C6-C7
30	2	308	CLA	C3-C5-C6-C7
30	6	310	CLA	C3-C5-C6-C7
30	8	305	CLA	C3-C5-C6-C7
30	16	303	CLA	C3-C5-C6-C7
30	A	829	CLA	CBA-CGA-O2A-C1
30	A	833	CLA	CBA-CGA-O2A-C1
30	A	836	CLA	CBA-CGA-O2A-C1
30	7	303	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	12	312	CLA	CBA-CGA-O2A-C1
30	14	310	CLA	CBA-CGA-O2A-C1
34	9	318	LHG	C24-C23-O8-C6
37	8	315	A86	C39-C38-O4-C34
30	5	309	CLA	O1A-CGA-O2A-C1
30	7	309	CLA	C5-C6-C7-C8
36	B	849	LMG	C11-C10-O7-C8
36	F	205	LMG	C11-C10-O7-C8
36	8	320	LMG	C11-C10-O7-C8
36	8	321	LMG	C11-C10-O7-C8
37	8	315	A86	O5-C38-O4-C34
30	B	802	CLA	CBD-CGD-O2D-CED
30	B	808	CLA	CBD-CGD-O2D-CED
30	B	838	CLA	CBD-CGD-O2D-CED
30	5	311	CLA	CBD-CGD-O2D-CED
30	8	305	CLA	CBD-CGD-O2D-CED
30	13	309	CLA	CBD-CGD-O2D-CED
38	6	311	KC1	CBD-CGD-O2D-CED
38	11	311	KC1	CBD-CGD-O2D-CED
35	9	317	LMT	O5B-C5B-C6B-O6B
36	3	317	LMG	C4-C5-C6-O5
30	A	820	CLA	O1A-CGA-O2A-C1
30	10	309	CLA	O1A-CGA-O2A-C1
36	B	847	LMG	O6-C5-C6-O5
36	F	205	LMG	O6-C5-C6-O5
36	3	317	LMG	O6-C5-C6-O5
30	12	308	CLA	O1D-CGD-O2D-CED
30	5	311	CLA	C3-C5-C6-C7
30	12	312	CLA	C3-C5-C6-C7
30	13	302	CLA	C3-C5-C6-C7
30	B	816	CLA	CBA-CGA-O2A-C1
30	15	307	CLA	CBA-CGA-O2A-C1
30	16	306	CLA	CBA-CGA-O2A-C1
36	3	317	LMG	C29-C28-O8-C9
35	11	303	LMT	O5B-C5B-C6B-O6B
36	A	856	LMG	O6-C5-C6-O5
38	5	310	KC1	CAA-CBA-CGA-O1A
38	6	308	KC1	CAA-CBA-CGA-O1A
38	7	308	KC1	CAA-CBA-CGA-O2A
38	8	313	KC1	CAA-CBA-CGA-O1A
38	11	311	KC1	CAA-CBA-CGA-O1A
38	14	306	KC1	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	9	315	A86	C39-C38-O4-C34
30	A	829	CLA	O1A-CGA-O2A-C1
30	A	836	CLA	O1A-CGA-O2A-C1
30	A	812	CLA	C4-C3-C5-C6
30	B	816	CLA	C4-C3-C5-C6
30	B	838	CLA	C4-C3-C5-C6
30	6	314	CLA	C4-C3-C5-C6
30	9	307	CLA	C4-C3-C5-C6
30	12	302	CLA	C4-C3-C5-C6
30	14	302	CLA	C4-C3-C5-C6
30	A	812	CLA	C2-C3-C5-C6
30	B	816	CLA	C2-C3-C5-C6
30	B	838	CLA	C2-C3-C5-C6
30	6	314	CLA	C2-C3-C5-C6
30	8	305	CLA	C2-C3-C5-C6
30	9	307	CLA	C2-C3-C5-C6
30	12	302	CLA	C2-C3-C5-C6
30	14	302	CLA	C2-C3-C5-C6
30	B	828	CLA	CBD-CGD-O2D-CED
36	F	205	LMG	O10-C28-O8-C9
30	6	314	CLA	C2A-CAA-CBA-CGA
30	8	308	CLA	C2A-CAA-CBA-CGA
30	14	312	CLA	C2A-CAA-CBA-CGA
30	16	307	CLA	C2A-CAA-CBA-CGA
36	6	301	LMG	O6-C5-C6-O5
30	7	303	CLA	O1A-CGA-O2A-C1
30	12	312	CLA	O1A-CGA-O2A-C1
36	7	320	LMG	O6-C1-O1-C7
30	A	811	CLA	O1D-CGD-O2D-CED
37	14	314	A86	C39-C38-O4-C34
30	10	303	CLA	C3-C5-C6-C7
30	A	805	CLA	CBA-CGA-O2A-C1
30	A	823	CLA	CBA-CGA-O2A-C1
30	12	310	CLA	CBA-CGA-O2A-C1
30	13	307	CLA	CBA-CGA-O2A-C1
35	15	301	LMT	O5B-C5B-C6B-O6B
36	8	320	LMG	C4-C5-C6-O5
30	B	822	CLA	O1D-CGD-O2D-CED
38	5	312	KC1	O1D-CGD-O2D-CED
30	A	833	CLA	O1A-CGA-O2A-C1
30	12	310	CLA	O1A-CGA-O2A-C1
38	9	310	KC1	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
38	10	310	KC1	CAA-CBA-CGA-O1A
38	10	310	KC1	CAA-CBA-CGA-O2A
38	11	305	KC1	CAA-CBA-CGA-O2A
38	13	305	KC1	CAA-CBA-CGA-O1A
38	14	306	KC1	CAA-CBA-CGA-O1A
38	14	308	KC1	CAA-CBA-CGA-O1A
38	14	308	KC1	CAA-CBA-CGA-O2A
37	7	319	A86	C35-C34-O4-C38
30	B	826	CLA	CBD-CGD-O2D-CED
30	B	816	CLA	O1A-CGA-O2A-C1
30	A	843	CLA	C3-C5-C6-C7
30	10	305	CLA	C3-C5-C6-C7
30	A	835	CLA	O1D-CGD-O2D-CED
30	A	807	CLA	CBA-CGA-O2A-C1
30	A	811	CLA	CBA-CGA-O2A-C1
30	A	832	CLA	CBA-CGA-O2A-C1
30	B	811	CLA	CBA-CGA-O2A-C1
30	B	813	CLA	CBA-CGA-O2A-C1
30	B	818	CLA	CBA-CGA-O2A-C1
30	B	826	CLA	CBA-CGA-O2A-C1
30	B	829	CLA	CBA-CGA-O2A-C1
30	2u	202	CLA	CBA-CGA-O2A-C1
30	1	301	CLA	CBA-CGA-O2A-C1
30	1	305	CLA	CBA-CGA-O2A-C1
30	2	309	CLA	CBA-CGA-O2A-C1
30	3	301	CLA	CBA-CGA-O2A-C1
30	3	306	CLA	CBA-CGA-O2A-C1
30	3	307	CLA	CBA-CGA-O2A-C1
30	5	308	CLA	CBA-CGA-O2A-C1
30	7	311	CLA	CBA-CGA-O2A-C1
30	8	303	CLA	CBA-CGA-O2A-C1
30	9	309	CLA	CBA-CGA-O2A-C1
30	11	310	CLA	CBA-CGA-O2A-C1
30	15	302	CLA	CBA-CGA-O2A-C1
30	15	304	CLA	CBA-CGA-O2A-C1
30	16	303	CLA	CBA-CGA-O2A-C1
30	B	810	CLA	CBD-CGD-O2D-CED
30	B	839	CLA	CBD-CGD-O2D-CED
30	12	303	CLA	CBD-CGD-O2D-CED
30	12	307	CLA	CBD-CGD-O2D-CED
36	A	856	LMG	C4-C5-C6-O5
37	5	301	A86	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	8	315	A86	C24-C25-C26-C27
37	10	302	A86	C1-C2-C3-C4
37	10	315	A86	C11-C10-C9-C8
37	10	317	A86	C3-C4-C5-C6
37	12	314	A86	C11-C10-C9-C8
37	14	317	A86	C11-C10-C9-C8
37	15	316	A86	C3-C4-C5-C6
37	15	317	A86	C24-C25-C26-C27
39	3	316	DD6	C11-C10-C9-C8
39	4	316	DD6	C24-C25-C26-C27
39	6	319	DD6	C11-C10-C9-C8
30	3	306	CLA	C10-C11-C12-C13
35	12	318	LMT	O5B-C5B-C6B-O6B
30	1	305	CLA	O1A-CGA-O2A-C1
36	B	847	LMG	C4-C5-C6-O5
36	F	205	LMG	C4-C5-C6-O5
37	8	318	A86	C39-C38-O4-C34
38	4	307	KC1	CAA-CBA-CGA-O1A
38	5	310	KC1	CAA-CBA-CGA-O2A
38	6	308	KC1	CAA-CBA-CGA-O2A
38	6	311	KC1	CAA-CBA-CGA-O1A
38	7	308	KC1	CAA-CBA-CGA-O1A
38	7	313	KC1	CAA-CBA-CGA-O2A
38	8	307	KC1	CAA-CBA-CGA-O2A
38	8	313	KC1	CAA-CBA-CGA-O2A
38	9	304	KC1	CAA-CBA-CGA-O2A
38	9	312	KC1	CAA-CBA-CGA-O1A
38	10	312	KC1	CAA-CBA-CGA-O1A
38	10	312	KC1	CAA-CBA-CGA-O2A
38	11	305	KC1	CAA-CBA-CGA-O1A
38	11	307	KC1	CAA-CBA-CGA-O1A
38	11	307	KC1	CAA-CBA-CGA-O2A
38	11	311	KC1	CAA-CBA-CGA-O2A
38	12	313	KC1	CAA-CBA-CGA-O2A
38	13	308	KC1	CAA-CBA-CGA-O1A
38	13	308	KC1	CAA-CBA-CGA-O2A
30	A	811	CLA	C8-C10-C11-C12
30	A	821	CLA	C10-C11-C12-C13
30	A	822	CLA	C8-C10-C11-C12
30	A	829	CLA	C10-C11-C12-C13
30	A	844	CLA	C10-C11-C12-C13
30	B	806	CLA	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	B	838	CLA	C8-C10-C11-C12
30	8	301	CLA	C10-C11-C12-C13
30	10	303	CLA	C15-C16-C17-C18
30	14	302	CLA	C13-C15-C16-C17
34	A	853	LHG	O2-C2-C3-O3
36	B	847	LMG	C28-C29-C30-C31
36	A	856	LMG	C2-C1-O1-C7
36	7	320	LMG	C2-C1-O1-C7
30	B	813	CLA	O1A-CGA-O2A-C1
30	8	303	CLA	O1A-CGA-O2A-C1
30	15	302	CLA	O1A-CGA-O2A-C1
30	B	811	CLA	C2-C3-C5-C6
30	1	305	CLA	C2-C3-C5-C6
30	2	309	CLA	C2-C3-C5-C6
30	5	303	CLA	C2-C3-C5-C6
30	6	309	CLA	C2-C3-C5-C6
30	A	816	CLA	C14-C13-C15-C16
30	A	833	CLA	C11-C10-C8-C9
30	B	828	CLA	C11-C12-C13-C14
30	F	202	CLA	C6-C7-C8-C9
30	1	307	CLA	C6-C7-C8-C9
30	3	307	CLA	C11-C12-C13-C14
30	4	302	CLA	C11-C12-C13-C14
30	10	308	CLA	C11-C10-C8-C9
30	11	309	CLA	C11-C10-C8-C9
30	12	304	CLA	C11-C12-C13-C14
30	16	303	CLA	C11-C12-C13-C14
38	10	306	KC1	O1D-CGD-O2D-CED
30	4	306	CLA	CBD-CGD-O2D-CED
30	5	308	CLA	CBD-CGD-O2D-CED
37	7	319	A86	C33-C34-O4-C38
37	11	315	A86	C35-C34-O4-C38
30	2	305	CLA	C15-C16-C17-C18
31	A	845	PQN	C23-C25-C26-C27
30	A	821	CLA	C2A-CAA-CBA-CGA
30	B	802	CLA	C2A-CAA-CBA-CGA
30	B	837	CLA	C2A-CAA-CBA-CGA
33	B	841	BCR	C7-C8-C9-C34
33	I	101	BCR	C37-C22-C23-C24
33	J	103	BCR	C37-C22-C23-C24
33	L	205	BCR	C7-C8-C9-C34
33	L	205	BCR	C37-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	M	101	BCR	C7-C8-C9-C34
37	1	309	A86	C7-C6-C8-C9
37	2	318	A86	C-C1-C24-C25
37	3	314	A86	C7-C6-C8-C9
37	4	312	A86	C7-C6-C8-C9
37	6	320	A86	C7-C6-C8-C9
37	8	318	A86	C7-C6-C8-C9
37	9	313	A86	C-C1-C24-C25
37	9	316	A86	C-C1-C24-C25
37	10	302	A86	C-C1-C24-C25
37	10	316	A86	C-C1-C24-C25
37	13	315	A86	C-C1-C24-C25
37	14	314	A86	C7-C6-C8-C9
37	14	315	A86	C7-C6-C8-C9
37	14	317	A86	C7-C6-C8-C9
37	14	318	A86	C7-C6-C8-C9
37	14	320	A86	C7-C6-C8-C9
37	15	315	A86	C-C1-C24-C25
37	15	321	A86	C7-C6-C8-C9
37	15	323	A86	C7-C6-C8-C9
37	16	312	A86	C7-C6-C8-C9
39	2	315	DD6	C-C1-C24-C25
39	2	317	DD6	C12-C11-C13-C14
39	3	312	DD6	C-C1-C24-C25
39	3	312	DD6	C7-C6-C8-C9
39	3	313	DD6	C-C1-C24-C25
39	3	313	DD6	C7-C6-C8-C9
39	3	316	DD6	C12-C11-C13-C14
39	4	313	DD6	C12-C11-C13-C14
39	5	313	DD6	C12-C11-C13-C14
39	5	314	DD6	C12-C11-C13-C14
39	6	318	DD6	C7-C6-C8-C9
39	6	321	DD6	C12-C11-C13-C14
39	7	317	DD6	C12-C11-C13-C14
39	7	317	DD6	C7-C6-C8-C9
39	8	316	DD6	C-C1-C24-C25
39	8	317	DD6	C-C1-C24-C25
39	9	314	DD6	C7-C6-C8-C9
39	10	313	DD6	C12-C11-C13-C14
39	10	314	DD6	C-C1-C24-C25
39	10	314	DD6	C12-C11-C13-C14
39	11	313	DD6	C12-C11-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
39	12	315	DD6	C-C1-C24-C25
39	15	318	DD6	C12-C11-C13-C14
39	15	319	DD6	C-C1-C24-C25
39	15	319	DD6	C12-C11-C13-C14
39	15	319	DD6	C7-C6-C8-C9
39	16	313	DD6	C-C1-C24-C25
39	16	313	DD6	C12-C11-C13-C14
33	A	851	BCR	C21-C22-C23-C24
37	2	318	A86	C2-C1-C24-C25
37	6	320	A86	C5-C6-C8-C9
37	7	315	A86	C2-C1-C24-C25
37	8	315	A86	C2-C1-C24-C25
37	8	318	A86	C5-C6-C8-C9
37	9	316	A86	C2-C1-C24-C25
37	10	302	A86	C2-C1-C24-C25
37	10	316	A86	C2-C1-C24-C25
37	13	315	A86	C2-C1-C24-C25
37	14	314	A86	C5-C6-C8-C9
37	14	315	A86	C5-C6-C8-C9
37	14	316	A86	C2-C1-C24-C25
37	14	317	A86	C5-C6-C8-C9
37	14	318	A86	C5-C6-C8-C9
37	14	320	A86	C5-C6-C8-C9
37	15	315	A86	C2-C1-C24-C25
37	15	323	A86	C5-C6-C8-C9
37	16	312	A86	C5-C6-C8-C9
39	3	313	DD6	C10-C11-C13-C14
39	3	316	DD6	C2-C1-C24-C25
39	4	313	DD6	C5-C6-C8-C9
39	6	318	DD6	C10-C11-C13-C14
39	6	319	DD6	C10-C11-C13-C14
39	6	319	DD6	C5-C6-C8-C9
39	7	302	DD6	C10-C11-C13-C14
39	7	318	DD6	C5-C6-C8-C9
39	8	316	DD6	C10-C11-C13-C14
39	16	313	DD6	C10-C11-C13-C14
30	A	832	CLA	O1A-CGA-O2A-C1
30	3	306	CLA	O1A-CGA-O2A-C1
30	16	303	CLA	O1A-CGA-O2A-C1
30	A	804	CLA	C8-C10-C11-C12
30	A	829	CLA	C8-C10-C11-C12
30	A	843	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	B	809	CLA	C13-C15-C16-C17
30	1	307	CLA	C5-C6-C7-C8
30	2	304	CLA	C13-C15-C16-C17
30	2	311	CLA	C10-C11-C12-C13
30	6	306	CLA	C13-C15-C16-C17
30	7	304	CLA	C10-C11-C12-C13
30	8	302	CLA	C13-C15-C16-C17
30	13	302	CLA	C13-C15-C16-C17
30	13	307	CLA	C10-C11-C12-C13
35	A	854	LMT	O5B-C5B-C6B-O6B
35	11	303	LMT	C4B-C5B-C6B-O6B
36	6	301	LMG	C4-C5-C6-O5
38	5	306	KC1	CAA-CBA-CGA-O1A
38	7	313	KC1	CAA-CBA-CGA-O1A
38	8	307	KC1	CAA-CBA-CGA-O1A
38	9	304	KC1	CAA-CBA-CGA-O1A
38	9	310	KC1	CAA-CBA-CGA-O2A
38	9	311	KC1	CAA-CBA-CGA-O1A
38	9	312	KC1	CAA-CBA-CGA-O2A
38	13	305	KC1	CAA-CBA-CGA-O2A
30	3	307	CLA	O1D-CGD-O2D-CED
38	13	305	KC1	O1D-CGD-O2D-CED
30	2u	202	CLA	C3-C5-C6-C7
30	4	302	CLA	C3-C5-C6-C7
30	9	307	CLA	C3-C5-C6-C7
30	A	831	CLA	CBA-CGA-O2A-C1
30	1	307	CLA	CBA-CGA-O2A-C1
30	3	303	CLA	CBA-CGA-O2A-C1
30	8	308	CLA	CBA-CGA-O2A-C1
30	9	303	CLA	CBA-CGA-O2A-C1
30	A	812	CLA	C13-C15-C16-C17
30	A	815	CLA	C5-C6-C7-C8
30	B	806	CLA	C10-C11-C12-C13
30	B	809	CLA	C10-C11-C12-C13
30	B	811	CLA	C5-C6-C7-C8
30	1	305	CLA	C15-C16-C17-C18
30	2	304	CLA	C10-C11-C12-C13
30	2	307	CLA	C10-C11-C12-C13
30	2	311	CLA	C8-C10-C11-C12
30	6	306	CLA	C8-C10-C11-C12
30	6	309	CLA	C10-C11-C12-C13
30	7	310	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	11	308	CLA	C8-C10-C11-C12
30	14	302	CLA	C10-C11-C12-C13
30	15	304	CLA	C8-C10-C11-C12
30	16	302	CLA	C8-C10-C11-C12
30	12	302	CLA	CBD-CGD-O2D-CED
30	A	812	CLA	C5-C6-C7-C8
30	A	816	CLA	C8-C10-C11-C12
30	A	826	CLA	C13-C15-C16-C17
30	A	828	CLA	C10-C11-C12-C13
30	A	839	CLA	C8-C10-C11-C12
30	B	805	CLA	C13-C15-C16-C17
30	B	810	CLA	C10-C11-C12-C13
30	B	813	CLA	C15-C16-C17-C18
30	B	819	CLA	C13-C15-C16-C17
30	B	851	CLA	C13-C15-C16-C17
30	2	301	CLA	C15-C16-C17-C18
30	2	303	CLA	C5-C6-C7-C8
30	3	302	CLA	C10-C11-C12-C13
30	4	306	CLA	C5-C6-C7-C8
30	5	304	CLA	C10-C11-C12-C13
30	5	307	CLA	C10-C11-C12-C13
30	5	309	CLA	C15-C16-C17-C18
30	7	303	CLA	C10-C11-C12-C13
30	7	307	CLA	C15-C16-C17-C18
30	8	302	CLA	C15-C16-C17-C18
30	11	310	CLA	C10-C11-C12-C13
30	12	312	CLA	C8-C10-C11-C12
30	7	311	CLA	O1A-CGA-O2A-C1
30	9	309	CLA	O1A-CGA-O2A-C1
36	5	318	LMG	C28-C29-C30-C31
36	7	320	LMG	C28-C29-C30-C31
30	B	833	CLA	CBD-CGD-O2D-CED
30	A	834	CLA	C5-C6-C7-C8
30	1	302	CLA	C13-C15-C16-C17
30	1	304	CLA	C10-C11-C12-C13
30	3	303	CLA	C8-C10-C11-C12
30	7	306	CLA	C5-C6-C7-C8
30	10	305	CLA	C15-C16-C17-C18
30	7	304	CLA	CBA-CGA-O2A-C1
35	B	852	LMT	O5B-C5B-C6B-O6B
38	3	311	KC1	CAA-CBA-CGA-O2A
38	4	307	KC1	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
38	5	306	KC1	CAA-CBA-CGA-O2A
38	6	311	KC1	CAA-CBA-CGA-O2A
38	9	311	KC1	CAA-CBA-CGA-O2A
38	12	313	KC1	CAA-CBA-CGA-O1A
30	A	803	CLA	C13-C15-C16-C17
30	1	302	CLA	C8-C10-C11-C12
30	7	307	CLA	C13-C15-C16-C17
30	12	306	CLA	C10-C11-C12-C13
30	13	302	CLA	C8-C10-C11-C12
30	15	302	CLA	C5-C6-C7-C8
30	16	301	CLA	C13-C15-C16-C17
30	A	809	CLA	CBD-CGD-O2D-CED
30	15	311	CLA	CBD-CGD-O2D-CED
30	14	303	CLA	C8-C10-C11-C12
30	B	813	CLA	C8-C10-C11-C12
30	3	305	CLA	C8-C10-C11-C12
30	7	303	CLA	C8-C10-C11-C12
30	9	309	CLA	C10-C11-C12-C13
30	15	313	CLA	C5-C6-C7-C8
30	6	309	CLA	C4-C3-C5-C6
30	1	302	CLA	O1D-CGD-O2D-CED
30	A	813	CLA	C6-C7-C8-C10
30	A	844	CLA	C11-C12-C13-C15
30	F	202	CLA	C11-C10-C8-C7
30	1	303	CLA	C12-C13-C15-C16
30	15	304	CLA	C11-C12-C13-C15
30	12	310	CLA	C3-C5-C6-C7
30	13	301	CLA	C3-C5-C6-C7
30	14	307	CLA	C3-C5-C6-C7
30	16	301	CLA	C3-C5-C6-C7
30	A	805	CLA	O1A-CGA-O2A-C1
30	A	823	CLA	O1A-CGA-O2A-C1
30	B	811	CLA	O1A-CGA-O2A-C1
30	2	309	CLA	O1A-CGA-O2A-C1
30	3	303	CLA	O1A-CGA-O2A-C1
30	3	307	CLA	O1A-CGA-O2A-C1
30	8	308	CLA	O1A-CGA-O2A-C1
30	11	310	CLA	O1A-CGA-O2A-C1
36	7	320	LMG	O10-C28-O8-C9
37	1	309	A86	C24-C25-C26-C27
37	2	319	A86	C11-C10-C9-C8
37	3	315	A86	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	4	315	A86	C24-C25-C26-C27
37	7	315	A86	C11-C10-C9-C8
37	7	315	A86	C24-C25-C26-C27
37	9	313	A86	C24-C25-C26-C27
37	9	316	A86	C24-C25-C26-C27
37	10	315	A86	C1-C2-C3-C4
37	10	315	A86	C24-C25-C26-C27
37	10	317	A86	C1-C2-C3-C4
37	11	314	A86	C24-C25-C26-C27
37	11	314	A86	C3-C4-C5-C6
37	11	316	A86	C11-C10-C9-C8
37	13	315	A86	C11-C10-C9-C8
37	13	315	A86	C24-C25-C26-C27
37	13	315	A86	C3-C4-C5-C6
37	14	316	A86	C24-C25-C26-C27
37	14	318	A86	C11-C10-C9-C8
37	14	319	A86	C3-C4-C5-C6
37	15	317	A86	C11-C10-C9-C8
39	4	316	DD6	C1-C2-C3-C4
39	7	318	DD6	C24-C25-C26-C27
39	11	313	DD6	C11-C10-C9-C8
39	11	313	DD6	C3-C4-C5-C6
30	B	817	CLA	C2A-CAA-CBA-CGA
30	2	313	CLA	C2A-CAA-CBA-CGA
30	15	307	CLA	C2A-CAA-CBA-CGA
30	15	314	CLA	C2A-CAA-CBA-CGA
38	5	306	KC1	O1D-CGD-O2D-CED
38	8	311	KC1	O1D-CGD-O2D-CED
38	11	307	KC1	O1D-CGD-O2D-CED
30	A	803	CLA	C10-C11-C12-C13
30	A	805	CLA	C5-C6-C7-C8
30	B	824	CLA	C13-C15-C16-C17
30	F	201	CLA	C15-C16-C17-C18
30	2u	202	CLA	C13-C15-C16-C17
30	5	304	CLA	C13-C15-C16-C17
30	9	307	CLA	C15-C16-C17-C18
30	10	309	CLA	C5-C6-C7-C8
30	11	308	CLA	C10-C11-C12-C13
30	14	302	CLA	C15-C16-C17-C18
35	11	303	LMT	O1'-C1-C2-C3
38	3	304	KC1	CAA-CBA-CGA-O2A
30	A	807	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	2u	202	CLA	O1A-CGA-O2A-C1
36	2u	204	LMG	O10-C28-O8-C9
30	13	301	CLA	CBD-CGD-O2D-CED
38	9	311	KC1	CBD-CGD-O2D-CED
35	A	854	LMT	C4B-C5B-C6B-O6B
36	5	318	LMG	O6-C1-O1-C7
30	B	807	CLA	C15-C16-C17-C18
30	1	303	CLA	C10-C11-C12-C13
30	6	309	CLA	C15-C16-C17-C18
31	A	845	PQN	C25-C26-C27-C28
38	13	306	KC1	O1D-CGD-O2D-CED
35	6	302	LMT	O1'-C1-C2-C3
36	B	849	LMG	C10-C11-C12-C13
33	L	201	BCR	C18-C19-C20-C21
37	12	316	A86	C33-C34-O4-C38
37	12	316	A86	C35-C34-O4-C38
37	14	301	A86	C33-C34-O4-C38
30	1	303	CLA	C3-C5-C6-C7
30	4	303	CLA	C3-C5-C6-C7
30	12	304	CLA	C3-C5-C6-C7
30	A	805	CLA	C8-C10-C11-C12
30	A	809	CLA	C5-C6-C7-C8
30	A	843	CLA	C13-C15-C16-C17
30	F	201	CLA	C13-C15-C16-C17
30	2	304	CLA	C8-C10-C11-C12
30	2	307	CLA	C13-C15-C16-C17
30	2	308	CLA	C10-C11-C12-C13
30	6	304	CLA	C13-C15-C16-C17
30	7	311	CLA	C15-C16-C17-C18
31	B	840	PQN	C23-C25-C26-C27
30	A	817	CLA	CBA-CGA-O2A-C1
30	B	833	CLA	CBA-CGA-O2A-C1
30	A	811	CLA	O1A-CGA-O2A-C1
30	A	831	CLA	O1A-CGA-O2A-C1
30	B	826	CLA	O1A-CGA-O2A-C1
30	1	301	CLA	O1A-CGA-O2A-C1
30	3	301	CLA	O1A-CGA-O2A-C1
30	7	304	CLA	O1A-CGA-O2A-C1
30	13	307	CLA	O1A-CGA-O2A-C1
30	15	304	CLA	O1A-CGA-O2A-C1
37	14	318	A86	O5-C38-O4-C34
30	F	202	CLA	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	5	311	CLA	C8-C10-C11-C12
30	6	310	CLA	C13-C15-C16-C17
30	8	303	CLA	C10-C11-C12-C13
30	9	305	CLA	C10-C11-C12-C13
30	9	308	CLA	C5-C6-C7-C8
30	13	302	CLA	C5-C6-C7-C8
30	13	302	CLA	C10-C11-C12-C13
30	A	820	CLA	O1D-CGD-O2D-CED
30	3	303	CLA	O1D-CGD-O2D-CED
30	11	310	CLA	O1D-CGD-O2D-CED
35	15	301	LMT	C4B-C5B-C6B-O6B
30	B	829	CLA	O1A-CGA-O2A-C1
30	1	307	CLA	O1A-CGA-O2A-C1
36	8	319	LMG	C11-C10-O7-C8
30	A	811	CLA	C10-C11-C12-C13
30	A	820	CLA	C8-C10-C11-C12
30	A	826	CLA	C10-C11-C12-C13
30	A	834	CLA	C15-C16-C17-C18
30	B	825	CLA	C13-C15-C16-C17
30	1	305	CLA	C13-C15-C16-C17
30	2	308	CLA	C13-C15-C16-C17
30	5	309	CLA	C8-C10-C11-C12
30	8	302	CLA	C5-C6-C7-C8
34	2	320	LHG	C4-O6-P-O3
34	5	317	LHG	C3-O3-P-O6
34	6	322	LHG	C4-O6-P-O3
34	9	318	LHG	C4-O6-P-O3
30	12	302	CLA	C3-C5-C6-C7
30	9	308	CLA	CBA-CGA-O2A-C1
30	12	308	CLA	CBA-CGA-O2A-C1
30	B	851	CLA	CBD-CGD-O2D-CED
30	B	832	CLA	C15-C16-C17-C18
30	16	303	CLA	C15-C16-C17-C18
35	9	317	LMT	C4B-C5B-C6B-O6B
38	7	308	KC1	O1D-CGD-O2D-CED
36	6	301	LMG	O9-C10-O7-C8
30	A	833	CLA	C5-C6-C7-C8
30	B	830	CLA	CBD-CGD-O2D-CED
30	8	301	CLA	O1D-CGD-O2D-CED
30	A	806	CLA	C2A-CAA-CBA-CGA
30	B	803	CLA	C2A-CAA-CBA-CGA
30	1	301	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	1	302	CLA	C2A-CAA-CBA-CGA
30	3	301	CLA	C2A-CAA-CBA-CGA
30	5	307	CLA	C2A-CAA-CBA-CGA
30	7	310	CLA	C2A-CAA-CBA-CGA
38	2	314	KC1	CAA-CBA-CGA-O2A
38	6	313	KC1	CAA-CBA-CGA-O1A
38	8	312	KC1	CAA-CBA-CGA-O2A
38	8	314	KC1	CAA-CBA-CGA-O2A
30	A	813	CLA	CBA-CGA-O2A-C1
30	B	819	CLA	CBA-CGA-O2A-C1
30	B	838	CLA	CBA-CGA-O2A-C1
30	6	309	CLA	CBA-CGA-O2A-C1
30	9	302	CLA	CBA-CGA-O2A-C1
30	5	304	CLA	C5-C6-C7-C8
30	13	302	CLA	O1D-CGD-O2D-CED
30	10	305	CLA	C8-C10-C11-C12
37	8	318	A86	C24-C25-C26-C27
37	11	315	A86	C11-C10-C9-C8
37	11	315	A86	C24-C25-C26-C27
37	12	316	A86	C11-C10-C9-C8
37	15	317	A86	C3-C4-C5-C6
37	15	320	A86	C1-C2-C3-C4
37	15	320	A86	C3-C4-C5-C6
37	15	323	A86	C3-C4-C5-C6
39	3	316	DD6	C1-C2-C3-C4
39	7	318	DD6	C11-C10-C9-C8
36	7	320	LMG	C11-C10-O7-C8
33	A	848	BCR	C16-C17-C18-C36
33	B	843	BCR	C20-C21-C22-C37
33	B	844	BCR	C16-C17-C18-C36
33	B	845	BCR	C11-C10-C9-C34
33	B	846	BCR	C11-C10-C9-C34
33	B	846	BCR	C20-C21-C22-C37
33	L	201	BCR	C20-C21-C22-C37
33	L	204	BCR	C20-C21-C22-C37
33	M	101	BCR	C20-C21-C22-C37
39	2	317	DD6	C9-C10-C11-C12
39	2	317	DD6	C4-C5-C6-C7
39	6	319	DD6	C9-C10-C11-C12
39	6	321	DD6	C4-C5-C6-C7
39	8	317	DD6	C9-C10-C11-C12
39	15	318	DD6	C-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
35	16	315	LMT	C5'-C4'-O1B-C1B
36	7	320	LMG	C31-C32-C33-C34
37	2	302	A86	O5-C38-O4-C34
36	14	321	LMG	C4-C5-C6-O5
30	15	306	CLA	O1D-CGD-O2D-CED
38	13	308	KC1	O1D-CGD-O2D-CED
38	1	308	KC1	C2A-CAA-CBA-CGA
38	4	308	KC1	C2A-CAA-CBA-CGA
38	4	310	KC1	C2A-CAA-CBA-CGA
38	13	311	KC1	C2A-CAA-CBA-CGA
38	13	312	KC1	C2A-CAA-CBA-CGA
38	14	311	KC1	C2A-CAA-CBA-CGA
30	B	851	CLA	C16-C17-C18-C20
30	10	308	CLA	C16-C17-C18-C19
30	16	302	CLA	C16-C17-C18-C20
30	16	305	CLA	CBA-CGA-O2A-C1
35	1	311	LMT	C7-C8-C9-C10
36	A	856	LMG	C30-C31-C32-C33
36	6	301	LMG	C13-C14-C15-C16
36	8	320	LMG	C33-C34-C35-C36
38	1	306	KC1	CAA-CBA-CGA-O2A
38	3	311	KC1	CAA-CBA-CGA-O1A
38	6	313	KC1	CAA-CBA-CGA-O2A
38	13	306	KC1	CAA-CBA-CGA-O1A
38	13	306	KC1	CAA-CBA-CGA-O2A
35	12	318	LMT	C4B-C5B-C6B-O6B
30	A	841	CLA	O1D-CGD-O2D-CED
30	B	833	CLA	O1A-CGA-O2A-C1
30	9	302	CLA	O1A-CGA-O2A-C1
34	A	852	LHG	C10-C11-C12-C13
34	A	852	LHG	C12-C13-C14-C15
30	A	828	CLA	C13-C15-C16-C17
30	A	830	CLA	C13-C15-C16-C17
36	B	847	LMG	C29-C30-C31-C32
30	A	823	CLA	O1D-CGD-O2D-CED
30	A	825	CLA	O1D-CGD-O2D-CED
33	A	849	BCR	C16-C17-C18-C19
33	A	850	BCR	C20-C21-C22-C23
33	B	843	BCR	C20-C21-C22-C23
33	B	845	BCR	C12-C13-C14-C15
33	F	204	BCR	C12-C13-C14-C15
33	J	102	BCR	C20-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	J	103	BCR	C11-C10-C9-C8
33	L	204	BCR	C11-C10-C9-C8
35	B	852	LMT	C2'-C1'-O1'-C1
35	9	317	LMT	C2'-C1'-O1'-C1
36	B	849	LMG	C2-C1-O1-C7
36	3	317	LMG	C2-C1-O1-C7
36	5	318	LMG	C2-C1-O1-C7
39	1	310	DD6	C24-C1-C2-C3
39	1	310	DD6	C9-C10-C11-C13
39	2	316	DD6	C24-C1-C2-C3
39	2	317	DD6	C4-C5-C6-C8
39	3	312	DD6	C4-C5-C6-C8
39	3	316	DD6	C9-C10-C11-C13
39	5	313	DD6	C4-C5-C6-C8
39	6	303	DD6	C24-C1-C2-C3
39	6	319	DD6	C9-C10-C11-C13
39	6	321	DD6	C9-C10-C11-C13
39	7	302	DD6	C9-C10-C11-C13
39	8	317	DD6	C24-C1-C2-C3
39	12	315	DD6	C24-C1-C2-C3
39	13	314	DD6	C4-C5-C6-C8
39	15	318	DD6	C4-C5-C6-C8
39	16	313	DD6	C4-C5-C6-C8
30	B	814	CLA	CBA-CGA-O2A-C1
30	B	834	CLA	CBA-CGA-O2A-C1
34	2	320	LHG	C11-C10-C9-C8
36	8	320	LMG	C16-C17-C18-C19
30	B	828	CLA	C10-C11-C12-C13
30	15	309	CLA	C10-C11-C12-C13
30	B	819	CLA	O1A-CGA-O2A-C1
30	B	838	CLA	O1A-CGA-O2A-C1
30	9	303	CLA	O1A-CGA-O2A-C1
30	B	821	CLA	C6-C7-C8-C9
30	5	302	CLA	C16-C17-C18-C19
30	10	308	CLA	C16-C17-C18-C20
30	13	301	CLA	C16-C17-C18-C19
30	16	302	CLA	C16-C17-C18-C19
30	A	826	CLA	C4-C3-C5-C6
30	B	834	CLA	C4-C3-C5-C6
30	9	301	CLA	C4-C3-C5-C6
34	A	852	LHG	C25-C26-C27-C28
36	B	847	LMG	C37-C38-C39-C40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	8	320	LMG	C32-C33-C34-C35
30	B	834	CLA	C2-C3-C5-C6
30	B	826	CLA	C6-C7-C8-C9
30	B	838	CLA	C6-C7-C8-C9
30	F	201	CLA	C6-C7-C8-C9
30	3	307	CLA	C6-C7-C8-C9
30	5	311	CLA	C11-C10-C8-C9
30	12	308	CLA	C11-C12-C13-C14
31	B	840	PQN	C21-C22-C23-C24
36	F	205	LMG	C10-C11-C12-C13
34	A	852	LHG	C32-C33-C34-C35
35	A	854	LMT	C3-C4-C5-C6
38	1	306	KC1	CAA-CBA-CGA-O1A
38	3	304	KC1	CAA-CBA-CGA-O1A
38	8	314	KC1	CAA-CBA-CGA-O1A
30	A	812	CLA	C2A-CAA-CBA-CGA
30	A	813	CLA	C2A-CAA-CBA-CGA
30	A	837	CLA	C2A-CAA-CBA-CGA
30	B	830	CLA	C2A-CAA-CBA-CGA
30	12	302	CLA	C2A-CAA-CBA-CGA
30	A	817	CLA	O1A-CGA-O2A-C1
30	5	308	CLA	O1A-CGA-O2A-C1
33	B	841	BCR	C37-C22-C23-C24
37	2	302	A86	C-C1-C24-C25
37	4	317	A86	C-C1-C24-C25
37	15	316	A86	C7-C6-C8-C9
39	6	303	DD6	C12-C11-C13-C14
39	10	313	DD6	C7-C6-C8-C9
39	12	315	DD6	C7-C6-C8-C9
35	A	854	LMT	C2-C3-C4-C5
36	7	320	LMG	C11-C12-C13-C14
36	8	320	LMG	C12-C13-C14-C15
34	A	852	LHG	O1-C1-C2-C3
34	A	853	LHG	O1-C1-C2-C3
34	5	317	LHG	O1-C1-C2-C3
34	6	322	LHG	O1-C1-C2-C3
33	L	201	BCR	C7-C8-C9-C10
33	L	204	BCR	C21-C22-C23-C24
33	L	205	BCR	C7-C8-C9-C10
37	2	302	A86	C2-C1-C24-C25
37	4	317	A86	C2-C1-C24-C25
37	8	318	A86	C2-C1-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	15	316	A86	C5-C6-C8-C9
37	15	322	A86	C5-C6-C8-C9
39	2	316	DD6	C5-C6-C8-C9
39	4	316	DD6	C2-C1-C24-C25
39	6	303	DD6	C5-C6-C8-C9
39	7	318	DD6	C10-C11-C13-C14
39	11	313	DD6	C10-C11-C13-C14
39	15	318	DD6	C2-C1-C24-C25
30	A	807	CLA	C3-C5-C6-C7
34	B	848	LHG	O9-C7-O7-C5
30	B	806	CLA	C13-C15-C16-C17
30	1	301	CLA	C10-C11-C12-C13
34	9	318	LHG	C24-C25-C26-C27
36	B	849	LMG	C29-C30-C31-C32
36	8	320	LMG	C30-C31-C32-C33
34	B	848	LHG	C7-C8-C9-C10
34	A	852	LHG	C24-C25-C26-C27
36	3	317	LMG	C14-C15-C16-C17
36	3	317	LMG	C29-C30-C31-C32
30	4	304	CLA	C11-C12-C13-C14
30	4	304	CLA	C11-C12-C13-C15
30	16	301	CLA	C16-C17-C18-C20
35	B	852	LMT	O5'-C1'-O1'-C1
36	A	856	LMG	O6-C1-O1-C7
30	3	307	CLA	C10-C11-C12-C13
30	5	308	CLA	C15-C16-C17-C18
30	7	307	CLA	C10-C11-C12-C13
30	11	309	CLA	C8-C10-C11-C12
35	7	321	LMT	C3-C4-C5-C6
36	B	847	LMG	C15-C16-C17-C18
36	B	849	LMG	C12-C13-C14-C15
38	8	306	KC1	O1D-CGD-O2D-CED
34	A	852	LHG	C13-C14-C15-C16
36	8	319	LMG	C36-C37-C38-C39
34	9	318	LHG	C23-C24-C25-C26
36	8	319	LMG	C28-C29-C30-C31
30	A	825	CLA	C8-C10-C11-C12
30	2	301	CLA	C8-C10-C11-C12
30	2	310	CLA	C5-C6-C7-C8
30	3	303	CLA	C5-C6-C7-C8
30	7	310	CLA	C15-C16-C17-C18
30	16	303	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
38	2	314	KC1	CAA-CBA-CGA-O1A
38	8	312	KC1	CAA-CBA-CGA-O1A
30	B	818	CLA	O1A-CGA-O2A-C1
34	9	318	LHG	C11-C10-C9-C8
30	9	303	CLA	O1D-CGD-O2D-CED
30	6	316	CLA	C3-C5-C6-C7
30	8	304	CLA	CBA-CGA-O2A-C1
34	2	320	LHG	C24-C23-O8-C6
34	A	852	LHG	C27-C28-C29-C30
30	5	302	CLA	O1D-CGD-O2D-CED
30	A	802	CLA	C3A-C2A-CAA-CBA
30	A	814	CLA	C3A-C2A-CAA-CBA
30	A	838	CLA	C3A-C2A-CAA-CBA
30	B	813	CLA	C3A-C2A-CAA-CBA
30	B	825	CLA	C3A-C2A-CAA-CBA
30	F	201	CLA	C3A-C2A-CAA-CBA
30	1	304	CLA	C3A-C2A-CAA-CBA
30	2	305	CLA	C3A-C2A-CAA-CBA
30	3	309	CLA	C3A-C2A-CAA-CBA
30	4	306	CLA	C3A-C2A-CAA-CBA
30	4	309	CLA	C3A-C2A-CAA-CBA
30	8	304	CLA	C3A-C2A-CAA-CBA
30	9	305	CLA	C3A-C2A-CAA-CBA
30	9	306	CLA	C3A-C2A-CAA-CBA
30	9	308	CLA	C3A-C2A-CAA-CBA
30	10	305	CLA	C3A-C2A-CAA-CBA
30	10	311	CLA	C3A-C2A-CAA-CBA
30	11	306	CLA	C3A-C2A-CAA-CBA
30	13	303	CLA	C3A-C2A-CAA-CBA
30	13	304	CLA	C3A-C2A-CAA-CBA
30	14	303	CLA	C3A-C2A-CAA-CBA
30	14	313	CLA	C3A-C2A-CAA-CBA
30	15	305	CLA	C3A-C2A-CAA-CBA
30	15	308	CLA	C3A-C2A-CAA-CBA
30	15	311	CLA	C3A-C2A-CAA-CBA
30	15	312	CLA	C3A-C2A-CAA-CBA
30	16	306	CLA	C3A-C2A-CAA-CBA
30	16	307	CLA	C3A-C2A-CAA-CBA
30	16	308	CLA	C3A-C2A-CAA-CBA
30	16	309	CLA	C3A-C2A-CAA-CBA
30	6	307	CLA	C10-C11-C12-C13
37	11	314	A86	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
39	3	312	DD6	C24-C25-C26-C27
35	11	303	LMT	C2-C1-O1'-C1'
35	A	855	LMT	C2-C3-C4-C5
36	B	847	LMG	C23-C24-C25-C26
30	A	810	CLA	O1D-CGD-O2D-CED
30	12	321	CLA	O1D-CGD-O2D-CED
36	14	321	LMG	O10-C28-O8-C9
30	A	820	CLA	C16-C17-C18-C20
36	3	317	LMG	C13-C14-C15-C16
36	14	321	LMG	C7-C8-C9-O8
36	3	317	LMG	C12-C13-C14-C15
33	B	844	BCR	C14-C15-C16-C17
30	3	305	CLA	C3-C5-C6-C7
30	10	307	CLA	C3-C5-C6-C7
36	8	319	LMG	C10-C11-C12-C13
30	12	308	CLA	O1A-CGA-O2A-C1
30	A	818	CLA	C4-C3-C5-C6
30	B	822	CLA	C4-C3-C5-C6
30	3	302	CLA	C4-C3-C5-C6
30	12	302	CLA	CBA-CGA-O2A-C1
30	13	301	CLA	CBA-CGA-O2A-C1
30	A	818	CLA	C2-C3-C5-C6
30	B	822	CLA	C2-C3-C5-C6
30	9	301	CLA	C2-C3-C5-C6
35	16	315	LMT	C3'-C4'-O1B-C1B
30	A	819	CLA	C2A-CAA-CBA-CGA
34	A	853	LHG	O1-C1-C2-O2
34	B	848	LHG	O1-C1-C2-O2
36	8	321	LMG	C28-C29-C30-C31
30	9	308	CLA	O1A-CGA-O2A-C1
30	7	304	CLA	C16-C17-C18-C20
30	B	811	CLA	C10-C11-C12-C13
30	B	829	CLA	C15-C16-C17-C18
30	11	304	CLA	C3-C5-C6-C7
36	6	301	LMG	C12-C13-C14-C15
30	A	813	CLA	O1A-CGA-O2A-C1
30	B	814	CLA	O1A-CGA-O2A-C1
30	B	834	CLA	O1A-CGA-O2A-C1
30	16	305	CLA	O1A-CGA-O2A-C1
35	11	303	LMT	C7-C8-C9-C10
36	A	856	LMG	C12-C13-C14-C15
36	3	317	LMG	C32-C33-C34-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	9	315	A86	O5-C38-O4-C34
36	8	321	LMG	O9-C10-O7-C8
30	A	815	CLA	C2-C1-O2A-CGA
30	1	302	CLA	C2-C1-O2A-CGA
36	B	849	LMG	C30-C31-C32-C33
35	8	322	LMT	C7-C8-C9-C10
30	13	301	CLA	C16-C17-C18-C20
33	A	847	BCR	C5-C6-C7-C8
33	A	848	BCR	C5-C6-C7-C8
33	A	849	BCR	C5-C6-C7-C8
33	A	850	BCR	C5-C6-C7-C8
33	A	850	BCR	C23-C24-C25-C26
33	A	850	BCR	C23-C24-C25-C30
33	A	851	BCR	C5-C6-C7-C8
33	A	851	BCR	C23-C24-C25-C26
33	B	841	BCR	C5-C6-C7-C8
33	B	841	BCR	C23-C24-C25-C26
33	B	842	BCR	C5-C6-C7-C8
33	B	843	BCR	C5-C6-C7-C8
33	B	844	BCR	C23-C24-C25-C26
33	B	846	BCR	C5-C6-C7-C8
33	B	846	BCR	C23-C24-C25-C26
33	B	846	BCR	C23-C24-C25-C30
33	J	102	BCR	C1-C6-C7-C8
33	J	102	BCR	C5-C6-C7-C8
33	J	103	BCR	C1-C6-C7-C8
33	J	103	BCR	C5-C6-C7-C8
33	J	103	BCR	C23-C24-C25-C26
33	J	103	BCR	C23-C24-C25-C30
33	L	201	BCR	C23-C24-C25-C26
33	L	201	BCR	C23-C24-C25-C30
33	L	204	BCR	C23-C24-C25-C30
33	L	205	BCR	C5-C6-C7-C8
33	M	101	BCR	C5-C6-C7-C8
33	2u	201	BCR	C1-C6-C7-C8
33	2u	201	BCR	C5-C6-C7-C8
33	2u	201	BCR	C23-C24-C25-C26
33	2u	201	BCR	C23-C24-C25-C30
30	A	819	CLA	CBA-CGA-O2A-C1
30	B	805	CLA	CBA-CGA-O2A-C1
30	1	302	CLA	CBA-CGA-O2A-C1
30	15	313	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	8	320	LMG	C29-C28-O8-C9
30	A	803	CLA	C15-C16-C17-C18
30	A	820	CLA	C13-C15-C16-C17
30	9	308	CLA	C10-C11-C12-C13
30	12	312	CLA	C10-C11-C12-C13
34	A	852	LHG	C8-C7-O7-C5
36	2u	204	LMG	O6-C5-C6-O5
30	A	833	CLA	C8-C10-C11-C12
30	A	834	CLA	C10-C11-C12-C13
30	B	838	CLA	O1D-CGD-O2D-CED
35	16	315	LMT	O5'-C5'-C6'-O6'
35	B	852	LMT	C6-C7-C8-C9
30	A	806	CLA	C4-C3-C5-C6
30	6	316	CLA	C4-C3-C5-C6
30	7	306	CLA	C4-C3-C5-C6
30	A	804	CLA	C11-C12-C13-C15
30	A	806	CLA	C2-C3-C5-C6
30	A	809	CLA	C6-C7-C8-C10
30	A	812	CLA	C11-C12-C13-C15
30	A	816	CLA	C12-C13-C15-C16
30	A	826	CLA	C2-C3-C5-C6
30	A	834	CLA	C2-C3-C5-C6
30	B	826	CLA	C6-C7-C8-C10
30	3	302	CLA	C2-C3-C5-C6
30	3	302	CLA	C6-C7-C8-C10
30	3	307	CLA	C6-C7-C8-C10
30	5	311	CLA	C11-C10-C8-C7
30	6	304	CLA	C12-C13-C15-C16
30	6	307	CLA	C11-C10-C8-C7
30	6	316	CLA	C2-C3-C5-C6
30	7	305	CLA	C2-C3-C5-C6
30	10	308	CLA	C11-C10-C8-C7
30	11	304	CLA	C12-C13-C15-C16
30	12	304	CLA	C11-C12-C13-C15
30	13	302	CLA	C6-C7-C8-C10
30	16	302	CLA	C2-C3-C5-C6
30	16	303	CLA	C11-C12-C13-C15
30	8	304	CLA	O1A-CGA-O2A-C1
30	15	313	CLA	O1A-CGA-O2A-C1
34	6	322	LHG	C11-C10-C9-C8
30	A	820	CLA	C15-C16-C17-C18
30	A	833	CLA	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	B	806	CLA	C5-C6-C7-C8
30	10	305	CLA	C13-C15-C16-C17
37	7	315	A86	C1-C2-C3-C4
37	7	315	A86	C3-C4-C5-C6
37	7	316	A86	C24-C25-C26-C27
37	11	316	A86	C3-C4-C5-C6
37	14	301	A86	C24-C25-C26-C27
39	2	315	DD6	C24-C25-C26-C27
39	6	321	DD6	C11-C10-C9-C8
39	8	316	DD6	C3-C4-C5-C6
30	B	809	CLA	O1D-CGD-O2D-CED
38	6	311	KC1	O1D-CGD-O2D-CED
36	8	319	LMG	O9-C10-O7-C8
30	A	825	CLA	CBA-CGA-O2A-C1
30	4	305	CLA	CBA-CGA-O2A-C1
30	5	311	CLA	CBA-CGA-O2A-C1
30	10	308	CLA	CBA-CGA-O2A-C1
36	14	321	LMG	C29-C28-O8-C9
35	16	315	LMT	C7-C8-C9-C10
36	B	849	LMG	C14-C15-C16-C17
36	B	849	LMG	C15-C16-C17-C18
30	A	818	CLA	C2A-CAA-CBA-CGA
30	B	829	CLA	C2A-CAA-CBA-CGA
30	5	308	CLA	C2A-CAA-CBA-CGA
30	9	302	CLA	C2A-CAA-CBA-CGA
30	9	303	CLA	C2A-CAA-CBA-CGA
30	13	301	CLA	C2A-CAA-CBA-CGA
30	13	309	CLA	C2A-CAA-CBA-CGA
30	B	809	CLA	C15-C16-C17-C18
30	B	833	CLA	C8-C10-C11-C12
30	B	834	CLA	C5-C6-C7-C8
30	B	834	CLA	C10-C11-C12-C13
30	12	312	CLA	C15-C16-C17-C18
31	A	845	PQN	C20-C21-C22-C23
35	A	854	LMT	C7-C8-C9-C10
30	A	818	CLA	C5-C6-C7-C8
30	B	804	CLA	O1D-CGD-O2D-CED
30	13	309	CLA	O1D-CGD-O2D-CED
30	B	808	CLA	C13-C15-C16-C17
38	1	308	KC1	C2B-C3B-CAB-CBB
38	2	312	KC1	C2B-C3B-CAB-CBB
38	2	314	KC1	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
38	3	304	KC1	C2B-C3B-CAB-CBB
38	3	308	KC1	C2B-C3B-CAB-CBB
38	3	311	KC1	C2B-C3B-CAB-CBB
38	4	307	KC1	C2B-C3B-CAB-CBB
38	5	306	KC1	C2B-C3B-CAB-CBB
38	5	312	KC1	C2B-C3B-CAB-CBB
38	6	308	KC1	C2B-C3B-CAB-CBB
38	6	311	KC1	C2B-C3B-CAB-CBB
38	6	313	KC1	C2B-C3B-CAB-CBB
38	8	306	KC1	C2B-C3B-CAB-CBB
38	8	311	KC1	C2B-C3B-CAB-CBB
38	8	314	KC1	C2B-C3B-CAB-CBB
38	9	304	KC1	C2B-C3B-CAB-CBB
38	9	310	KC1	C2B-C3B-CAB-CBB
38	9	312	KC1	C2B-C3B-CAB-CBB
38	10	306	KC1	C2B-C3B-CAB-CBB
38	11	305	KC1	C2B-C3B-CAB-CBB
38	11	307	KC1	C2B-C3B-CAB-CBB
38	11	312	KC1	C2B-C3B-CAB-CBB
38	12	305	KC1	C2B-C3B-CAB-CBB
38	12	313	KC1	C2B-C3B-CAB-CBB
38	13	308	KC1	C2B-C3B-CAB-CBB
38	13	312	KC1	C2B-C3B-CAB-CBB
38	14	311	KC1	C2B-C3B-CAB-CBB
38	16	304	KC1	C2B-C3B-CAB-CBB
30	11	308	CLA	C3-C5-C6-C7
38	10	310	KC1	CBD-CGD-O2D-CED
30	A	824	CLA	CBA-CGA-O2A-C1
30	15	309	CLA	CBA-CGA-O2A-C1
30	B	821	CLA	C6-C7-C8-C10
35	9	317	LMT	O5'-C1'-O1'-C1
30	A	828	CLA	C15-C16-C17-C18
30	7	309	CLA	C13-C15-C16-C17
30	B	831	CLA	O1D-CGD-O2D-CED
30	5	303	CLA	O1D-CGD-O2D-CED
30	11	309	CLA	O1D-CGD-O2D-CED
36	8	319	LMG	C35-C36-C37-C38
36	14	321	LMG	C29-C30-C31-C32
34	B	848	LHG	C8-C7-O7-C5
35	15	301	LMT	C3-C4-C5-C6
36	B	847	LMG	C16-C17-C18-C19
36	B	847	LMG	C40-C41-C42-C43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	7	320	LMG	C33-C34-C35-C36
37	14	314	A86	O5-C38-O4-C34
38	2	312	KC1	C4B-C3B-CAB-CBB
38	2	314	KC1	C4B-C3B-CAB-CBB
38	3	304	KC1	C4B-C3B-CAB-CBB
38	3	308	KC1	C4B-C3B-CAB-CBB
38	3	311	KC1	C4B-C3B-CAB-CBB
38	4	307	KC1	C4B-C3B-CAB-CBB
38	5	306	KC1	C4B-C3B-CAB-CBB
38	5	312	KC1	C4B-C3B-CAB-CBB
38	6	308	KC1	C4B-C3B-CAB-CBB
38	6	311	KC1	C4B-C3B-CAB-CBB
38	6	313	KC1	C4B-C3B-CAB-CBB
38	8	306	KC1	C4B-C3B-CAB-CBB
38	8	311	KC1	C4B-C3B-CAB-CBB
38	8	313	KC1	C4B-C3B-CAB-CBB
38	8	314	KC1	C4B-C3B-CAB-CBB
38	9	304	KC1	C4B-C3B-CAB-CBB
38	9	310	KC1	C4B-C3B-CAB-CBB
38	9	312	KC1	C4B-C3B-CAB-CBB
38	10	306	KC1	C4B-C3B-CAB-CBB
38	11	305	KC1	C4B-C3B-CAB-CBB
38	11	307	KC1	C4B-C3B-CAB-CBB
38	11	312	KC1	C4B-C3B-CAB-CBB
38	12	305	KC1	C4B-C3B-CAB-CBB
38	12	313	KC1	C4B-C3B-CAB-CBB
38	13	312	KC1	C4B-C3B-CAB-CBB
38	14	311	KC1	C4B-C3B-CAB-CBB
38	16	304	KC1	C4B-C3B-CAB-CBB
30	A	810	CLA	C13-C15-C16-C17
30	B	811	CLA	C8-C10-C11-C12
30	B	822	CLA	C10-C11-C12-C13
30	5	308	CLA	C8-C10-C11-C12
30	15	302	CLA	C10-C11-C12-C13
30	A	826	CLA	CBD-CGD-O2D-CED
30	1	301	CLA	CBD-CGD-O2D-CED
30	1	302	CLA	O1A-CGA-O2A-C1
30	A	833	CLA	C3-C5-C6-C7
36	A	856	LMG	C31-C32-C33-C34
36	B	847	LMG	C32-C33-C34-C35
30	8	303	CLA	C13-C15-C16-C17
36	F	205	LMG	O7-C8-C9-O8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	8	319	LMG	O7-C8-C9-O8
30	13	301	CLA	O1A-CGA-O2A-C1
30	B	851	CLA	C16-C17-C18-C19
30	1	307	CLA	C15-C16-C17-C18
30	6	305	CLA	C13-C15-C16-C17
30	8	301	CLA	C8-C10-C11-C12
30	12	302	CLA	C15-C16-C17-C18
30	A	834	CLA	C4-C3-C5-C6
30	2	303	CLA	C4-C3-C5-C6
30	5	309	CLA	C4-C3-C5-C6
30	7	305	CLA	C4-C3-C5-C6
30	16	302	CLA	C4-C3-C5-C6
30	A	804	CLA	C11-C12-C13-C14
30	A	812	CLA	C11-C12-C13-C14
30	A	813	CLA	C6-C7-C8-C9
30	A	825	CLA	C11-C10-C8-C9
30	A	839	CLA	C11-C12-C13-C14
30	A	842	CLA	C14-C13-C15-C16
30	1	303	CLA	C14-C13-C15-C16
30	3	302	CLA	C6-C7-C8-C9
30	6	304	CLA	C14-C13-C15-C16
30	7	309	CLA	C6-C7-C8-C9
30	7	311	CLA	C6-C7-C8-C9
30	8	301	CLA	C11-C12-C13-C14
30	13	302	CLA	C6-C7-C8-C9
30	16	303	CLA	C11-C10-C8-C9
35	7	321	LMT	O5B-C5B-C6B-O6B
36	8	319	LMG	O6-C5-C6-O5
30	A	828	CLA	C3-C5-C6-C7
30	8	301	CLA	C3-C5-C6-C7
30	B	821	CLA	C2A-CAA-CBA-CGA
30	B	826	CLA	C2A-CAA-CBA-CGA
30	9	308	CLA	C2A-CAA-CBA-CGA
30	10	307	CLA	C2A-CAA-CBA-CGA
30	16	301	CLA	C2A-CAA-CBA-CGA
36	8	320	LMG	C11-C12-C13-C14
37	8	318	A86	O5-C38-O4-C34
37	10	315	A86	C7-C6-C8-C9
37	11	314	A86	C7-C6-C8-C9
37	14	319	A86	C7-C6-C8-C9
38	11	311	KC1	O1D-CGD-O2D-CED
30	B	805	CLA	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	B	826	CLA	C13-C15-C16-C17
30	7	307	CLA	C8-C10-C11-C12
30	11	309	CLA	C10-C11-C12-C13
33	A	847	BCR	C7-C8-C9-C10
33	A	850	BCR	C21-C22-C23-C24
33	B	846	BCR	C21-C22-C23-C24
37	10	315	A86	C5-C6-C8-C9
37	11	314	A86	C5-C6-C8-C9
39	3	316	DD6	C5-C6-C8-C9
39	12	317	DD6	C10-C11-C13-C14
30	A	819	CLA	O1A-CGA-O2A-C1
30	4	305	CLA	O1A-CGA-O2A-C1
30	6	309	CLA	O1A-CGA-O2A-C1
30	A	804	CLA	C1A-C2A-CAA-CBA
30	A	810	CLA	C1A-C2A-CAA-CBA
30	A	816	CLA	C1A-C2A-CAA-CBA
30	A	819	CLA	C1A-C2A-CAA-CBA
30	A	825	CLA	C1A-C2A-CAA-CBA
30	A	833	CLA	C1A-C2A-CAA-CBA
30	A	835	CLA	C1A-C2A-CAA-CBA
30	A	840	CLA	C1A-C2A-CAA-CBA
30	A	842	CLA	C1A-C2A-CAA-CBA
30	B	805	CLA	C1A-C2A-CAA-CBA
30	B	813	CLA	C1A-C2A-CAA-CBA
30	B	814	CLA	C1A-C2A-CAA-CBA
30	B	818	CLA	C1A-C2A-CAA-CBA
30	B	826	CLA	C1A-C2A-CAA-CBA
30	B	828	CLA	C1A-C2A-CAA-CBA
30	B	829	CLA	C1A-C2A-CAA-CBA
30	B	836	CLA	C1A-C2A-CAA-CBA
30	B	838	CLA	C1A-C2A-CAA-CBA
30	B	839	CLA	C1A-C2A-CAA-CBA
30	F	201	CLA	C1A-C2A-CAA-CBA
30	2	303	CLA	C1A-C2A-CAA-CBA
30	2	308	CLA	C1A-C2A-CAA-CBA
30	3	301	CLA	C1A-C2A-CAA-CBA
30	3	306	CLA	C1A-C2A-CAA-CBA
30	3	309	CLA	C1A-C2A-CAA-CBA
30	4	305	CLA	C1A-C2A-CAA-CBA
30	4	306	CLA	C1A-C2A-CAA-CBA
30	5	308	CLA	C1A-C2A-CAA-CBA
30	5	309	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	5	311	CLA	C1A-C2A-CAA-CBA
30	6	314	CLA	C1A-C2A-CAA-CBA
30	6	317	CLA	C1A-C2A-CAA-CBA
30	7	305	CLA	C1A-C2A-CAA-CBA
30	8	301	CLA	C1A-C2A-CAA-CBA
30	8	303	CLA	C1A-C2A-CAA-CBA
30	8	304	CLA	C1A-C2A-CAA-CBA
30	9	302	CLA	C1A-C2A-CAA-CBA
30	9	303	CLA	C1A-C2A-CAA-CBA
30	9	306	CLA	C1A-C2A-CAA-CBA
30	9	309	CLA	C1A-C2A-CAA-CBA
30	10	303	CLA	C1A-C2A-CAA-CBA
30	10	308	CLA	C1A-C2A-CAA-CBA
30	10	309	CLA	C1A-C2A-CAA-CBA
30	11	309	CLA	C1A-C2A-CAA-CBA
30	11	310	CLA	C1A-C2A-CAA-CBA
30	12	308	CLA	C1A-C2A-CAA-CBA
30	12	310	CLA	C1A-C2A-CAA-CBA
30	13	301	CLA	C1A-C2A-CAA-CBA
30	13	304	CLA	C1A-C2A-CAA-CBA
30	13	307	CLA	C1A-C2A-CAA-CBA
30	14	305	CLA	C1A-C2A-CAA-CBA
30	14	312	CLA	C1A-C2A-CAA-CBA
30	15	302	CLA	C1A-C2A-CAA-CBA
30	15	303	CLA	C1A-C2A-CAA-CBA
30	15	305	CLA	C1A-C2A-CAA-CBA
30	15	307	CLA	C1A-C2A-CAA-CBA
30	15	309	CLA	C1A-C2A-CAA-CBA
30	15	312	CLA	C1A-C2A-CAA-CBA
30	15	314	CLA	C1A-C2A-CAA-CBA
30	16	301	CLA	C1A-C2A-CAA-CBA
30	16	309	CLA	C1A-C2A-CAA-CBA
30	16	310	CLA	C1A-C2A-CAA-CBA
30	5	302	CLA	C16-C17-C18-C20
30	16	301	CLA	C16-C17-C18-C19
37	14	315	A86	C1-C2-C3-C4
37	15	322	A86	C24-C25-C26-C27
39	2	315	DD6	C11-C10-C9-C8
39	3	312	DD6	C11-C10-C9-C8
39	7	302	DD6	C3-C4-C5-C6
30	A	822	CLA	O1D-CGD-O2D-CED
30	A	821	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	B	813	CLA	C10-C11-C12-C13
30	2	307	CLA	C15-C16-C17-C18
30	5	308	CLA	C13-C15-C16-C17
30	9	308	CLA	C13-C15-C16-C17
30	B	838	CLA	C3-C5-C6-C7
30	3	306	CLA	O1D-CGD-O2D-CED
30	15	303	CLA	O1D-CGD-O2D-CED
30	A	825	CLA	O1A-CGA-O2A-C1
35	B	852	LMT	C1-C2-C3-C4
30	B	837	CLA	C5-C6-C7-C8
30	L	202	CLA	C10-C11-C12-C13
30	10	307	CLA	C15-C16-C17-C18
30	F	202	CLA	C15-C16-C17-C18
34	B	848	LHG	C1-C2-C3-O3
30	A	814	CLA	C4-C3-C5-C6
30	1	304	CLA	C4-C3-C5-C6
36	8	320	LMG	C29-C30-C31-C32
30	B	805	CLA	O1A-CGA-O2A-C1
36	8	320	LMG	C13-C14-C15-C16
30	4	302	CLA	C13-C15-C16-C17
30	11	308	CLA	C13-C15-C16-C17
34	B	848	LHG	C4-C5-C6-O8
36	A	856	LMG	C7-C8-C9-O8
36	6	301	LMG	C7-C8-C9-O8
36	8	320	LMG	O1-C7-C8-C9
38	5	305	KC1	CAA-CBA-CGA-O1A
30	A	830	CLA	C15-C16-C17-C18
30	B	821	CLA	C5-C6-C7-C8
30	B	802	CLA	O1D-CGD-O2D-CED
30	B	808	CLA	O1D-CGD-O2D-CED
30	B	802	CLA	C5-C6-C7-C8
30	7	310	CLA	C13-C15-C16-C17
35	7	301	LMT	C9-C10-C11-C12
36	B	847	LMG	C21-C22-C23-C24
30	12	304	CLA	CAA-CBA-CGA-O2A
30	5	311	CLA	O1A-CGA-O2A-C1
30	B	819	CLA	C3-C5-C6-C7
30	15	303	CLA	C10-C11-C12-C13
30	2	311	CLA	CBD-CGD-O2D-CED
30	12	308	CLA	C10-C11-C12-C13
38	14	308	KC1	C2C-C3C-CAC-CBC
30	B	810	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	B	828	CLA	O1D-CGD-O2D-CED
30	16	302	CLA	C10-C11-C12-C13
33	B	843	BCR	C35-C13-C14-C15
33	F	204	BCR	C35-C13-C14-C15
35	6	302	LMT	O5B-C5B-C6B-O6B
30	A	811	CLA	C4-C3-C5-C6
30	A	820	CLA	C4-C3-C5-C6
30	A	844	CLA	C4-C3-C5-C6
30	2	310	CLA	C4-C3-C5-C6
30	12	306	CLA	C4-C3-C5-C6
30	16	306	CLA	C4-C3-C5-C6
30	A	836	CLA	C6-C7-C8-C9
30	A	824	CLA	O1A-CGA-O2A-C1
30	15	309	CLA	O1A-CGA-O2A-C1
30	B	833	CLA	O1D-CGD-O2D-CED
30	A	834	CLA	CBA-CGA-O2A-C1
30	5	302	CLA	CBA-CGA-O2A-C1
30	6	310	CLA	CBA-CGA-O2A-C1
30	13	303	CLA	CBA-CGA-O2A-C1
35	A	857	LMT	O5B-C5B-C6B-O6B
36	B	849	LMG	C16-C17-C18-C19
30	10	311	CLA	CBD-CGD-O2D-CED
38	1	306	KC1	CBD-CGD-O2D-CED
38	8	307	KC1	CBD-CGD-O2D-CED
30	A	826	CLA	C8-C10-C11-C12
30	B	838	CLA	C5-C6-C7-C8
35	7	321	LMT	C6-C7-C8-C9
36	F	205	LMG	C7-C8-O7-C10
30	1	303	CLA	C2A-CAA-CBA-CGA
30	3	306	CLA	C2A-CAA-CBA-CGA
30	7	303	CLA	C2A-CAA-CBA-CGA
36	8	320	LMG	O9-C10-O7-C8
30	7	311	CLA	C13-C15-C16-C17
30	5	304	CLA	C2-C1-O2A-CGA
30	6	306	CLA	C2-C1-O2A-CGA
30	12	304	CLA	C2-C1-O2A-CGA
35	B	852	LMT	C5-C6-C7-C8
36	5	318	LMG	O6-C5-C6-O5
35	11	303	LMT	C6-C7-C8-C9
35	11	303	LMT	C11-C10-C9-C8
30	8	305	CLA	O1D-CGD-O2D-CED
30	3	301	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	10	304	CLA	C10-C11-C12-C13
30	A	816	CLA	CBA-CGA-O2A-C1
30	11	306	CLA	CBA-CGA-O2A-C1
30	3	307	CLA	C2C-C3C-CAC-CBC
30	12	303	CLA	O1D-CGD-O2D-CED
30	10	308	CLA	O1A-CGA-O2A-C1
30	12	302	CLA	O1A-CGA-O2A-C1
38	5	305	KC1	CAA-CBA-CGA-O2A
31	B	840	PQN	C15-C16-C17-C18
30	12	307	CLA	O1D-CGD-O2D-CED
33	A	850	BCR	C11-C10-C9-C8
33	B	841	BCR	C20-C21-C22-C23
33	F	204	BCR	C11-C10-C9-C8
39	1	310	DD6	C4-C5-C6-C8
39	7	302	DD6	C24-C1-C2-C3
34	A	852	LHG	O7-C5-C6-O8
36	F	205	LMG	O1-C7-C8-O7
36	7	320	LMG	O7-C8-C9-O8
34	A	852	LHG	C26-C27-C28-C29
30	A	815	CLA	C10-C11-C12-C13
30	B	812	CLA	C5-C6-C7-C8
30	B	813	CLA	C13-C15-C16-C17
30	6	310	CLA	O1A-CGA-O2A-C1
30	13	303	CLA	O1A-CGA-O2A-C1
36	8	319	LMG	C32-C33-C34-C35
30	A	839	CLA	C4-C3-C5-C6
30	B	807	CLA	C4-C3-C5-C6
30	13	302	CLA	C4-C3-C5-C6
30	A	804	CLA	C12-C13-C15-C16
30	A	806	CLA	C11-C12-C13-C15
30	A	811	CLA	C2-C3-C5-C6
30	A	816	CLA	C11-C10-C8-C7
30	A	820	CLA	C2-C3-C5-C6
30	A	822	CLA	C12-C13-C15-C16
30	A	825	CLA	C11-C10-C8-C7
30	A	835	CLA	C12-C13-C15-C16
30	A	839	CLA	C2-C3-C5-C6
30	A	839	CLA	C11-C12-C13-C15
30	A	841	CLA	C11-C10-C8-C7
30	A	842	CLA	C12-C13-C15-C16
30	A	844	CLA	C2-C3-C5-C6
30	B	811	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	B	822	CLA	C11-C12-C13-C15
30	B	828	CLA	C11-C12-C13-C15
30	B	835	CLA	C6-C7-C8-C10
30	B	838	CLA	C12-C13-C15-C16
30	1	307	CLA	C11-C10-C8-C7
30	2	301	CLA	C11-C10-C8-C7
30	2	301	CLA	C12-C13-C15-C16
30	2	311	CLA	C11-C12-C13-C15
30	6	304	CLA	C11-C12-C13-C15
30	7	309	CLA	C6-C7-C8-C10
30	7	311	CLA	C6-C7-C8-C10
30	8	301	CLA	C11-C12-C13-C15
30	8	303	CLA	C11-C12-C13-C15
30	9	303	CLA	C11-C10-C8-C7
30	11	308	CLA	C11-C12-C13-C15
30	11	308	CLA	C12-C13-C15-C16
30	12	304	CLA	C11-C10-C8-C7
30	12	306	CLA	C2-C3-C5-C6
30	12	312	CLA	C11-C10-C8-C7
30	15	304	CLA	C6-C7-C8-C10
30	15	304	CLA	C12-C13-C15-C16
30	16	303	CLA	C6-C7-C8-C10
30	16	303	CLA	C11-C10-C8-C7
30	16	306	CLA	C2-C3-C5-C6
30	A	813	CLA	C3-C5-C6-C7
36	14	321	LMG	O6-C5-C6-O5
30	A	807	CLA	C11-C12-C13-C14
30	A	829	CLA	C6-C7-C8-C9
30	A	835	CLA	C14-C13-C15-C16
30	A	841	CLA	C11-C10-C8-C9
30	B	802	CLA	C11-C12-C13-C14
30	B	811	CLA	C11-C10-C8-C9
30	B	822	CLA	C11-C12-C13-C14
30	B	829	CLA	C14-C13-C15-C16
30	B	835	CLA	C6-C7-C8-C9
30	L	202	CLA	C11-C12-C13-C14
30	1	307	CLA	C11-C10-C8-C9
30	2	301	CLA	C14-C13-C15-C16
30	2	311	CLA	C11-C12-C13-C14
30	6	304	CLA	C11-C12-C13-C14
30	7	307	CLA	C11-C10-C8-C9
30	8	303	CLA	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	11	308	CLA	C11-C12-C13-C14
30	11	310	CLA	C14-C13-C15-C16
30	12	304	CLA	C11-C10-C8-C9
30	12	312	CLA	C11-C10-C8-C9
30	14	303	CLA	C11-C10-C8-C9
30	15	304	CLA	C6-C7-C8-C9
30	16	303	CLA	C6-C7-C8-C9
39	8	317	DD6	C3-C4-C5-C6
30	15	307	CLA	CBD-CGD-O2D-CED
30	1	303	CLA	CBA-CGA-O2A-C1
30	4	302	CLA	CBA-CGA-O2A-C1
30	10	303	CLA	CBA-CGA-O2A-C1
30	4	303	CLA	C5-C6-C7-C8
33	J	102	BCR	C7-C8-C9-C34
37	9	315	A86	C7-C6-C8-C9
37	11	316	A86	C-C1-C24-C25
37	14	319	A86	C-C1-C24-C25
37	16	312	A86	C-C1-C24-C25
39	6	318	DD6	C12-C11-C13-C14
33	B	841	BCR	C21-C22-C23-C24
37	2u	203	A86	C5-C6-C8-C9
37	9	315	A86	C5-C6-C8-C9
37	11	316	A86	C2-C1-C24-C25
37	14	319	A86	C2-C1-C24-C25
37	14	319	A86	C5-C6-C8-C9
37	15	317	A86	C5-C6-C8-C9
37	16	312	A86	C2-C1-C24-C25
39	2	317	DD6	C2-C1-C24-C25
39	2	317	DD6	C10-C11-C13-C14
39	4	316	DD6	C10-C11-C13-C14
39	7	317	DD6	C10-C11-C13-C14
39	13	314	DD6	C5-C6-C8-C9
30	B	831	CLA	C3-C5-C6-C7
34	A	853	LHG	C1-C2-C3-O3
30	8	304	CLA	C10-C11-C12-C13
36	5	318	LMG	C31-C32-C33-C34
30	A	834	CLA	O1A-CGA-O2A-C1
30	B	828	CLA	CBA-CGA-O2A-C1
30	9	301	CLA	CBA-CGA-O2A-C1
30	11	309	CLA	CBA-CGA-O2A-C1
30	B	817	CLA	C10-C11-C12-C13
30	A	813	CLA	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
35	8	322	LMT	C4-C5-C6-C7
35	11	303	LMT	C1-C2-C3-C4
34	A	852	LHG	C19-C20-C21-C22
34	B	848	LHG	O6-C4-C5-C6
34	6	322	LHG	O6-C4-C5-C6
30	2	305	CLA	CBA-CGA-O2A-C1
30	8	309	CLA	CBA-CGA-O2A-C1
30	9	307	CLA	CBA-CGA-O2A-C1
30	15	311	CLA	O1D-CGD-O2D-CED
30	A	830	CLA	C4-C3-C5-C6
30	B	830	CLA	C4-C3-C5-C6
30	B	837	CLA	C4-C3-C5-C6
30	8	303	CLA	C4-C3-C5-C6
30	10	305	CLA	C4-C3-C5-C6
30	11	309	CLA	C4-C3-C5-C6
30	12	308	CLA	C4-C3-C5-C6
30	B	807	CLA	C2-C3-C5-C6
30	B	830	CLA	O1D-CGD-O2D-CED
30	8	302	CLA	C3-C5-C6-C7
30	15	302	CLA	C16-C17-C18-C19
34	9	318	LHG	C9-C10-C11-C12
30	15	304	CLA	C10-C11-C12-C13
30	A	828	CLA	CBA-CGA-O2A-C1
30	6	304	CLA	CBA-CGA-O2A-C1
30	11	308	CLA	CBA-CGA-O2A-C1
30	12	304	CLA	CBA-CGA-O2A-C1
30	1	303	CLA	C3A-C2A-CAA-CBA
30	8	308	CLA	C3A-C2A-CAA-CBA
30	11	304	CLA	C3A-C2A-CAA-CBA
30	A	806	CLA	C10-C11-C12-C13
30	A	816	CLA	C10-C11-C12-C13
37	2	318	A86	C24-C25-C26-C27
37	5	315	A86	C24-C25-C26-C27
37	9	313	A86	C11-C10-C9-C8
37	12	314	A86	C24-C25-C26-C27
39	3	312	DD6	C3-C4-C5-C6
39	3	313	DD6	C11-C10-C9-C8
39	16	313	DD6	C24-C25-C26-C27
37	1	309	A86	O-C13-C14-C15
37	5	316	A86	O-C13-C14-C15
37	8	315	A86	O-C13-C14-C15
37	14	316	A86	O-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	15	320	A86	O-C13-C14-C15
37	16	314	A86	O-C13-C14-C15
30	A	820	CLA	C3-C5-C6-C7
30	B	809	CLA	C3-C5-C6-C7
30	L	202	CLA	CBA-CGA-O2A-C1
30	8	305	CLA	CBA-CGA-O2A-C1
30	A	804	CLA	C10-C11-C12-C13
30	16	301	CLA	C5-C6-C7-C8
36	F	205	LMG	O1-C7-C8-C9
36	3	317	LMG	C7-C8-C9-O8
36	8	319	LMG	C7-C8-C9-O8
36	B	849	LMG	C17-C18-C19-C20
33	L	201	BCR	C14-C15-C16-C17
34	9	318	LHG	C29-C30-C31-C32
30	B	833	CLA	C3-C5-C6-C7
30	6	306	CLA	C3-C5-C6-C7
30	11	306	CLA	O1A-CGA-O2A-C1
30	F	202	CLA	C13-C15-C16-C17
30	1	303	CLA	C4-C3-C5-C6
30	15	309	CLA	C4-C3-C5-C6
30	7	306	CLA	C2-C3-C5-C6
38	2	306	KC1	CAA-CBA-CGA-O2A
38	12	309	KC1	CAA-CBA-CGA-O1A
38	12	309	KC1	CAA-CBA-CGA-O2A
30	3	303	CLA	C10-C11-C12-C13
30	A	836	CLA	C3-C5-C6-C7
30	12	321	CLA	C3-C5-C6-C7
30	10	308	CLA	C2A-CAA-CBA-CGA
30	11	309	CLA	C2A-CAA-CBA-CGA
34	5	317	LHG	O1-C1-C2-O2
30	B	830	CLA	C13-C15-C16-C17
30	10	307	CLA	CBA-CGA-O2A-C1
36	B	847	LMG	C38-C39-C40-C41
38	6	313	KC1	C3A-C2A-CAA-CBA
38	7	308	KC1	C3A-C2A-CAA-CBA
38	8	311	KC1	C3A-C2A-CAA-CBA
38	8	312	KC1	C3A-C2A-CAA-CBA
38	10	306	KC1	C3A-C2A-CAA-CBA
38	11	312	KC1	C3A-C2A-CAA-CBA
38	12	305	KC1	C3A-C2A-CAA-CBA
38	13	306	KC1	C3A-C2A-CAA-CBA
38	13	310	KC1	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	A	801	CL0	C16-C17-C18-C20
30	15	313	CLA	C10-C11-C12-C13
30	B	826	CLA	O1D-CGD-O2D-CED
38	2	306	KC1	CAA-CBA-CGA-O1A
35	A	854	LMT	C11-C10-C9-C8
30	B	851	CLA	O1D-CGD-O2D-CED
30	A	816	CLA	O1A-CGA-O2A-C1
30	2	305	CLA	O1A-CGA-O2A-C1
35	B	852	LMT	C4-C5-C6-C7
35	1	311	LMT	C9-C10-C11-C12
30	B	807	CLA	C3-C5-C6-C7
36	B	847	LMG	O1-C7-C8-O7
36	2u	204	LMG	O1-C7-C8-O7
36	5	318	LMG	O7-C8-C9-O8
36	6	301	LMG	O7-C8-C9-O8
30	A	830	CLA	CBA-CGA-O2A-C1
30	B	827	CLA	CBA-CGA-O2A-C1
36	14	321	LMG	C16-C17-C18-C19
37	13	313	A86	C24-C25-C26-C27
37	16	314	A86	C33-C34-O4-C38
30	A	820	CLA	C16-C17-C18-C19
30	B	809	CLA	C16-C17-C18-C20
37	2u	203	A86	C10-C11-C13-C14
37	2u	205	A86	C10-C11-C13-C14
37	1	309	A86	C10-C11-C13-C14
37	2	302	A86	C10-C11-C13-C14
37	7	316	A86	C10-C11-C13-C14
37	9	316	A86	C10-C11-C13-C14
37	12	314	A86	C10-C11-C13-C14
37	14	318	A86	C10-C11-C13-C14
37	15	320	A86	C10-C11-C13-C14
37	16	312	A86	C10-C11-C13-C14
36	2u	204	LMG	C11-C12-C13-C14
30	7	311	CLA	C4-C3-C5-C6
30	A	832	CLA	C2-C1-O2A-CGA
30	A	835	CLA	C2-C1-O2A-CGA
30	B	805	CLA	C2-C1-O2A-CGA
30	3	307	CLA	C2-C1-O2A-CGA
30	4	303	CLA	C2-C1-O2A-CGA
30	6	307	CLA	C2-C1-O2A-CGA
30	6	317	CLA	C2-C1-O2A-CGA
30	7	305	CLA	C2-C1-O2A-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	7	311	CLA	C2-C1-O2A-CGA
30	16	301	CLA	C2-C1-O2A-CGA
30	13	302	CLA	C2-C3-C5-C6
30	8	305	CLA	O1A-CGA-O2A-C1
30	B	818	CLA	C8-C10-C11-C12
30	A	806	CLA	C11-C12-C13-C14
30	A	811	CLA	C11-C12-C13-C14
30	B	808	CLA	C11-C10-C8-C9
30	B	813	CLA	C11-C12-C13-C14
30	B	828	CLA	C6-C7-C8-C9
30	1	302	CLA	C11-C10-C8-C9
30	2	304	CLA	C14-C13-C15-C16
30	5	307	CLA	C14-C13-C15-C16
30	6	314	CLA	C11-C12-C13-C14
30	7	303	CLA	C11-C12-C13-C14
30	8	301	CLA	C11-C10-C8-C9
30	9	308	CLA	C6-C7-C8-C9
30	9	308	CLA	C14-C13-C15-C16
30	10	303	CLA	C11-C10-C8-C9
30	11	310	CLA	C6-C7-C8-C9
30	13	303	CLA	C11-C12-C13-C14
30	14	307	CLA	C11-C10-C8-C9
30	15	302	CLA	C14-C13-C15-C16
30	15	304	CLA	C14-C13-C15-C16
31	A	845	PQN	C21-C22-C23-C24
30	15	305	CLA	CBD-CGD-O2D-CED
38	16	304	KC1	C1A-C2A-CAA-CBA
30	B	828	CLA	O1A-CGA-O2A-C1
30	9	301	CLA	O1A-CGA-O2A-C1
30	A	825	CLA	C10-C11-C12-C13
30	A	810	CLA	C2A-CAA-CBA-CGA
30	F	203	CLA	C2A-CAA-CBA-CGA
33	A	848	BCR	C23-C24-C25-C30
33	A	851	BCR	C23-C24-C25-C30
33	B	841	BCR	C1-C6-C7-C8
33	B	843	BCR	C23-C24-C25-C26
33	B	844	BCR	C1-C6-C7-C8
33	B	844	BCR	C5-C6-C7-C8
33	B	845	BCR	C1-C6-C7-C8
33	B	845	BCR	C5-C6-C7-C8
33	F	204	BCR	C1-C6-C7-C8
33	F	204	BCR	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	I	101	BCR	C5-C6-C7-C8
33	L	201	BCR	C1-C6-C7-C8
33	L	201	BCR	C5-C6-C7-C8
33	L	204	BCR	C1-C6-C7-C8
33	L	204	BCR	C5-C6-C7-C8
33	L	205	BCR	C23-C24-C25-C26
33	L	205	BCR	C23-C24-C25-C30
33	M	101	BCR	C23-C24-C25-C26
33	M	101	BCR	C23-C24-C25-C30
30	13	303	CLA	C13-C15-C16-C17
37	15	317	A86	C7-C6-C8-C9
39	7	317	DD6	C-C1-C24-C25
33	A	849	BCR	C21-C22-C23-C24
33	2u	201	BCR	C21-C22-C23-C24
37	15	321	A86	C5-C6-C8-C9
39	11	313	DD6	C5-C6-C8-C9
36	5	318	LMG	C10-C11-C12-C13
33	B	842	BCR	C14-C15-C16-C17
30	7	304	CLA	C16-C17-C18-C19
34	A	852	LHG	C7-C8-C9-C10
36	8	319	LMG	C34-C35-C36-C37
30	4	302	CLA	C10-C11-C12-C13
30	1	303	CLA	O1A-CGA-O2A-C1
30	5	308	CLA	O1D-CGD-O2D-CED
38	6	312	KC1	CAA-CBA-CGA-O1A
38	6	312	KC1	CAA-CBA-CGA-O2A
30	B	817	CLA	CAA-CBA-CGA-O2A
36	8	320	LMG	C18-C19-C20-C21
30	A	807	CLA	C11-C12-C13-C15
30	A	811	CLA	C11-C12-C13-C15
30	A	814	CLA	C2-C3-C5-C6
30	A	829	CLA	C6-C7-C8-C10
30	A	830	CLA	C2-C3-C5-C6
30	A	833	CLA	C11-C10-C8-C7
30	A	839	CLA	C12-C13-C15-C16
30	B	802	CLA	C11-C12-C13-C15
30	B	808	CLA	C11-C10-C8-C7
30	B	819	CLA	C12-C13-C15-C16
30	B	828	CLA	C6-C7-C8-C10
30	B	829	CLA	C12-C13-C15-C16
30	B	830	CLA	C12-C13-C15-C16
30	L	202	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	2u	202	CLA	C6-C7-C8-C10
30	2u	202	CLA	C11-C12-C13-C15
30	2	304	CLA	C12-C13-C15-C16
30	2	309	CLA	C12-C13-C15-C16
30	5	307	CLA	C12-C13-C15-C16
30	6	314	CLA	C11-C12-C13-C15
30	7	307	CLA	C11-C10-C8-C7
30	7	309	CLA	C12-C13-C15-C16
30	8	301	CLA	C11-C10-C8-C7
30	8	305	CLA	C12-C13-C15-C16
30	9	308	CLA	C6-C7-C8-C10
30	9	308	CLA	C12-C13-C15-C16
30	10	303	CLA	C11-C10-C8-C7
30	11	309	CLA	C12-C13-C15-C16
30	11	310	CLA	C12-C13-C15-C16
30	13	301	CLA	C6-C7-C8-C10
30	13	303	CLA	C11-C12-C13-C15
30	14	303	CLA	C11-C10-C8-C7
30	14	307	CLA	C11-C10-C8-C7
30	15	302	CLA	C12-C13-C15-C16
30	B	801	CLA	C3-C5-C6-C7
30	13	301	CLA	O1D-CGD-O2D-CED
30	6	310	CLA	C10-C11-C12-C13
37	2	319	A86	C1-C2-C3-C4
37	4	317	A86	C24-C25-C26-C27
37	5	301	A86	C24-C25-C26-C27
37	15	321	A86	C11-C10-C9-C8
39	4	316	DD6	C3-C4-C5-C6
39	5	313	DD6	C3-C4-C5-C6
39	5	314	DD6	C24-C25-C26-C27
39	6	318	DD6	C3-C4-C5-C6
39	8	316	DD6	C24-C25-C26-C27
39	10	314	DD6	C3-C4-C5-C6
39	12	315	DD6	C24-C25-C26-C27
30	B	808	CLA	C5-C6-C7-C8
30	B	829	CLA	C10-C11-C12-C13
30	5	307	CLA	C15-C16-C17-C18
36	7	320	LMG	C13-C14-C15-C16
33	B	842	BCR	C20-C21-C22-C37
33	B	844	BCR	C35-C13-C14-C15
33	B	844	BCR	C20-C21-C22-C37
33	L	204	BCR	C35-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	M	101	BCR	C16-C17-C18-C36
38	14	308	KC1	C4C-C3C-CAC-CBC
39	2	316	DD6	C9-C10-C11-C12
39	7	317	DD6	C4-C5-C6-C7
39	7	318	DD6	C9-C10-C11-C12
30	A	802	CLA	C3-C5-C6-C7
38	5	306	KC1	C2A-CAA-CBA-CGA
30	A	840	CLA	CBD-CGD-O2D-CED
36	B	847	LMG	C31-C32-C33-C34
30	4	306	CLA	O1D-CGD-O2D-CED
35	A	854	LMT	C6-C7-C8-C9
30	A	808	CLA	CAD-CBD-CGD-O2D
30	A	812	CLA	CAD-CBD-CGD-O2D
30	A	815	CLA	CAD-CBD-CGD-O2D
30	A	821	CLA	CAD-CBD-CGD-O2D
30	A	827	CLA	CAD-CBD-CGD-O2D
30	A	834	CLA	CAD-CBD-CGD-O2D
30	B	821	CLA	CAD-CBD-CGD-O2D
30	B	831	CLA	CAD-CBD-CGD-O2D
30	B	837	CLA	CAD-CBD-CGD-O2D
30	J	101	CLA	CAD-CBD-CGD-O2D
30	1	307	CLA	CAD-CBD-CGD-O2D
30	2	301	CLA	CAD-CBD-CGD-O2D
30	4	305	CLA	CAD-CBD-CGD-O2D
30	4	306	CLA	CAD-CBD-CGD-O2D
30	5	303	CLA	CAD-CBD-CGD-O2D
30	5	307	CLA	CAD-CBD-CGD-O2D
30	5	311	CLA	CAD-CBD-CGD-O2D
30	6	306	CLA	CAD-CBD-CGD-O2D
30	6	309	CLA	CAD-CBD-CGD-O2D
30	8	304	CLA	CAD-CBD-CGD-O2D
30	10	307	CLA	CAD-CBD-CGD-O2D
30	12	306	CLA	CAD-CBD-CGD-O2D
30	13	309	CLA	CAD-CBD-CGD-O2D
30	14	302	CLA	CAD-CBD-CGD-O2D
30	15	311	CLA	CAD-CBD-CGD-O2D
30	16	302	CLA	CAD-CBD-CGD-O2D
30	16	308	CLA	CAD-CBD-CGD-O2D
30	16	310	CLA	CAD-CBD-CGD-O2D
37	3	315	A86	C28-C27-C29-C30
37	5	315	A86	C28-C27-C29-C30
37	7	315	A86	C28-C27-C29-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	15	317	A86	C28-C27-C29-C30
38	2	306	KC1	CAD-CBD-CGD-O2D
38	7	308	KC1	C2B-C3B-CAB-CBB
38	9	310	KC1	CAD-CBD-CGD-O2D
38	11	305	KC1	CAD-CBD-CGD-O2D
38	12	309	KC1	C2B-C3B-CAB-CBB
38	14	308	KC1	C2B-C3B-CAB-CBB
38	14	311	KC1	CAD-CBD-CGD-O2D
38	16	304	KC1	CAD-CBD-CGD-O2D
38	8	306	KC1	CAA-CBA-CGA-O1A
30	6	307	CLA	C8-C10-C11-C12
30	12	304	CLA	C10-C11-C12-C13
35	7	321	LMT	C4-C5-C6-C7
33	A	847	BCR	C22-C23-C24-C25
30	15	308	CLA	CBD-CGD-O2D-CED
30	4	306	CLA	CBA-CGA-O2A-C1
30	A	813	CLA	C4-C3-C5-C6
30	6	317	CLA	C4-C3-C5-C6
30	3	307	CLA	C4C-C3C-CAC-CBC
35	15	301	LMT	O5'-C1'-O1'-C1
30	7	311	CLA	C2-C3-C5-C6
36	3	317	LMG	C28-C29-C30-C31
34	9	318	LHG	C4-C5-C6-O8
36	B	847	LMG	O1-C7-C8-C9
36	8	321	LMG	C7-C8-C9-O8
37	2	318	A86	C12-C11-C13-O
37	3	315	A86	C12-C11-C13-O
37	4	314	A86	C12-C11-C13-O
37	5	301	A86	C12-C11-C13-O
37	7	315	A86	C12-C11-C13-O
37	10	302	A86	C12-C11-C13-O
37	10	317	A86	C12-C11-C13-O
37	11	301	A86	C12-C11-C13-O
37	12	316	A86	C12-C11-C13-O
37	13	313	A86	C12-C11-C13-O
37	14	316	A86	C12-C11-C13-O
37	15	317	A86	C12-C11-C13-O
37	16	312	A86	C12-C11-C13-O
30	16	306	CLA	CBD-CGD-O2D-CED
30	A	828	CLA	O1A-CGA-O2A-C1
30	B	827	CLA	O1A-CGA-O2A-C1
34	2	320	LHG	O10-C23-O8-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	B	848	LHG	O6-C4-C5-O7
34	6	322	LHG	O6-C4-C5-O7
30	A	829	CLA	C13-C15-C16-C17
30	B	803	CLA	C10-C11-C12-C13
30	6	317	CLA	C13-C15-C16-C17
30	A	841	CLA	C3-C5-C6-C7
38	1	306	KC1	C4B-C3B-CAB-CBB
38	13	308	KC1	C4B-C3B-CAB-CBB
38	14	306	KC1	C4B-C3B-CAB-CBB
30	A	822	CLA	C2A-CAA-CBA-CGA
38	8	312	KC1	CBD-CGD-O2D-CED
30	15	302	CLA	C16-C17-C18-C20
30	12	302	CLA	O1D-CGD-O2D-CED
30	A	806	CLA	CHA-CBD-CGD-O1D
30	A	806	CLA	CHA-CBD-CGD-O2D
30	A	821	CLA	CHA-CBD-CGD-O1D
30	A	839	CLA	CHA-CBD-CGD-O1D
30	A	841	CLA	CHA-CBD-CGD-O2D
30	B	807	CLA	CHA-CBD-CGD-O2D
30	B	808	CLA	CHA-CBD-CGD-O1D
30	B	824	CLA	CHA-CBD-CGD-O1D
30	4	304	CLA	CHA-CBD-CGD-O1D
30	4	304	CLA	CHA-CBD-CGD-O2D
30	4	309	CLA	CHA-CBD-CGD-O1D
30	4	309	CLA	CHA-CBD-CGD-O2D
30	5	304	CLA	CHA-CBD-CGD-O1D
30	5	304	CLA	CHA-CBD-CGD-O2D
30	6	314	CLA	CHA-CBD-CGD-O1D
30	6	315	CLA	CHA-CBD-CGD-O1D
30	6	315	CLA	CHA-CBD-CGD-O2D
30	7	312	CLA	CHA-CBD-CGD-O1D
30	8	308	CLA	CHA-CBD-CGD-O1D
30	8	308	CLA	CHA-CBD-CGD-O2D
30	9	301	CLA	CHA-CBD-CGD-O1D
30	9	301	CLA	CHA-CBD-CGD-O2D
30	13	304	CLA	CHA-CBD-CGD-O1D
30	13	307	CLA	CHA-CBD-CGD-O1D
30	13	307	CLA	CHA-CBD-CGD-O2D
30	14	304	CLA	CHA-CBD-CGD-O1D
30	14	304	CLA	CHA-CBD-CGD-O2D
30	15	305	CLA	CHA-CBD-CGD-O1D
30	15	310	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	15	313	CLA	CHA-CBD-CGD-O1D
30	15	313	CLA	CHA-CBD-CGD-O2D
30	16	306	CLA	CHA-CBD-CGD-O1D
30	16	306	CLA	CHA-CBD-CGD-O2D
30	16	308	CLA	CHA-CBD-CGD-O1D
38	3	308	KC1	CHA-CBD-CGD-O1D
38	5	306	KC1	CHA-CBD-CGD-O1D
38	5	306	KC1	CHA-CBD-CGD-O2D
38	6	312	KC1	CHA-CBD-CGD-O1D
38	6	312	KC1	CHA-CBD-CGD-O2D
38	11	307	KC1	CHA-CBD-CGD-O1D
38	11	311	KC1	CHA-CBD-CGD-O1D
38	11	311	KC1	CHA-CBD-CGD-O2D
38	12	309	KC1	CHA-CBD-CGD-O1D
38	12	309	KC1	CHA-CBD-CGD-O2D
38	12	311	KC1	CHA-CBD-CGD-O1D
38	12	311	KC1	CHA-CBD-CGD-O2D
38	13	306	KC1	CHA-CBD-CGD-O1D
38	13	306	KC1	CHA-CBD-CGD-O2D
30	2	304	CLA	C3-C5-C6-C7
30	4	302	CLA	O1A-CGA-O2A-C1
30	8	309	CLA	O1A-CGA-O2A-C1
30	9	307	CLA	O1A-CGA-O2A-C1
30	10	303	CLA	O1A-CGA-O2A-C1
30	12	304	CLA	O1A-CGA-O2A-C1
30	5	311	CLA	O1D-CGD-O2D-CED
33	L	205	BCR	C12-C13-C14-C15
39	5	314	DD6	C4-C5-C6-C8
39	7	318	DD6	C4-C5-C6-C8
34	9	318	LHG	O7-C5-C6-O8
36	3	317	LMG	O7-C8-C9-O8
30	A	813	CLA	CBD-CGD-O2D-CED
30	A	830	CLA	O1A-CGA-O2A-C1
30	10	307	CLA	O1A-CGA-O2A-C1
30	11	308	CLA	O1A-CGA-O2A-C1
36	8	320	LMG	O10-C28-O8-C9
36	14	321	LMG	C17-C18-C19-C20
37	2	318	A86	C10-C11-C13-O
37	3	315	A86	C13-C14-C15-O1
37	5	301	A86	C13-C14-C15-O1
37	5	316	A86	C13-C14-C15-O1
37	7	315	A86	C10-C11-C13-O

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	10	302	A86	C10-C11-C13-O
37	10	302	A86	C13-C14-C15-O1
37	10	316	A86	C13-C14-C15-O1
37	11	301	A86	C10-C11-C13-O
37	11	301	A86	C13-C14-C15-O1
37	11	314	A86	C13-C14-C15-O1
37	11	316	A86	C13-C14-C15-O1
37	12	314	A86	C10-C11-C13-O
37	12	314	A86	C13-C14-C15-O1
37	12	316	A86	C10-C11-C13-O
37	13	313	A86	C10-C11-C13-O
37	14	316	A86	C13-C14-C15-O1
37	14	317	A86	C13-C14-C15-O1
37	14	318	A86	C10-C11-C13-O
37	14	318	A86	C13-C14-C15-O1
37	15	315	A86	C13-C14-C15-O1
37	15	321	A86	C13-C14-C15-O1
37	16	312	A86	C10-C11-C13-O
35	7	301	LMT	C7-C8-C9-C10
30	15	302	CLA	C3-C5-C6-C7
34	6	322	LHG	C8-C7-O7-C5
30	B	813	CLA	C4-C3-C5-C6
30	L	202	CLA	O1A-CGA-O2A-C1
30	5	302	CLA	O1A-CGA-O2A-C1
30	B	830	CLA	C2-C3-C5-C6
34	A	852	LHG	O9-C7-O7-C5
30	B	819	CLA	C11-C10-C8-C9
30	B	819	CLA	C14-C13-C15-C16
30	B	830	CLA	C14-C13-C15-C16
30	13	301	CLA	C6-C7-C8-C9
30	A	809	CLA	O1D-CGD-O2D-CED
30	A	813	CLA	O1D-CGD-O2D-CED
36	8	320	LMG	C15-C16-C17-C18
36	A	856	LMG	O10-C28-O8-C9
38	8	306	KC1	CAA-CBA-CGA-O2A
30	10	303	CLA	C2A-CAA-CBA-CGA
30	F	202	CLA	C8-C10-C11-C12
33	B	843	BCR	C36-C18-C19-C20
37	13	313	A86	C7-C6-C8-C9
37	15	316	A86	C-C1-C24-C25
39	3	313	DD6	C12-C11-C13-C14
39	6	319	DD6	C12-C11-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	B	847	LMG	C17-C18-C19-C20
30	2u	202	CLA	C5-C6-C7-C8
30	8	305	CLA	C13-C15-C16-C17
30	15	313	CLA	C13-C15-C16-C17
33	A	848	BCR	C21-C22-C23-C24
33	J	102	BCR	C7-C8-C9-C10
37	13	313	A86	C5-C6-C8-C9
37	15	316	A86	C2-C1-C24-C25
39	3	316	DD6	C10-C11-C13-C14
39	4	313	DD6	C10-C11-C13-C14
39	6	318	DD6	C2-C1-C24-C25
39	15	318	DD6	C10-C11-C13-C14
39	15	319	DD6	C10-C11-C13-C14
30	A	814	CLA	C3-C5-C6-C7
35	1	311	LMT	O1'-C1-C2-C3
30	A	823	CLA	C1A-C2A-CAA-CBA
30	A	836	CLA	C1A-C2A-CAA-CBA
30	1	305	CLA	C1A-C2A-CAA-CBA
30	3	310	CLA	C1A-C2A-CAA-CBA
30	7	311	CLA	C1A-C2A-CAA-CBA
30	8	309	CLA	C1A-C2A-CAA-CBA
30	11	304	CLA	C1A-C2A-CAA-CBA
30	4	304	CLA	C10-C11-C12-C13
30	6	305	CLA	C15-C16-C17-C18
30	A	821	CLA	C2-C1-O2A-CGA
30	13	302	CLA	C2-C1-O2A-CGA
30	15	304	CLA	C2-C1-O2A-CGA
30	10	308	CLA	CBD-CGD-O2D-CED
35	12	301	LMT	C4B-C5B-C6B-O6B
30	4	309	CLA	CBA-CGA-O2A-C1
36	6	301	LMG	C11-C12-C13-C14
37	2	319	A86	C3-C4-C5-C6
34	6	322	LHG	C3-O3-P-O6
35	A	857	LMT	C2-C3-C4-C5
36	B	847	LMG	C12-C13-C14-C15
38	9	311	KC1	O1D-CGD-O2D-CED
35	11	317	LMT	C3'-C4'-O1B-C1B
30	A	807	CLA	CAA-CBA-CGA-O2A
30	A	829	CLA	C15-C16-C17-C18
29	A	801	CL0	C3-C5-C6-C7
30	B	835	CLA	C3-C5-C6-C7
30	2	311	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	1	304	CLA	C2-C3-C5-C6
30	2	303	CLA	C2-C3-C5-C6
30	5	309	CLA	C2-C3-C5-C6
30	6	304	CLA	O1A-CGA-O2A-C1
34	A	852	LHG	C3-O3-P-O4
34	2	320	LHG	C4-O6-P-O4
34	5	317	LHG	C3-O3-P-O5
34	6	322	LHG	C3-O3-P-O4
34	6	322	LHG	C4-O6-P-O4
34	9	318	LHG	C4-O6-P-O4
30	15	309	CLA	C16-C17-C18-C20
36	6	301	LMG	C10-C11-C12-C13
30	A	839	CLA	C10-C11-C12-C13
34	6	322	LHG	C24-C23-O8-C6
30	B	839	CLA	O1D-CGD-O2D-CED
30	A	819	CLA	CAA-CBA-CGA-O2A
30	B	804	CLA	C2A-CAA-CBA-CGA
30	15	304	CLA	C3-C5-C6-C7
30	11	309	CLA	O1A-CGA-O2A-C1
36	14	321	LMG	C30-C31-C32-C33
30	A	806	CLA	CAD-CBD-CGD-O1D
30	B	834	CLA	CAD-CBD-CGD-O1D
30	4	304	CLA	CAD-CBD-CGD-O1D
30	4	309	CLA	CAD-CBD-CGD-O1D
30	5	304	CLA	CAD-CBD-CGD-O1D
30	6	315	CLA	CAD-CBD-CGD-O1D
30	7	312	CLA	CAD-CBD-CGD-O1D
30	8	308	CLA	CAD-CBD-CGD-O1D
30	13	304	CLA	CAD-CBD-CGD-O1D
30	14	312	CLA	CAD-CBD-CGD-O1D
37	15	317	A86	C26-C27-C29-C30
37	16	312	A86	C26-C27-C29-C30
38	6	312	KC1	CAD-CBD-CGD-O1D
38	12	311	KC1	CAD-CBD-CGD-O1D
30	1	304	CLA	CBD-CGD-O2D-CED
30	7	305	CLA	C16-C17-C18-C20
30	6	309	CLA	CBD-CGD-O2D-CED
30	A	802	CLA	C6-C7-C8-C10
30	A	807	CLA	C3A-C2A-CAA-CBA
30	A	820	CLA	C11-C12-C13-C15
30	B	801	CLA	C11-C10-C8-C7
30	B	813	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	B	819	CLA	C11-C10-C8-C7
30	B	851	CLA	C11-C10-C8-C7
30	F	202	CLA	C11-C12-C13-C15
30	F	202	CLA	C12-C13-C15-C16
30	3	307	CLA	C11-C12-C13-C15
30	4	302	CLA	C12-C13-C15-C16
30	6	310	CLA	C12-C13-C15-C16
30	6	317	CLA	C12-C13-C15-C16
30	7	310	CLA	C12-C13-C15-C16
30	9	305	CLA	C11-C12-C13-C15
30	9	309	CLA	C12-C13-C15-C16
30	11	309	CLA	C11-C10-C8-C7
30	11	310	CLA	C6-C7-C8-C10
30	12	302	CLA	C11-C12-C13-C15
30	12	304	CLA	C3A-C2A-CAA-CBA
33	2u	201	BCR	C19-C20-C21-C22
36	2u	204	LMG	C28-C29-C30-C31
30	3	305	CLA	O1A-CGA-O2A-C1
30	A	829	CLA	C2A-CAA-CBA-CGA
30	4	305	CLA	C2A-CAA-CBA-CGA
30	12	302	CLA	CAA-CBA-CGA-O2A
36	F	205	LMG	C7-C8-C9-O8
36	2u	204	LMG	O1-C7-C8-C9
36	6	301	LMG	O1-C7-C8-C9
36	8	319	LMG	O1-C7-C8-C9
30	6	316	CLA	O1A-CGA-O2A-C1
34	B	848	LHG	O7-C5-C6-O8
36	A	856	LMG	O7-C8-C9-O8
36	8	321	LMG	O7-C8-C9-O8
36	14	321	LMG	O7-C8-C9-O8
30	A	812	CLA	CBA-CGA-O2A-C1
30	4	306	CLA	O1A-CGA-O2A-C1
30	4	309	CLA	O1A-CGA-O2A-C1
30	5	307	CLA	C5-C6-C7-C8
30	B	816	CLA	C3-C5-C6-C7
30	A	827	CLA	O1A-CGA-O2A-C1
30	9	305	CLA	C15-C16-C17-C18
30	A	803	CLA	C4-C3-C5-C6
30	A	828	CLA	C4-C3-C5-C6
30	F	202	CLA	C4-C3-C5-C6
30	B	837	CLA	C2-C3-C5-C6
37	2	319	A86	C13-C14-C15-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	4	312	A86	C13-C14-C15-C20
37	7	319	A86	C13-C14-C15-C20
37	8	318	A86	C13-C14-C15-C20
37	14	314	A86	C13-C14-C15-C20
37	14	320	A86	C13-C14-C15-C20
37	15	315	A86	C13-C14-C15-C20
37	15	316	A86	C13-C14-C15-C20
37	15	317	A86	C13-C14-C15-C20
37	15	323	A86	C13-C14-C15-C20
30	B	801	CLA	C11-C10-C8-C9
30	B	838	CLA	C14-C13-C15-C16
30	F	202	CLA	C11-C10-C8-C9
30	2u	202	CLA	C11-C12-C13-C14
30	2	309	CLA	C14-C13-C15-C16
30	4	302	CLA	C14-C13-C15-C16
30	4	304	CLA	C11-C10-C8-C9
30	6	307	CLA	C11-C10-C8-C9
30	6	310	CLA	C14-C13-C15-C16
30	7	303	CLA	C11-C10-C8-C9
30	7	307	CLA	C14-C13-C15-C16
30	7	309	CLA	C14-C13-C15-C16
30	8	305	CLA	C14-C13-C15-C16
30	10	303	CLA	C14-C13-C15-C16
30	11	309	CLA	C14-C13-C15-C16
30	15	302	CLA	C6-C7-C8-C9
30	15	304	CLA	C11-C12-C13-C14
38	8	312	KC1	O1D-CGD-O2D-CED
38	10	310	KC1	O1D-CGD-O2D-CED
33	A	850	BCR	C22-C23-C24-C25
36	8	320	LMG	C14-C15-C16-C17
30	7	305	CLA	C3-C5-C6-C7
30	6	307	CLA	CAA-CBA-CGA-O2A
34	A	852	LHG	O1-C1-C2-O2
34	A	852	LHG	C31-C32-C33-C34
37	2u	203	A86	C6-C8-C9-C10
37	2u	205	A86	C6-C8-C9-C10
37	2	302	A86	C1-C24-C25-C26
37	4	314	A86	C6-C8-C9-C10
37	9	315	A86	C1-C24-C25-C26
37	10	301	A86	C1-C24-C25-C26
37	10	302	A86	C1-C24-C25-C26
37	10	302	A86	C6-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	11	301	A86	C6-C8-C9-C10
37	13	313	A86	C6-C8-C9-C10
37	15	315	A86	C1-C24-C25-C26
37	15	315	A86	C6-C8-C9-C10
37	15	320	A86	C6-C8-C9-C10
37	15	323	A86	C6-C8-C9-C10
37	16	312	A86	C6-C8-C9-C10
39	2	315	DD6	C6-C8-C9-C10
39	10	313	DD6	C6-C8-C9-C10
39	1	310	DD6	C3-C4-C5-C6
30	A	805	CLA	C11-C12-C13-C14
34	A	852	LHG	C28-C29-C30-C31
30	A	812	CLA	O1A-CGA-O2A-C1
36	7	320	LMG	O9-C10-O7-C8
30	A	831	CLA	C5-C6-C7-C8
30	B	833	CLA	C10-C11-C12-C13
30	2	307	CLA	CAA-CBA-CGA-O2A
34	B	848	LHG	C10-C11-C12-C13
30	11	309	CLA	C2-C3-C5-C6
30	12	308	CLA	C2-C3-C5-C6
30	6	306	CLA	C5-C6-C7-C8
34	B	848	LHG	O10-C23-C24-C25
36	A	856	LMG	C29-C30-C31-C32
36	B	847	LMG	C18-C19-C20-C21
30	A	814	CLA	C10-C11-C12-C13
30	A	823	CLA	C1-C2-C3-C4
30	4	301	CLA	C1-C2-C3-C4
30	4	305	CLA	C3-C5-C6-C7
30	4	304	CLA	CAA-CBA-CGA-O2A
30	5	304	CLA	CAA-CBA-CGA-O2A
30	A	809	CLA	C2A-CAA-CBA-CGA
30	A	805	CLA	C2-C1-O2A-CGA
30	A	809	CLA	C2-C1-O2A-CGA
30	A	843	CLA	C2-C1-O2A-CGA
30	B	811	CLA	C2-C1-O2A-CGA
30	B	812	CLA	C2-C1-O2A-CGA
30	B	821	CLA	C2-C1-O2A-CGA
30	2	307	CLA	C2-C1-O2A-CGA
30	5	311	CLA	C2-C1-O2A-CGA
30	6	314	CLA	C2-C1-O2A-CGA
30	9	302	CLA	C2-C1-O2A-CGA
36	14	321	LMG	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	2	302	A86	C35-C34-O4-C38
35	12	301	LMT	C1-C2-C3-C4
36	3	317	LMG	C10-C11-C12-C13
37	2u	203	A86	C12-C11-C13-C14
37	5	301	A86	C12-C11-C13-C14
37	12	314	A86	C12-C11-C13-C14
37	14	316	A86	C12-C11-C13-C14
37	14	318	A86	C12-C11-C13-C14
37	16	312	A86	C12-C11-C13-C14
35	A	854	LMT	C5'-C4'-O1B-C1B
36	14	321	LMG	C12-C13-C14-C15
30	A	827	CLA	CBA-CGA-O2A-C1
30	6	316	CLA	CBA-CGA-O2A-C1
30	8	301	CLA	CBA-CGA-O2A-C1
30	15	305	CLA	O1D-CGD-O2D-CED
30	4	305	CLA	C5-C6-C7-C8
30	6	314	CLA	C13-C15-C16-C17
30	13	301	CLA	C8-C10-C11-C12
35	11	303	LMT	C5-C6-C7-C8
30	15	313	CLA	C3-C5-C6-C7
33	A	848	BCR	C23-C24-C25-C26
33	B	845	BCR	C23-C24-C25-C26
33	I	101	BCR	C1-C6-C7-C8
30	A	813	CLA	C2-C3-C5-C6
30	A	828	CLA	C2-C3-C5-C6
30	B	813	CLA	C2-C3-C5-C6
30	2	310	CLA	C2-C3-C5-C6
30	6	317	CLA	C2-C3-C5-C6
35	12	320	LMT	C5-C6-C7-C8
30	1	301	CLA	C5-C6-C7-C8
30	B	813	CLA	C16-C17-C18-C20
36	14	321	LMG	C11-C10-O7-C8
36	8	320	LMG	O6-C1-O1-C7
30	3	305	CLA	C2A-CAA-CBA-CGA
33	A	848	BCR	C20-C21-C22-C23
33	B	845	BCR	C20-C21-C22-C23
37	8	318	A86	C11-C13-C14-C15
39	2	315	DD6	C24-C1-C2-C3
39	3	313	DD6	C9-C10-C11-C13
39	10	313	DD6	C24-C1-C2-C3
39	12	317	DD6	C24-C1-C2-C3
30	A	841	CLA	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	A	852	LHG	C3-O3-P-O6
34	A	853	LHG	C3-O3-P-O6
34	9	318	LHG	C3-O3-P-O6
30	10	311	CLA	O1D-CGD-O2D-CED
30	A	816	CLA	C4-C3-C5-C6
30	11	310	CLA	C4-C3-C5-C6
35	16	315	LMT	C6-C7-C8-C9
30	A	834	CLA	C11-C12-C13-C15
30	B	838	CLA	C6-C7-C8-C10
30	F	201	CLA	C6-C7-C8-C10
30	7	303	CLA	C11-C10-C8-C7
30	7	307	CLA	C12-C13-C15-C16
31	A	845	PQN	C21-C22-C23-C25
31	B	840	PQN	C21-C22-C23-C25
36	B	849	LMG	C28-C29-C30-C31
30	A	822	CLA	C14-C13-C15-C16
30	B	838	CLA	C11-C10-C8-C9
30	B	851	CLA	C11-C10-C8-C9
30	F	202	CLA	C11-C12-C13-C14
30	F	202	CLA	C14-C13-C15-C16
30	2	301	CLA	C11-C10-C8-C9
30	6	317	CLA	C14-C13-C15-C16
30	7	310	CLA	C14-C13-C15-C16
30	9	303	CLA	C11-C10-C8-C9
30	9	305	CLA	C11-C12-C13-C14
30	12	302	CLA	C11-C12-C13-C14
30	A	816	CLA	C15-C16-C17-C18
30	15	304	CLA	C13-C15-C16-C17
34	A	853	LHG	C8-C7-O7-C5
37	3	315	A86	C3-C4-C5-C6
37	6	320	A86	C11-C10-C9-C8
37	10	317	A86	C24-C25-C26-C27
39	6	303	DD6	C11-C10-C9-C8
30	B	809	CLA	C16-C17-C18-C19
30	7	305	CLA	C16-C17-C18-C19
30	8	302	CLA	CBD-CGD-O2D-CED
30	B	827	CLA	C2A-CAA-CBA-CGA
30	15	302	CLA	C2A-CAA-CBA-CGA
37	14	301	A86	C35-C34-O4-C38
34	9	318	LHG	C5-C4-O6-P
30	12	310	CLA	C8-C10-C11-C12
36	6	301	LMG	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	B	808	CLA	C10-C11-C12-C13
30	10	305	CLA	C2-C3-C5-C6
30	15	309	CLA	C2-C3-C5-C6
30	A	816	CLA	C16-C17-C18-C19
30	A	829	CLA	C16-C17-C18-C20
30	A	838	CLA	CBA-CGA-O2A-C1
30	3	305	CLA	CBA-CGA-O2A-C1
38	11	311	KC1	C2B-C3B-CAB-CBB
30	2	310	CLA	O1A-CGA-O2A-C1
30	13	304	CLA	CAA-CBA-CGA-O2A
38	3	308	KC1	CAA-CBA-CGA-O1A
29	A	801	CL0	CAA-CBA-CGA-O2A
30	11	304	CLA	C13-C15-C16-C17
33	F	204	BCR	C6-C7-C8-C9
33	J	102	BCR	C6-C7-C8-C9
30	A	826	CLA	O1D-CGD-O2D-CED
34	A	853	LHG	C24-C23-O8-C6
30	A	803	CLA	C2A-CAA-CBA-CGA
30	2	308	CLA	C2A-CAA-CBA-CGA
30	8	301	CLA	C2A-CAA-CBA-CGA
30	15	309	CLA	C16-C17-C18-C19
37	6	320	A86	C3-C4-C5-C6
37	11	301	A86	C24-C25-C26-C27
37	15	315	A86	C11-C10-C9-C8
39	5	314	DD6	C3-C4-C5-C6
39	7	302	DD6	C11-C10-C9-C8
39	7	314	DD6	C11-C10-C9-C8
39	7	314	DD6	C1-C2-C3-C4
39	10	314	DD6	C24-C25-C26-C27
39	15	319	DD6	C24-C25-C26-C27
30	A	838	CLA	O1A-CGA-O2A-C1
30	2	311	CLA	O1A-CGA-O2A-C1
30	7	309	CLA	O1A-CGA-O2A-C1
35	A	854	LMT	C9-C10-C11-C12
36	5	318	LMG	C30-C31-C32-C33
34	A	852	LHG	O6-C4-C5-O7
30	A	826	CLA	C16-C17-C18-C20
38	1	308	KC1	C4B-C3B-CAB-CBB
38	12	309	KC1	C4B-C3B-CAB-CBB
30	3	302	CLA	C3-C5-C6-C7
30	7	309	CLA	C3-C5-C6-C7
30	A	805	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	6	305	CLA	C4-C3-C5-C6
30	B	819	CLA	C10-C11-C12-C13
30	6	306	CLA	CAA-CBA-CGA-O2A
30	A	831	CLA	C2-C1-O2A-CGA
30	L	202	CLA	C2-C1-O2A-CGA
30	4	306	CLA	C2-C1-O2A-CGA
30	5	309	CLA	C2-C1-O2A-CGA
30	9	301	CLA	C2-C1-O2A-CGA
30	12	310	CLA	C2-C1-O2A-CGA
30	16	306	CLA	C2-C1-O2A-CGA
30	A	825	CLA	C11-C12-C13-C14
30	A	815	CLA	C13-C15-C16-C17
30	9	306	CLA	CAA-CBA-CGA-O1A
30	15	303	CLA	CAA-CBA-CGA-O2A
35	A	854	LMT	O1'-C1-C2-C3
30	A	837	CLA	C3A-C2A-CAA-CBA
30	B	812	CLA	C3A-C2A-CAA-CBA
30	B	851	CLA	C3A-C2A-CAA-CBA
30	4	304	CLA	C3A-C2A-CAA-CBA
30	6	307	CLA	C3A-C2A-CAA-CBA
30	14	302	CLA	C3A-C2A-CAA-CBA
30	15	304	CLA	C3A-C2A-CAA-CBA
37	10	316	A86	C11-C10-C9-C8
35	A	857	LMT	C2-C1-O1'-C1'
37	4	312	A86	O-C13-C14-C15
37	9	316	A86	O-C13-C14-C15
37	10	315	A86	O-C13-C14-C15
37	14	314	A86	O-C13-C14-C15
37	14	317	A86	O-C13-C14-C15
37	15	317	A86	O-C13-C14-C15
30	J	101	CLA	CAA-CBA-CGA-O2A
30	15	306	CLA	CAA-CBA-CGA-O2A
30	2	311	CLA	C4-C3-C5-C6
35	1	311	LMT	C5-C6-C7-C8
30	A	805	CLA	C6-C7-C8-C9
30	A	816	CLA	C6-C7-C8-C9
30	3	305	CLA	C6-C7-C8-C9
30	A	835	CLA	C5-C6-C7-C8
30	8	301	CLA	O1A-CGA-O2A-C1
36	A	856	LMG	C32-C33-C34-C35
33	L	204	BCR	C11-C10-C9-C34
36	7	320	LMG	C7-C8-C9-O8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	2u	203	A86	C-C1-C2-C3
37	2u	203	A86	C4-C5-C6-C7
37	2u	205	A86	C-C1-C2-C3
37	2u	205	A86	C4-C5-C6-C7
37	3	314	A86	C-C1-C2-C3
37	4	314	A86	C-C1-C2-C3
37	4	314	A86	C4-C5-C6-C7
37	7	319	A86	C-C1-C2-C3
37	7	319	A86	C4-C5-C6-C7
37	8	318	A86	C-C1-C2-C3
37	10	301	A86	C25-C26-C27-C28
37	11	301	A86	C-C1-C2-C3
37	11	301	A86	C4-C5-C6-C7
37	14	320	A86	C-C1-C2-C3
37	15	322	A86	C-C1-C2-C3
39	10	313	DD6	C9-C10-C11-C12
30	2	305	CLA	C3-C5-C6-C7
30	9	306	CLA	CAA-CBA-CGA-O2A
30	A	844	CLA	C2A-CAA-CBA-CGA
30	B	822	CLA	C2A-CAA-CBA-CGA
30	1	304	CLA	C8-C10-C11-C12
30	12	304	CLA	CAA-CBA-CGA-O1A
38	3	308	KC1	CAA-CBA-CGA-O2A
38	12	311	KC1	CAA-CBA-CGA-O1A
30	2	310	CLA	CBA-CGA-O2A-C1
30	2	311	CLA	CBA-CGA-O2A-C1
30	7	309	CLA	CBA-CGA-O2A-C1
30	15	305	CLA	CAA-CBA-CGA-O1A
33	B	841	BCR	C36-C18-C19-C20
33	L	201	BCR	C11-C12-C13-C35
30	6	314	CLA	CBD-CGD-O2D-CED
37	4	312	A86	C5-C6-C8-C9
30	15	306	CLA	CAA-CBA-CGA-O1A
30	A	842	CLA	C13-C15-C16-C17
30	A	802	CLA	C1A-C2A-CAA-CBA
30	A	814	CLA	C1A-C2A-CAA-CBA
30	A	817	CLA	C1A-C2A-CAA-CBA
30	B	820	CLA	C1A-C2A-CAA-CBA
30	B	825	CLA	C1A-C2A-CAA-CBA
30	1	303	CLA	C1A-C2A-CAA-CBA
30	4	309	CLA	C1A-C2A-CAA-CBA
30	15	310	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
35	11	317	LMT	C5'-C4'-O1B-C1B
30	A	803	CLA	C2-C3-C5-C6
30	A	812	CLA	C6-C7-C8-C10
30	5	302	CLA	C11-C10-C8-C7
30	5	309	CLA	C11-C10-C8-C7
30	13	302	CLA	C11-C10-C8-C7
30	16	303	CLA	C12-C13-C15-C16
31	A	845	PQN	C17-C18-C20-C21
30	A	842	CLA	O1A-CGA-O2A-C1
30	J	101	CLA	CAA-CBA-CGA-O1A
39	6	303	DD6	C3-C4-C5-C6
34	A	852	LHG	C34-C35-C36-C37
30	13	304	CLA	CAA-CBA-CGA-O1A
35	12	301	LMT	O1'-C1-C2-C3
30	6	310	CLA	C2A-CAA-CBA-CGA
30	9	306	CLA	C2A-CAA-CBA-CGA
30	B	808	CLA	C8-C10-C11-C12
30	B	828	CLA	C8-C10-C11-C12
30	10	308	CLA	C15-C16-C17-C18
38	1	306	KC1	O1D-CGD-O2D-CED
30	B	801	CLA	C5-C6-C7-C8
30	6	304	CLA	C10-C11-C12-C13
30	A	842	CLA	CBA-CGA-O2A-C1
38	1	306	KC1	C3A-C2A-CAA-CBA
38	2	306	KC1	C3A-C2A-CAA-CBA
38	3	304	KC1	C3A-C2A-CAA-CBA
38	5	306	KC1	C3A-C2A-CAA-CBA
38	9	311	KC1	C3A-C2A-CAA-CBA
38	10	312	KC1	C3A-C2A-CAA-CBA
38	14	306	KC1	C3A-C2A-CAA-CBA
30	B	814	CLA	CBD-CGD-O2D-CED
30	A	816	CLA	C16-C17-C18-C20
30	A	844	CLA	C16-C17-C18-C19
30	B	825	CLA	C5-C6-C7-C8
30	9	305	CLA	C13-C15-C16-C17
30	B	824	CLA	C4-C3-C5-C6
30	B	826	CLA	C4-C3-C5-C6
30	12	303	CLA	C4-C3-C5-C6
30	12	312	CLA	C4-C3-C5-C6
30	5	311	CLA	C10-C11-C12-C13
38	14	306	KC1	C2C-C3C-CAC-CBC
30	16	302	CLA	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	16	306	CLA	O1D-CGD-O2D-CED
33	A	847	BCR	C11-C10-C9-C8
33	A	849	BCR	C11-C10-C9-C8
33	B	842	BCR	C11-C10-C9-C8
37	2u	203	A86	C24-C1-C2-C3
37	2u	203	A86	C4-C5-C6-C8
37	2u	205	A86	C24-C1-C2-C3
37	2u	205	A86	C4-C5-C6-C8
37	3	314	A86	C24-C1-C2-C3
37	4	314	A86	C24-C1-C2-C3
37	4	314	A86	C4-C5-C6-C8
37	7	319	A86	C24-C1-C2-C3
37	7	319	A86	C4-C5-C6-C8
37	9	316	A86	C13-C14-C15-C16
37	10	301	A86	C25-C26-C27-C29
37	11	301	A86	C24-C1-C2-C3
37	11	301	A86	C4-C5-C6-C8
37	14	301	A86	C13-C14-C15-C16
37	14	320	A86	C24-C1-C2-C3
37	15	322	A86	C24-C1-C2-C3
37	16	312	A86	C13-C14-C15-C16
37	16	314	A86	C13-C14-C15-C16
39	3	312	DD6	C24-C1-C2-C3
39	5	313	DD6	C24-C1-C2-C3
30	F	203	CLA	CAA-CBA-CGA-O2A
36	2u	204	LMG	O7-C8-C9-O8
38	8	310	KC1	CAA-CBA-CGA-O2A
33	A	847	BCR	C15-C16-C17-C18
33	A	848	BCR	C15-C16-C17-C18
37	5	315	A86	C11-C10-C9-C8
37	14	316	A86	C11-C10-C9-C8
37	15	317	A86	C1-C2-C3-C4
39	3	316	DD6	C24-C25-C26-C27
30	F	203	CLA	CAA-CBA-CGA-O1A
30	12	304	CLA	C13-C15-C16-C17
30	10	305	CLA	O1A-CGA-O2A-C1
37	2	319	A86	C10-C11-C13-C14
37	3	314	A86	C10-C11-C13-C14
37	4	312	A86	C10-C11-C13-C14
37	4	314	A86	C10-C11-C13-C14
37	8	318	A86	C10-C11-C13-C14
37	10	302	A86	C10-C11-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	10	317	A86	C10-C11-C13-C14
37	11	301	A86	C10-C11-C13-C14
37	11	314	A86	C10-C11-C13-C14
37	13	313	A86	C10-C11-C13-C14
37	13	315	A86	C10-C11-C13-C14
37	15	321	A86	C10-C11-C13-C14
30	15	307	CLA	O1D-CGD-O2D-CED
30	2	305	CLA	C4-C3-C5-C6
35	A	854	LMT	C3'-C4'-O1B-C1B
30	A	810	CLA	C2-C1-O2A-CGA
30	A	813	CLA	C2-C1-O2A-CGA
30	A	818	CLA	C2-C1-O2A-CGA
30	B	814	CLA	C2-C1-O2A-CGA
30	B	829	CLA	C2-C1-O2A-CGA
30	B	830	CLA	C2-C1-O2A-CGA
30	1	304	CLA	C2-C1-O2A-CGA
30	6	309	CLA	C2-C1-O2A-CGA
30	7	303	CLA	C2-C1-O2A-CGA
30	7	306	CLA	C2-C1-O2A-CGA
30	9	309	CLA	C2-C1-O2A-CGA
30	A	816	CLA	C2-C3-C5-C6
30	F	202	CLA	C2-C3-C5-C6
30	6	305	CLA	C2-C3-C5-C6
35	12	318	LMT	C4-C5-C6-C7
30	A	829	CLA	C14-C13-C15-C16
30	A	831	CLA	C6-C7-C8-C9
30	B	822	CLA	C11-C10-C8-C9
30	13	302	CLA	C11-C10-C8-C9
30	B	835	CLA	C5-C6-C7-C8
38	4	310	KC1	C1A-C2A-CAA-CBA
38	9	312	KC1	C1A-C2A-CAA-CBA
38	10	310	KC1	C1A-C2A-CAA-CBA
30	A	840	CLA	O1D-CGD-O2D-CED
30	5	302	CLA	C10-C11-C12-C13
30	2	301	CLA	C2A-CAA-CBA-CGA
30	15	310	CLA	CAA-CBA-CGA-O2A
33	A	847	BCR	C23-C24-C25-C30
33	A	849	BCR	C23-C24-C25-C30
33	B	842	BCR	C23-C24-C25-C30
33	B	843	BCR	C23-C24-C25-C30
33	B	845	BCR	C23-C24-C25-C30
33	F	204	BCR	C23-C24-C25-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	I	101	BCR	C23-C24-C25-C30
33	J	102	BCR	C23-C24-C25-C30
37	3	314	A86	C24-C25-C26-C27
37	6	320	A86	C1-C2-C3-C4
37	9	315	A86	C1-C2-C3-C4
37	14	314	A86	C3-C4-C5-C6
39	9	314	DD6	C24-C25-C26-C27
30	A	810	CLA	C4-C3-C5-C6
30	2	304	CLA	C4-C3-C5-C6
30	12	310	CLA	C4-C3-C5-C6
30	14	307	CLA	C4-C3-C5-C6
37	10	317	A86	C35-C34-O4-C38
39	4	313	DD6	C2-C1-C24-C25
30	2	311	CLA	C2-C3-C5-C6
30	8	303	CLA	C2-C3-C5-C6
30	11	310	CLA	C2-C3-C5-C6
30	14	312	CLA	CAA-CBA-CGA-O2A
30	B	805	CLA	C8-C10-C11-C12
36	3	317	LMG	C8-C7-O1-C1
38	12	305	KC1	CAA-CBA-CGA-O2A
30	B	832	CLA	C16-C17-C18-C20
30	6	314	CLA	C10-C11-C12-C13
30	6	317	CLA	C10-C11-C12-C13
35	7	301	LMT	O5B-C1B-O1B-C4'
38	8	307	KC1	O1D-CGD-O2D-CED
30	14	309	CLA	CAA-CBA-CGA-O2A
30	L	202	CLA	C2A-CAA-CBA-CGA
30	A	833	CLA	CBD-CGD-O2D-CED
30	5	307	CLA	CBA-CGA-O2A-C1
30	14	307	CLA	C8-C10-C11-C12
30	13	307	CLA	C3-C5-C6-C7
30	3	310	CLA	CAA-CBA-CGA-O2A
30	15	310	CLA	CAA-CBA-CGA-O1A
38	12	311	KC1	CAA-CBA-CGA-O2A
30	B	826	CLA	C15-C16-C17-C18
36	B	847	LMG	C35-C36-C37-C38
36	A	856	LMG	O8-C28-C29-C30
30	11	308	CLA	C4-C3-C5-C6
30	A	805	CLA	C2-C3-C5-C6
30	A	810	CLA	C2-C3-C5-C6
30	1	302	CLA	C11-C10-C8-C7
30	15	304	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	15	312	CLA	CBD-CGD-O2D-CED
34	6	322	LHG	O1-C1-C2-O2
33	A	849	BCR	C19-C20-C21-C22
37	10	317	A86	C11-C10-C9-C8
39	13	314	DD6	C24-C25-C26-C27
38	12	305	KC1	CAA-CBA-CGA-O1A
30	13	309	CLA	CAA-CBA-CGA-O2A
30	1	301	CLA	O1D-CGD-O2D-CED
30	10	309	CLA	CBD-CGD-O2D-CED
30	B	829	CLA	C13-C15-C16-C17
30	2	304	CLA	C5-C6-C7-C8
30	15	311	CLA	CAA-CBA-CGA-O2A
30	B	838	CLA	C2A-CAA-CBA-CGA
35	11	318	LMT	O5B-C1B-O1B-C4'
30	B	808	CLA	C15-C16-C17-C18
30	A	829	CLA	C16-C17-C18-C19
38	8	310	KC1	CAA-CBA-CGA-O1A
36	8	319	LMG	C37-C38-C39-C40
30	7	303	CLA	C15-C16-C17-C18
33	A	847	BCR	C35-C13-C14-C15
33	B	842	BCR	C11-C10-C9-C34
33	B	845	BCR	C20-C21-C22-C37
39	4	313	DD6	C4-C5-C6-C7
39	6	319	DD6	C4-C5-C6-C7
30	B	821	CLA	CAA-CBA-CGA-O2A
30	2	308	CLA	CAA-CBA-CGA-O2A
30	A	830	CLA	C3-C5-C6-C7
30	B	808	CLA	C4-C3-C5-C6
30	B	812	CLA	C4-C3-C5-C6
30	B	829	CLA	C4-C3-C5-C6
30	5	307	CLA	C4-C3-C5-C6
30	9	308	CLA	C4-C3-C5-C6
30	13	307	CLA	C4-C3-C5-C6
30	1	301	CLA	C8-C10-C11-C12
30	16	308	CLA	CAA-CBA-CGA-O2A
30	B	826	CLA	C2-C3-C5-C6
30	1	303	CLA	C2-C3-C5-C6
30	12	310	CLA	C2-C3-C5-C6
30	A	803	CLA	CBA-CGA-O2A-C1
30	B	813	CLA	C4C-C3C-CAC-CBC
30	A	802	CLA	C6-C7-C8-C9
30	A	812	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	A	816	CLA	C11-C10-C8-C9
30	A	820	CLA	C11-C12-C13-C14
30	A	828	CLA	C6-C7-C8-C9
30	A	834	CLA	C11-C12-C13-C14
30	A	839	CLA	C14-C13-C15-C16
30	B	813	CLA	C11-C10-C8-C9
30	B	825	CLA	C14-C13-C15-C16
30	B	826	CLA	C14-C13-C15-C16
30	2u	202	CLA	C6-C7-C8-C9
30	9	307	CLA	C6-C7-C8-C9
30	16	303	CLA	C14-C13-C15-C16
30	A	812	CLA	C3A-C2A-CAA-CBA
30	A	818	CLA	C3A-C2A-CAA-CBA
30	B	802	CLA	C3A-C2A-CAA-CBA
30	B	803	CLA	C3A-C2A-CAA-CBA
30	6	306	CLA	C3A-C2A-CAA-CBA
30	6	309	CLA	C3A-C2A-CAA-CBA
30	12	312	CLA	C3A-C2A-CAA-CBA
30	15	310	CLA	C3A-C2A-CAA-CBA
30	B	831	CLA	O1A-CGA-O2A-C1
30	A	814	CLA	CAA-CBA-CGA-O2A
30	B	813	CLA	CAA-CBA-CGA-O2A
30	2	313	CLA	CAA-CBA-CGA-O2A
30	13	309	CLA	CAA-CBA-CGA-O1A
30	15	305	CLA	CAA-CBA-CGA-O2A
30	A	811	CLA	CAD-CBD-CGD-O2D
30	A	818	CLA	CAD-CBD-CGD-O2D
30	A	831	CLA	CAD-CBD-CGD-O2D
30	A	832	CLA	CAD-CBD-CGD-O2D
30	B	810	CLA	CAD-CBD-CGD-O2D
30	B	813	CLA	CAD-CBD-CGD-O2D
30	B	851	CLA	CAD-CBD-CGD-O2D
30	F	202	CLA	CAD-CBD-CGD-O2D
30	F	203	CLA	CAD-CBD-CGD-O2D
30	2	304	CLA	CAD-CBD-CGD-O2D
30	2	308	CLA	CAD-CBD-CGD-O2D
30	2	311	CLA	CAD-CBD-CGD-O2D
30	3	307	CLA	CAD-CBD-CGD-O2D
30	3	310	CLA	CAD-CBD-CGD-O2D
30	4	311	CLA	CAD-CBD-CGD-O2D
30	5	308	CLA	CAD-CBD-CGD-O2D
30	9	302	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	9	306	CLA	CAD-CBD-CGD-O2D
30	9	308	CLA	CAD-CBD-CGD-O2D
30	10	305	CLA	CAD-CBD-CGD-O2D
30	10	311	CLA	CAD-CBD-CGD-O2D
30	11	309	CLA	CAD-CBD-CGD-O2D
30	12	304	CLA	CAD-CBD-CGD-O2D
30	12	321	CLA	CAD-CBD-CGD-O2D
30	14	310	CLA	CAD-CBD-CGD-O2D
30	15	303	CLA	CAD-CBD-CGD-O2D
30	15	307	CLA	CAD-CBD-CGD-O2D
30	16	303	CLA	CAD-CBD-CGD-O2D
30	16	305	CLA	CAD-CBD-CGD-O2D
34	B	848	LHG	C4-C5-O7-C7
34	B	848	LHG	C6-C5-O7-C7
37	12	316	A86	C28-C27-C29-C30
37	14	317	A86	C28-C27-C29-C30
37	15	323	A86	C28-C27-C29-C30
38	3	304	KC1	CAD-CBD-CGD-O2D
38	3	311	KC1	CAD-CBD-CGD-O2D
38	10	312	KC1	CAD-CBD-CGD-O2D
38	13	311	KC1	CAD-CBD-CGD-O2D
30	B	813	CLA	C2C-C3C-CAC-CBC
30	A	810	CLA	C10-C11-C12-C13
30	10	309	CLA	C10-C11-C12-C13
39	2	317	DD6	C24-C25-C26-C27
34	A	853	LHG	O9-C7-O7-C5
30	2	309	CLA	C2-C1-O2A-CGA
30	16	310	CLA	CAA-CBA-CGA-O2A
30	A	828	CLA	CAA-CBA-CGA-O2A
30	A	830	CLA	CAA-CBA-CGA-O2A
30	B	830	CLA	CAA-CBA-CGA-O2A
30	2	303	CLA	CAA-CBA-CGA-O2A
30	7	312	CLA	CAA-CBA-CGA-O2A
30	11	310	CLA	CAA-CBA-CGA-O2A
36	B	847	LMG	O7-C10-C11-C12
36	3	317	LMG	C31-C32-C33-C34
33	M	101	BCR	C22-C23-C24-C25
30	B	825	CLA	C4-C3-C5-C6
30	B	832	CLA	C4-C3-C5-C6
30	4	303	CLA	C4-C3-C5-C6
30	7	309	CLA	C4-C3-C5-C6
30	8	308	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	3	310	CLA	CAA-CBA-CGA-O1A
30	14	309	CLA	CAA-CBA-CGA-O1A
30	2	304	CLA	C2-C3-C5-C6
30	5	307	CLA	C2-C3-C5-C6
30	12	303	CLA	C2-C3-C5-C6
30	12	312	CLA	C2-C3-C5-C6
30	14	307	CLA	C2-C3-C5-C6
30	A	806	CLA	CAA-CBA-CGA-O2A
30	B	809	CLA	CAA-CBA-CGA-O2A
30	11	306	CLA	CAA-CBA-CGA-O2A
34	A	852	LHG	O8-C23-C24-C25
37	3	314	A86	C5-C6-C8-C9
39	2	316	DD6	C2-C1-C24-C25
39	2	316	DD6	C10-C11-C13-C14
39	9	314	DD6	C5-C6-C8-C9
34	A	852	LHG	C4-C5-C6-O8
37	2	319	A86	C12-C11-C13-O
37	3	314	A86	C12-C11-C13-O
37	4	312	A86	C12-C11-C13-O
37	12	314	A86	C12-C11-C13-O
37	14	318	A86	C12-C11-C13-O
37	15	322	A86	C12-C11-C13-O
39	7	314	DD6	C13-C14-C15-O1
39	9	314	DD6	C13-C14-C15-O1
30	A	837	CLA	CAA-CBA-CGA-O2A
30	14	304	CLA	CAA-CBA-CGA-O2A
30	B	826	CLA	C8-C10-C11-C12
30	B	803	CLA	CAA-CBA-CGA-O2A
30	1	303	CLA	CAA-CBA-CGA-O2A
30	10	307	CLA	CAA-CBA-CGA-O2A
30	14	312	CLA	CAA-CBA-CGA-O1A
30	15	311	CLA	CAA-CBA-CGA-O1A
30	16	310	CLA	CAA-CBA-CGA-O1A
30	B	817	CLA	O2A-C1-C2-C3
30	B	821	CLA	O2A-C1-C2-C3
30	B	830	CLA	O2A-C1-C2-C3
30	2	301	CLA	O2A-C1-C2-C3
30	6	317	CLA	O2A-C1-C2-C3
30	15	304	CLA	O2A-C1-C2-C3
30	5	307	CLA	O1A-CGA-O2A-C1
38	11	311	KC1	C4B-C3B-CAB-CBB
30	10	303	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	A	837	CLA	CAA-CBA-CGA-O1A
29	A	801	CL0	C16-C17-C18-C19
30	A	826	CLA	C16-C17-C18-C19
30	B	813	CLA	C16-C17-C18-C19
30	A	803	CLA	CHA-CBD-CGD-O2D
30	A	804	CLA	CHA-CBD-CGD-O1D
30	A	807	CLA	CHA-CBD-CGD-O1D
30	A	807	CLA	CHA-CBD-CGD-O2D
30	A	809	CLA	CHA-CBD-CGD-O1D
30	A	809	CLA	CHA-CBD-CGD-O2D
30	A	828	CLA	CHA-CBD-CGD-O1D
30	A	831	CLA	CHA-CBD-CGD-O2D
30	A	839	CLA	CHA-CBD-CGD-O2D
30	B	804	CLA	CHA-CBD-CGD-O1D
30	B	815	CLA	CHA-CBD-CGD-O2D
30	B	820	CLA	CHA-CBD-CGD-O1D
30	B	822	CLA	CHA-CBD-CGD-O1D
30	B	822	CLA	CHA-CBD-CGD-O2D
30	F	201	CLA	CHA-CBD-CGD-O1D
30	F	201	CLA	CHA-CBD-CGD-O2D
30	7	310	CLA	CHA-CBD-CGD-O1D
30	7	310	CLA	CHA-CBD-CGD-O2D
30	7	312	CLA	CHA-CBD-CGD-O2D
30	8	301	CLA	CHA-CBD-CGD-O2D
30	8	305	CLA	CHA-CBD-CGD-O2D
30	9	302	CLA	CHA-CBD-CGD-O1D
30	9	305	CLA	CHA-CBD-CGD-O1D
30	11	306	CLA	CHA-CBD-CGD-O1D
30	11	306	CLA	CHA-CBD-CGD-O2D
30	13	304	CLA	CHA-CBD-CGD-O2D
30	14	303	CLA	CHA-CBD-CGD-O1D
30	14	307	CLA	CHA-CBD-CGD-O1D
30	14	307	CLA	CHA-CBD-CGD-O2D
30	15	308	CLA	CHA-CBD-CGD-O1D
30	15	312	CLA	CHA-CBD-CGD-O2D
38	1	306	KC1	CHA-CBD-CGD-O2D
38	1	308	KC1	CHA-CBD-CGD-O1D
38	1	308	KC1	CHA-CBD-CGD-O2D
38	8	310	KC1	CHA-CBD-CGD-O1D
38	8	310	KC1	CHA-CBD-CGD-O2D
38	13	312	KC1	CHA-CBD-CGD-O1D
38	13	312	KC1	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
38	14	306	KC1	CHA-CBD-CGD-O1D
30	2	313	CLA	CAA-CBA-CGA-O1A
30	14	304	CLA	CAA-CBA-CGA-O1A
30	B	823	CLA	C4-C3-C5-C6
30	B	808	CLA	C2-C3-C5-C6
30	8	308	CLA	C2-C3-C5-C6
30	A	841	CLA	C8-C10-C11-C12
38	16	311	KC1	C4C-C3C-CAC-CBC
30	B	804	CLA	CAA-CBA-CGA-O2A
30	2u	202	CLA	CAA-CBA-CGA-O2A
30	12	308	CLA	CAA-CBA-CGA-O2A
30	16	301	CLA	CAA-CBA-CGA-O2A
30	16	306	CLA	CAA-CBA-CGA-O2A
36	5	318	LMG	O8-C28-C29-C30
36	3	317	LMG	O1-C7-C8-O7
37	10	317	A86	C33-C34-O4-C38
30	A	833	CLA	O1D-CGD-O2D-CED
30	1	301	CLA	CAA-CBA-CGA-O2A
30	1	307	CLA	CAA-CBA-CGA-O2A
30	3	305	CLA	CAA-CBA-CGA-O2A
30	10	311	CLA	CAA-CBA-CGA-O2A
37	2u	203	A86	C13-C14-C15-O1
37	1	309	A86	C13-C14-C15-O1
37	2	319	A86	C13-C14-C15-O1
37	3	314	A86	C10-C11-C13-O
37	4	312	A86	C10-C11-C13-O
37	4	314	A86	C10-C11-C13-O
37	8	315	A86	C13-C14-C15-O1
37	8	318	A86	C10-C11-C13-O
37	8	318	A86	C13-C14-C15-O1
37	9	316	A86	C10-C11-C13-O
37	10	301	A86	C13-C14-C15-O1
37	10	317	A86	C10-C11-C13-O
37	11	314	A86	C10-C11-C13-O
37	11	315	A86	C13-C14-C15-O1
37	13	313	A86	C13-C14-C15-O1
37	13	315	A86	C10-C11-C13-O
37	13	315	A86	C13-C14-C15-O1
37	14	314	A86	C13-C14-C15-O1
37	14	315	A86	C13-C14-C15-O1
37	14	319	A86	C13-C14-C15-O1
37	15	317	A86	C10-C11-C13-O

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	15	321	A86	C10-C11-C13-O
37	15	323	A86	C10-C11-C13-O
30	4	309	CLA	C5-C6-C7-C8
30	6	317	CLA	C8-C10-C11-C12
30	16	301	CLA	CBA-CGA-O2A-C1
30	2u	202	CLA	C4-C3-C5-C6
30	6	314	CLA	O1D-CGD-O2D-CED
30	A	826	CLA	C15-C16-C17-C18
36	8	319	LMG	O9-C10-C11-C12
30	A	826	CLA	C11-C10-C8-C7
30	A	827	CLA	C12-C13-C15-C16
30	B	825	CLA	C12-C13-C15-C16
30	5	304	CLA	C11-C12-C13-C15
30	5	308	CLA	C12-C13-C15-C16
30	8	301	CLA	C12-C13-C15-C16
30	13	302	CLA	C11-C12-C13-C15
30	15	302	CLA	C6-C7-C8-C10
30	B	807	CLA	CAA-CBA-CGA-O2A
30	6	316	CLA	CAA-CBA-CGA-O2A
30	13	301	CLA	CAA-CBA-CGA-O2A
30	B	851	CLA	C14-C13-C15-C16
30	1	307	CLA	C11-C12-C13-C14
30	5	302	CLA	C11-C10-C8-C9
30	5	308	CLA	C14-C13-C15-C16
30	8	302	CLA	C6-C7-C8-C9
30	9	309	CLA	C14-C13-C15-C16
30	13	302	CLA	C11-C12-C13-C14
31	A	845	PQN	C19-C18-C20-C21
34	B	848	LHG	O8-C23-C24-C25
39	1	310	DD6	C24-C25-C26-C27
39	4	313	DD6	C1-C2-C3-C4
36	B	847	LMG	C20-C21-C22-C23
30	15	308	CLA	CAA-CBA-CGA-O2A
30	16	308	CLA	CAA-CBA-CGA-O1A
30	4	301	CLA	CAA-CBA-CGA-O2A
30	8	301	CLA	CAA-CBA-CGA-O2A
30	B	832	CLA	C16-C17-C18-C19
30	9	301	CLA	C16-C17-C18-C20
30	A	843	CLA	C2A-CAA-CBA-CGA
30	B	807	CLA	C2A-CAA-CBA-CGA
30	14	305	CLA	C2A-CAA-CBA-CGA
30	B	831	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	L	203	CLA	CAA-CBA-CGA-O1A
30	2	304	CLA	C15-C16-C17-C18
30	1	307	CLA	C4-C3-C5-C6
30	F	202	CLA	O1A-CGA-O2A-C1
30	A	822	CLA	C2-C3-C5-C6
30	B	813	CLA	CAA-CBA-CGA-O1A
30	10	307	CLA	CAA-CBA-CGA-O1A
30	11	310	CLA	CAA-CBA-CGA-O1A
37	2	318	A86	C5-C6-C8-C9
37	11	301	A86	C2-C1-C24-C25
39	6	318	DD6	C5-C6-C8-C9
30	2	305	CLA	C13-C15-C16-C17
30	A	837	CLA	C1A-C2A-CAA-CBA
30	B	803	CLA	C1A-C2A-CAA-CBA
30	B	812	CLA	C1A-C2A-CAA-CBA
30	B	851	CLA	C1A-C2A-CAA-CBA
30	6	307	CLA	C1A-C2A-CAA-CBA
30	8	308	CLA	C1A-C2A-CAA-CBA
30	14	302	CLA	C1A-C2A-CAA-CBA
30	14	309	CLA	C1A-C2A-CAA-CBA
30	15	304	CLA	C1A-C2A-CAA-CBA
34	A	852	LHG	C33-C34-C35-C36
30	B	809	CLA	CAA-CBA-CGA-O1A
30	B	817	CLA	CAA-CBA-CGA-O1A
30	15	308	CLA	O1D-CGD-O2D-CED
30	B	802	CLA	C2-C1-O2A-CGA
30	2	303	CLA	C2-C1-O2A-CGA
30	8	301	CLA	C2-C1-O2A-CGA
30	A	814	CLA	CAA-CBA-CGA-O1A
30	2	303	CLA	CAA-CBA-CGA-O1A
30	7	312	CLA	CAA-CBA-CGA-O1A
30	A	814	CLA	C2A-CAA-CBA-CGA
30	7	307	CLA	C16-C17-C18-C19
30	B	821	CLA	CAA-CBA-CGA-O1A
30	1	303	CLA	CAA-CBA-CGA-O1A
30	11	306	CLA	CAA-CBA-CGA-O1A
30	A	839	CLA	C5-C6-C7-C8
30	7	311	CLA	C5-C6-C7-C8
30	3	302	CLA	O1A-CGA-O2A-C1
30	15	312	CLA	O1D-CGD-O2D-CED
30	A	808	CLA	CAA-CBA-CGA-O2A
30	B	835	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
35	A	854	LMT	C4-C5-C6-C7
30	A	806	CLA	CAA-CBA-CGA-O1A
30	2	308	CLA	CAA-CBA-CGA-O1A
30	12	308	CLA	CAA-CBA-CGA-O1A
30	13	301	CLA	CAA-CBA-CGA-O1A
30	A	844	CLA	C15-C16-C17-C18
30	1	305	CLA	C10-C11-C12-C13
30	12	302	CLA	C5-C6-C7-C8
34	A	853	LHG	C3-O3-P-O5
34	9	318	LHG	C10-C11-C12-C13
36	B	847	LMG	C24-C25-C26-C27
30	B	803	CLA	CAA-CBA-CGA-O1A
34	A	852	LHG	O10-C23-C24-C25
30	A	841	CLA	CAA-CBA-CGA-O2A
30	2	301	CLA	C13-C15-C16-C17
30	6	314	CLA	O1A-CGA-O2A-C1
39	11	313	DD6	C9-C10-C11-C12
33	A	847	BCR	C23-C24-C25-C26
33	A	849	BCR	C23-C24-C25-C26
33	B	842	BCR	C23-C24-C25-C26
33	F	204	BCR	C23-C24-C25-C26
33	J	102	BCR	C23-C24-C25-C26
30	9	303	CLA	C13-C15-C16-C17
30	12	303	CLA	C15-C16-C17-C18
39	7	314	DD6	C11-C13-C14-C15
39	10	313	DD6	C11-C13-C14-C15
39	12	317	DD6	C11-C13-C14-C15
39	13	314	DD6	C11-C13-C14-C15
39	16	313	DD6	C11-C13-C14-C15
30	A	828	CLA	CAA-CBA-CGA-O1A
30	1	301	CLA	CAA-CBA-CGA-O1A
30	B	851	CLA	O1A-CGA-O2A-C1
30	7	306	CLA	C16-C17-C18-C20
30	6	316	CLA	CAA-CBA-CGA-O1A
30	16	301	CLA	CAA-CBA-CGA-O1A
30	16	306	CLA	CAA-CBA-CGA-O1A
36	7	320	LMG	O9-C10-C11-C12
30	2	301	CLA	C5-C6-C7-C8
30	16	303	CLA	C5-C6-C7-C8
35	8	322	LMT	C6-C7-C8-C9
30	A	816	CLA	CAA-CBA-CGA-O2A
30	10	303	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	F	202	CLA	CBA-CGA-O2A-C1
30	B	812	CLA	C2-C3-C5-C6
30	10	311	CLA	CAA-CBA-CGA-O1A
30	15	308	CLA	CAA-CBA-CGA-O1A
30	A	814	CLA	CAD-CBD-CGD-O1D
30	A	828	CLA	CAD-CBD-CGD-O1D
30	A	839	CLA	CAD-CBD-CGD-O1D
30	B	805	CLA	CAD-CBD-CGD-O1D
30	B	818	CLA	CAD-CBD-CGD-O1D
30	B	828	CLA	CAD-CBD-CGD-O1D
30	2u	202	CLA	CAD-CBD-CGD-O1D
30	1	304	CLA	CAD-CBD-CGD-O1D
30	8	303	CLA	CAD-CBD-CGD-O1D
30	9	301	CLA	CAD-CBD-CGD-O1D
30	9	305	CLA	CAD-CBD-CGD-O1D
30	13	303	CLA	CAD-CBD-CGD-O1D
30	14	307	CLA	CAD-CBD-CGD-O1D
37	7	315	A86	C26-C27-C29-C30
37	12	316	A86	C26-C27-C29-C30
37	15	323	A86	C26-C27-C29-C30
38	13	312	KC1	CAD-CBD-CGD-O1D
30	B	830	CLA	CAA-CBA-CGA-O1A
30	B	839	CLA	CAA-CBA-CGA-O2A
36	8	319	LMG	O7-C10-C11-C12
30	A	809	CLA	C10-C11-C12-C13
30	A	842	CLA	C5-C6-C7-C8
30	A	804	CLA	C14-C13-C15-C16
30	A	826	CLA	C11-C10-C8-C9
30	A	827	CLA	C14-C13-C15-C16
30	A	839	CLA	C11-C10-C8-C9
30	B	851	CLA	C6-C7-C8-C9
30	2	309	CLA	C6-C7-C8-C9
30	5	302	CLA	C6-C7-C8-C9
30	6	306	CLA	C11-C10-C8-C9
30	8	301	CLA	C14-C13-C15-C16
30	14	307	CLA	C14-C13-C15-C16
35	9	317	LMT	C4-C5-C6-C7
30	2u	202	CLA	CAA-CBA-CGA-O1A
36	5	318	LMG	O10-C28-C29-C30
30	6	314	CLA	CBA-CGA-O2A-C1
30	A	813	CLA	CAA-CBA-CGA-O2A
30	B	836	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	2	305	CLA	CAA-CBA-CGA-O2A
30	3	303	CLA	CAA-CBA-CGA-O2A
36	B	849	LMG	C33-C34-C35-C36
30	15	304	CLA	C4C-C3C-CAC-CBC
30	A	826	CLA	CAA-CBA-CGA-O2A
30	A	839	CLA	CAA-CBA-CGA-O2A
30	8	305	CLA	CAA-CBA-CGA-O2A
30	16	307	CLA	CAA-CBA-CGA-O2A
30	A	808	CLA	CAA-CBA-CGA-O1A
30	B	807	CLA	CAA-CBA-CGA-O1A
30	7	307	CLA	C16-C17-C18-C20
36	B	847	LMG	C41-C42-C43-C44
30	A	807	CLA	C12-C13-C15-C16
30	B	838	CLA	C11-C10-C8-C7
30	F	202	CLA	C6-C7-C8-C10
30	1	307	CLA	C11-C12-C13-C15
30	2	309	CLA	C6-C7-C8-C10
30	8	305	CLA	C3A-C2A-CAA-CBA
30	1	307	CLA	CAA-CBA-CGA-O1A
30	8	301	CLA	CAA-CBA-CGA-O1A
30	B	806	CLA	CAA-CBA-CGA-O2A
30	B	810	CLA	CAA-CBA-CGA-O2A
30	B	812	CLA	CAA-CBA-CGA-O2A
30	1	305	CLA	CAA-CBA-CGA-O2A
30	2	304	CLA	CAA-CBA-CGA-O2A
30	10	309	CLA	CAA-CBA-CGA-O2A
30	13	307	CLA	CAA-CBA-CGA-O2A
36	6	301	LMG	O7-C10-C11-C12
33	M	101	BCR	C17-C18-C19-C20
39	1	310	DD6	C5-C6-C8-C9
39	2	315	DD6	C10-C11-C13-C14
39	3	312	DD6	C10-C11-C13-C14
30	4	301	CLA	CAA-CBA-CGA-O1A
30	14	302	CLA	CAA-CBA-CGA-O1A
37	2u	203	A86	C3-C4-C5-C6
39	6	321	DD6	C24-C25-C26-C27
35	15	301	LMT	C5'-C4'-O1B-C1B
30	A	844	CLA	C16-C17-C18-C20
35	6	302	LMT	C2-C1-O1'-C1'
37	2	319	A86	O-C13-C14-C15
37	4	314	A86	O-C13-C14-C15
37	4	317	A86	O-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	5	301	A86	O-C13-C14-C15
37	8	318	A86	O-C13-C14-C15
37	10	316	A86	O-C13-C14-C15
37	12	314	A86	O-C13-C14-C15
37	12	316	A86	O-C13-C14-C15
37	15	321	A86	O-C13-C14-C15
30	2	301	CLA	CAA-CBA-CGA-O2A
30	10	304	CLA	CAA-CBA-CGA-O2A
34	9	318	LHG	O7-C7-C8-C9
36	2u	204	LMG	O8-C28-C29-C30
35	B	850	LMT	O5'-C1'-O1'-C1
31	B	840	PQN	C18-C20-C21-C22
30	B	806	CLA	CAA-CBA-CGA-O1A
30	B	810	CLA	CAA-CBA-CGA-O1A
30	B	835	CLA	CAA-CBA-CGA-O1A
30	B	836	CLA	CAA-CBA-CGA-O1A
30	2	304	CLA	CAA-CBA-CGA-O1A
30	3	305	CLA	CAA-CBA-CGA-O1A
30	10	303	CLA	CAA-CBA-CGA-O1A
30	16	307	CLA	CAA-CBA-CGA-O1A
30	B	851	CLA	CBA-CGA-O2A-C1
30	L	203	CLA	CAA-CBA-CGA-O2A
30	2	307	CLA	C8-C10-C11-C12
36	2u	204	LMG	C4-C5-C6-O5
30	5	307	CLA	CAA-CBA-CGA-O2A
30	9	308	CLA	CAA-CBA-CGA-O2A
30	14	302	CLA	CAA-CBA-CGA-O2A
38	16	311	KC1	C2C-C3C-CAC-CBC
30	2u	202	CLA	C8-C10-C11-C12
30	14	302	CLA	C8-C10-C11-C12
30	A	826	CLA	CAA-CBA-CGA-O1A
30	B	804	CLA	CAA-CBA-CGA-O1A
30	3	303	CLA	CAA-CBA-CGA-O1A
30	11	310	CLA	C13-C15-C16-C17
36	B	849	LMG	C11-C12-C13-C14
30	7	307	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

235 monomers are involved in 440 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	A	813	CLA	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	B	843	BCR	2	0
30	2	307	CLA	3	0
30	3	306	CLA	2	0
30	B	837	CLA	2	0
30	12	310	CLA	2	0
30	A	824	CLA	1	0
30	A	834	CLA	2	0
30	A	843	CLA	2	0
30	14	302	CLA	2	0
30	1	301	CLA	2	0
30	B	839	CLA	3	0
30	B	806	CLA	7	0
30	A	841	CLA	2	0
30	A	819	CLA	3	0
30	2	305	CLA	2	0
33	L	204	BCR	4	0
34	5	317	LHG	1	0
30	J	101	CLA	1	0
30	A	830	CLA	4	0
31	A	845	PQN	5	0
30	A	811	CLA	3	0
30	A	802	CLA	3	0
30	14	312	CLA	1	0
30	A	842	CLA	4	0
38	5	312	KC1	1	0
33	J	102	BCR	3	0
30	A	803	CLA	2	0
39	6	318	DD6	1	0
30	3	305	CLA	1	0
30	6	307	CLA	1	0
30	16	307	CLA	2	0
37	7	315	A86	1	0
30	A	814	CLA	3	0
35	11	303	LMT	1	0
33	L	201	BCR	2	0
30	A	826	CLA	4	0
30	14	305	CLA	1	0
30	12	302	CLA	1	0
30	B	831	CLA	2	0
37	11	315	A86	1	0
33	M	101	BCR	3	0
30	9	301	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	A	829	CLA	10	0
36	A	856	LMG	2	0
30	B	820	CLA	2	0
30	A	823	CLA	1	0
30	3	302	CLA	1	0
30	8	308	CLA	1	0
30	7	303	CLA	1	0
30	B	830	CLA	2	0
30	B	816	CLA	2	0
30	A	805	CLA	3	0
30	3	303	CLA	2	0
30	10	309	CLA	2	0
30	A	809	CLA	1	0
30	4	311	CLA	2	0
33	B	842	BCR	1	0
36	3	317	LMG	2	0
30	10	304	CLA	1	0
30	A	821	CLA	2	0
30	A	832	CLA	1	0
30	1	303	CLA	3	0
39	6	321	DD6	1	0
30	10	303	CLA	3	0
30	B	817	CLA	5	0
30	B	807	CLA	2	0
30	11	310	CLA	4	0
30	12	312	CLA	1	0
30	B	838	CLA	7	0
30	5	307	CLA	2	0
30	2	308	CLA	1	0
30	B	802	CLA	2	0
30	A	828	CLA	2	0
35	12	301	LMT	2	0
30	B	821	CLA	2	0
37	14	320	A86	1	0
30	7	311	CLA	2	0
33	J	103	BCR	4	0
30	A	844	CLA	1	0
39	13	314	DD6	1	0
30	A	804	CLA	4	0
30	B	828	CLA	5	0
30	15	307	CLA	1	0
30	10	308	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	12	308	CLA	4	0
30	9	307	CLA	4	0
30	B	823	CLA	1	0
30	B	826	CLA	5	0
30	1	307	CLA	2	0
30	15	303	CLA	3	0
30	B	803	CLA	1	0
33	B	841	BCR	1	0
30	3	310	CLA	2	0
30	8	302	CLA	2	0
30	8	305	CLA	2	0
30	6	306	CLA	2	0
30	B	819	CLA	2	0
30	11	308	CLA	2	0
34	A	853	LHG	1	0
30	4	305	CLA	1	0
30	A	833	CLA	6	0
33	A	847	BCR	3	0
38	5	310	KC1	1	0
36	8	319	LMG	1	0
37	4	315	A86	1	0
30	2	311	CLA	1	0
30	6	314	CLA	2	0
30	B	827	CLA	5	0
30	2	304	CLA	1	0
30	8	303	CLA	2	0
35	11	318	LMT	2	0
38	12	309	KC1	1	0
30	L	202	CLA	5	0
30	A	810	CLA	5	0
30	B	813	CLA	7	0
30	L	203	CLA	2	0
30	B	822	CLA	2	0
30	9	305	CLA	2	0
37	14	317	A86	1	0
30	7	306	CLA	3	0
30	16	301	CLA	6	0
30	B	824	CLA	3	0
33	B	845	BCR	2	0
30	9	308	CLA	2	0
30	A	807	CLA	2	0
36	B	847	LMG	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	2	303	CLA	4	0
30	B	804	CLA	2	0
30	B	835	CLA	4	0
30	2	301	CLA	1	0
30	7	309	CLA	6	0
30	9	302	CLA	1	0
38	3	304	KC1	1	0
30	A	835	CLA	2	0
38	16	304	KC1	1	0
33	B	844	BCR	2	0
30	4	302	CLA	1	0
30	A	822	CLA	3	0
35	6	302	LMT	2	0
30	13	307	CLA	4	0
30	B	815	CLA	2	0
30	A	820	CLA	6	0
35	7	321	LMT	1	0
30	B	836	CLA	4	0
30	15	313	CLA	4	0
30	B	809	CLA	7	0
33	A	850	BCR	2	0
36	B	849	LMG	1	0
30	7	304	CLA	1	0
35	11	317	LMT	2	0
33	F	204	BCR	3	0
30	A	816	CLA	4	0
30	B	834	CLA	2	0
39	6	319	DD6	1	0
30	3	301	CLA	1	0
30	1	302	CLA	3	0
30	A	839	CLA	6	0
30	12	303	CLA	2	0
37	8	315	A86	1	0
30	15	308	CLA	1	0
30	B	825	CLA	1	0
30	11	306	CLA	2	0
30	A	806	CLA	5	0
30	B	805	CLA	2	0
36	8	321	LMG	1	0
30	B	801	CLA	4	0
35	7	301	LMT	1	0
30	B	808	CLA	2	0

Continued on next page...

Continued from previous page...

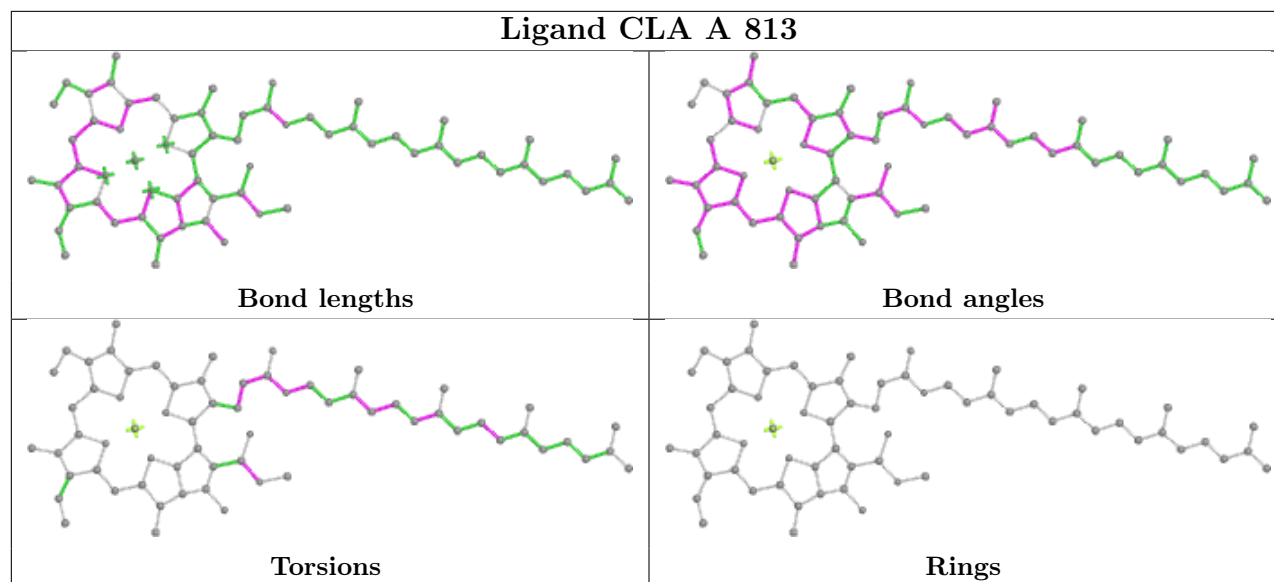
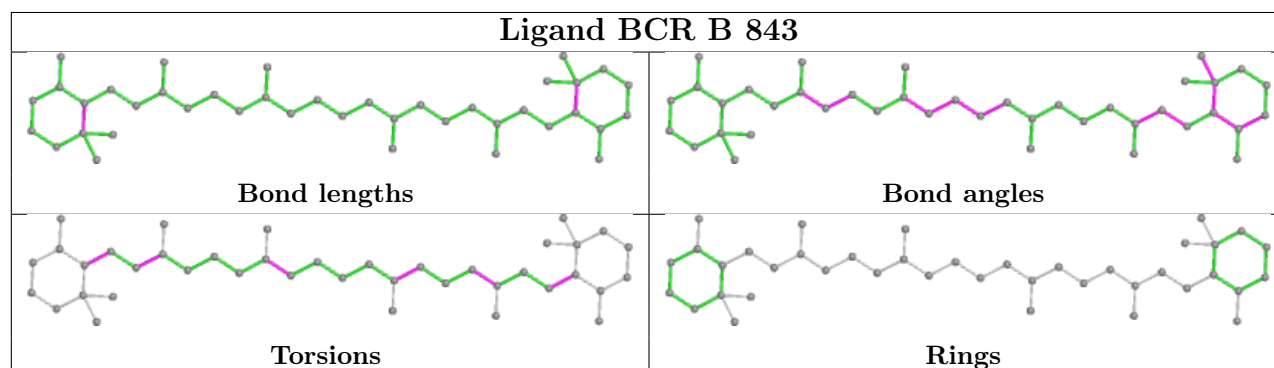
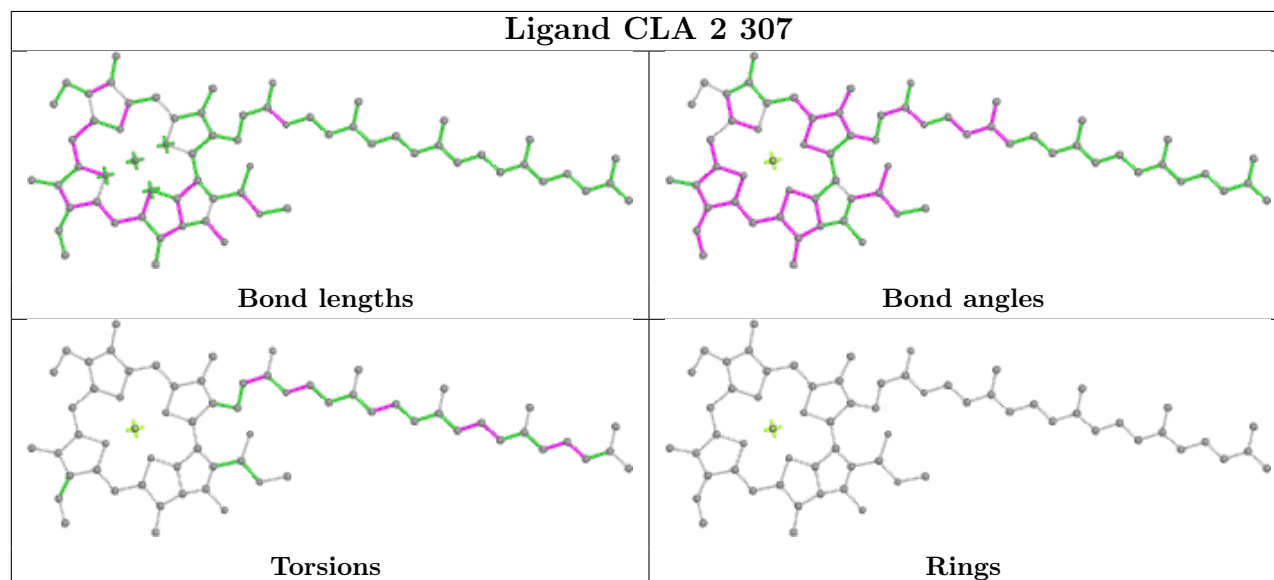
Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	F	202	CLA	3	0
36	14	321	LMG	2	0
30	A	817	CLA	3	0
30	2	310	CLA	1	0
30	10	305	CLA	1	0
33	B	846	BCR	4	0
30	A	838	CLA	1	0
35	A	857	LMT	1	0
30	B	833	CLA	1	0
38	4	310	KC1	1	0
30	15	304	CLA	2	0
35	12	319	LMT	1	0
30	B	818	CLA	1	0
30	1	304	CLA	2	0
30	9	306	CLA	2	0
30	6	316	CLA	5	0
30	A	836	CLA	3	0
30	B	811	CLA	4	0
30	10	307	CLA	1	0
33	A	848	BCR	2	0
35	A	855	LMT	2	0
30	5	304	CLA	2	0
30	15	302	CLA	4	0
30	5	303	CLA	4	0
30	15	309	CLA	2	0
30	F	201	CLA	6	0
30	A	831	CLA	5	0
33	A	849	BCR	4	0
30	16	302	CLA	1	0
39	10	313	DD6	1	0
30	14	307	CLA	1	0
30	11	304	CLA	3	0
30	16	309	CLA	1	0
30	16	310	CLA	1	0
37	9	316	A86	1	0
30	16	303	CLA	1	0
30	5	308	CLA	2	0
30	B	851	CLA	1	0
30	16	306	CLA	1	0
33	L	205	BCR	4	0
30	12	321	CLA	2	0
30	4	301	CLA	3	0

Continued on next page...

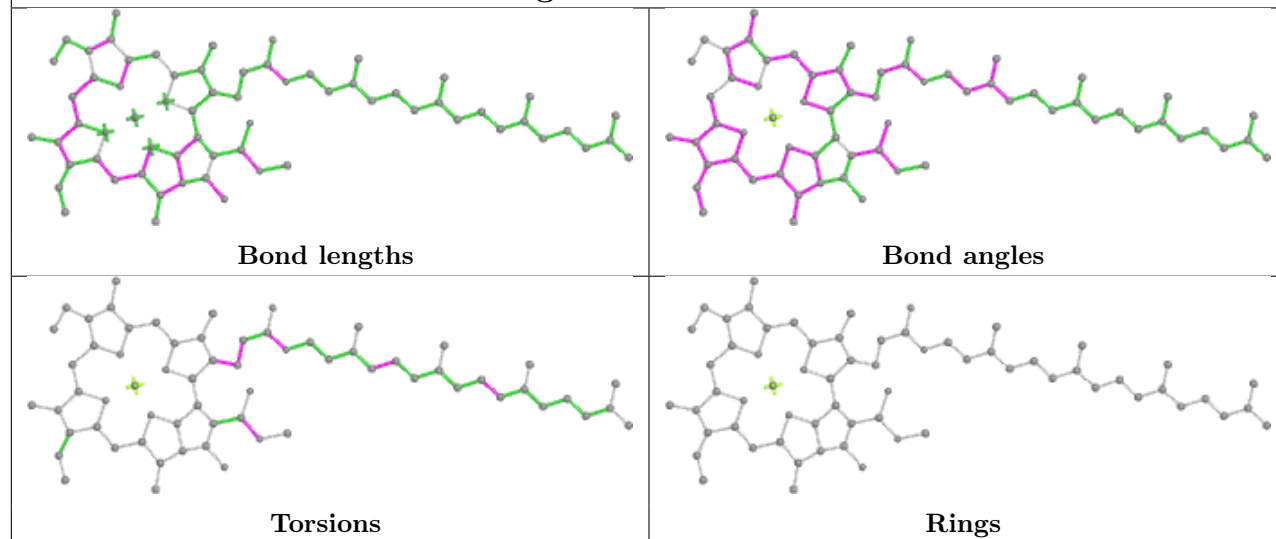
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	A	801	CL0	3	0
30	14	303	CLA	3	0
30	8	301	CLA	1	0
30	6	309	CLA	3	0
30	A	837	CLA	1	0
30	A	840	CLA	1	0
30	5	302	CLA	3	0
30	B	812	CLA	2	0
30	13	301	CLA	5	0
30	4	309	CLA	1	0
33	I	101	BCR	2	0
34	A	852	LHG	1	0
36	6	301	LMG	1	0
30	A	812	CLA	4	0
30	13	302	CLA	3	0
33	A	851	BCR	2	0
37	11	316	A86	1	0
30	7	307	CLA	2	0
30	4	306	CLA	6	0
31	B	840	PQN	1	0
35	12	320	LMT	1	0
30	A	818	CLA	1	0
37	5	315	A86	1	0
30	2	309	CLA	2	0

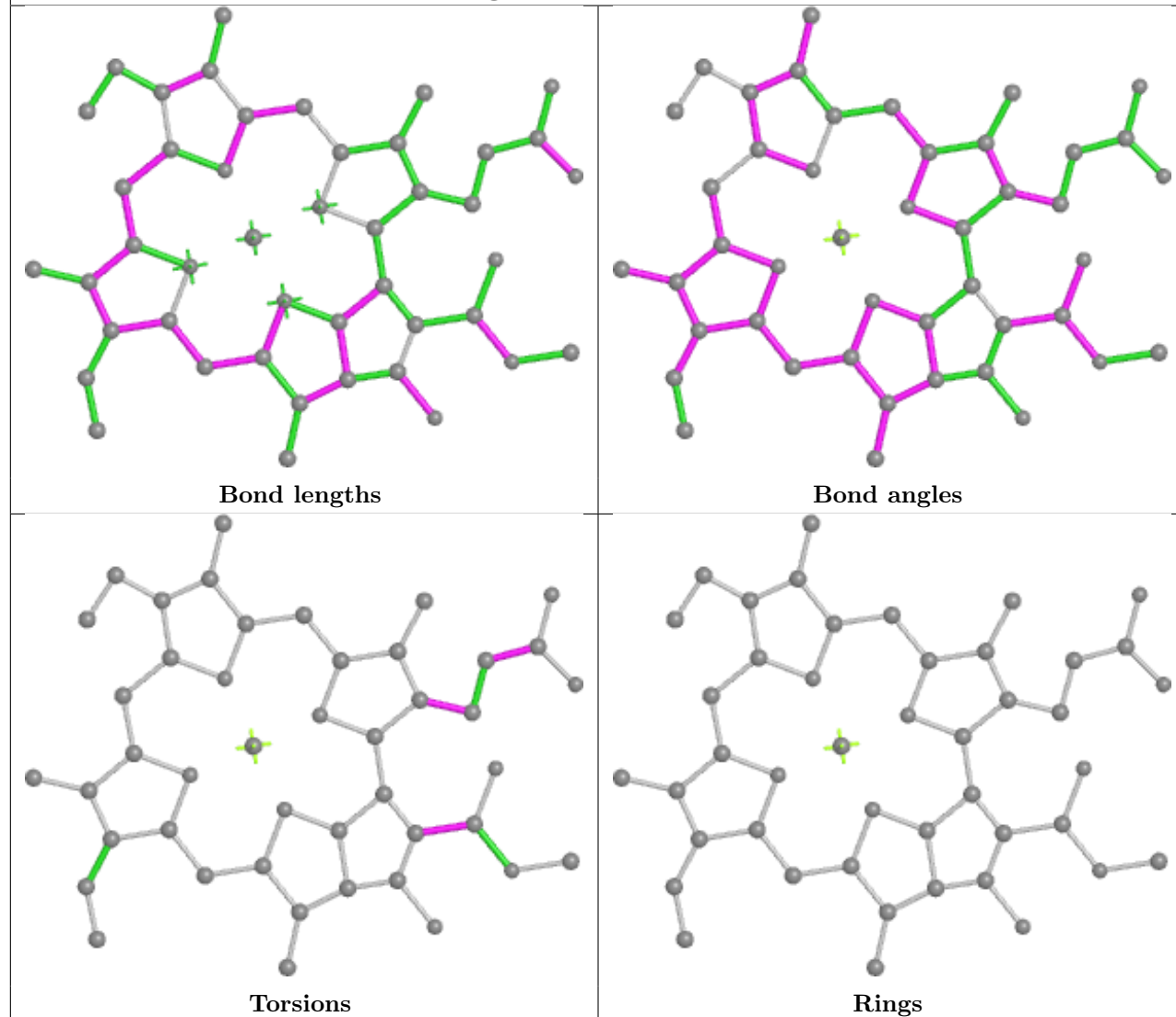
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand CLA A 813**Ligand BCR B 843****Ligand CLA 2 307**

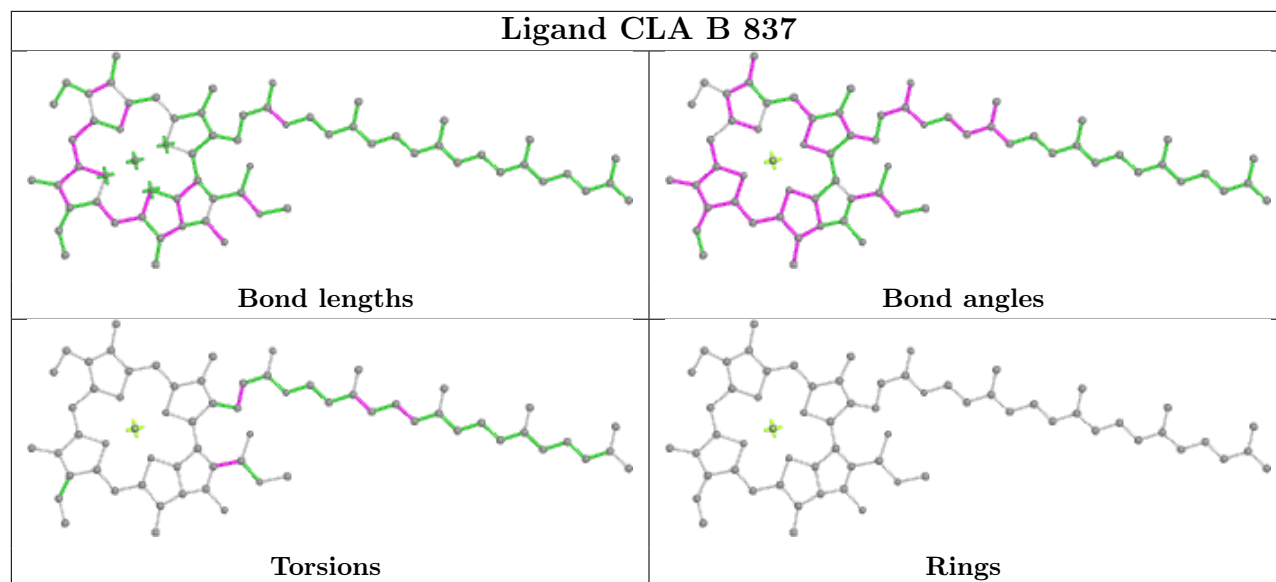
Ligand CLA 3 306



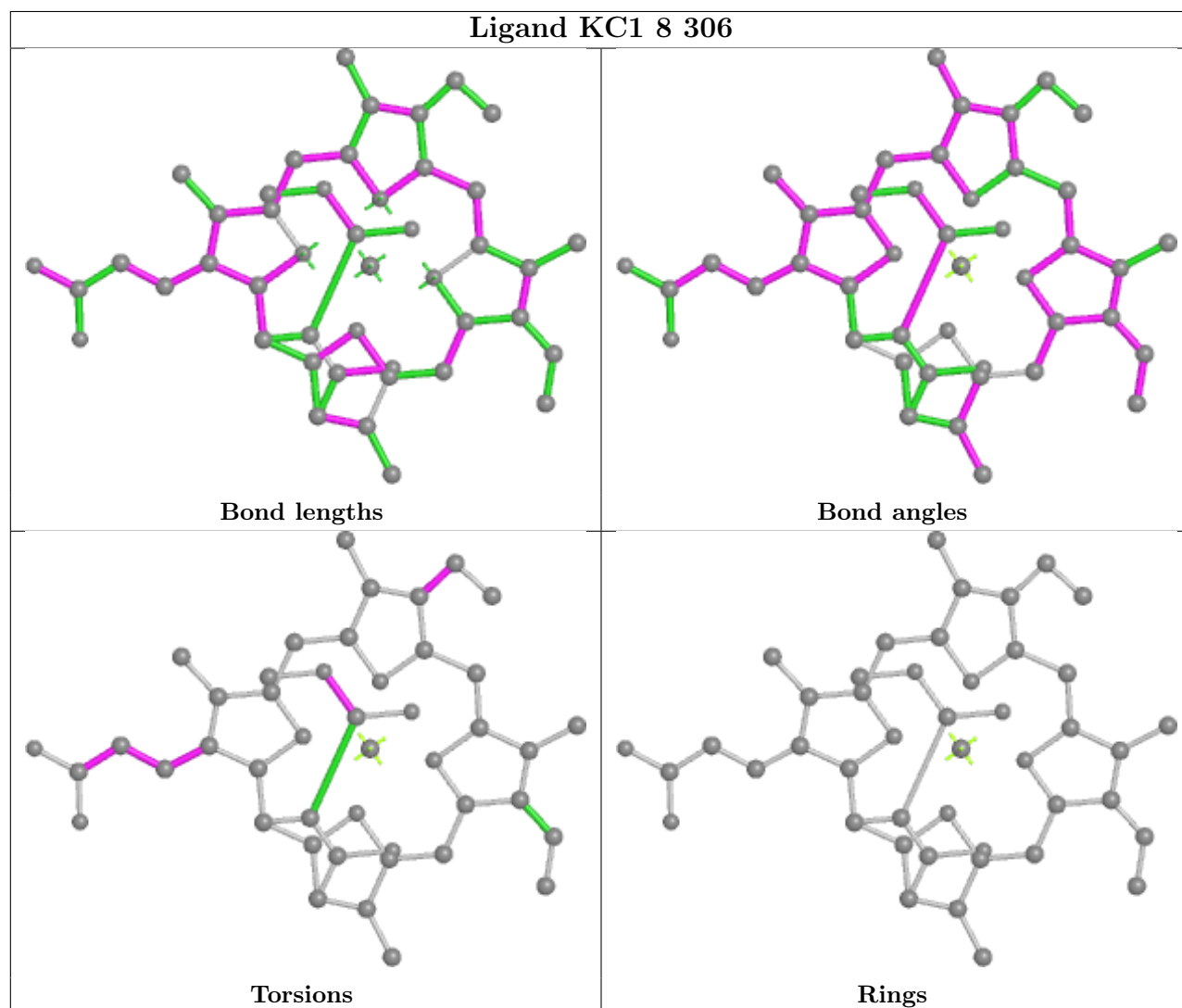
Ligand CLA 15 310

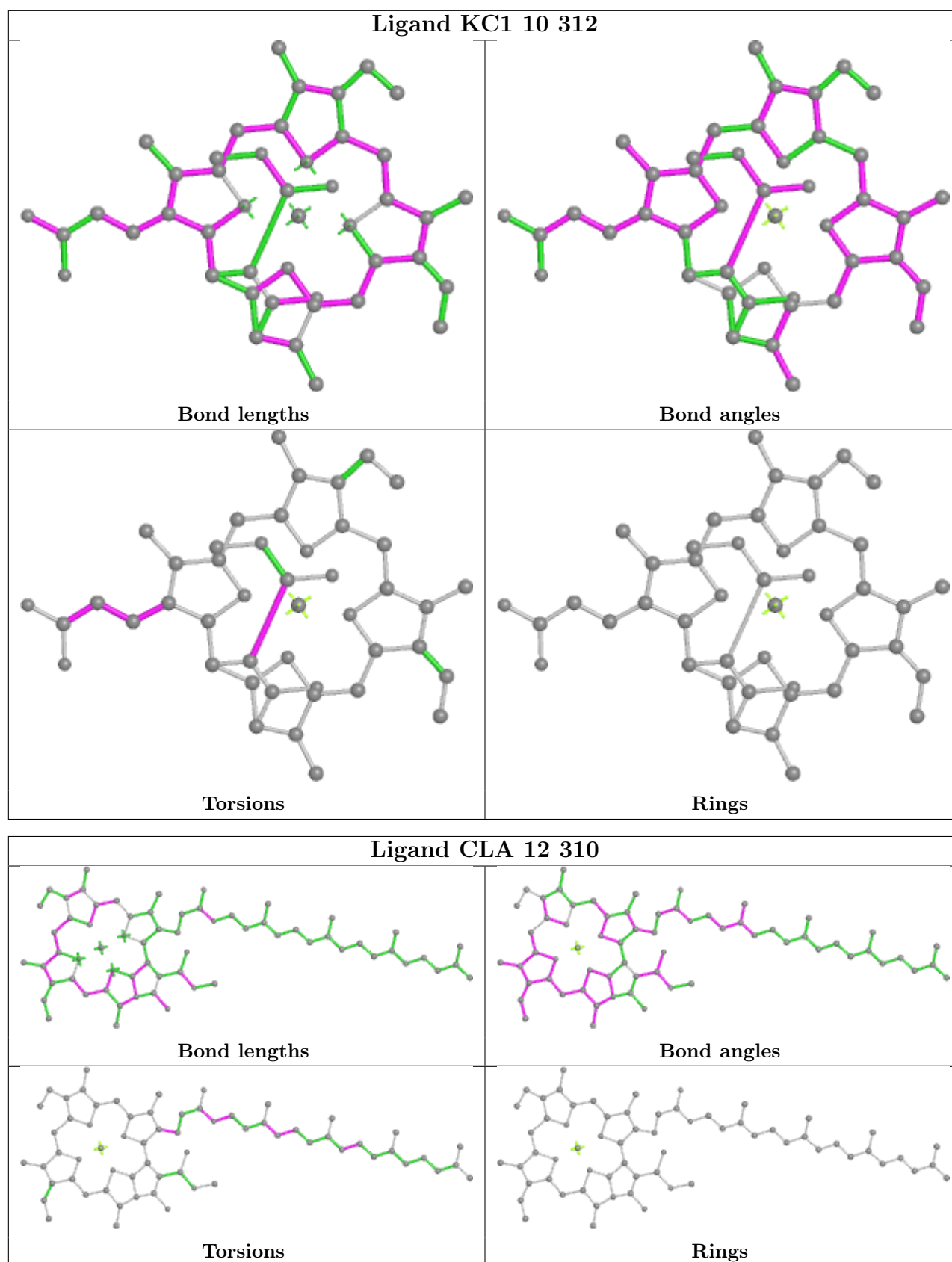


Ligand CLA B 837

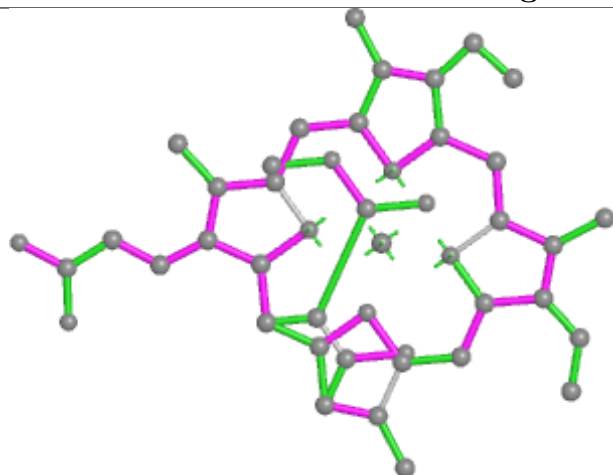


Ligand KC1 8 306

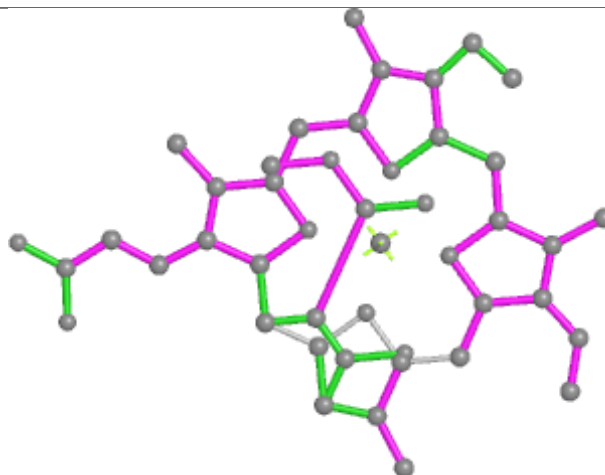




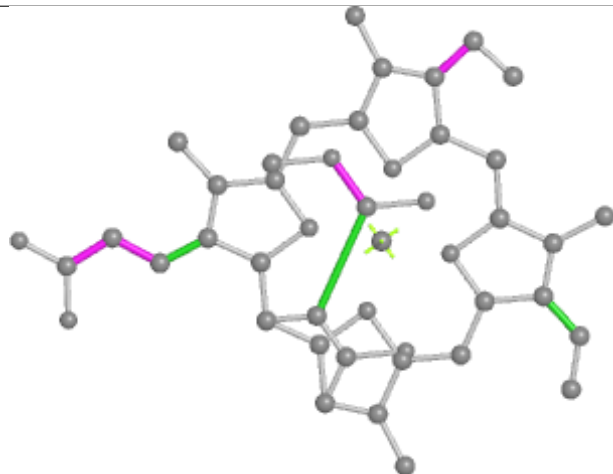
Ligand KC1 2 314



Bond lengths



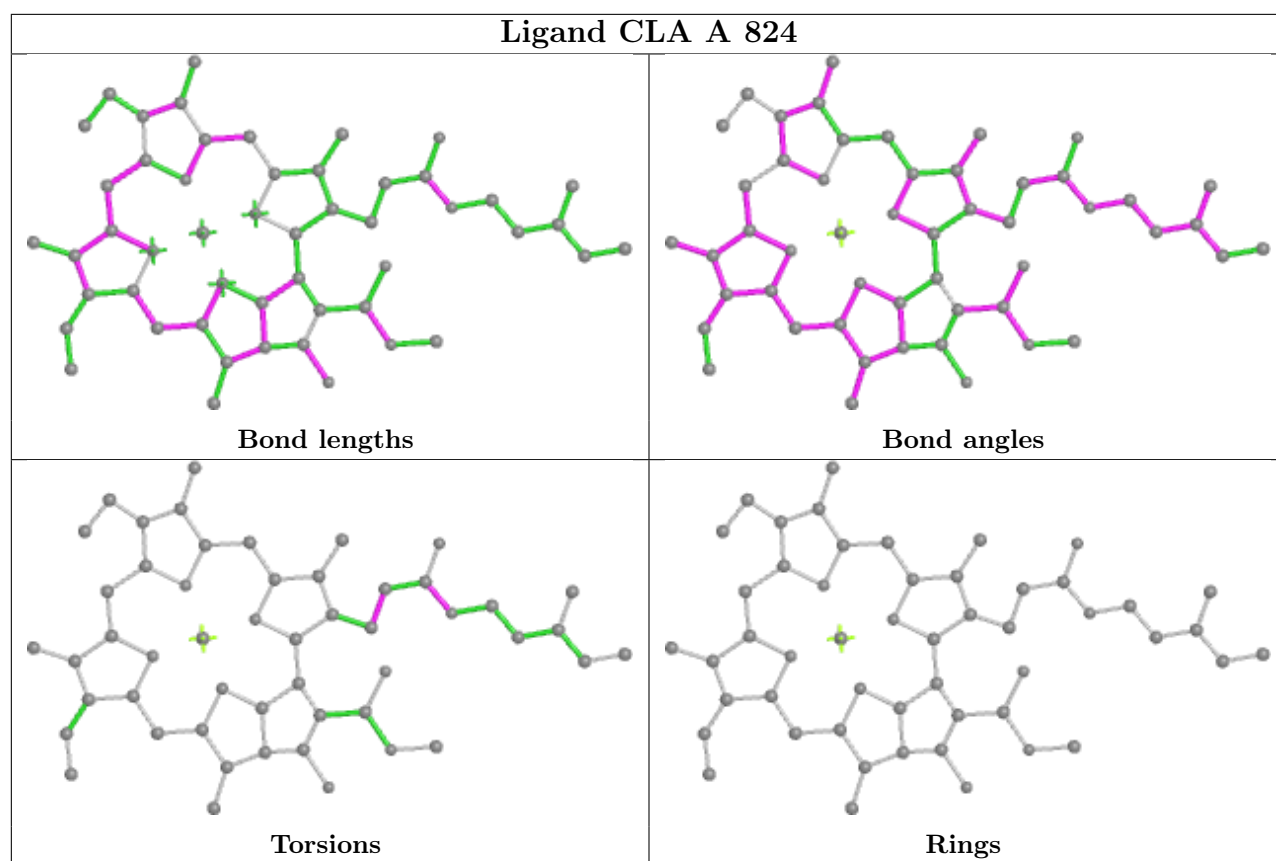
Bond angles



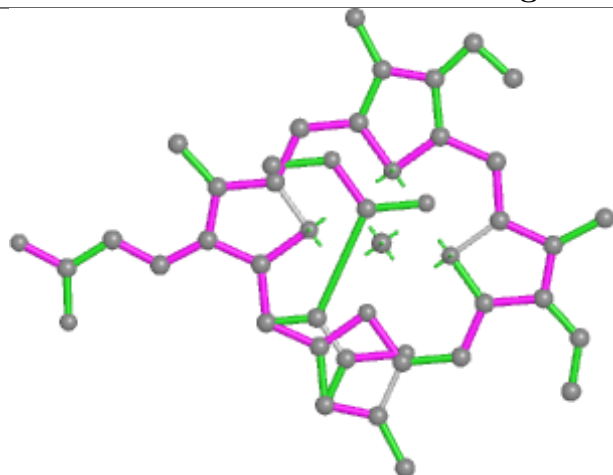
Torsions



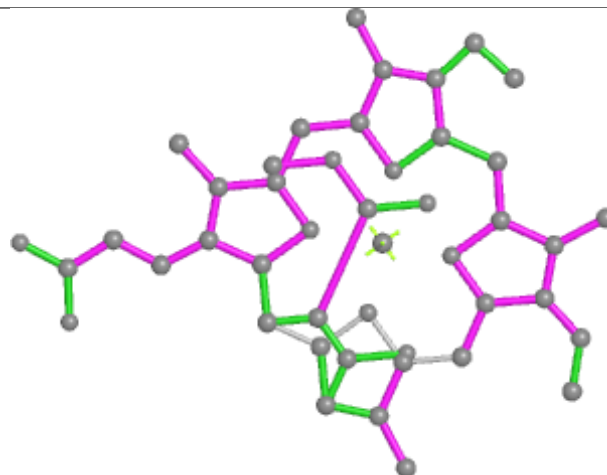
Rings



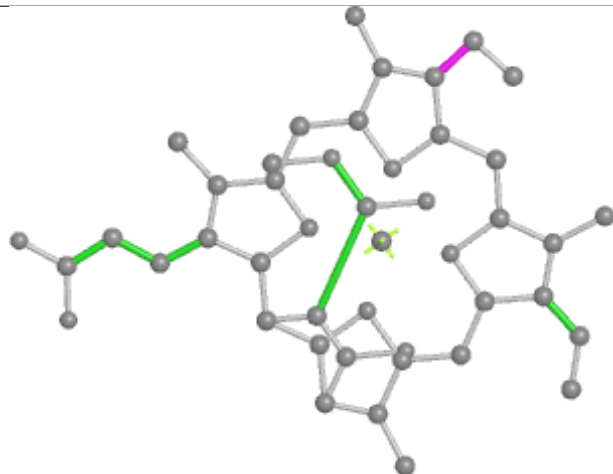
Ligand KC1 2 312



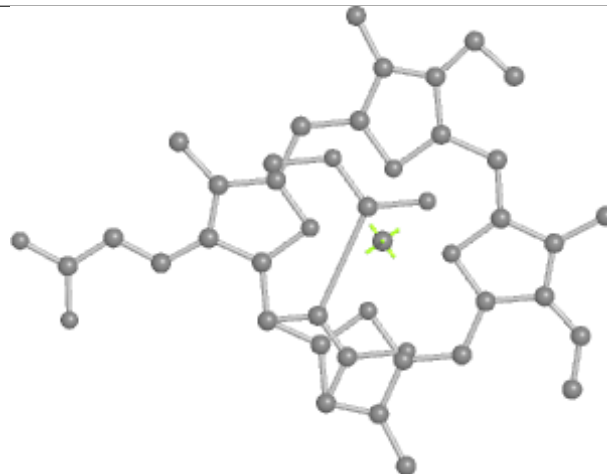
Bond lengths



Bond angles

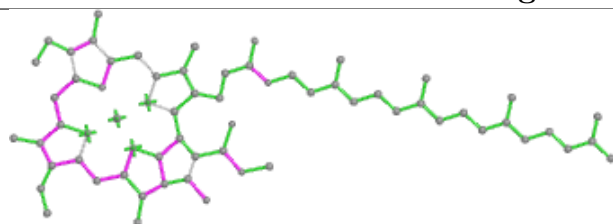


Torsions

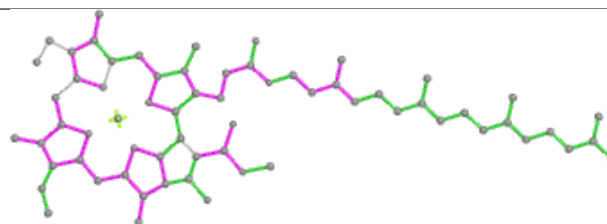


Rings

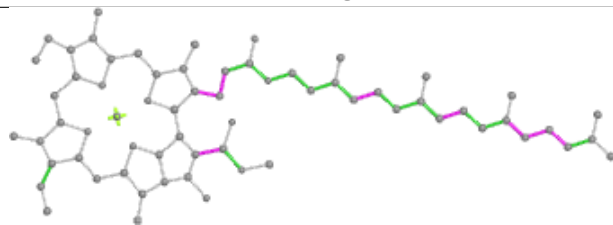
Ligand CLA 7 310



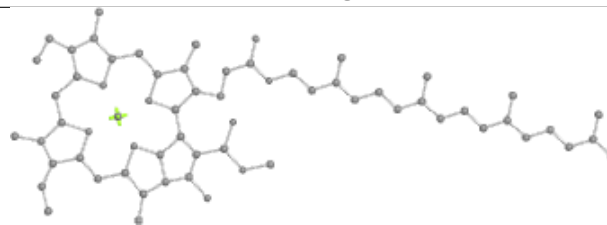
Bond lengths



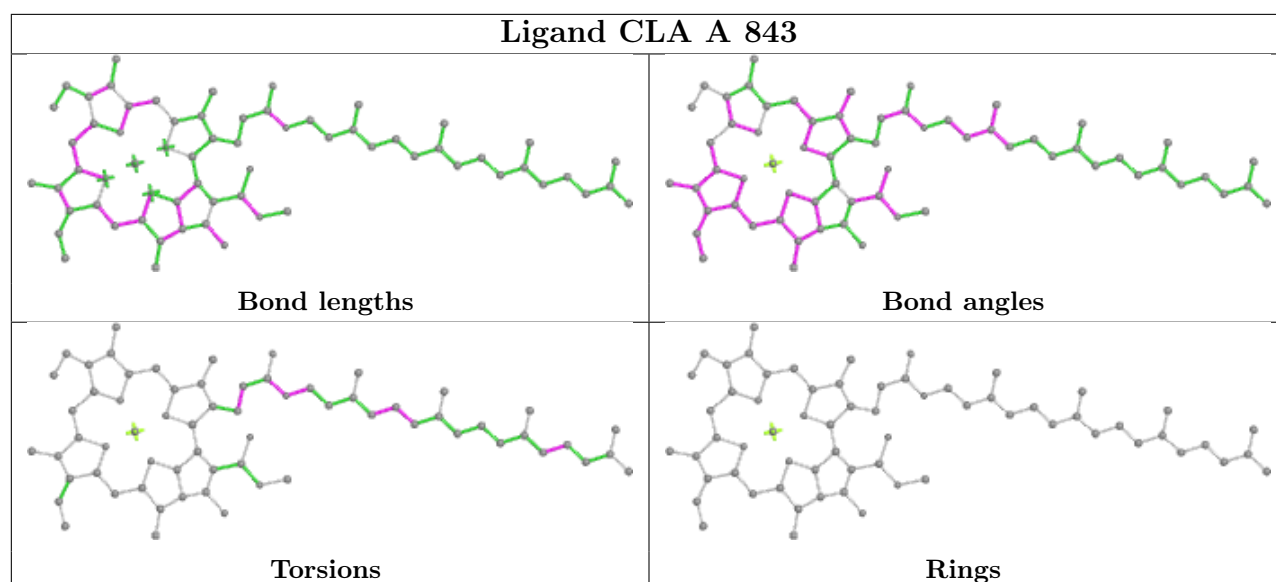
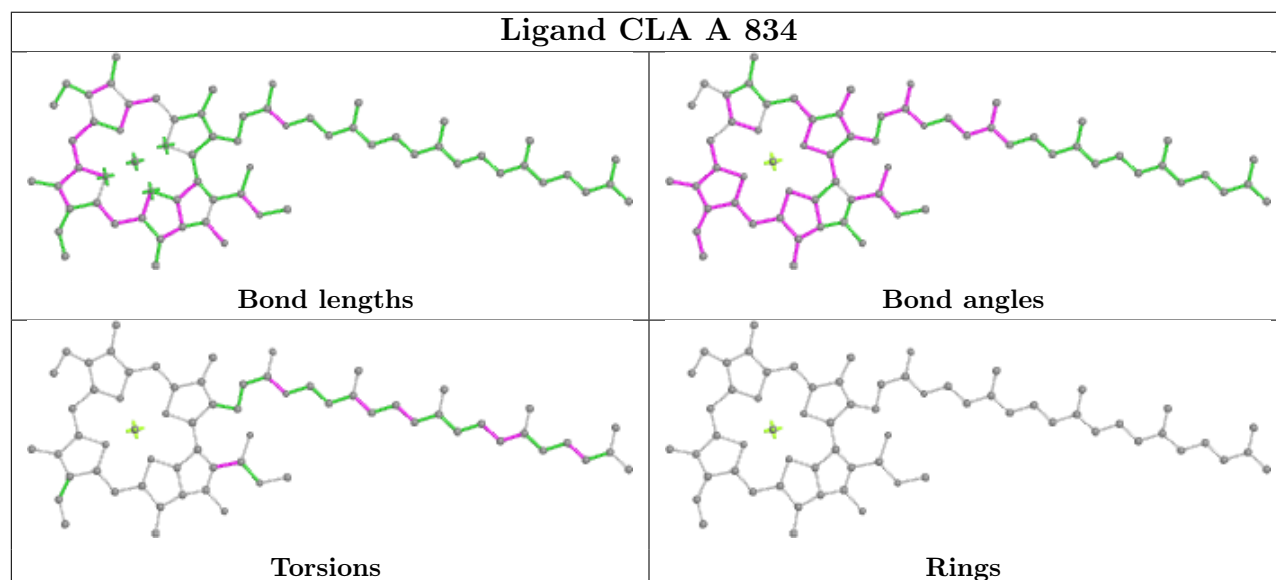
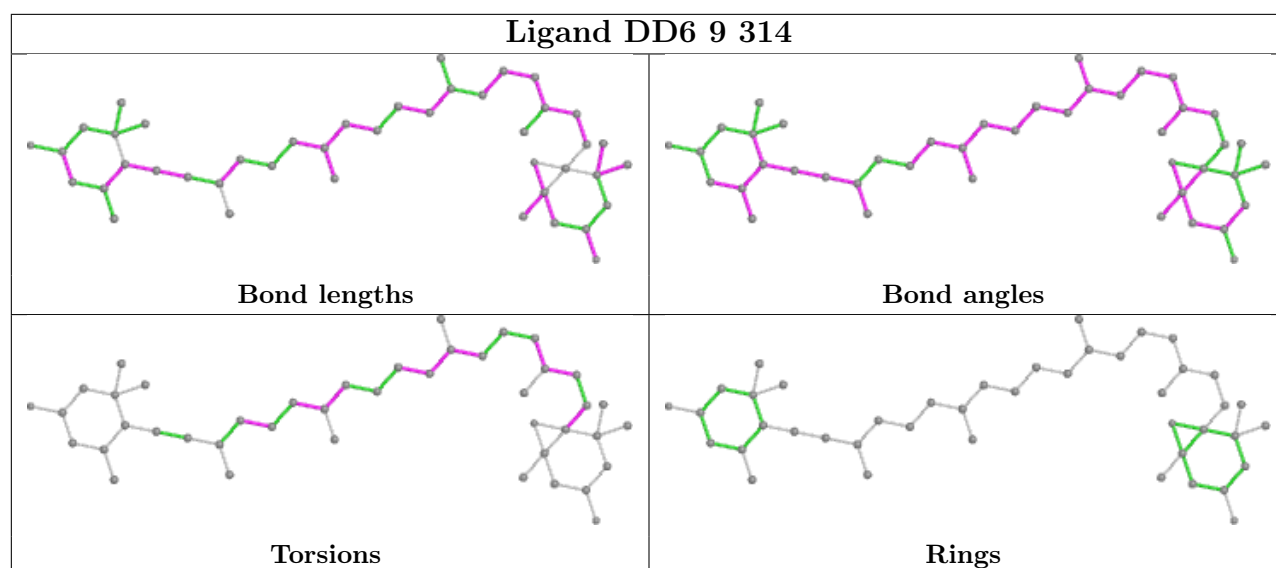
Bond angles

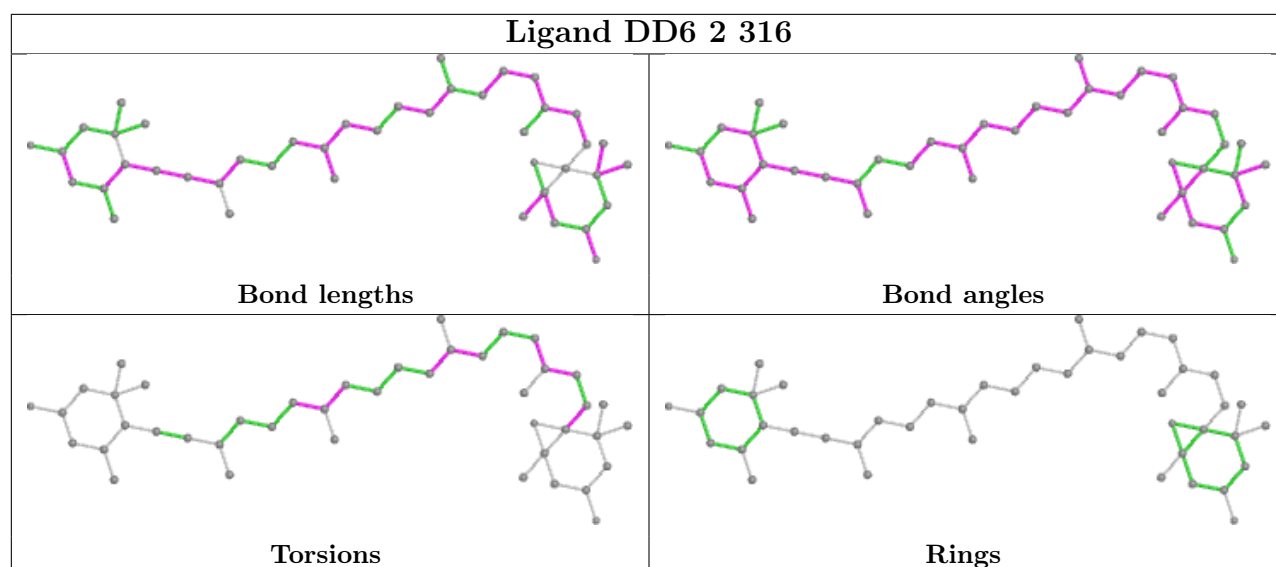
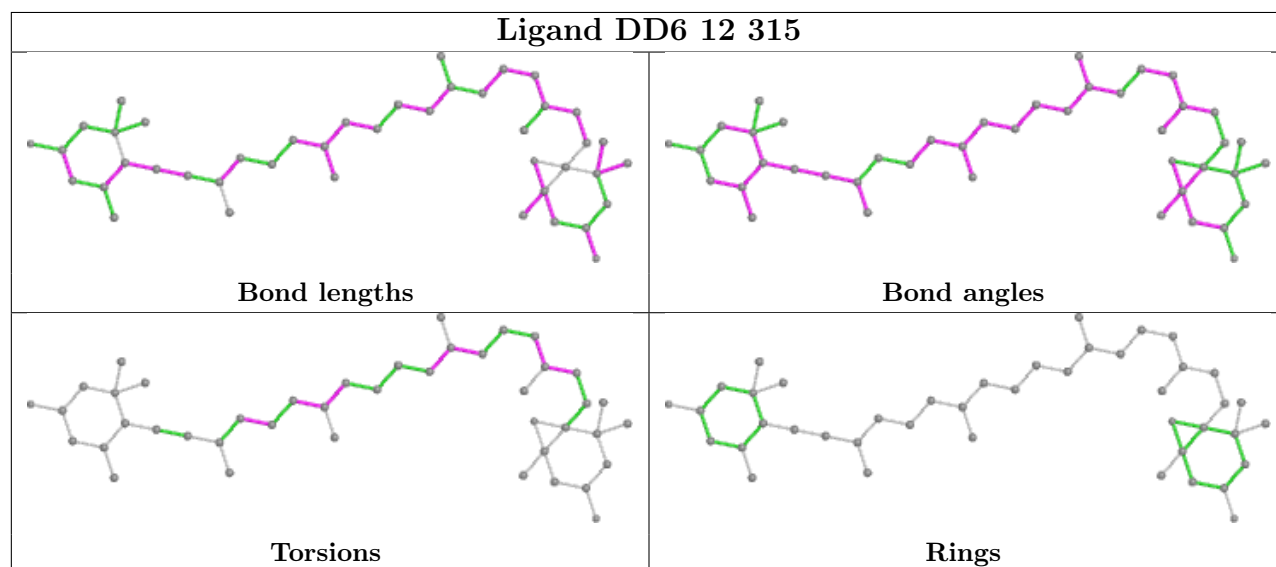
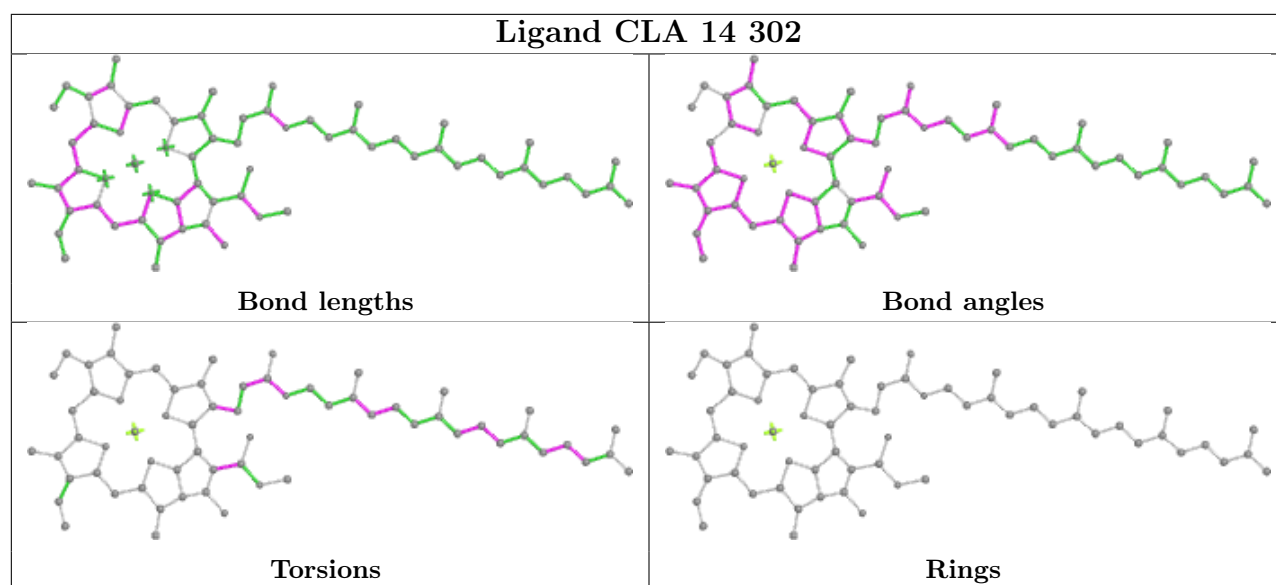


Torsions

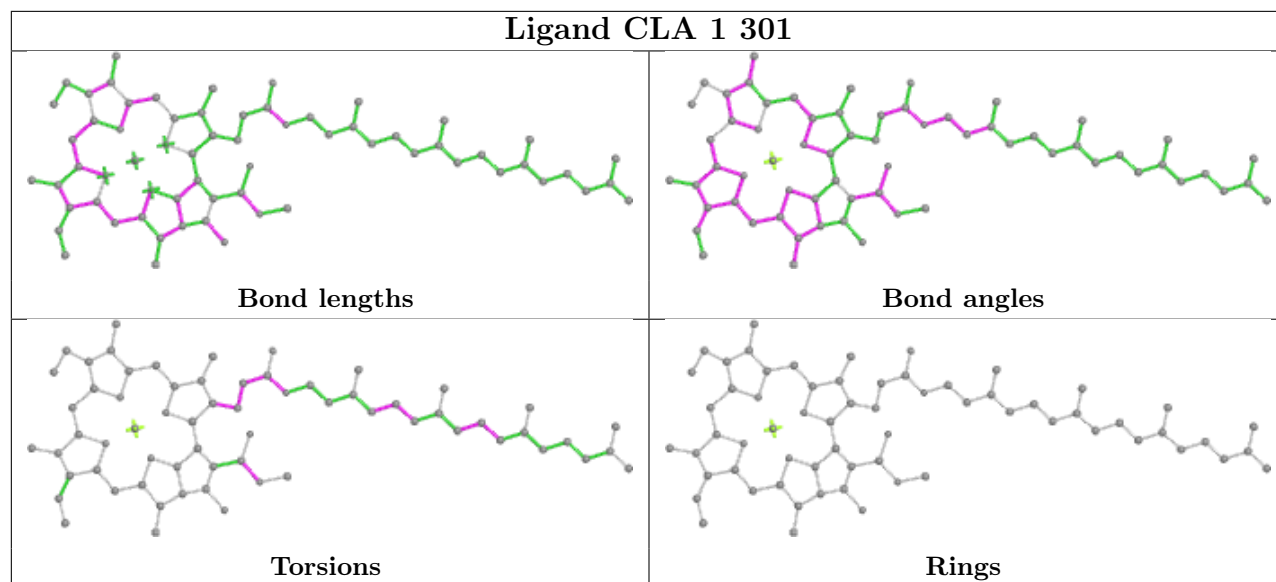


Rings

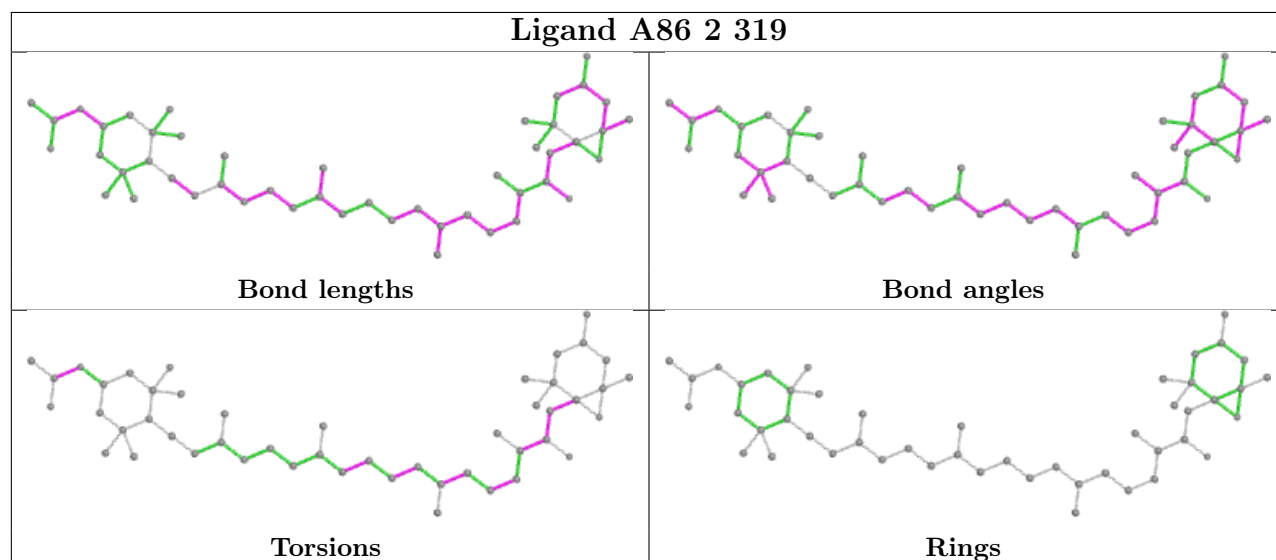




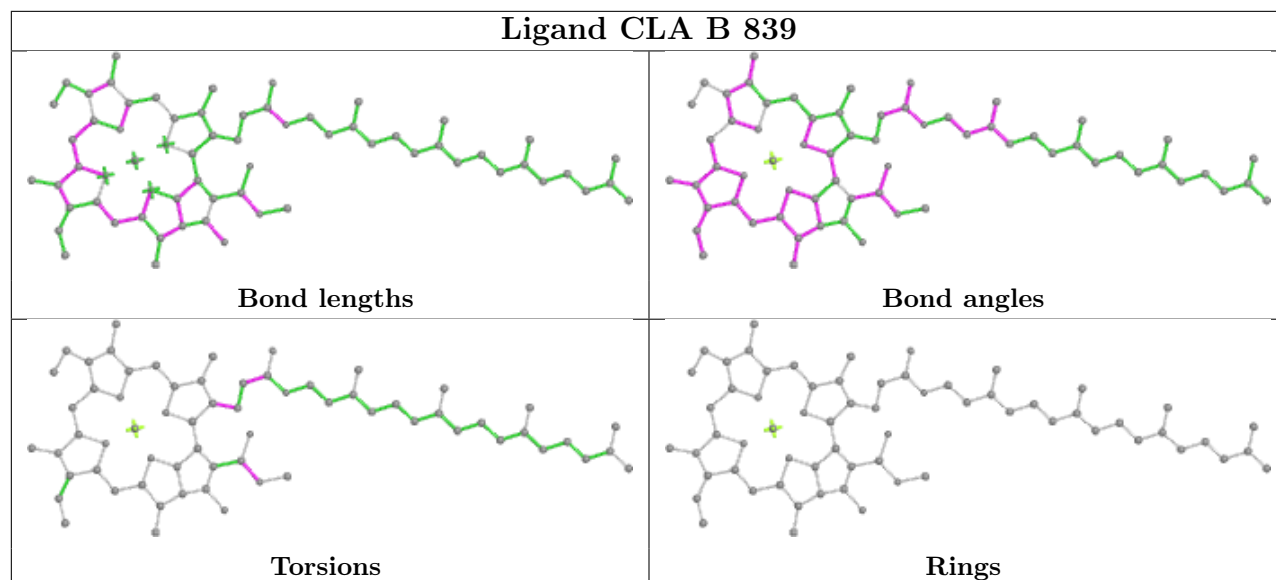
Ligand CLA 1 301



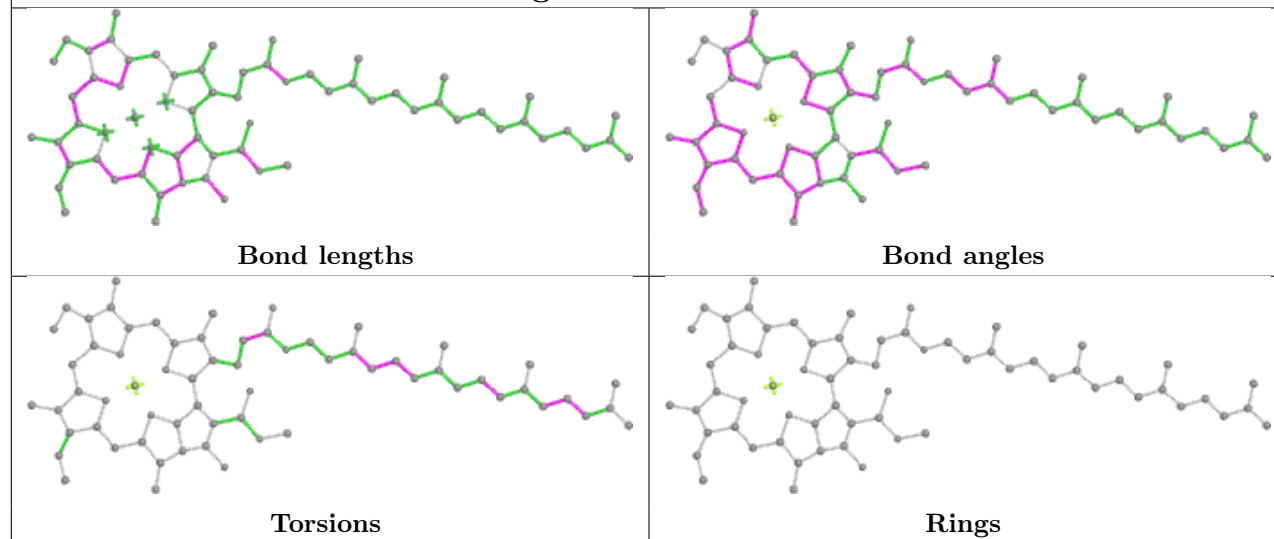
Ligand A86 2 319



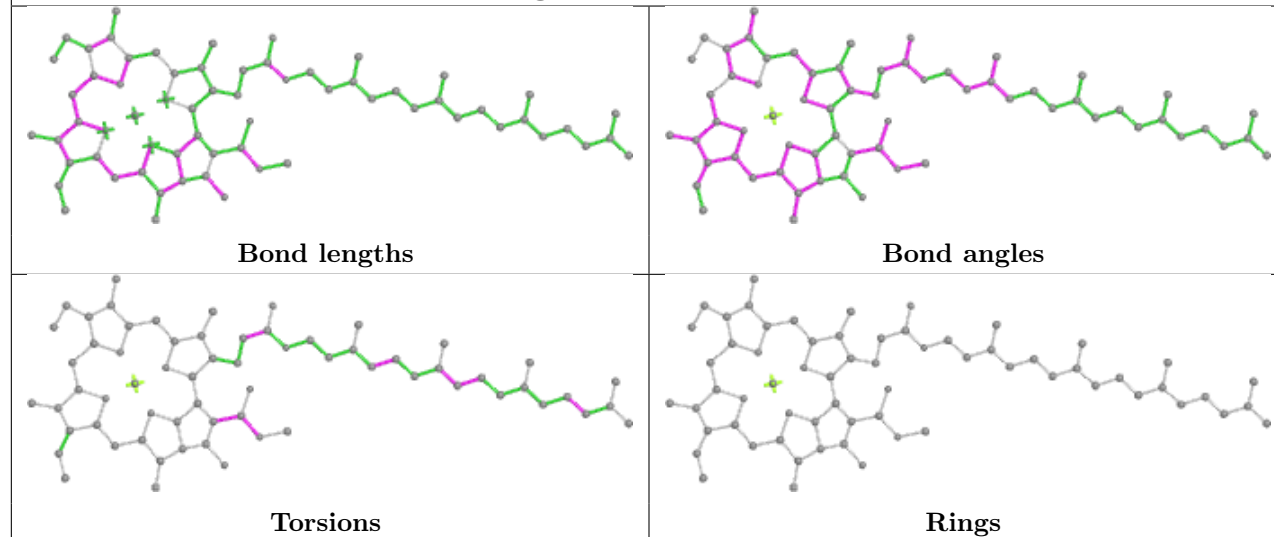
Ligand CLA B 839

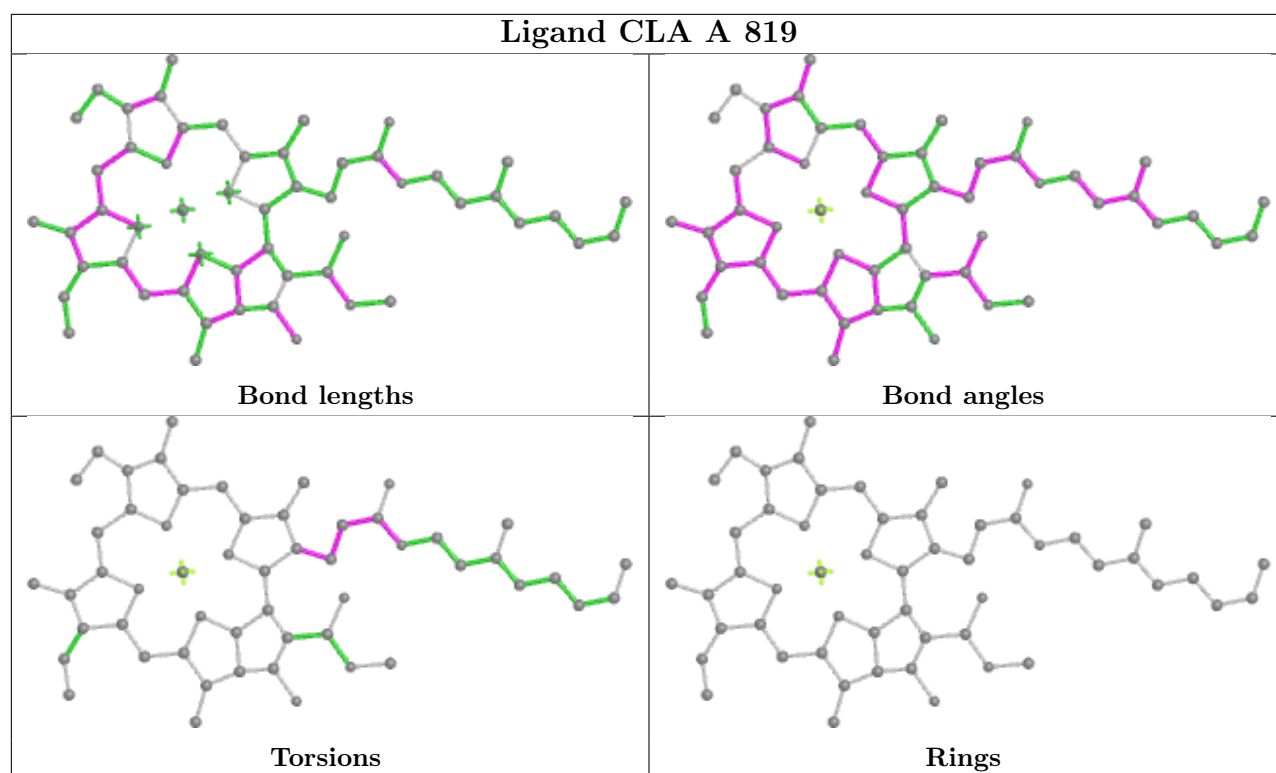


Ligand CLA B 806

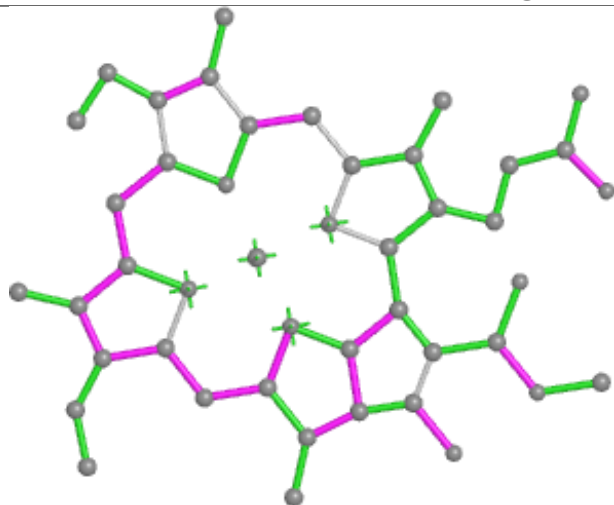


Ligand CLA A 841

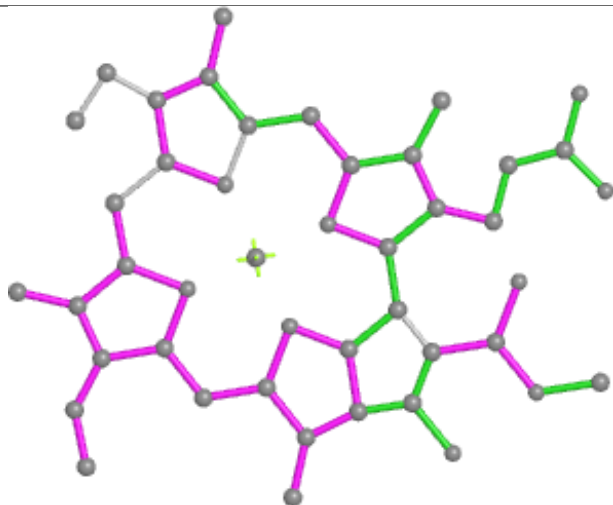




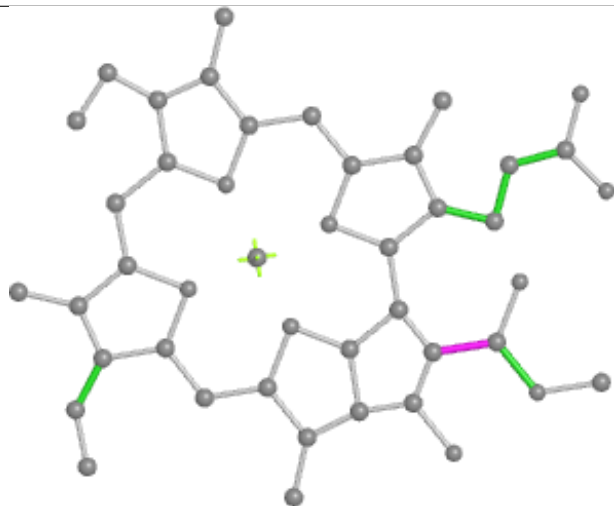
Ligand CLA 6 315



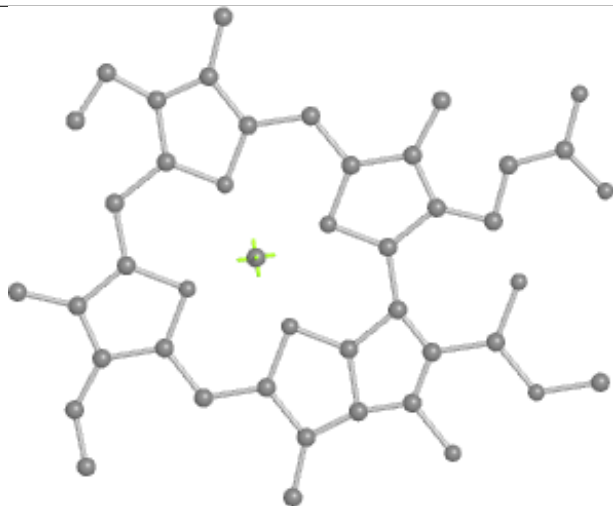
Bond lengths



Bond angles

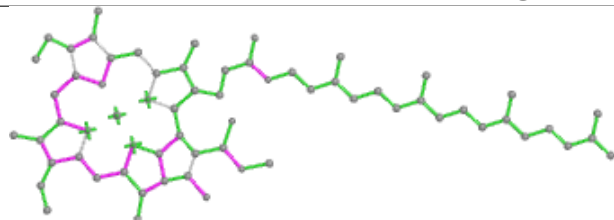


Torsions

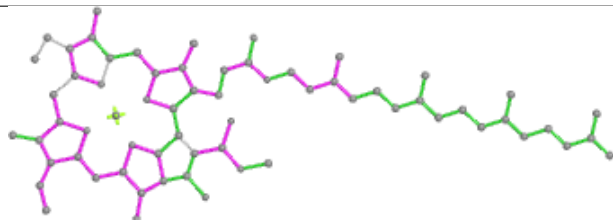


Rings

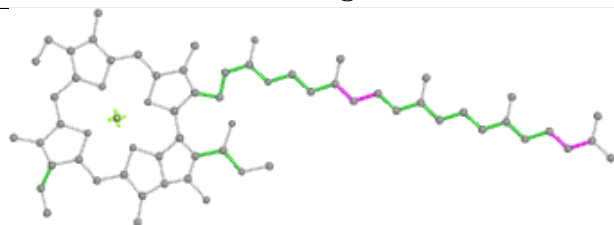
Ligand CLA B 832



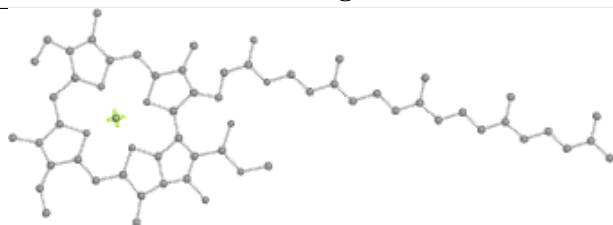
Bond lengths



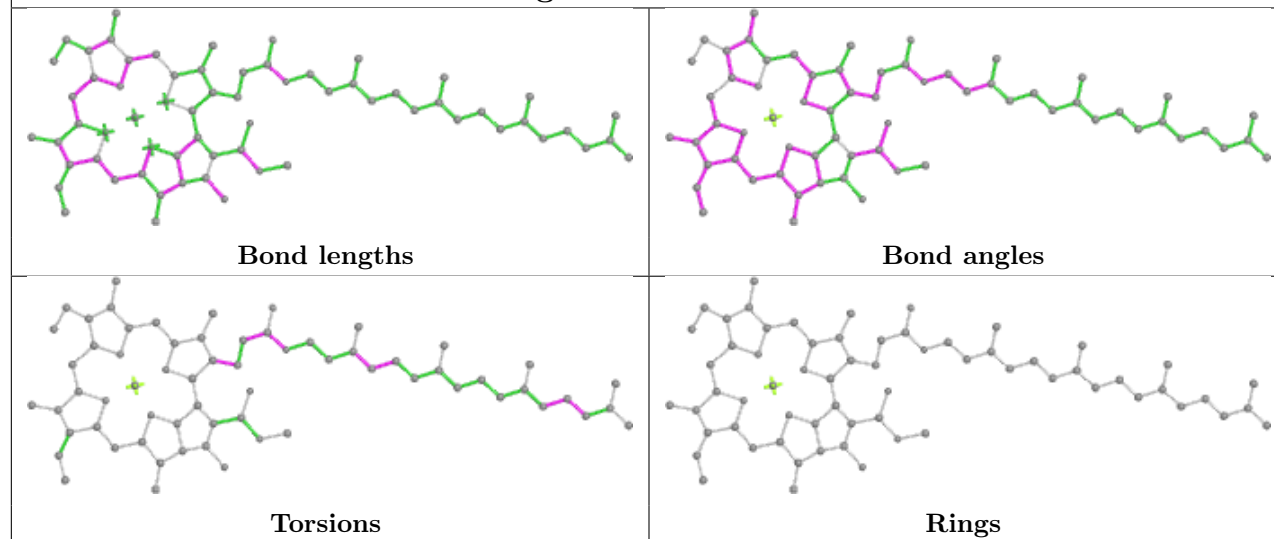
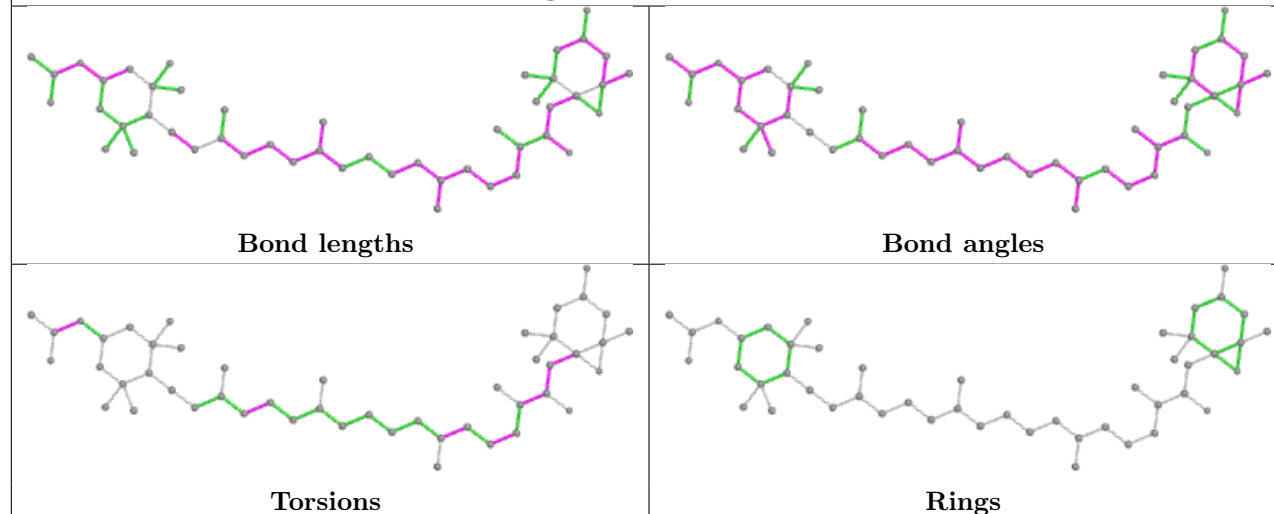
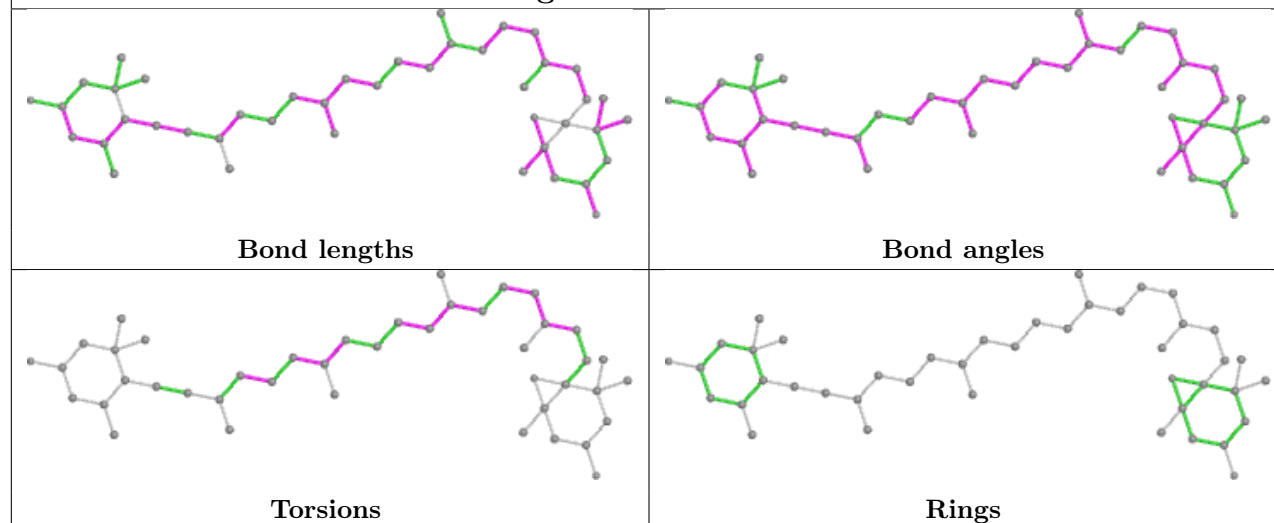
Bond angles

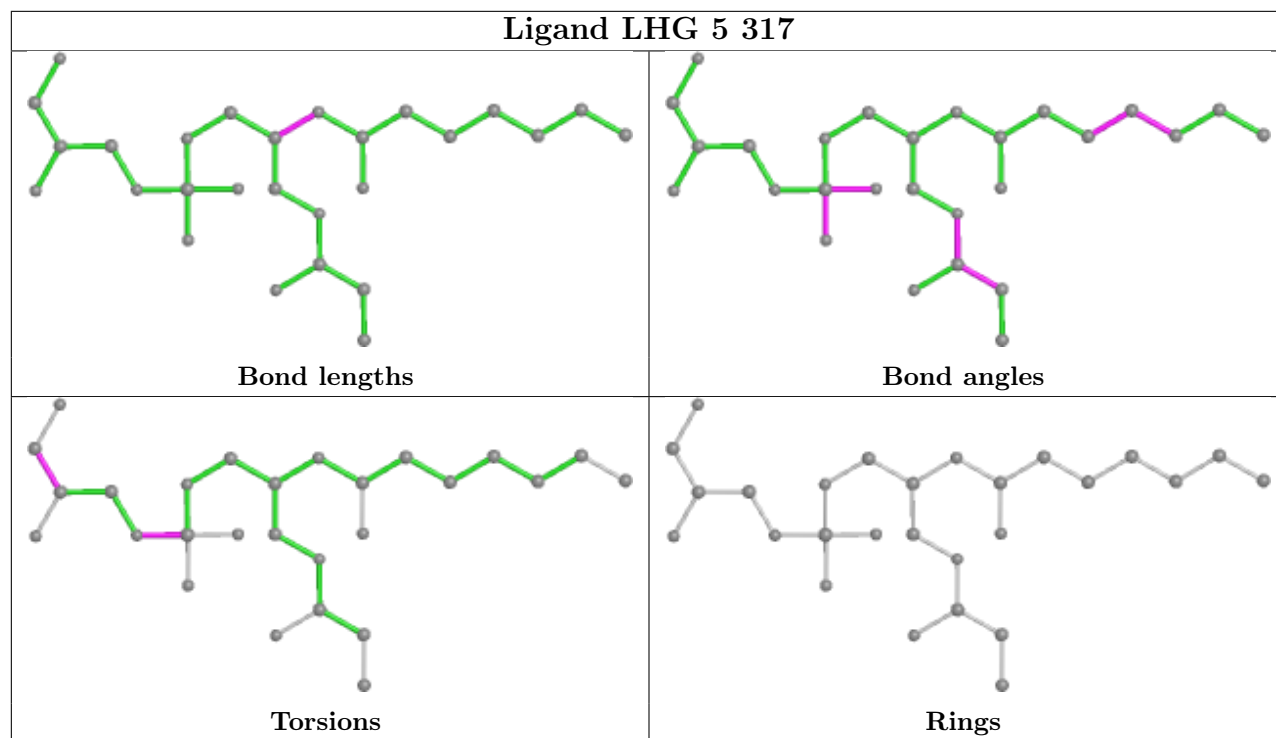
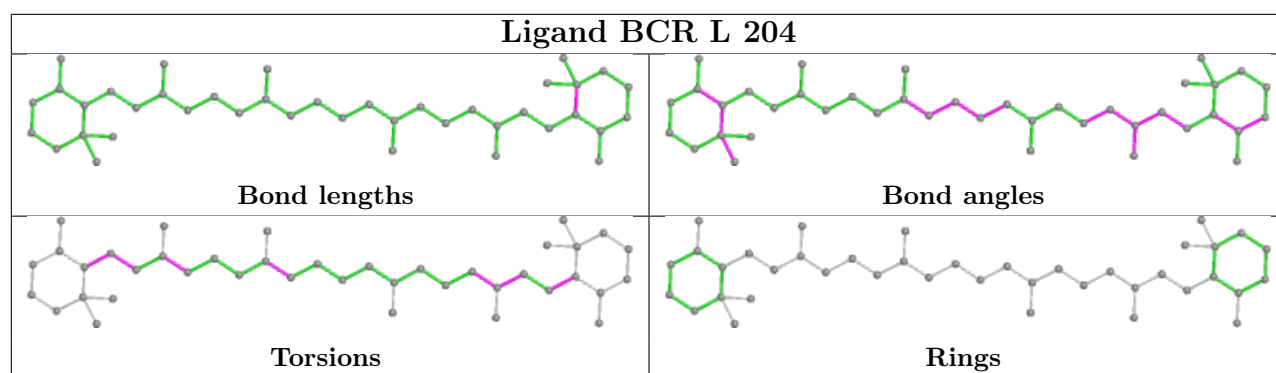


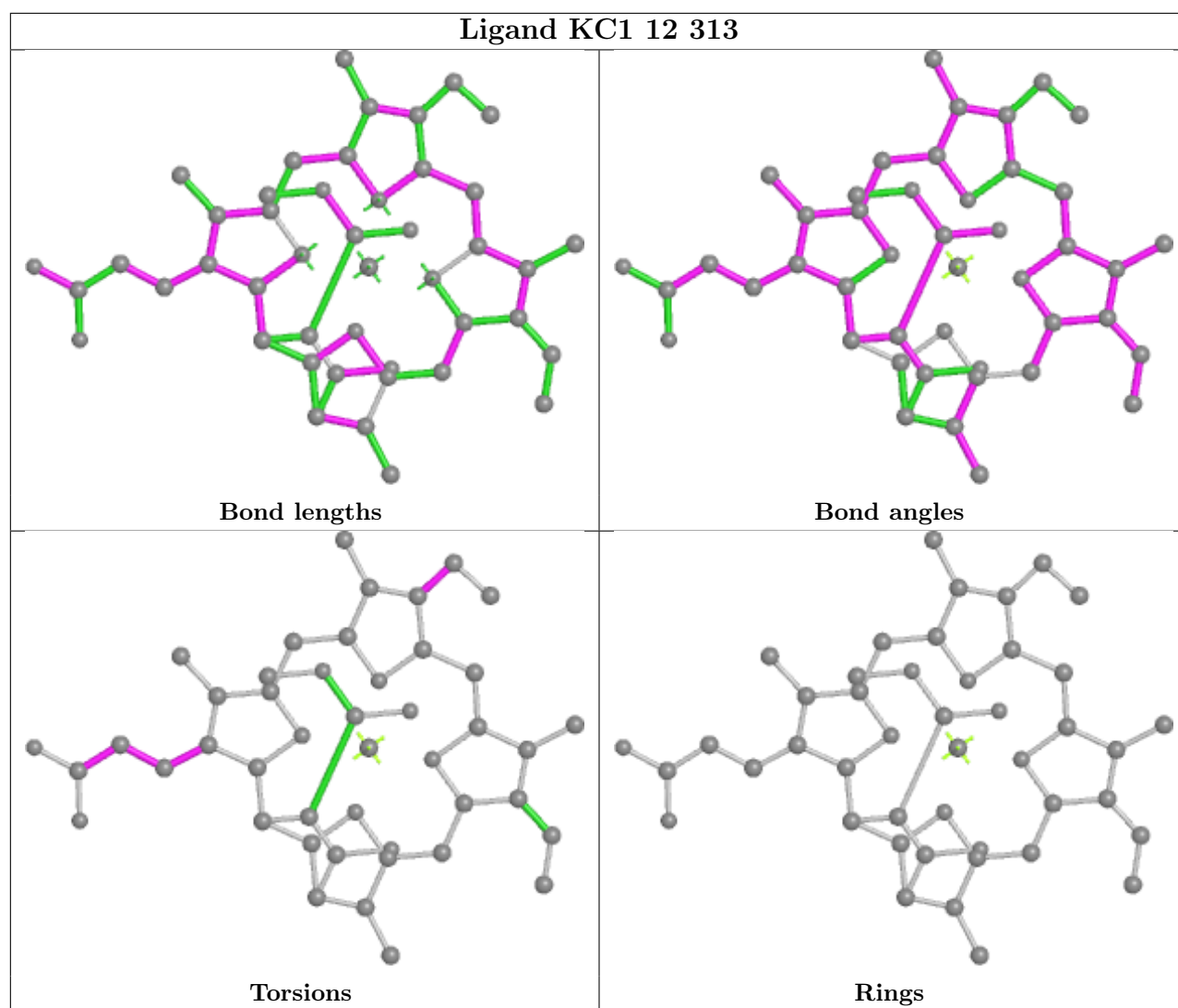
Torsions



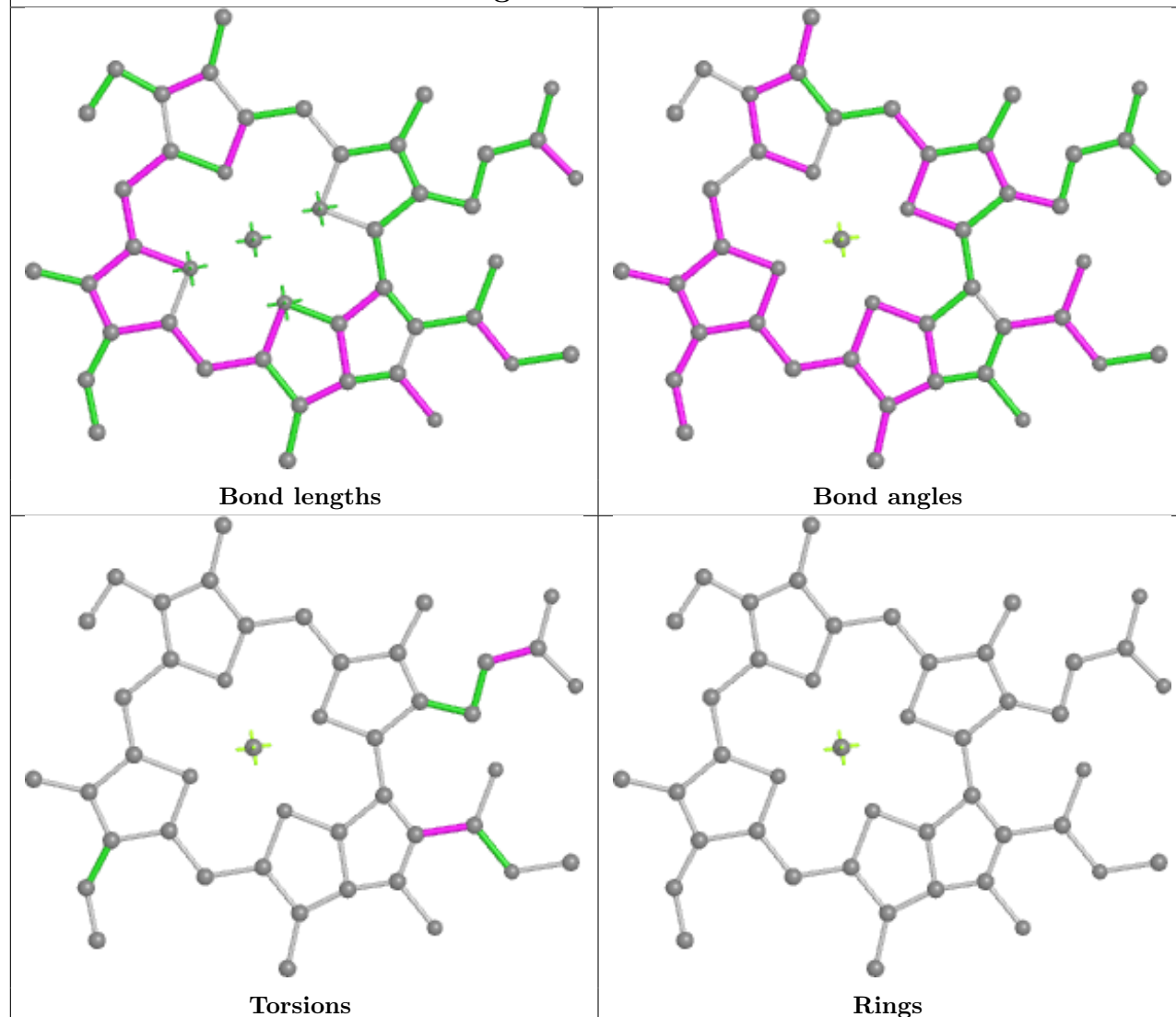
Rings

Ligand CLA 2 305**Ligand A86 5 301****Ligand DD6 3 312**

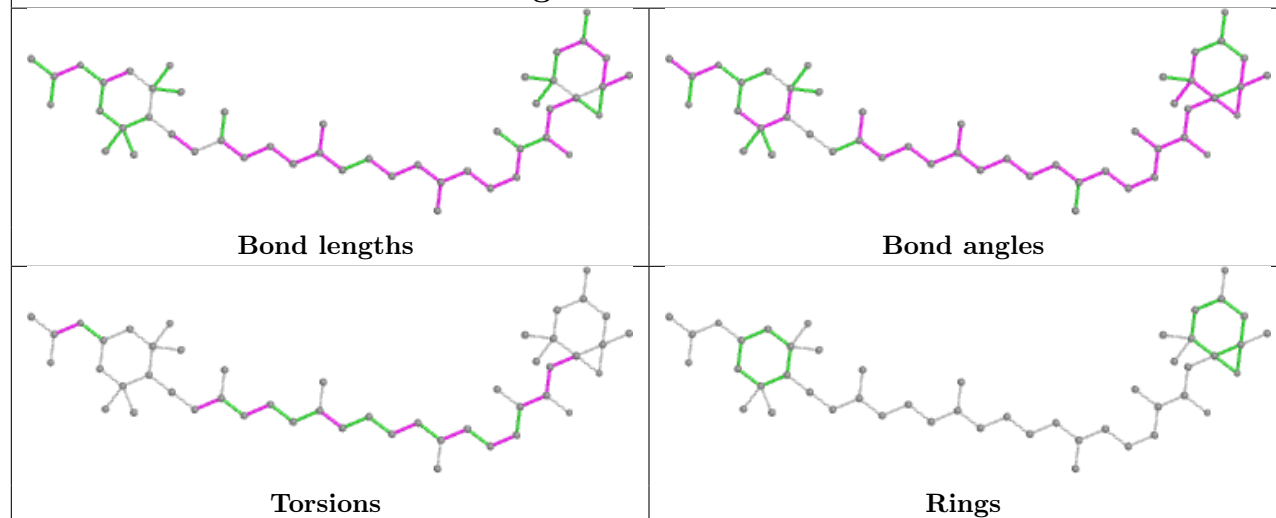


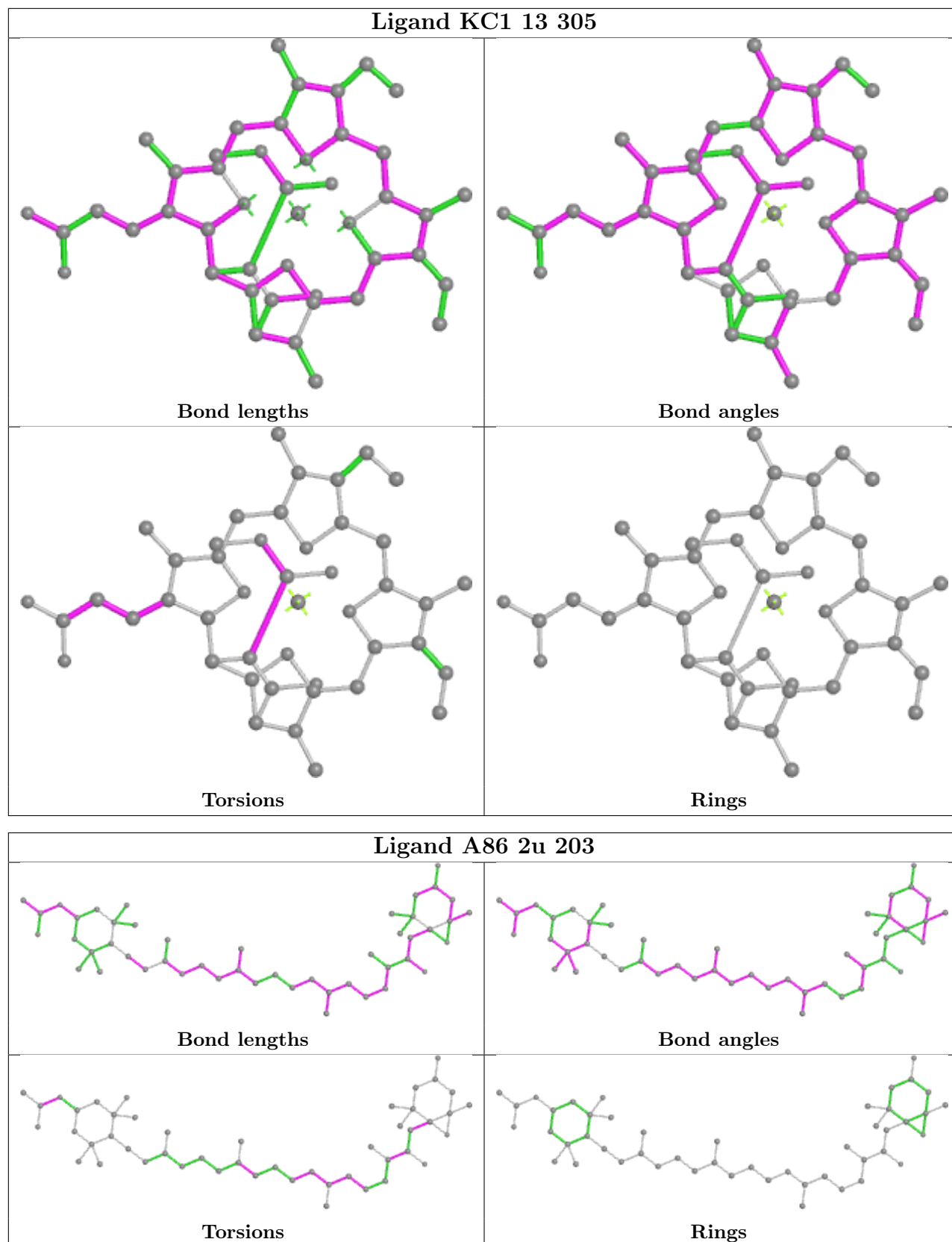


Ligand CLA J 101

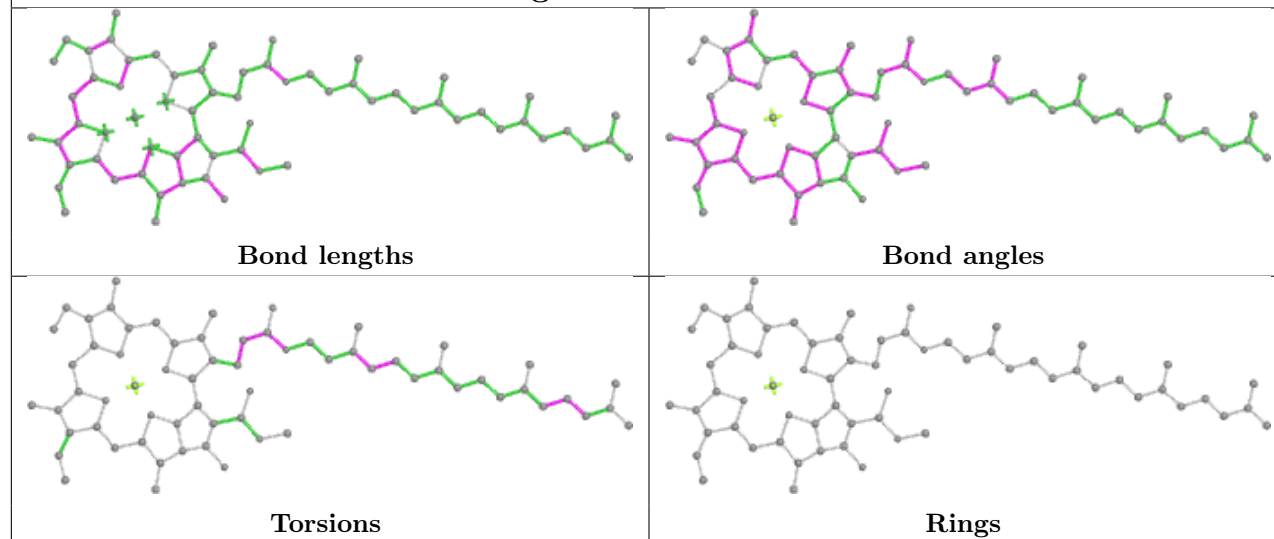


Ligand A86 15 322

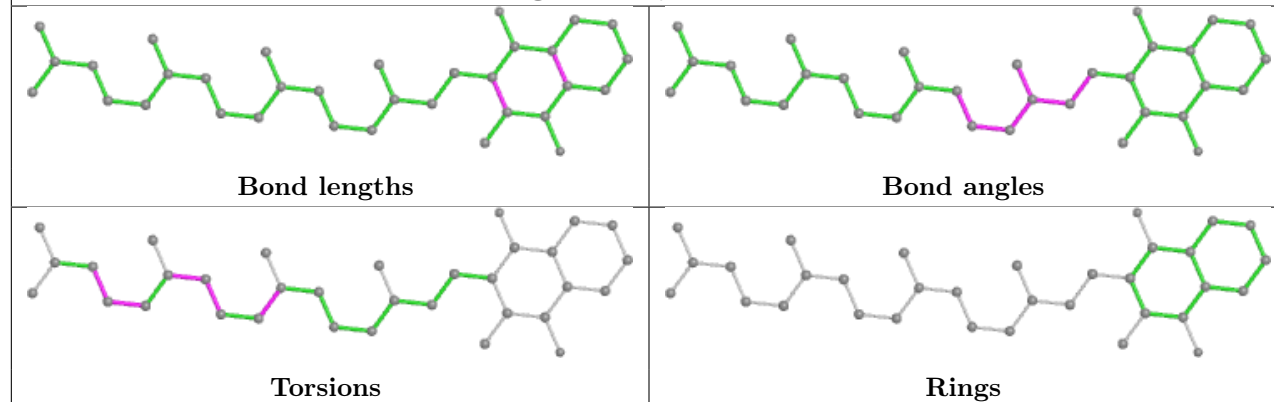




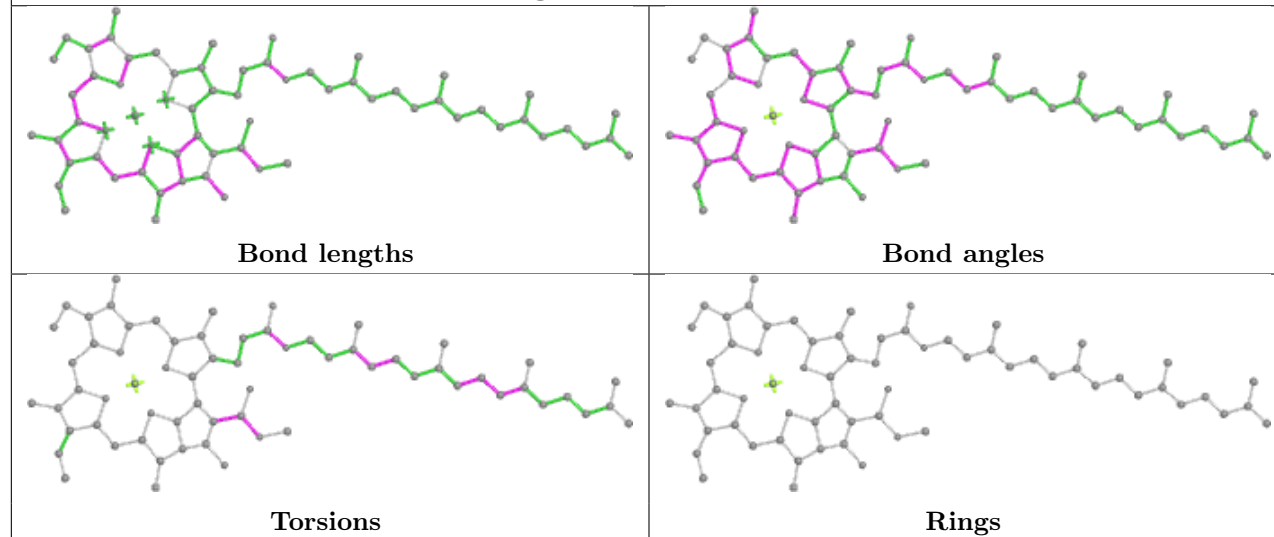
Ligand CLA A 830

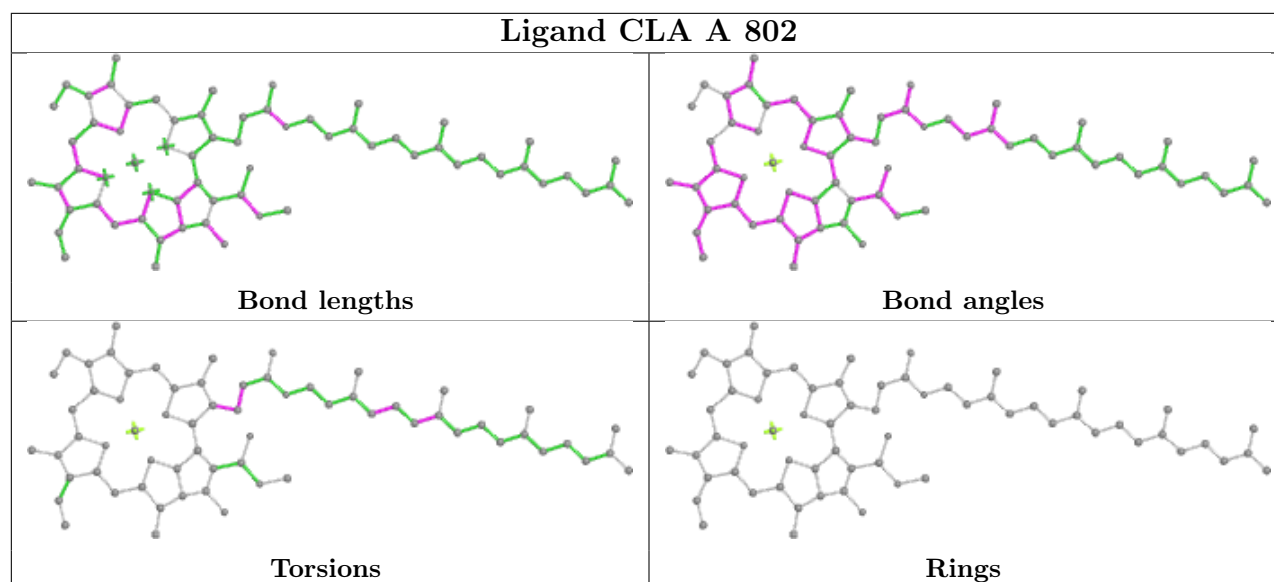
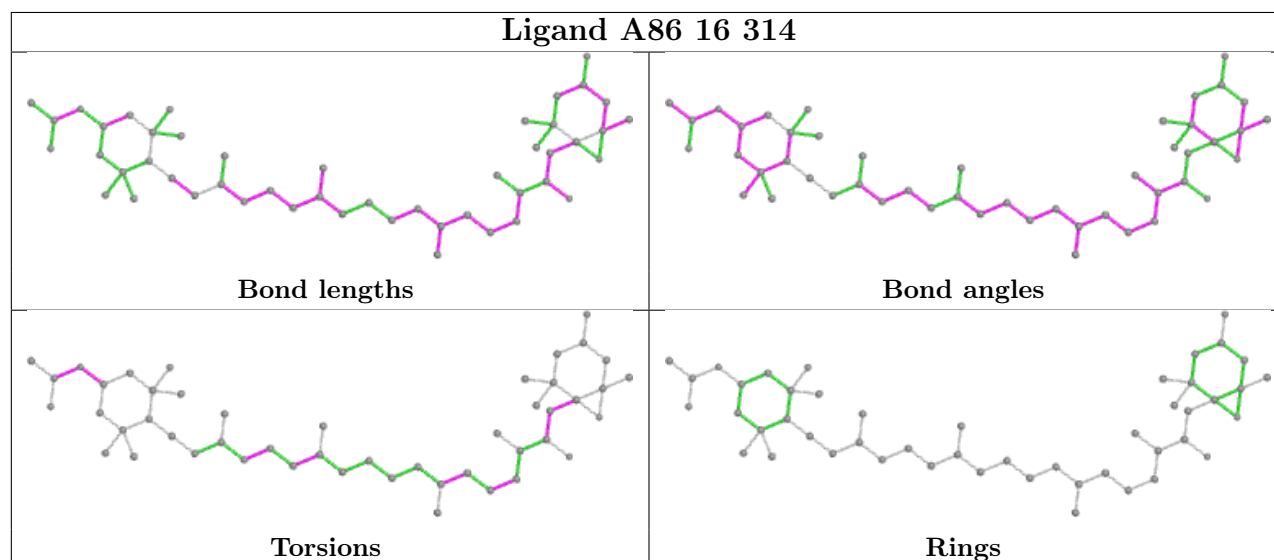
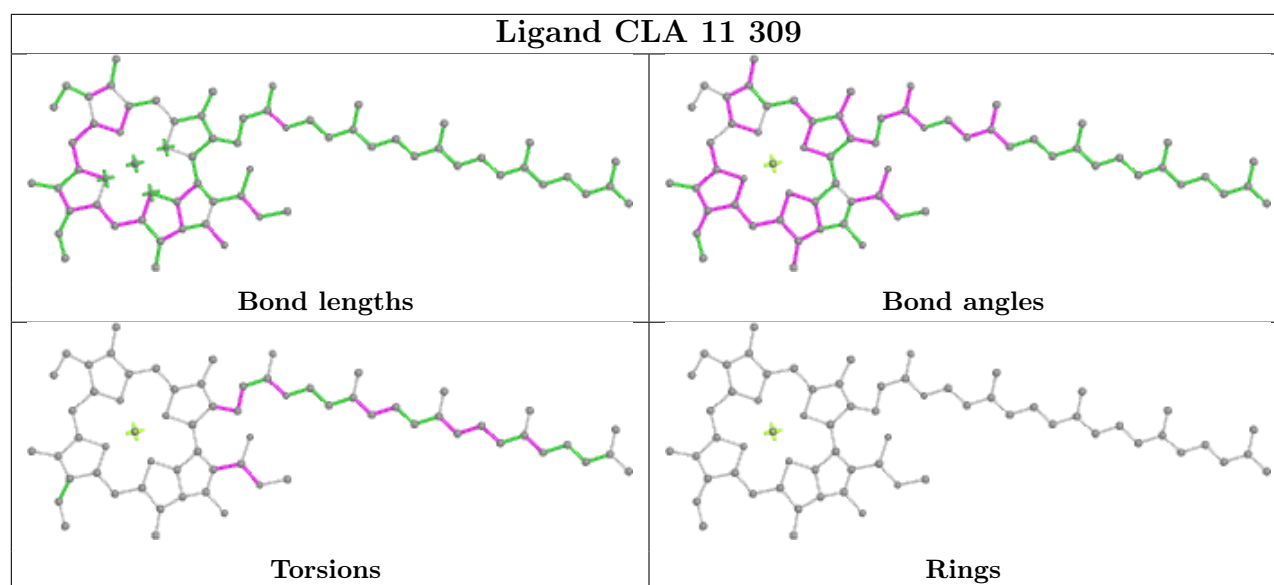


Ligand PQN A 845

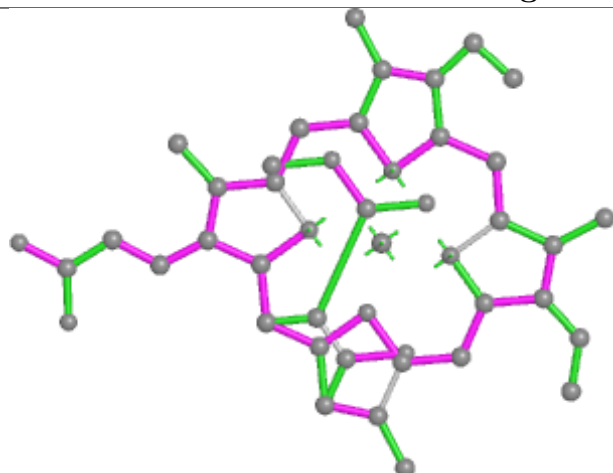


Ligand CLA A 811

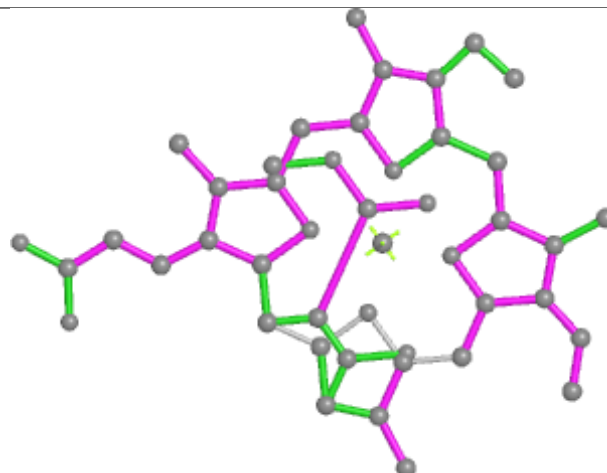




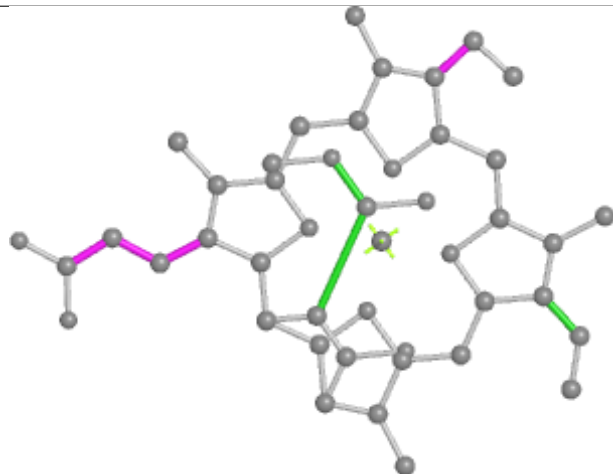
Ligand KC1 4 307



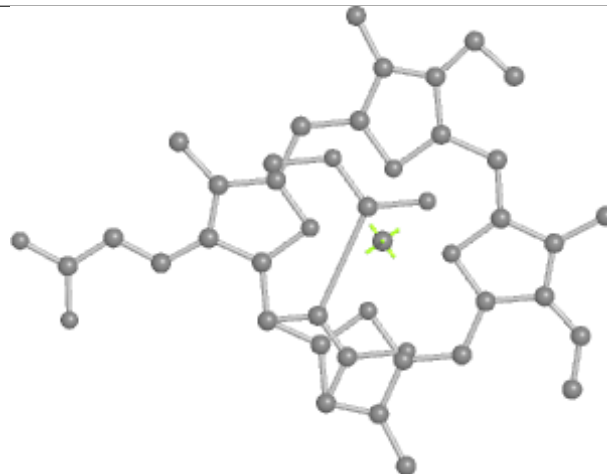
Bond lengths



Bond angles

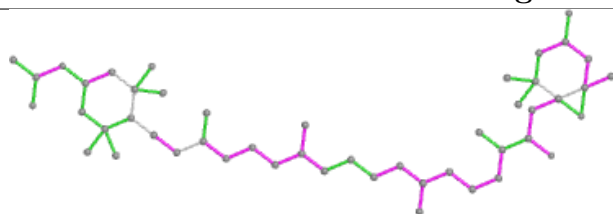


Torsions

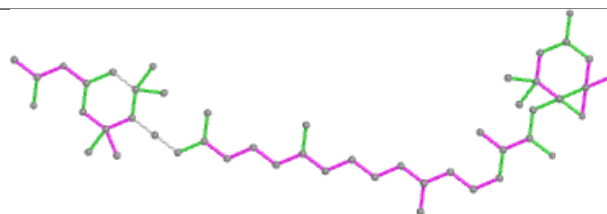


Rings

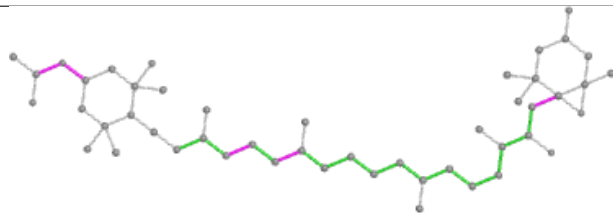
Ligand A86 14 301



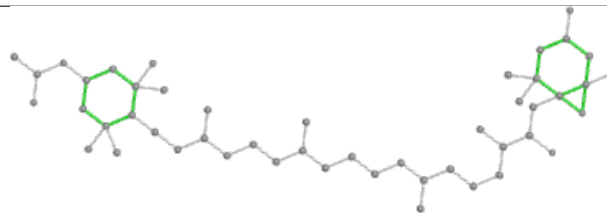
Bond lengths



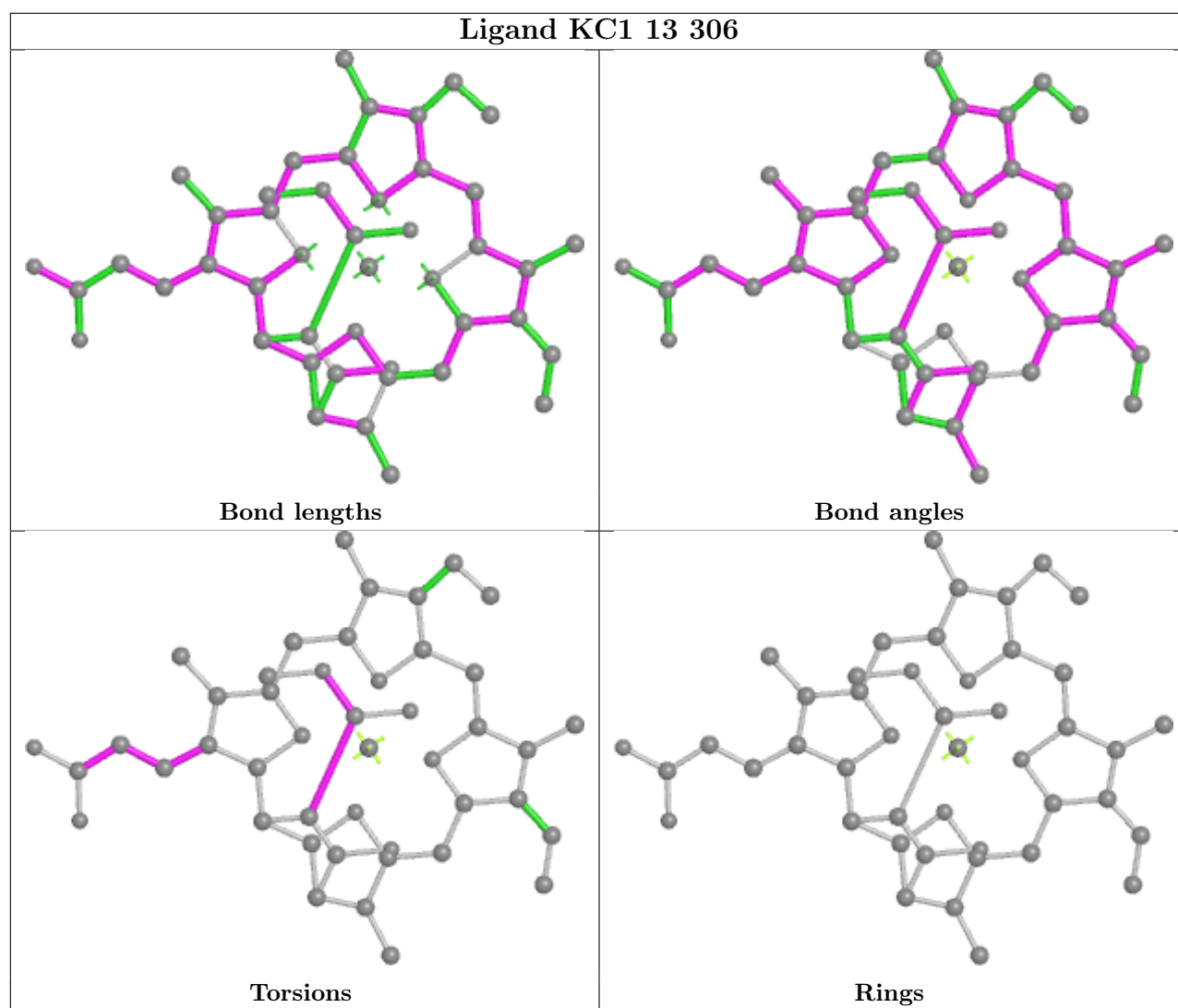
Bond angles

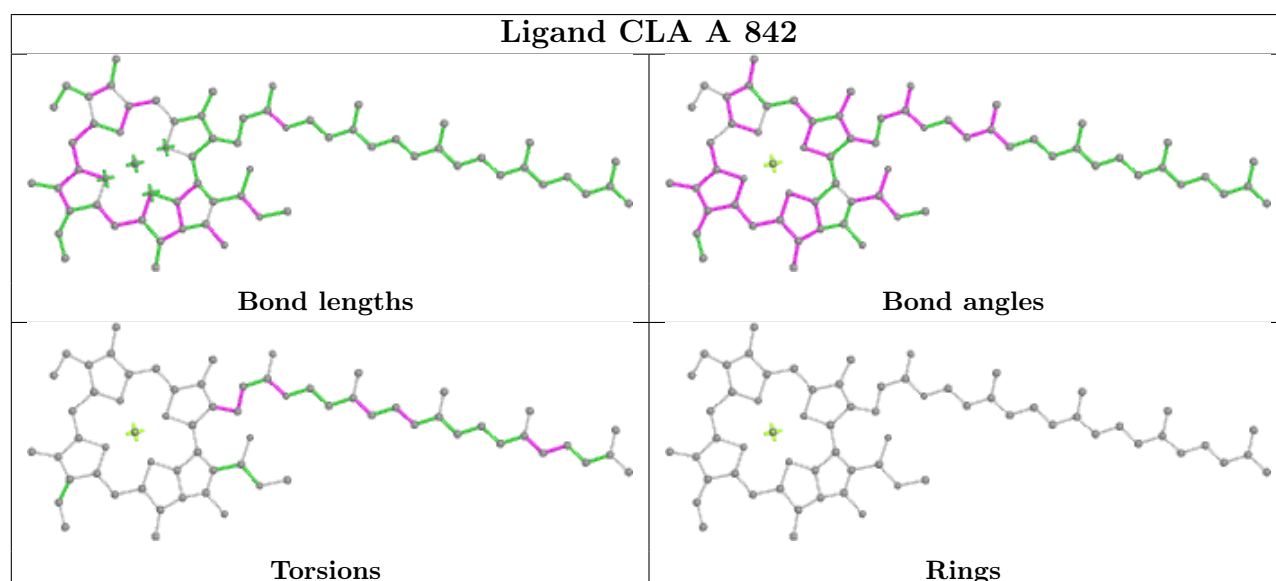
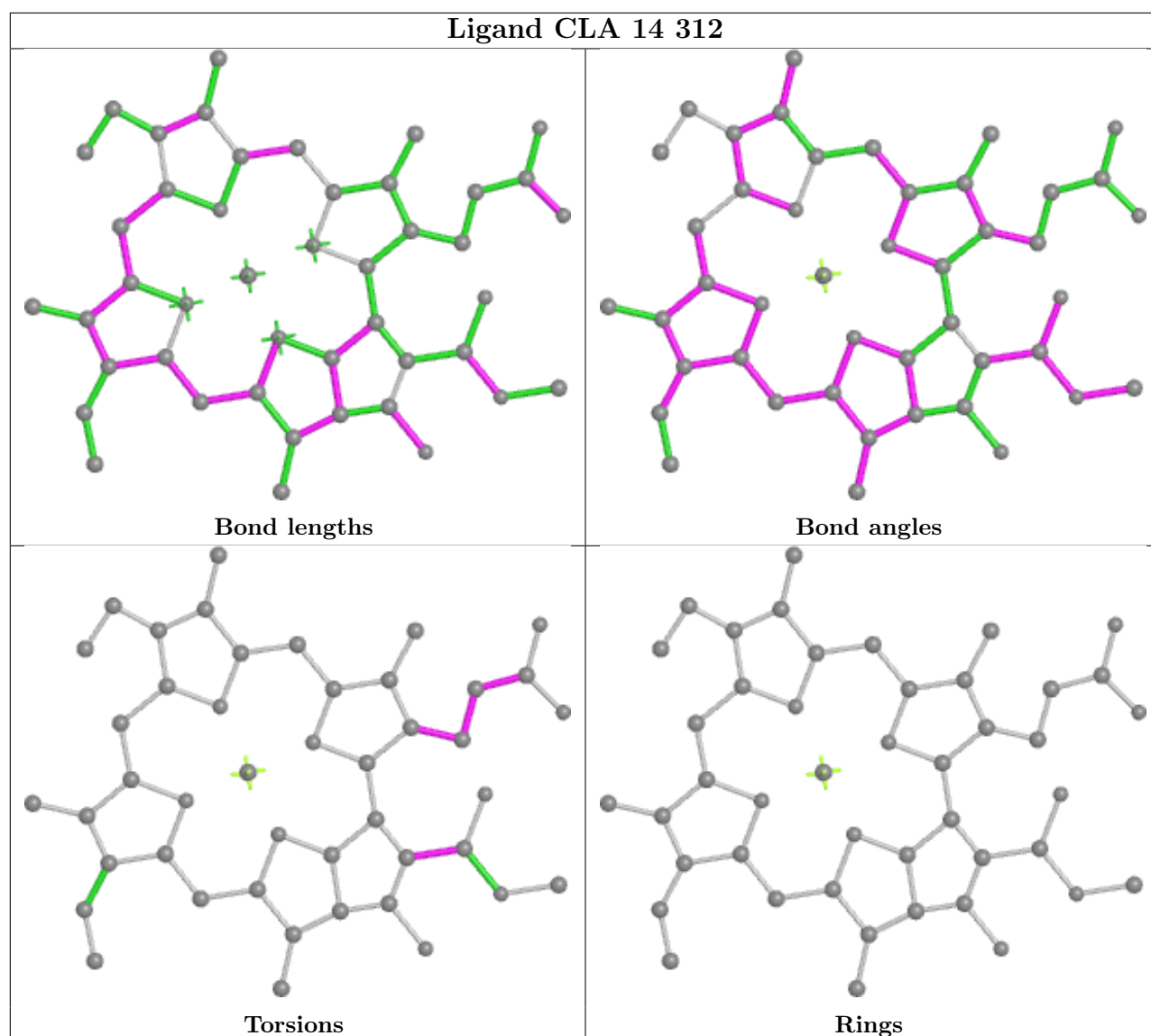


Torsions

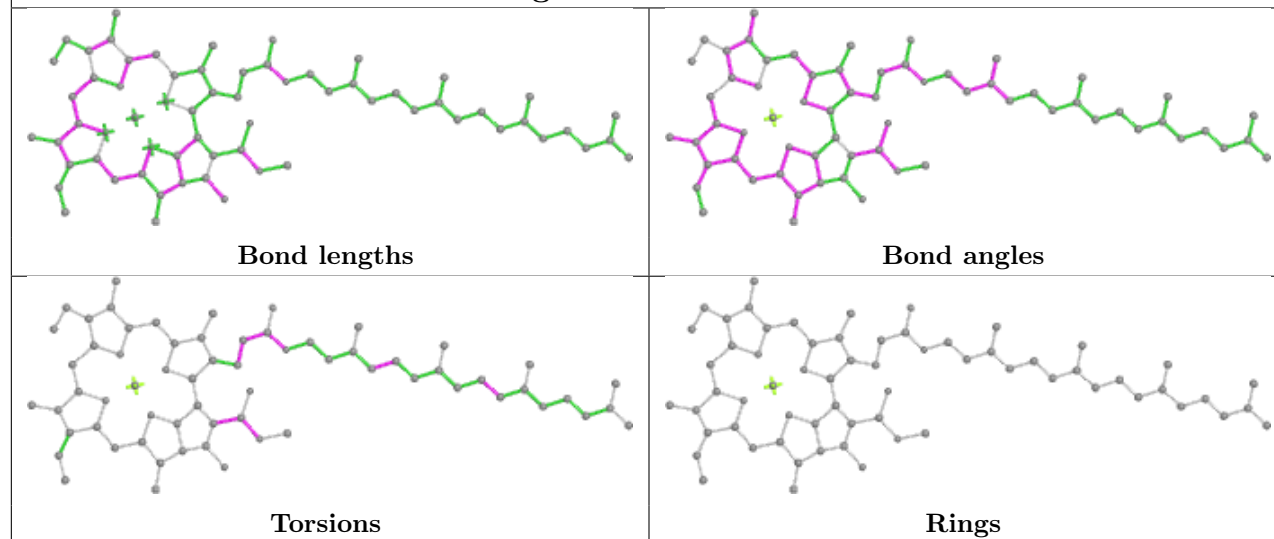


Rings

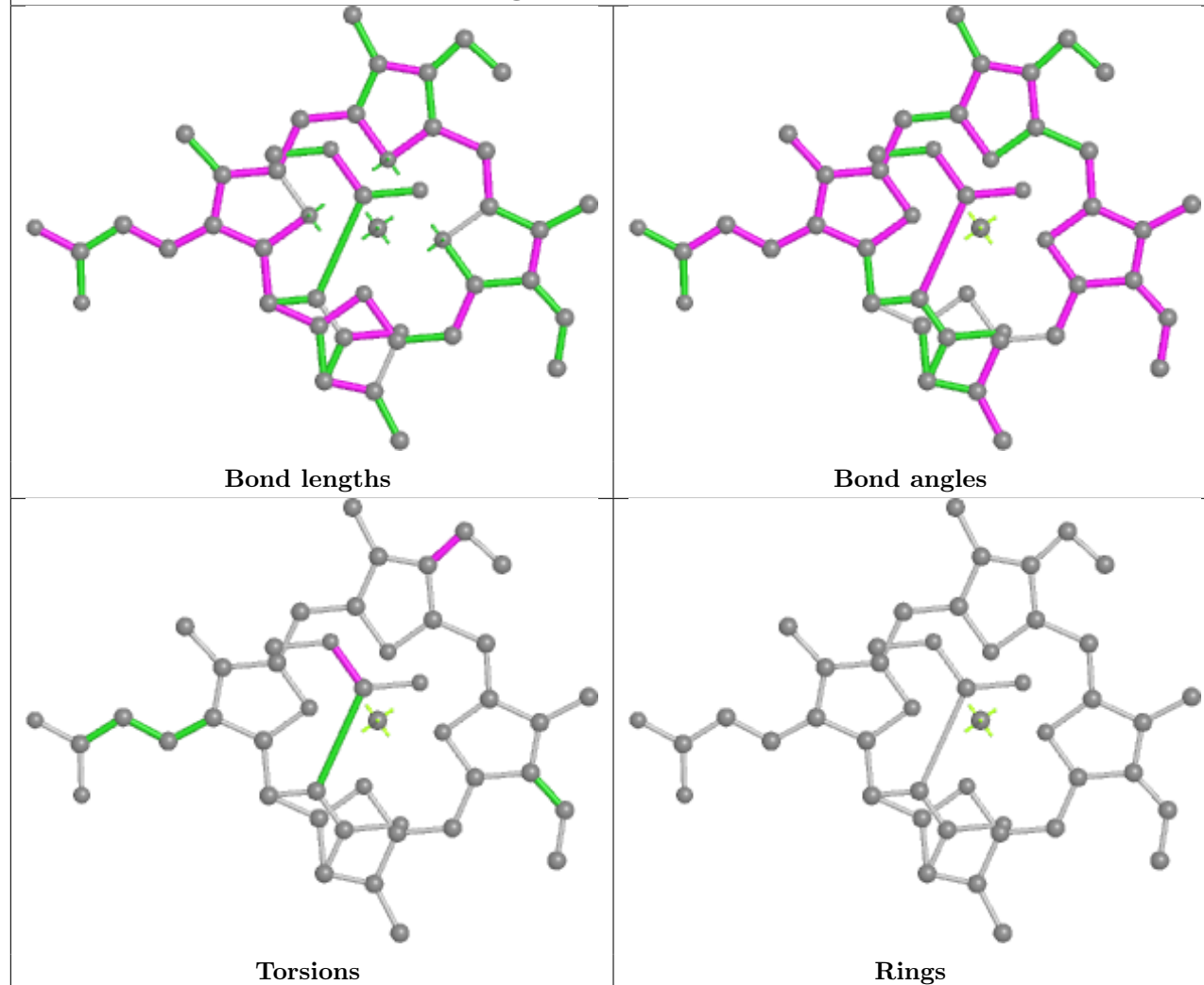


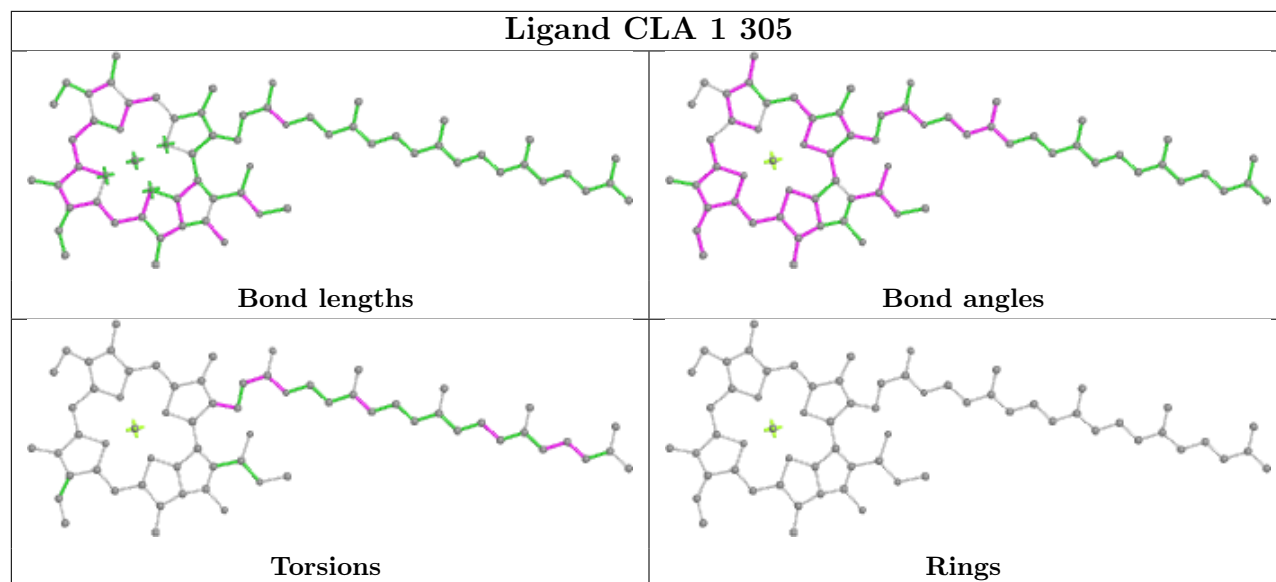
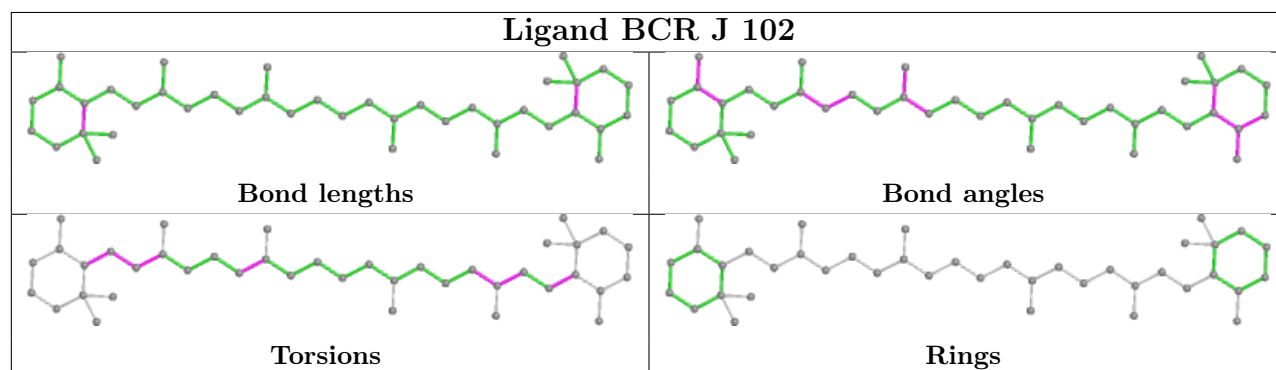
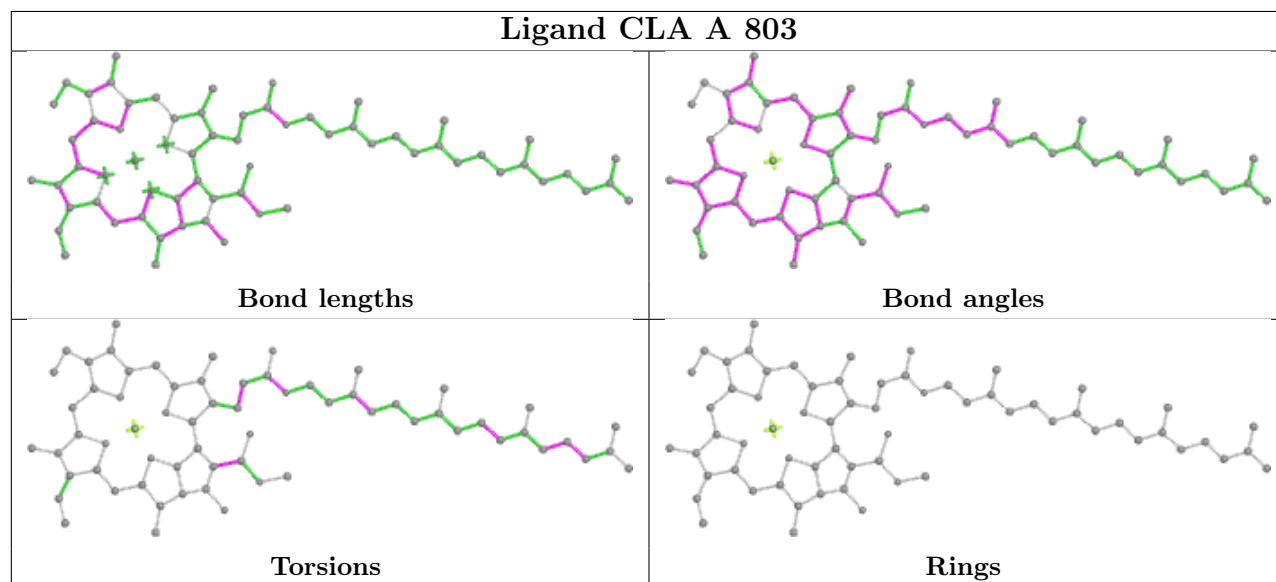


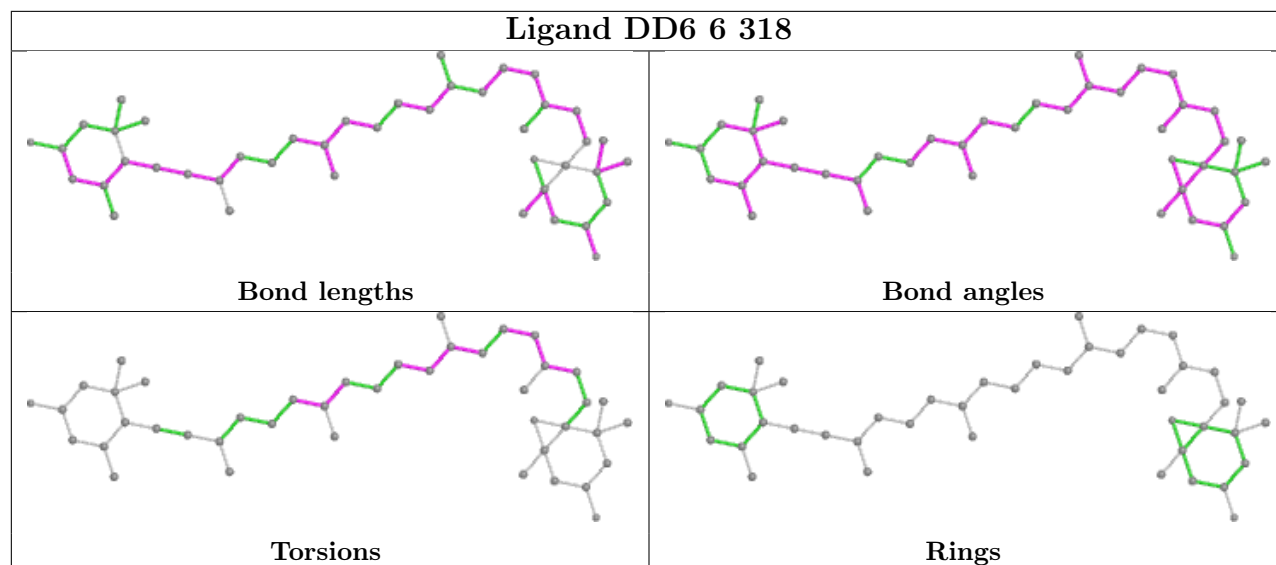
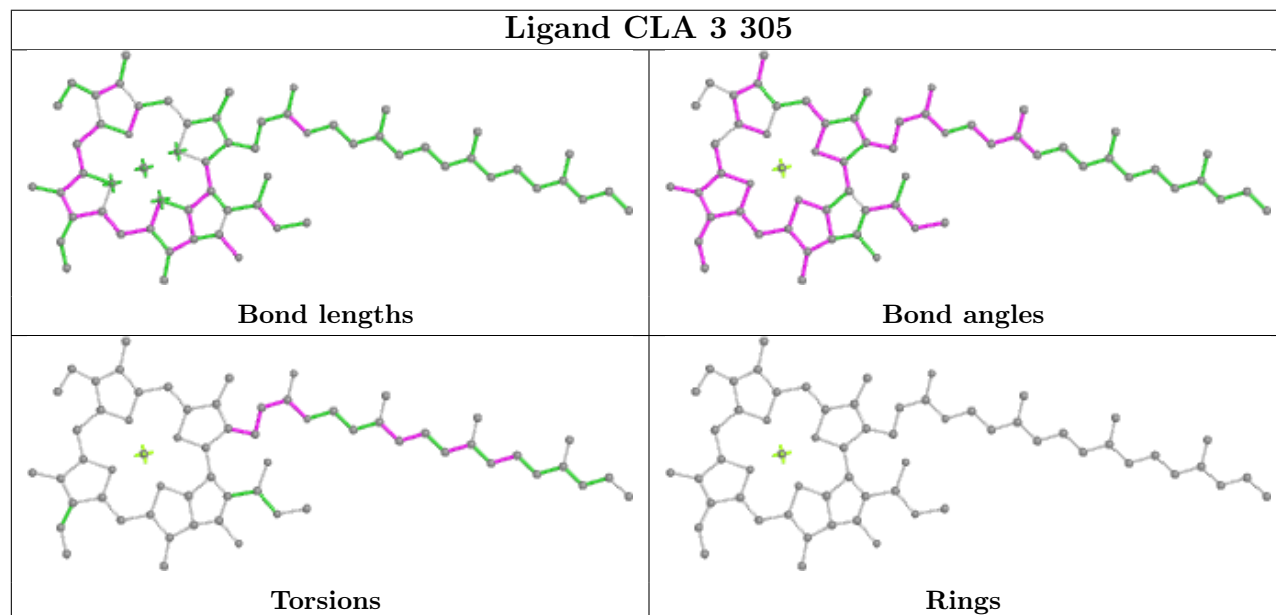
Ligand CLA B 810

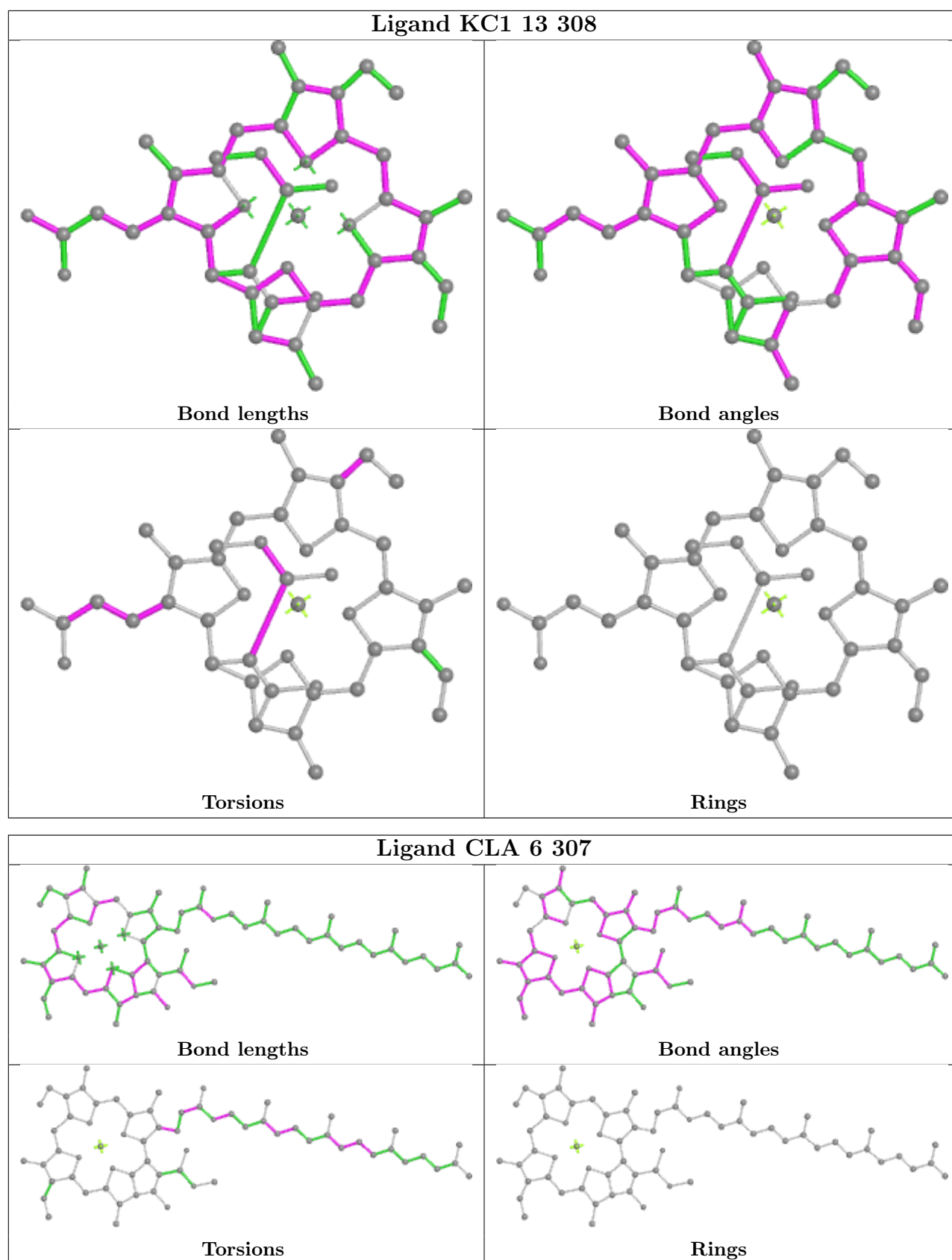


Ligand KC1 5 312

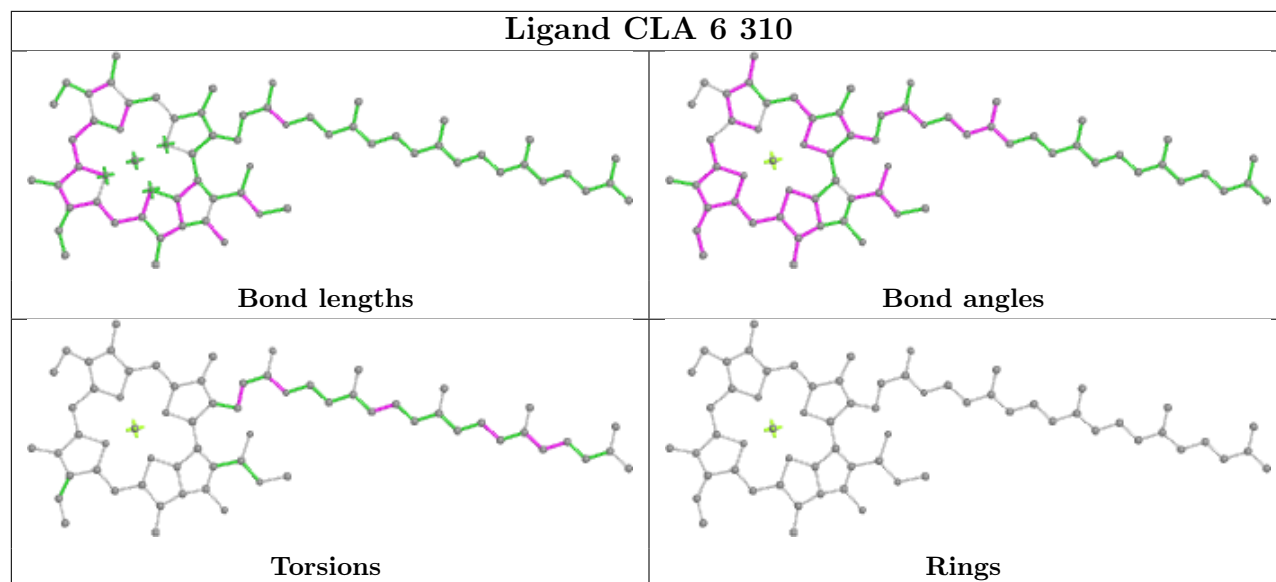


Ligand CLA 1 305**Ligand BCR J 102****Ligand CLA A 803**

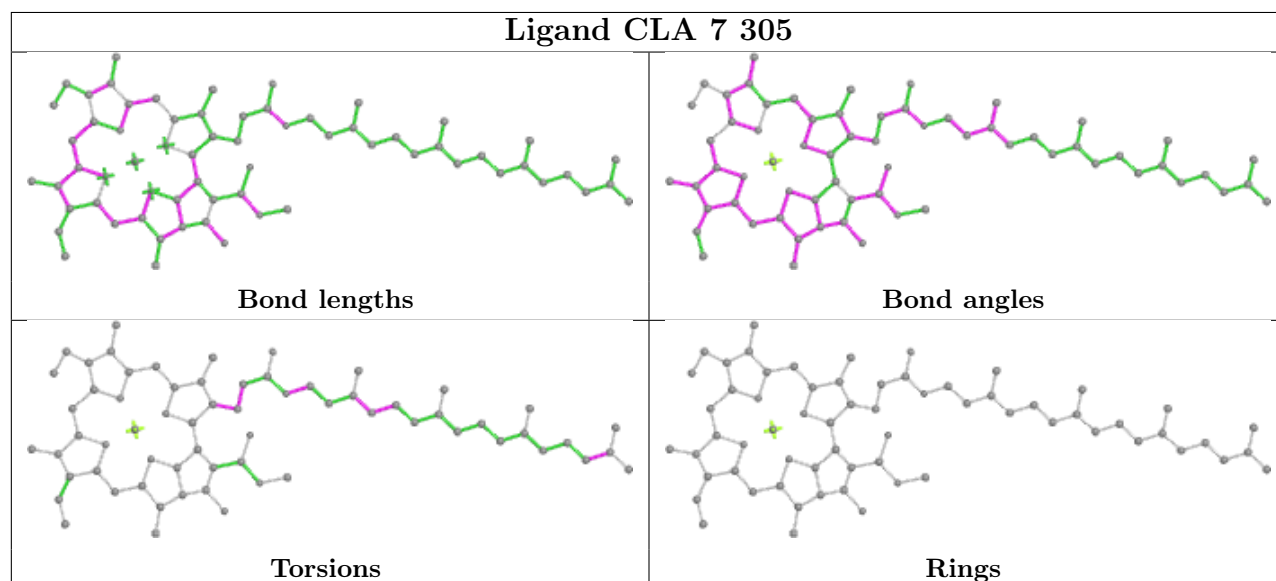
Ligand DD6 6 318**Ligand CLA 3 305**



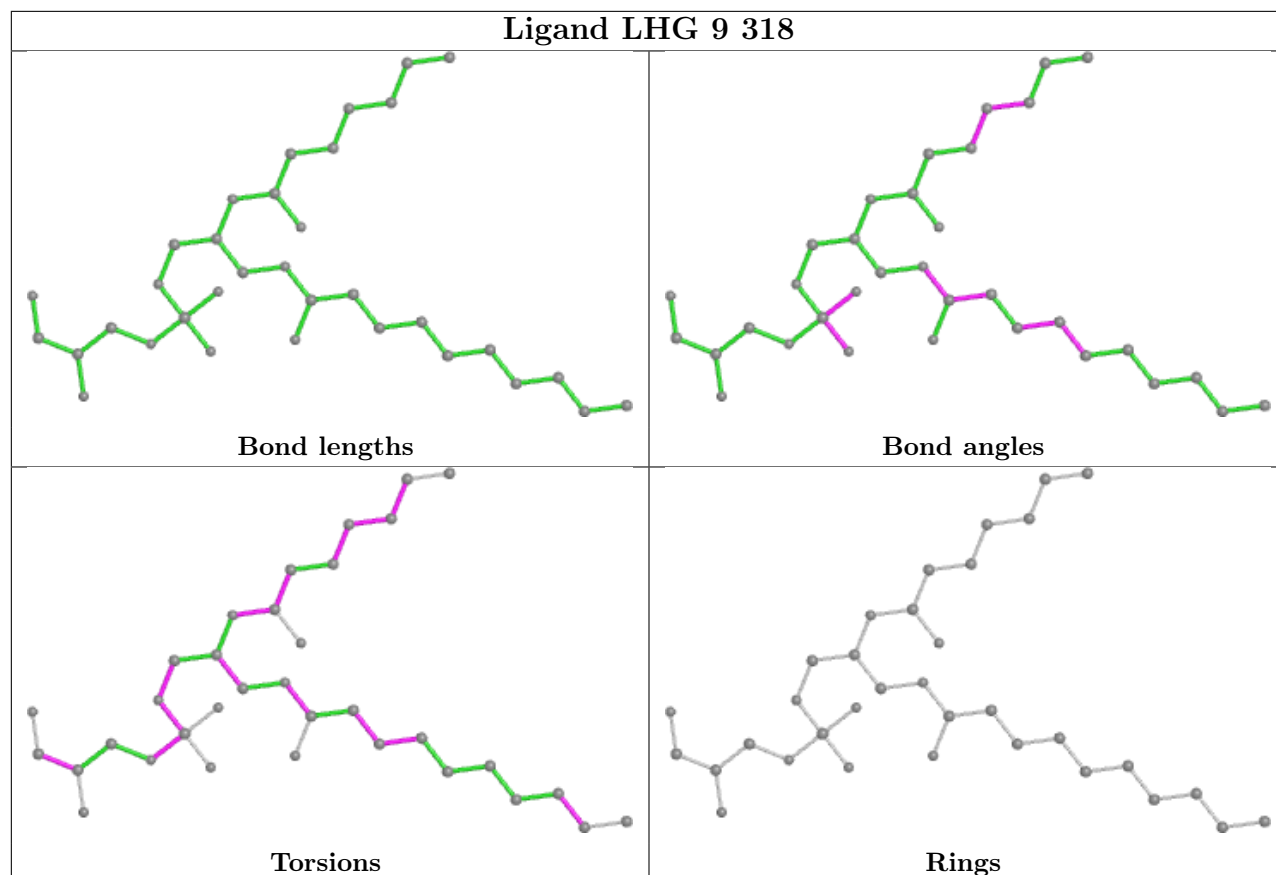
Ligand CLA 6 310



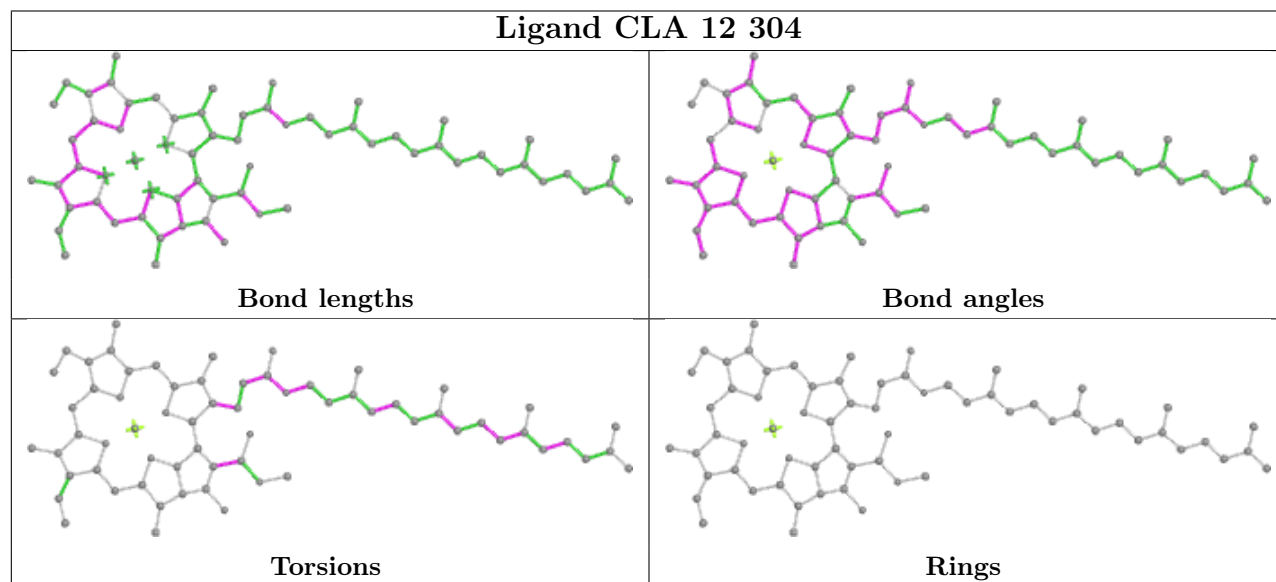
Ligand CLA 7 305



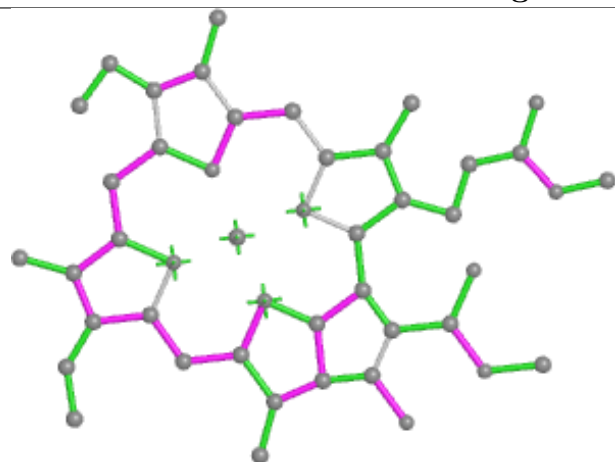
Ligand LHG 9 318



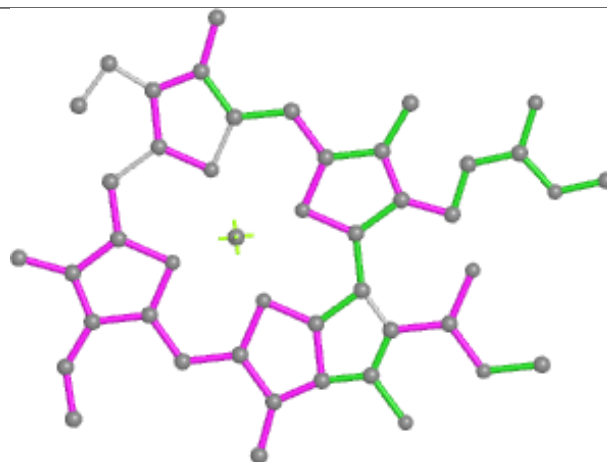
Ligand CLA 12 304



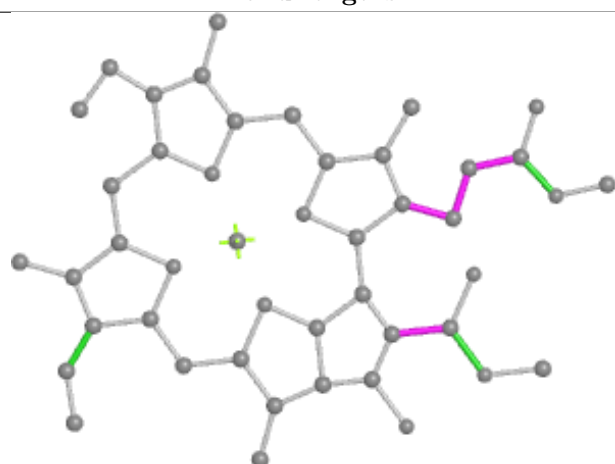
Ligand CLA 16 307



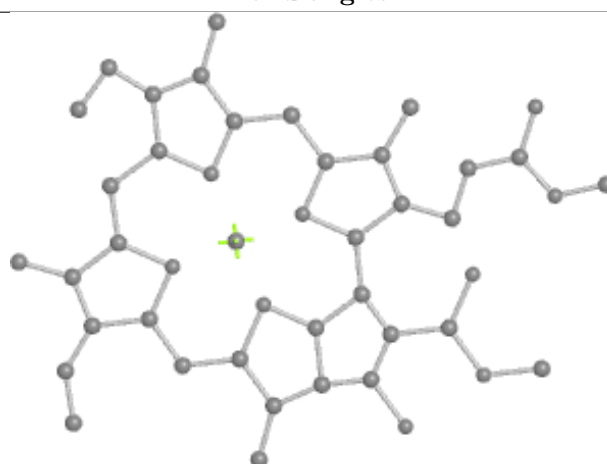
Bond lengths



Bond angles

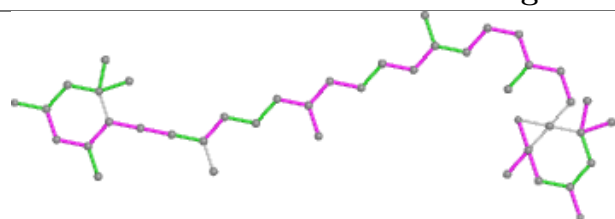


Torsions

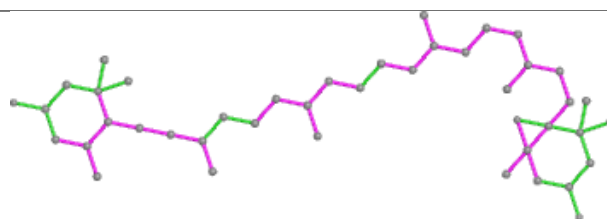


Rings

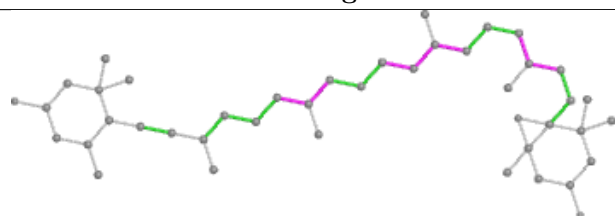
Ligand DD6 5 313



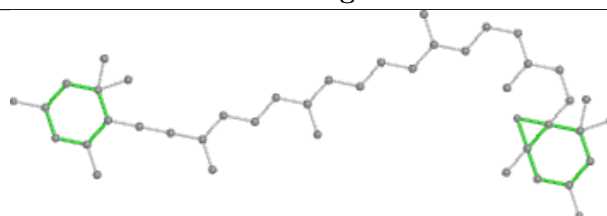
Bond lengths



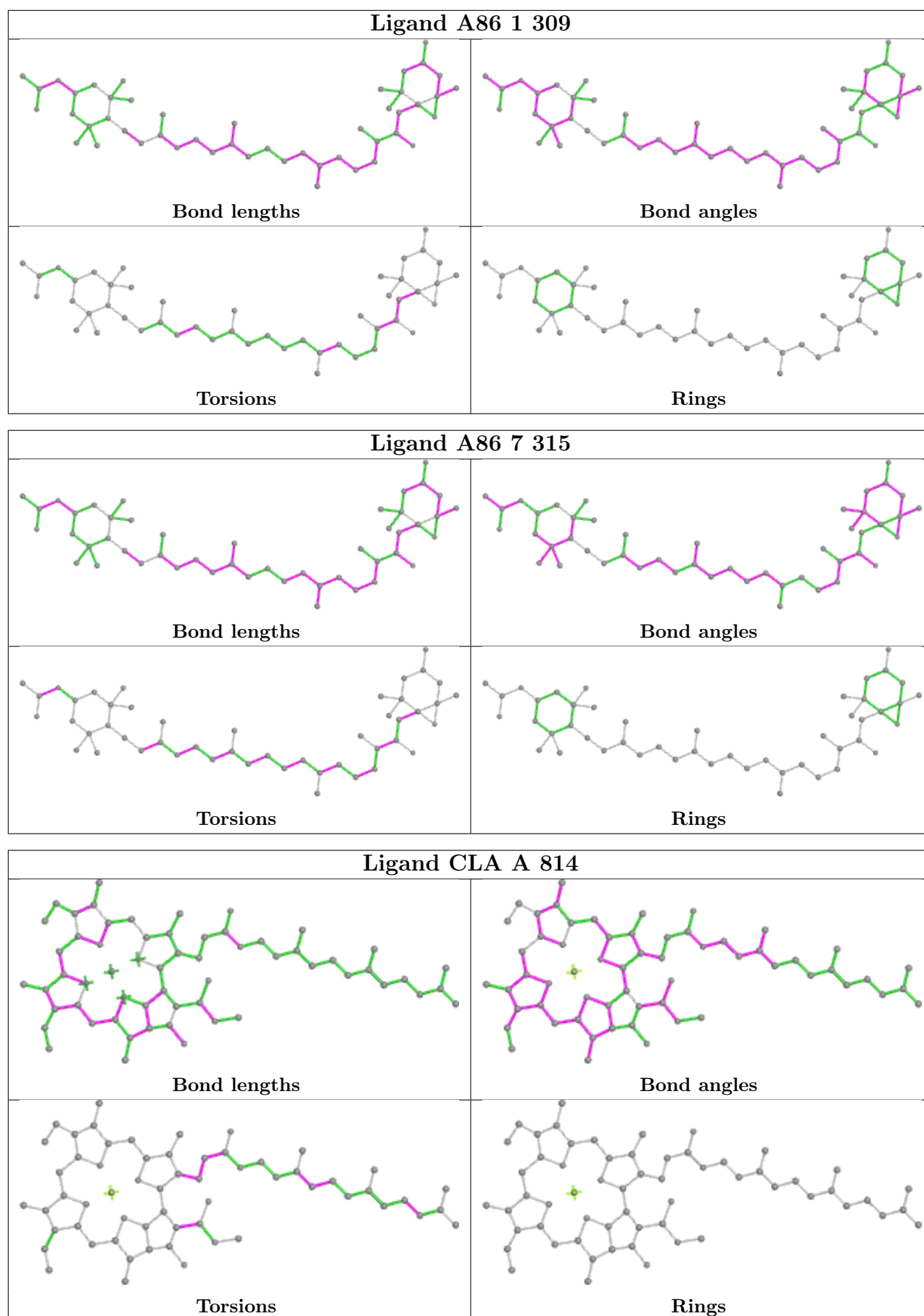
Bond angles

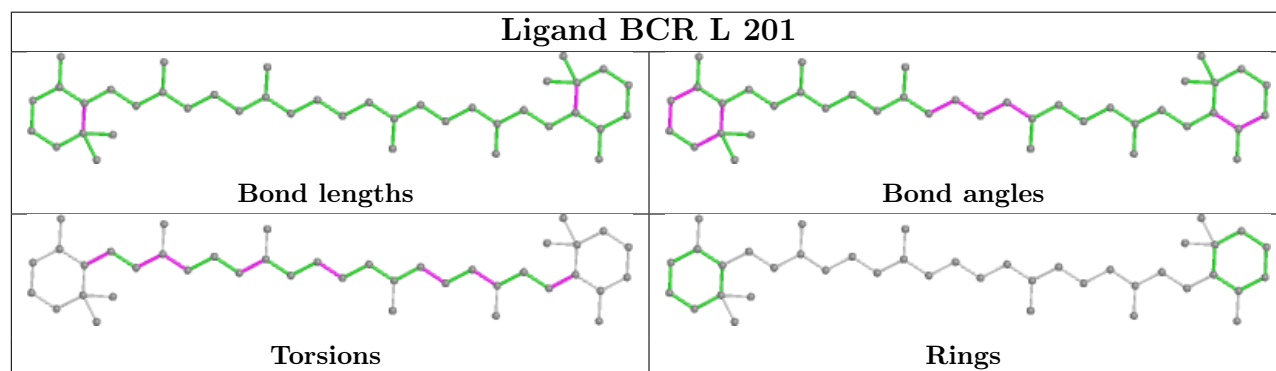
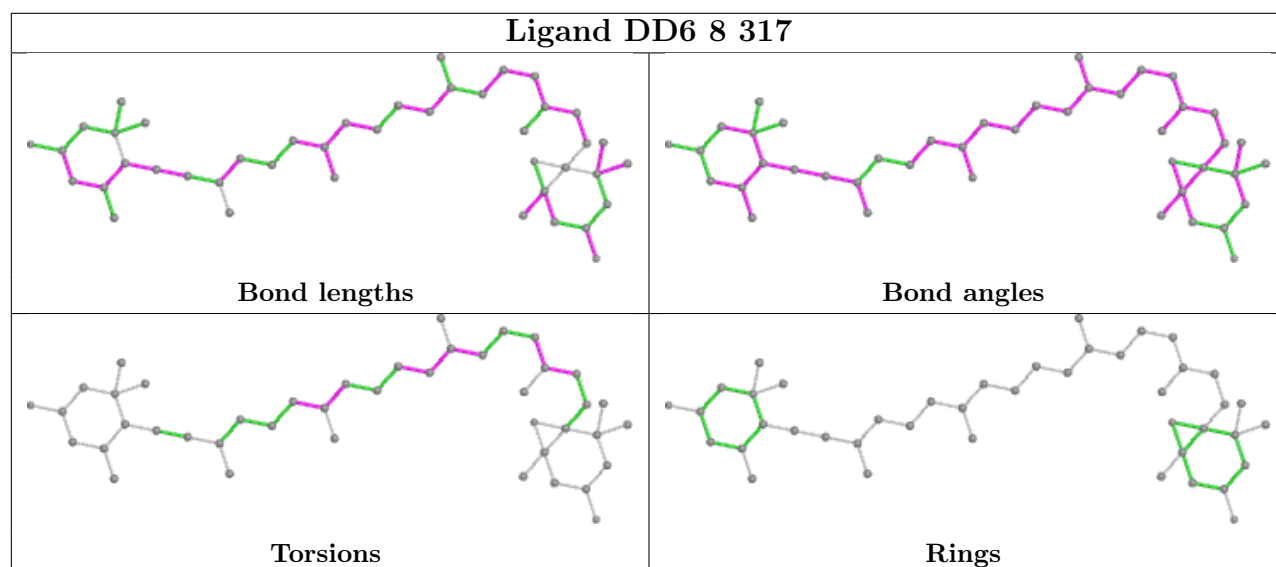
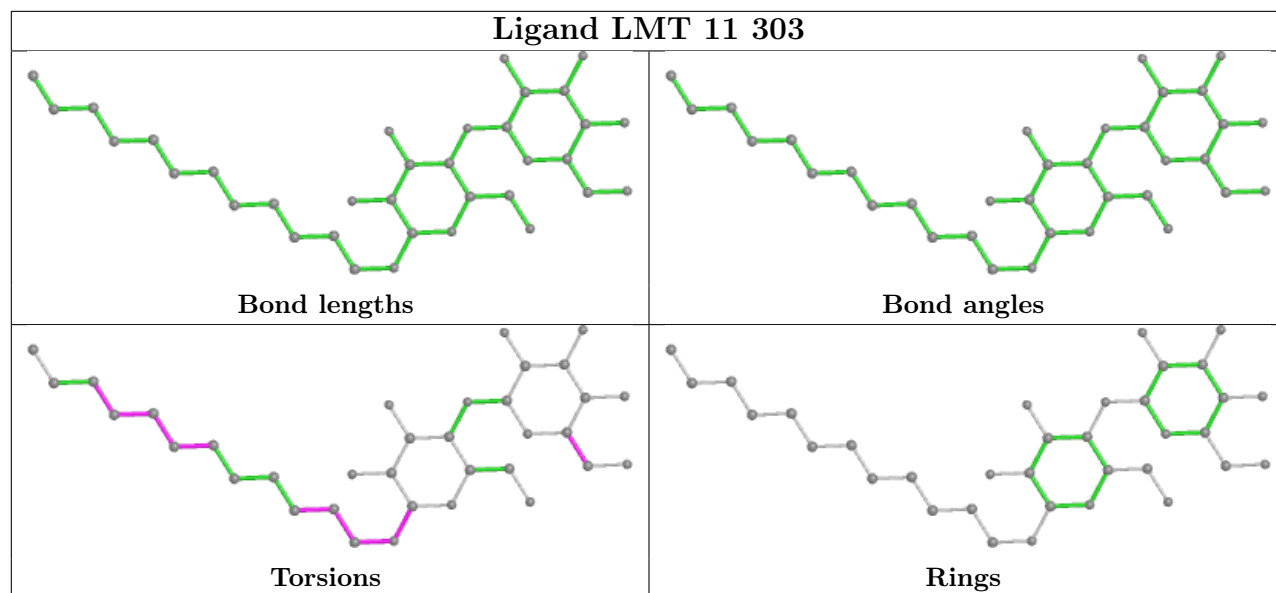


Torsions

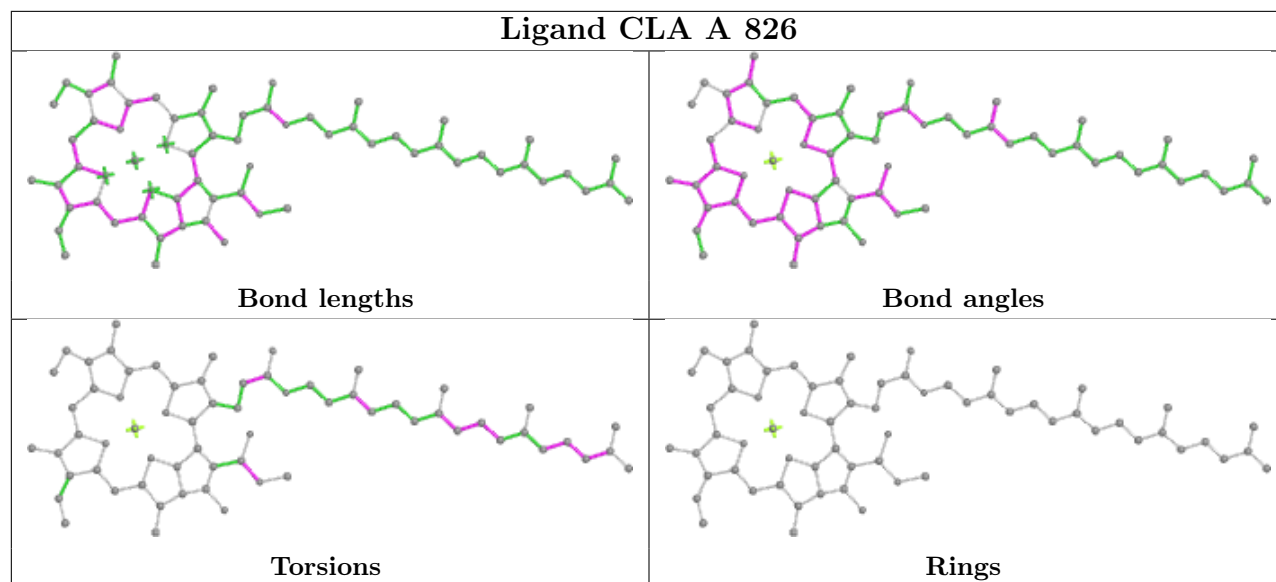


Rings

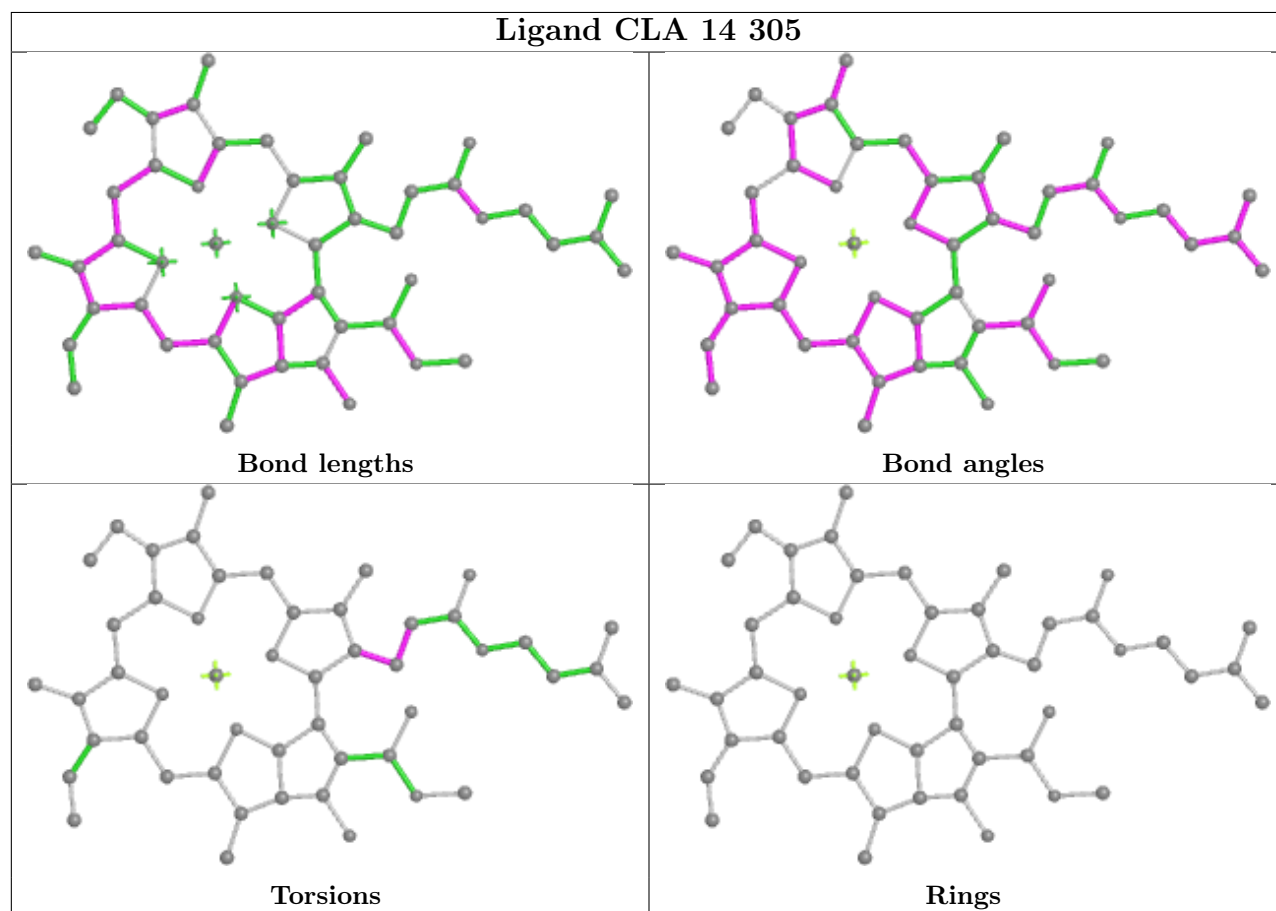




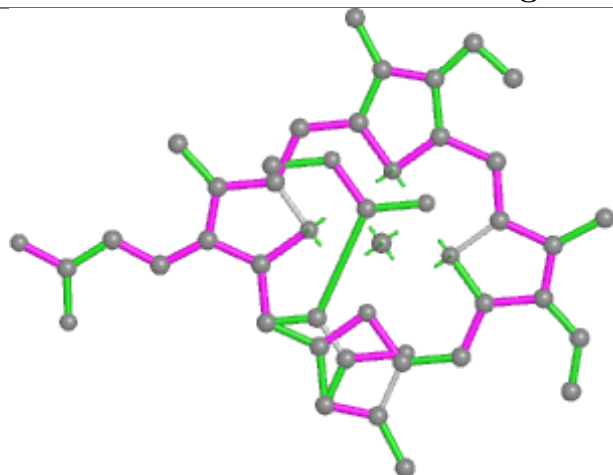
Ligand CLA A 826



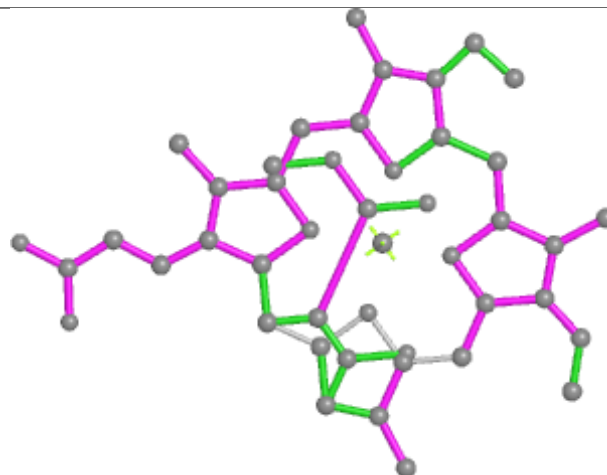
Ligand CLA 14 305



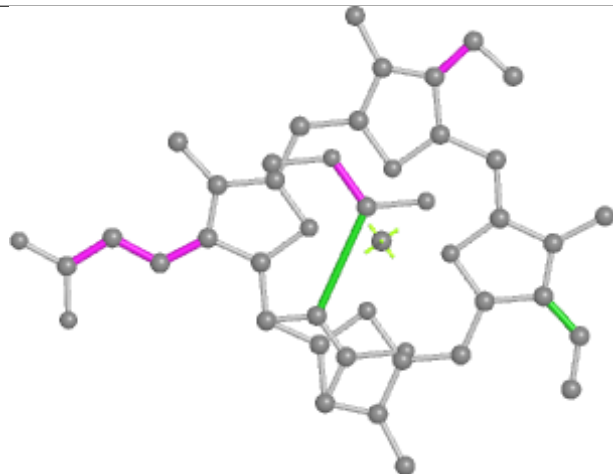
Ligand KC1 8 312



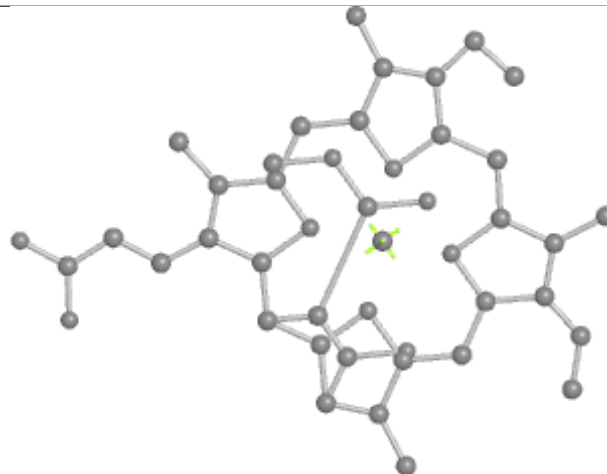
Bond lengths



Bond angles

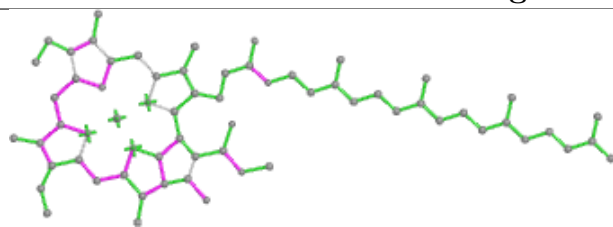


Torsions

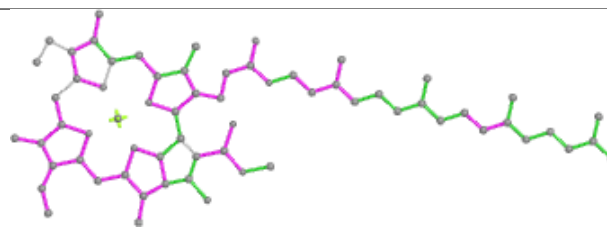


Rings

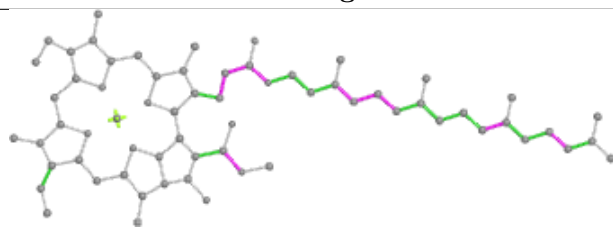
Ligand CLA 12 302



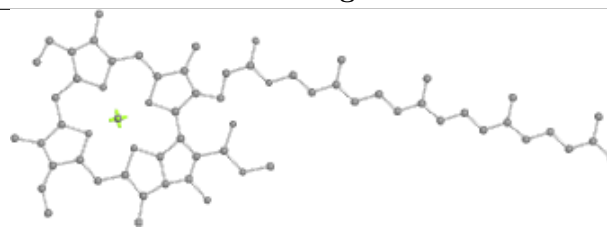
Bond lengths



Bond angles

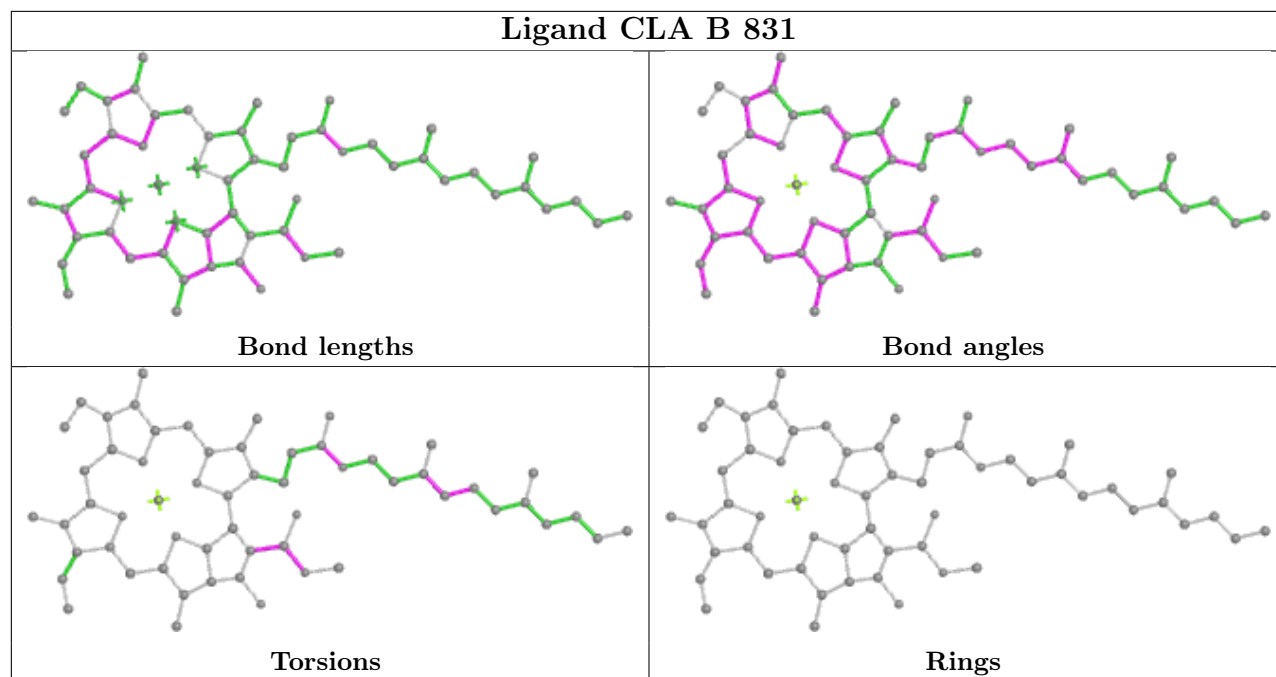


Torsions

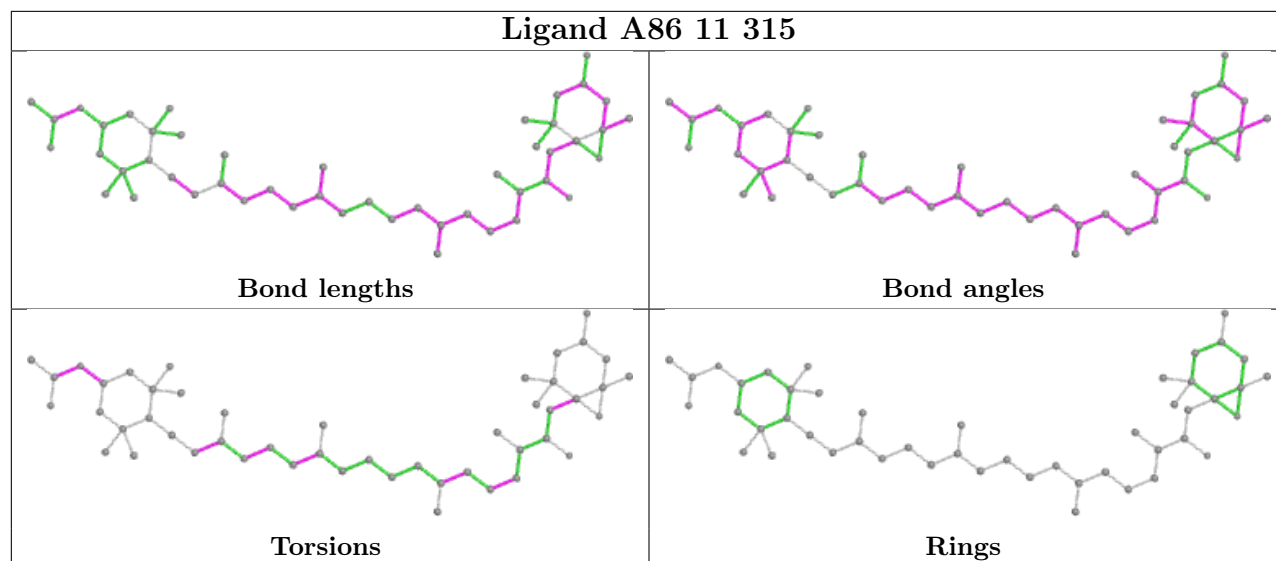


Rings

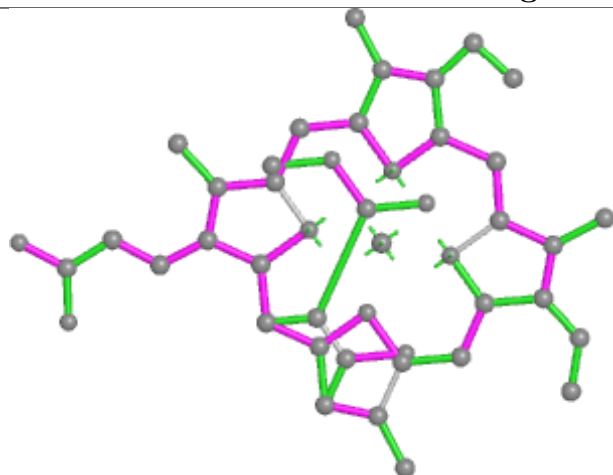
Ligand CLA B 831



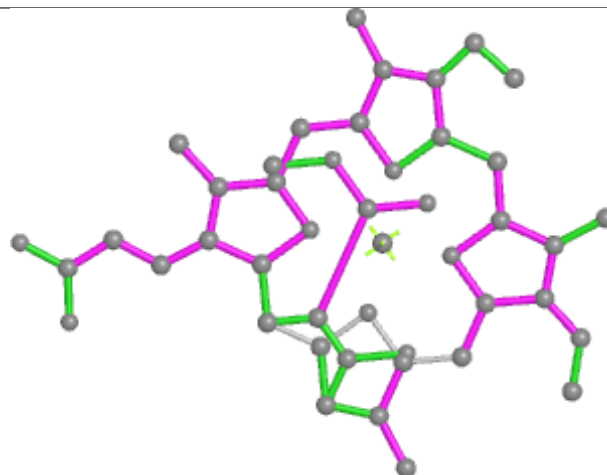
Ligand A86 11 315



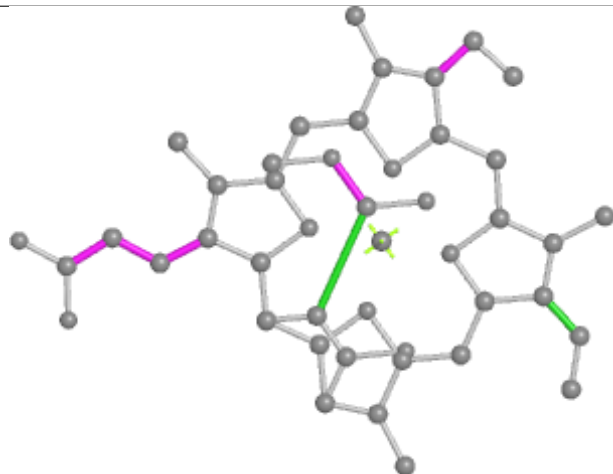
Ligand KC1 7 308



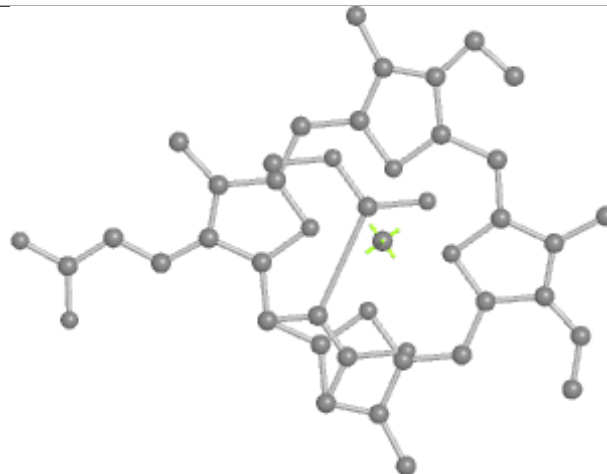
Bond lengths



Bond angles

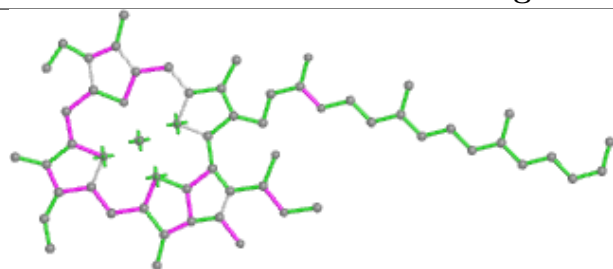


Torsions

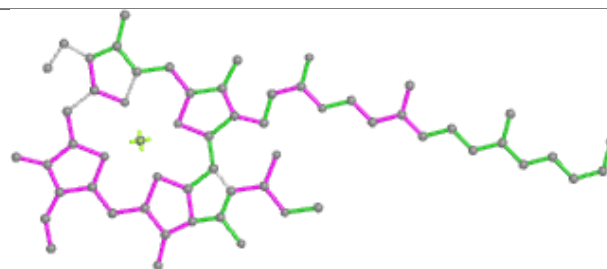


Rings

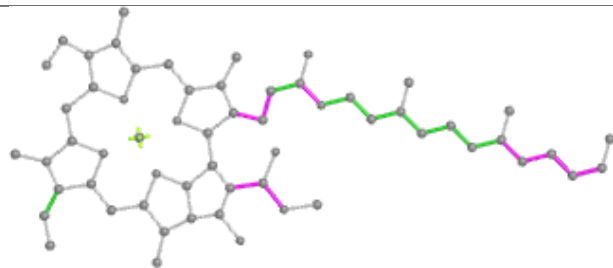
Ligand CLA A 825



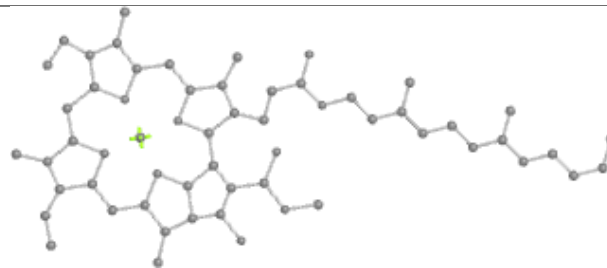
Bond lengths



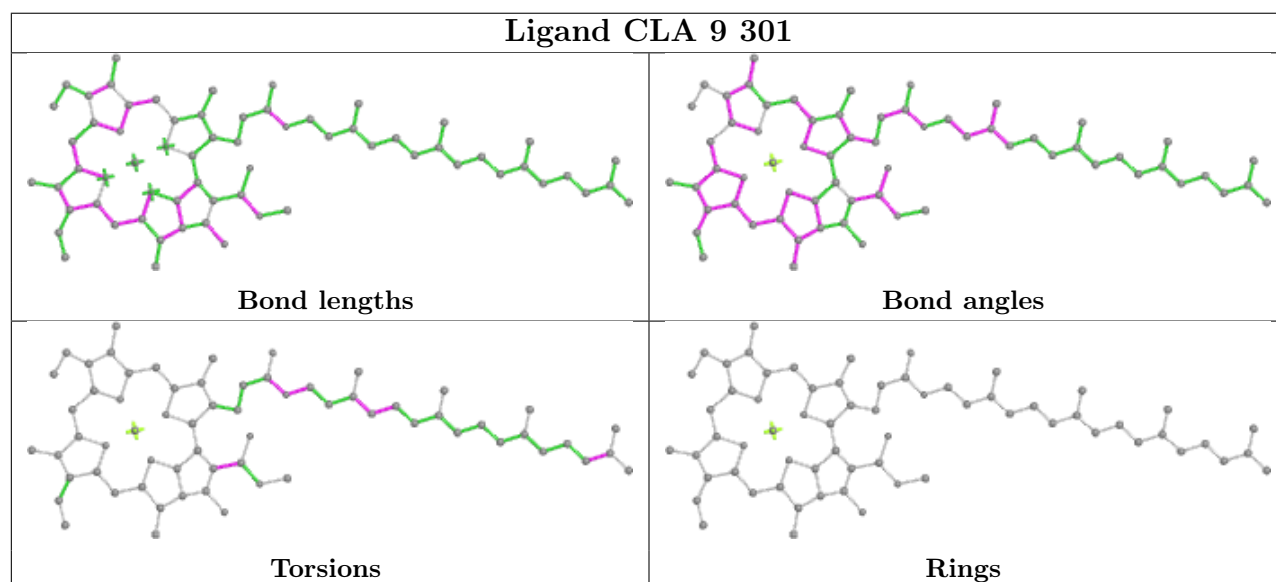
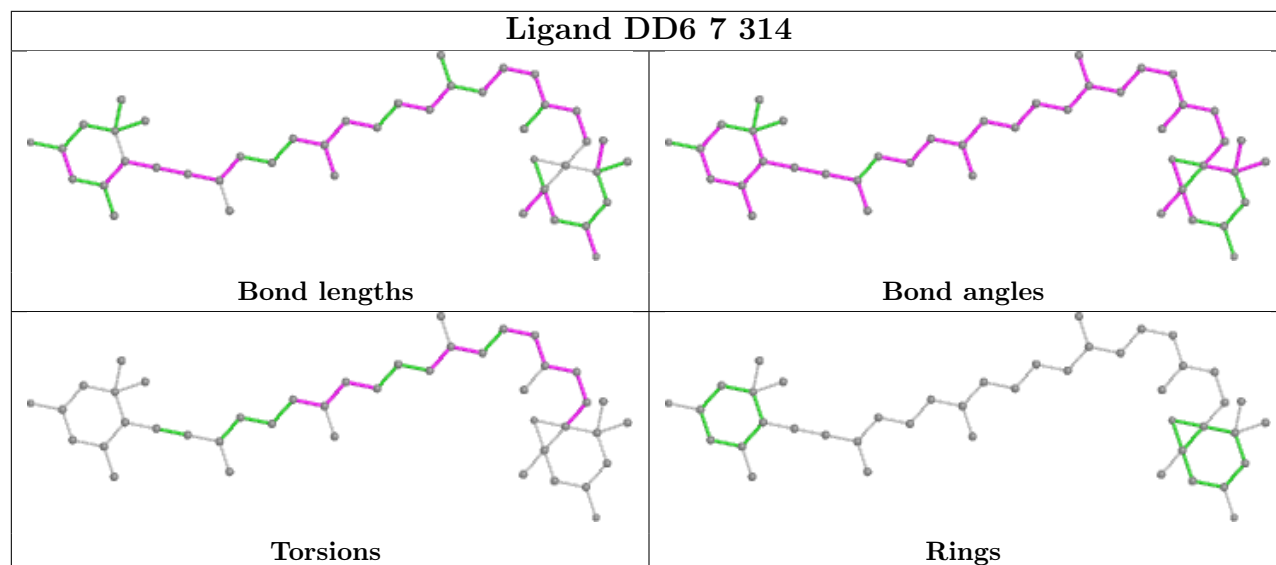
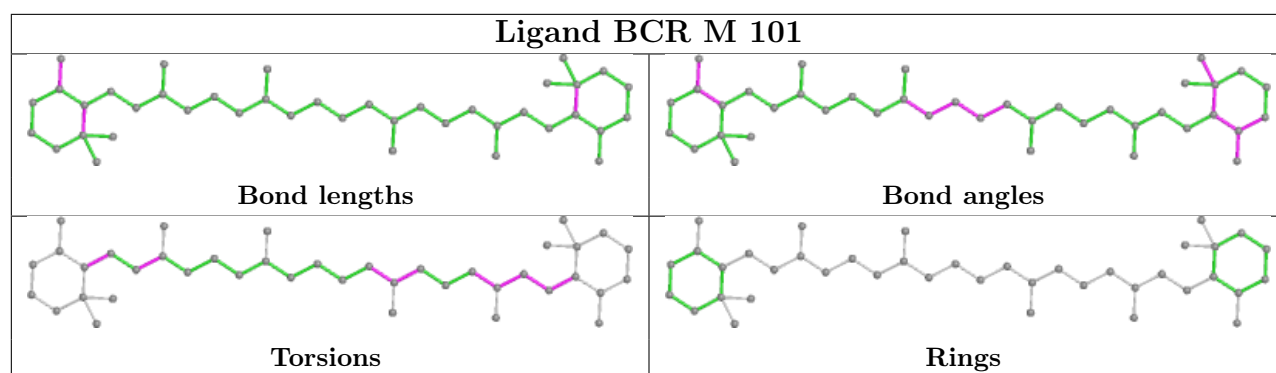
Bond angles

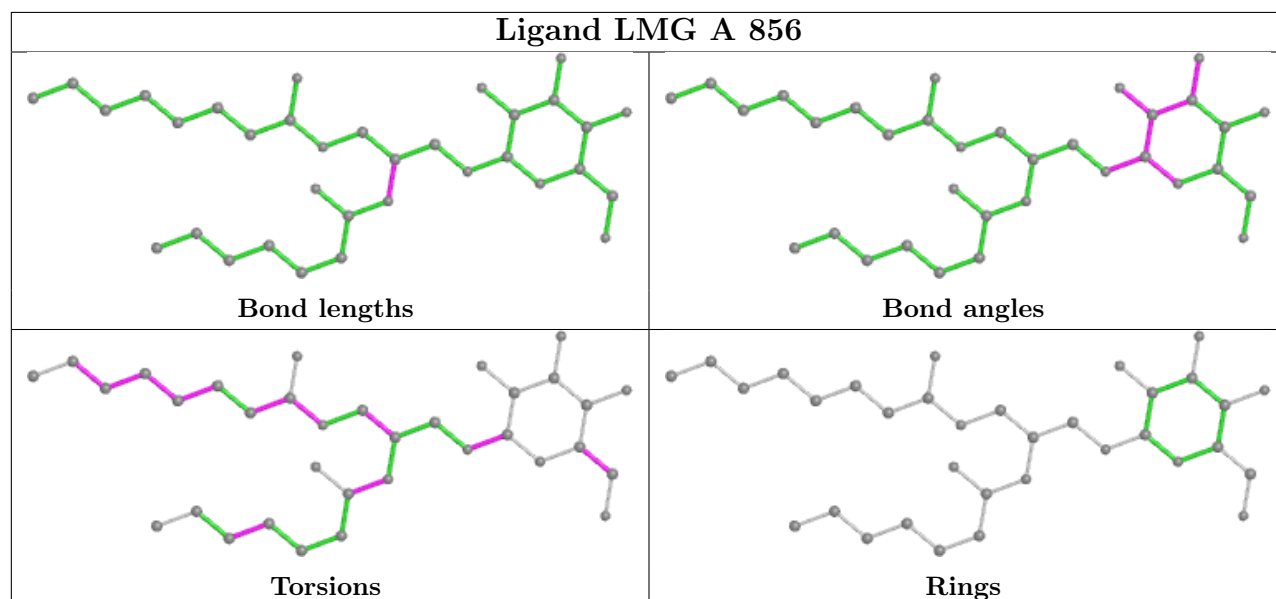
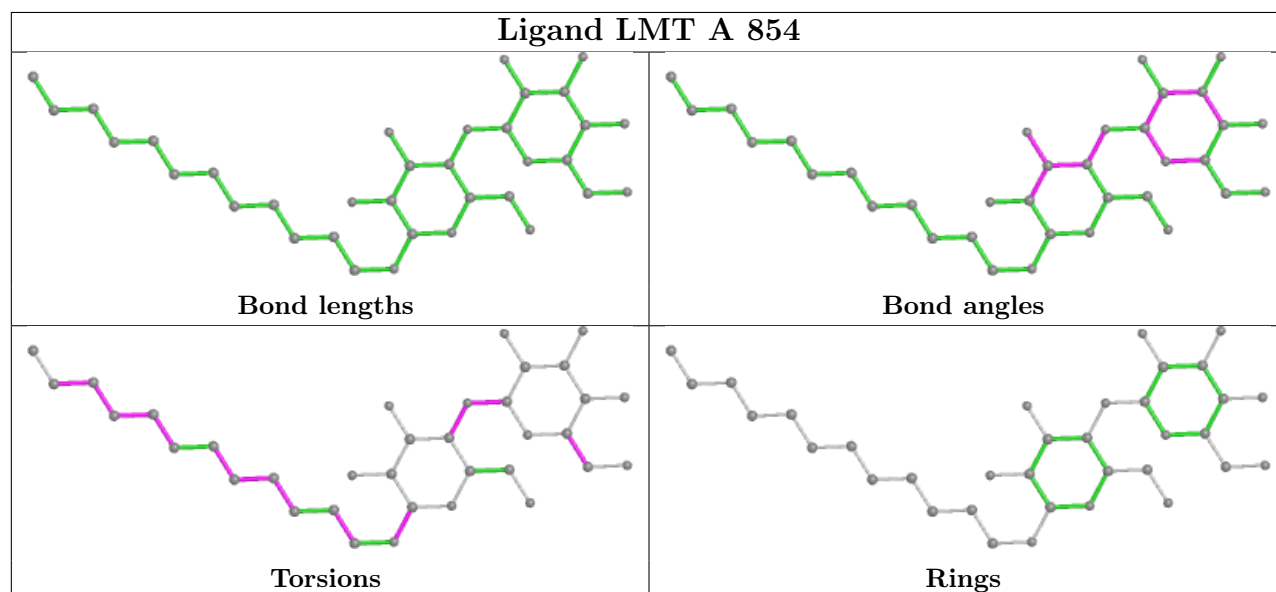
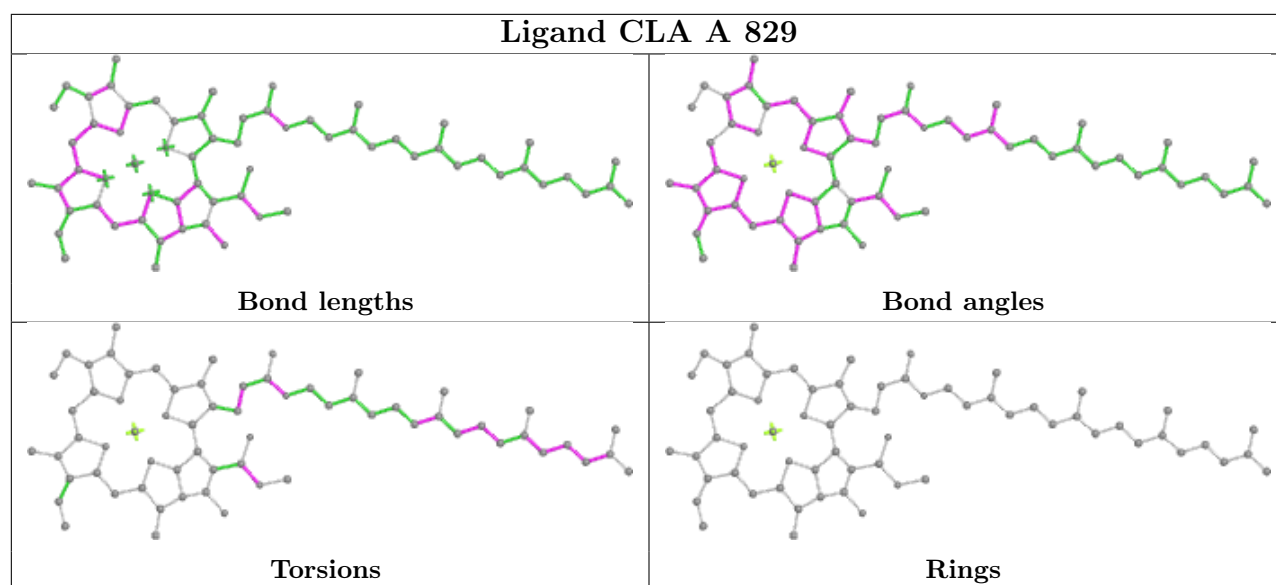


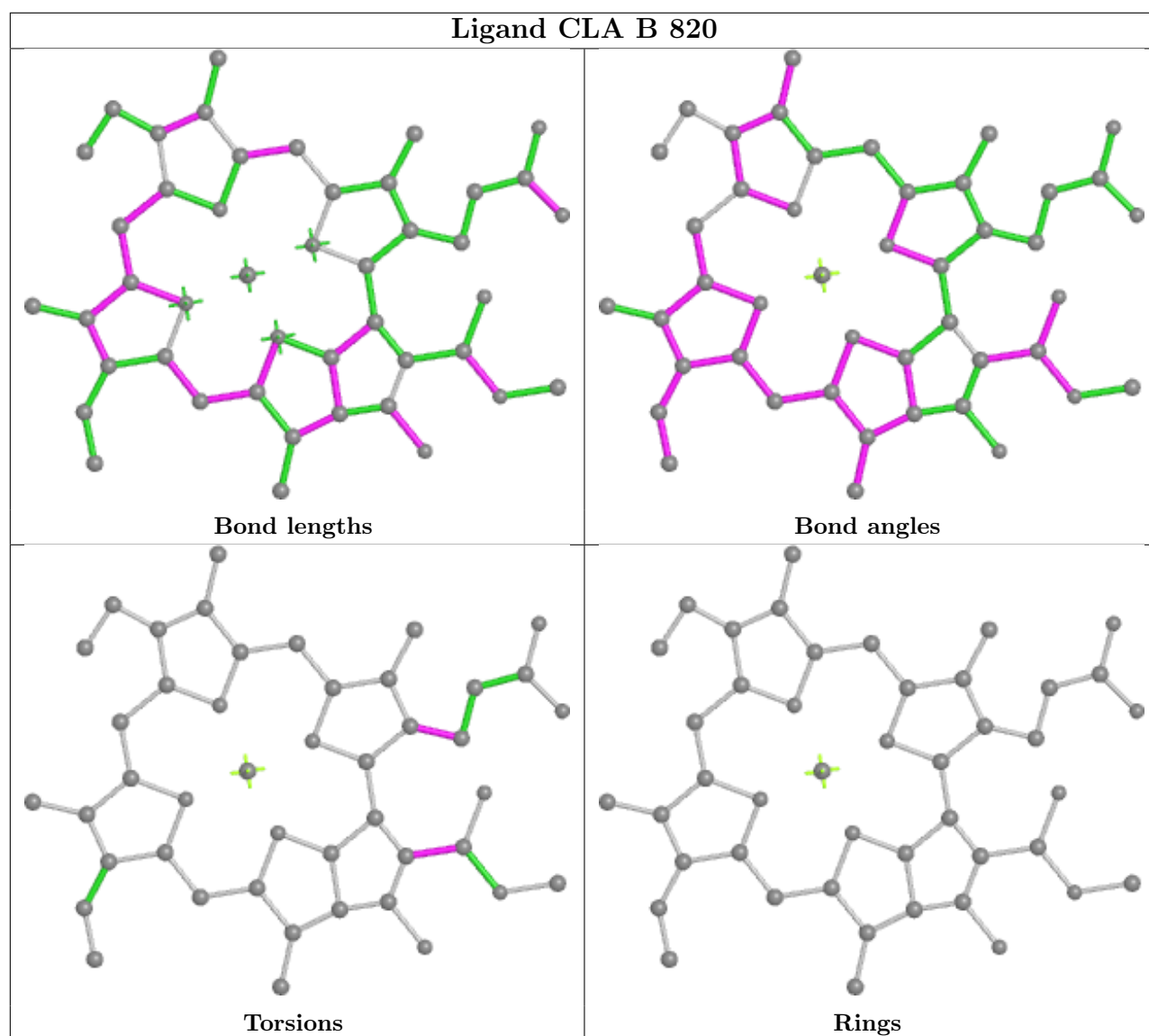
Torsions



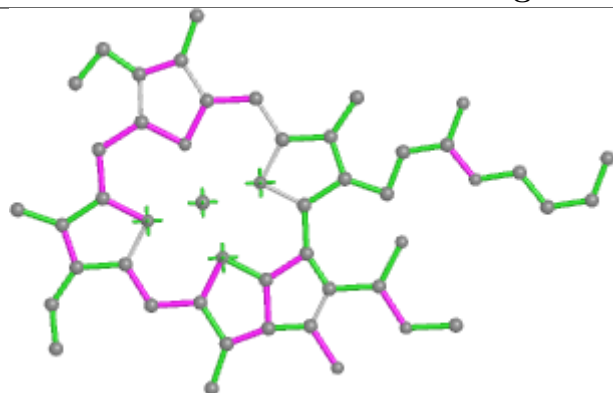
Rings



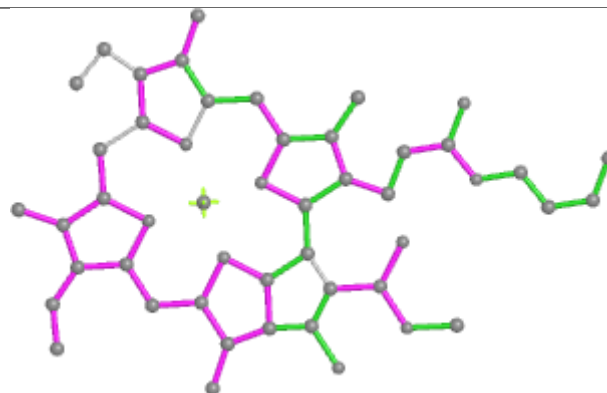




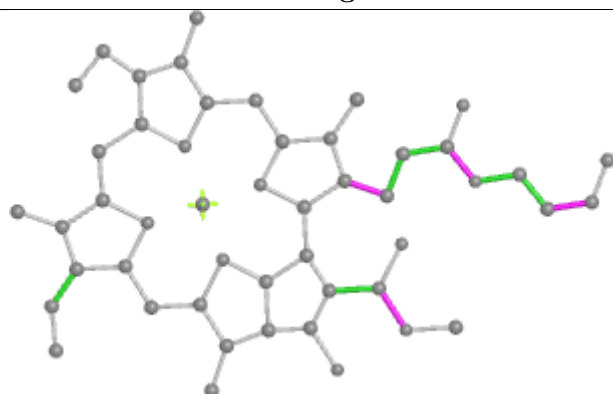
Ligand CLA A 823



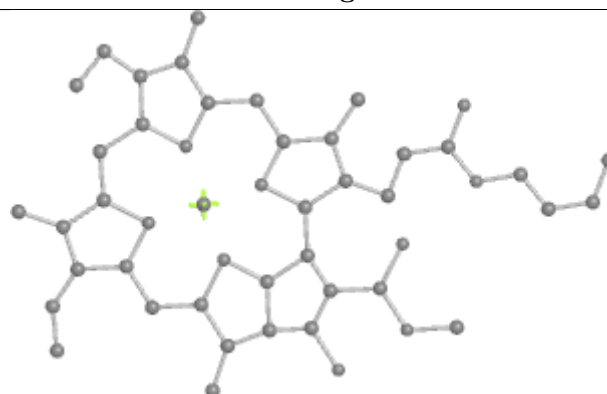
Bond lengths



Bond angles

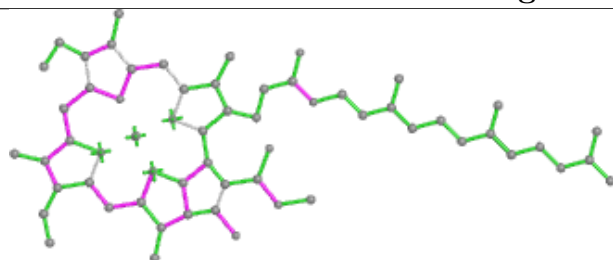


Torsions

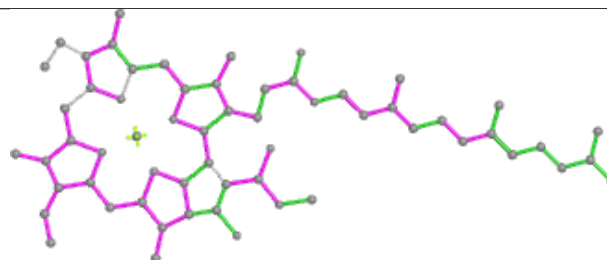


Rings

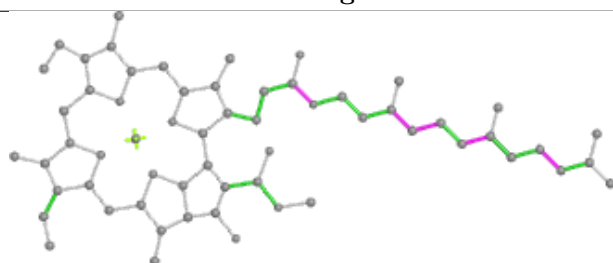
Ligand CLA 3 302



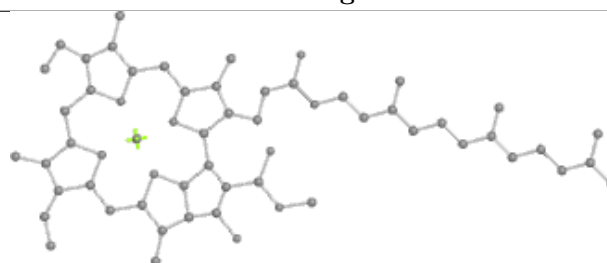
Bond lengths



Bond angles

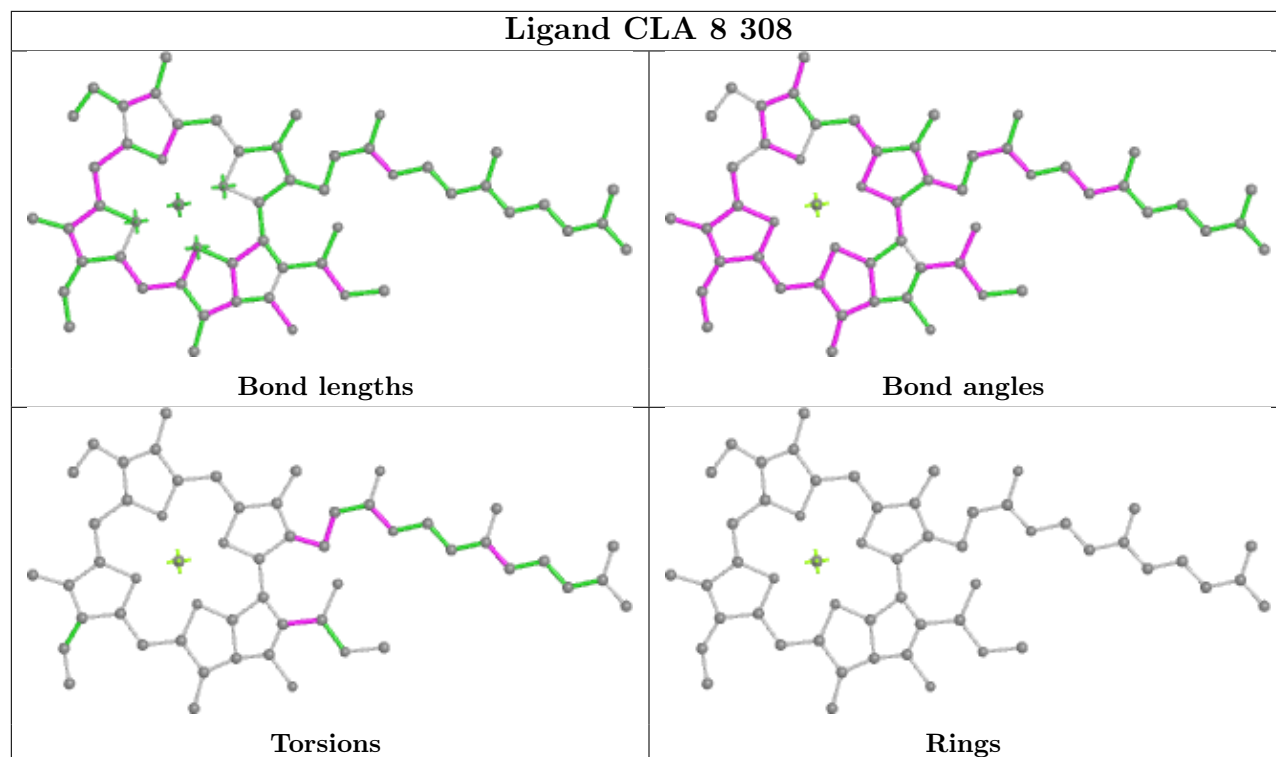


Torsions

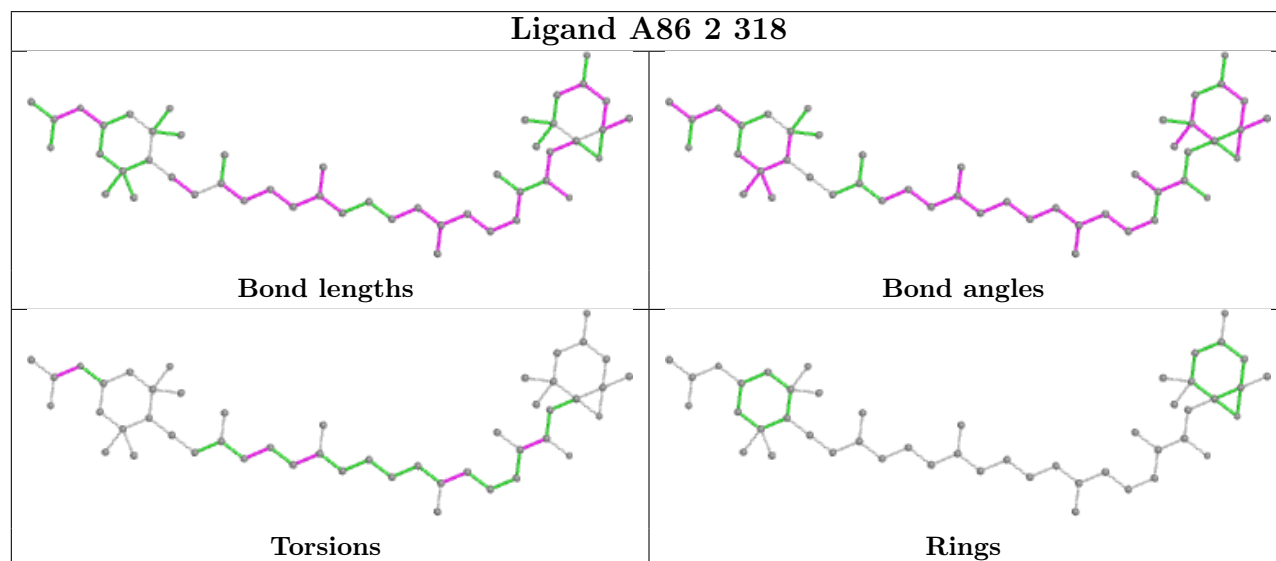


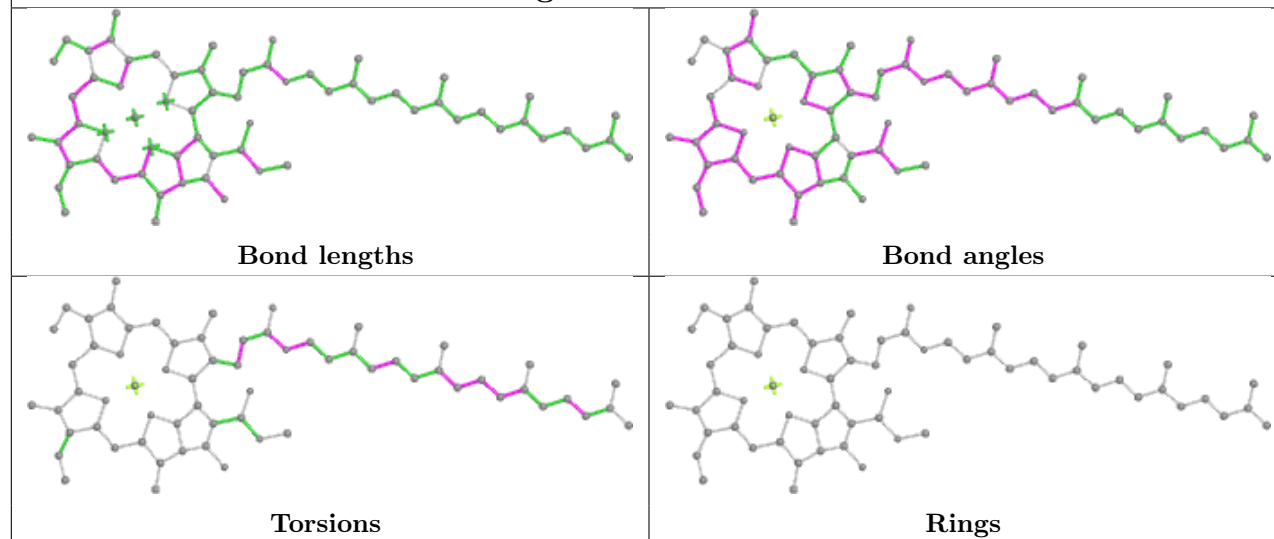
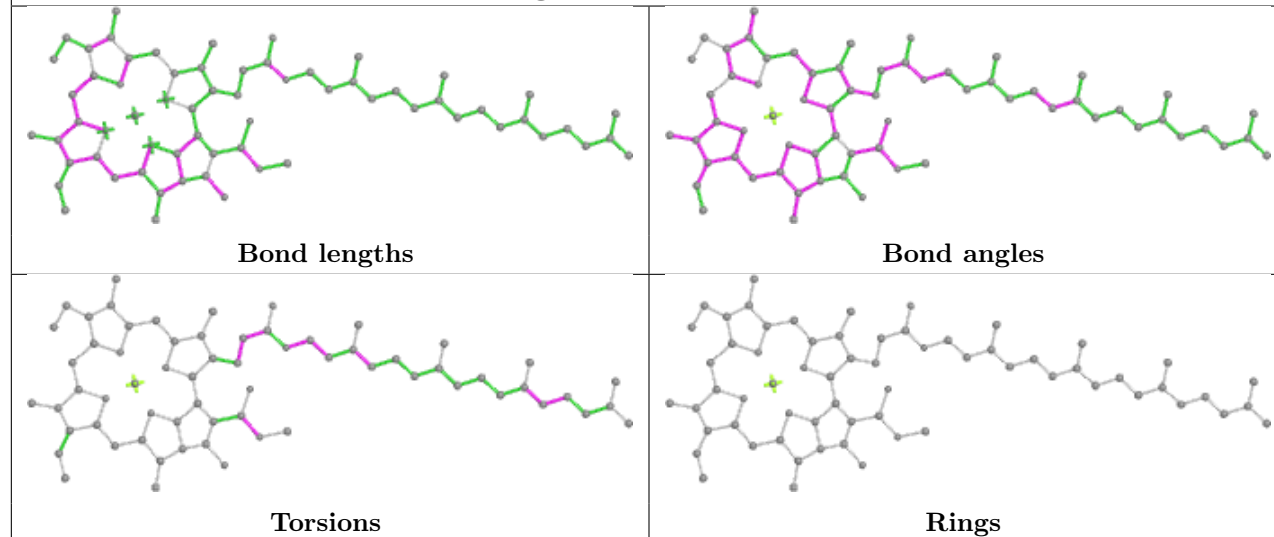
Rings

Ligand CLA 8 308

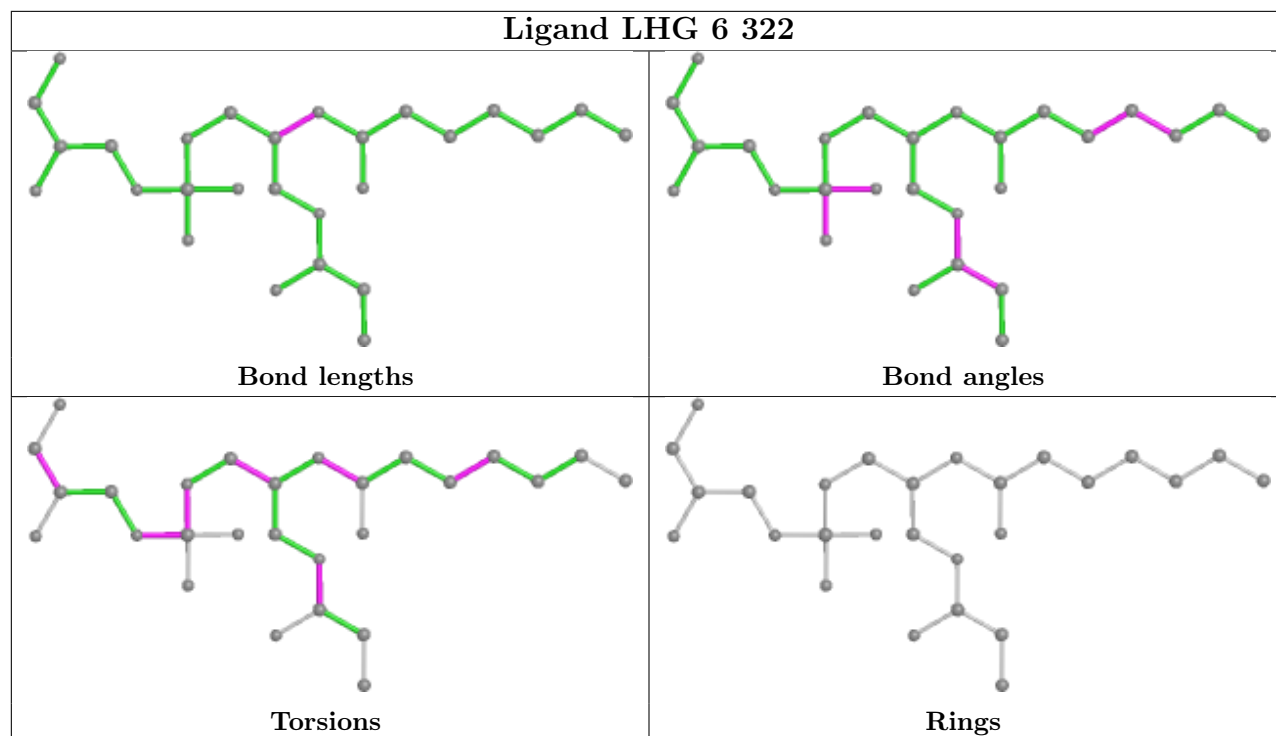


Ligand A86 2 318

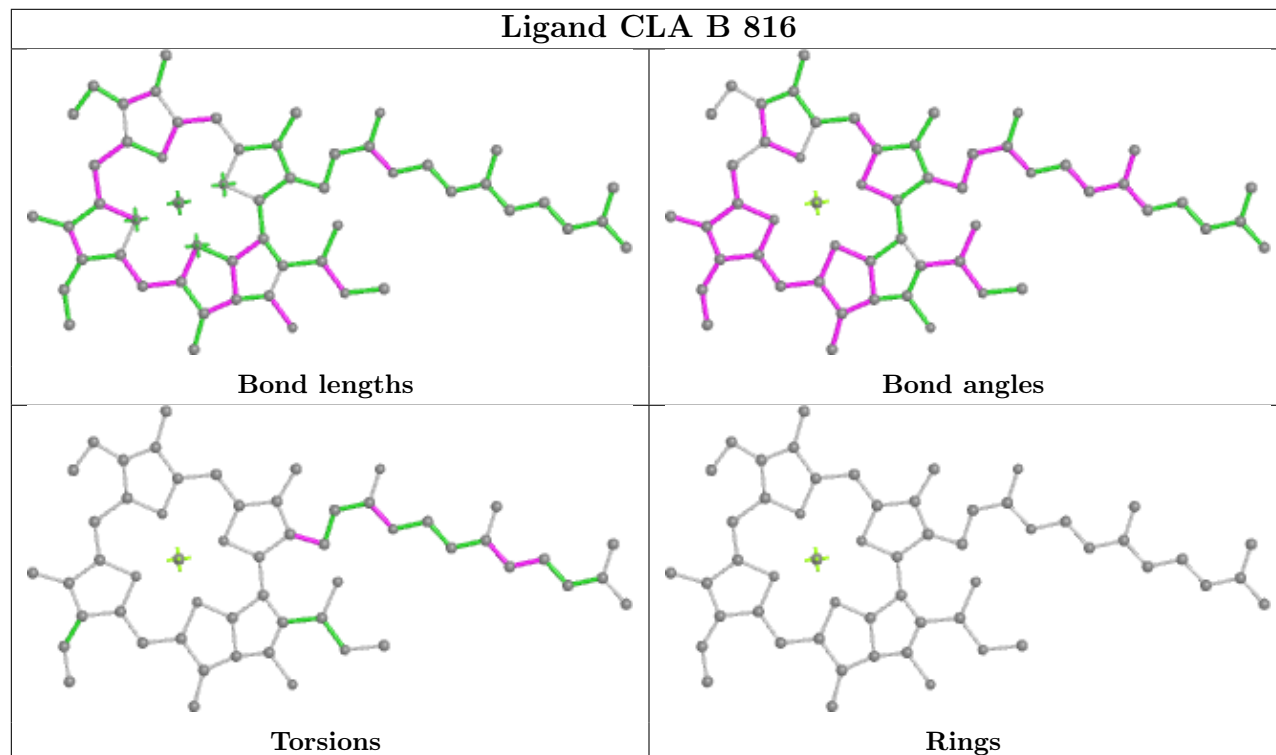


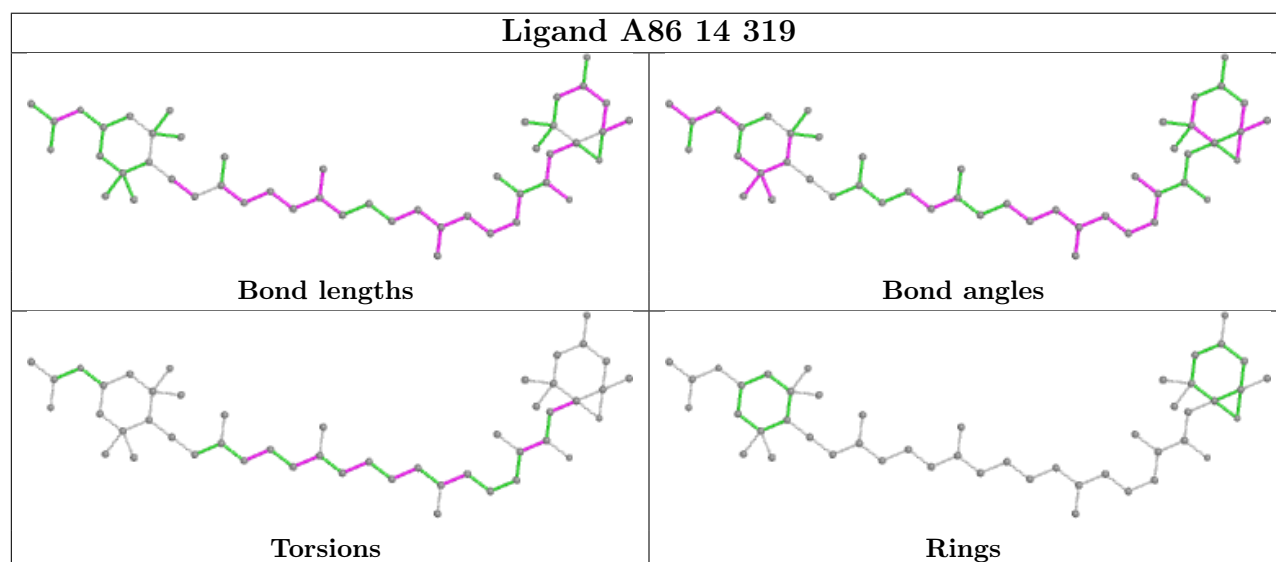
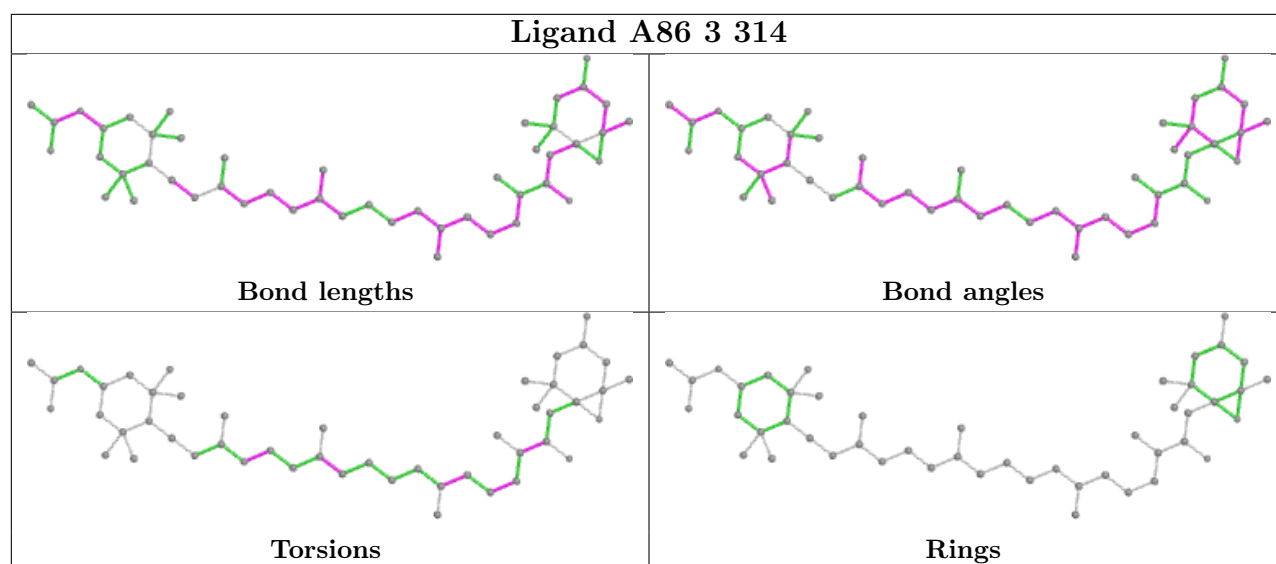
Ligand CLA 7 303**Ligand CLA B 830**

Ligand LHG 6 322

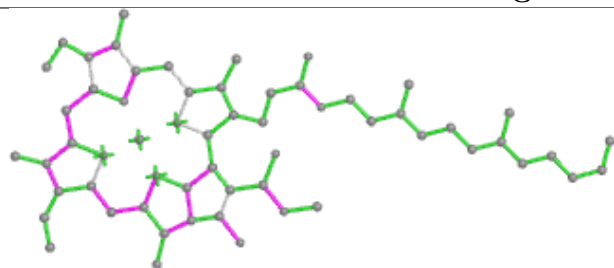


Ligand CLA B 816

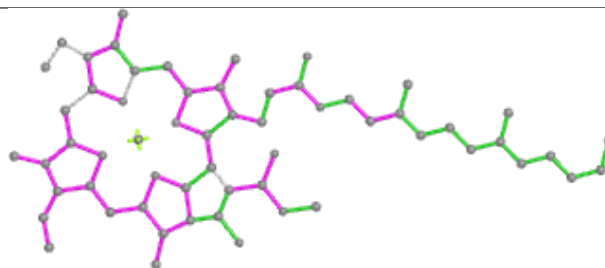




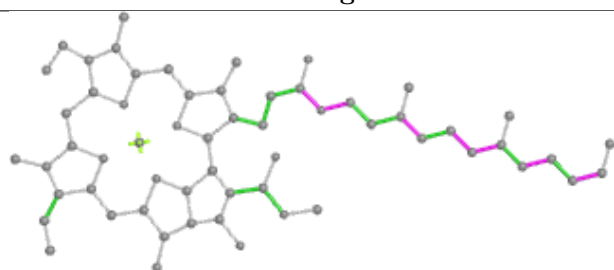
Ligand CLA A 805



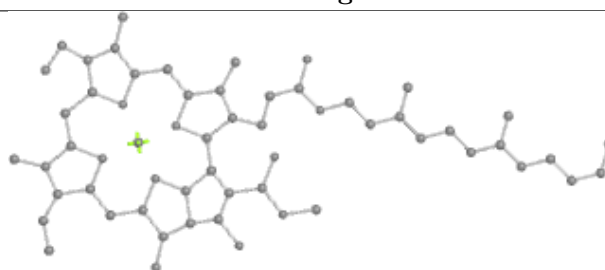
Bond lengths



Bond angles

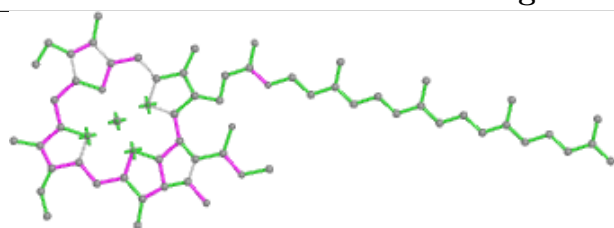


Torsions

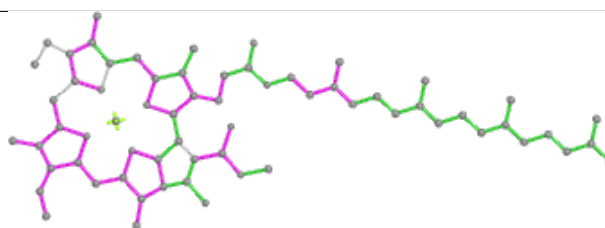


Rings

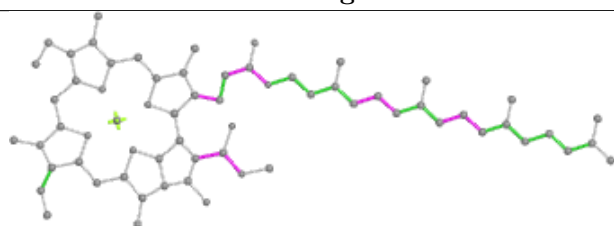
Ligand CLA 3 303



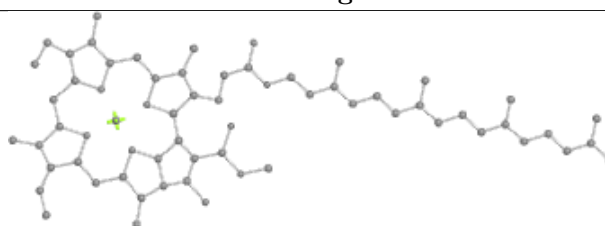
Bond lengths



Bond angles

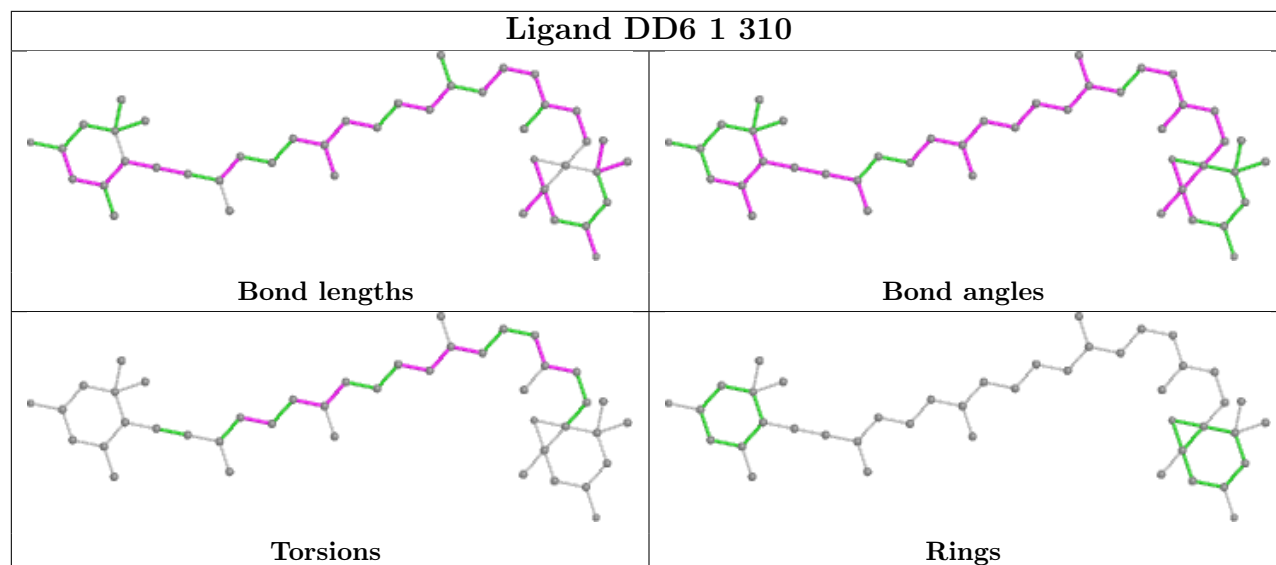


Torsions

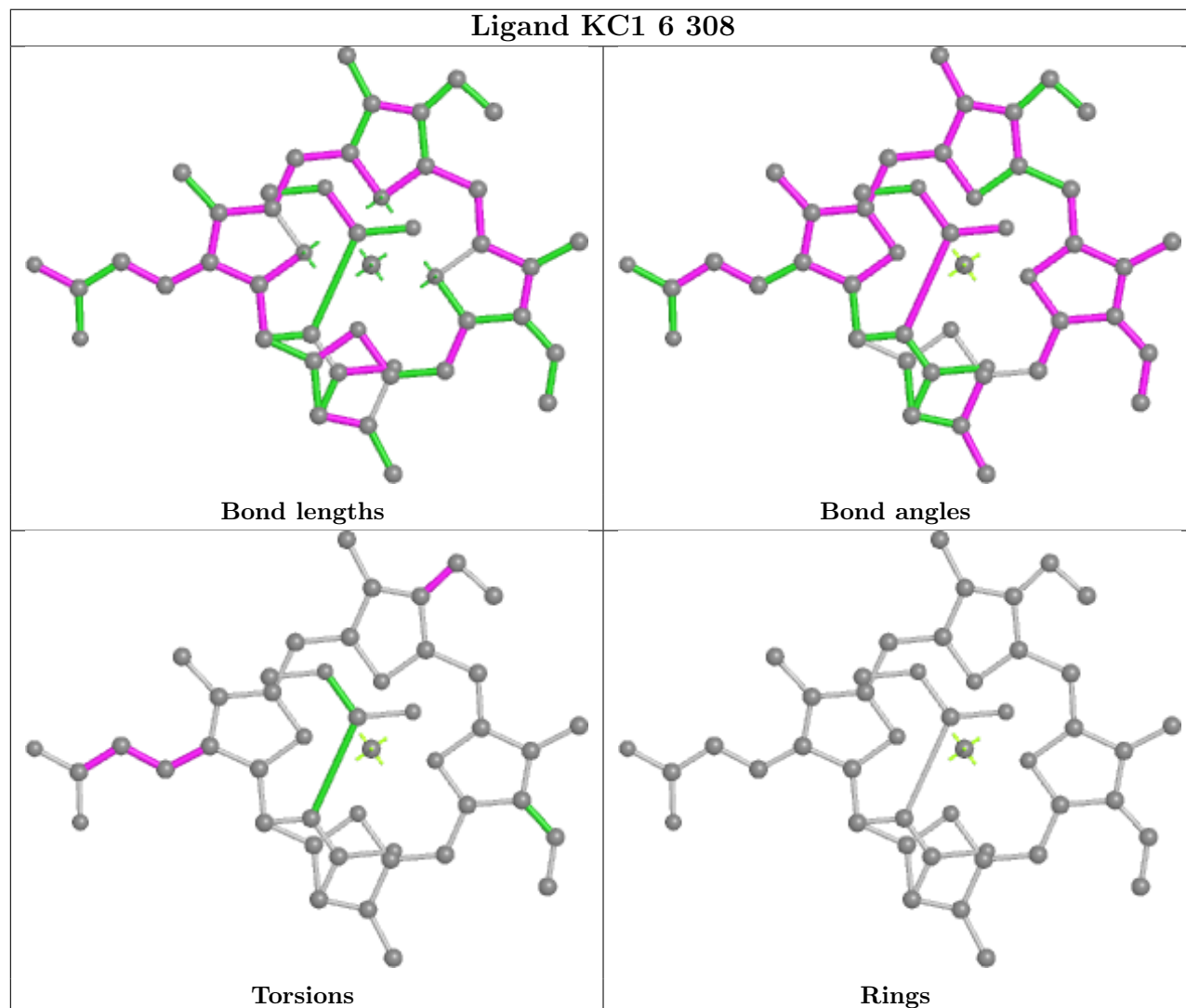


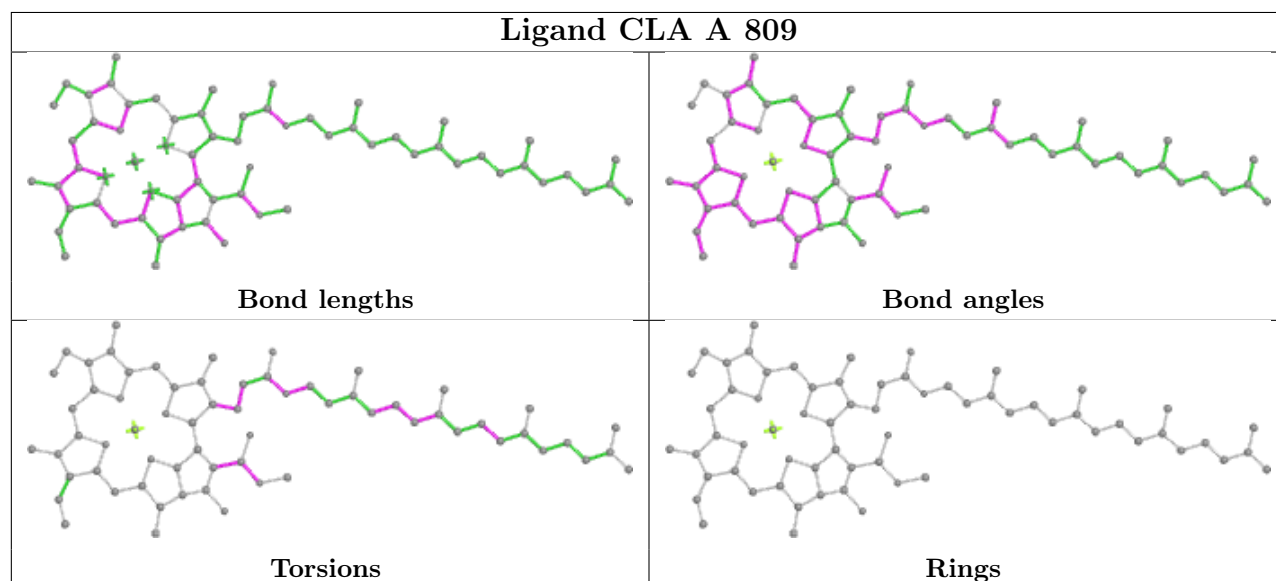
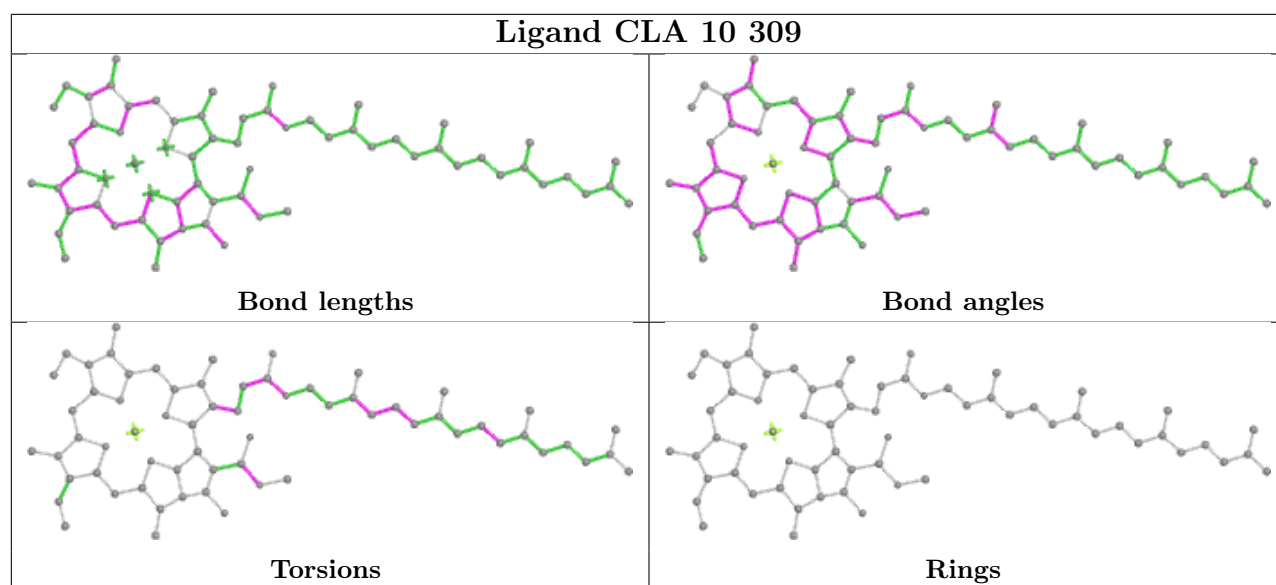
Rings

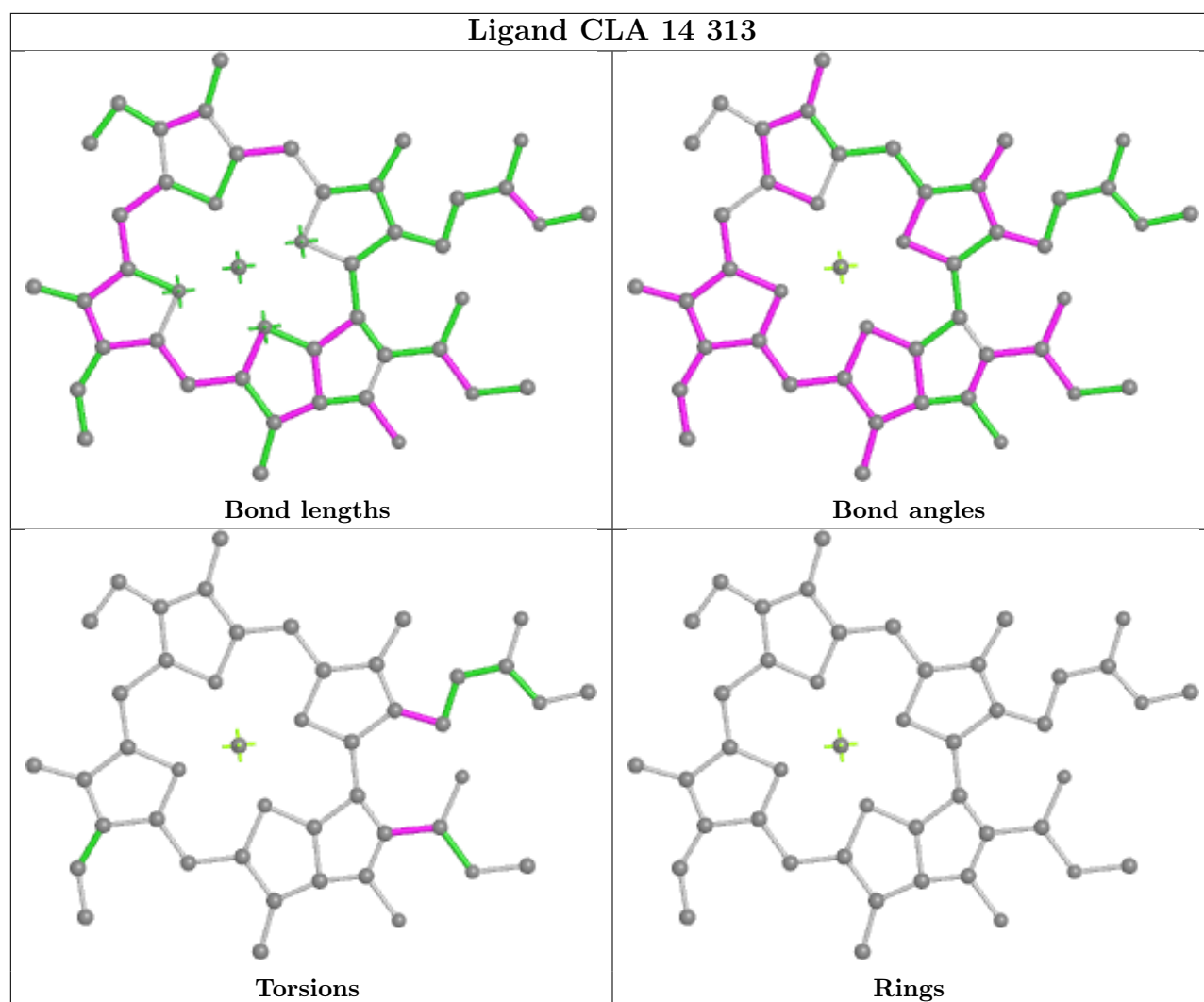
Ligand DD6 1 310

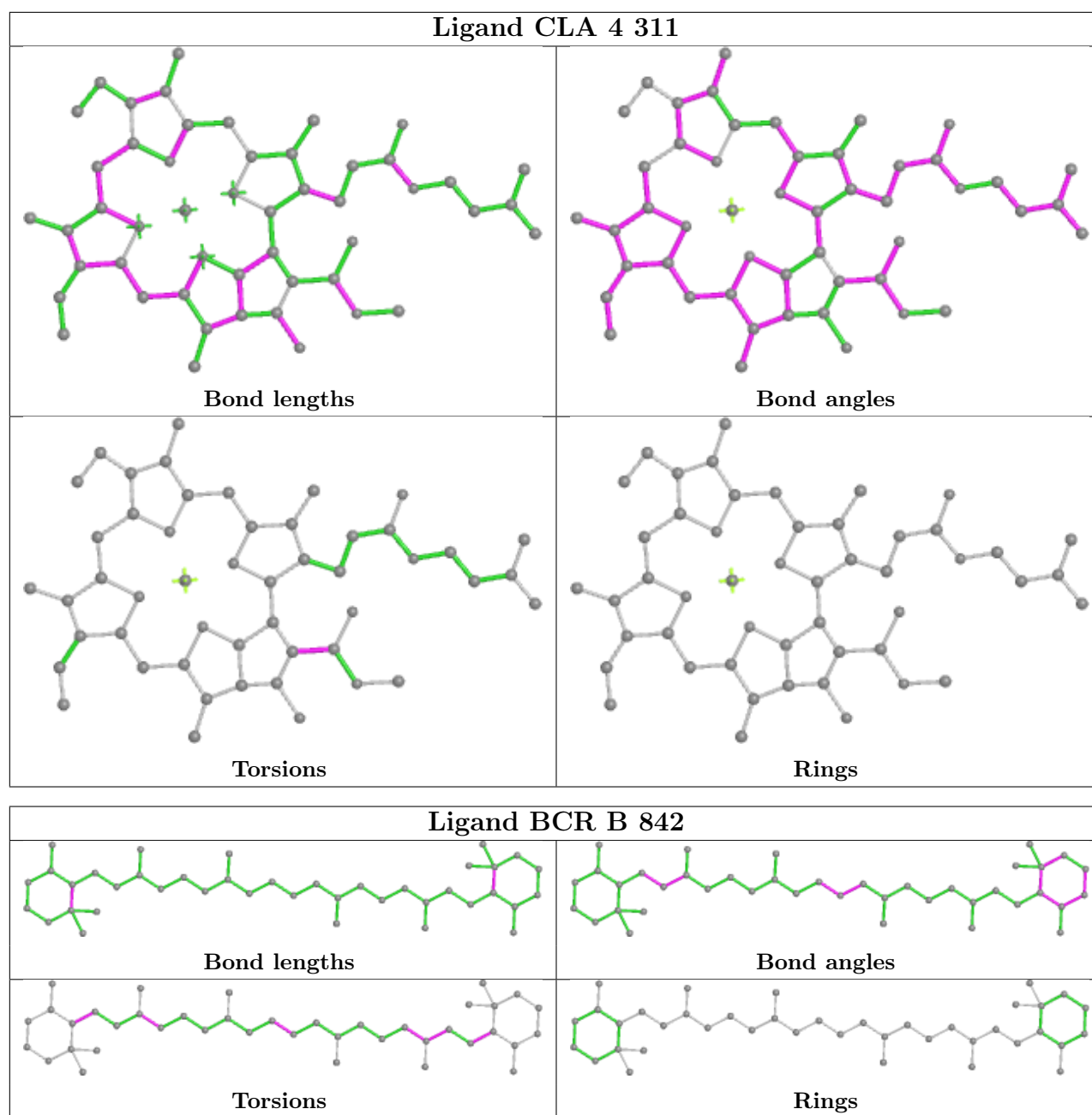


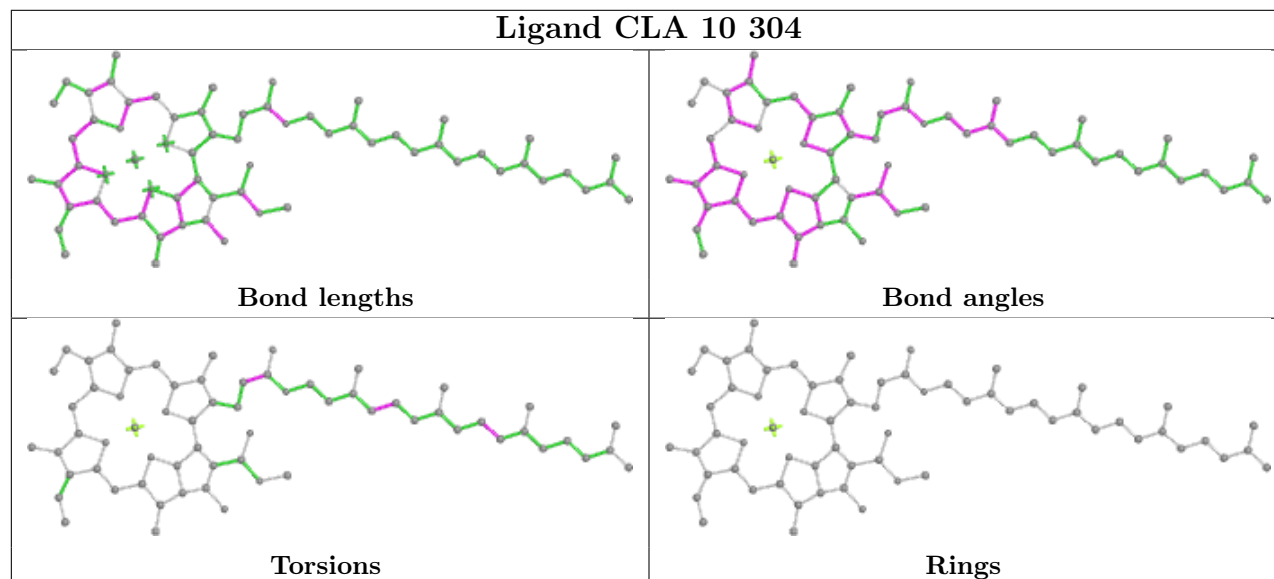
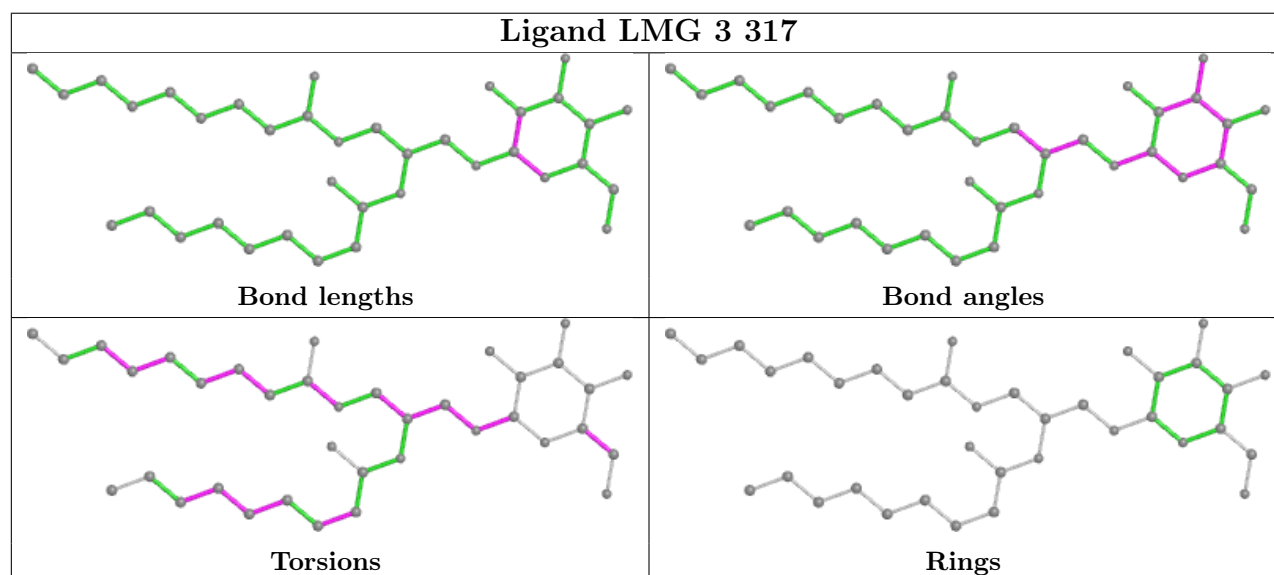
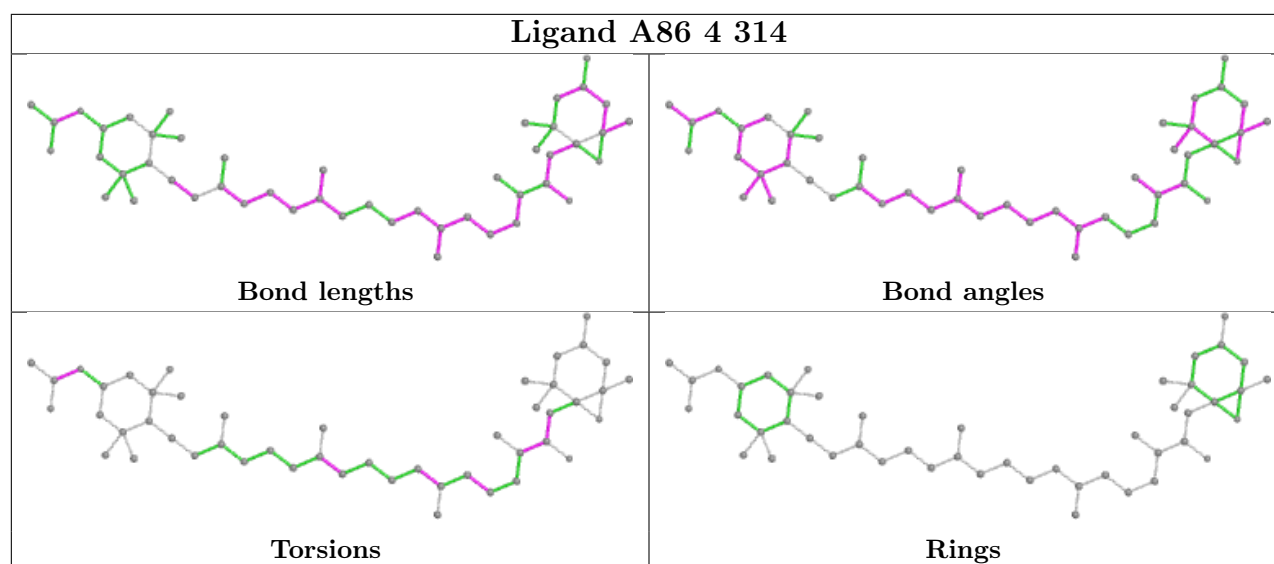
Ligand KC1 6 308



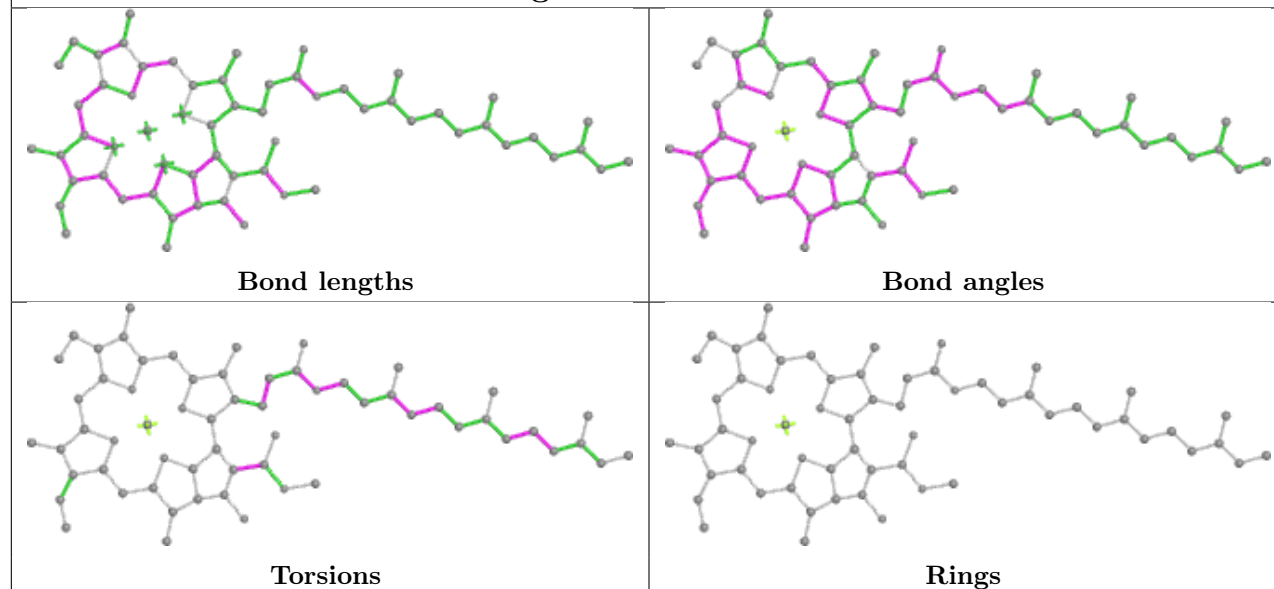




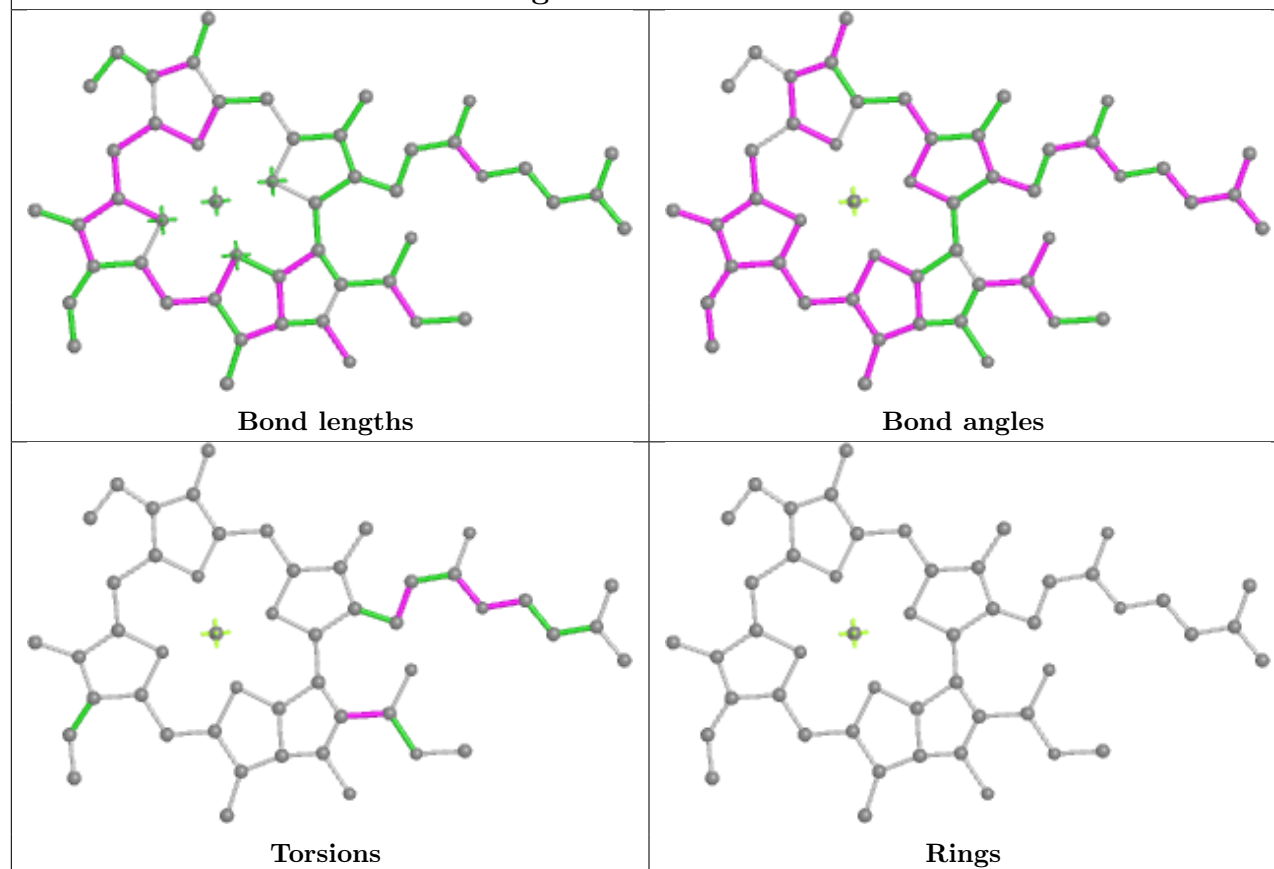




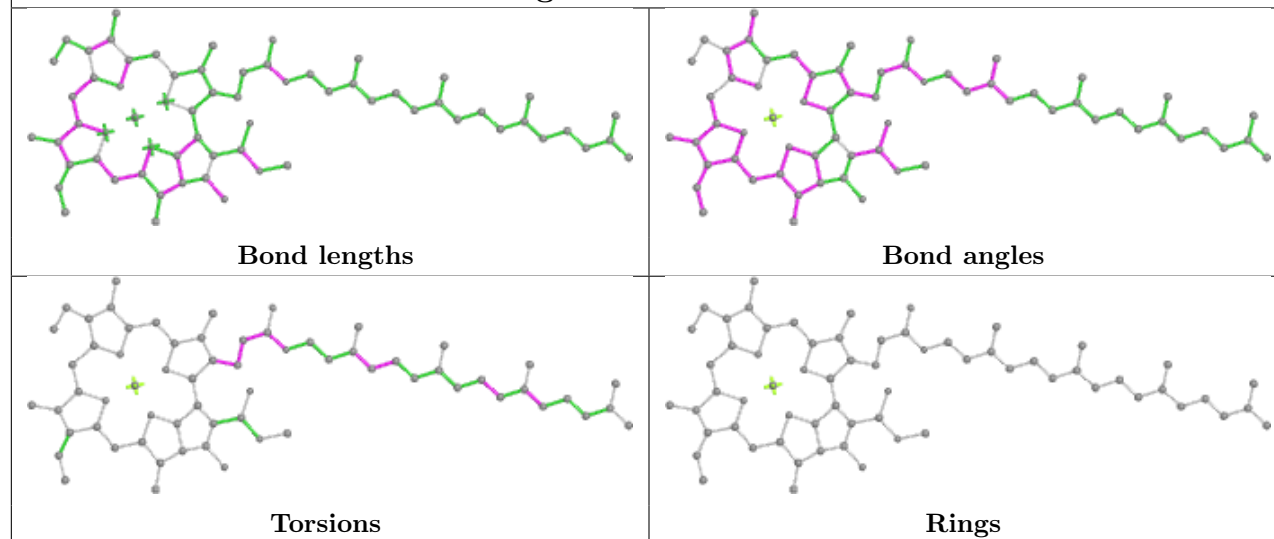
Ligand CLA A 821



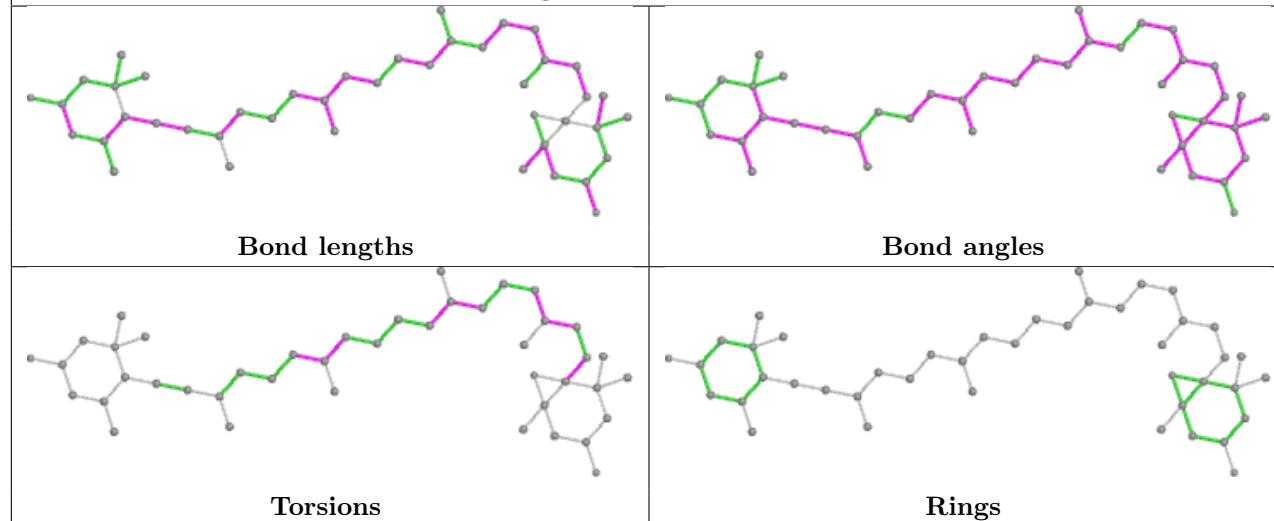
Ligand CLA A 832



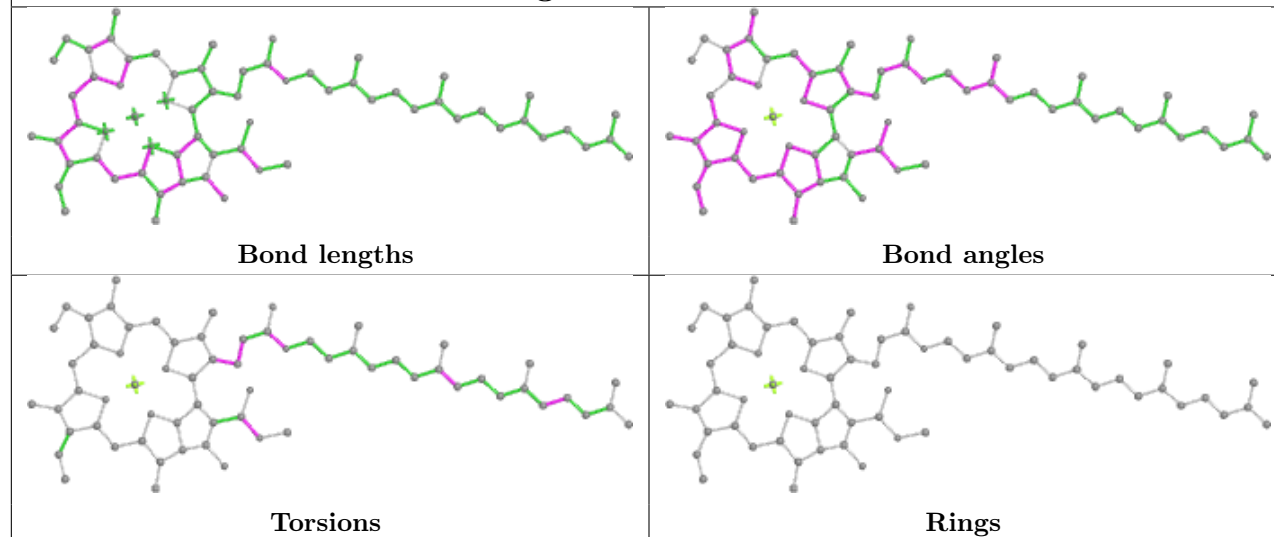
Ligand CLA 1 303

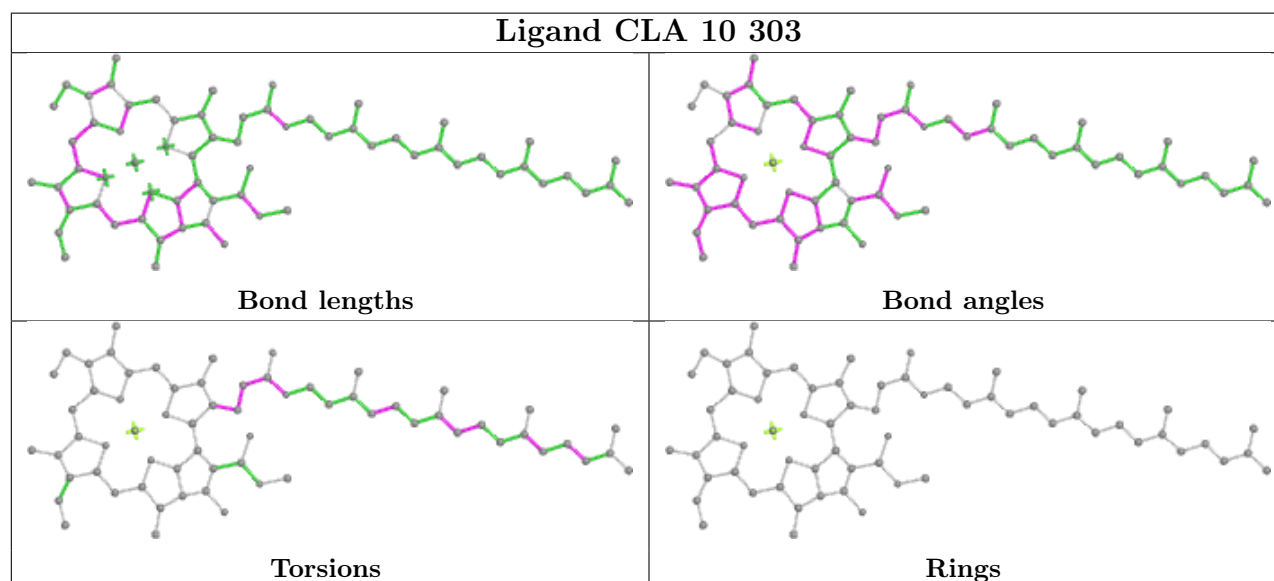
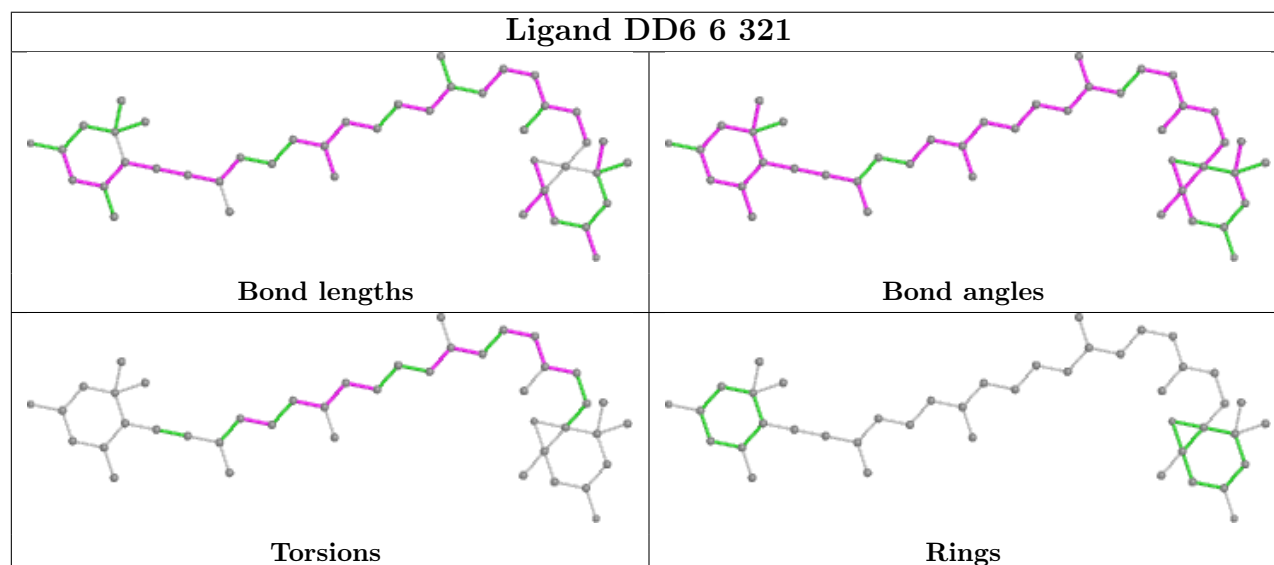
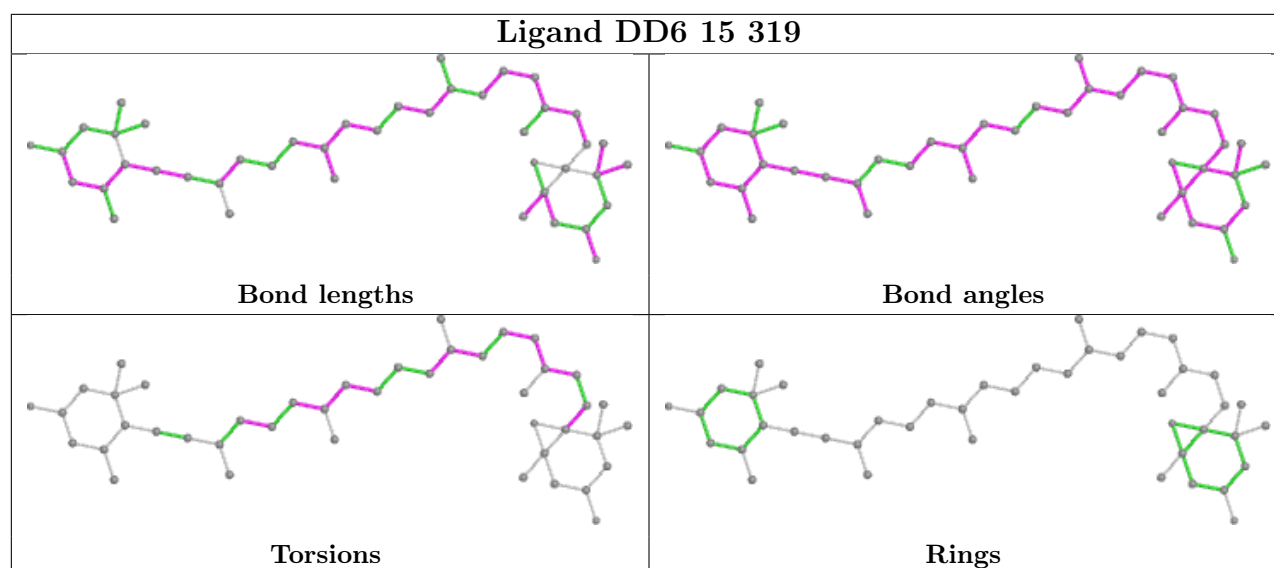


Ligand DD6 7 317

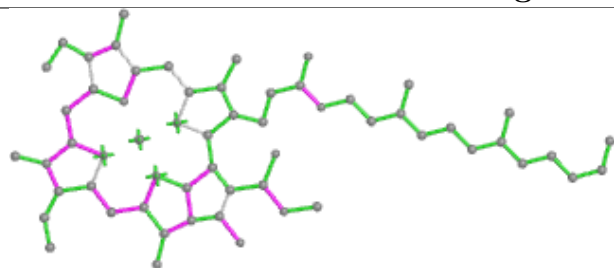


Ligand CLA 9 303

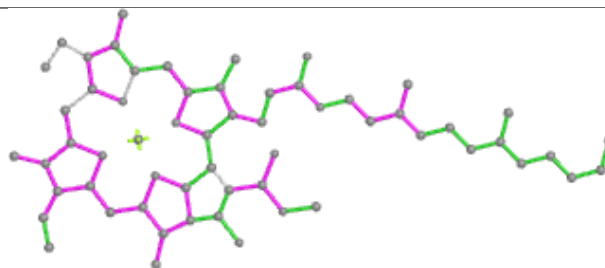




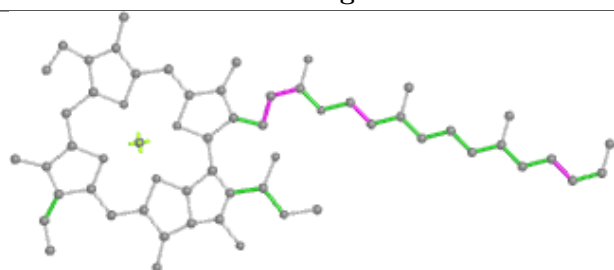
Ligand CLA B 817



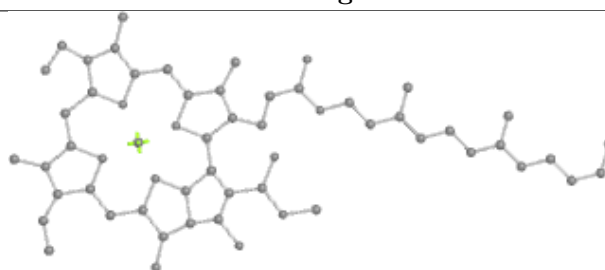
Bond lengths



Bond angles

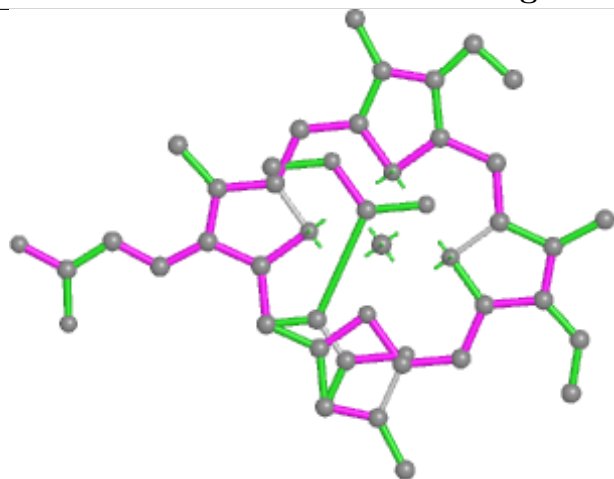


Torsions

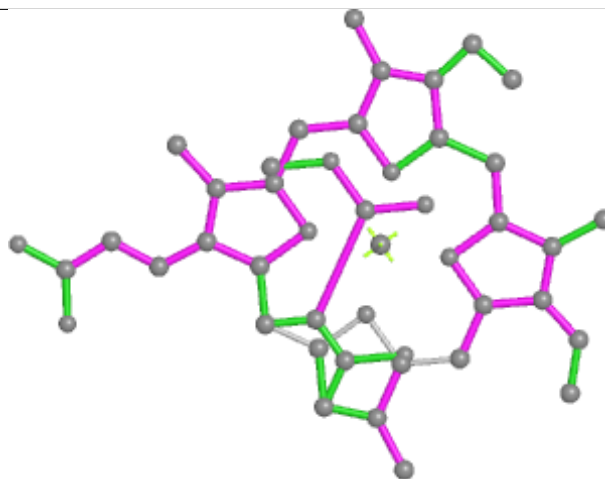


Rings

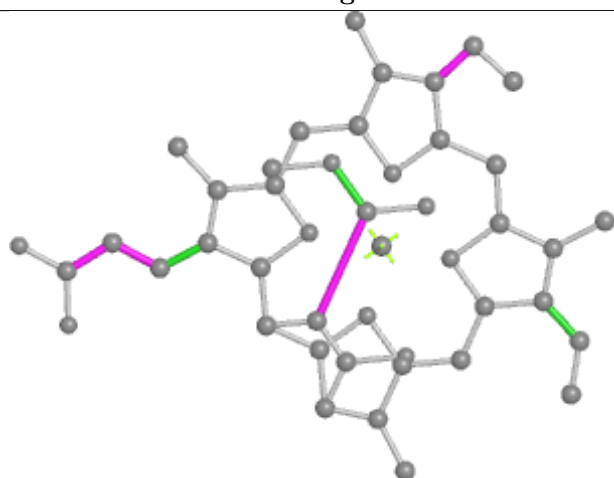
Ligand KC1 3 311



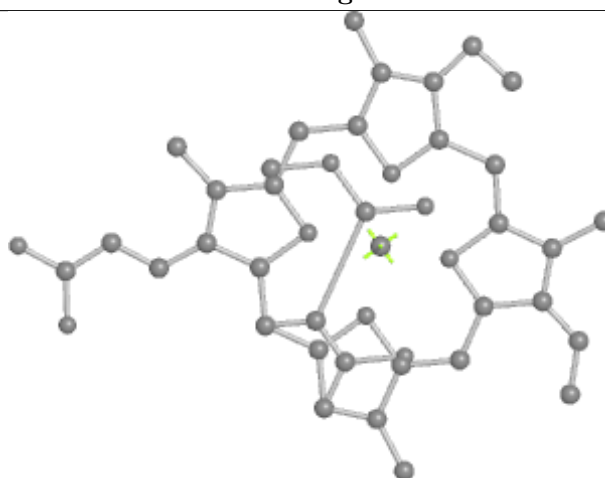
Bond lengths



Bond angles

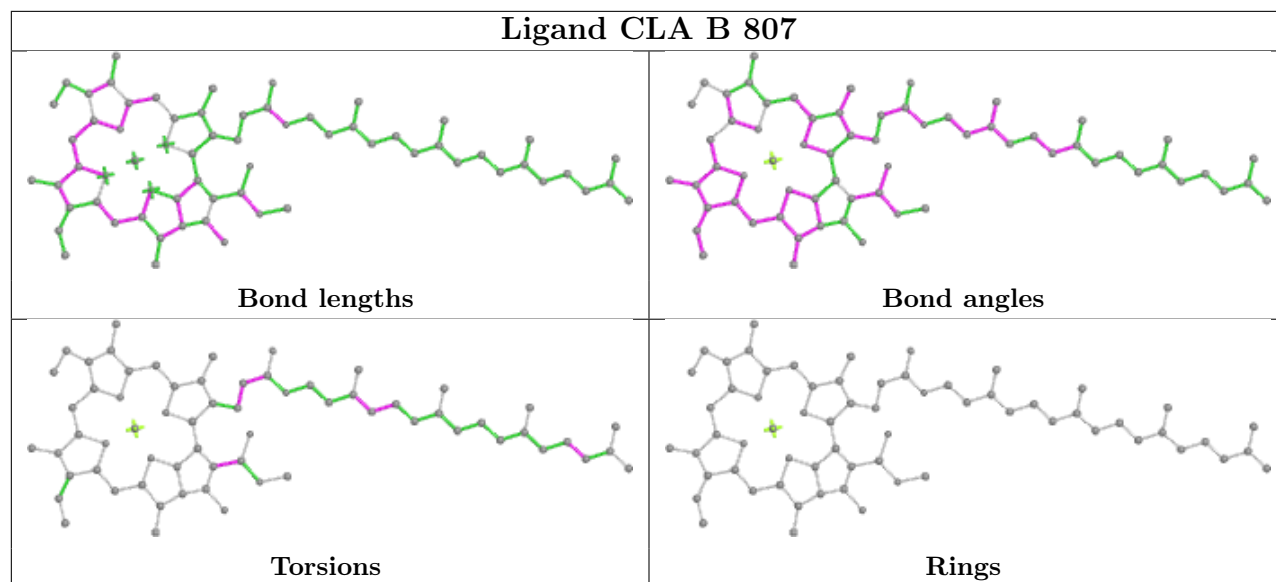


Torsions

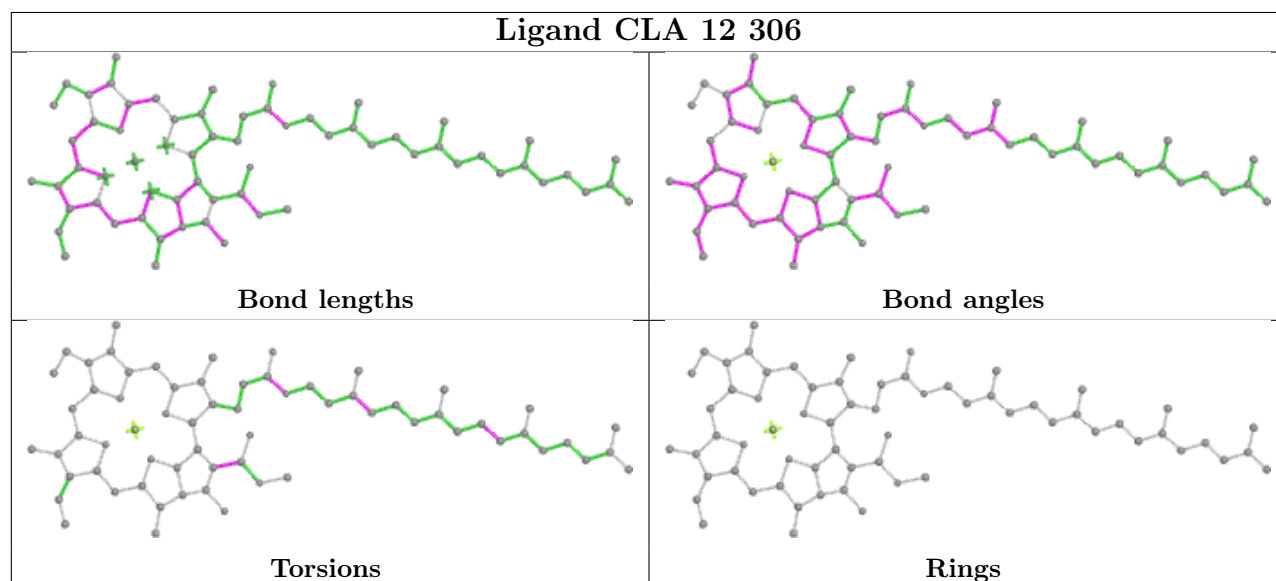


Rings

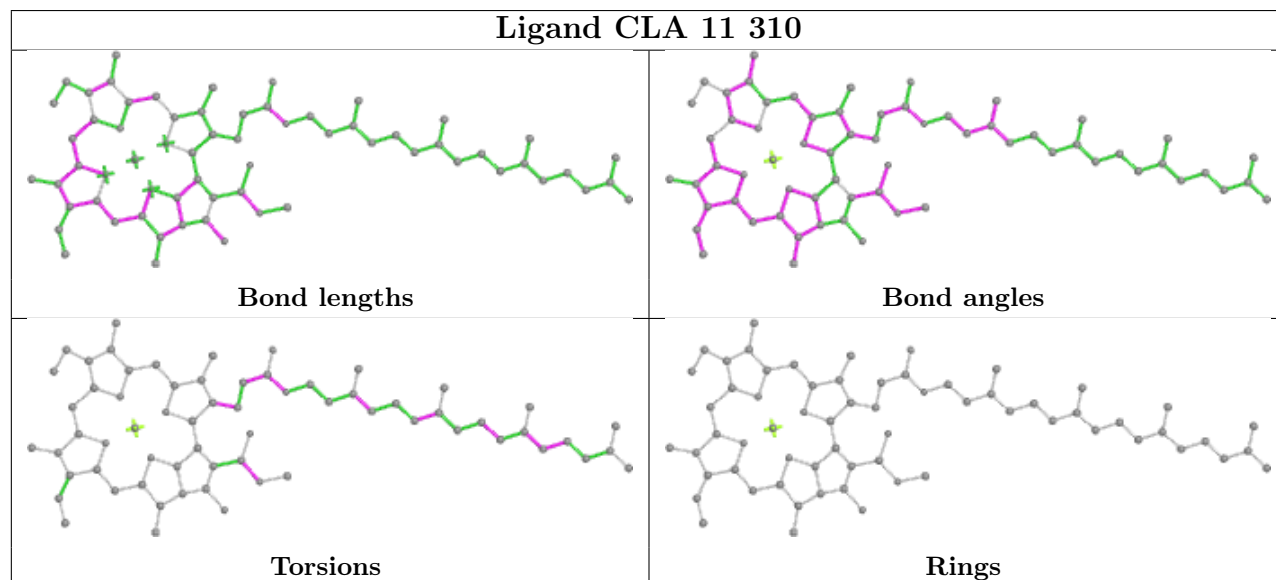
Ligand CLA B 807



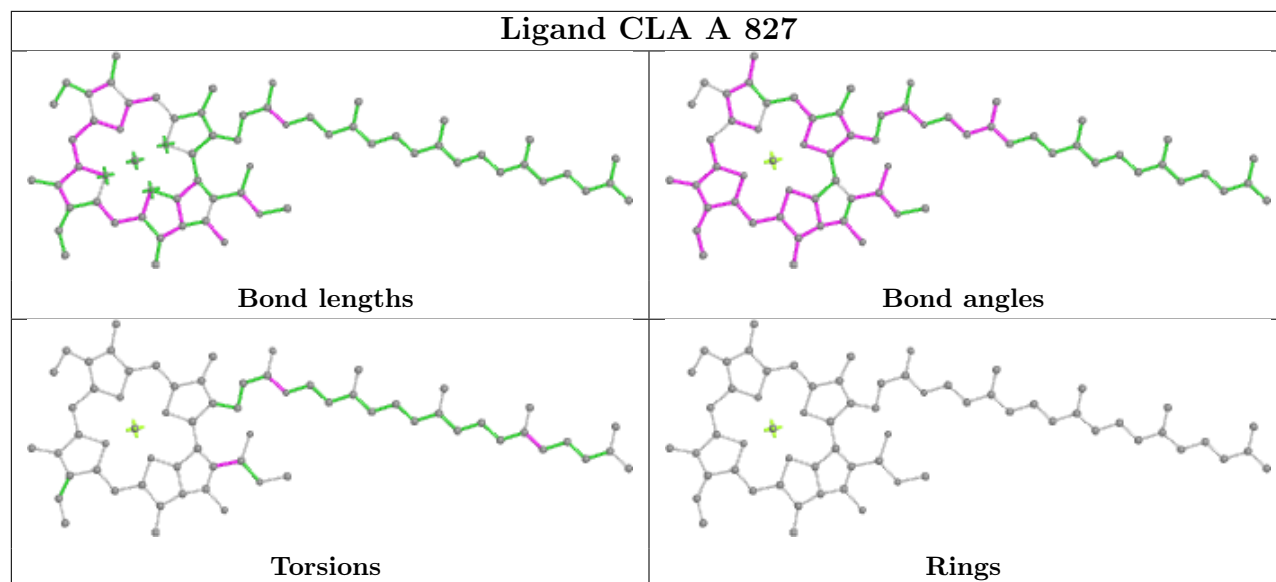
Ligand CLA 12 306



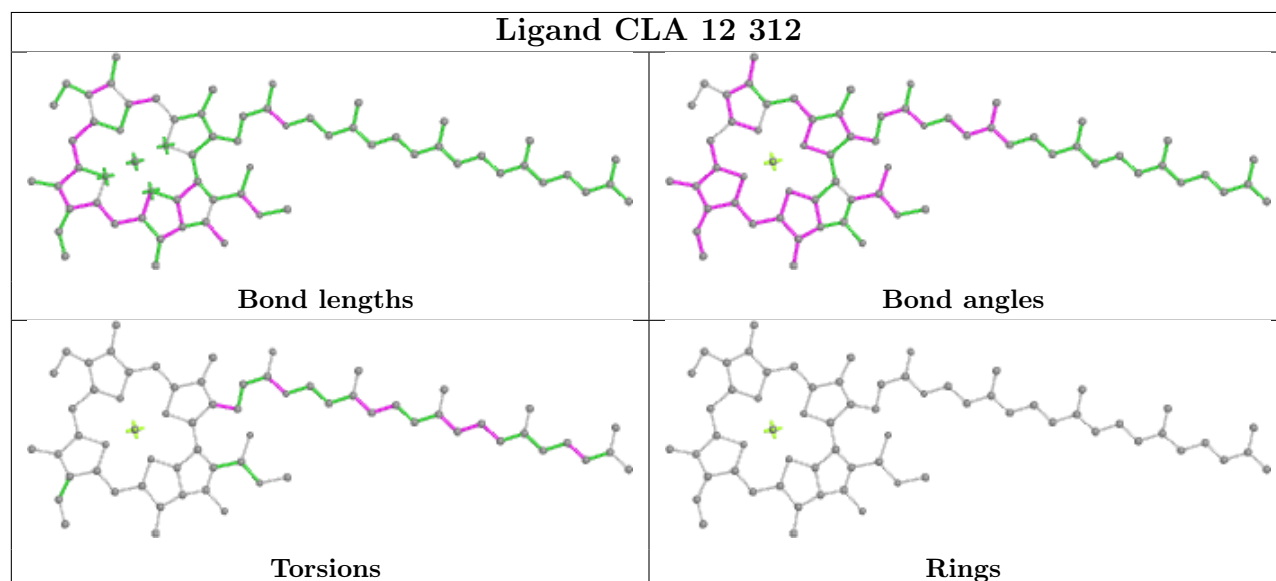
Ligand CLA 11 310



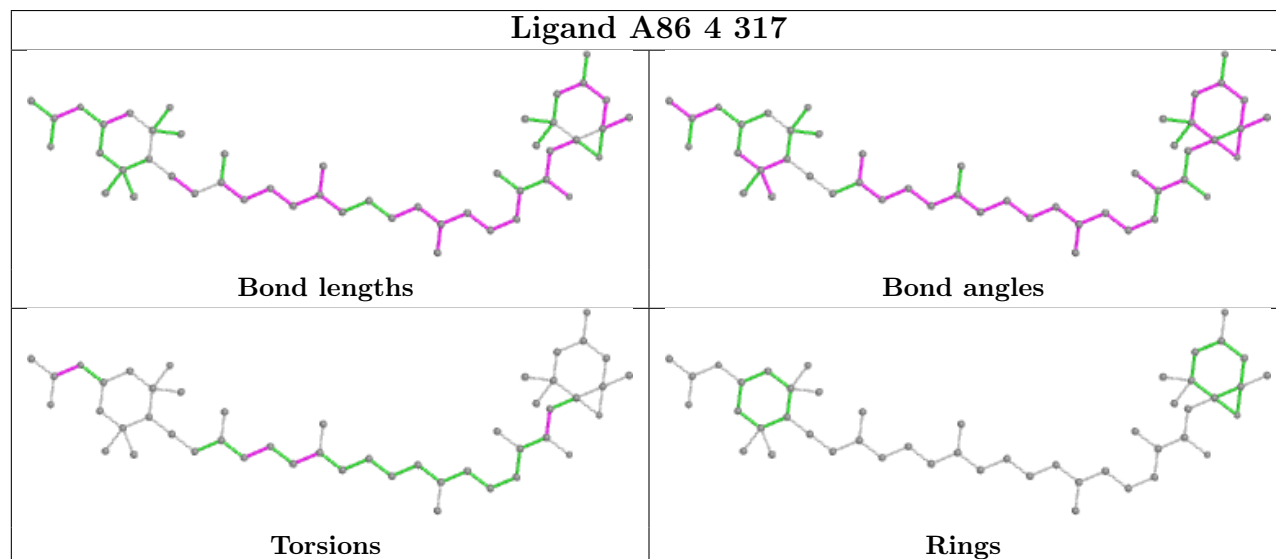
Ligand CLA A 827



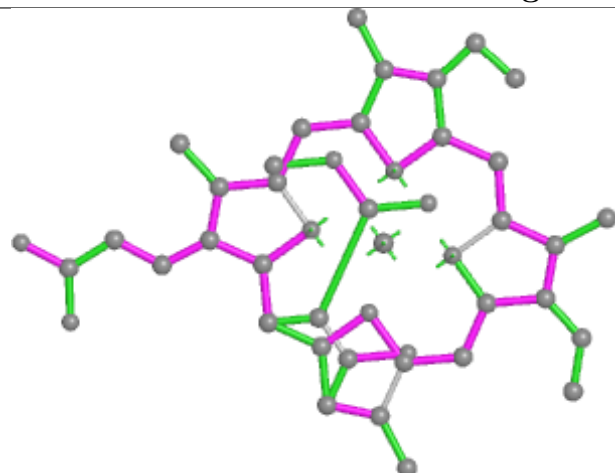
Ligand CLA 12 312



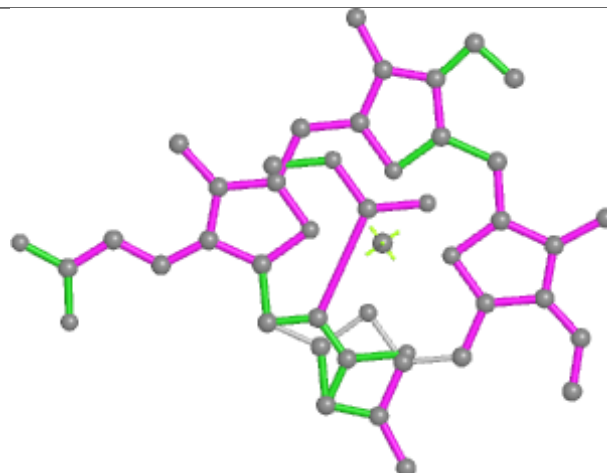
Ligand A86 4 317



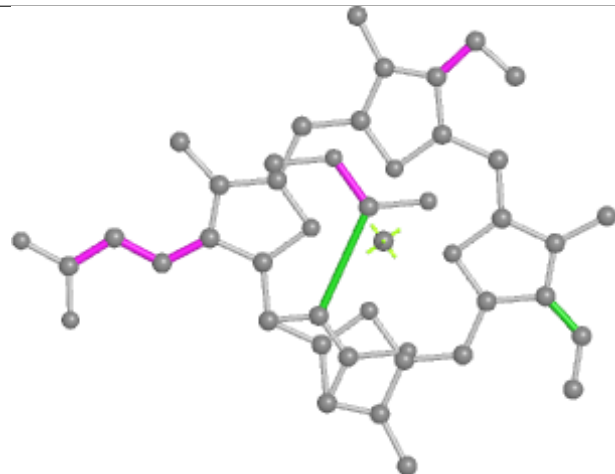
Ligand KC1 9 311



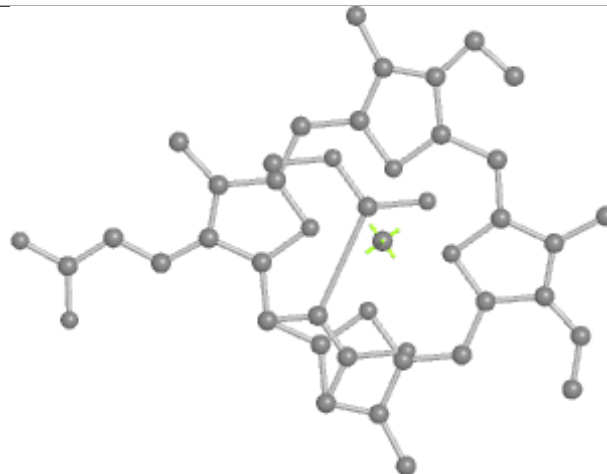
Bond lengths



Bond angles

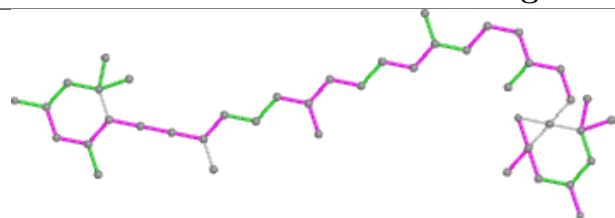


Torsions

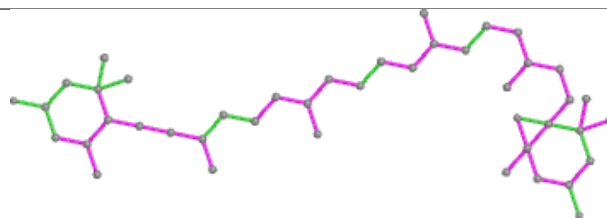


Rings

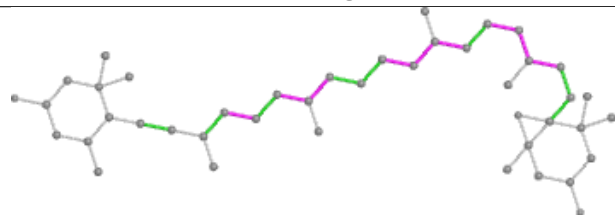
Ligand DD6 7 302



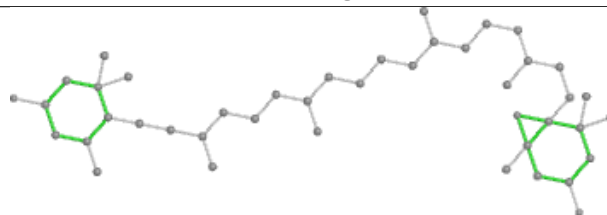
Bond lengths



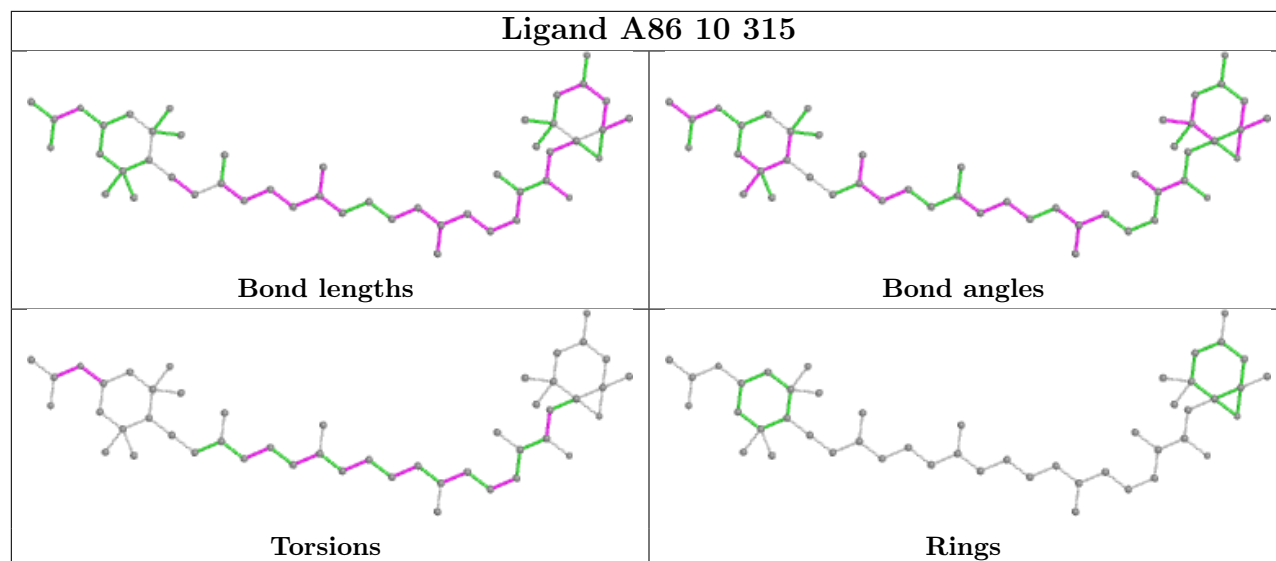
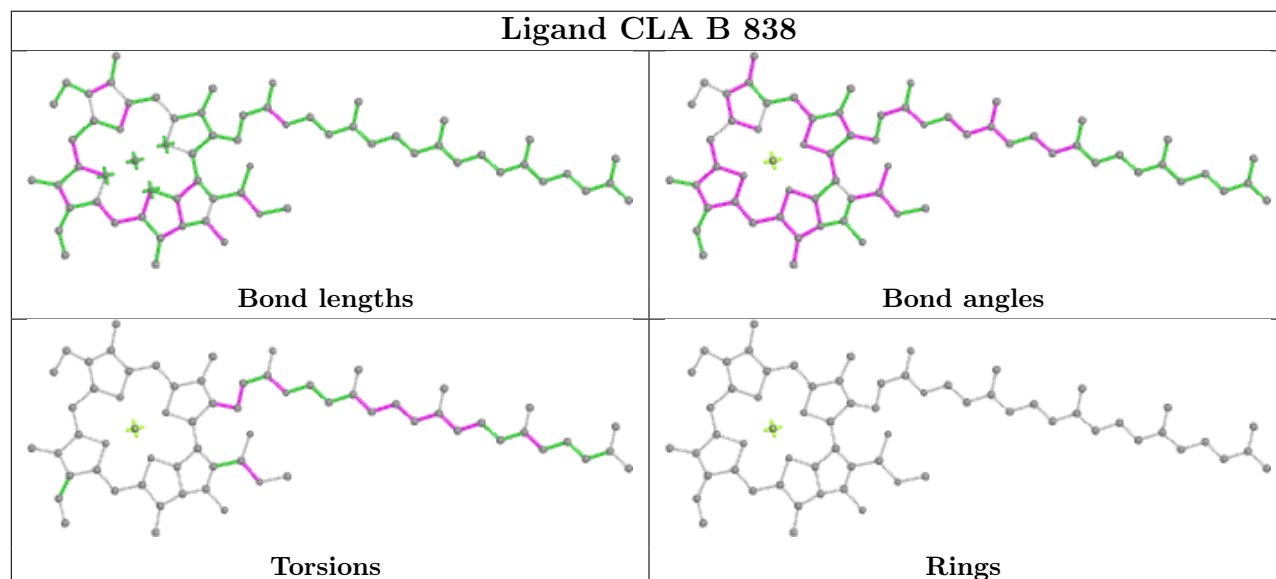
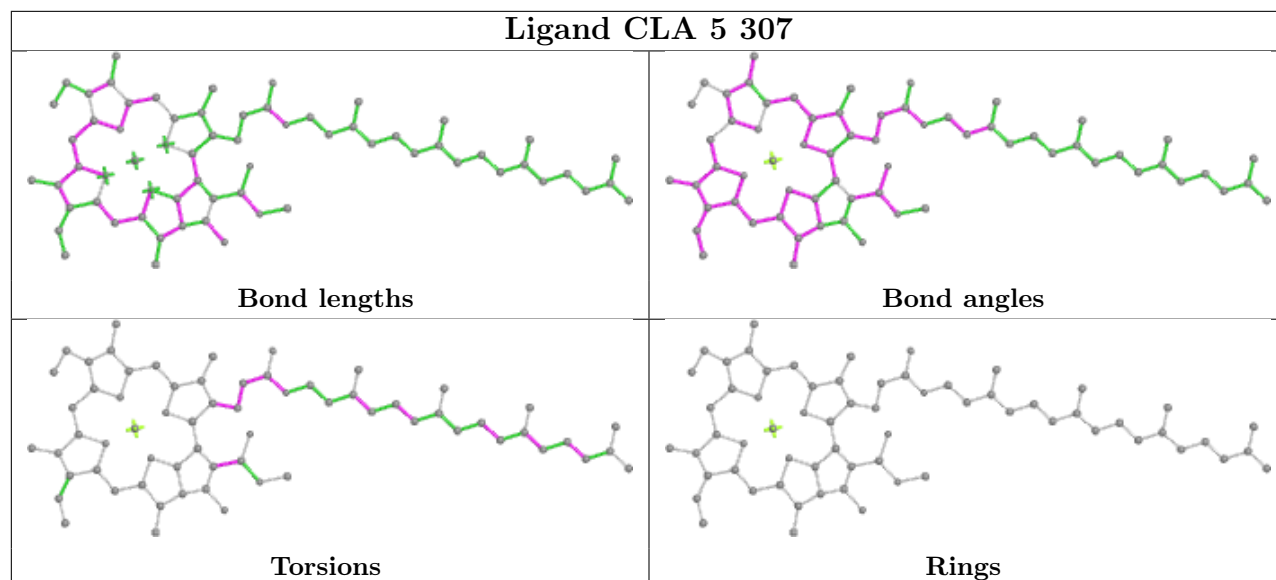
Bond angles



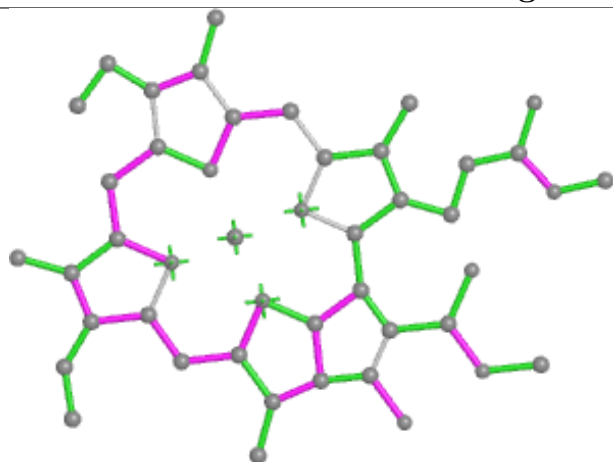
Torsions



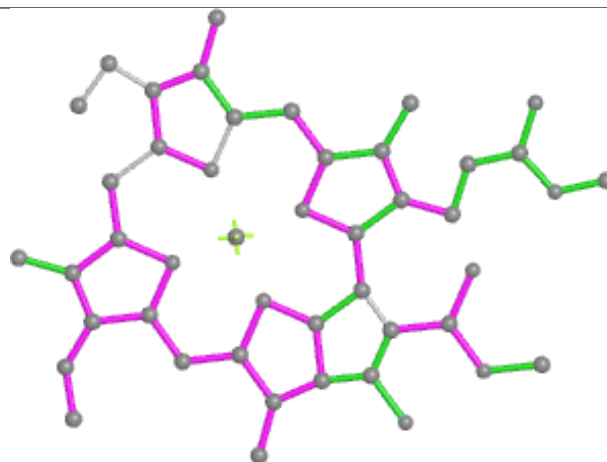
Rings

Ligand A86 10 315**Ligand CLA B 838****Ligand CLA 5 307**

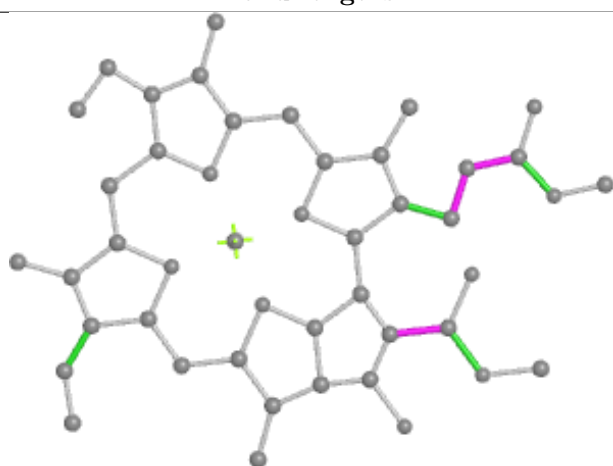
Ligand CLA 7 312



Bond lengths



Bond angles

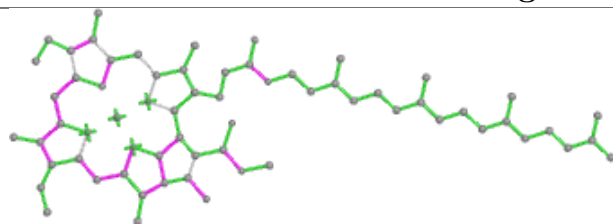


Torsions

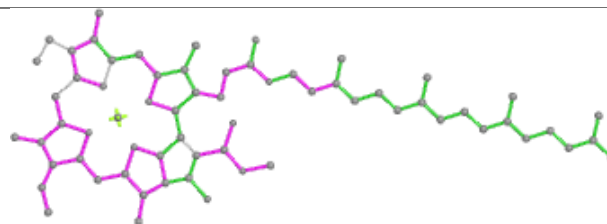


Rings

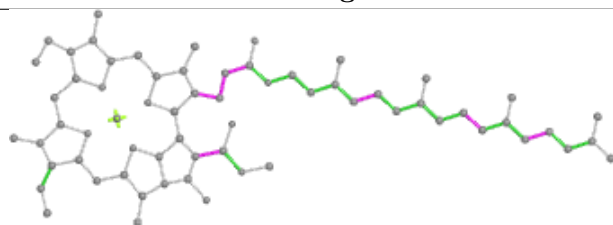
Ligand CLA 2 308



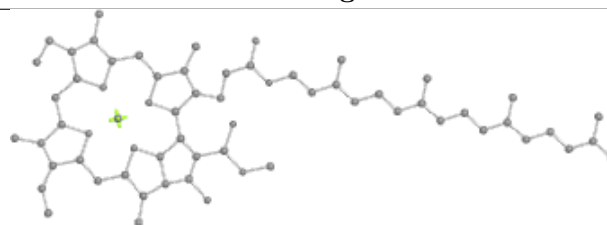
Bond lengths



Bond angles

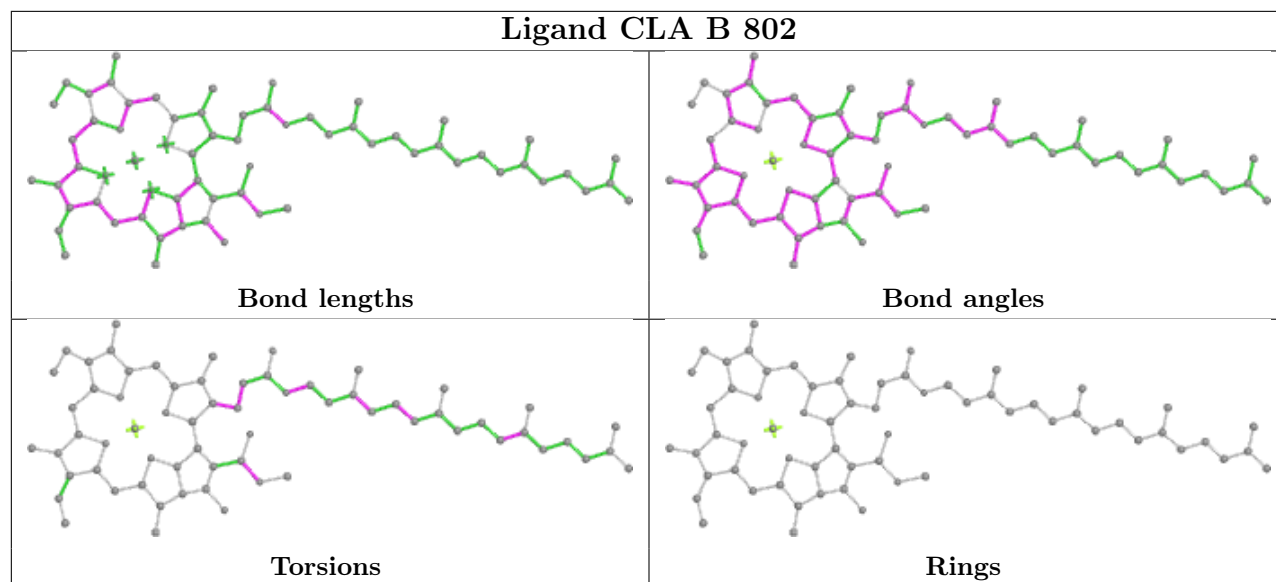


Torsions

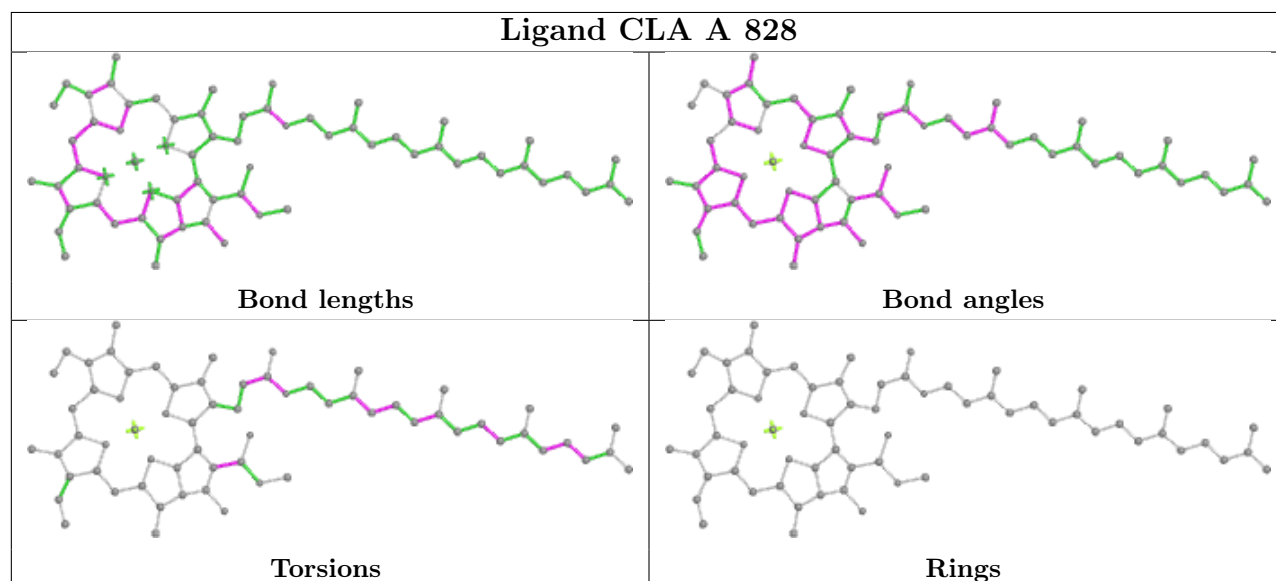


Rings

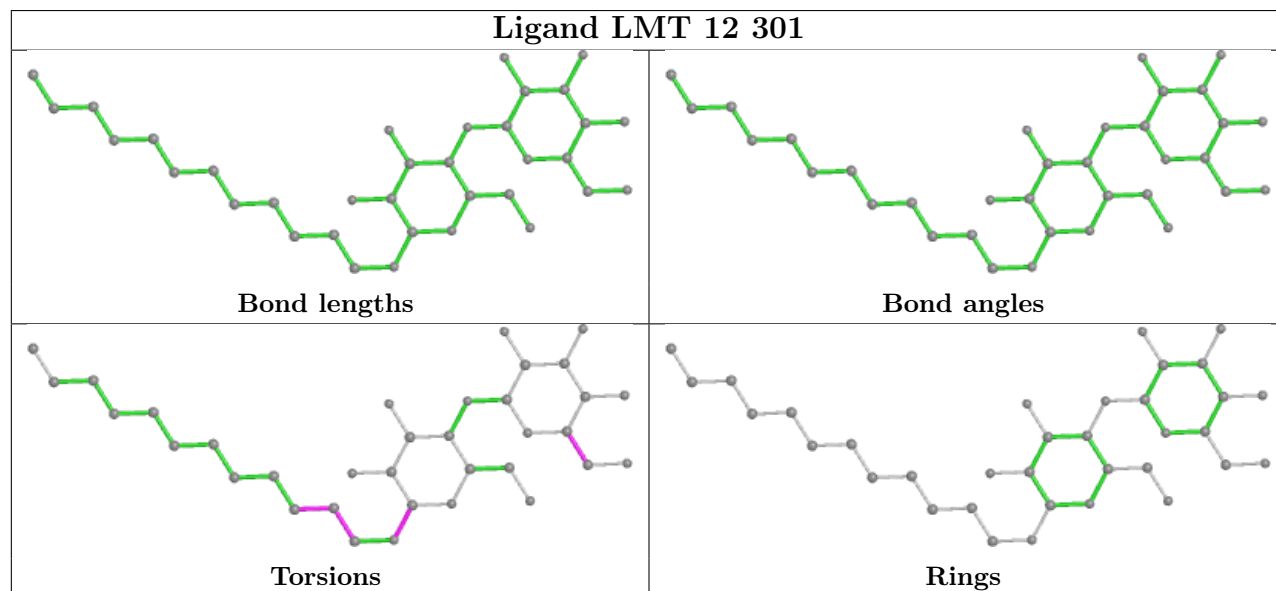
Ligand CLA B 802

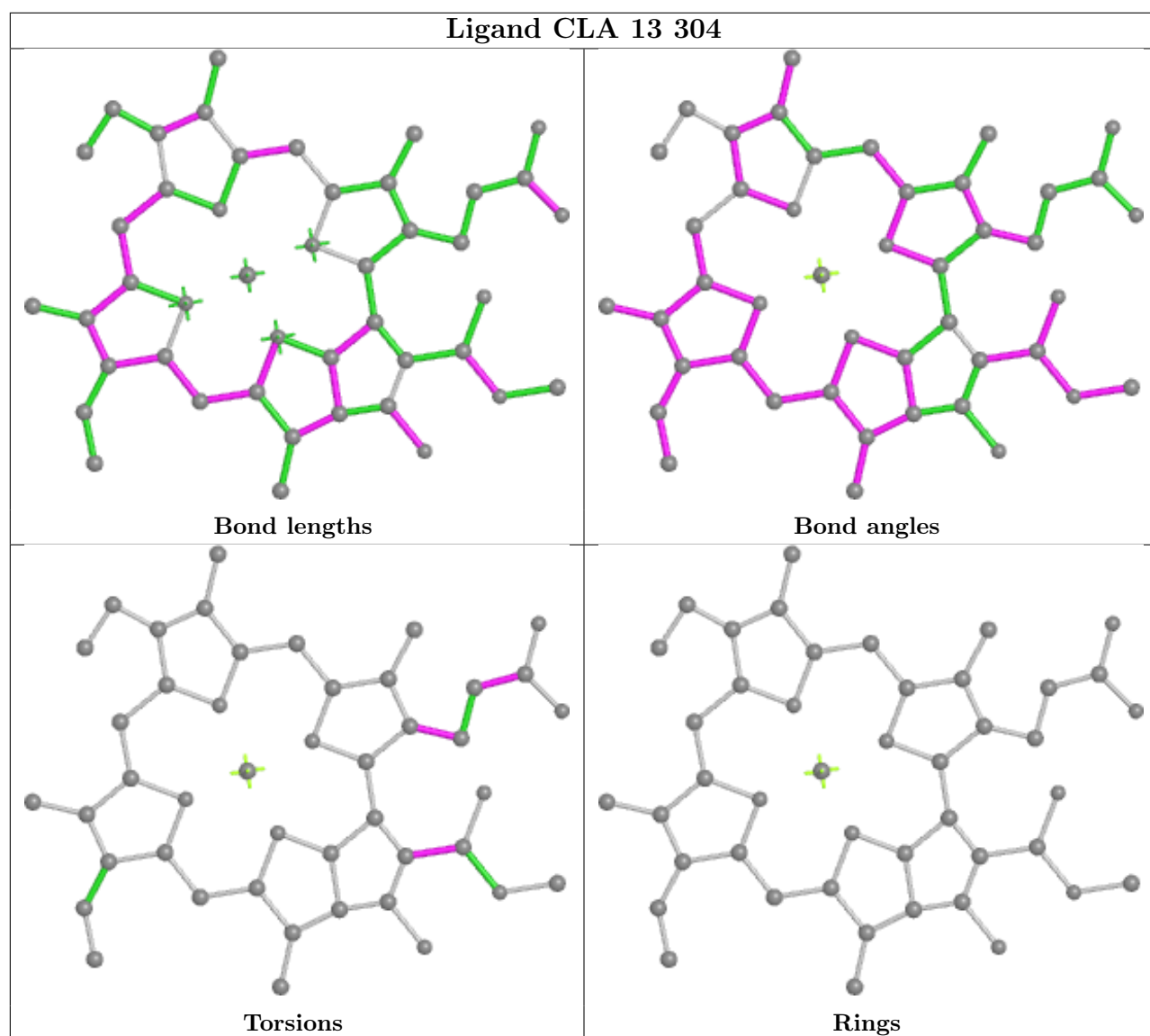


Ligand CLA A 828

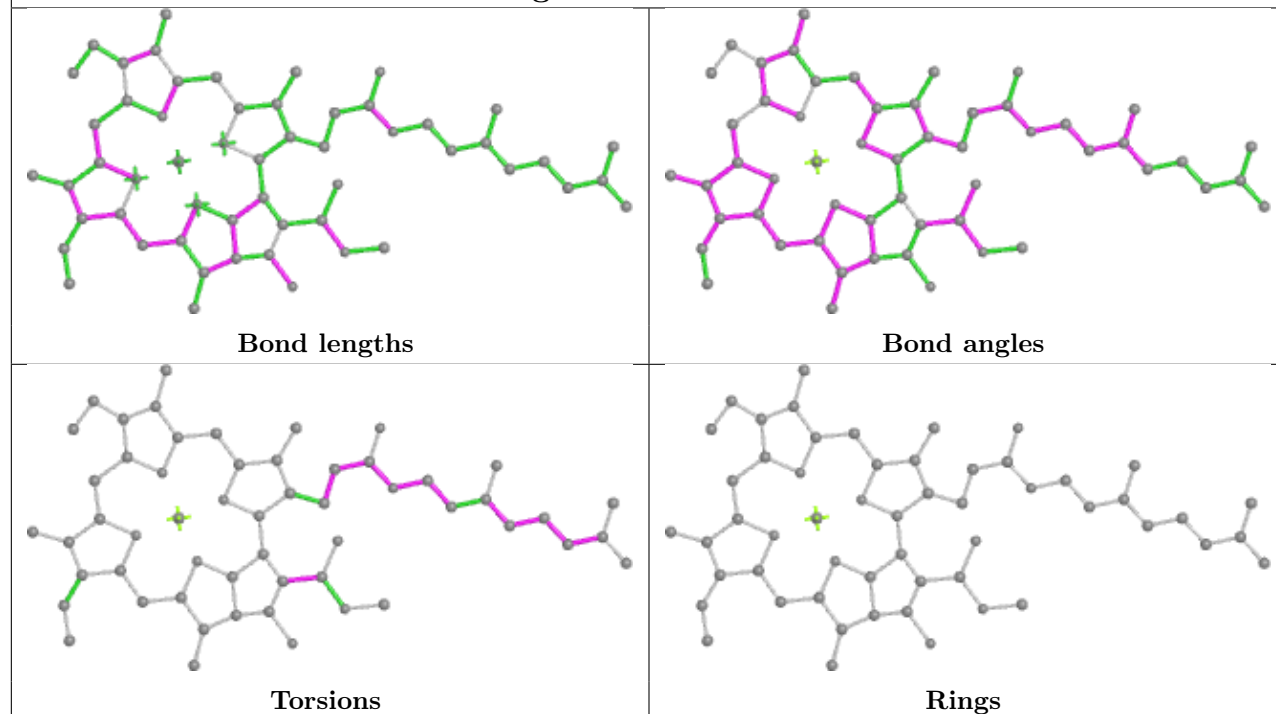


Ligand LMT 12 301

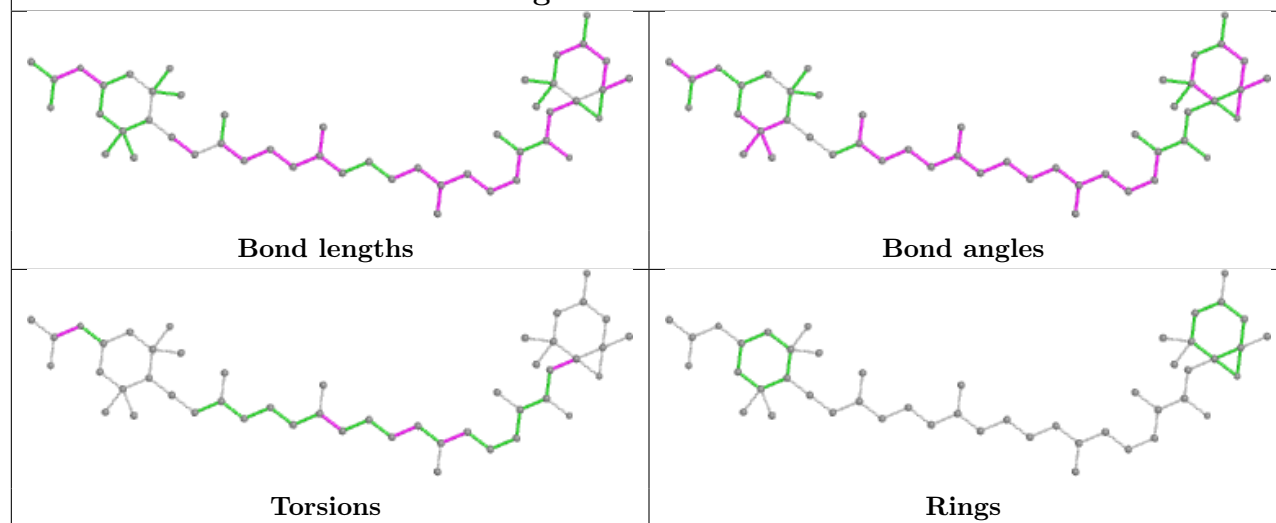




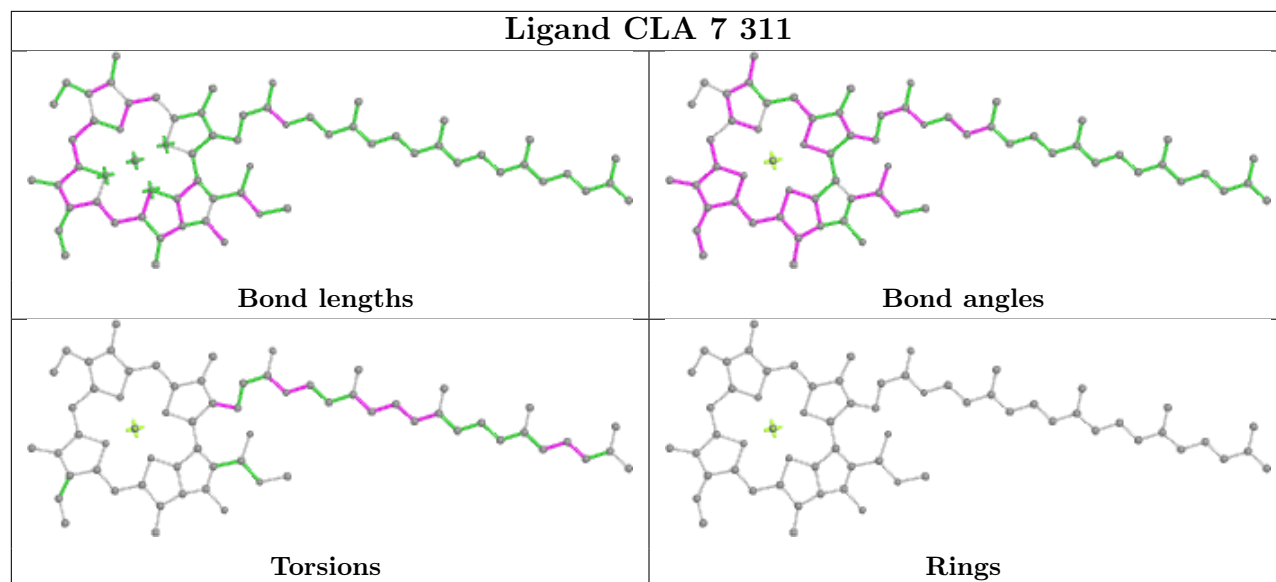
Ligand CLA B 821



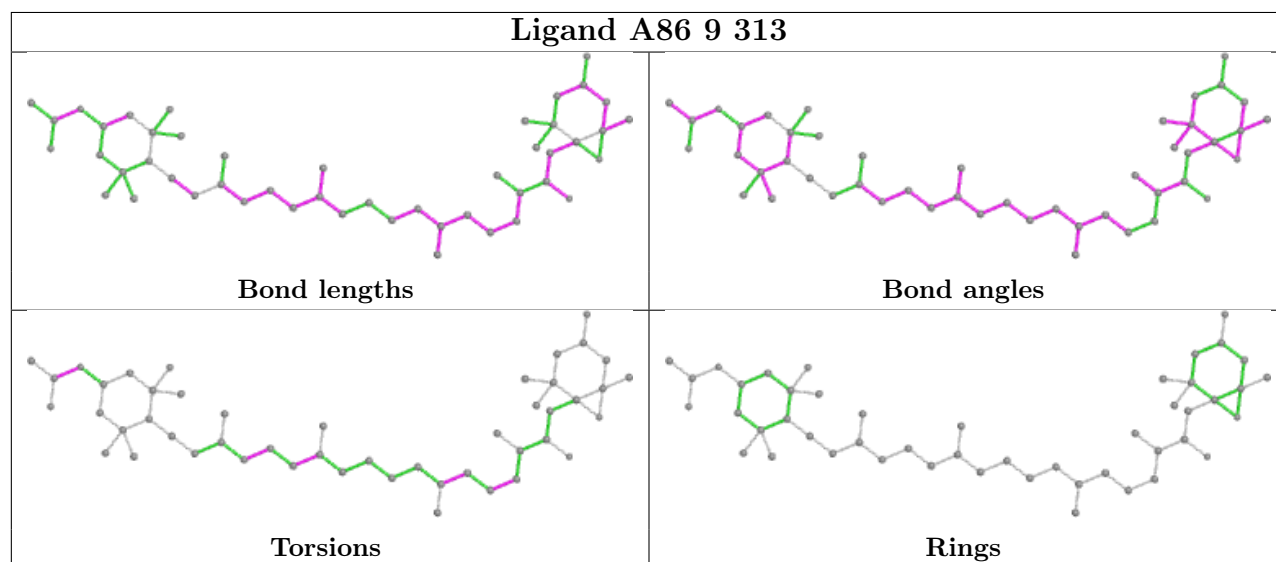
Ligand A86 14 320



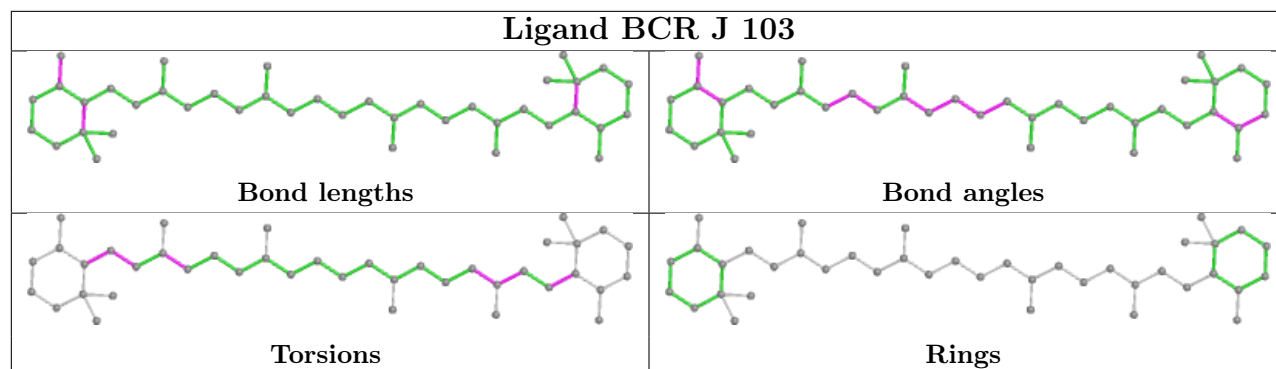
Ligand CLA 7 311



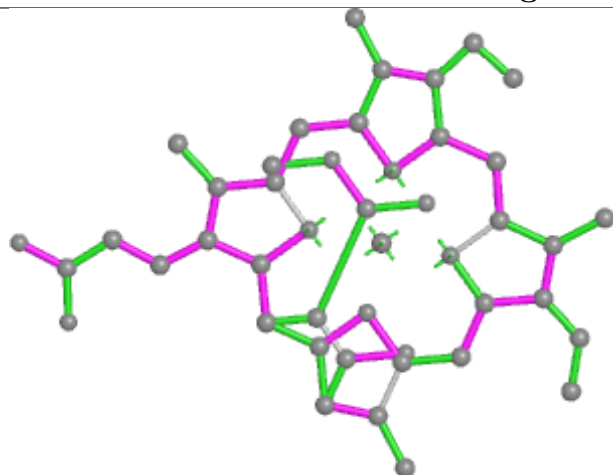
Ligand A86 9 313



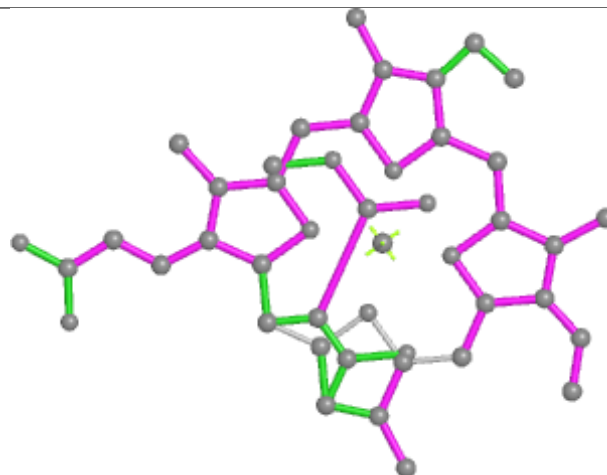
Ligand BCR J 103



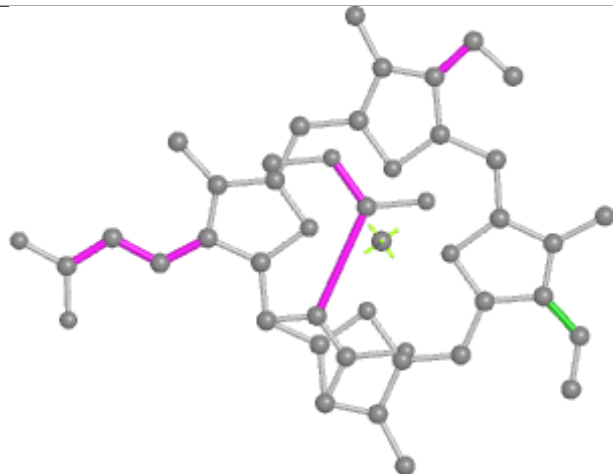
Ligand KC1 6 311



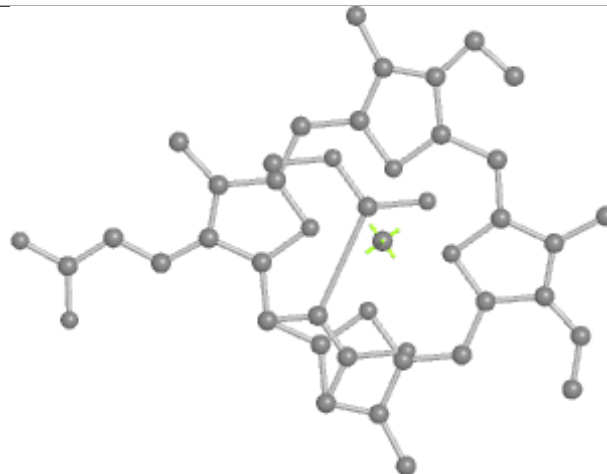
Bond lengths



Bond angles

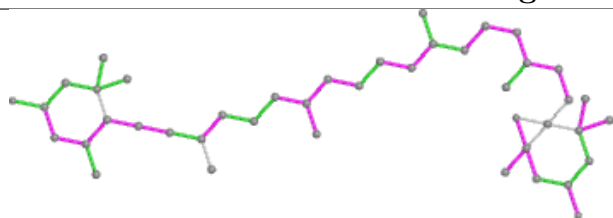


Torsions

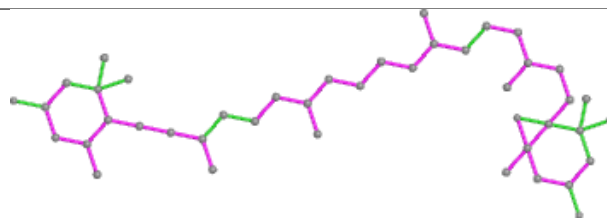


Rings

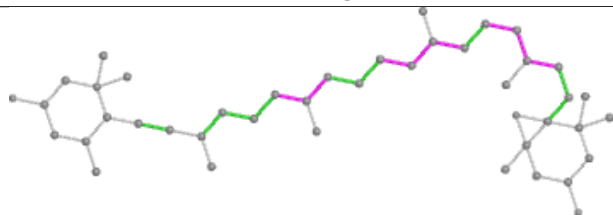
Ligand DD6 6 303



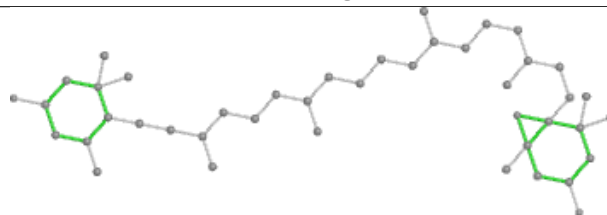
Bond lengths



Bond angles

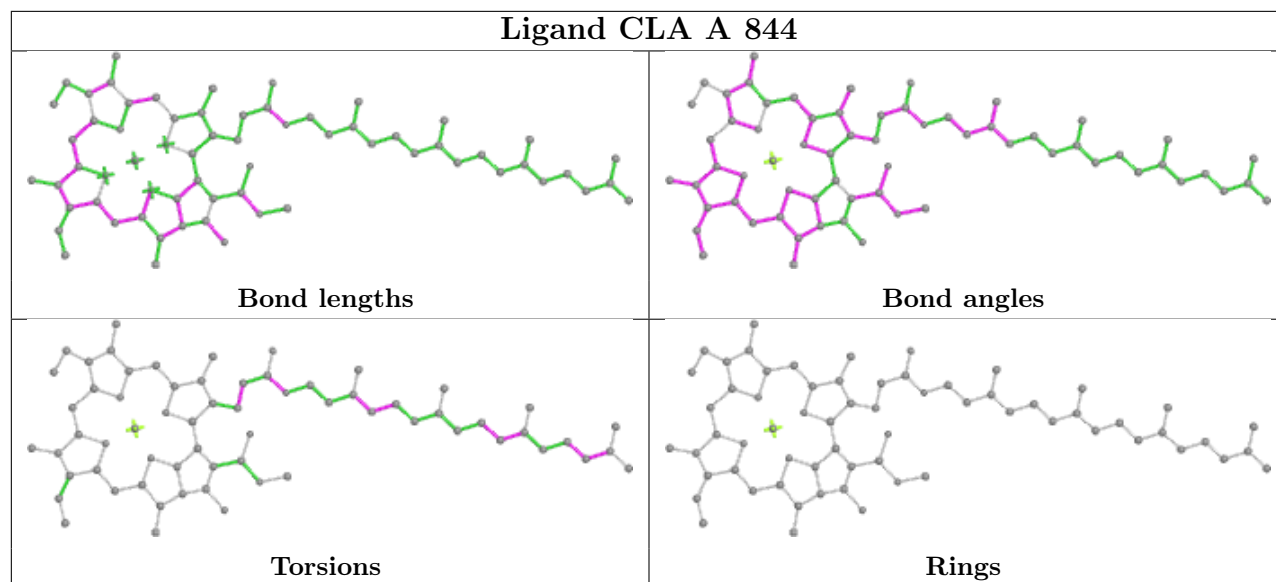


Torsions

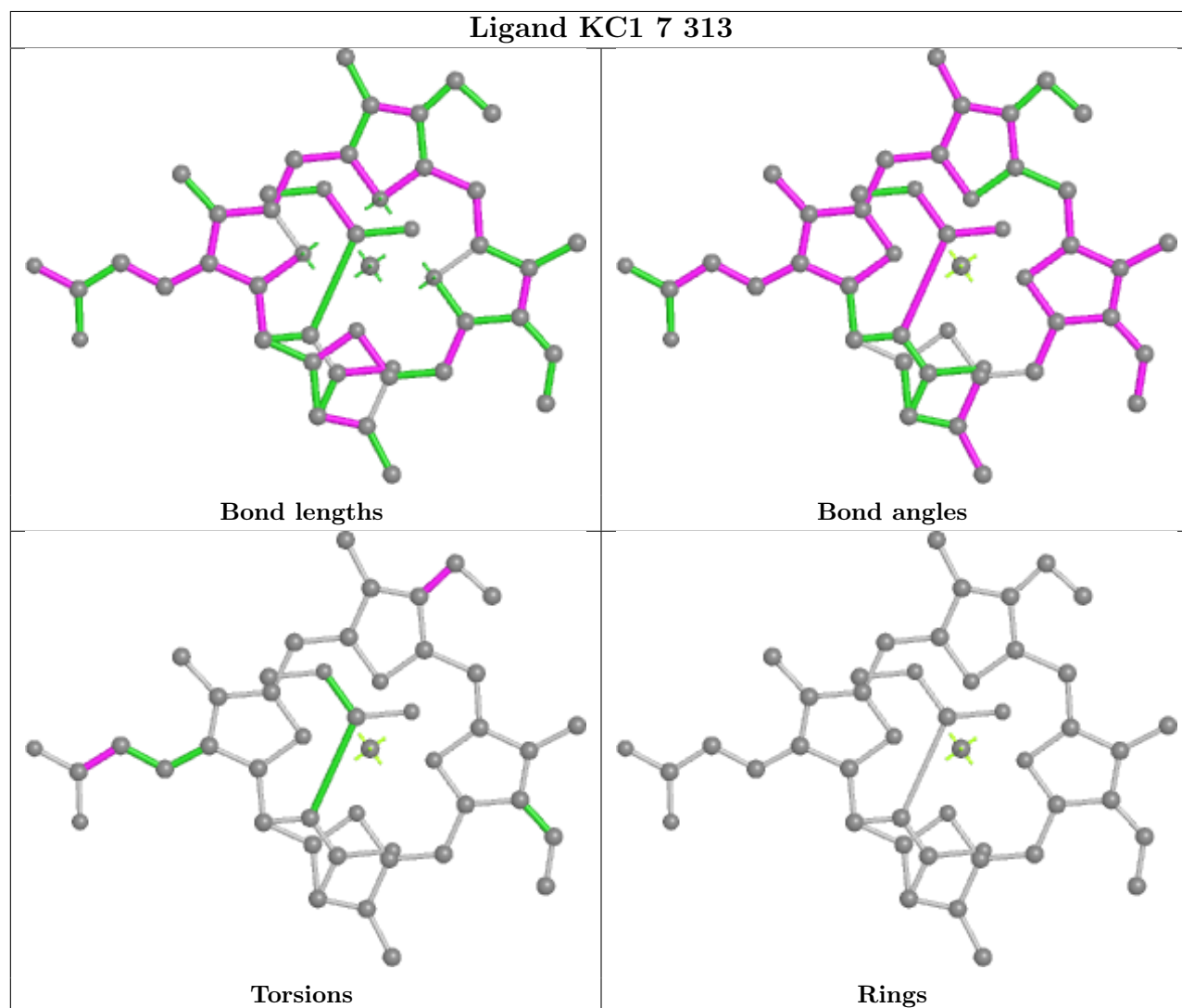


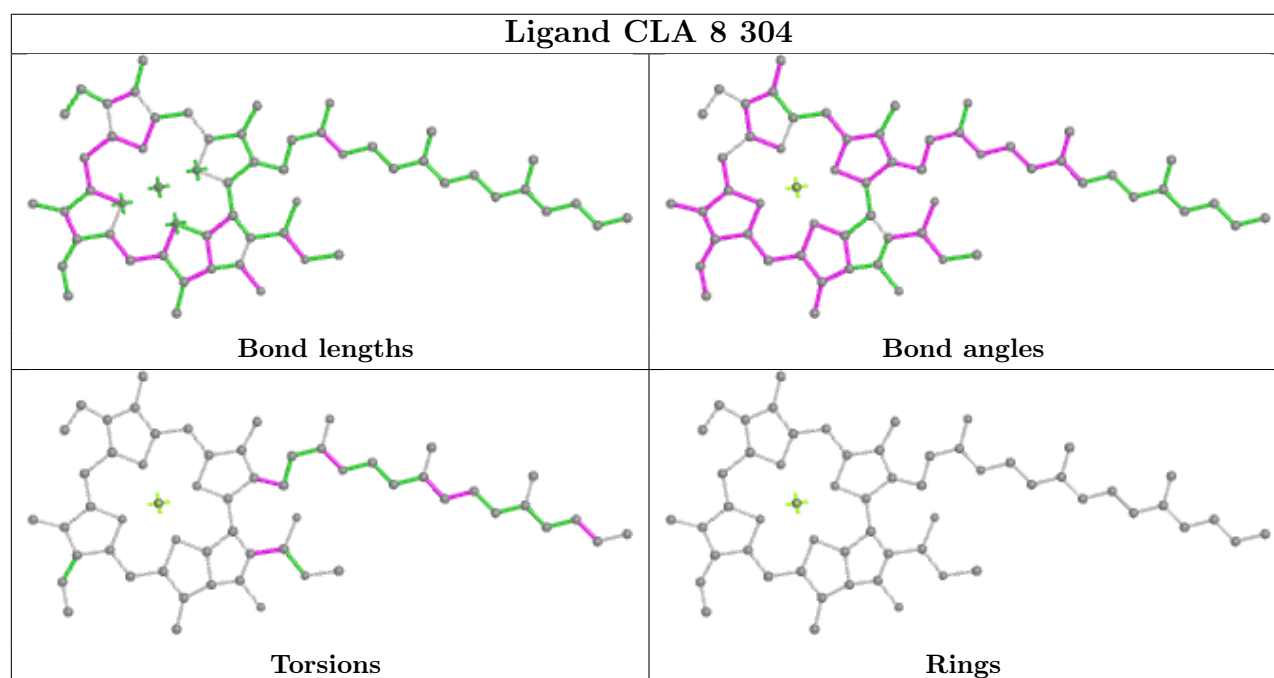
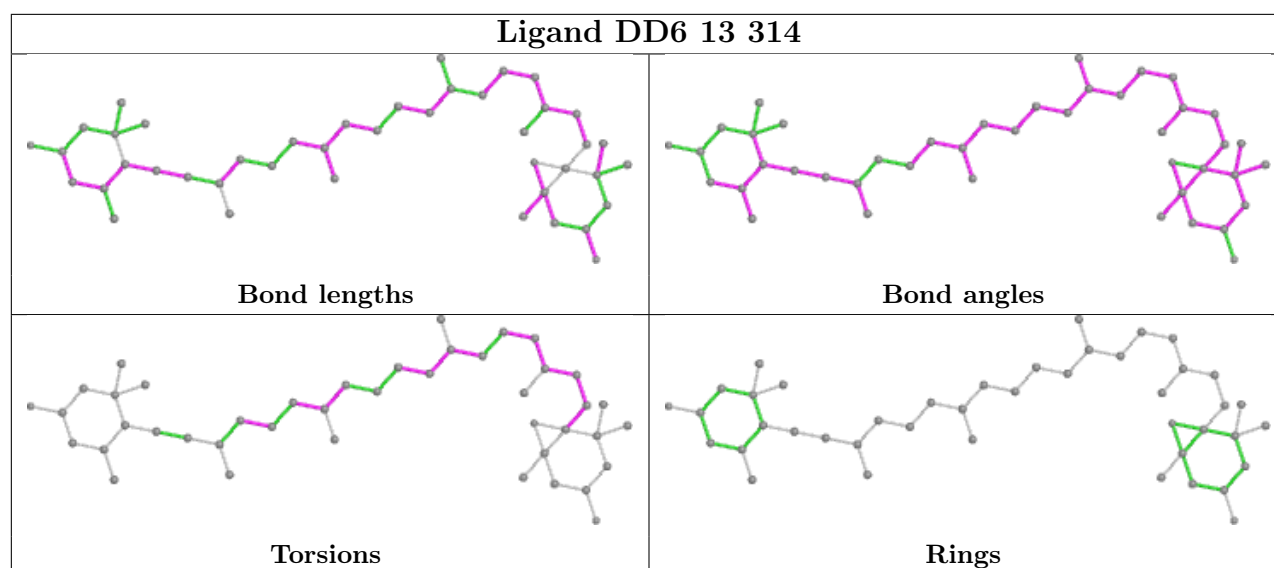
Rings

Ligand CLA A 844

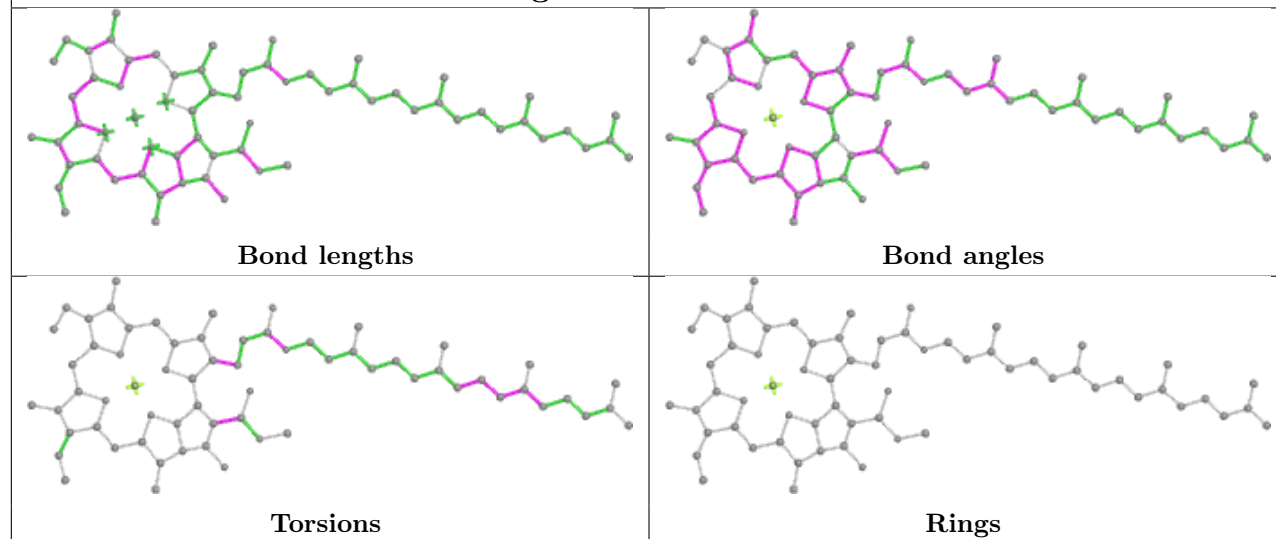


Ligand KC1 7 313

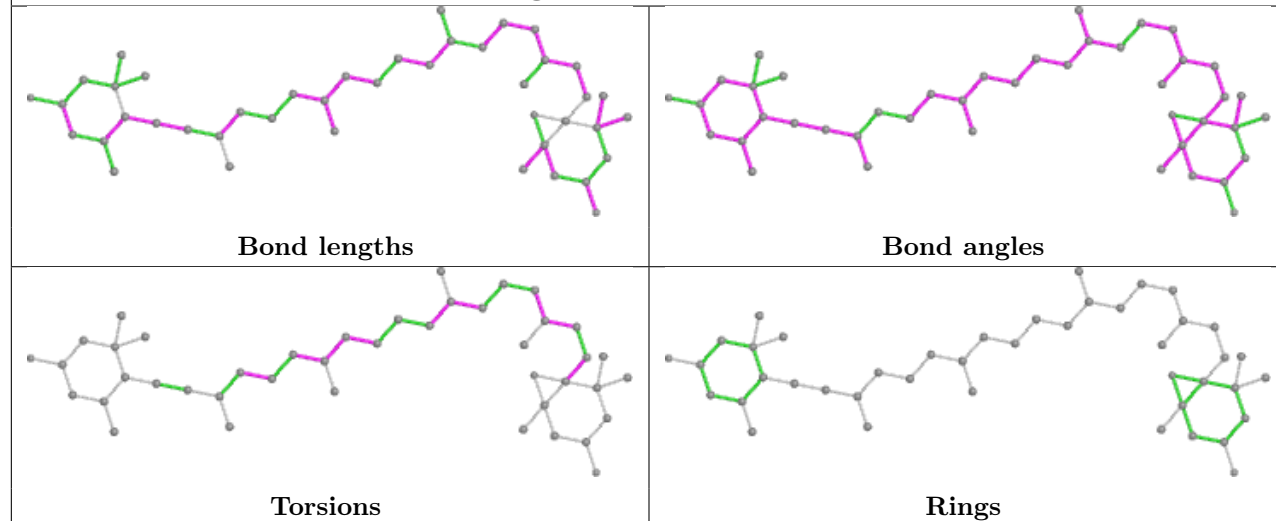


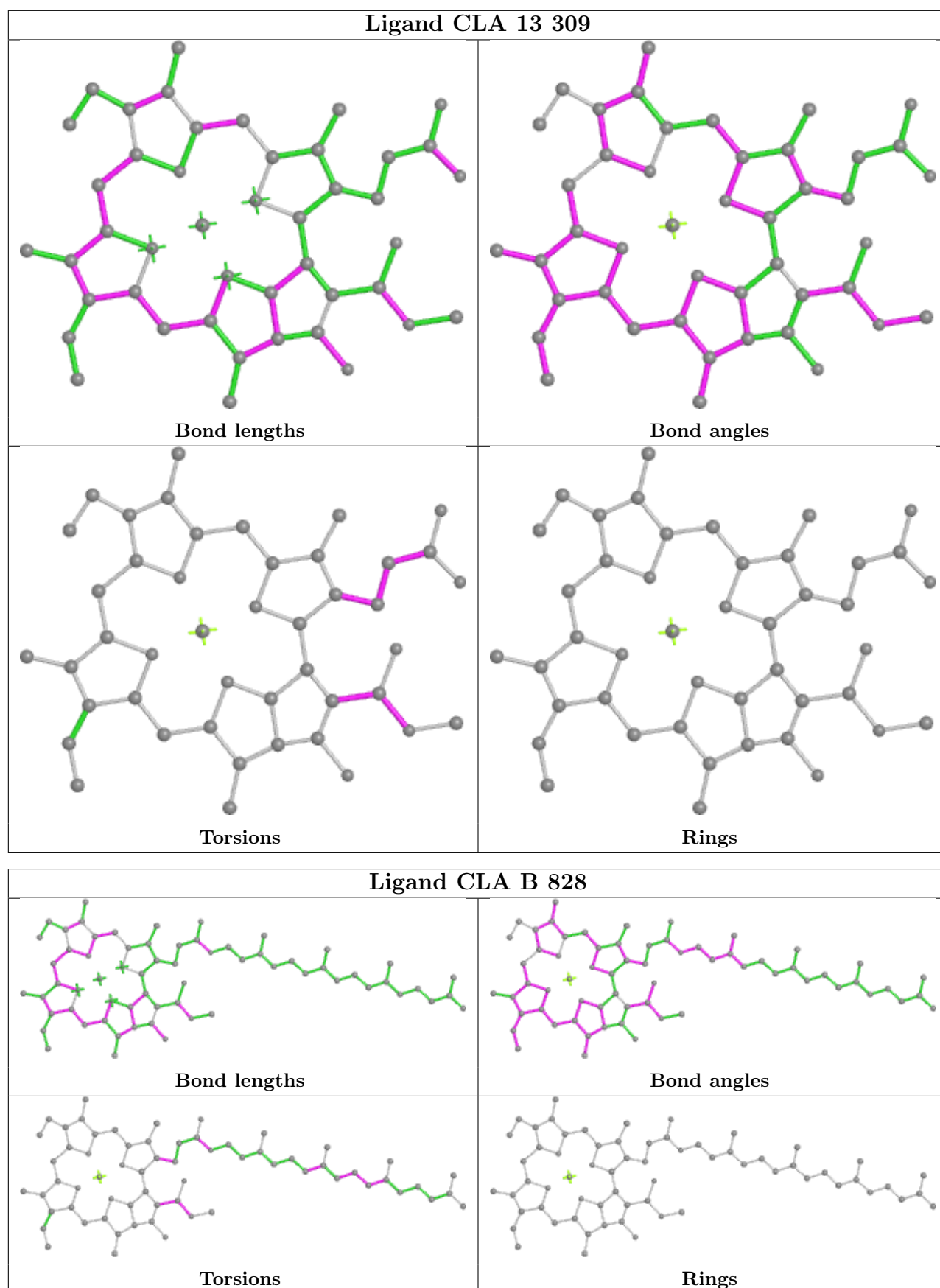


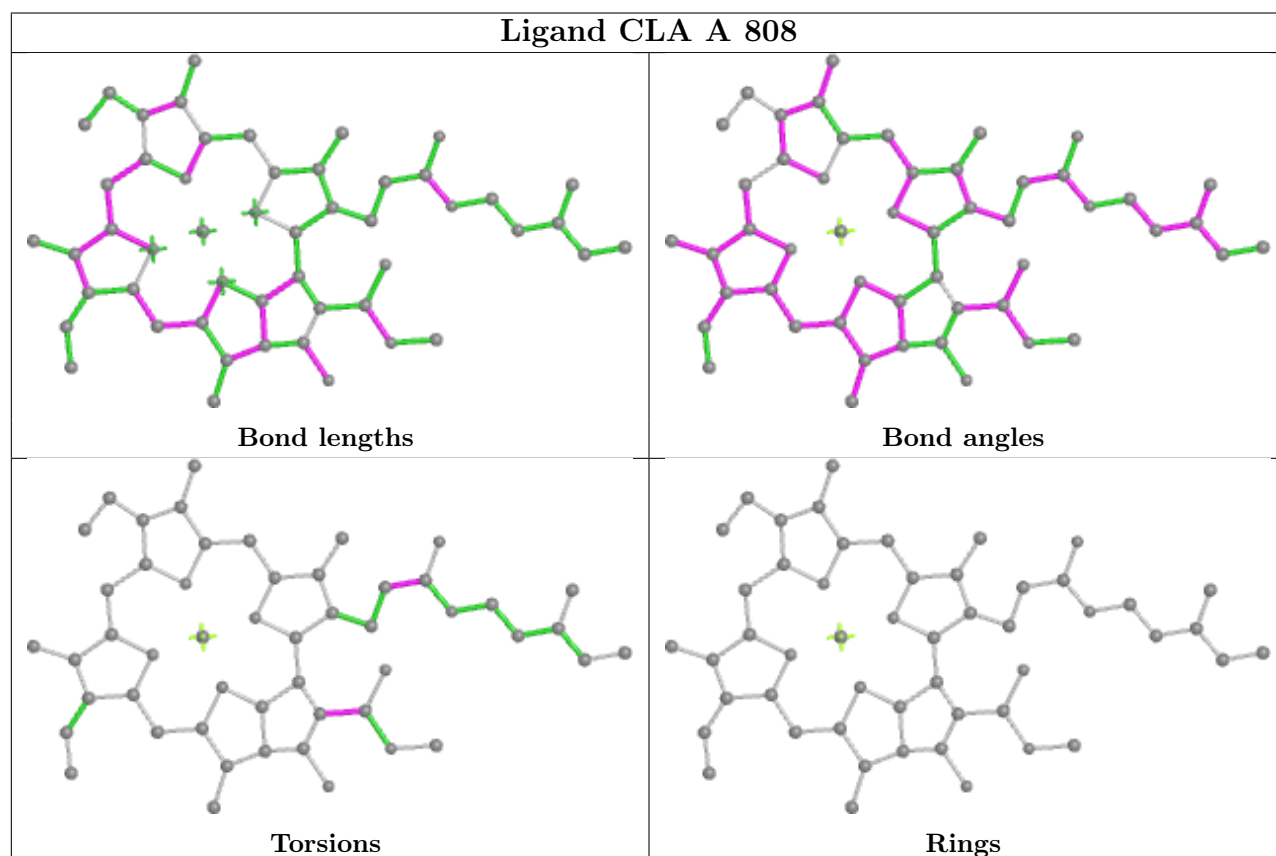
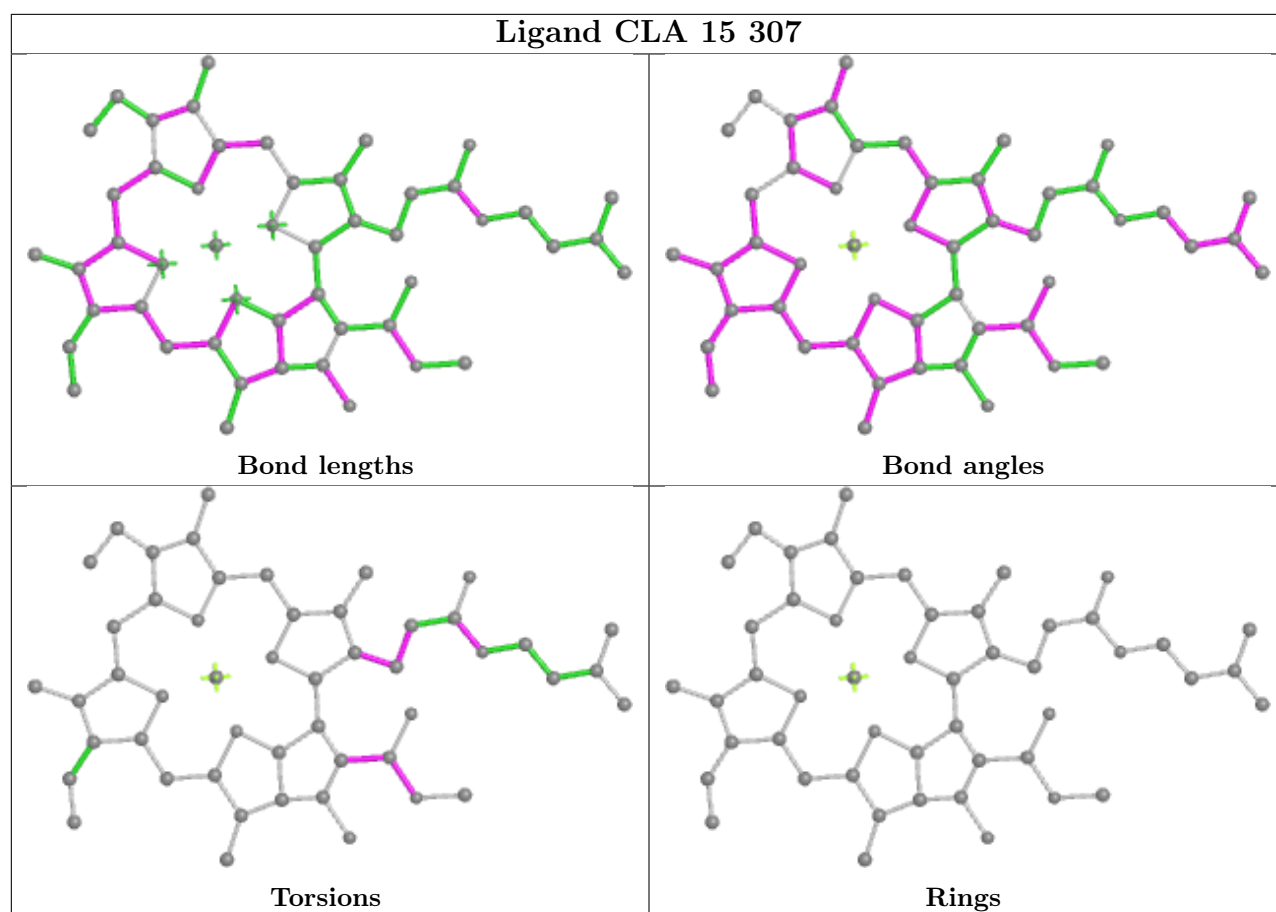
Ligand CLA A 804

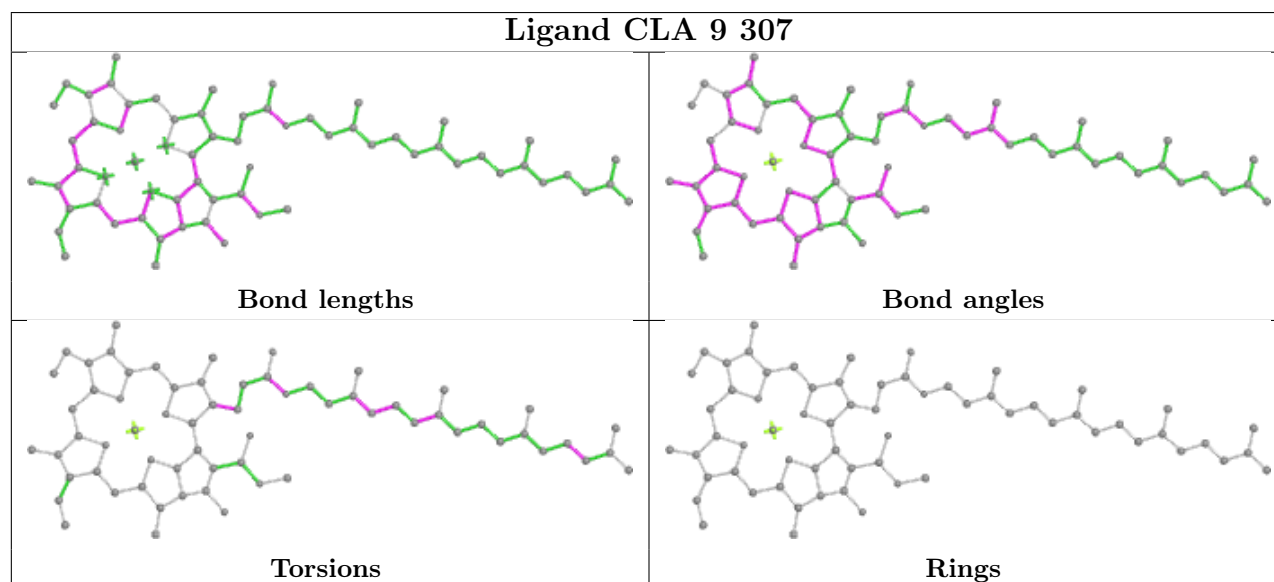
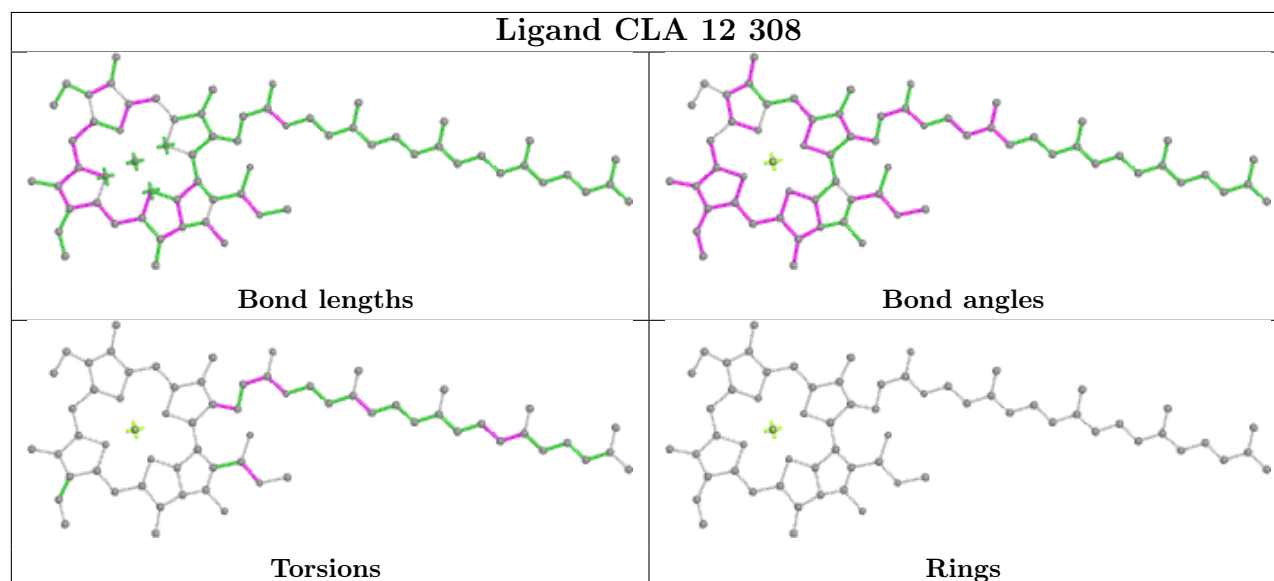
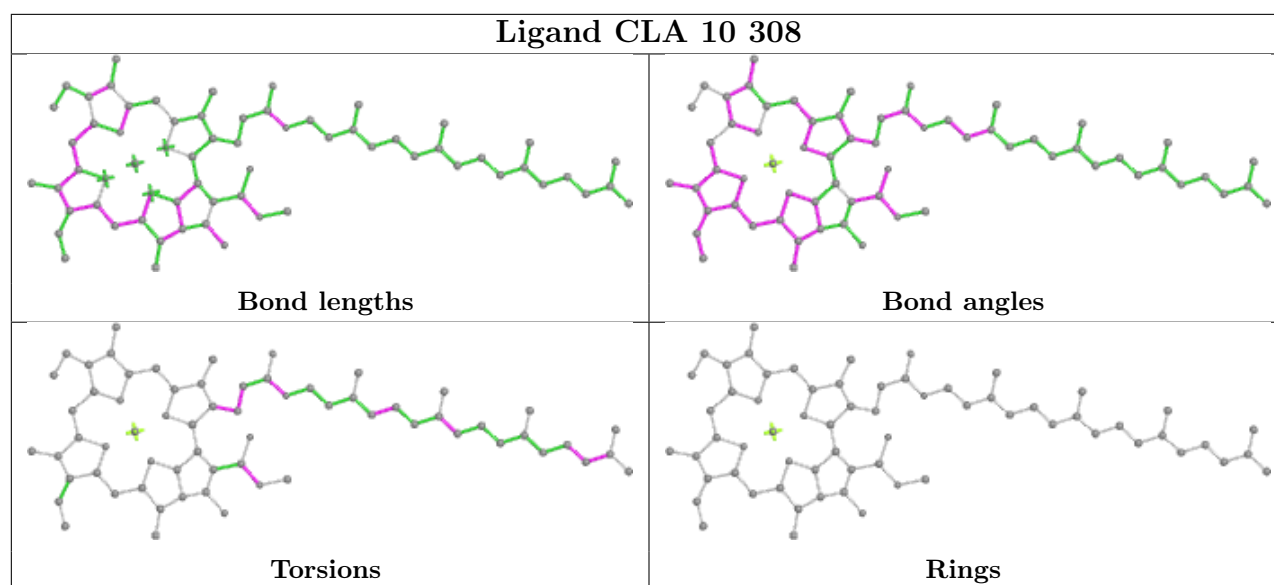


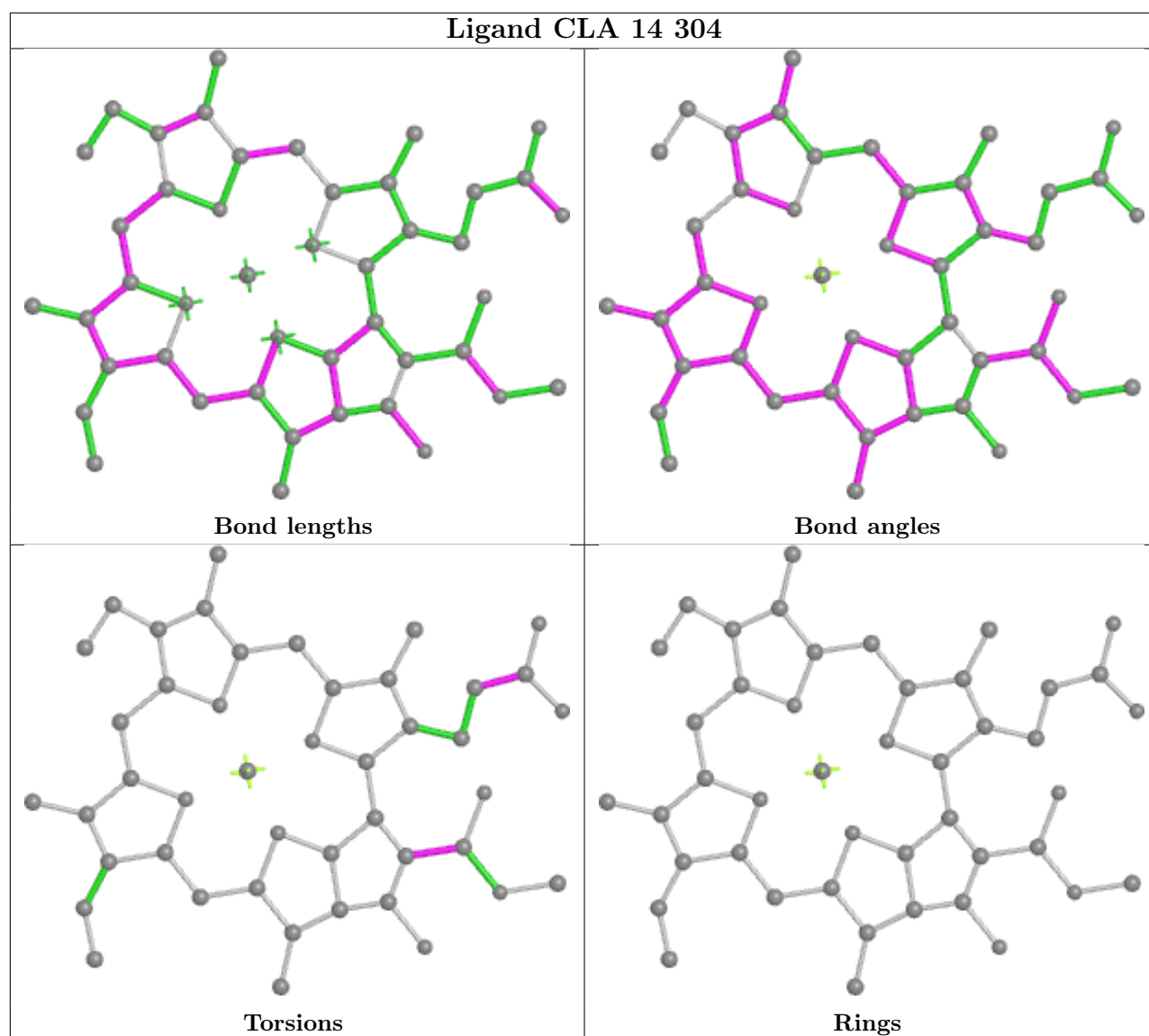
Ligand DD6 15 318



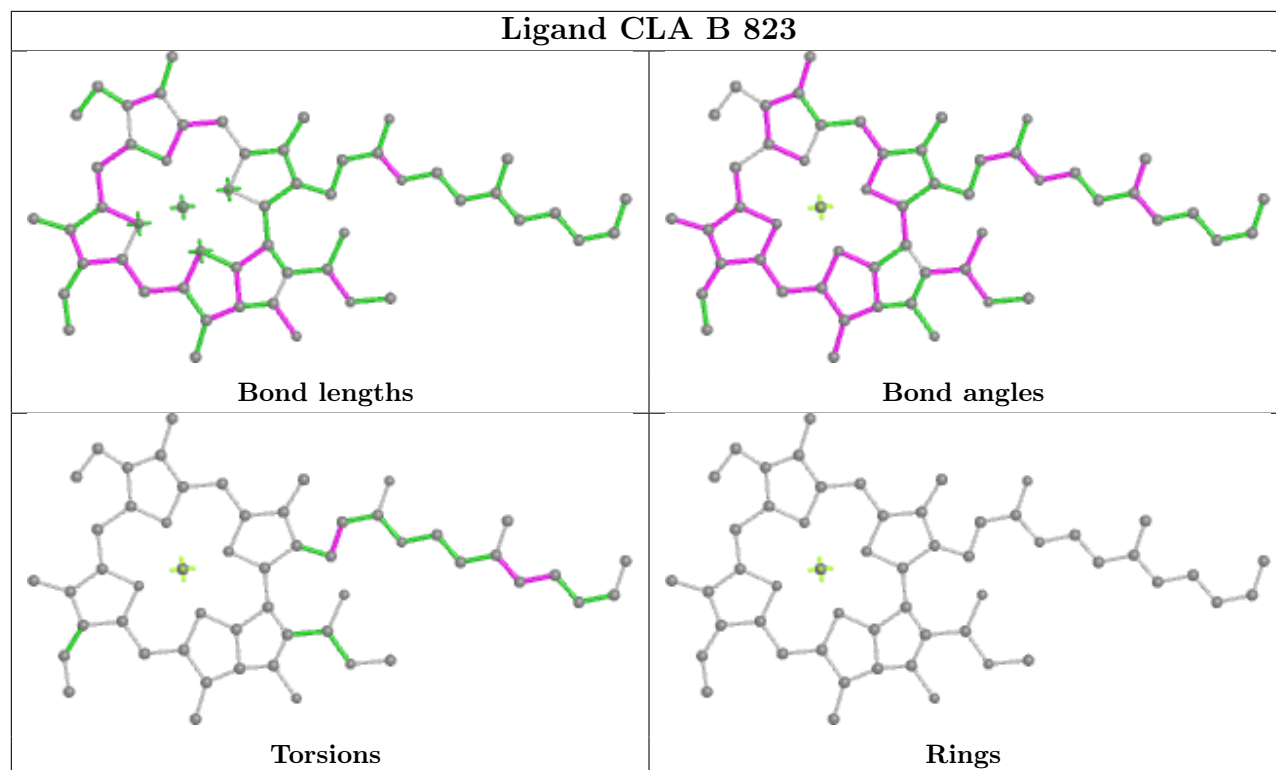




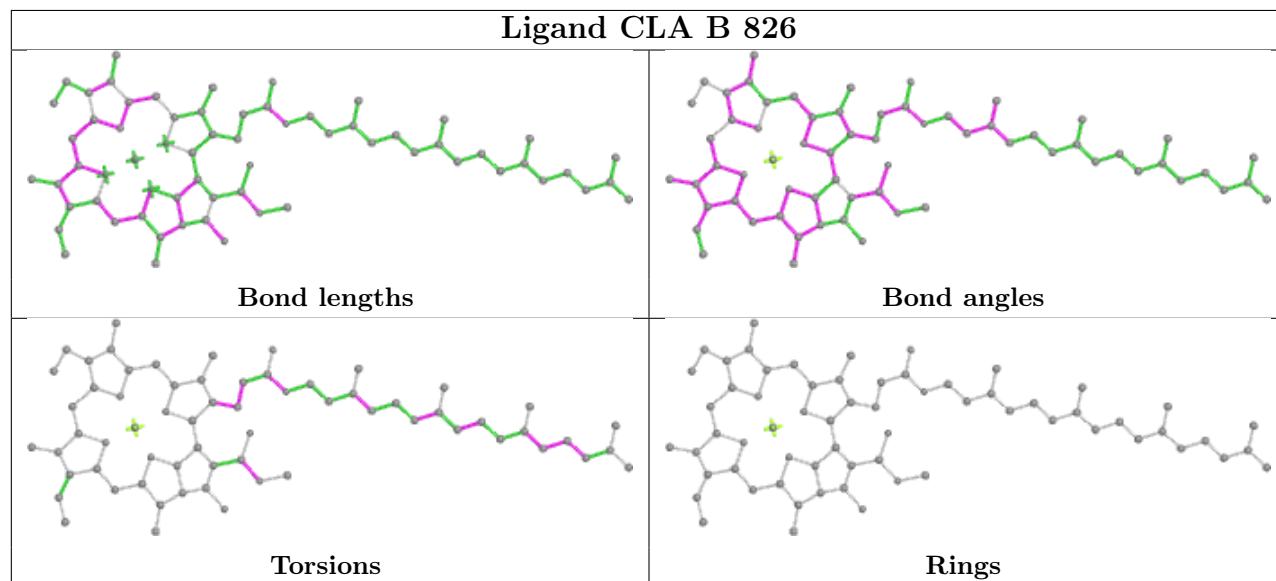




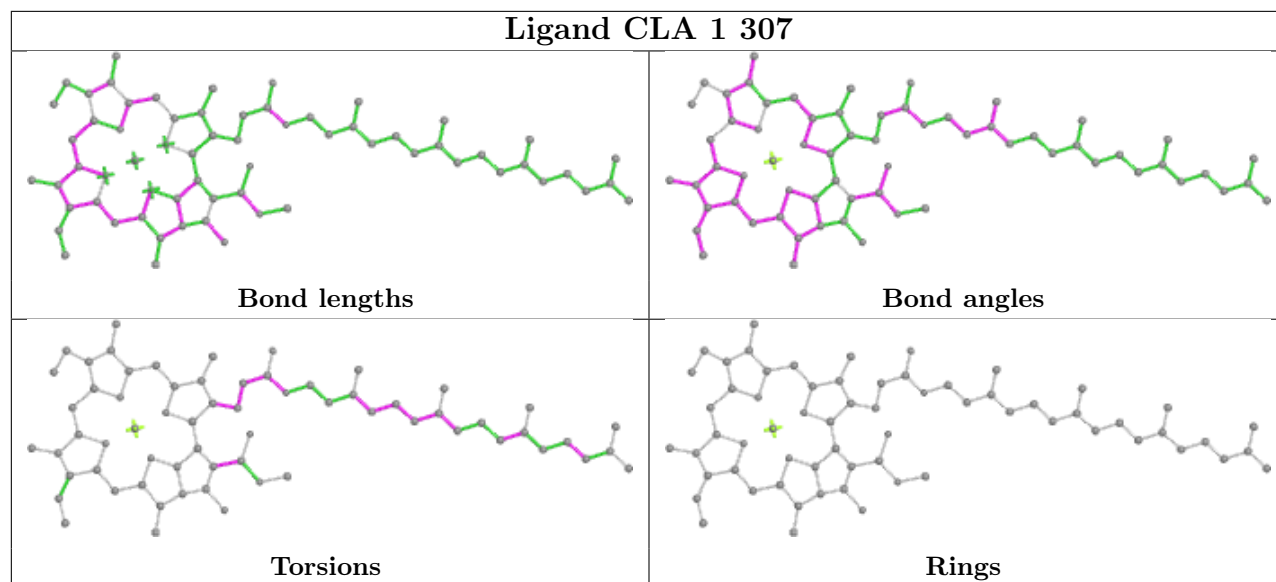
Ligand CLA B 823



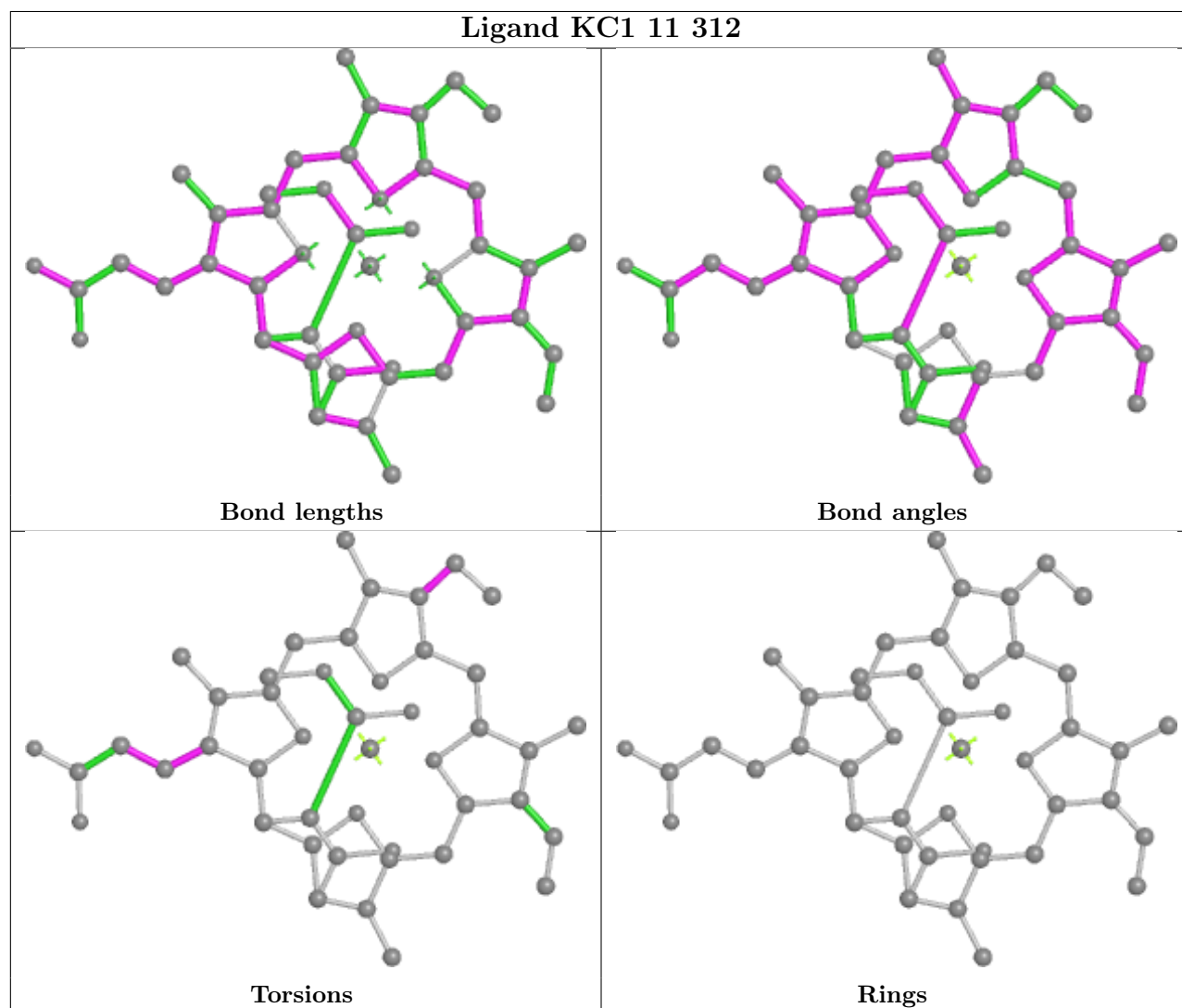
Ligand CLA B 826

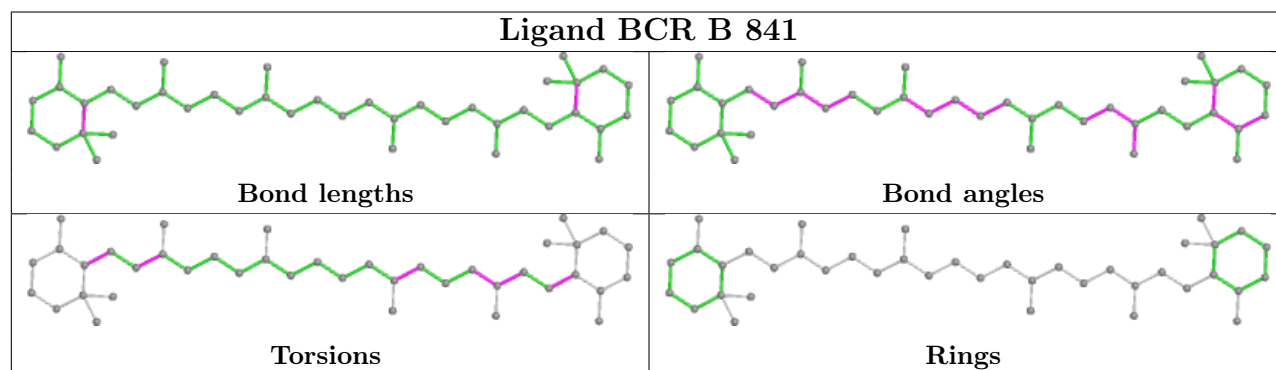
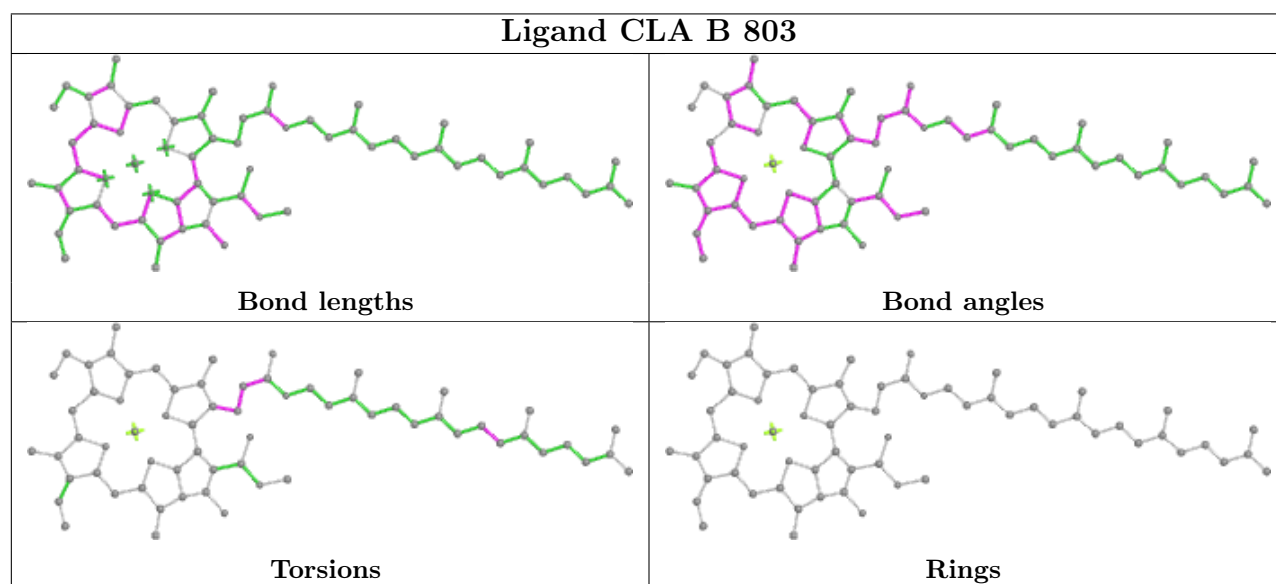
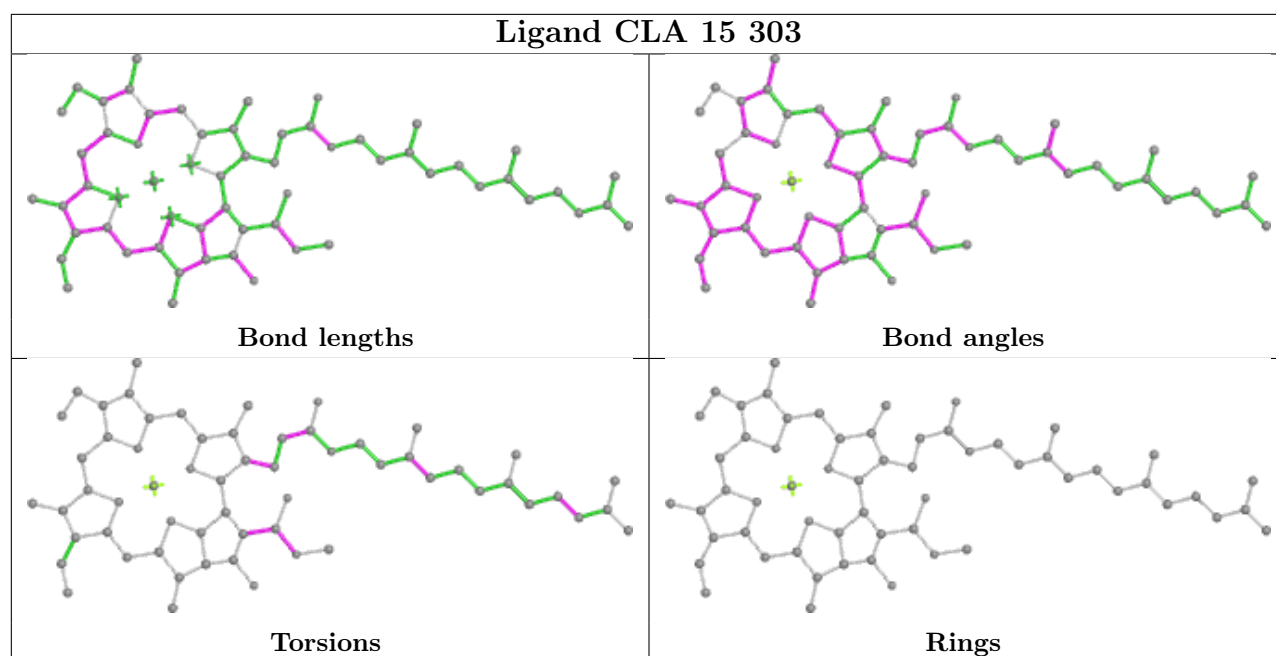


Ligand CLA 1 307

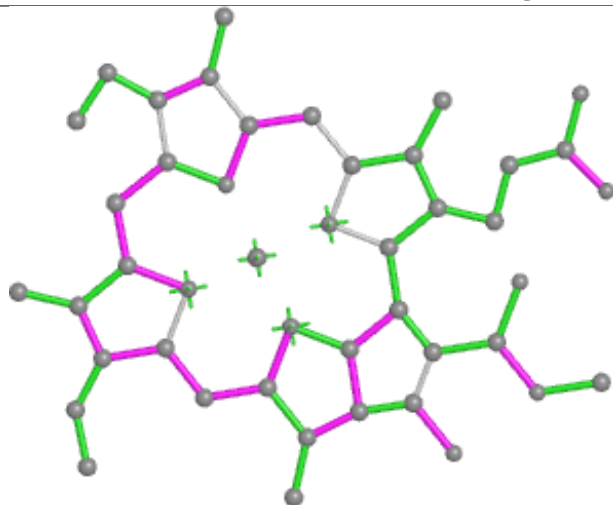


Ligand KC1 11 312

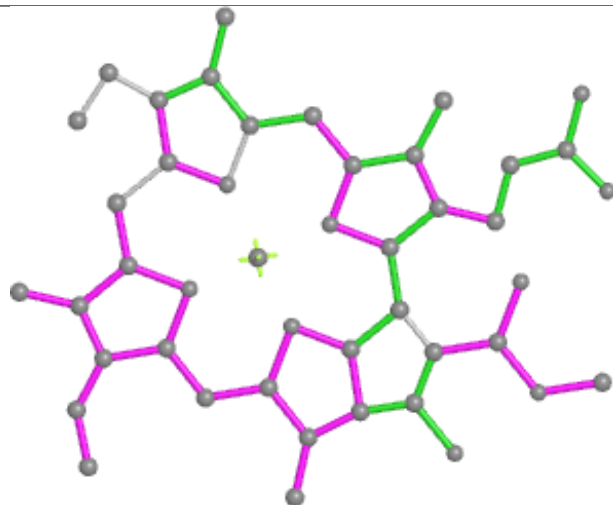




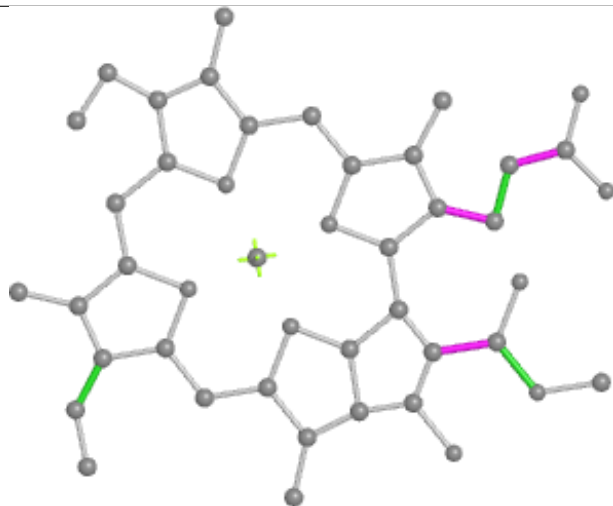
Ligand CLA 3 310



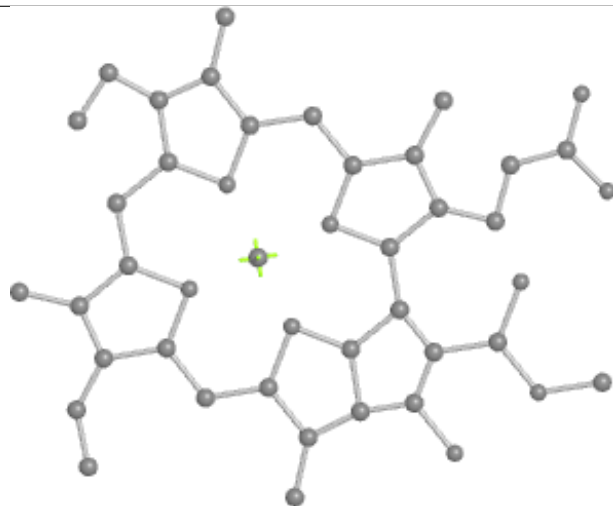
Bond lengths



Bond angles

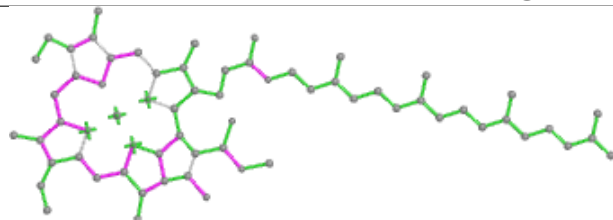


Torsions

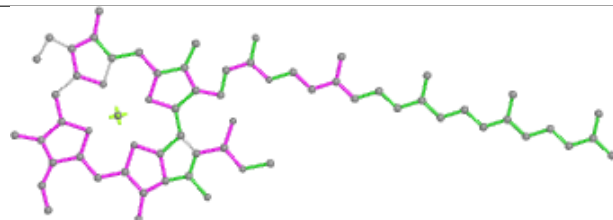


Rings

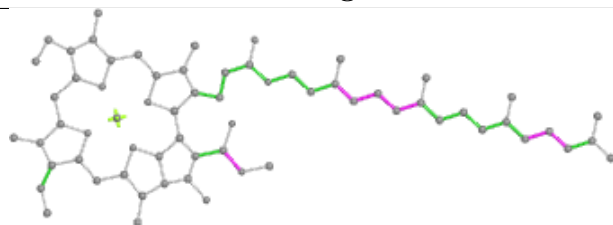
Ligand CLA 8 302



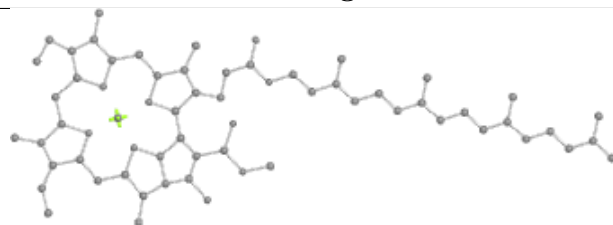
Bond lengths



Bond angles

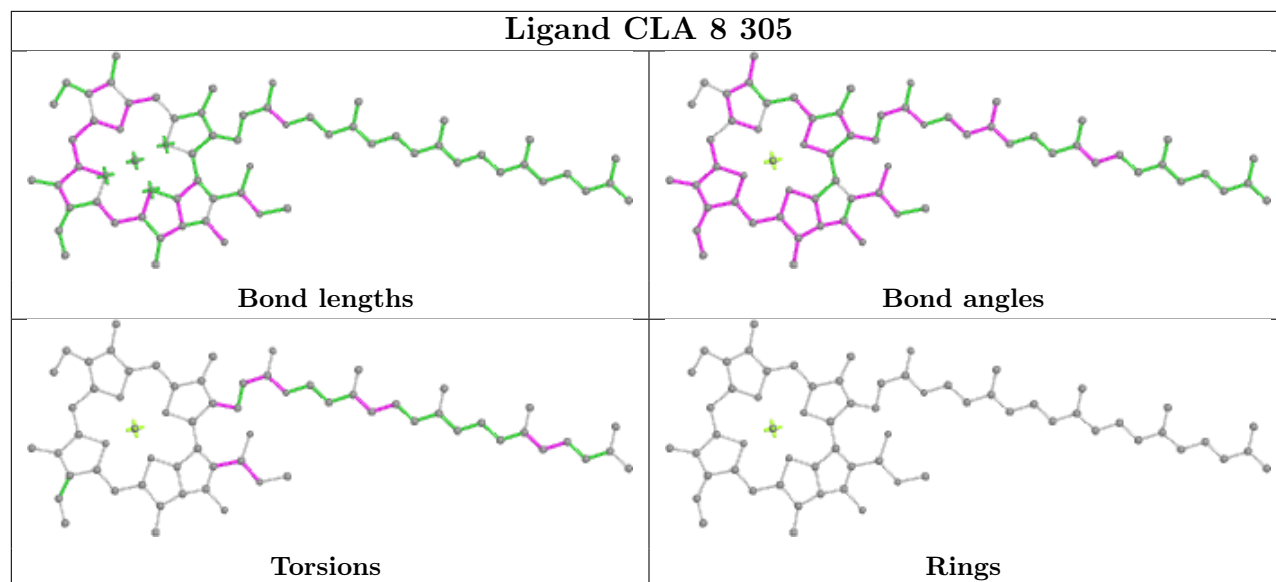


Torsions

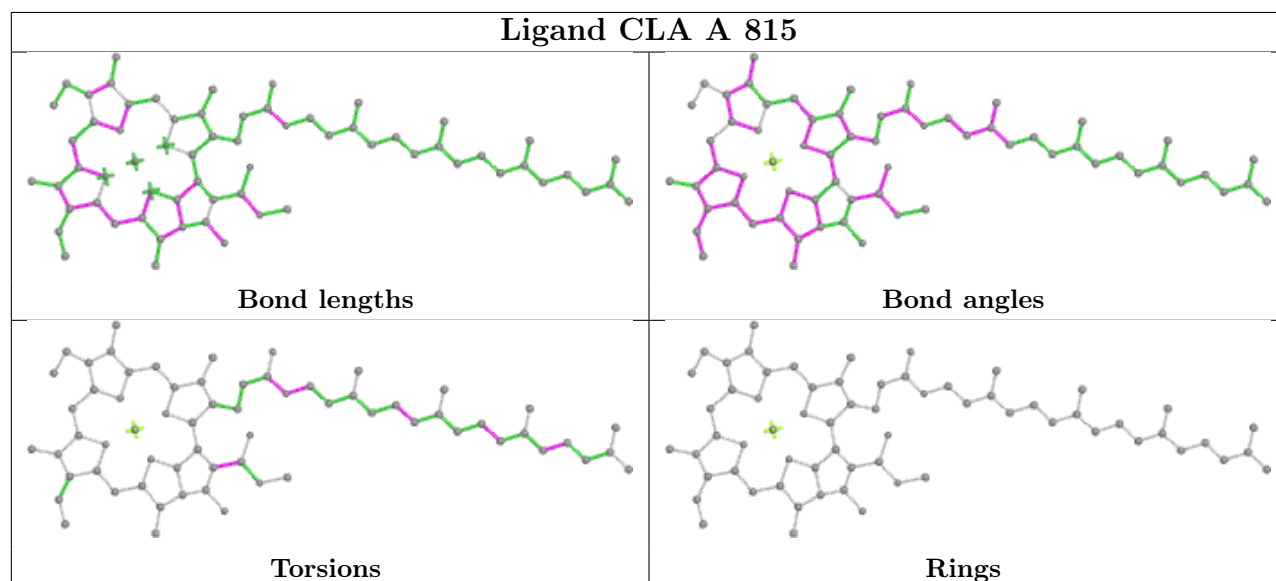


Rings

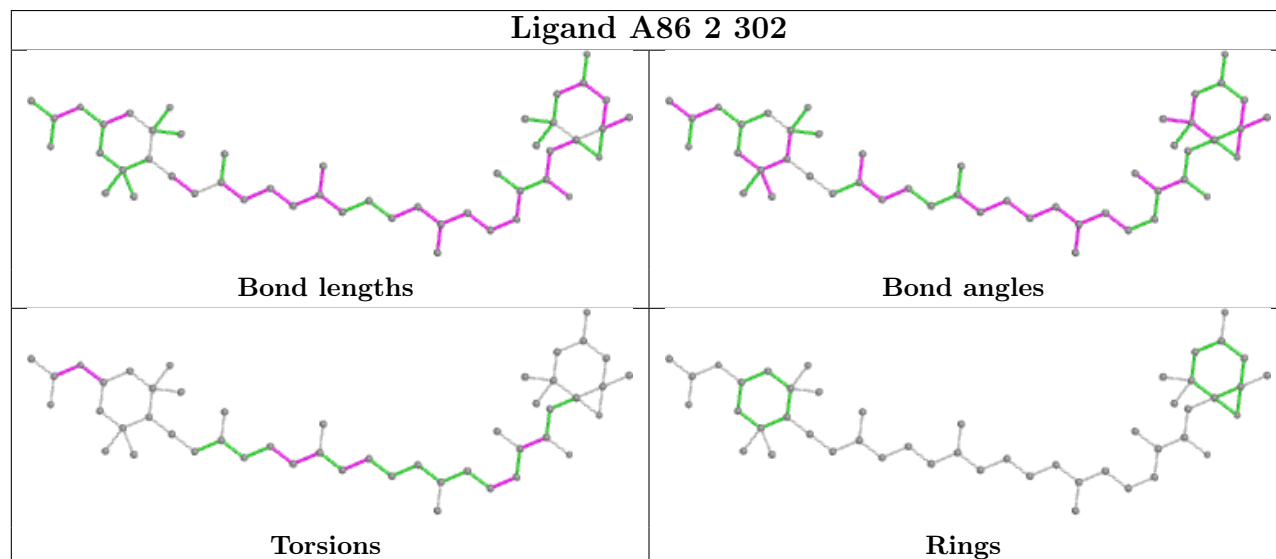
Ligand CLA 8 305



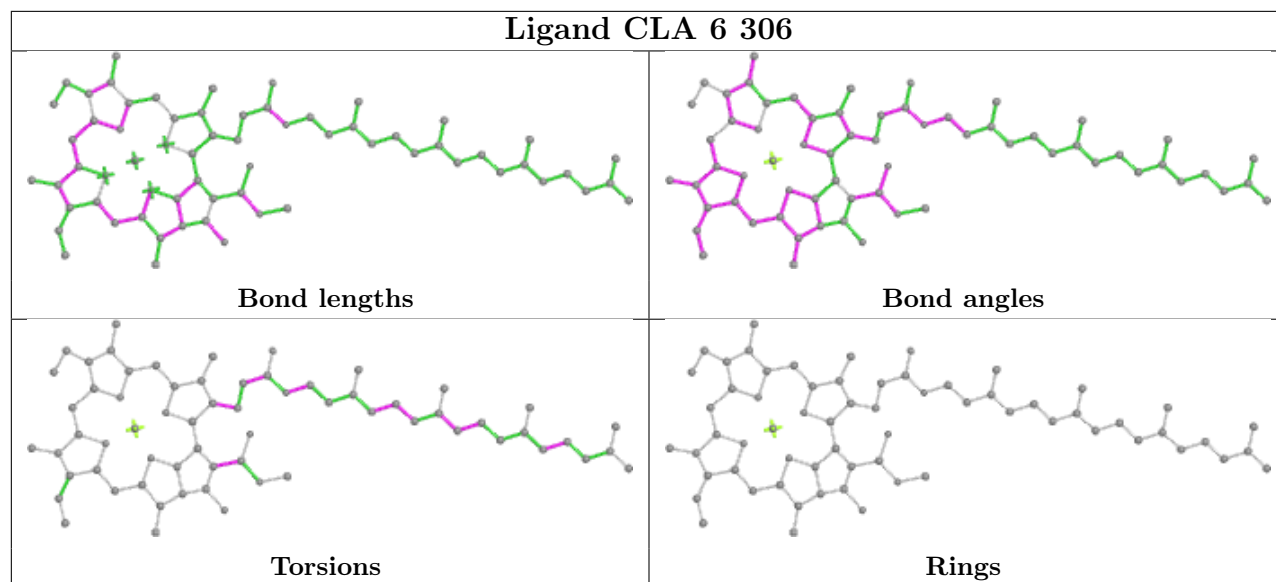
Ligand CLA A 815



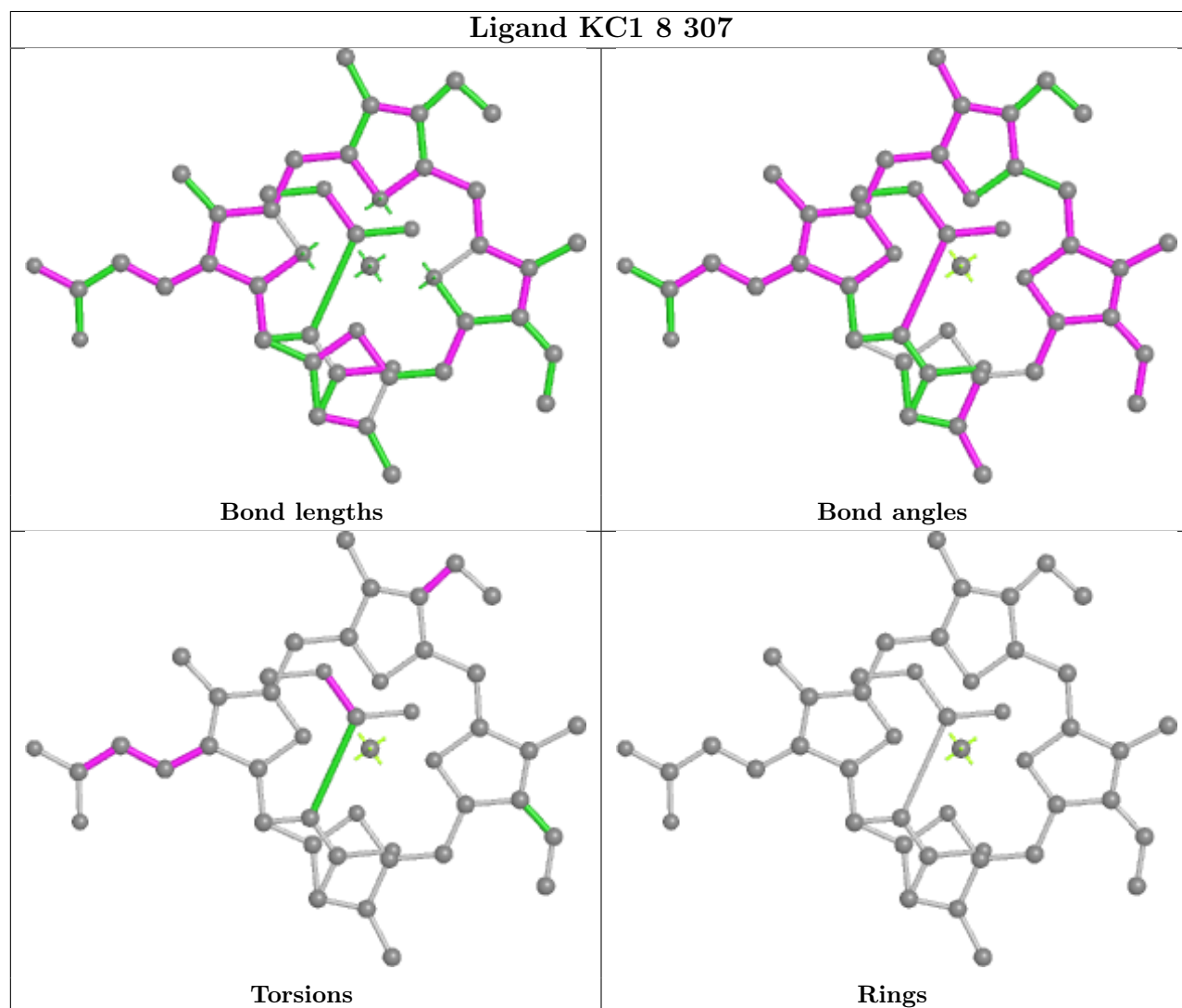
Ligand A86 2 302

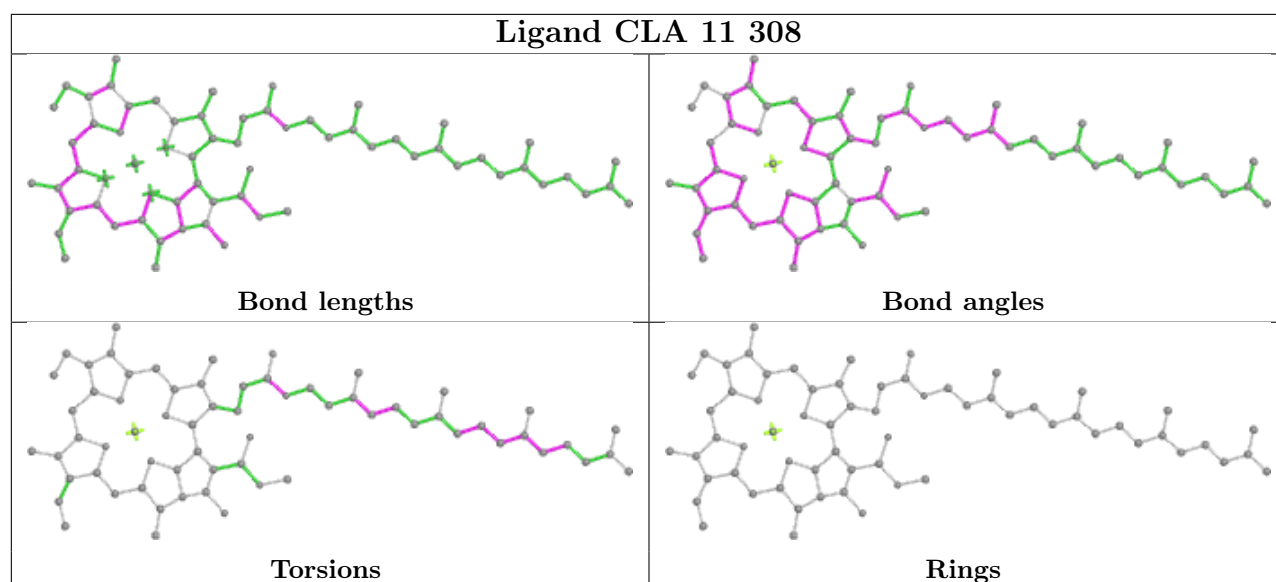
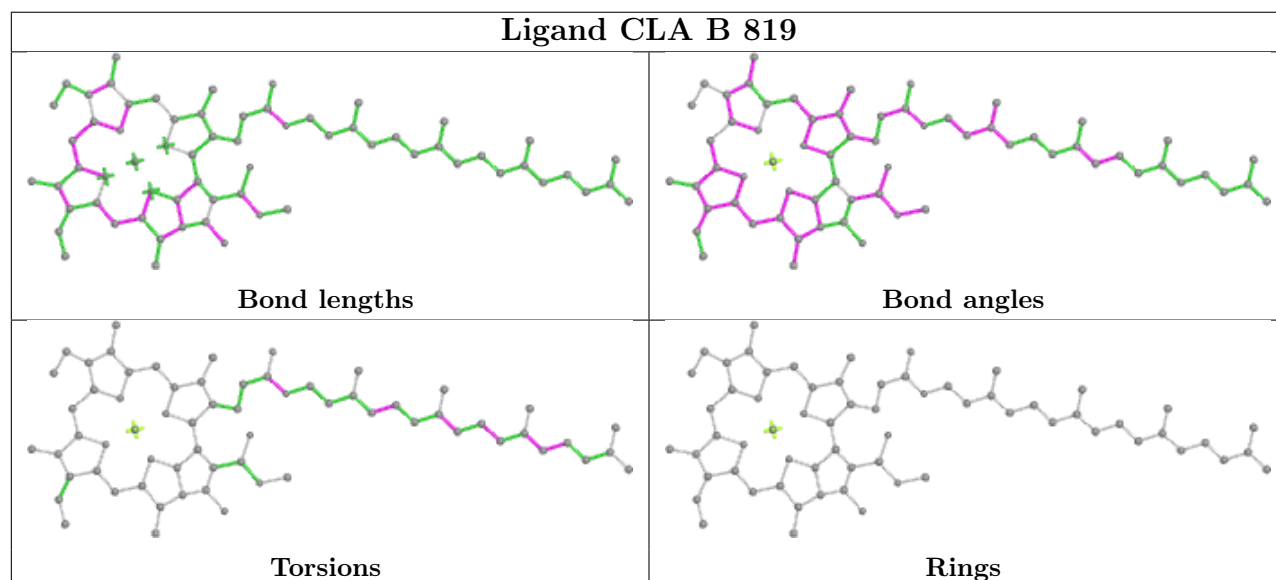
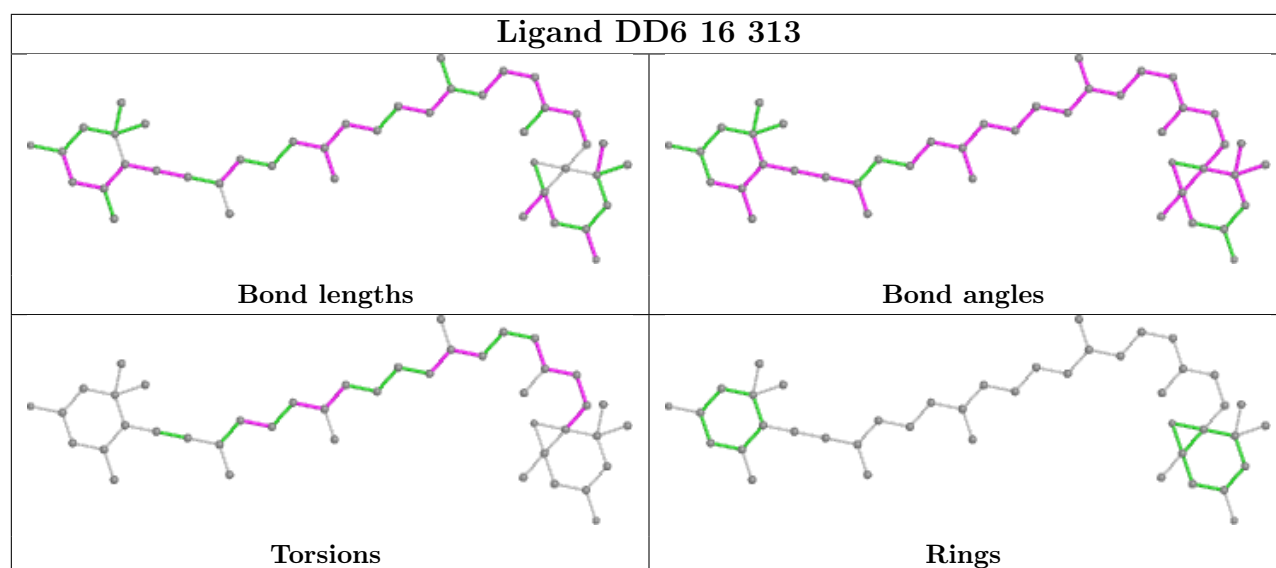


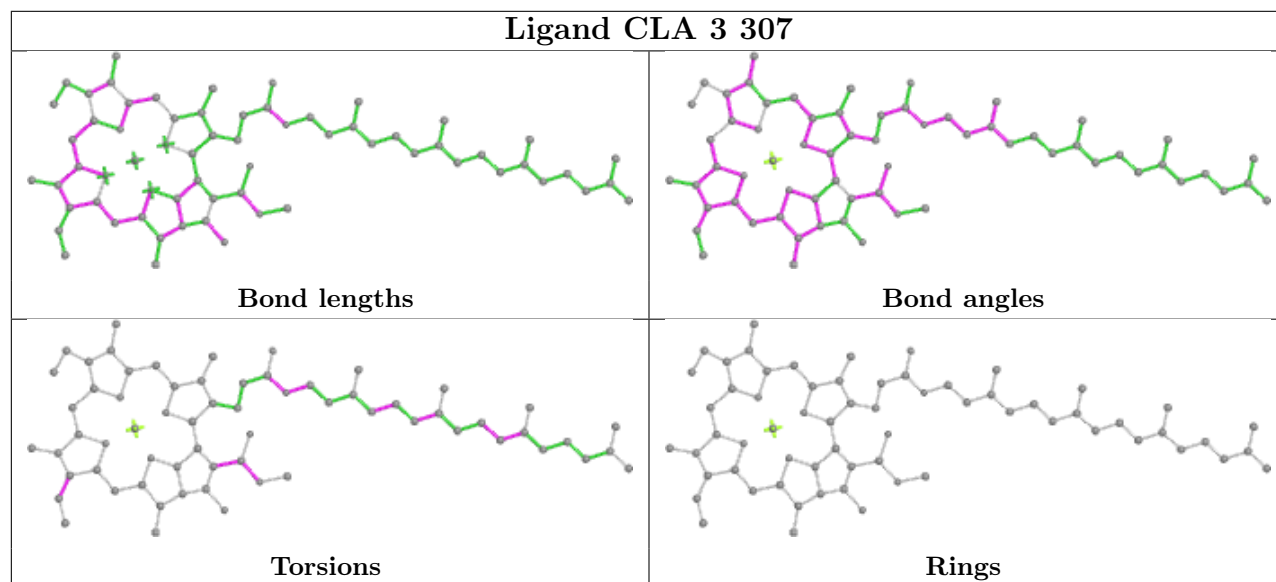
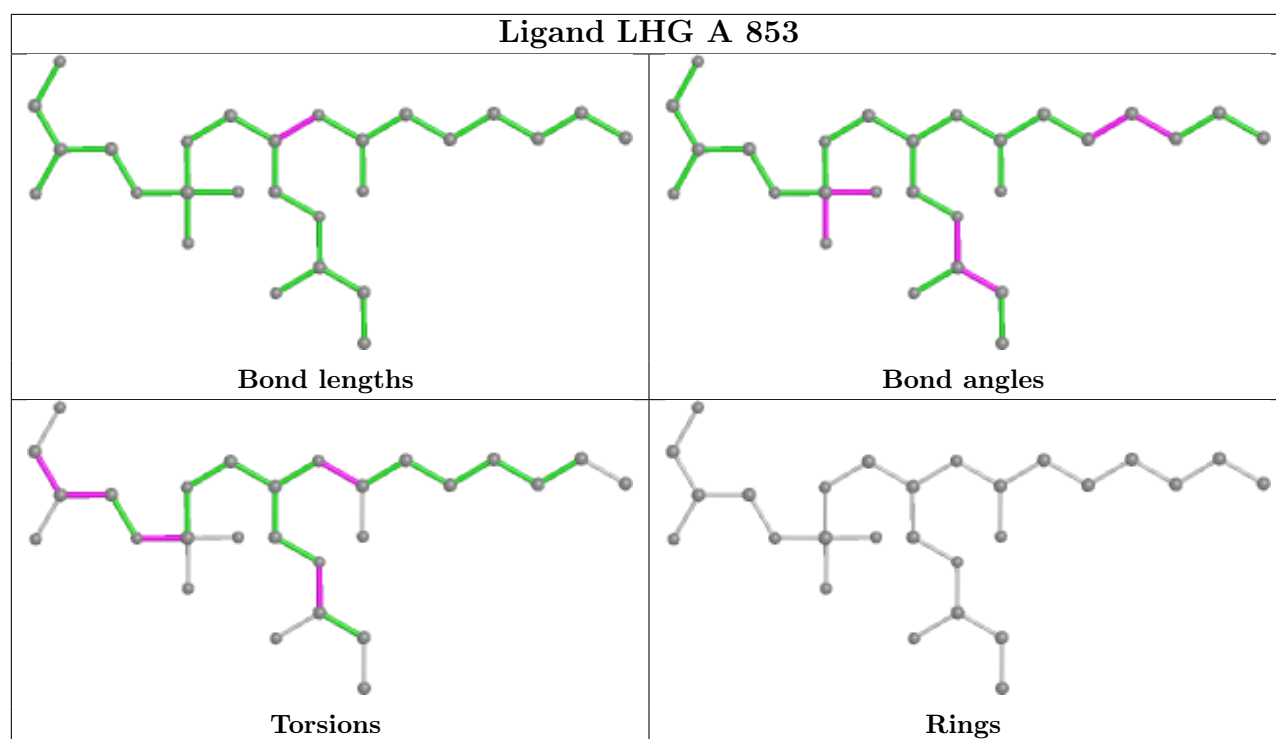
Ligand CLA 6 306

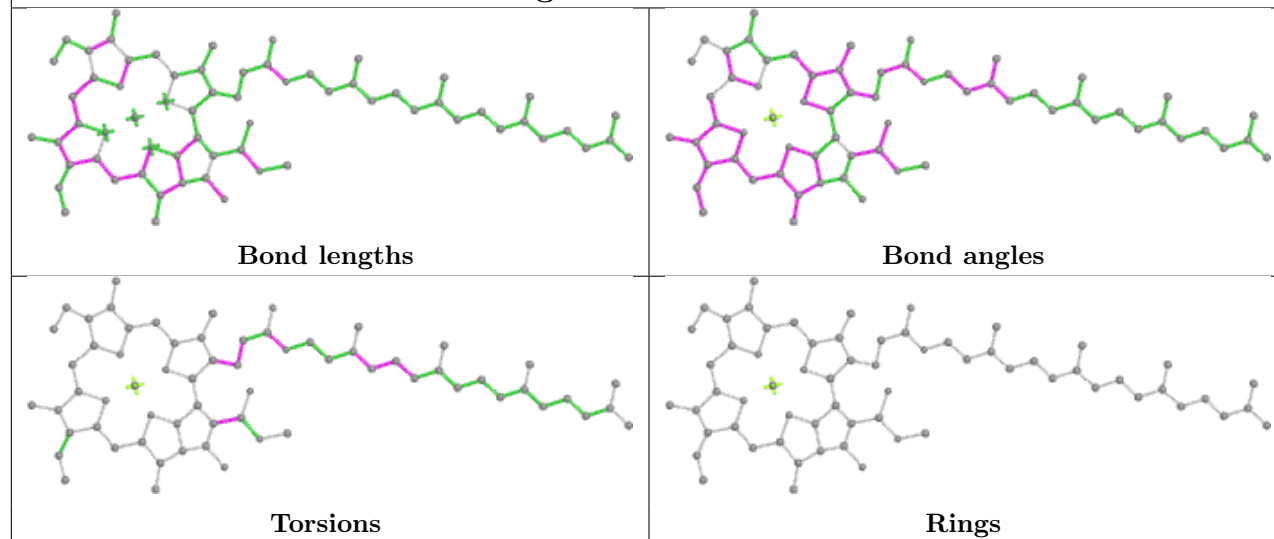
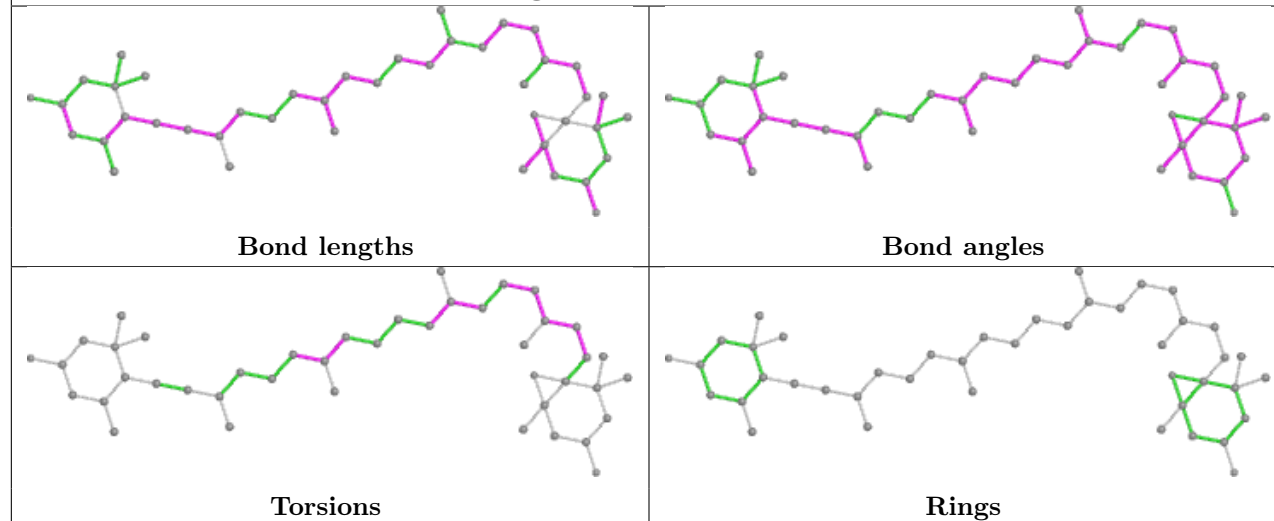


Ligand KC1 8 307

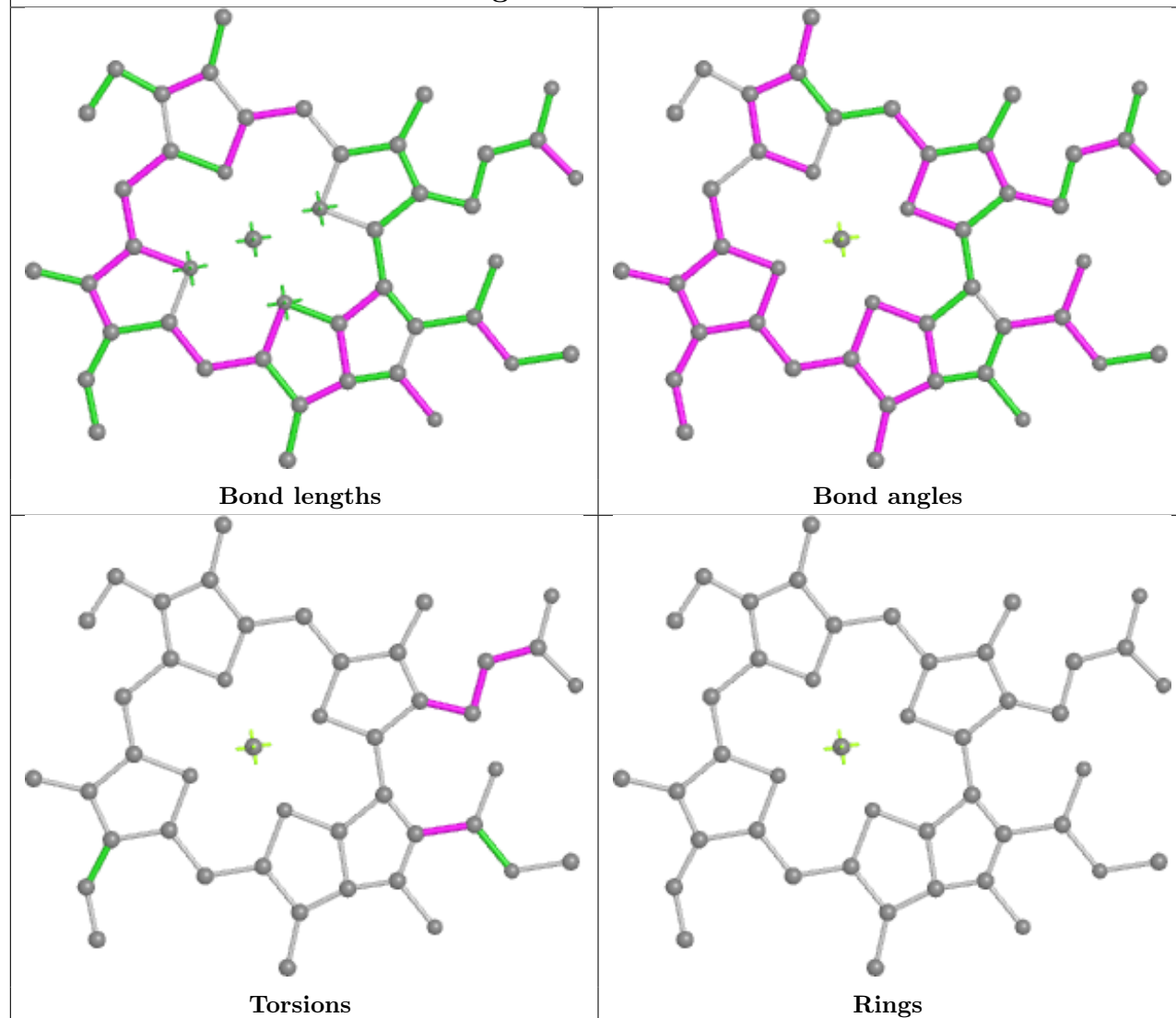




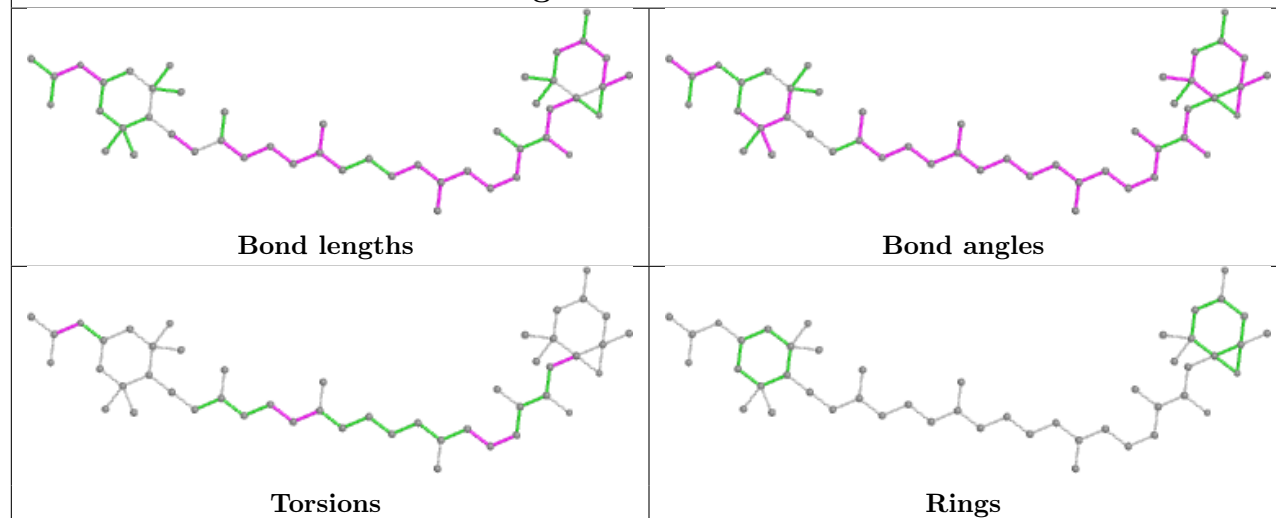


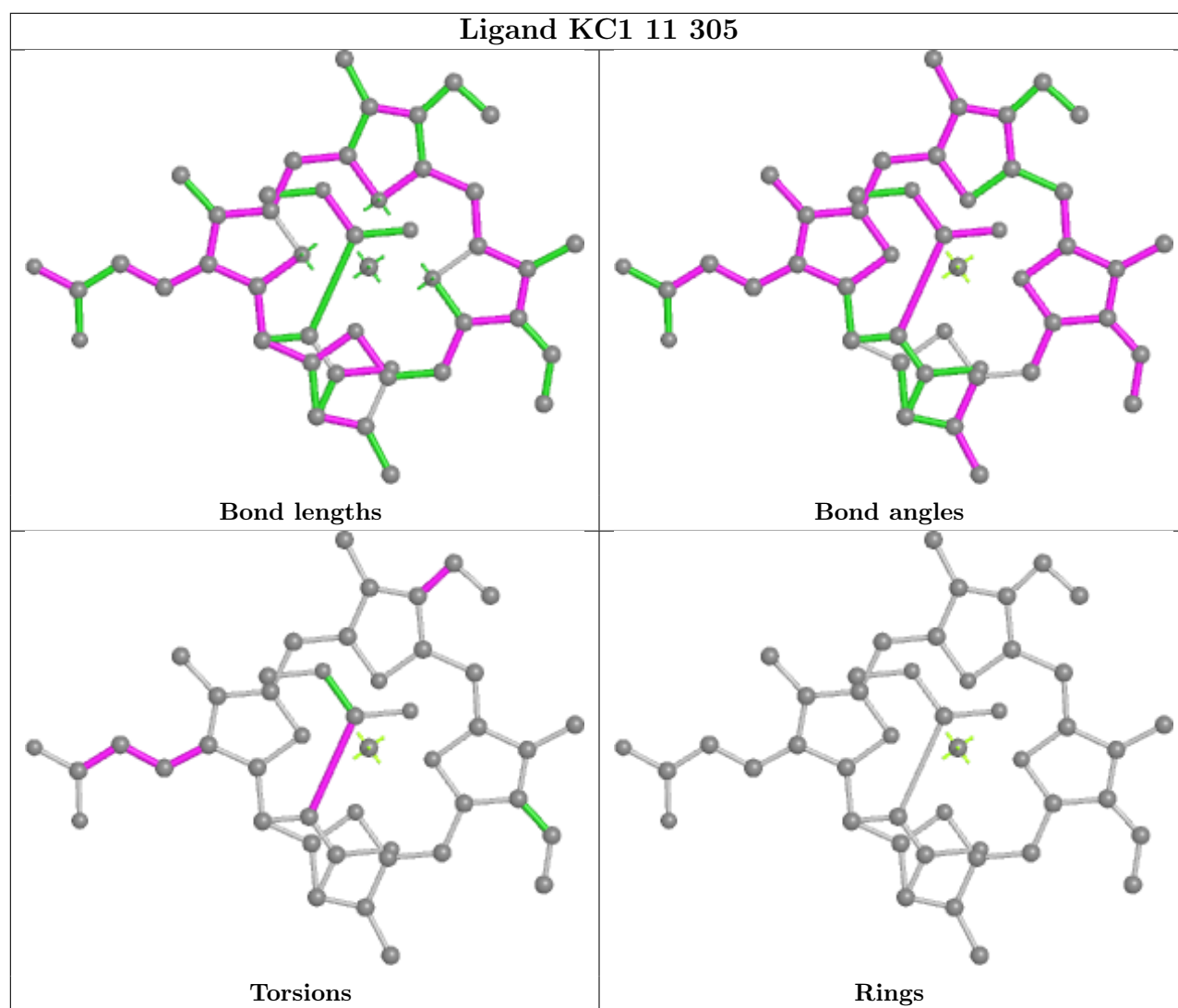
Ligand CLA 4 305**Ligand DD6 12 317**

Ligand CLA F 203

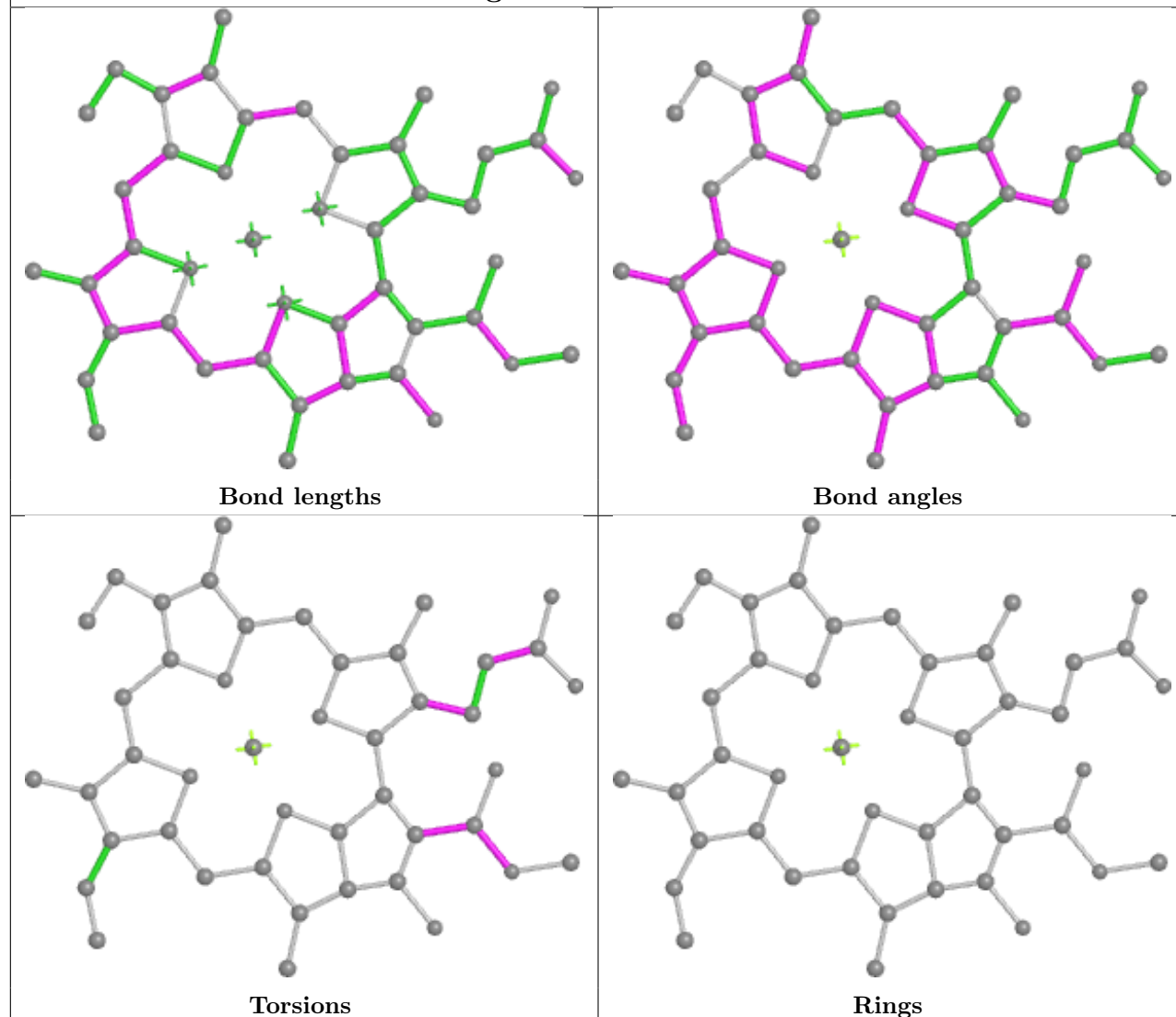


Ligand A86 15 315

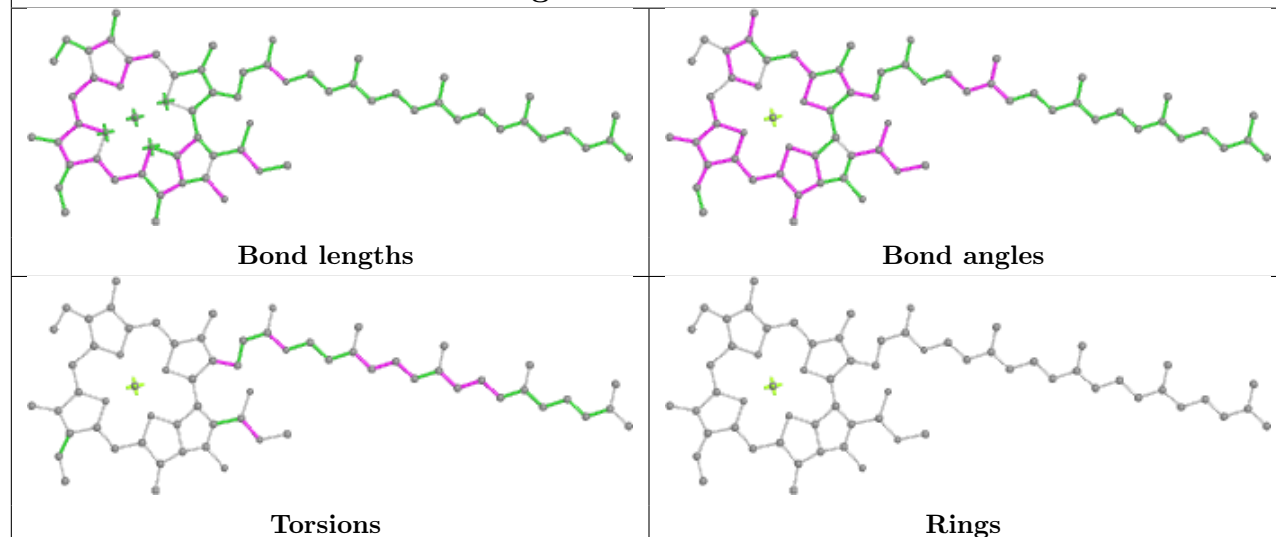


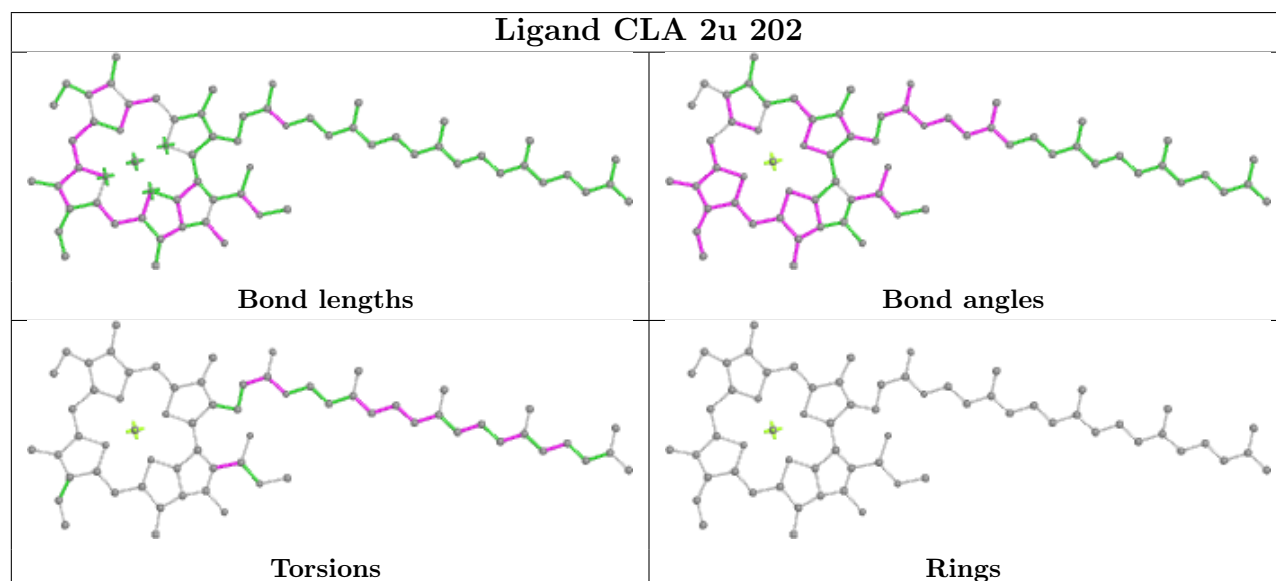
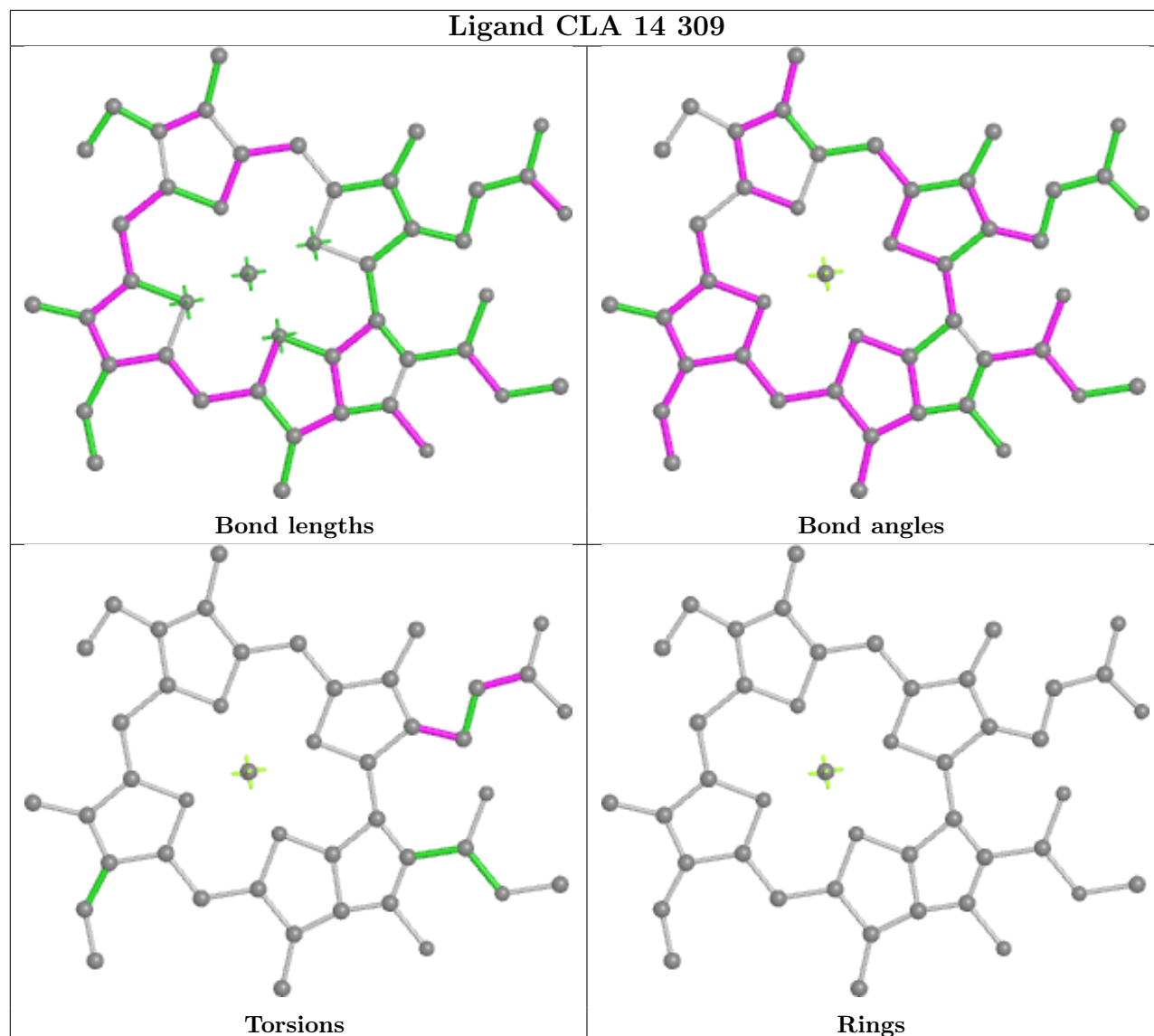


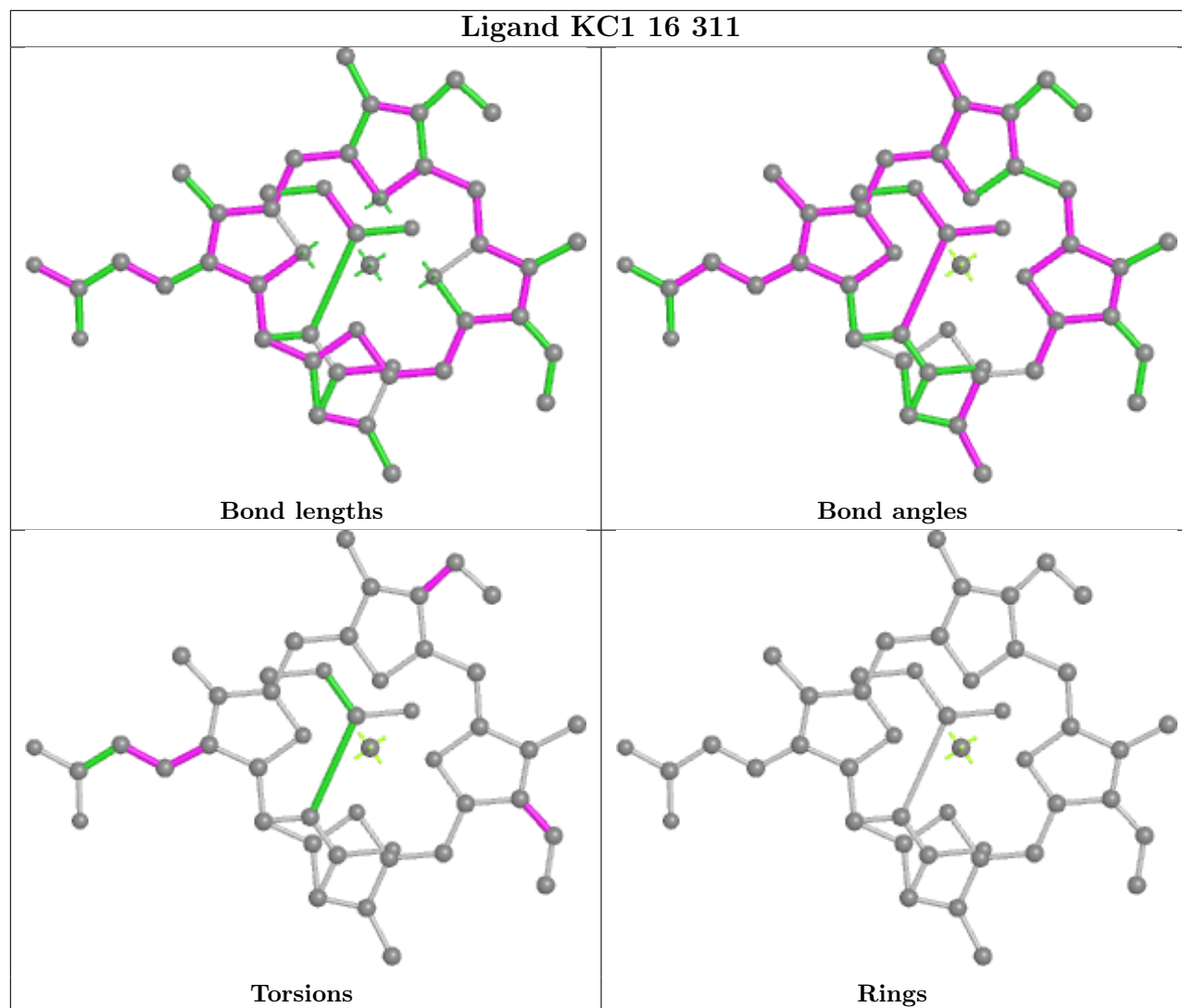
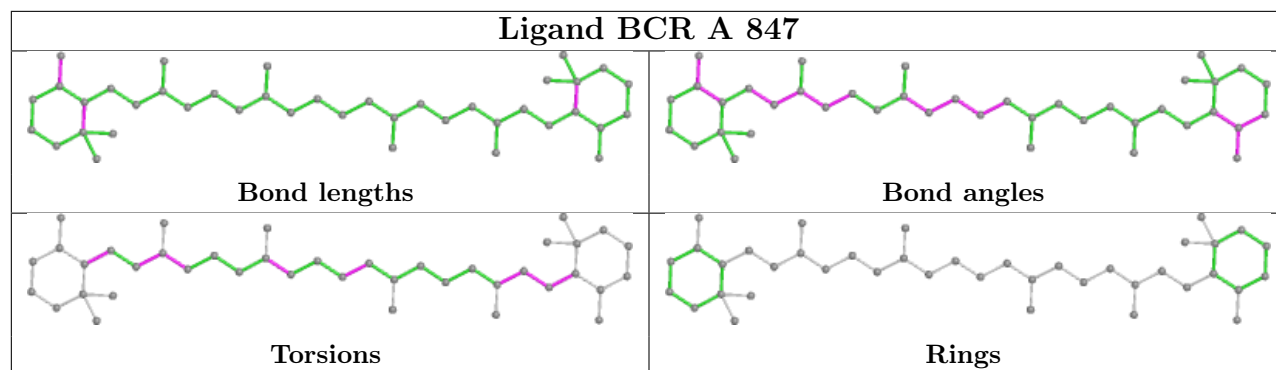
Ligand CLA 15 311



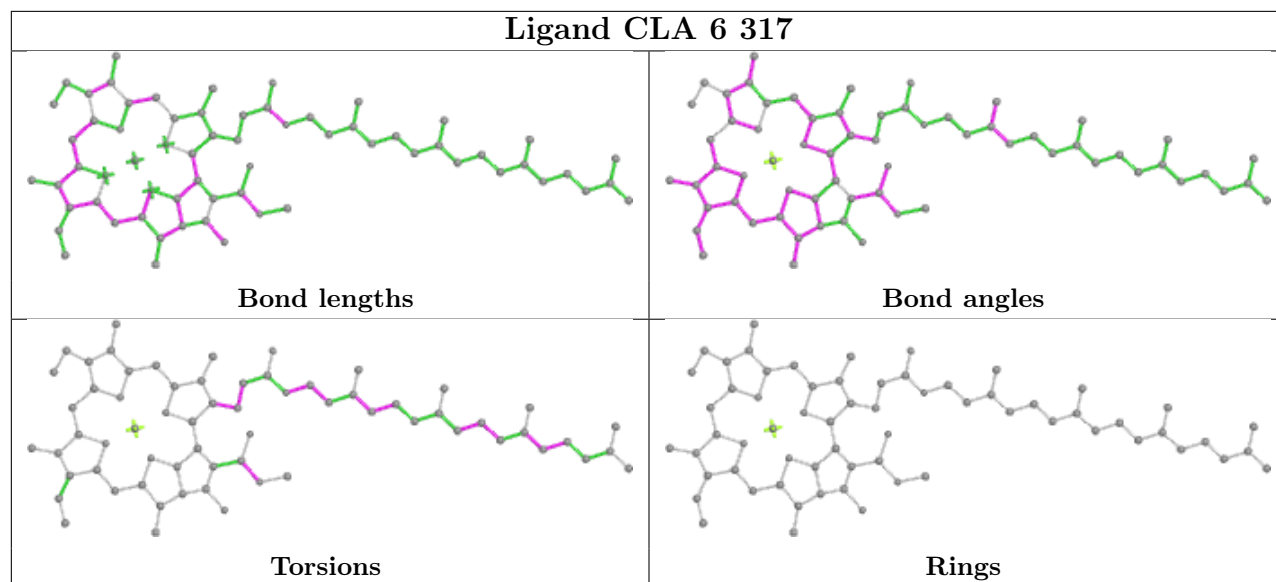
Ligand CLA A 833



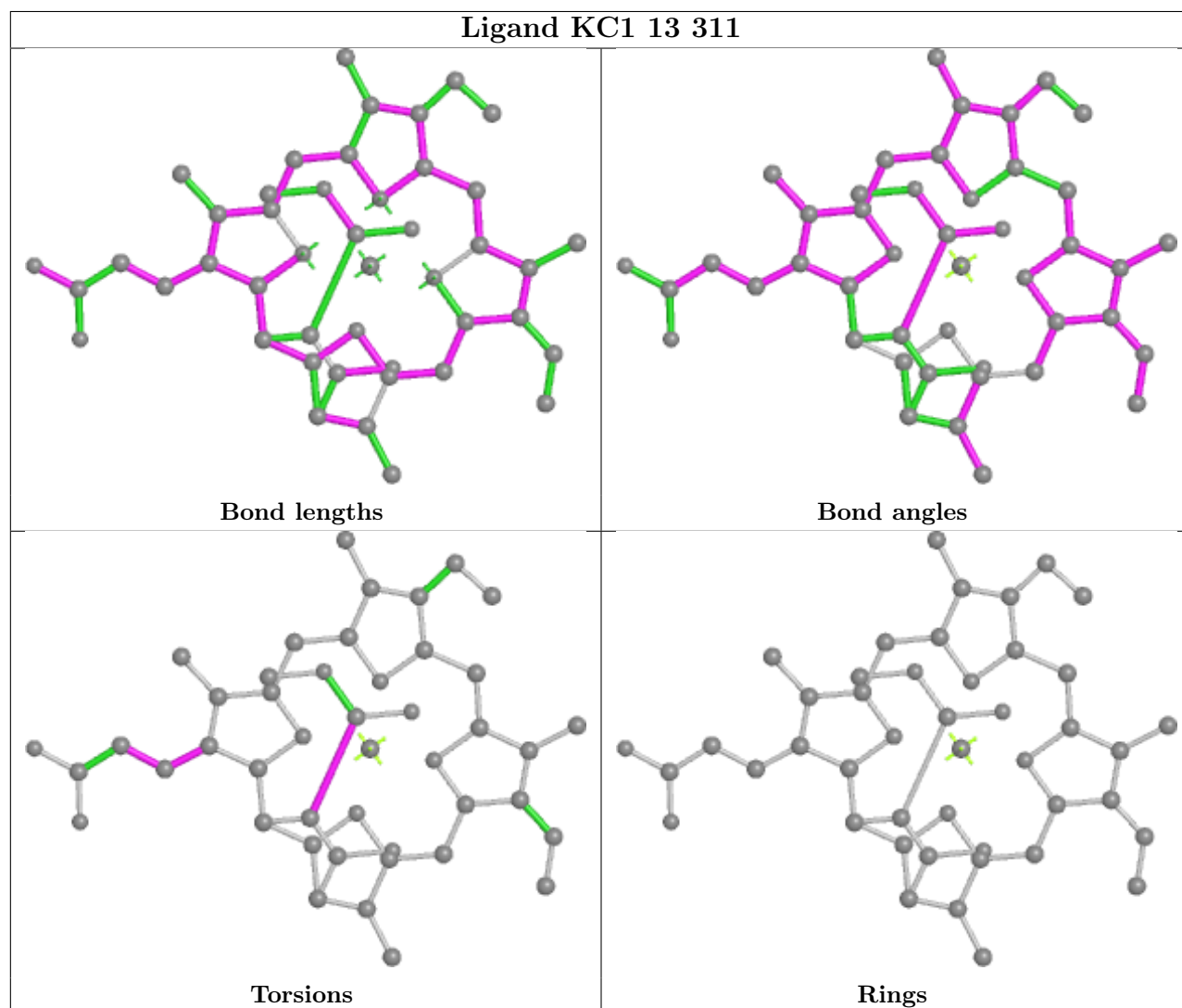




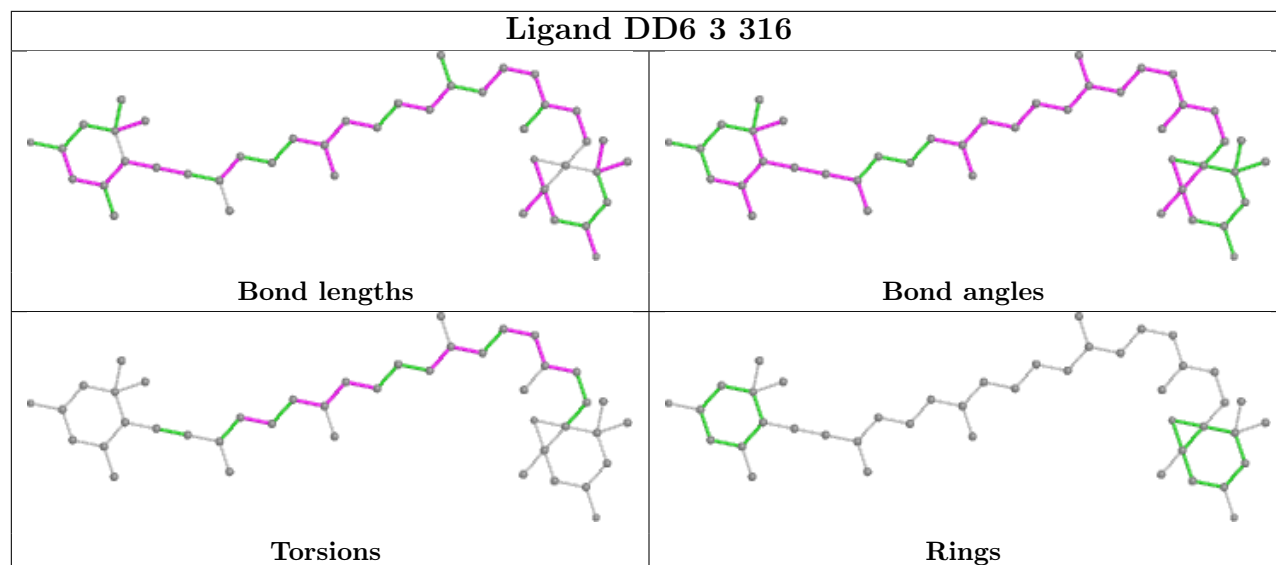
Ligand CLA 6 317



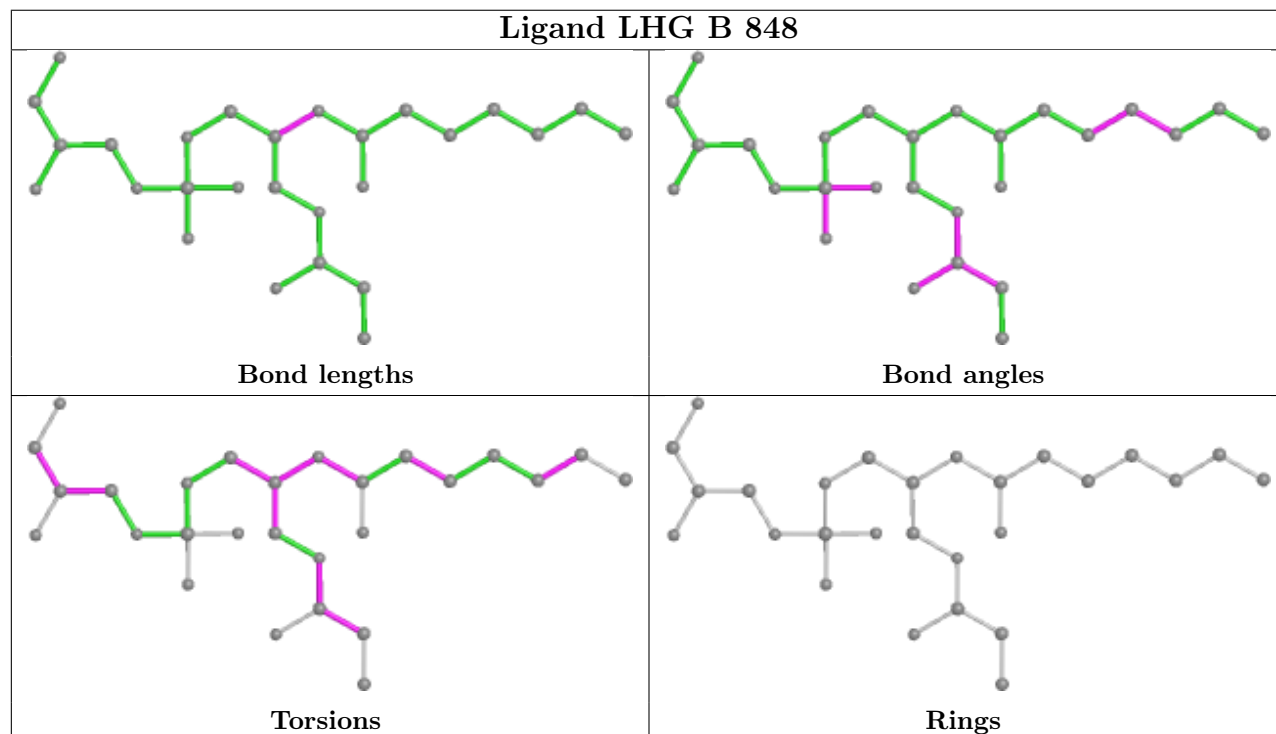
Ligand KC1 13 311



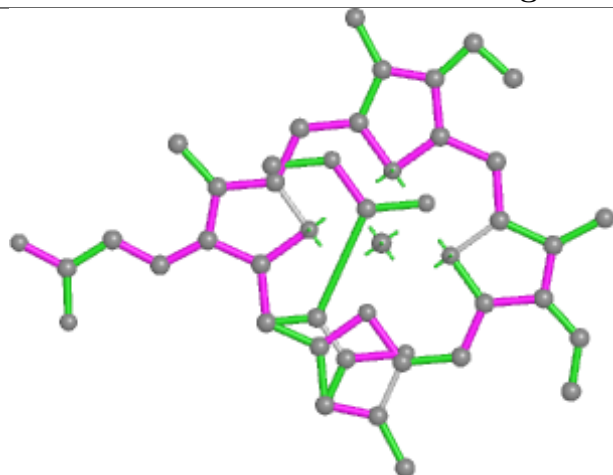
Ligand DD6 3 316



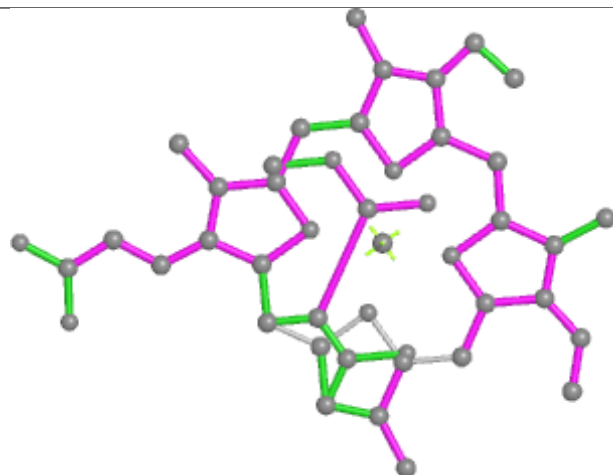
Ligand LHG B 848



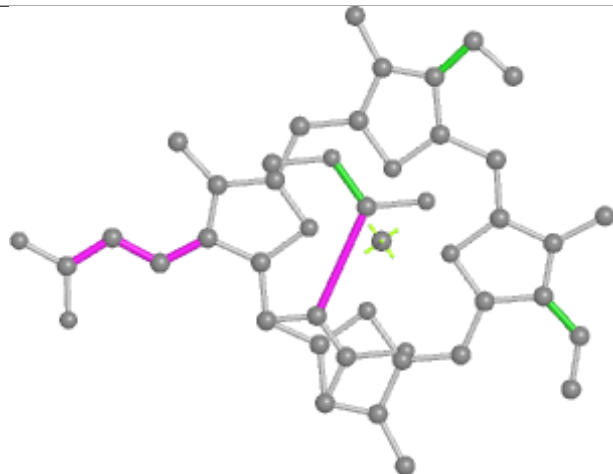
Ligand KC1 5 310



Bond lengths



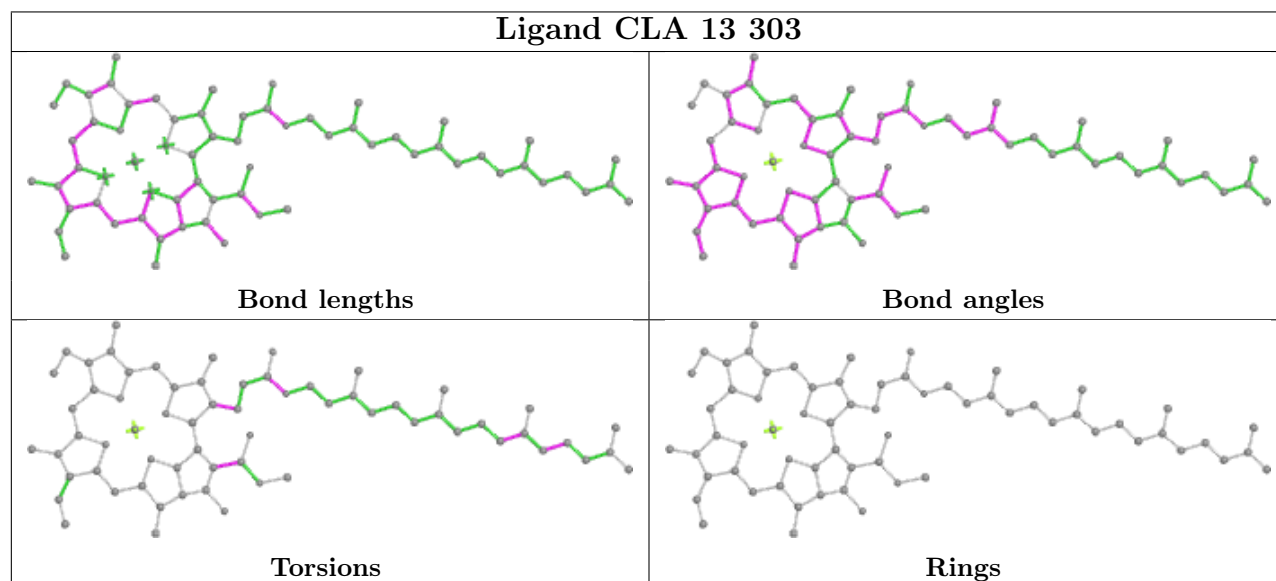
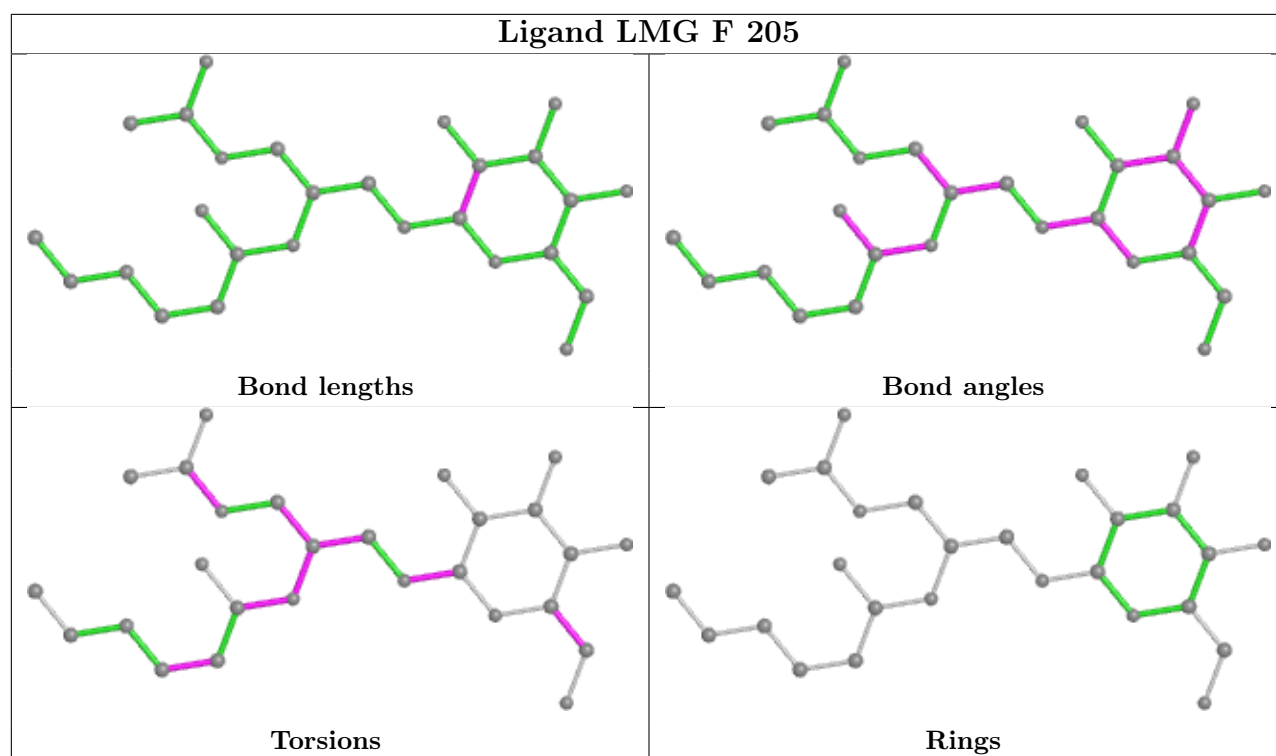
Bond angles

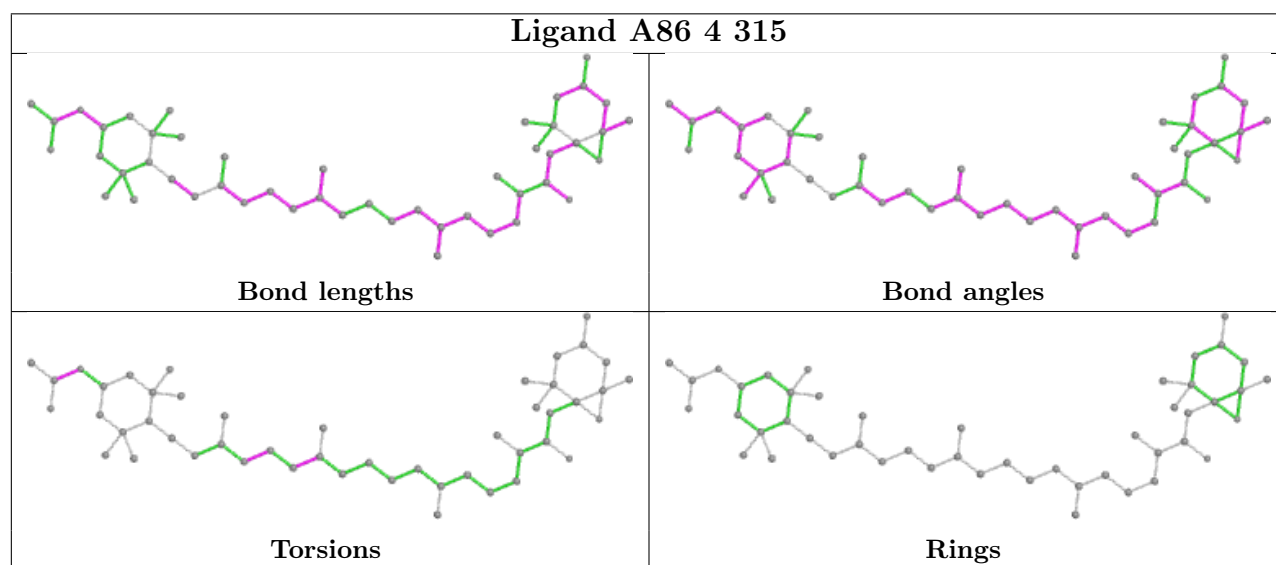
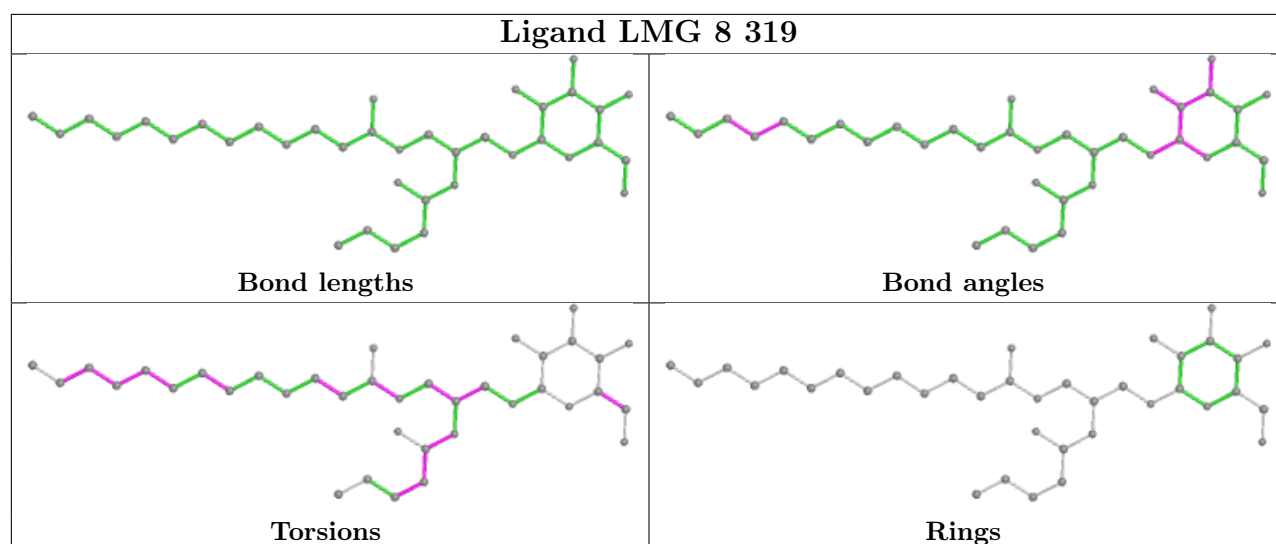


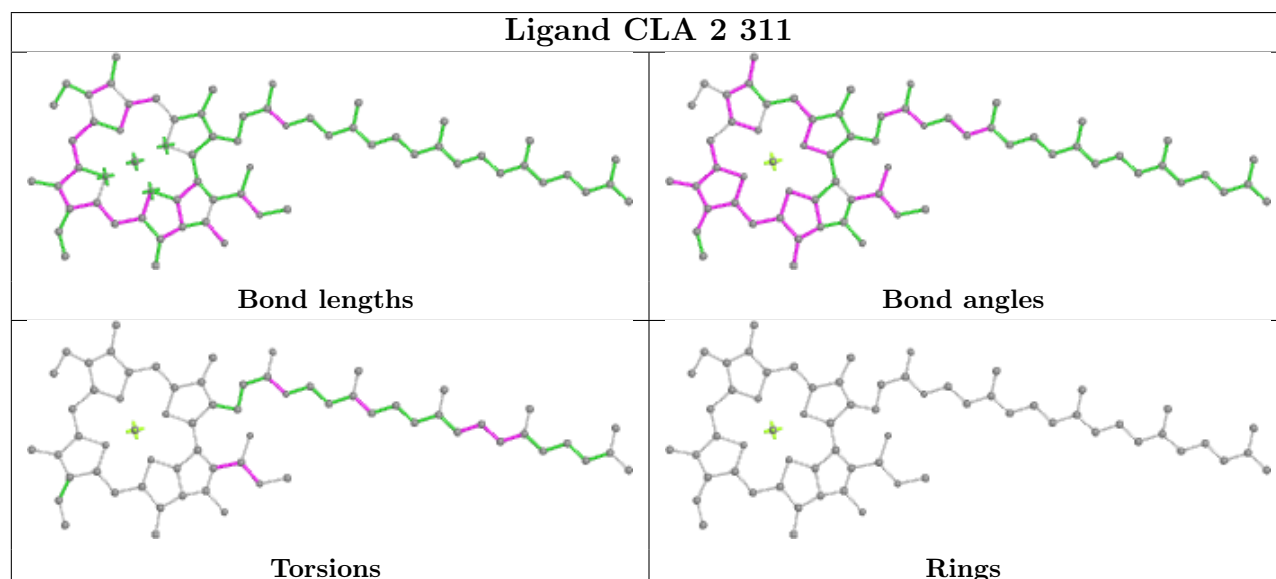
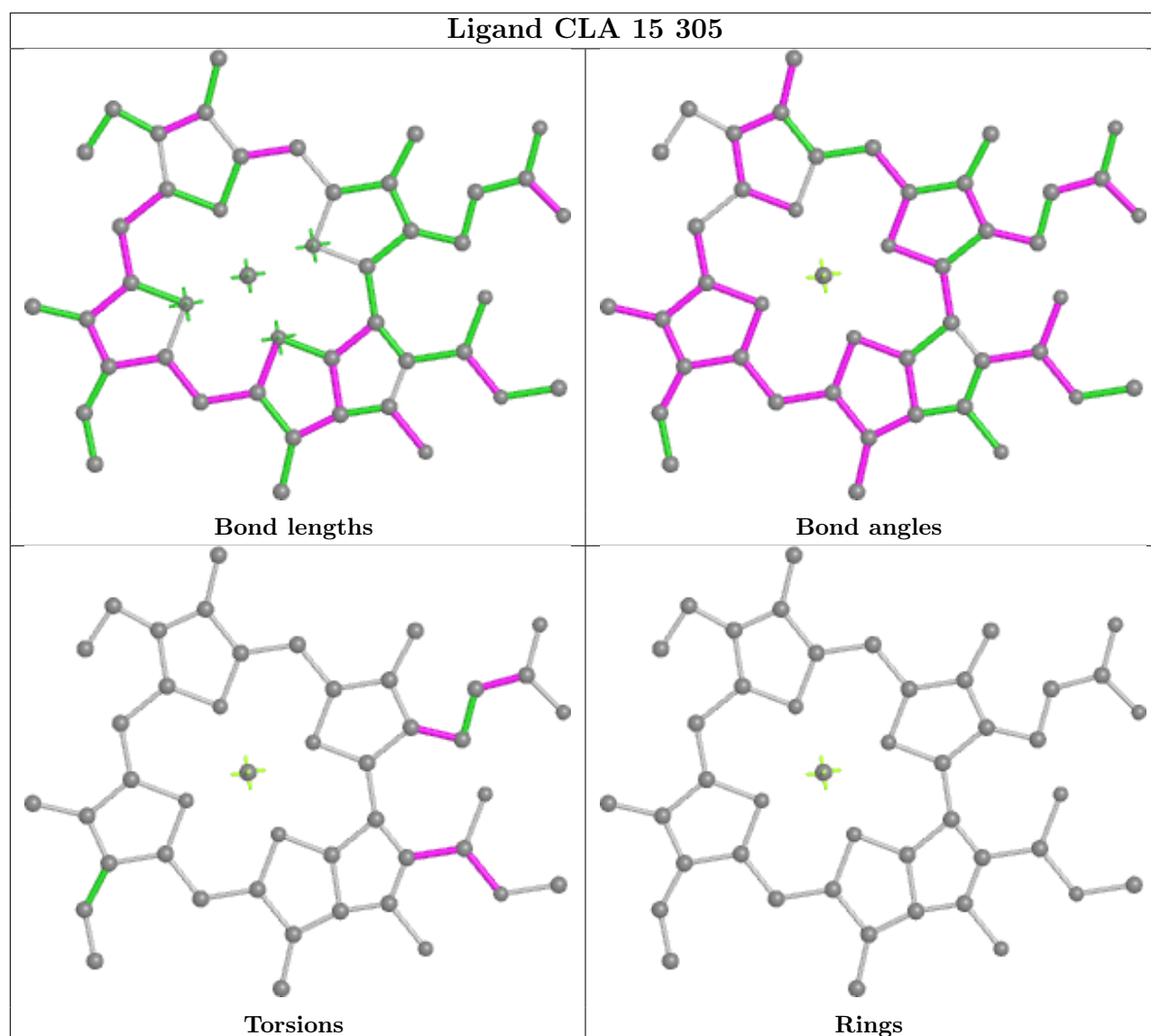
Torsions



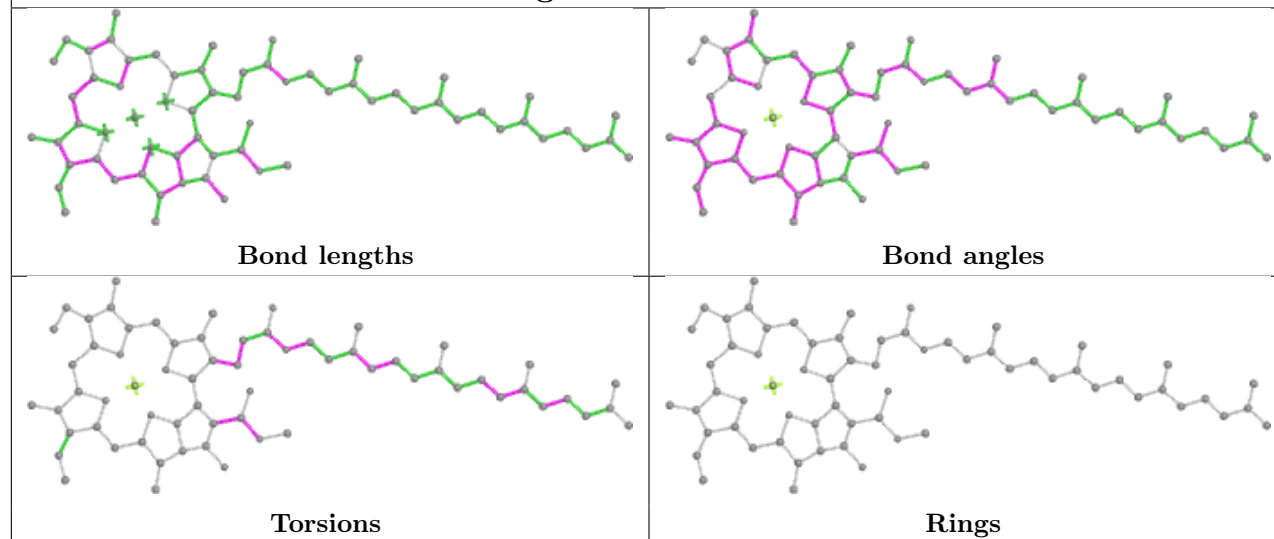
Rings



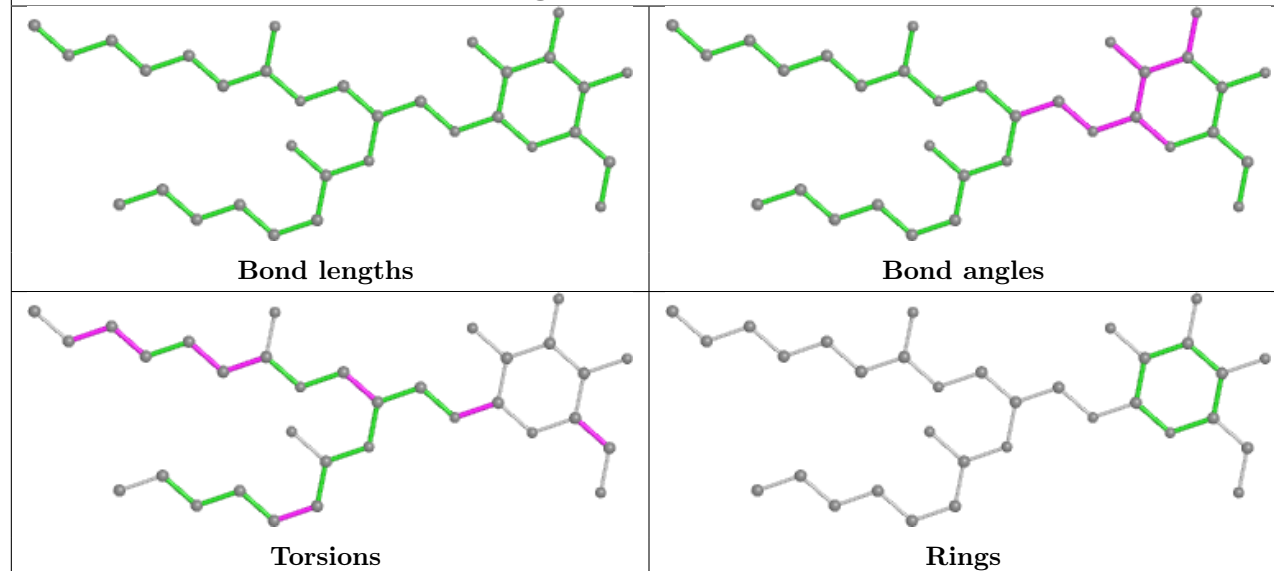




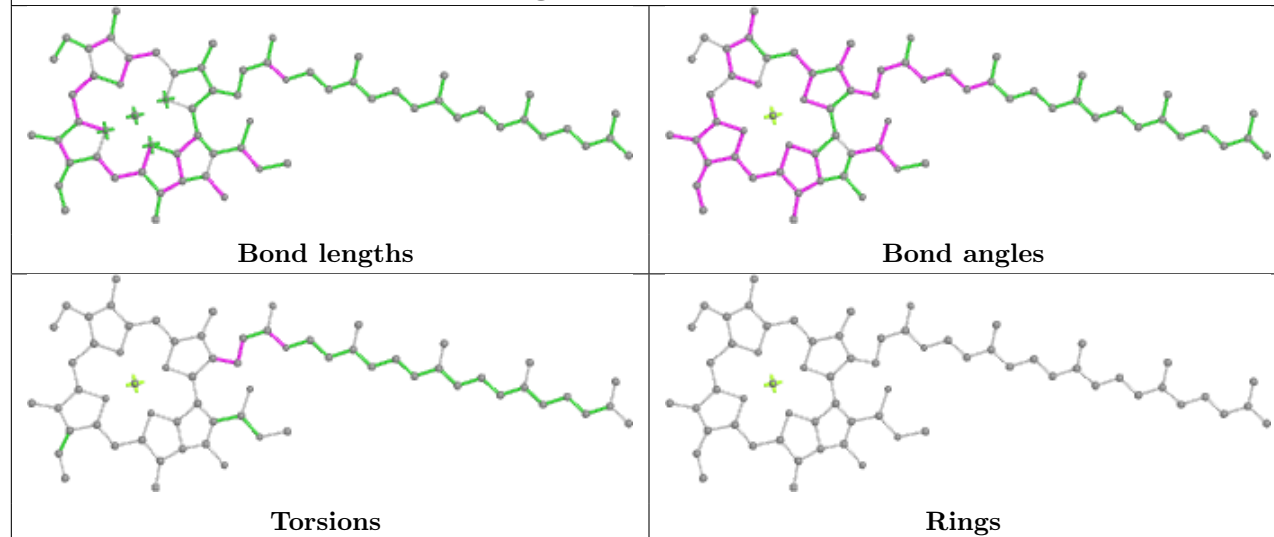
Ligand CLA 6 314



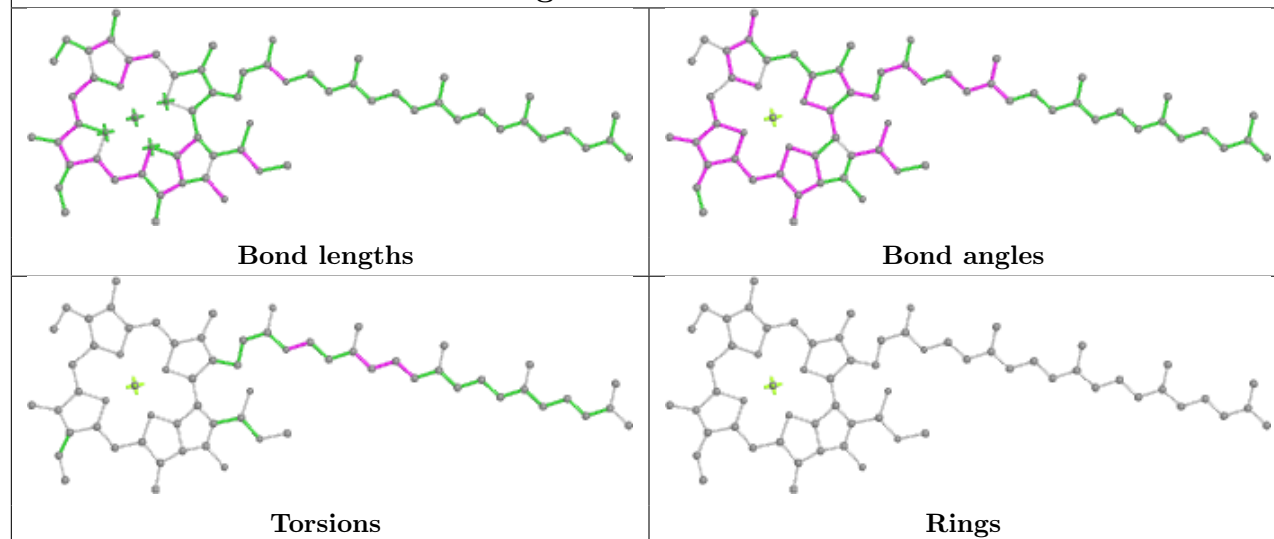
Ligand LMG 5 318



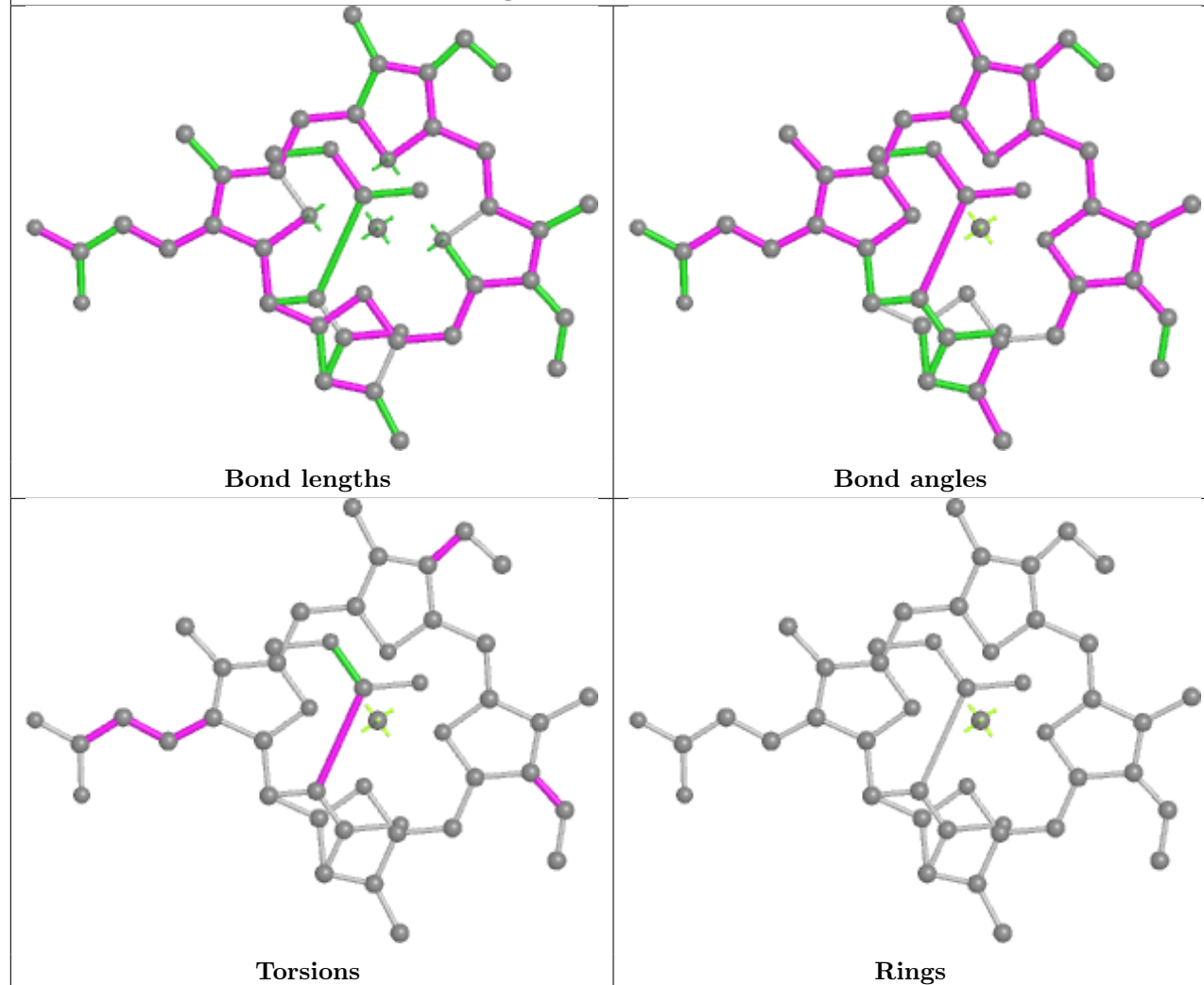
Ligand CLA B 827



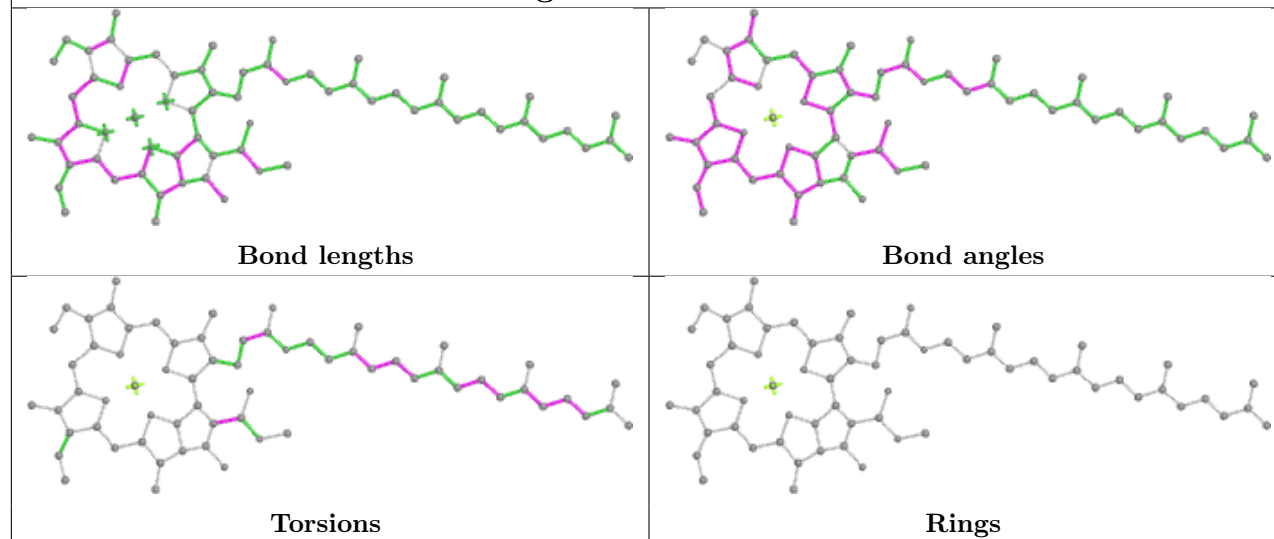
Ligand CLA 4 303



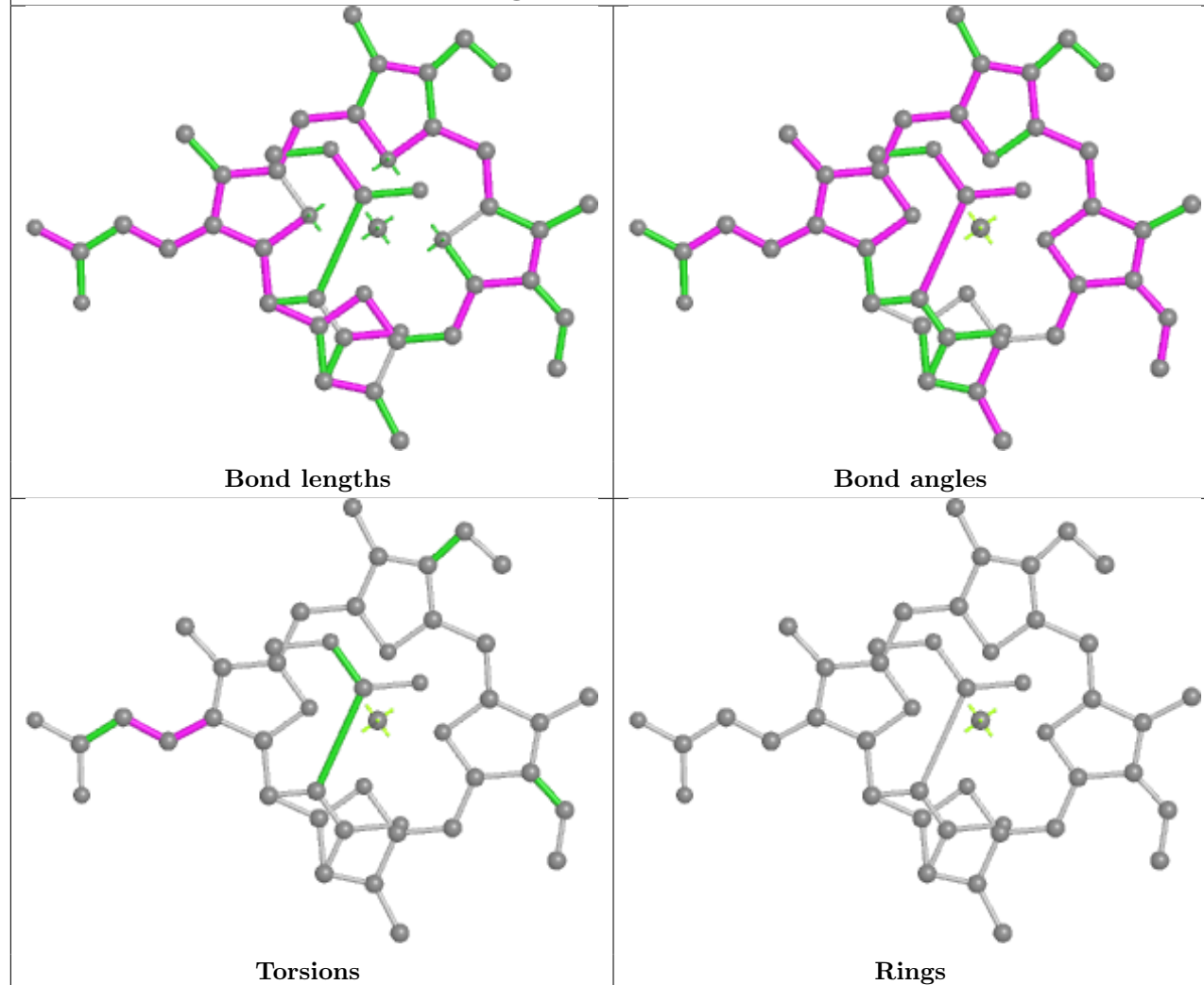
Ligand KC1 14 306



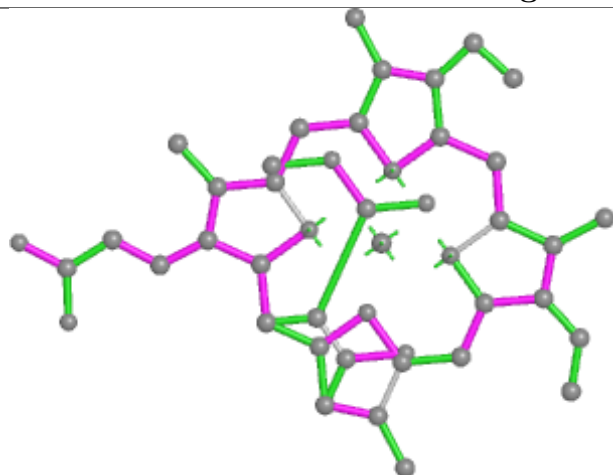
Ligand CLA 2 304



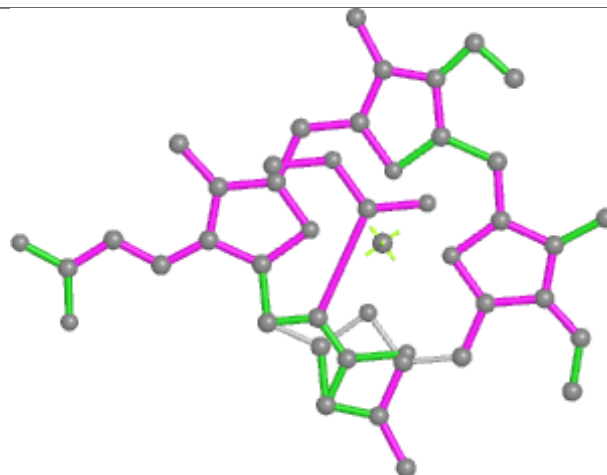
Ligand KC1 4 308



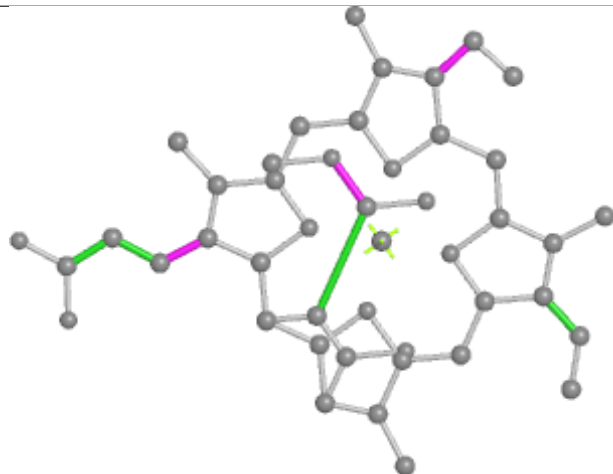
Ligand KC1 8 311



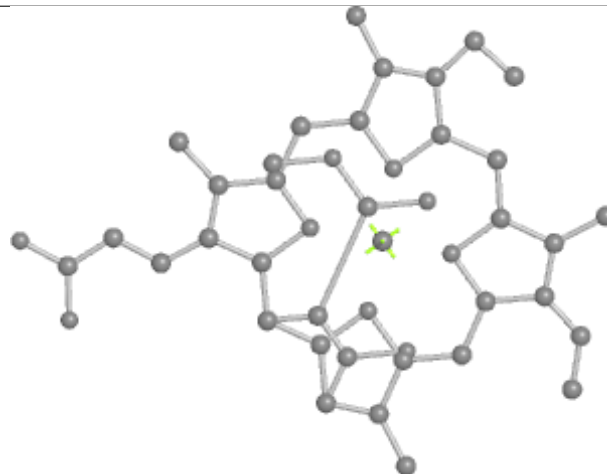
Bond lengths



Bond angles

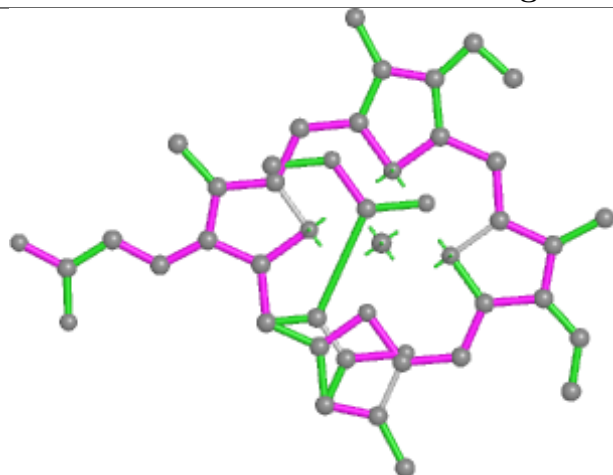


Torsions

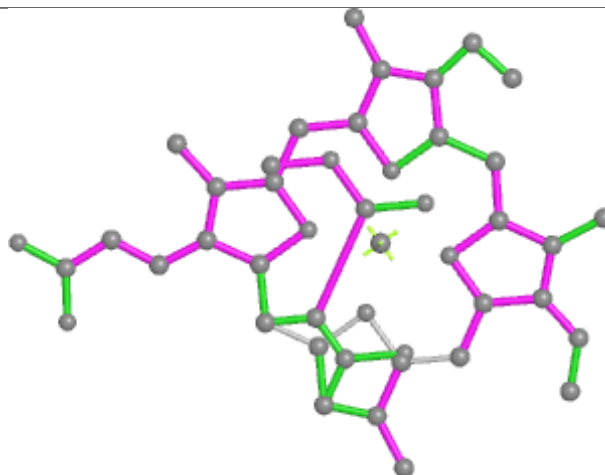


Rings

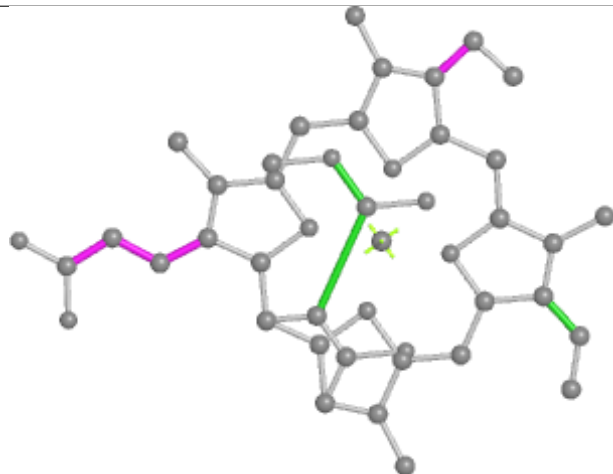
Ligand KC1 9 312



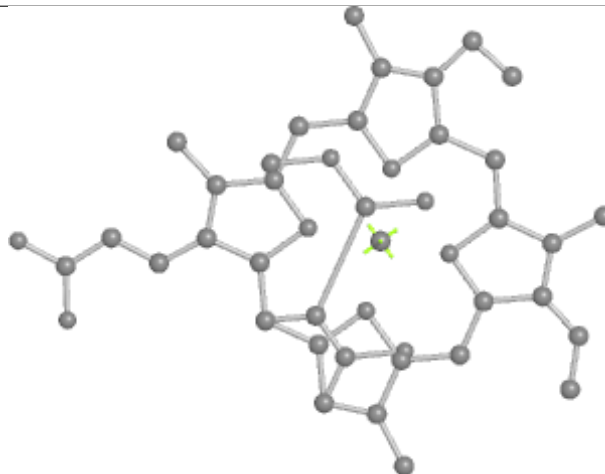
Bond lengths



Bond angles

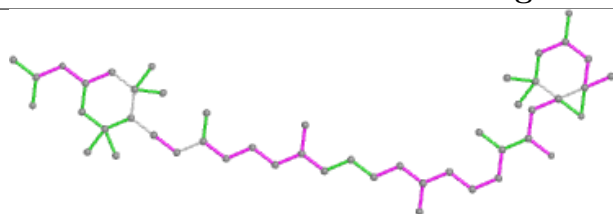


Torsions

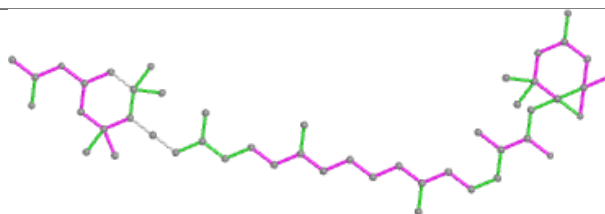


Rings

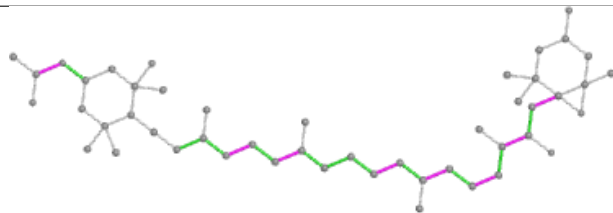
Ligand A86 15 316



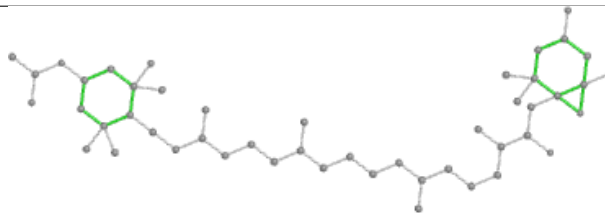
Bond lengths



Bond angles

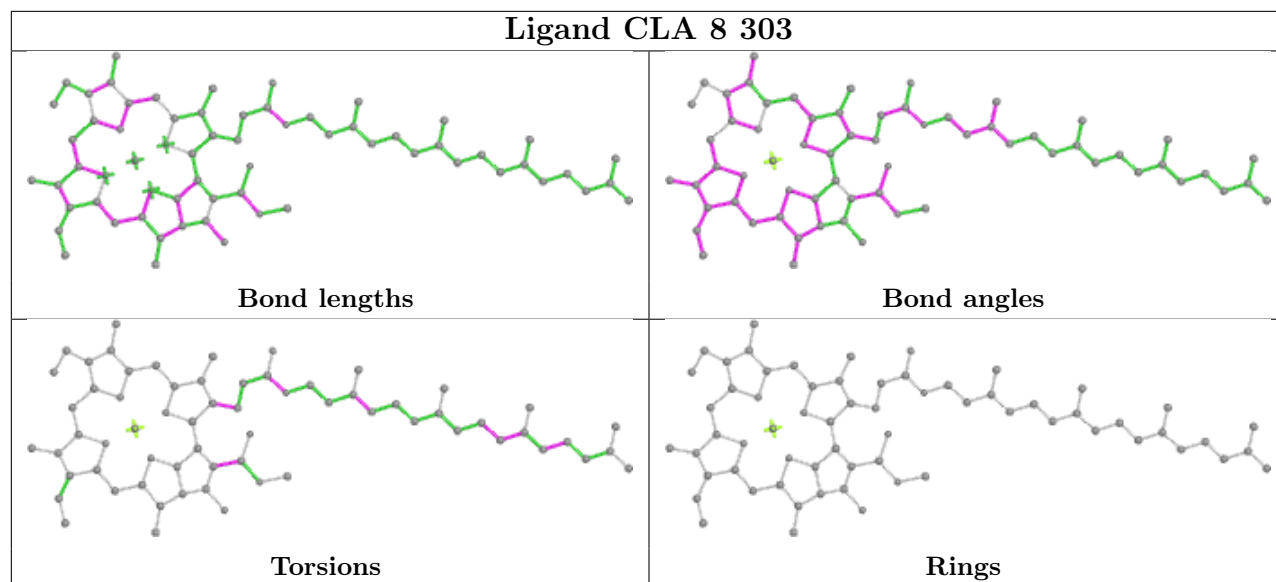


Torsions

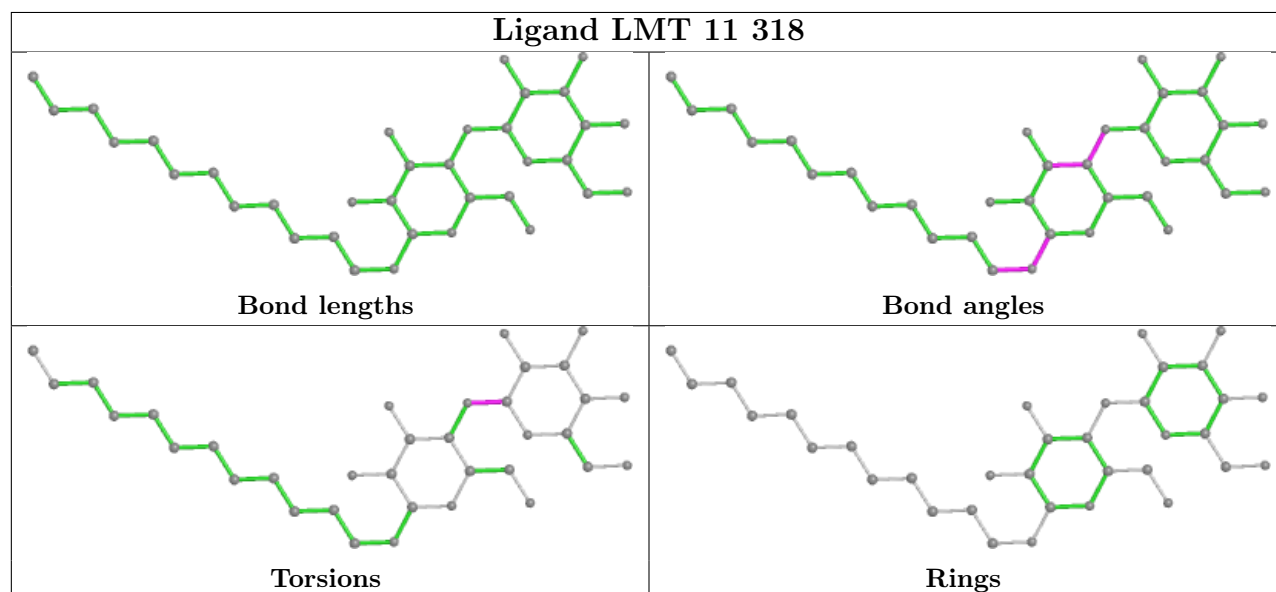


Rings

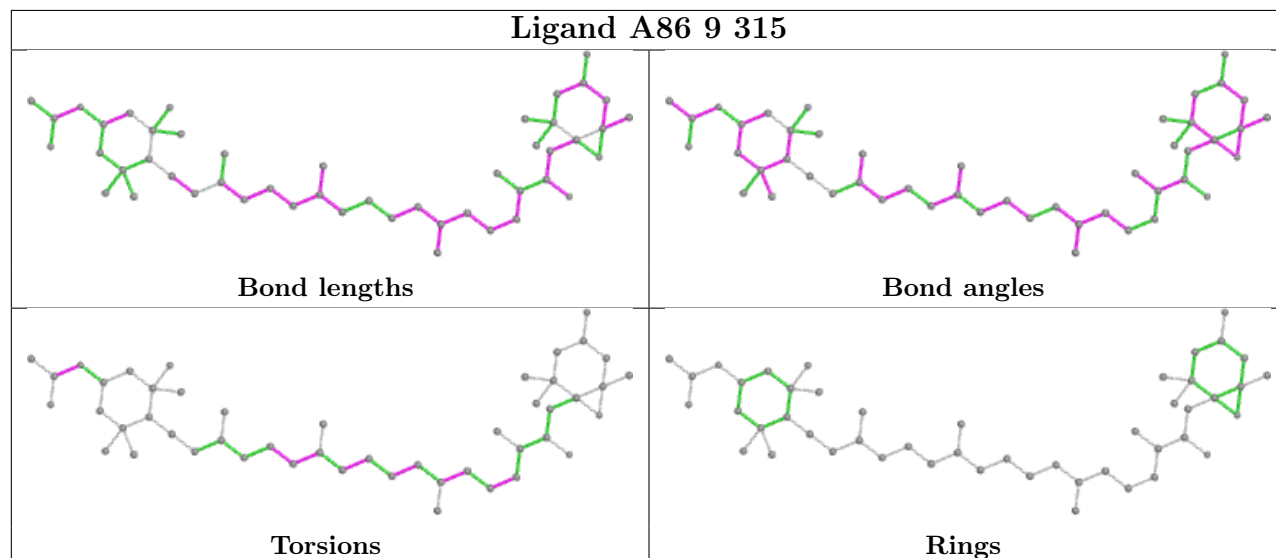
Ligand CLA 8 303



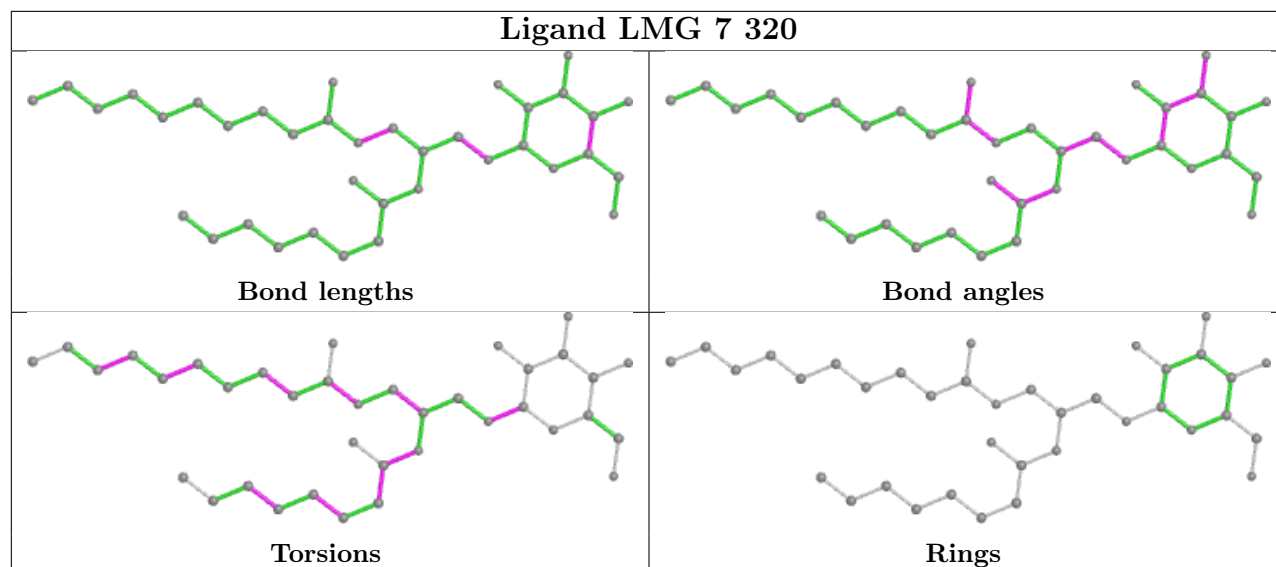
Ligand LMT 11 318



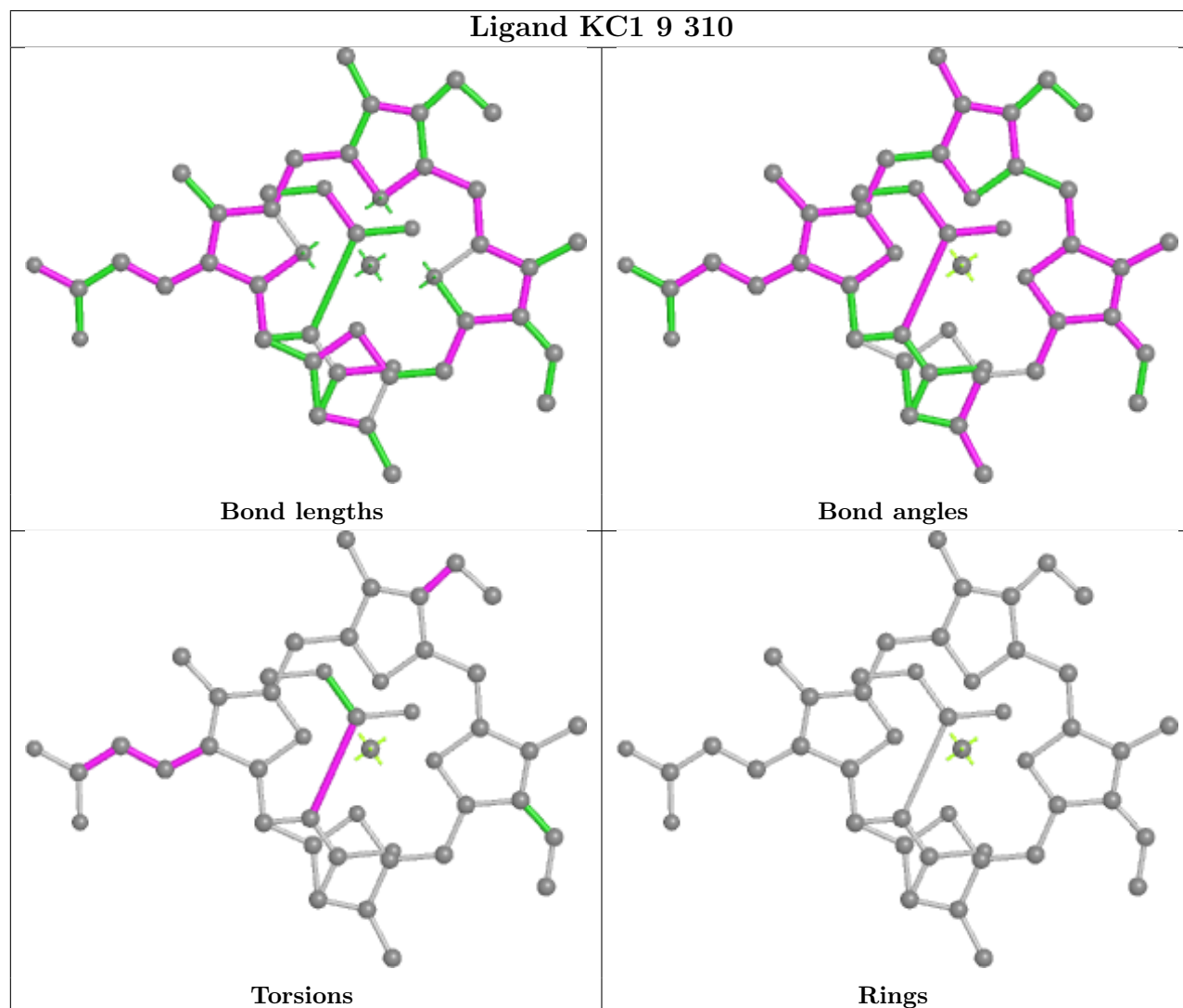
Ligand A86 9 315



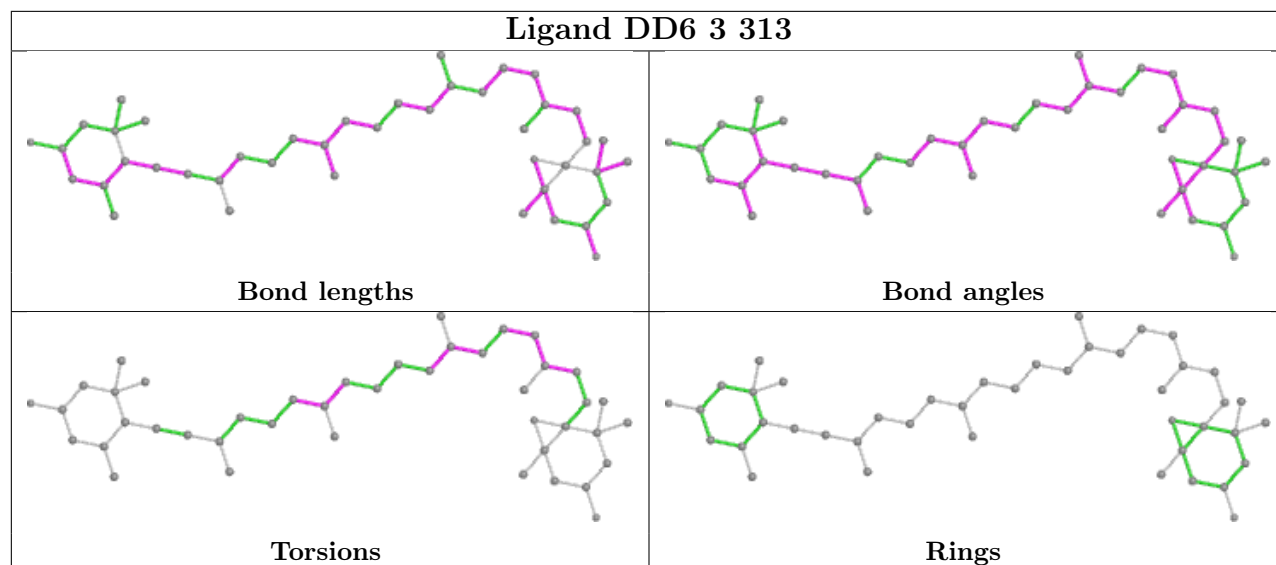
Ligand LMG 7 320



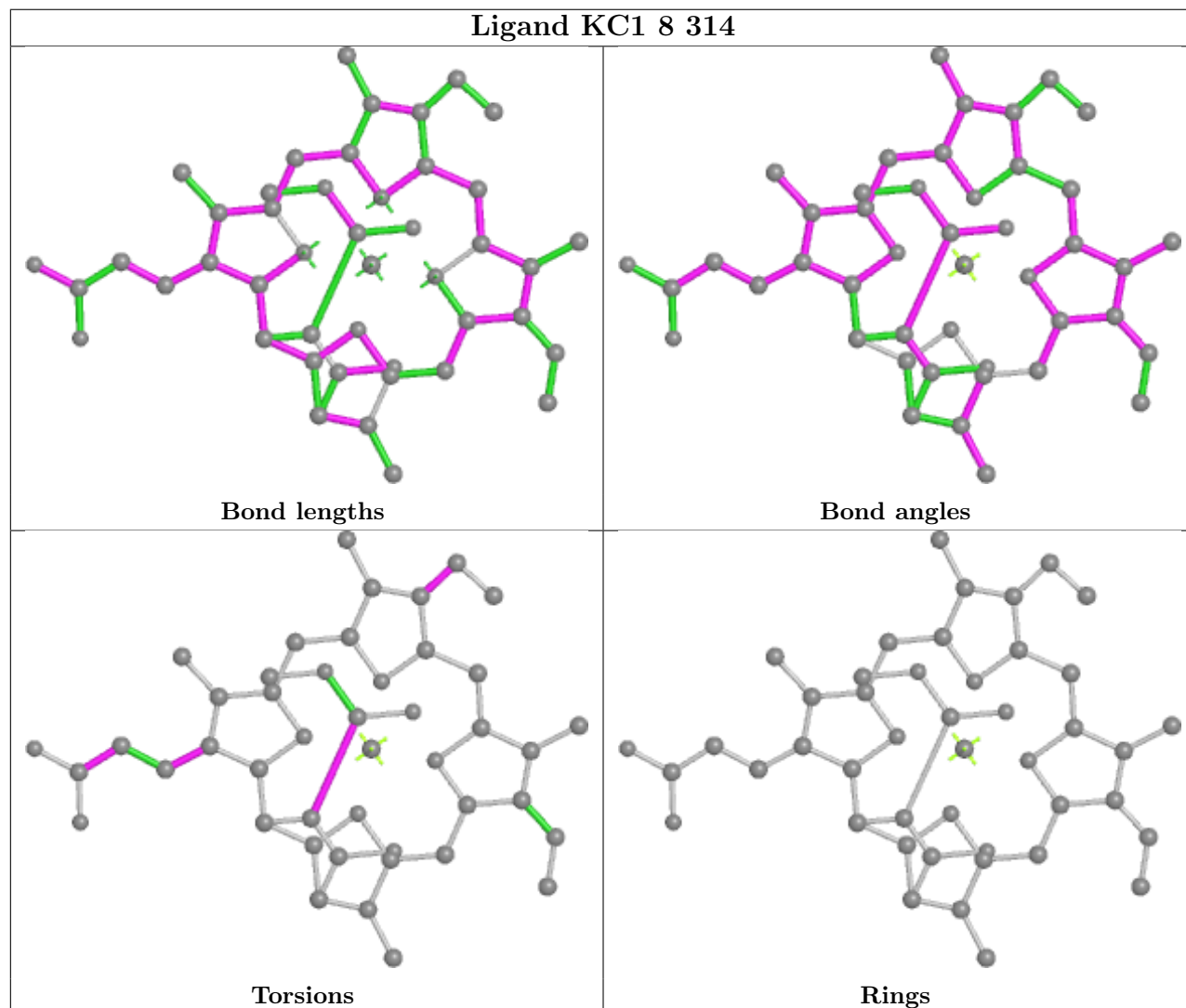
Ligand KC1 9 310

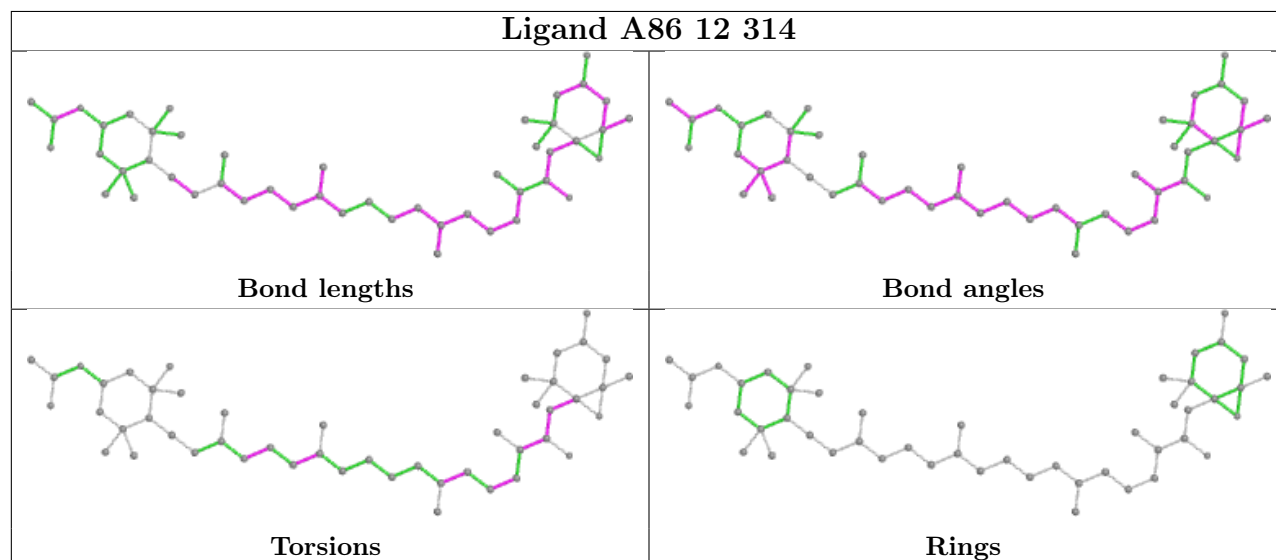
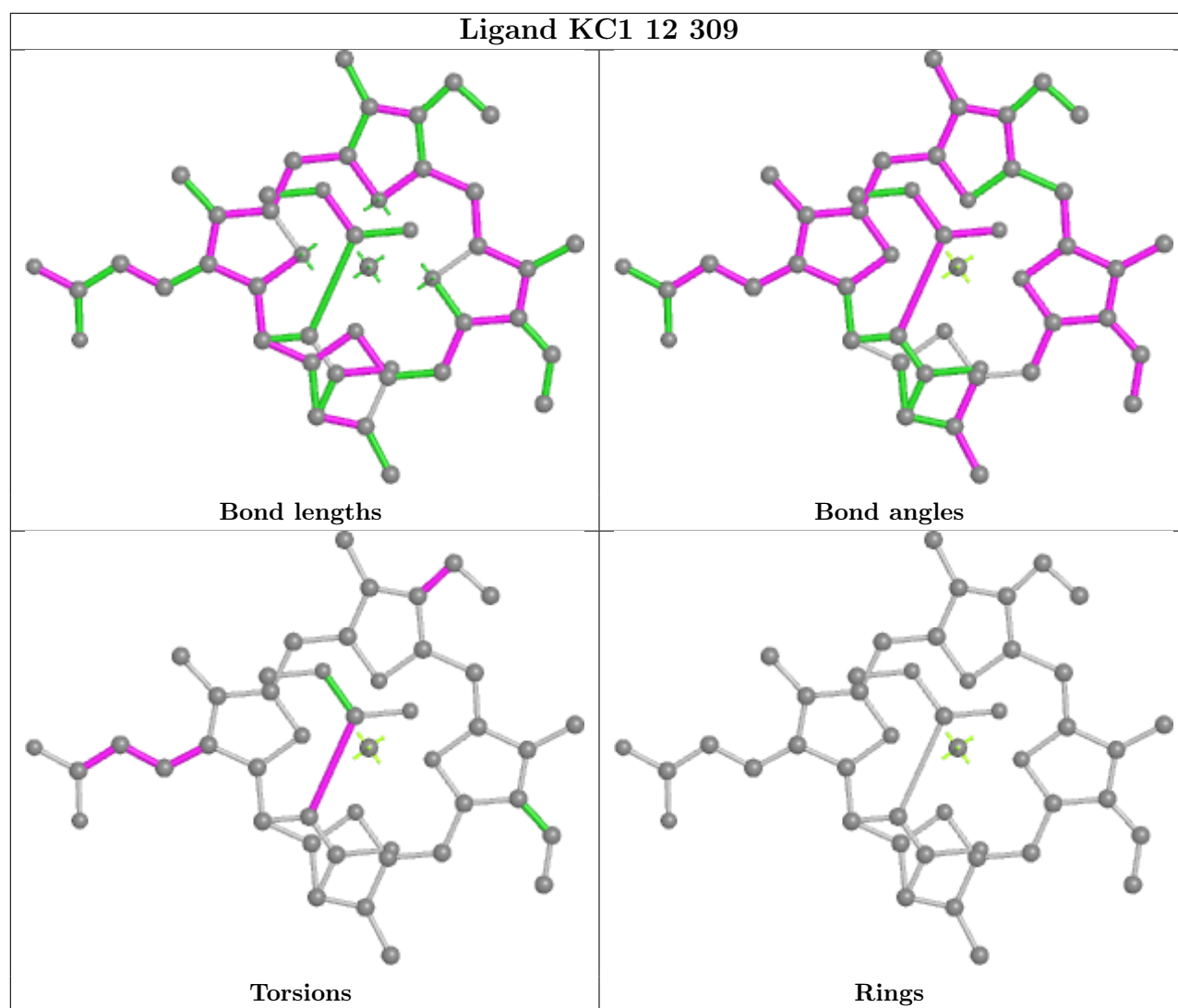


Ligand DD6 3 313

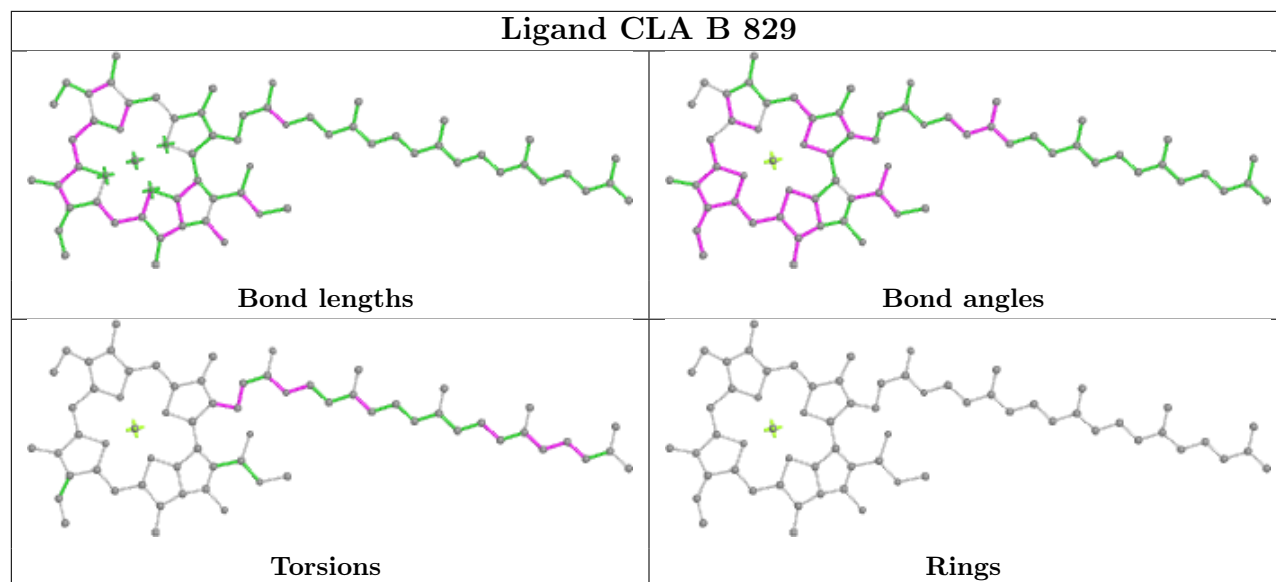


Ligand KC1 8 314

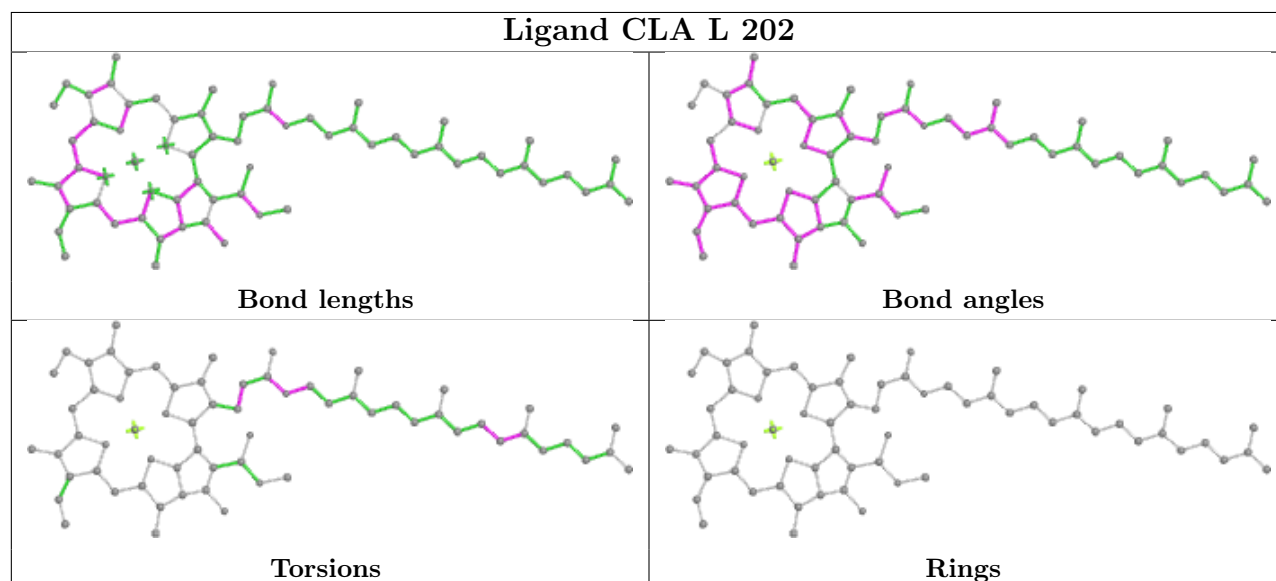




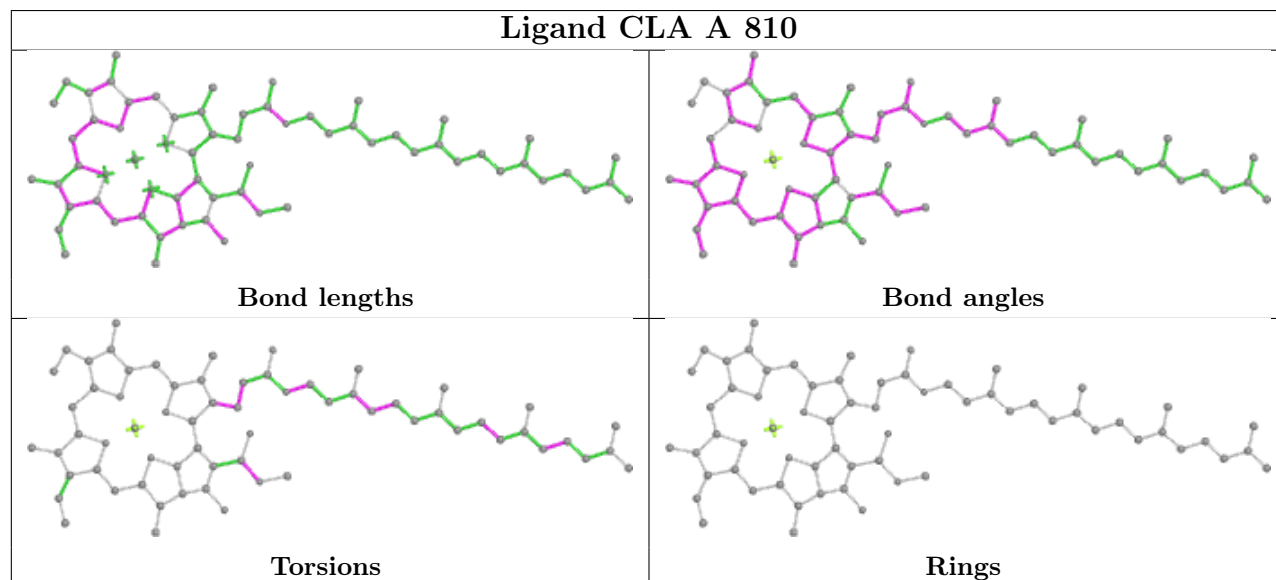
Ligand CLA B 829



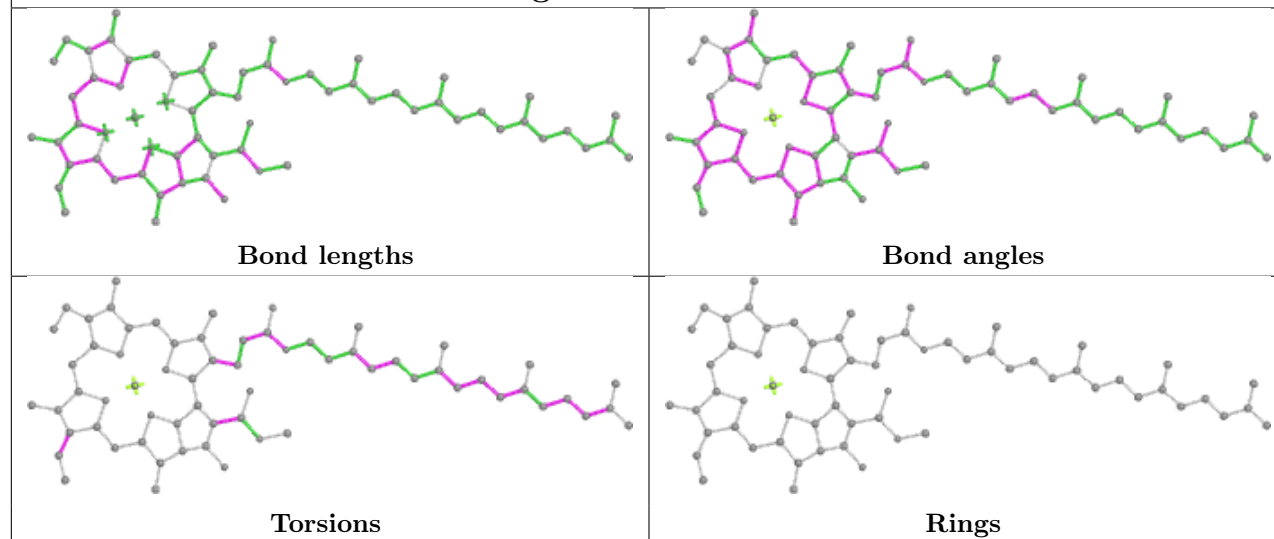
Ligand CLA L 202



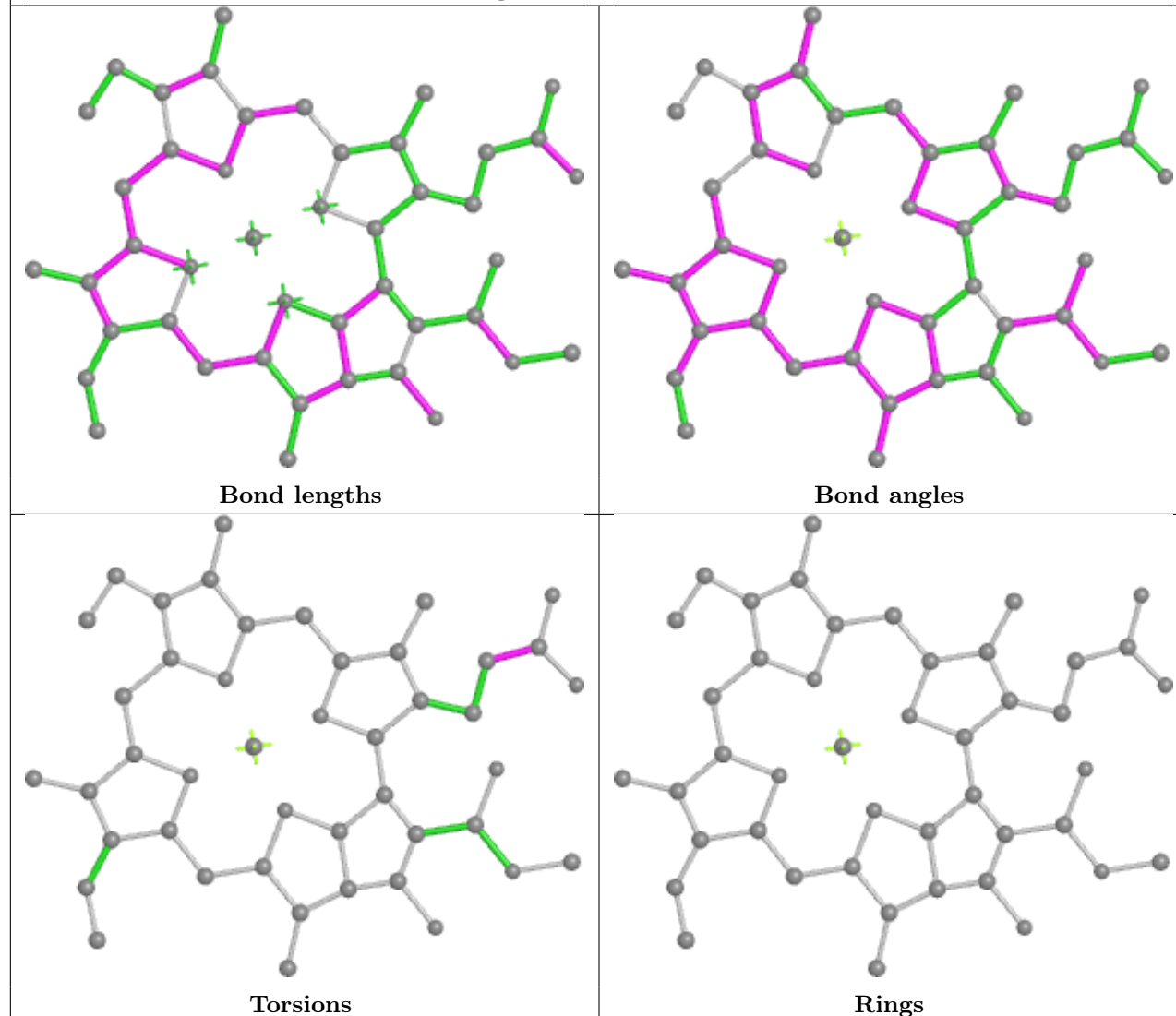
Ligand CLA A 810

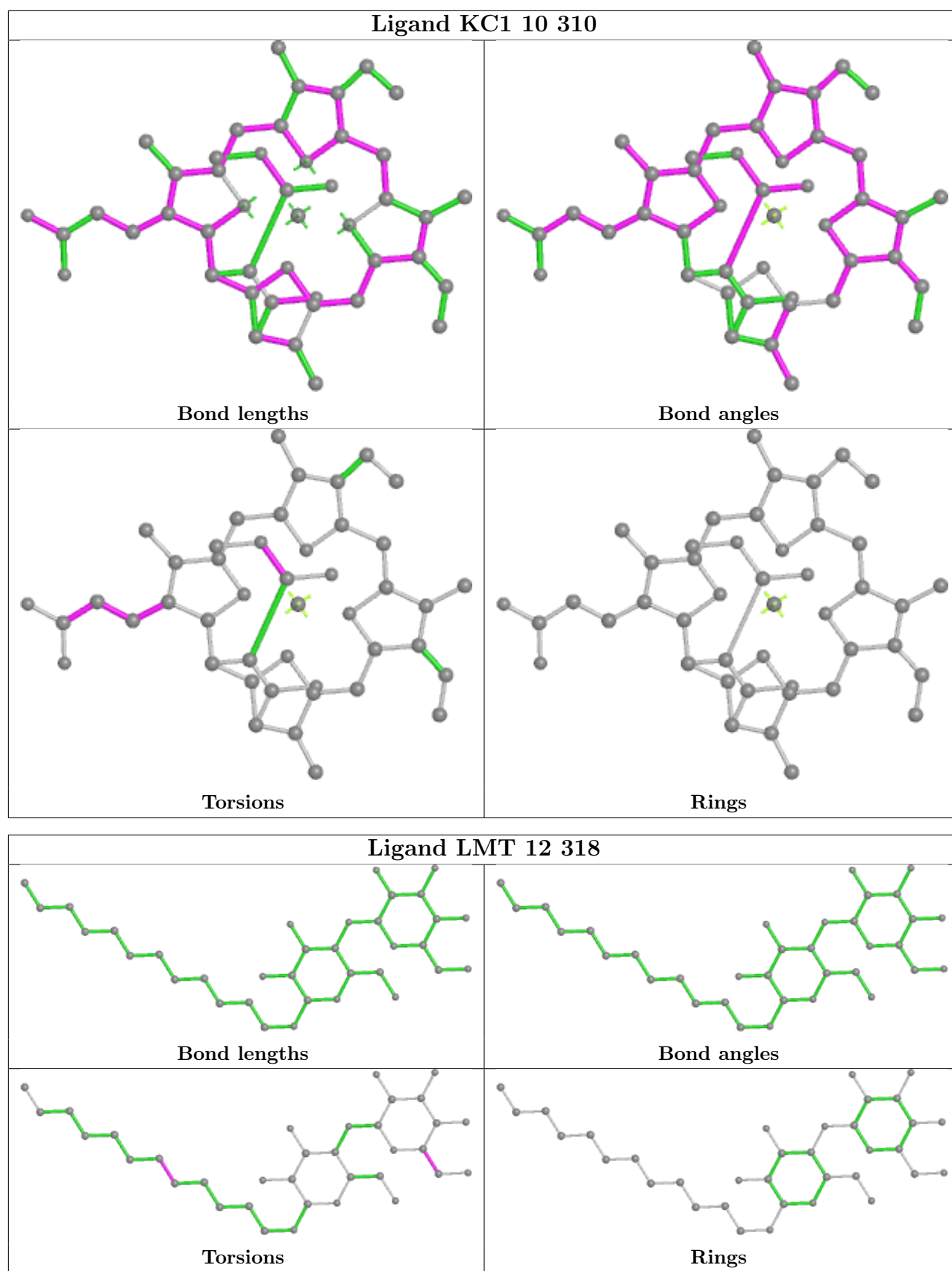


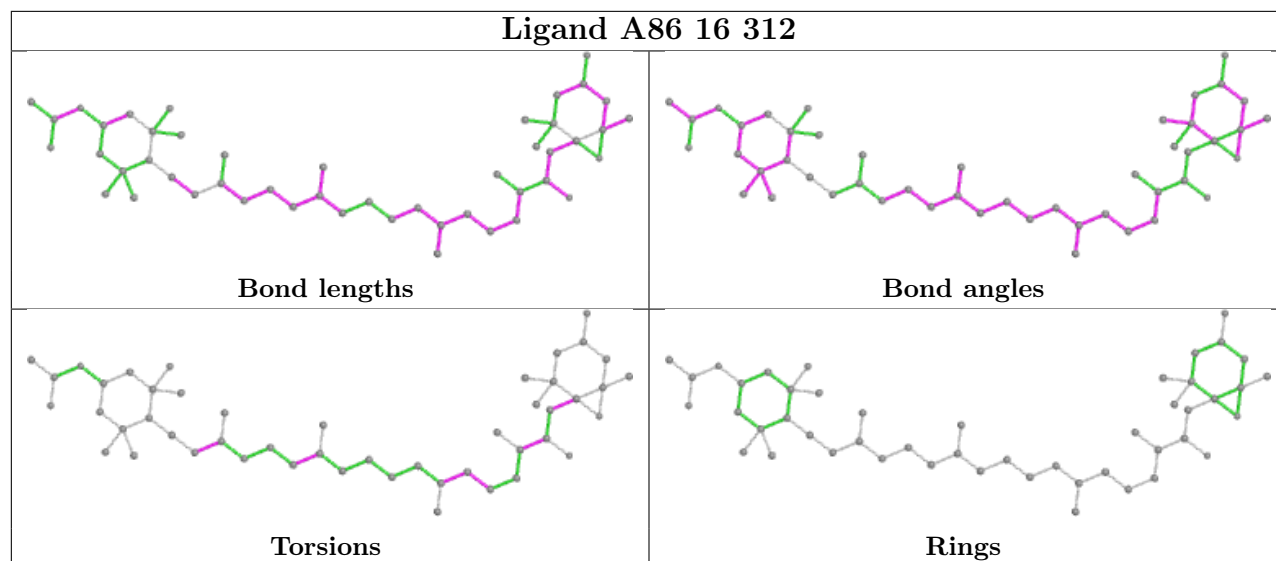
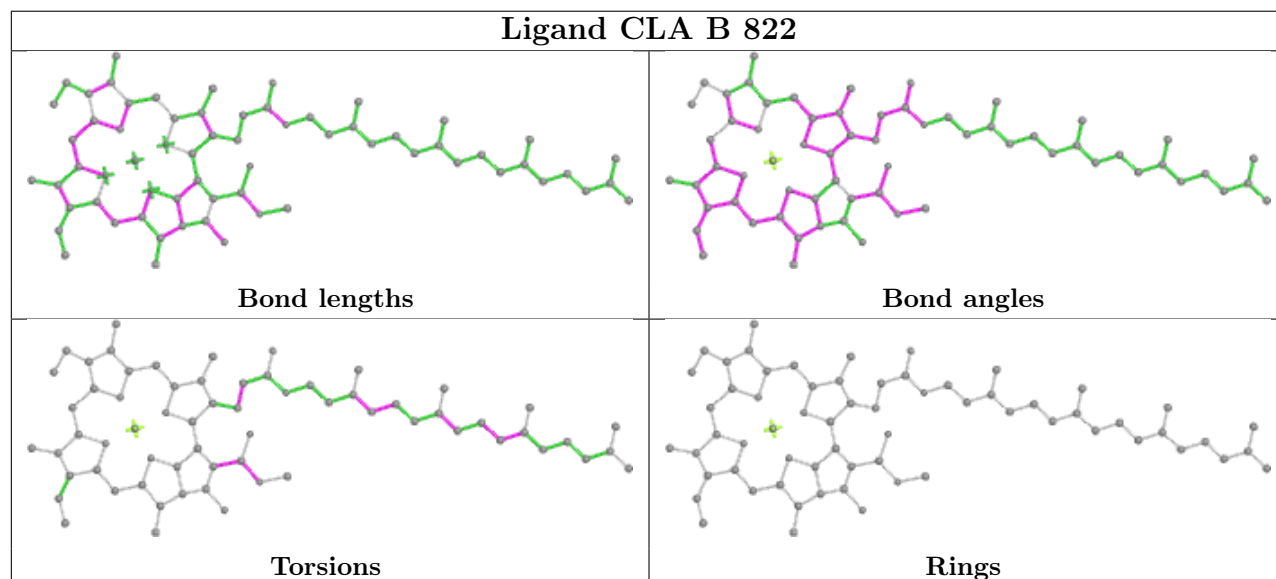
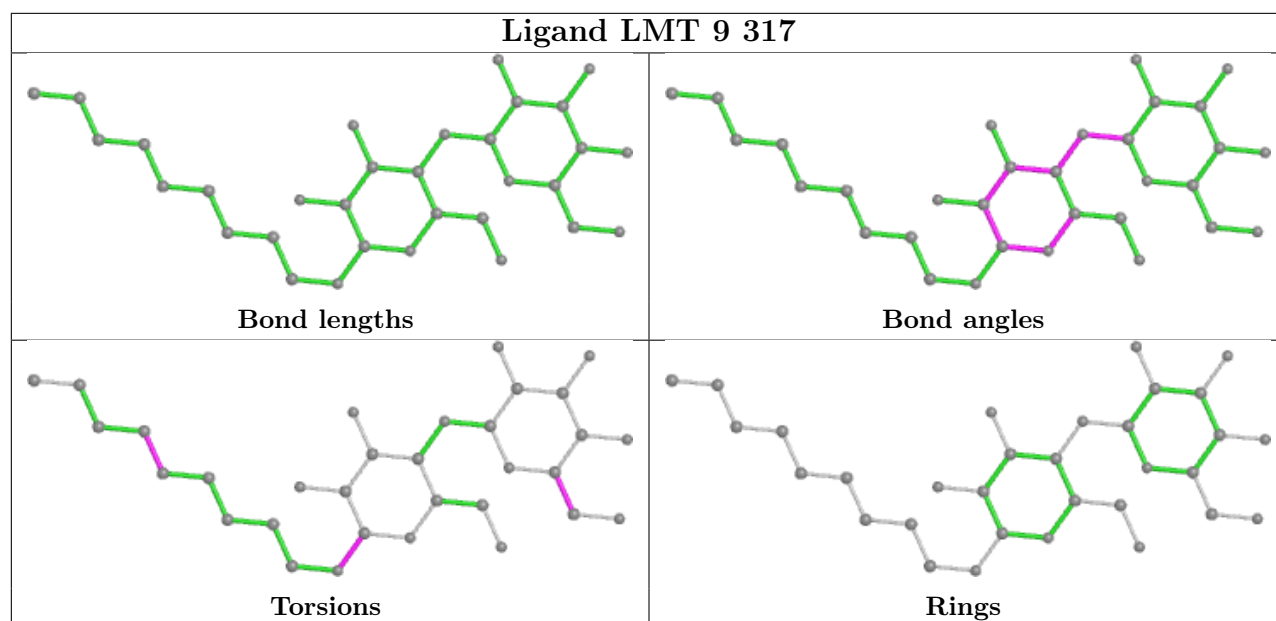
Ligand CLA B 813

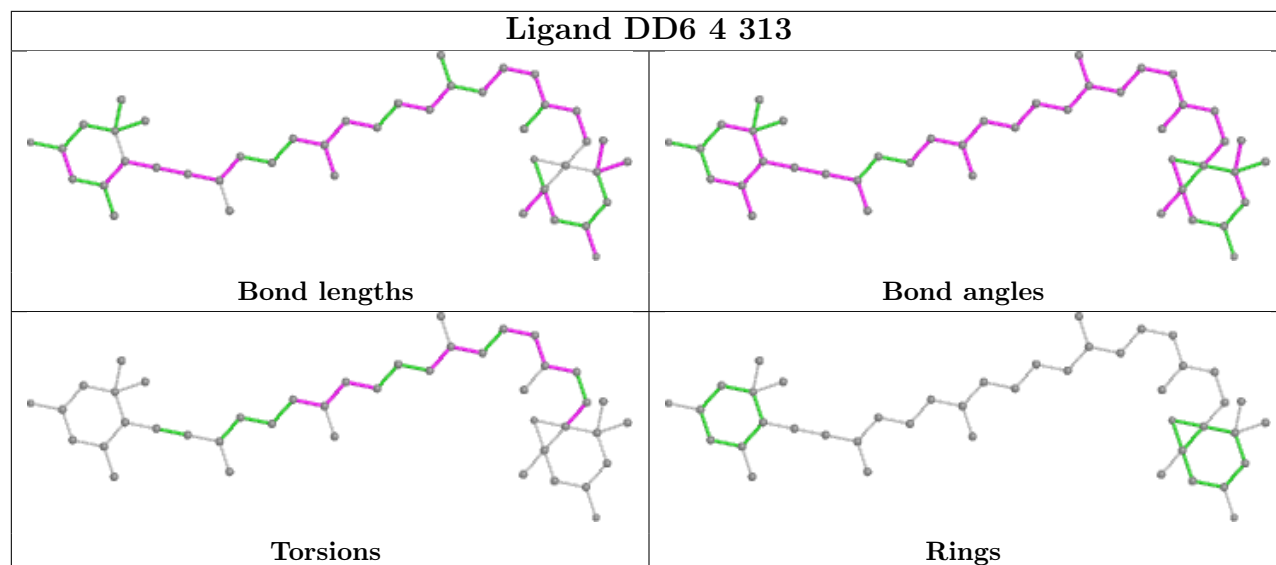
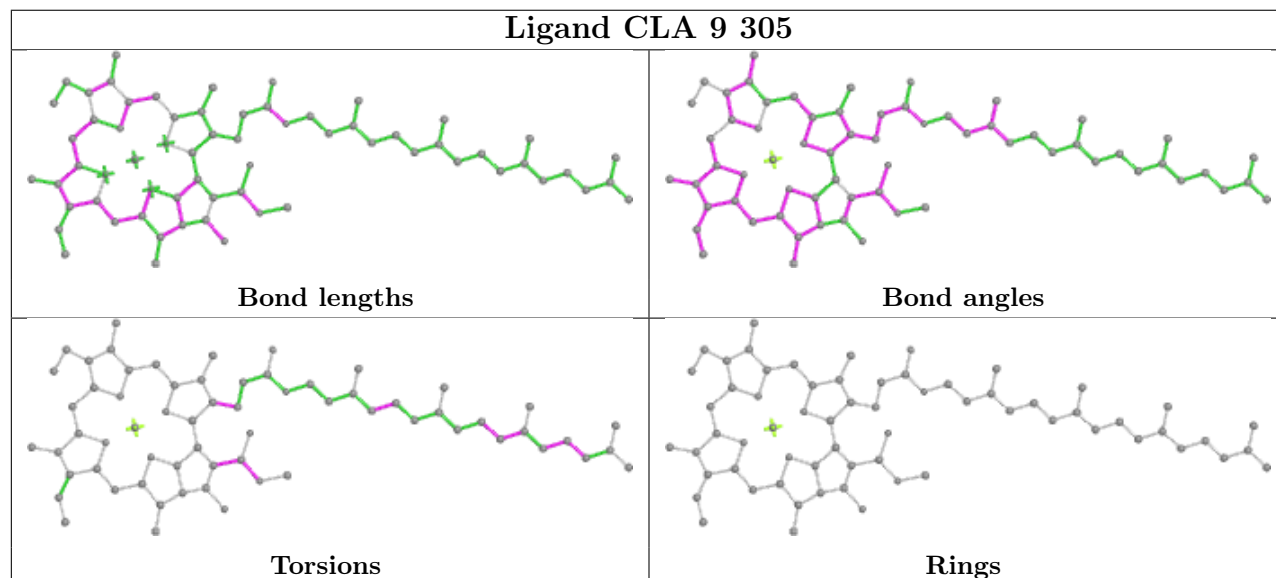
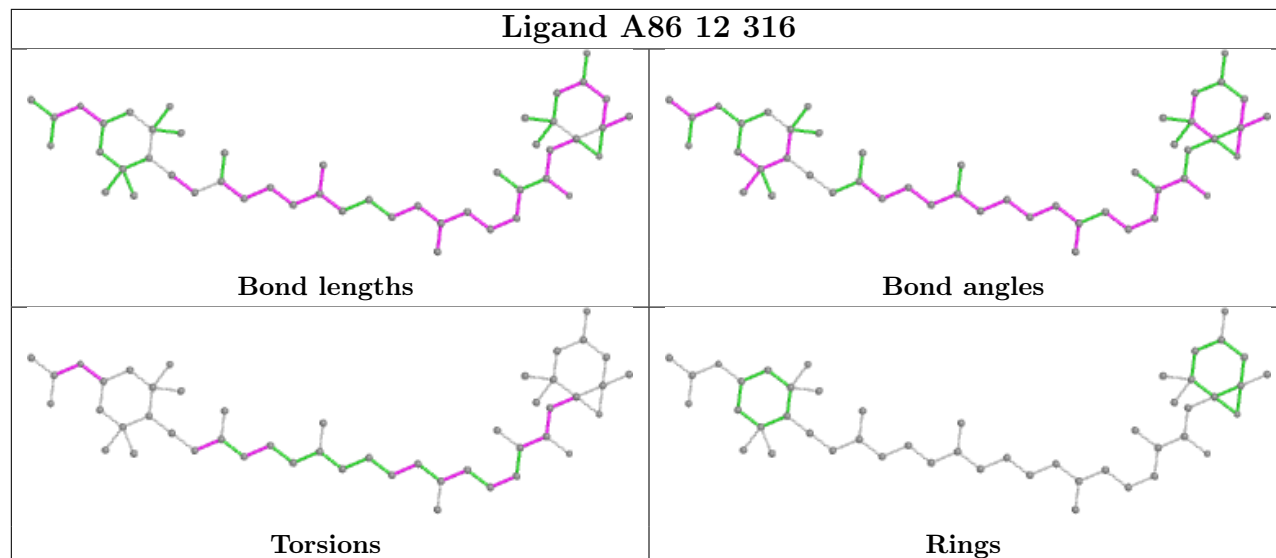


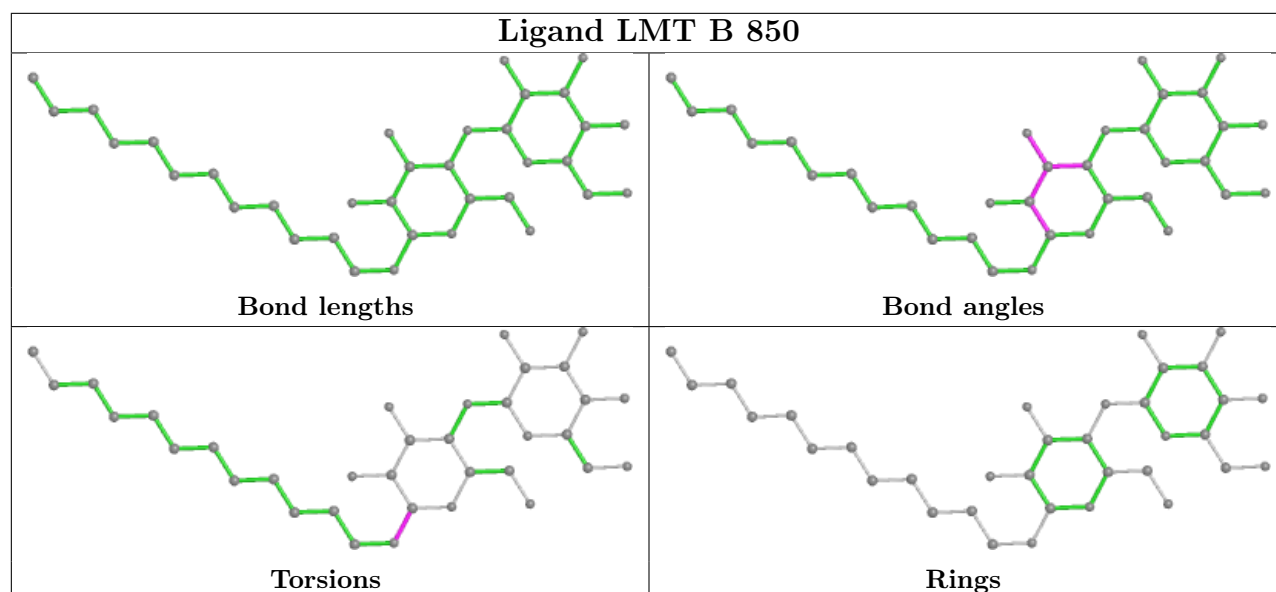
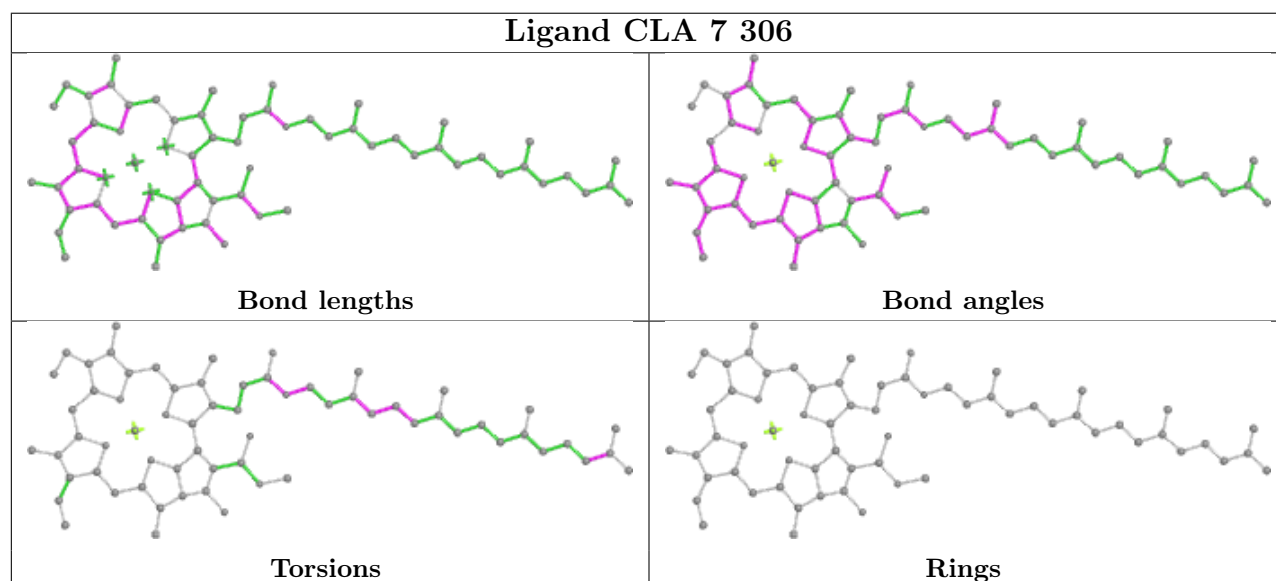
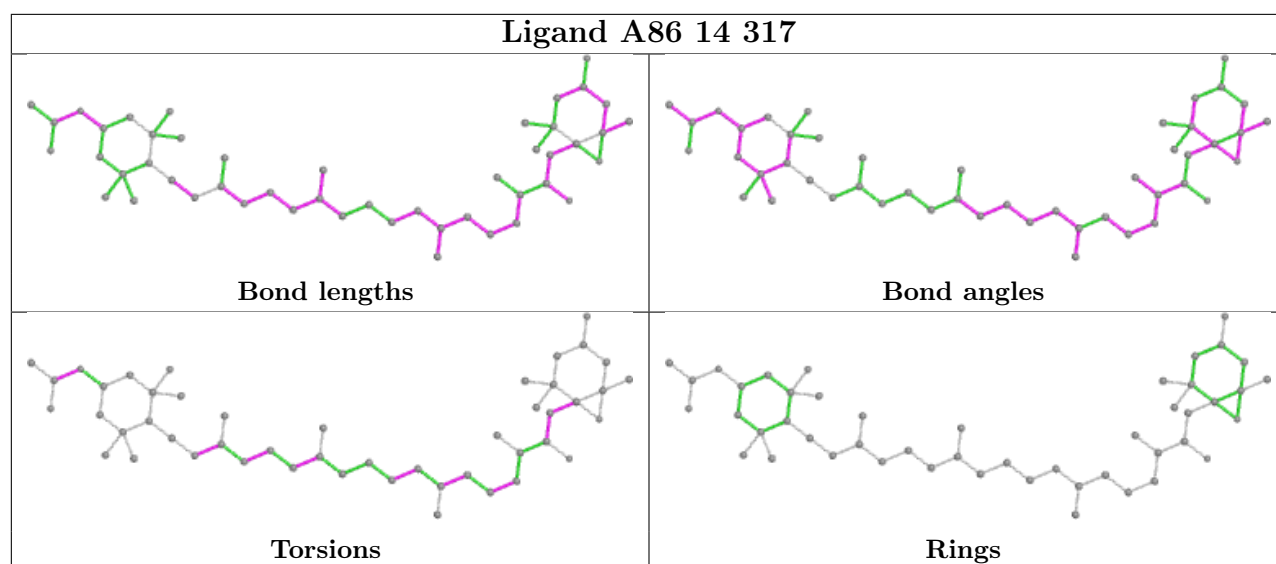
Ligand CLA L 203

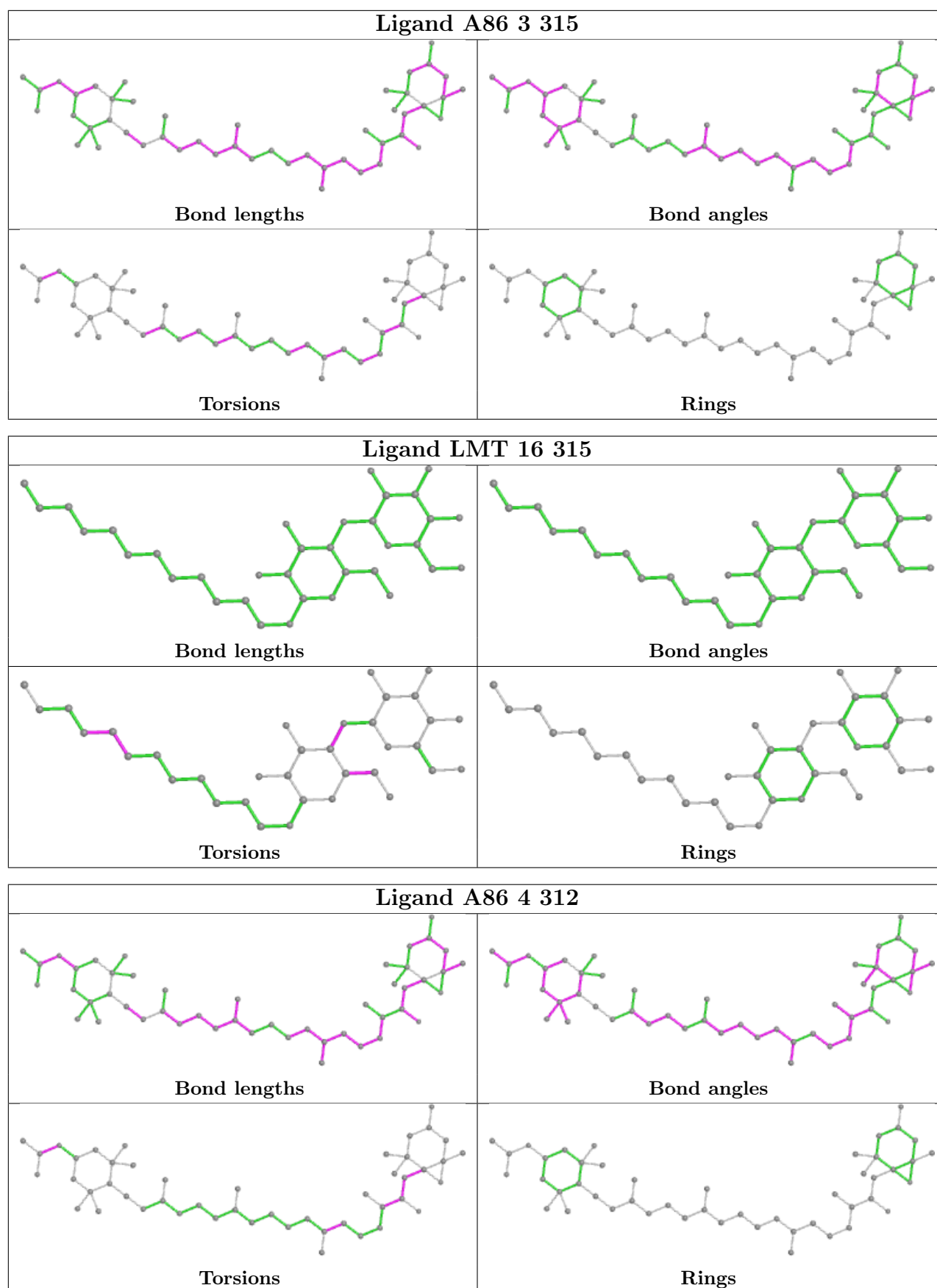


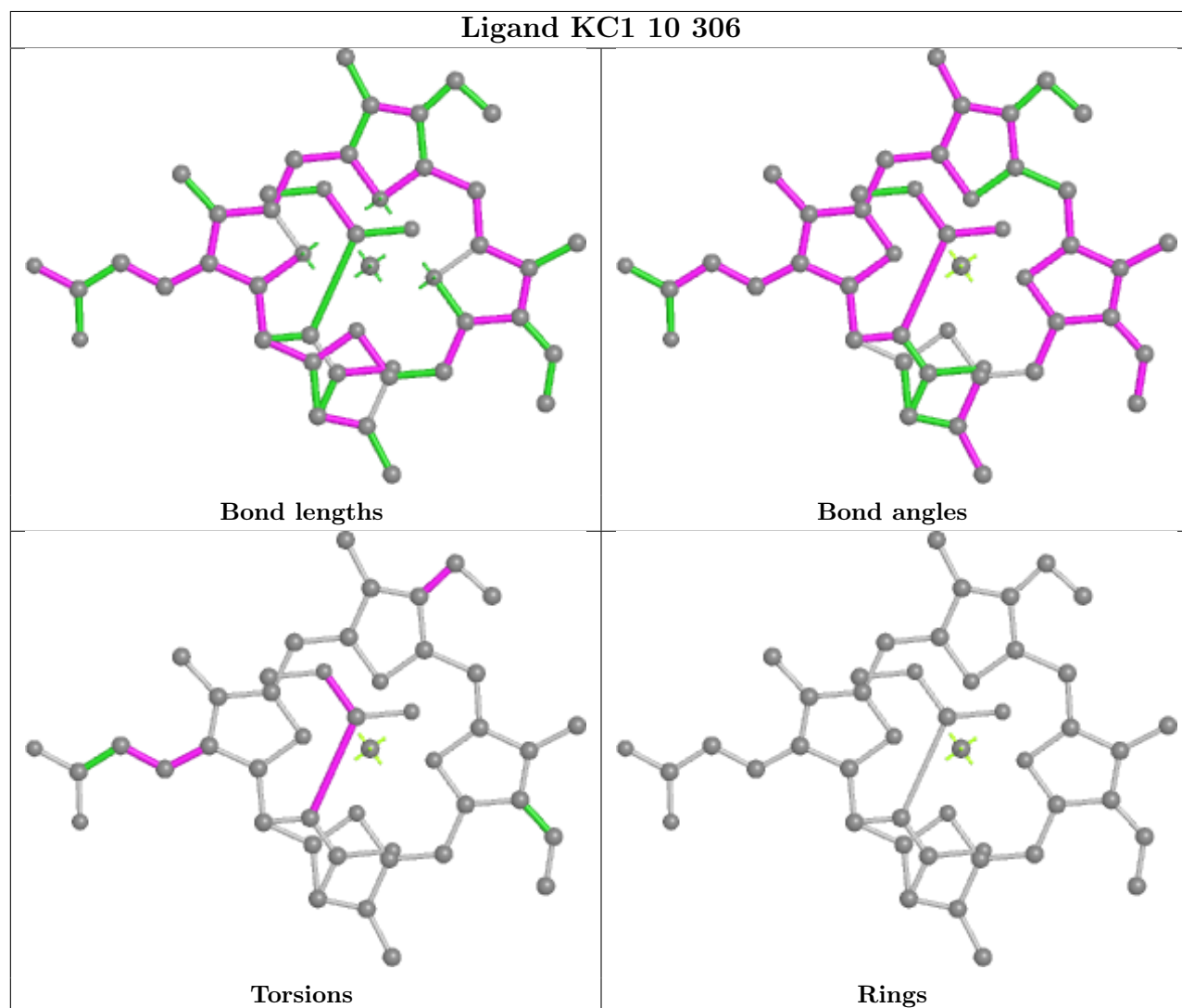
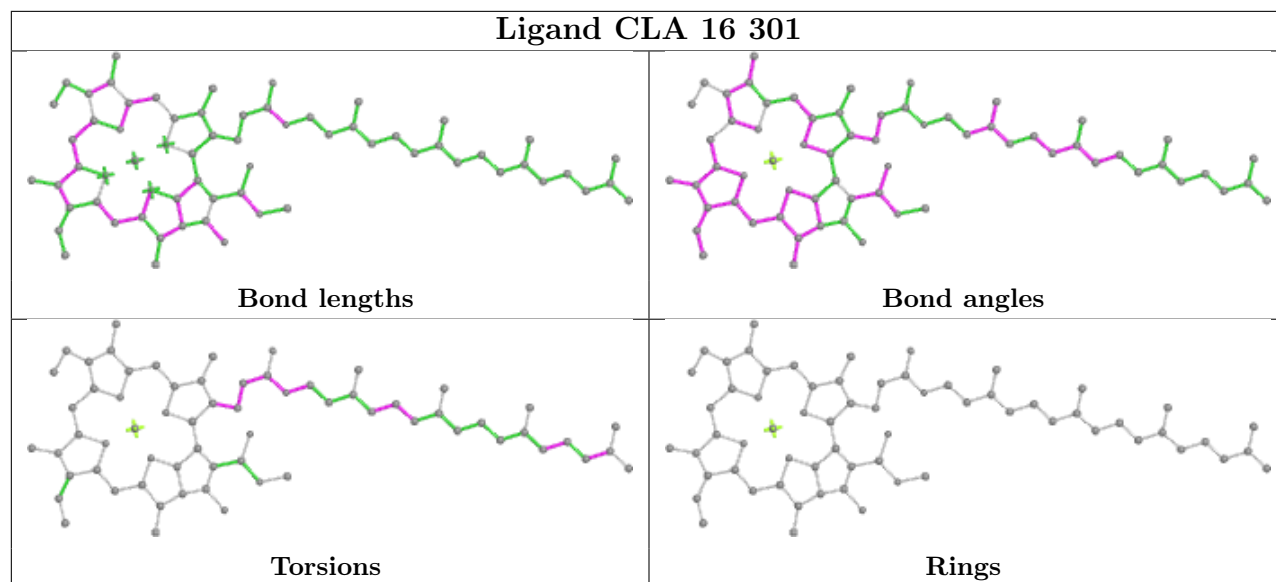


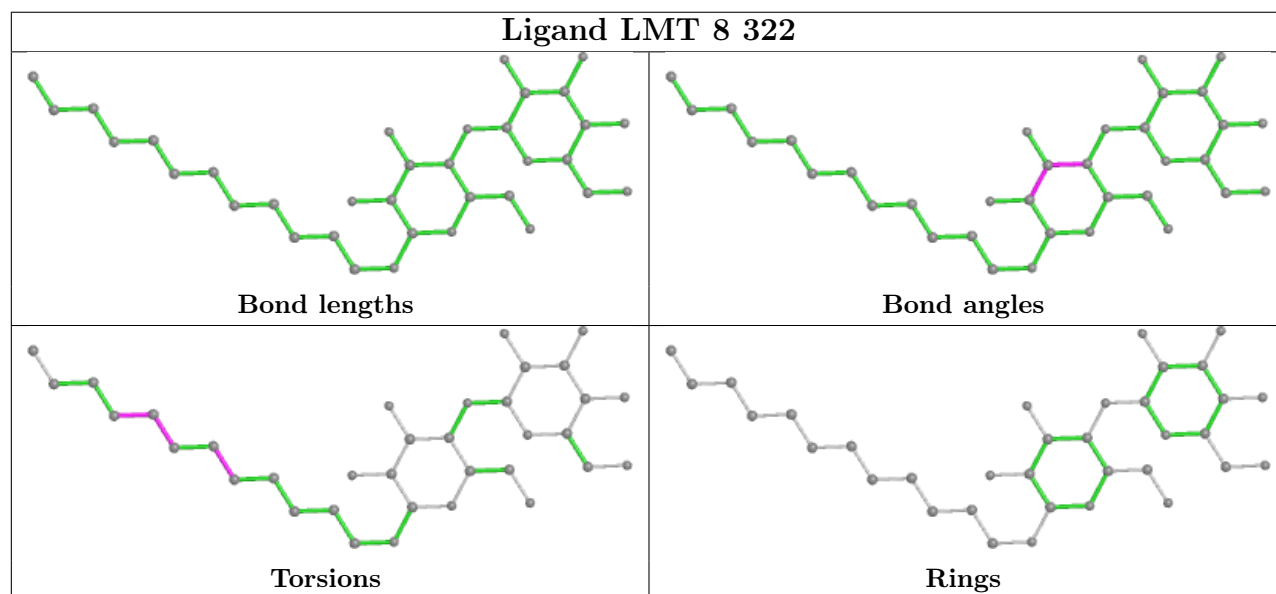
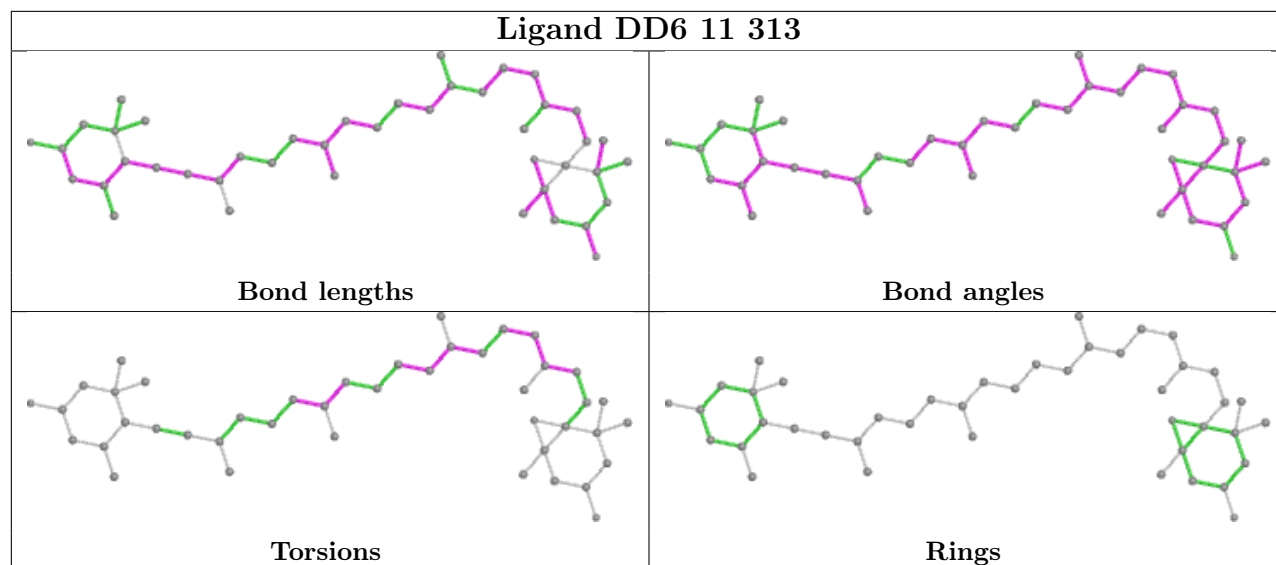
Ligand A86 16 312**Ligand CLA B 822****Ligand LMT 9 317**

Ligand DD6 4 313**Ligand CLA 9 305****Ligand A86 12 316**

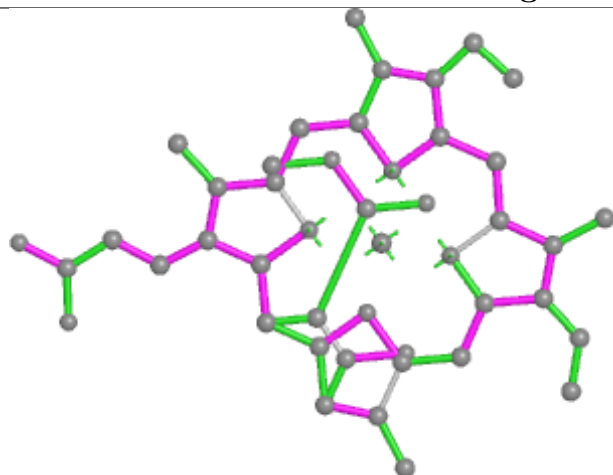




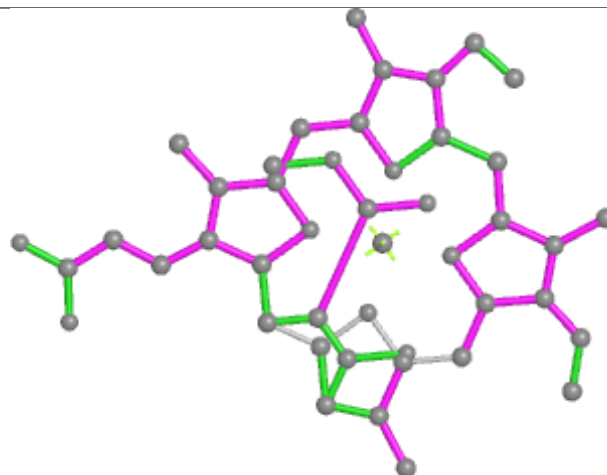




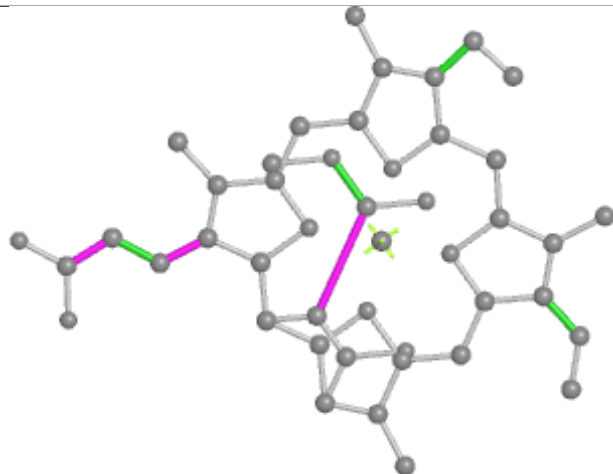
Ligand KC1 6 312



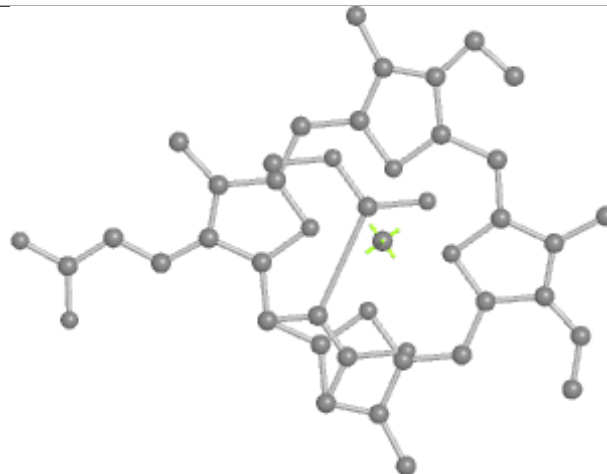
Bond lengths



Bond angles

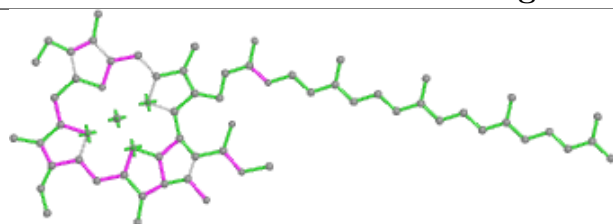


Torsions

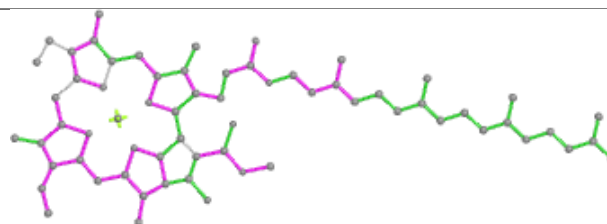


Rings

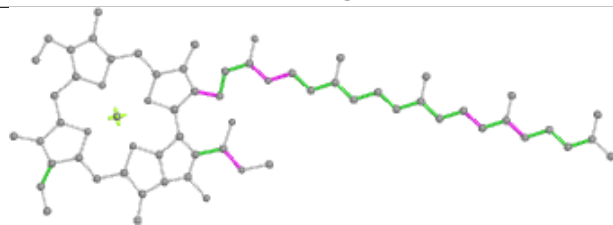
Ligand CLA 9 309



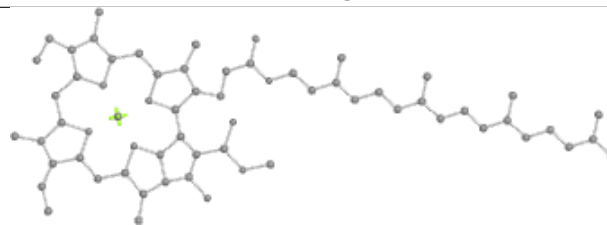
Bond lengths



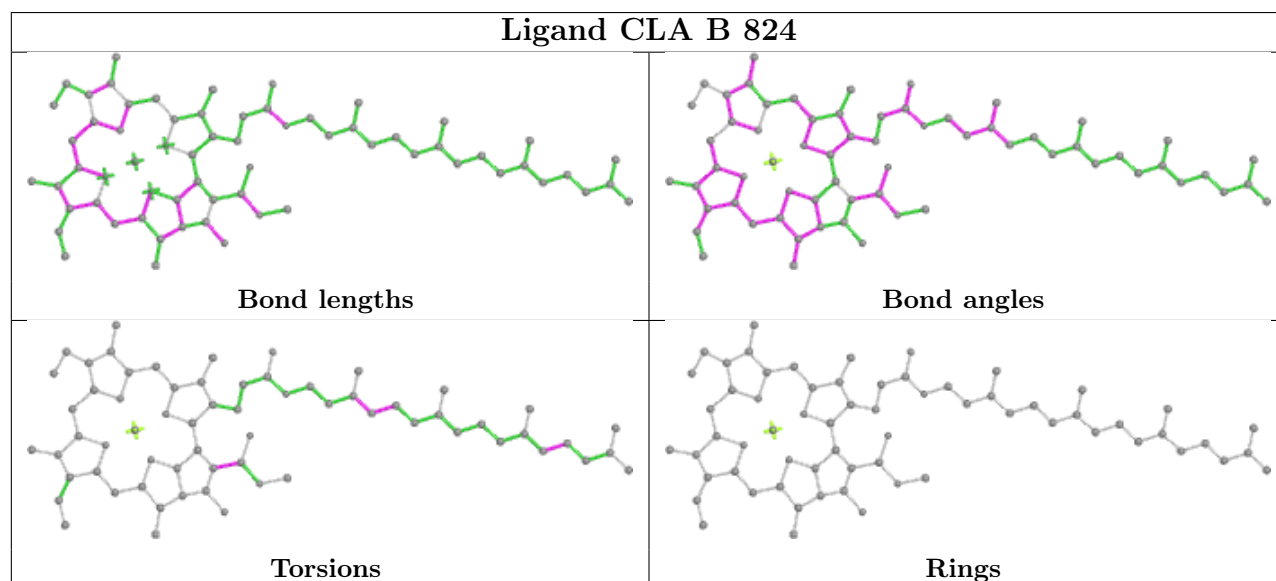
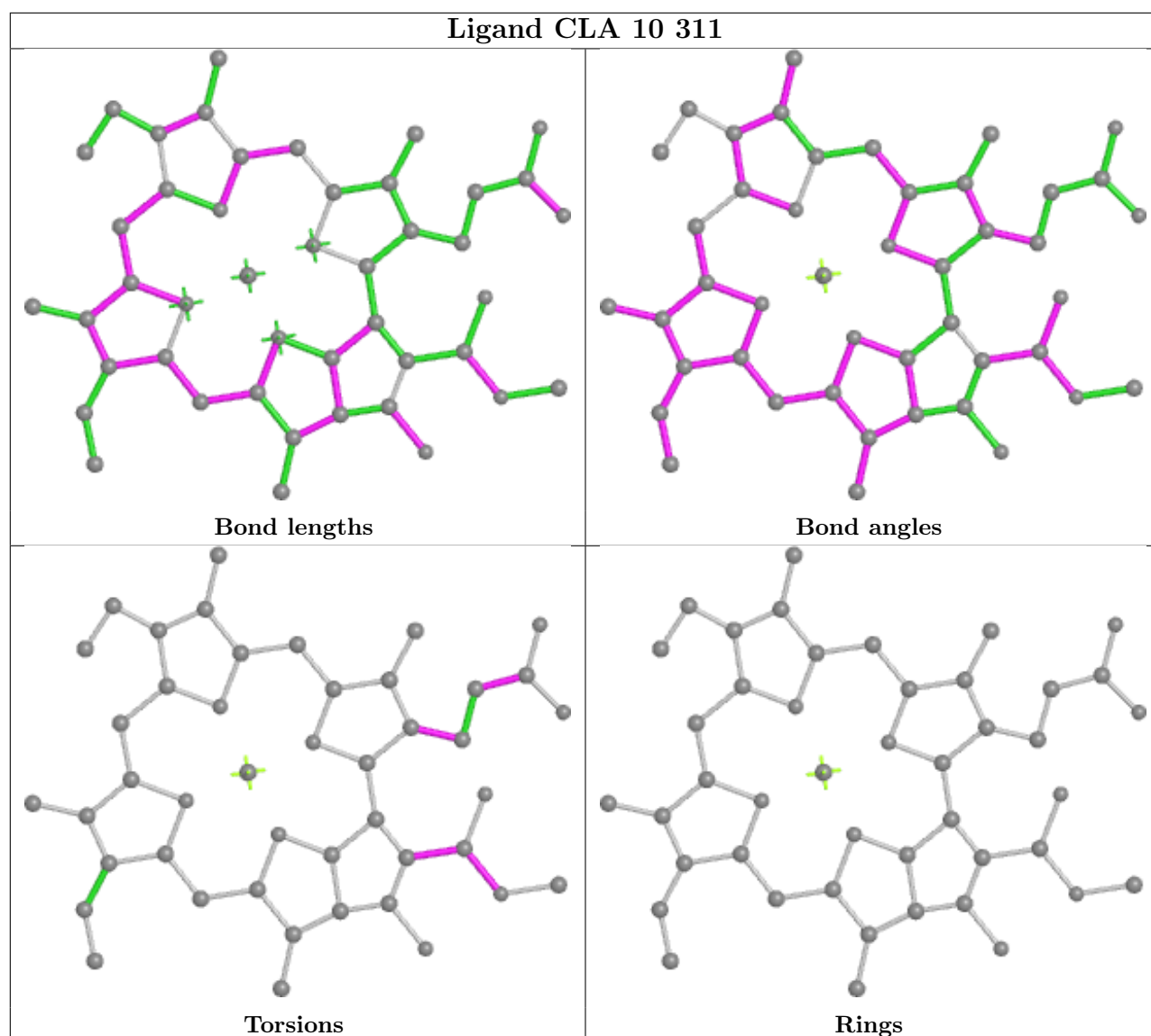
Bond angles



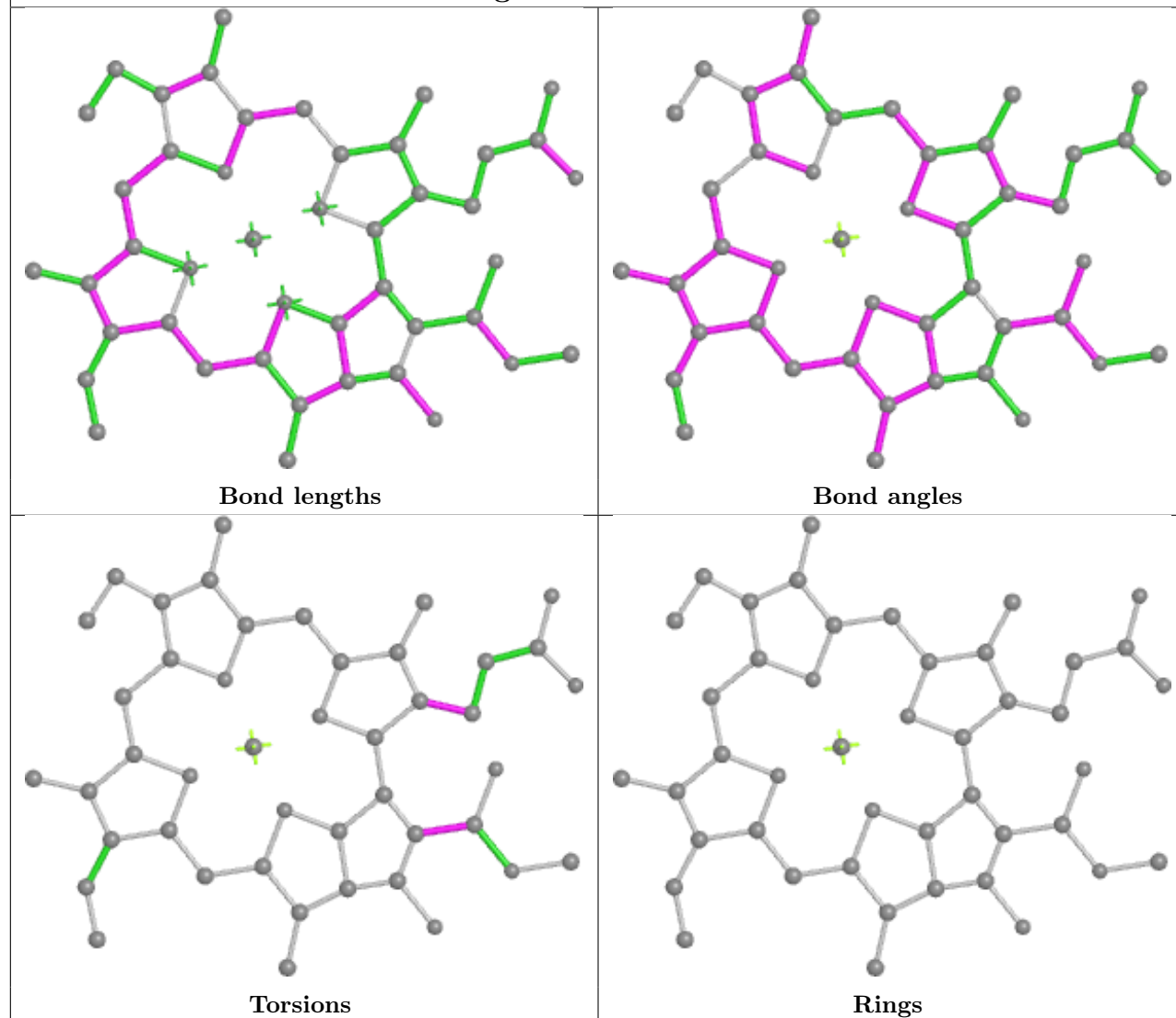
Torsions



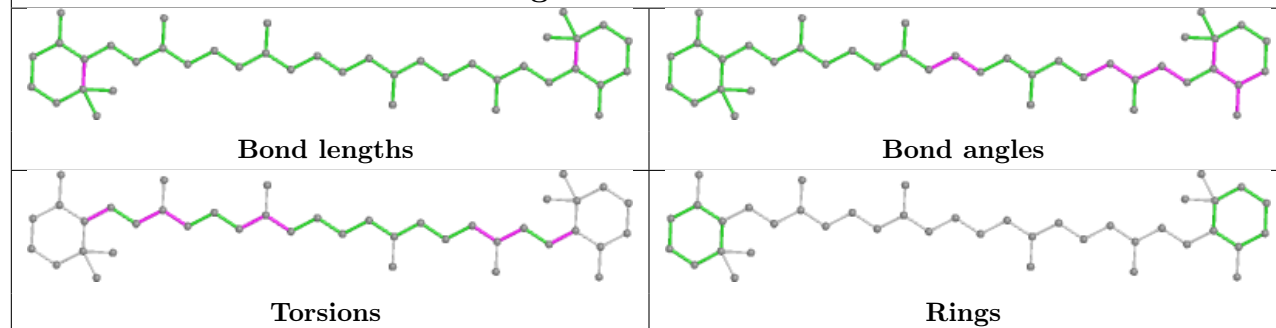
Rings



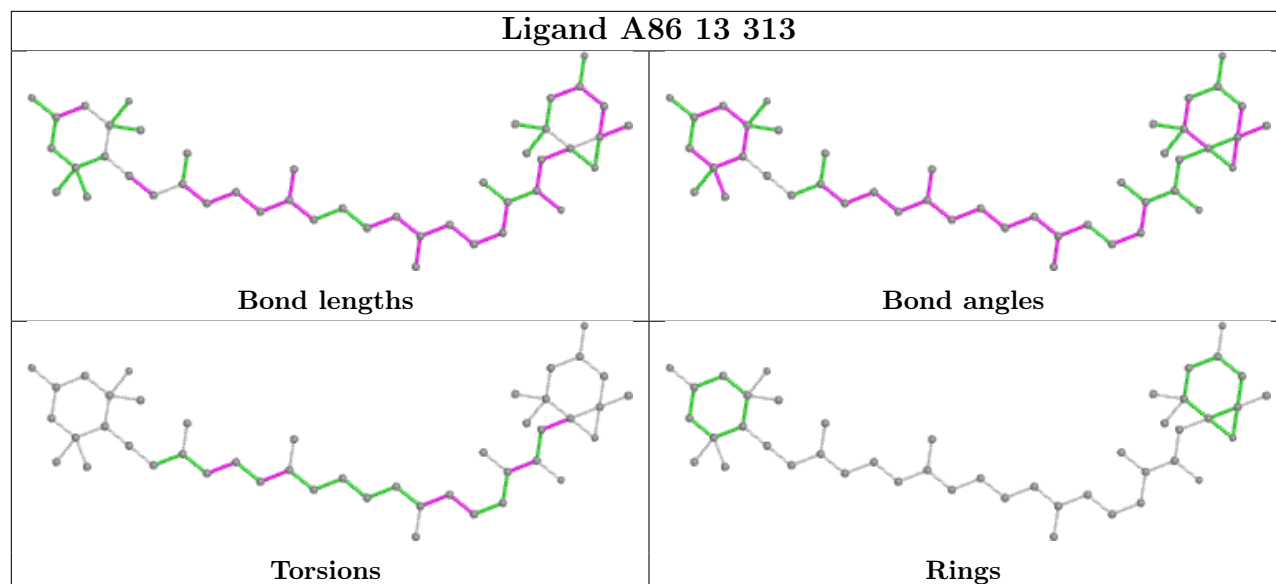
Ligand CLA 3 309



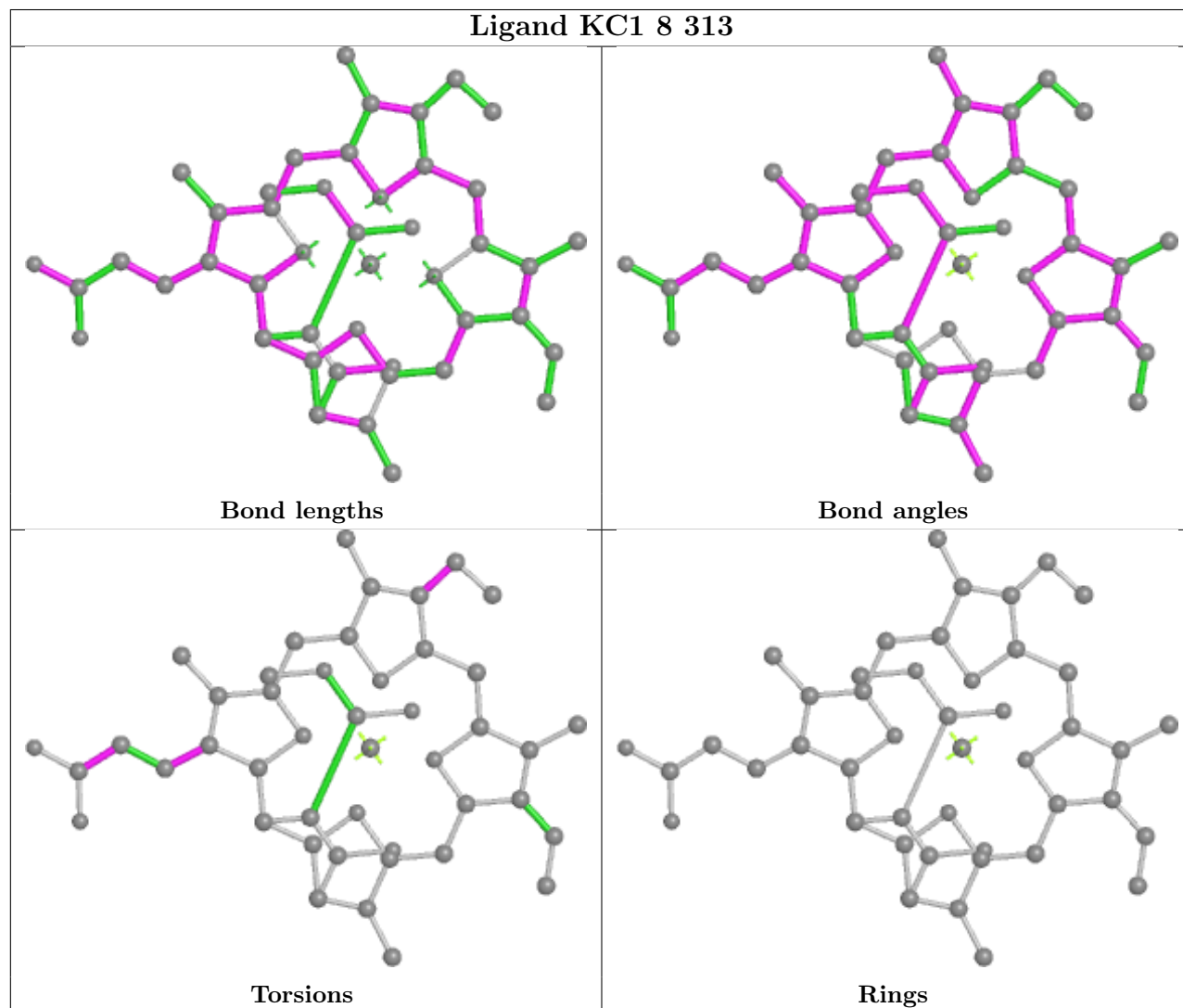
Ligand BCR B 845

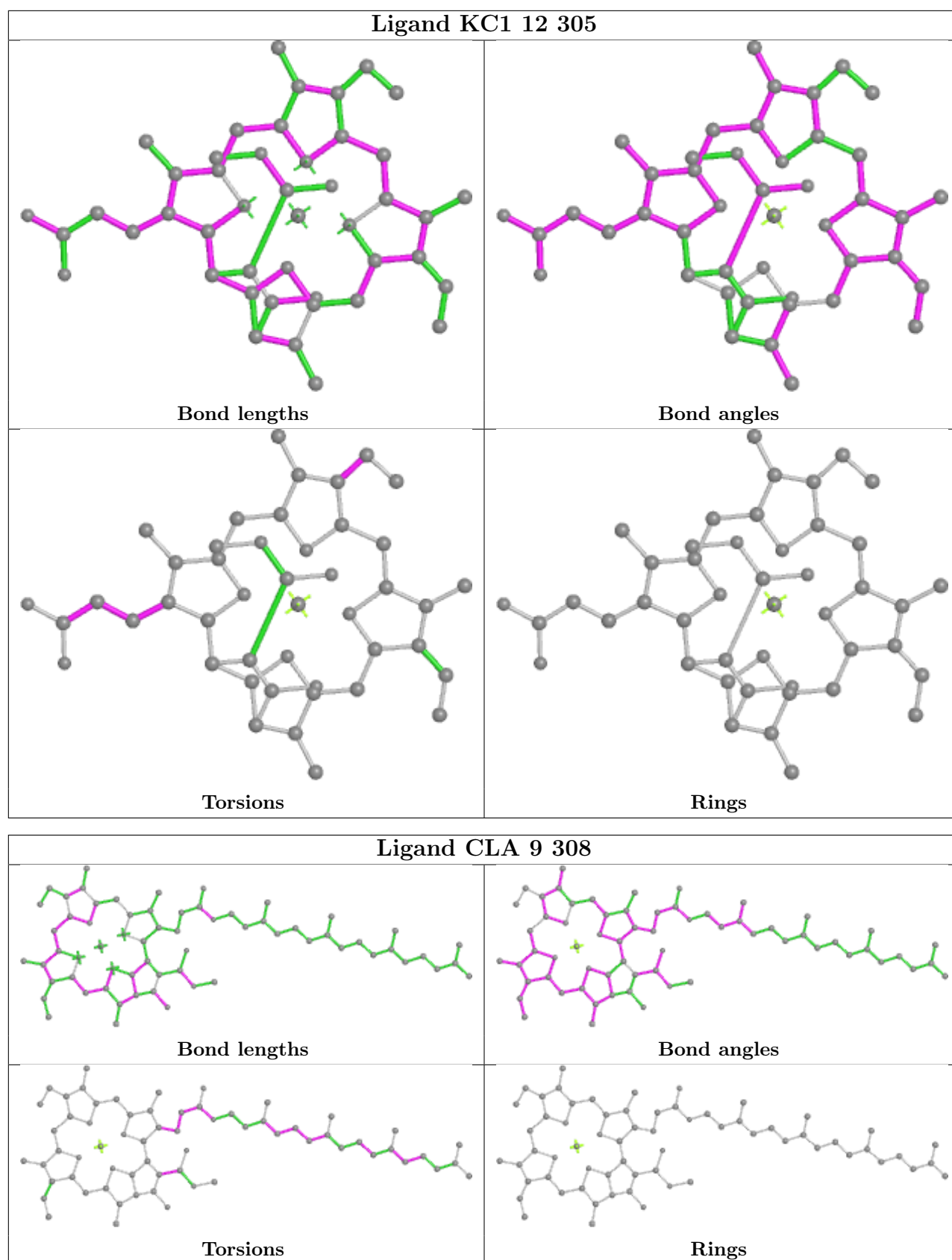


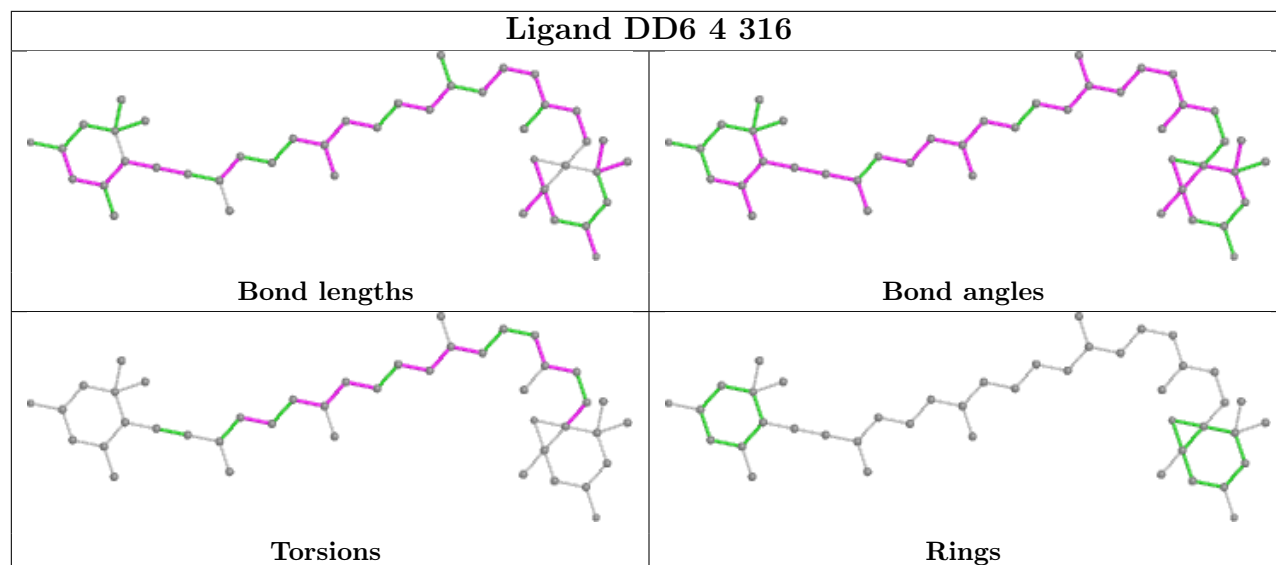
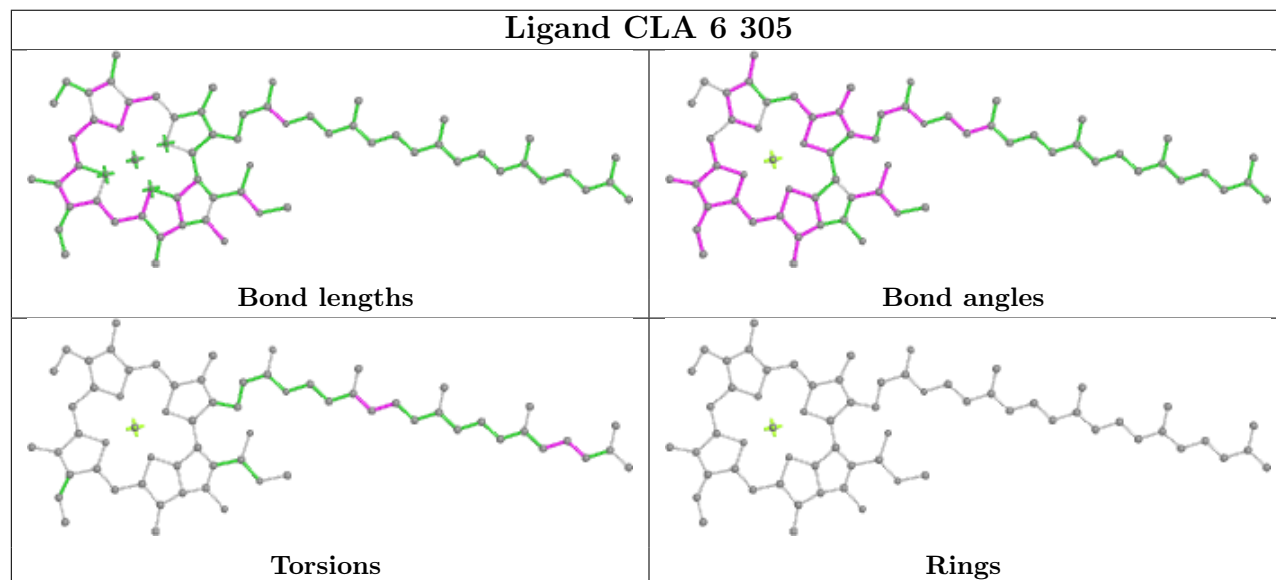
Ligand A86 13 313

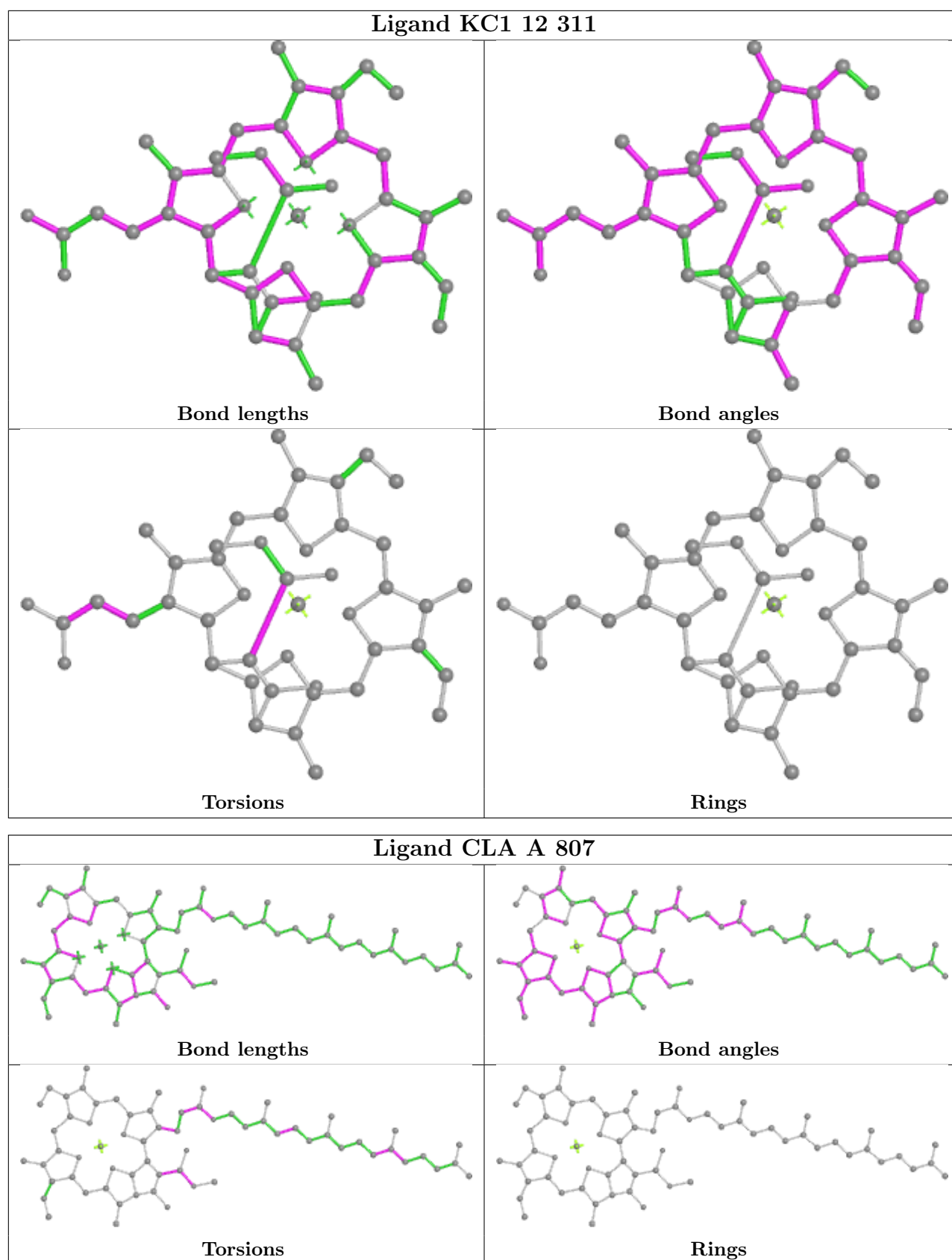


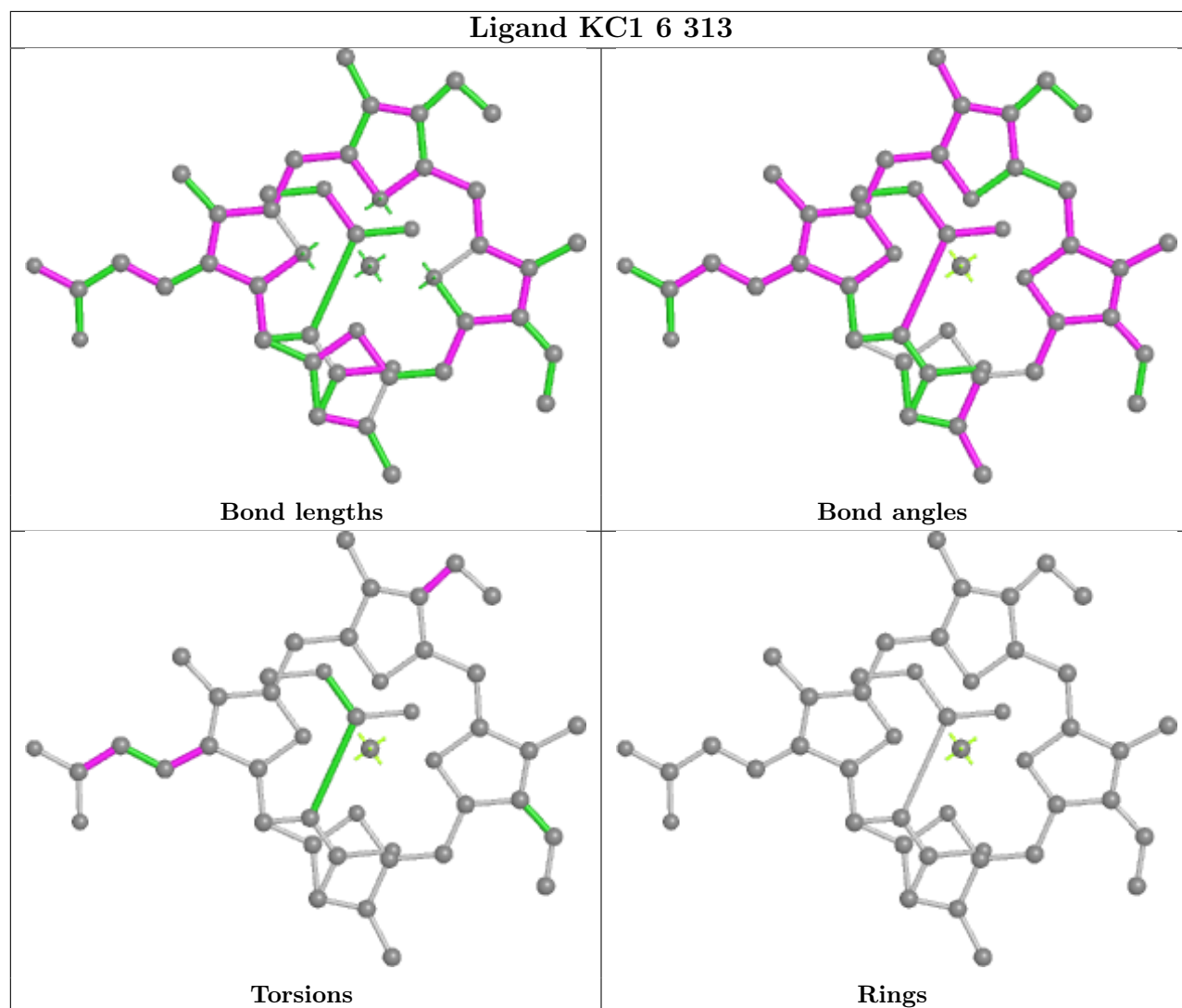
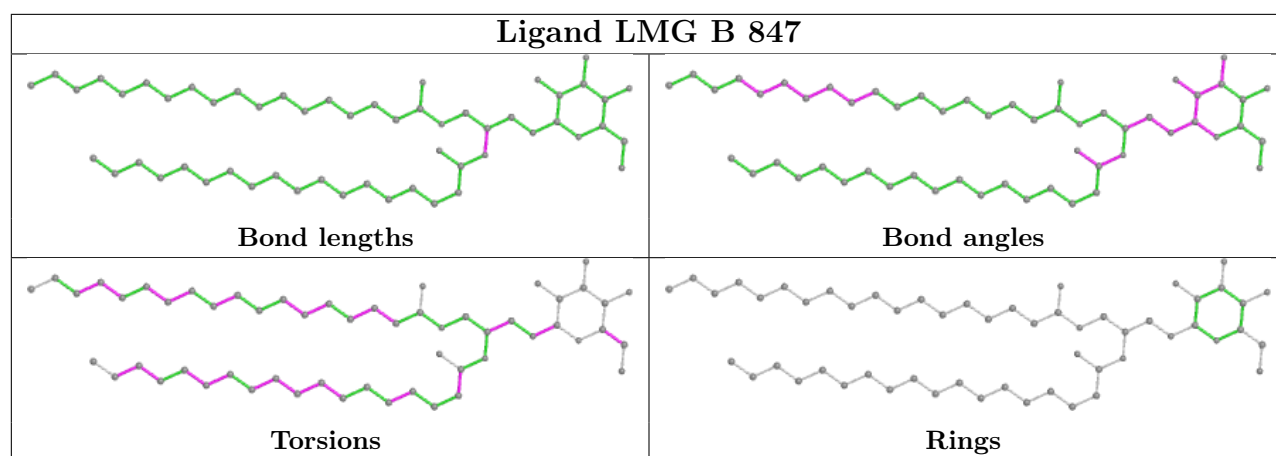
Ligand KC1 8 313

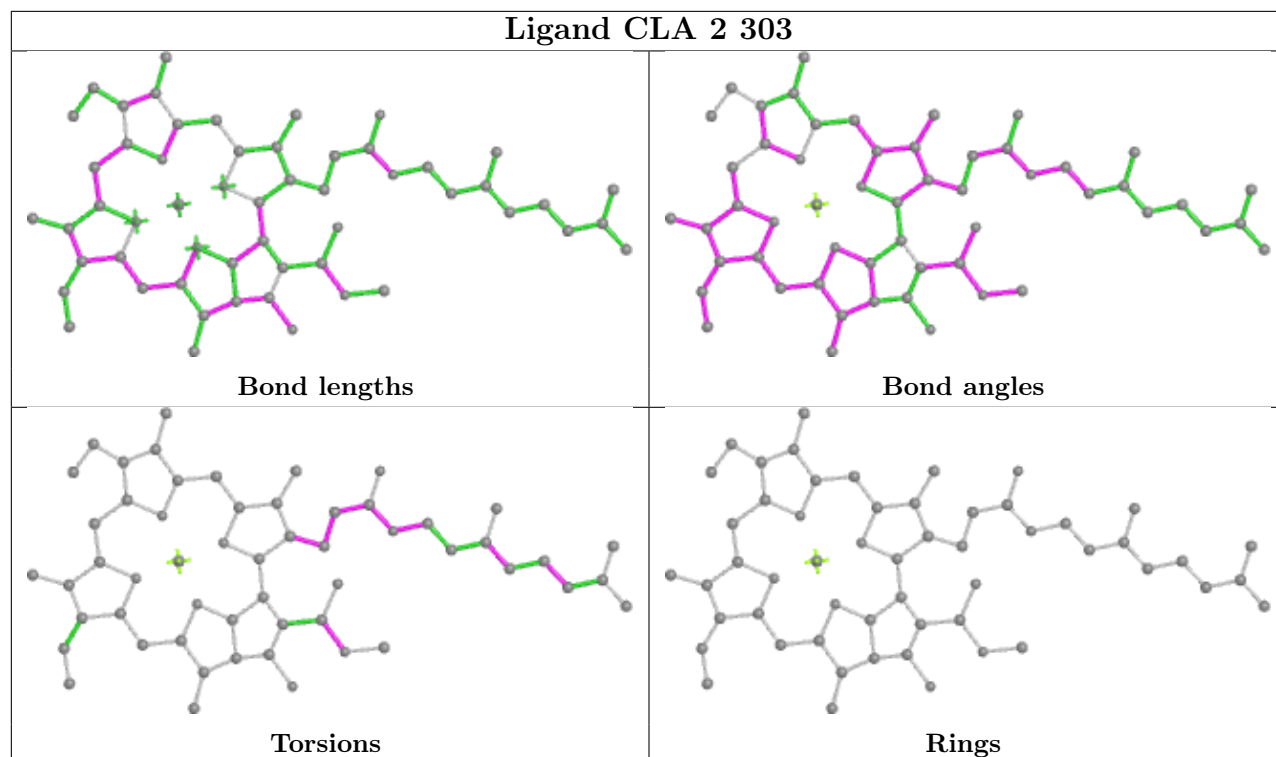
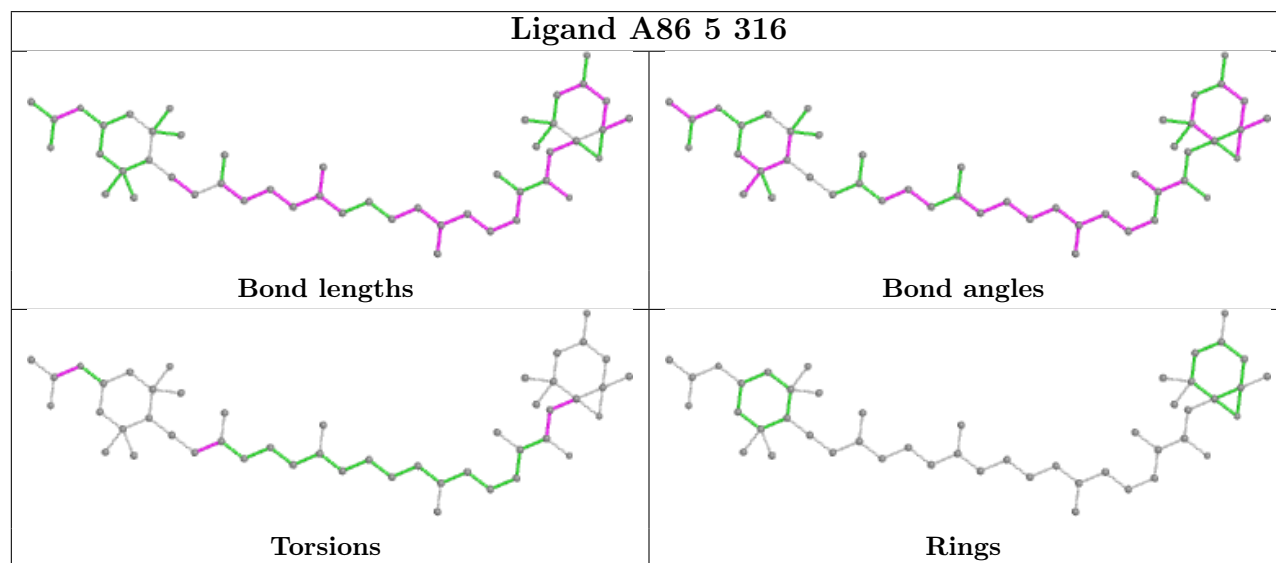


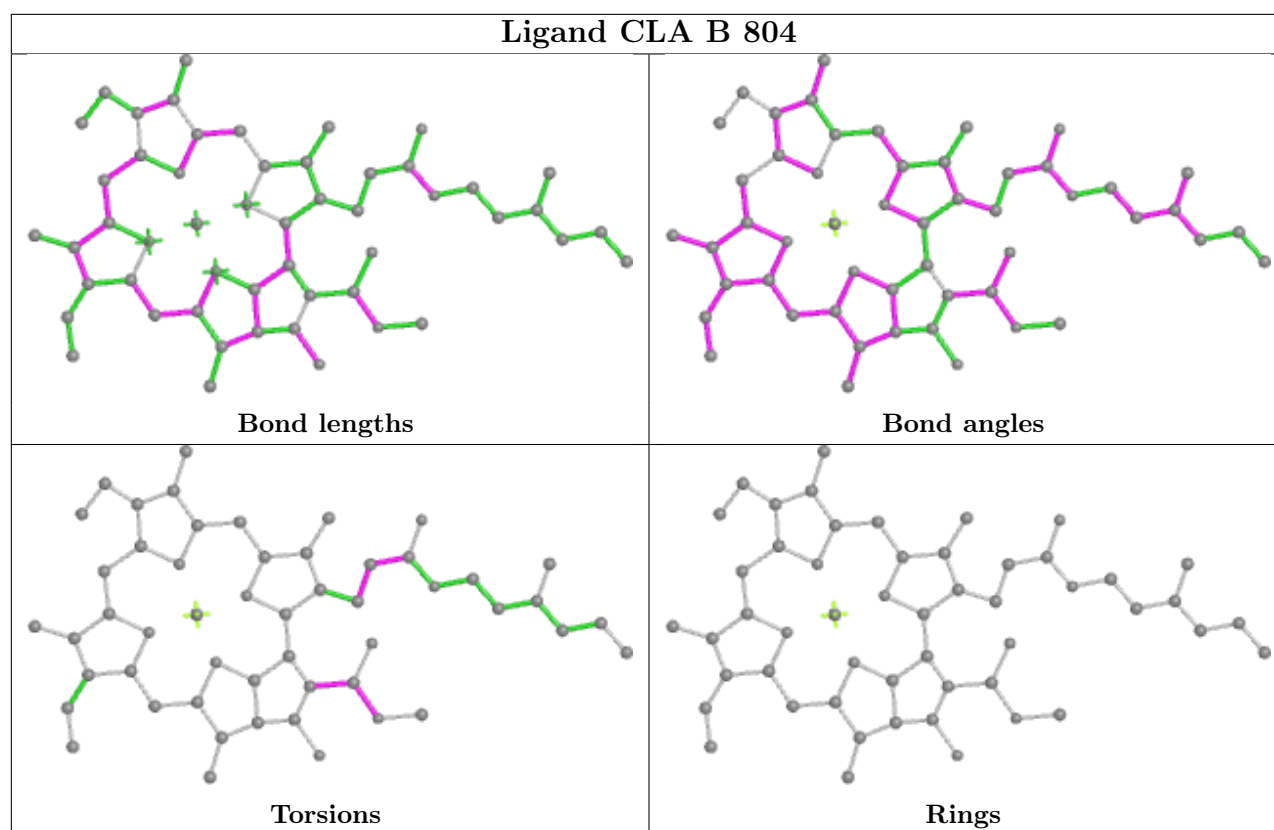


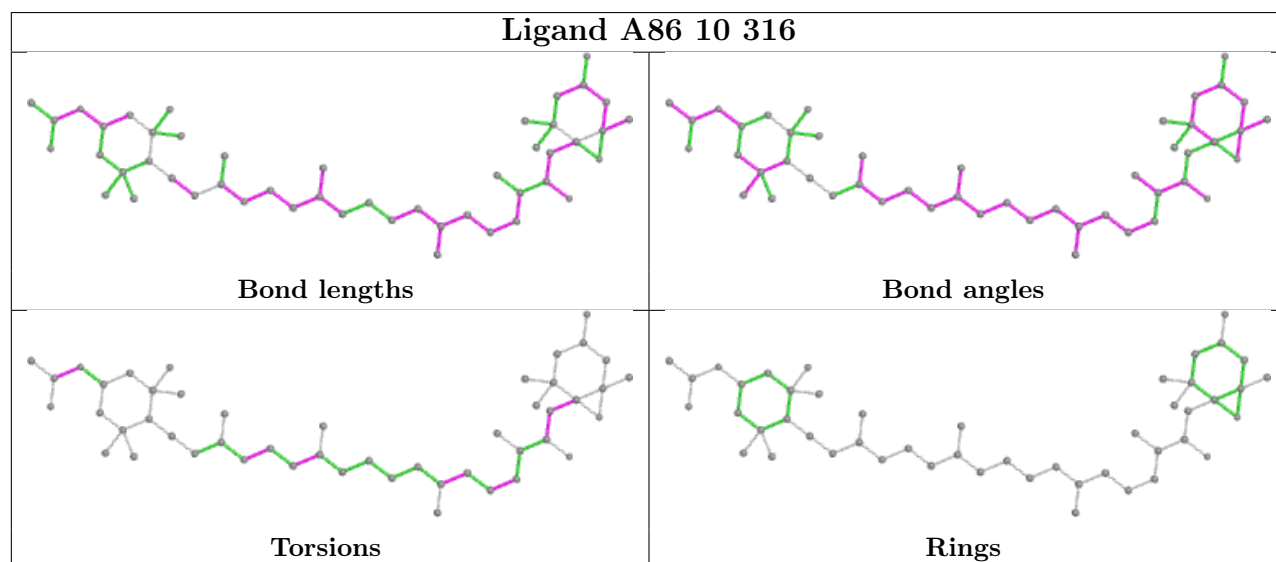
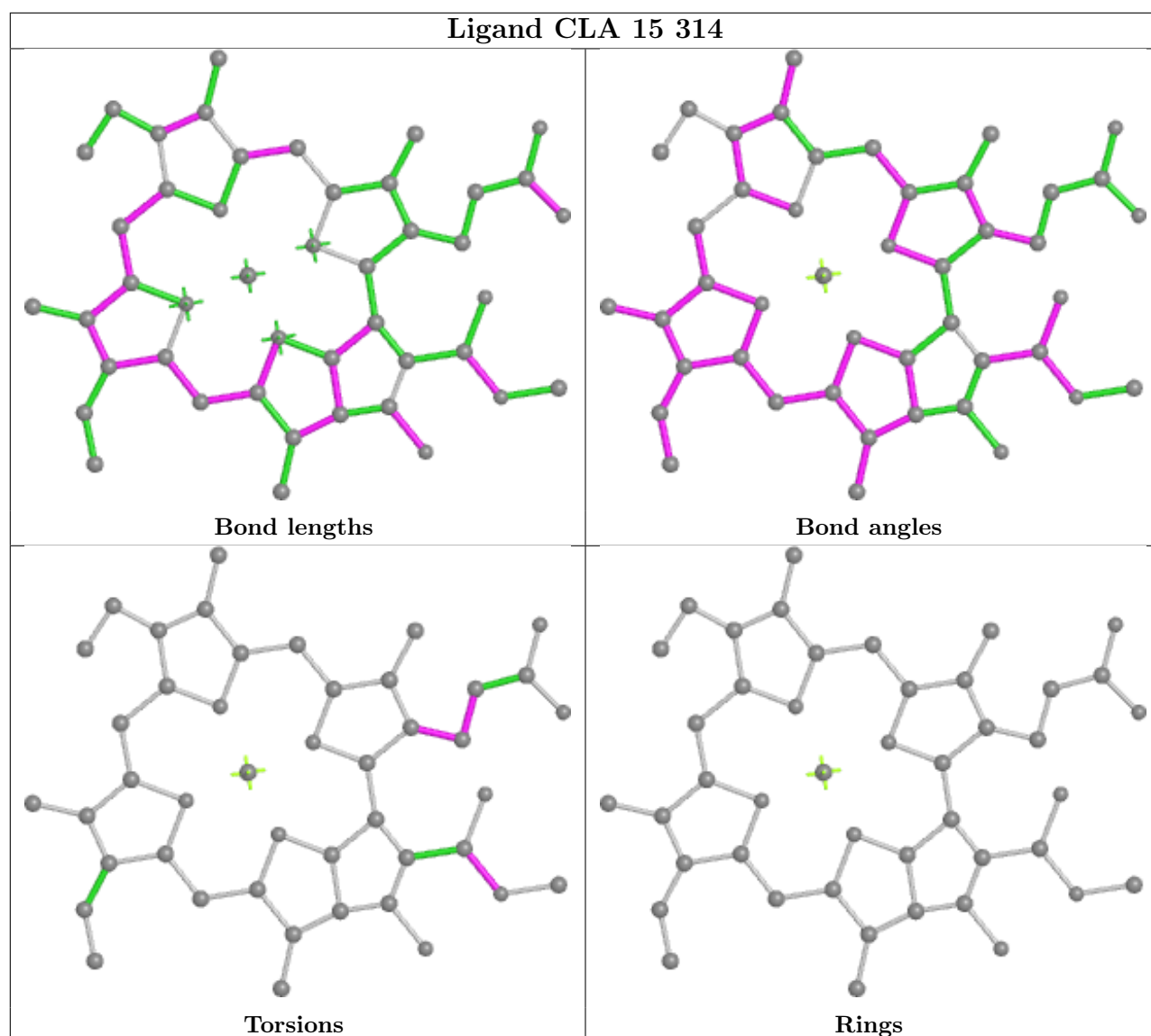
Ligand DD6 4 316**Ligand CLA 6 305**

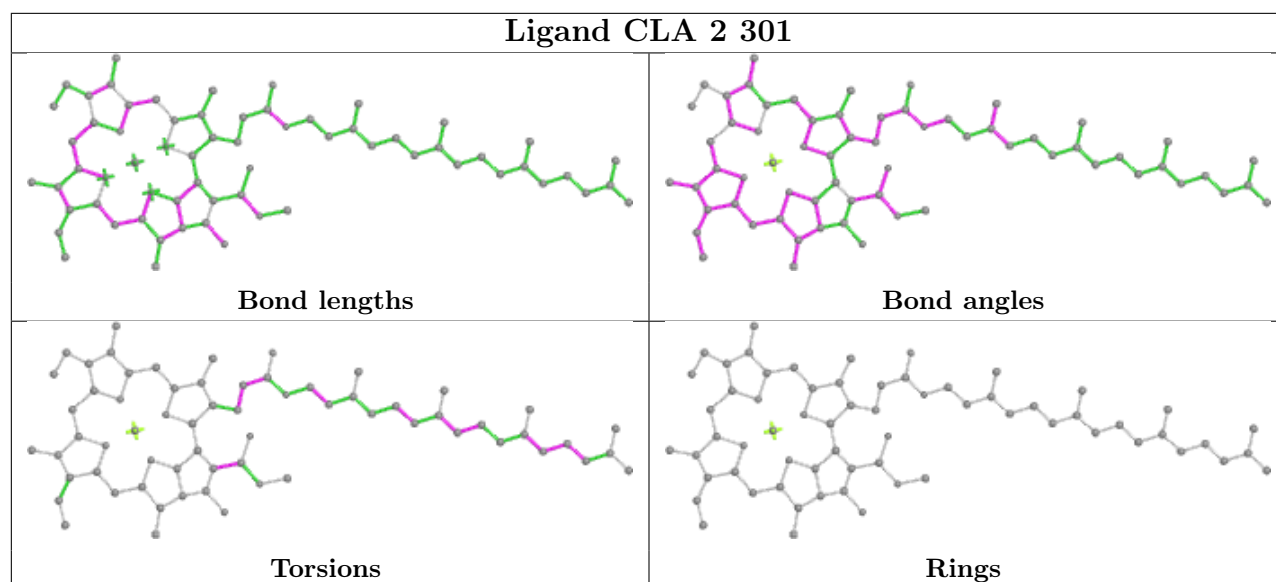
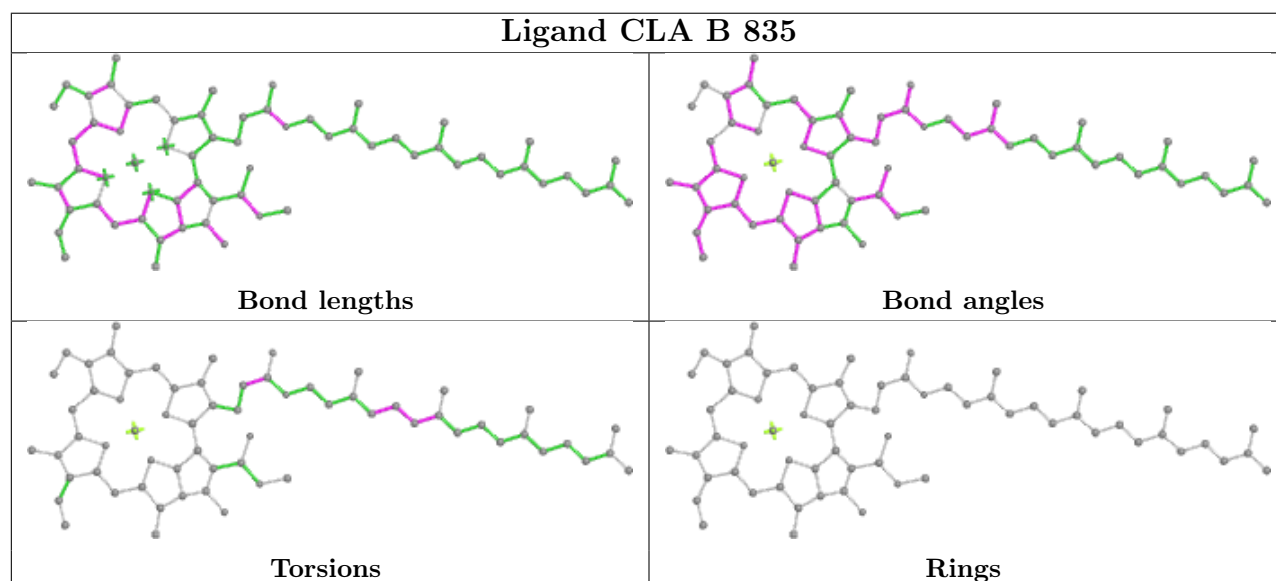
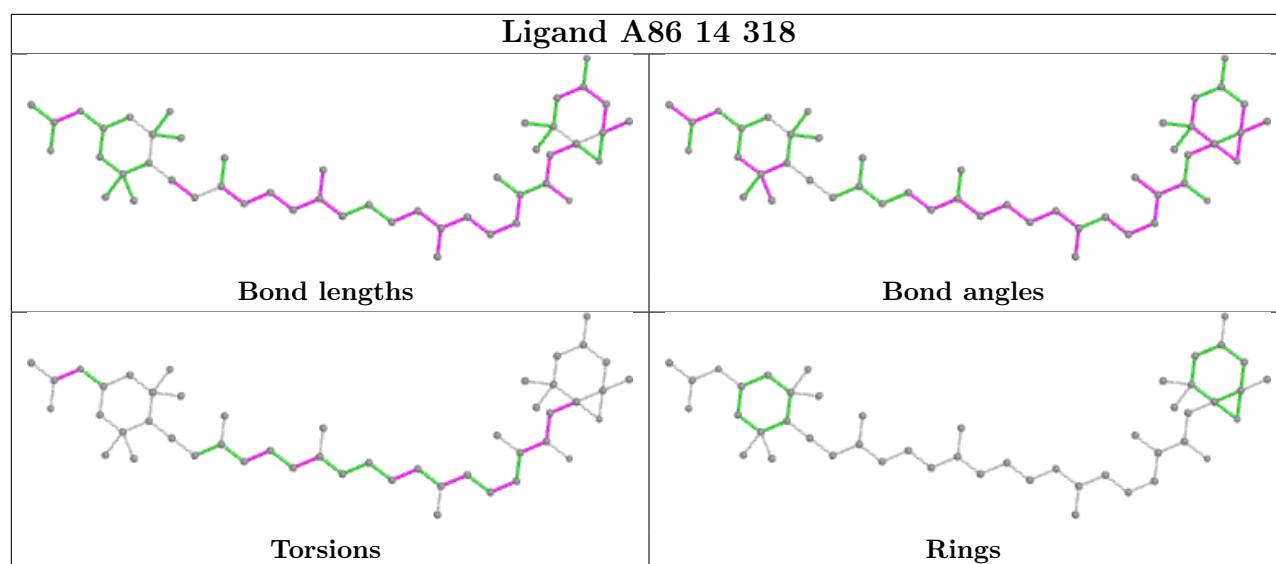




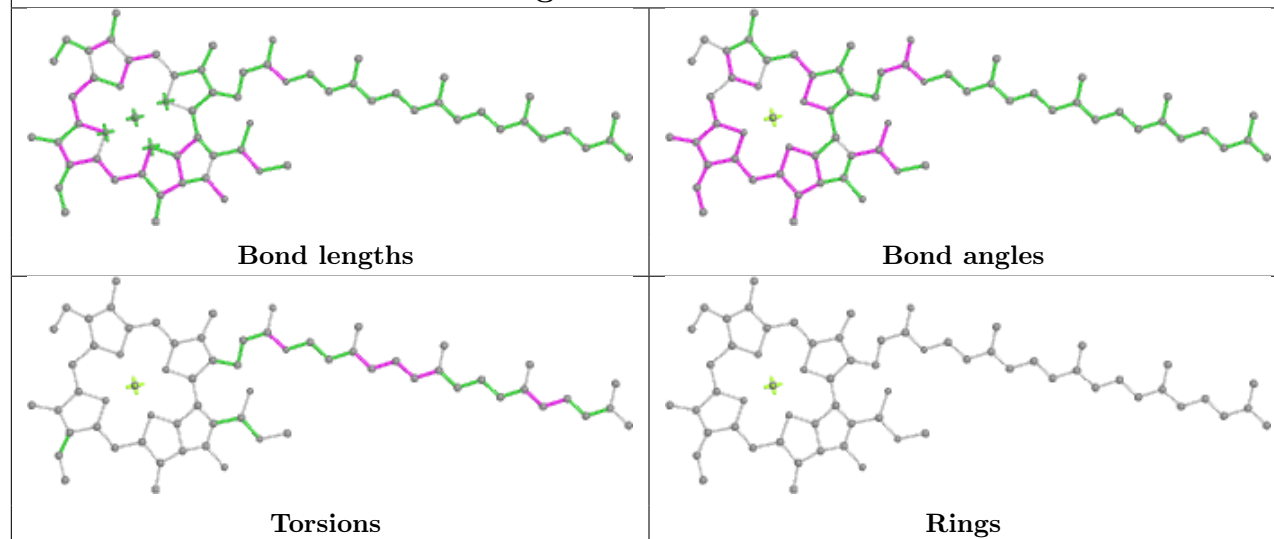
Ligand CLA 2 303**Ligand A86 5 316**



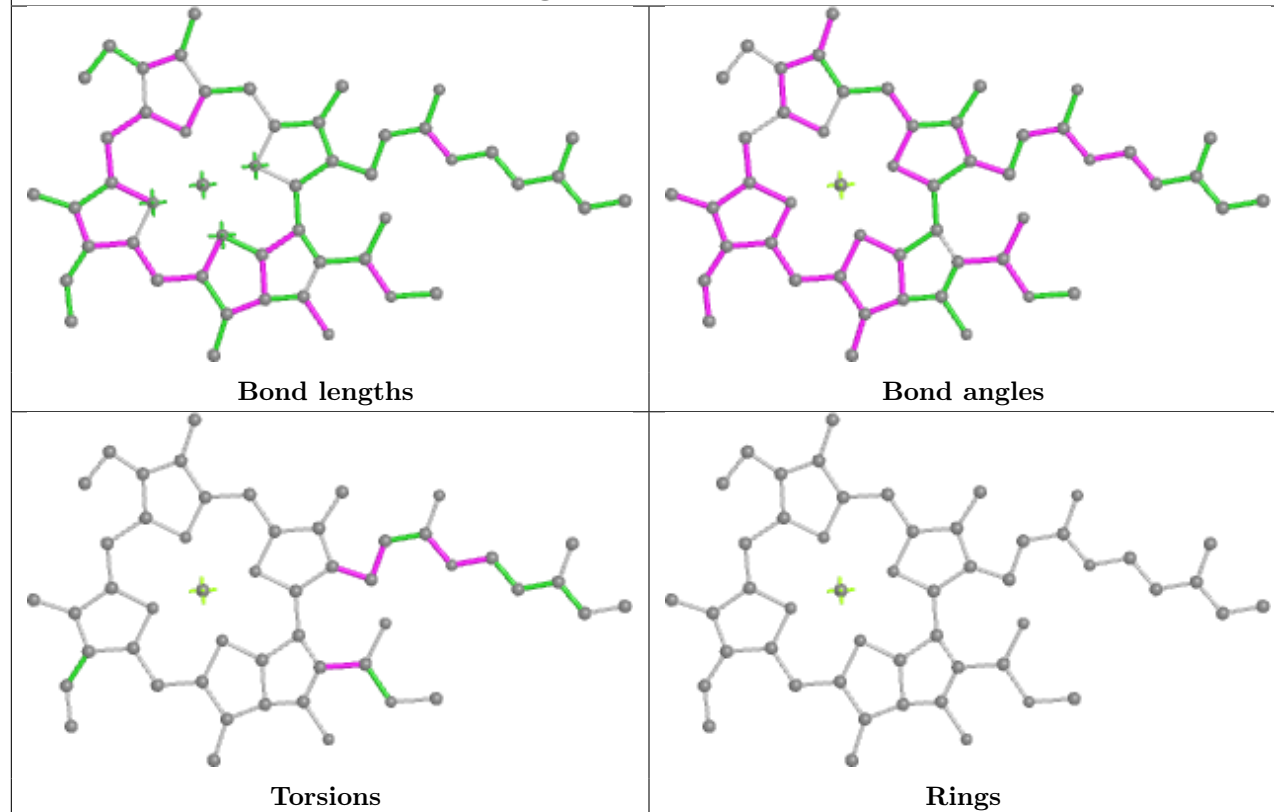


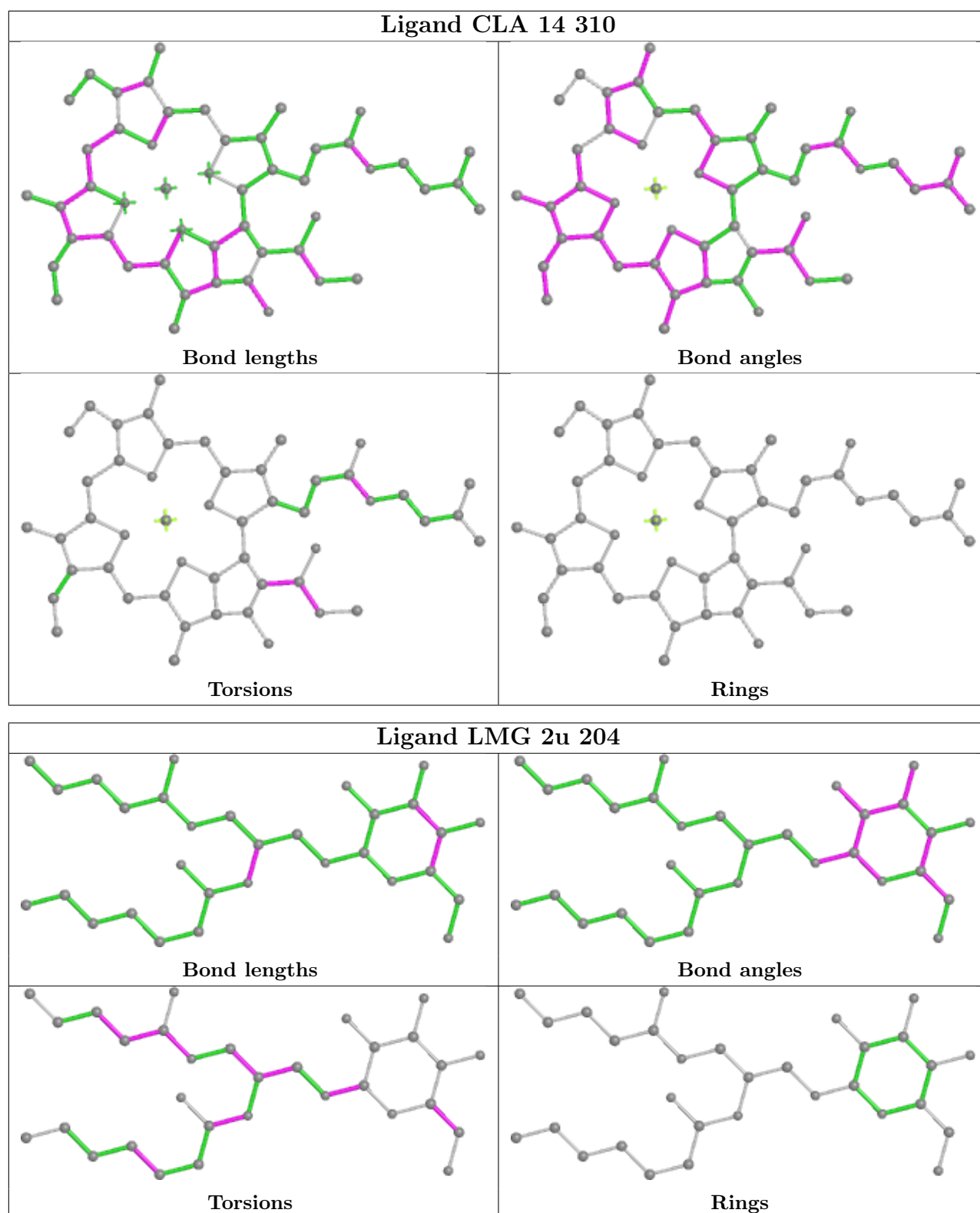


Ligand CLA 7 309

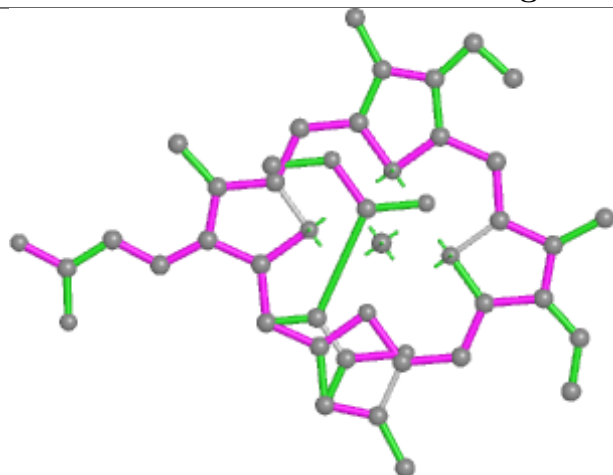


Ligand CLA 9 302

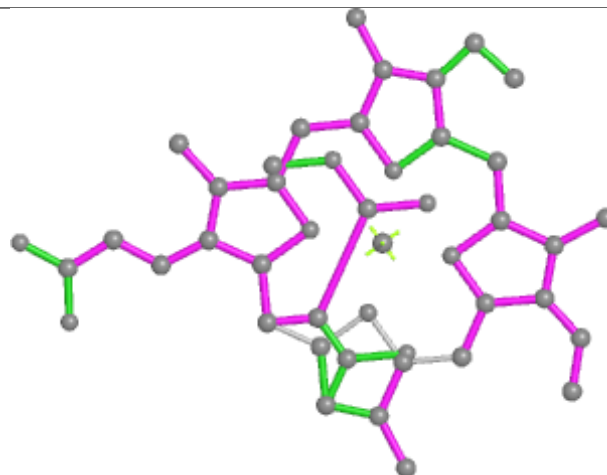




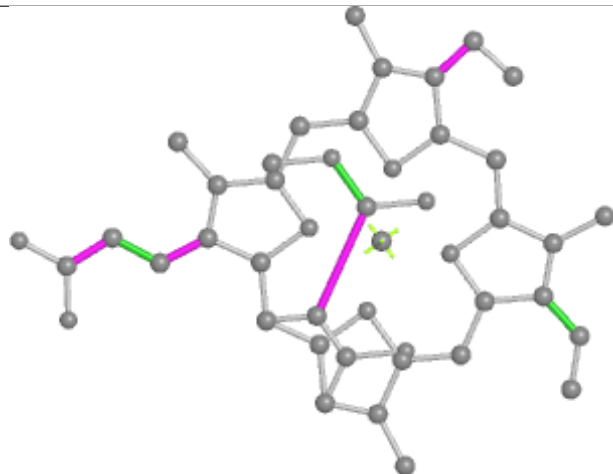
Ligand KC1 3 304



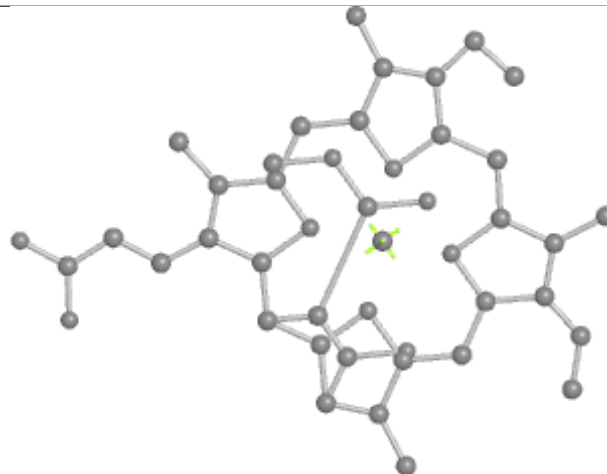
Bond lengths



Bond angles

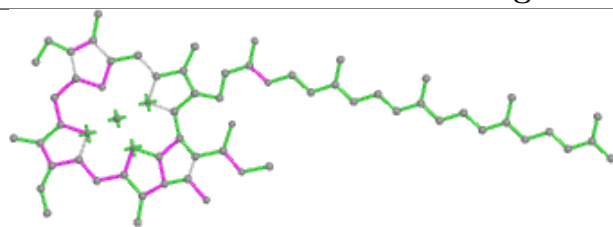


Torsions

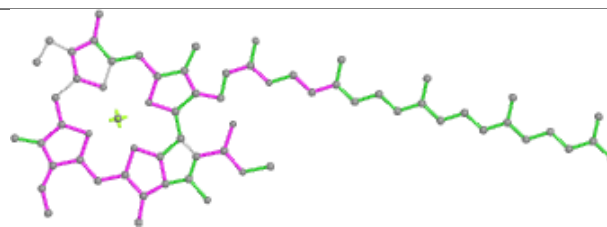


Rings

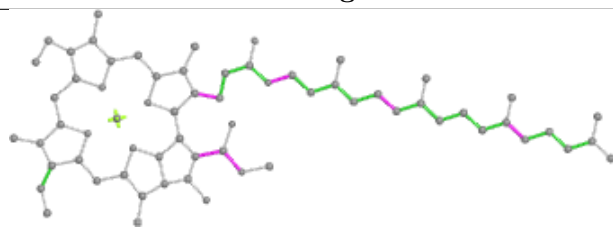
Ligand CLA A 835



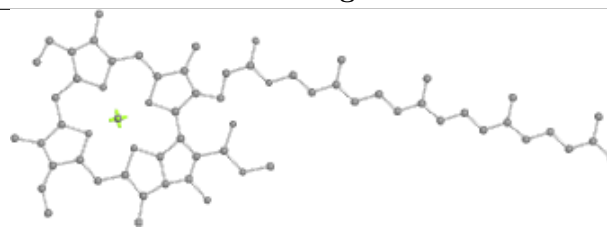
Bond lengths



Bond angles

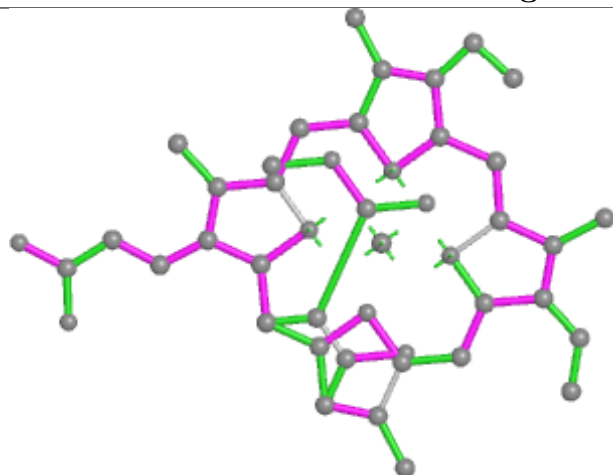


Torsions

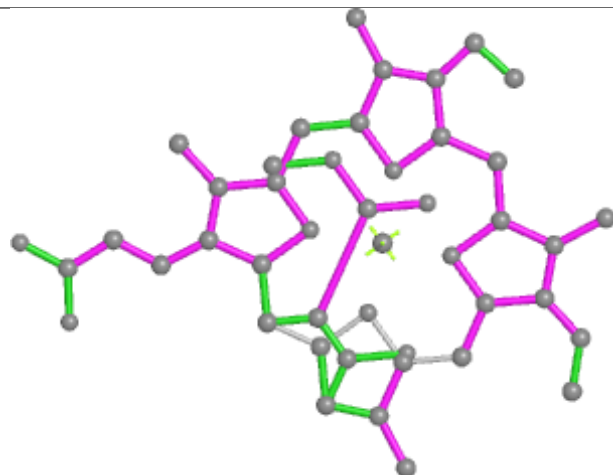


Rings

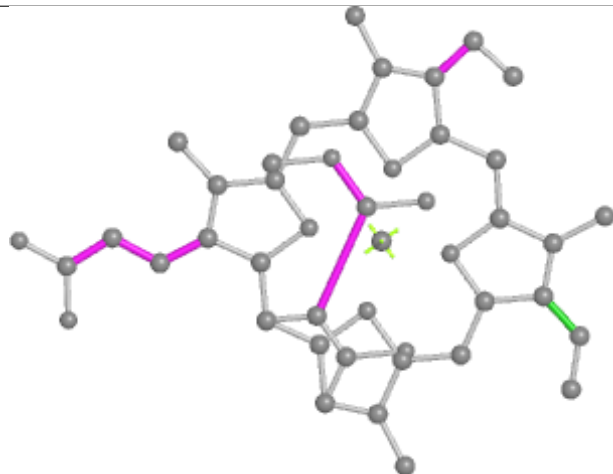
Ligand KC1 1 306



Bond lengths



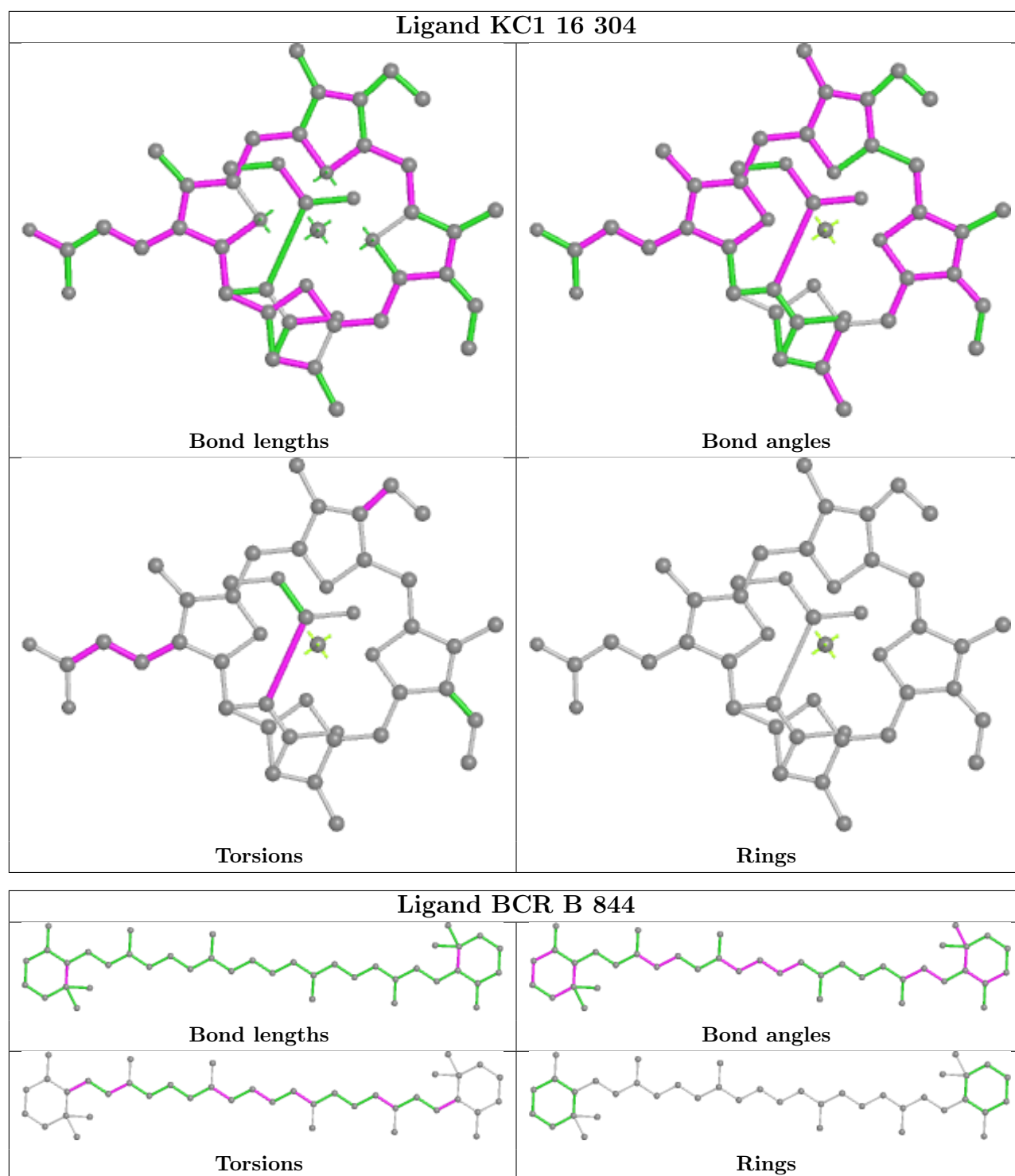
Bond angles

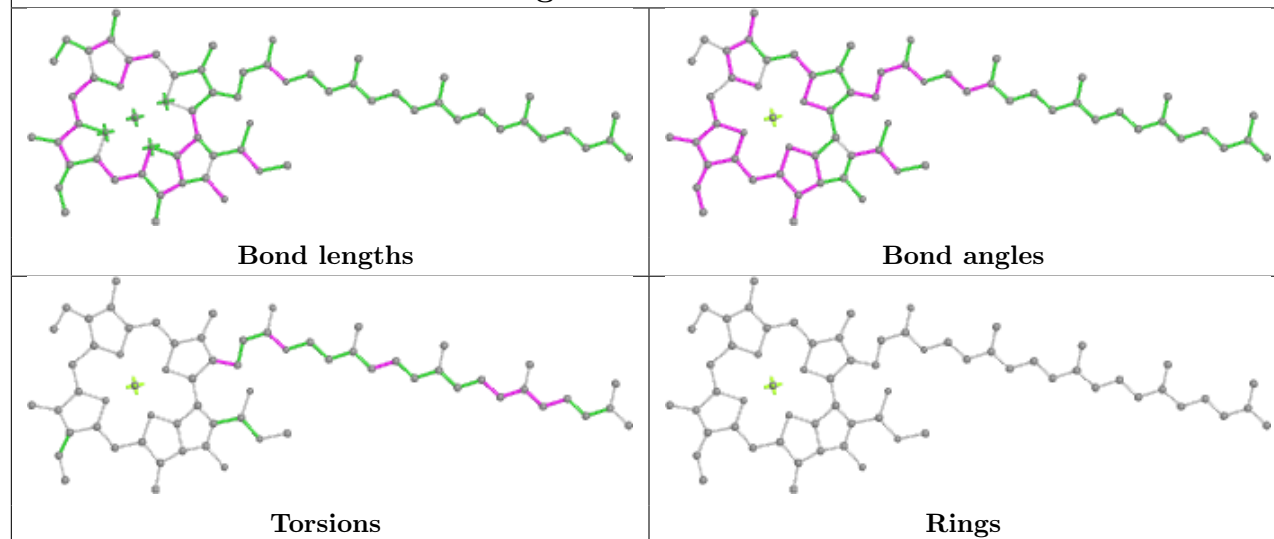
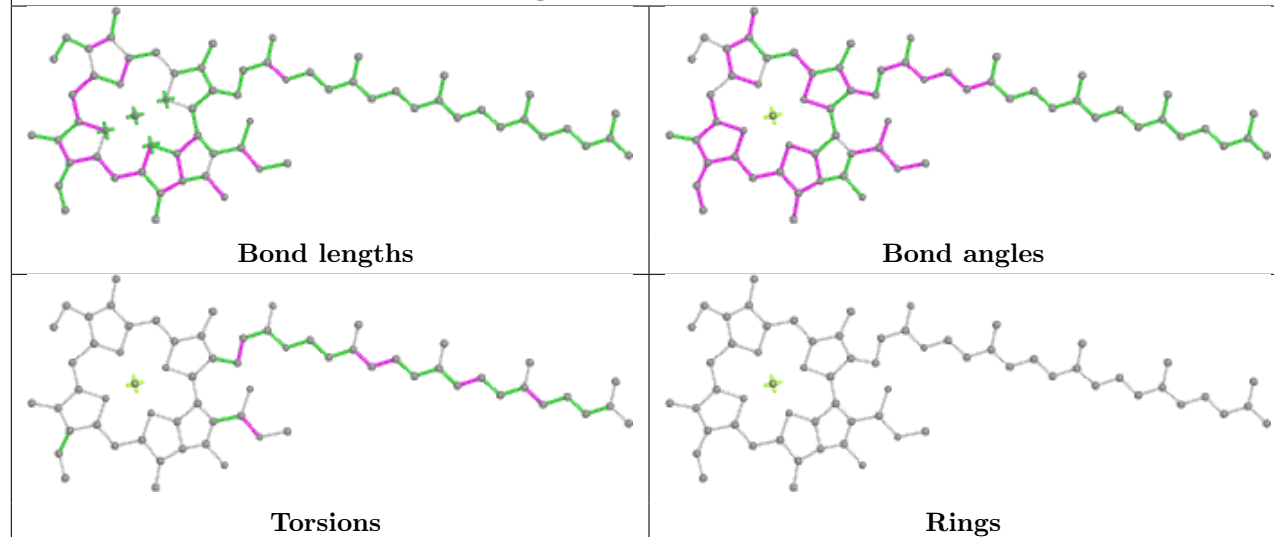


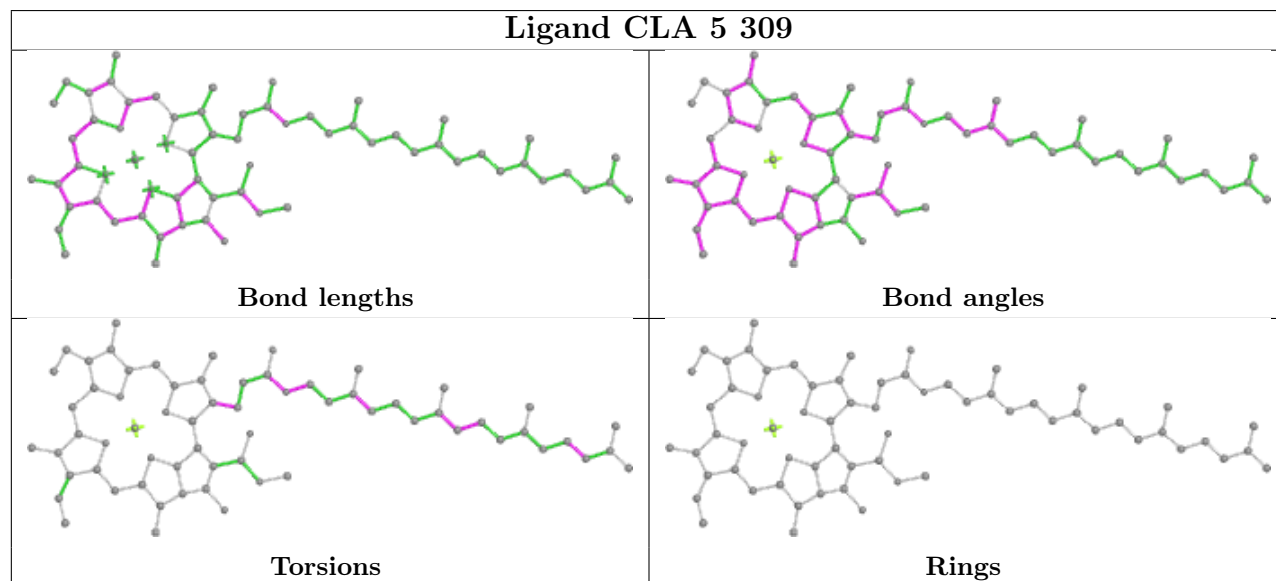
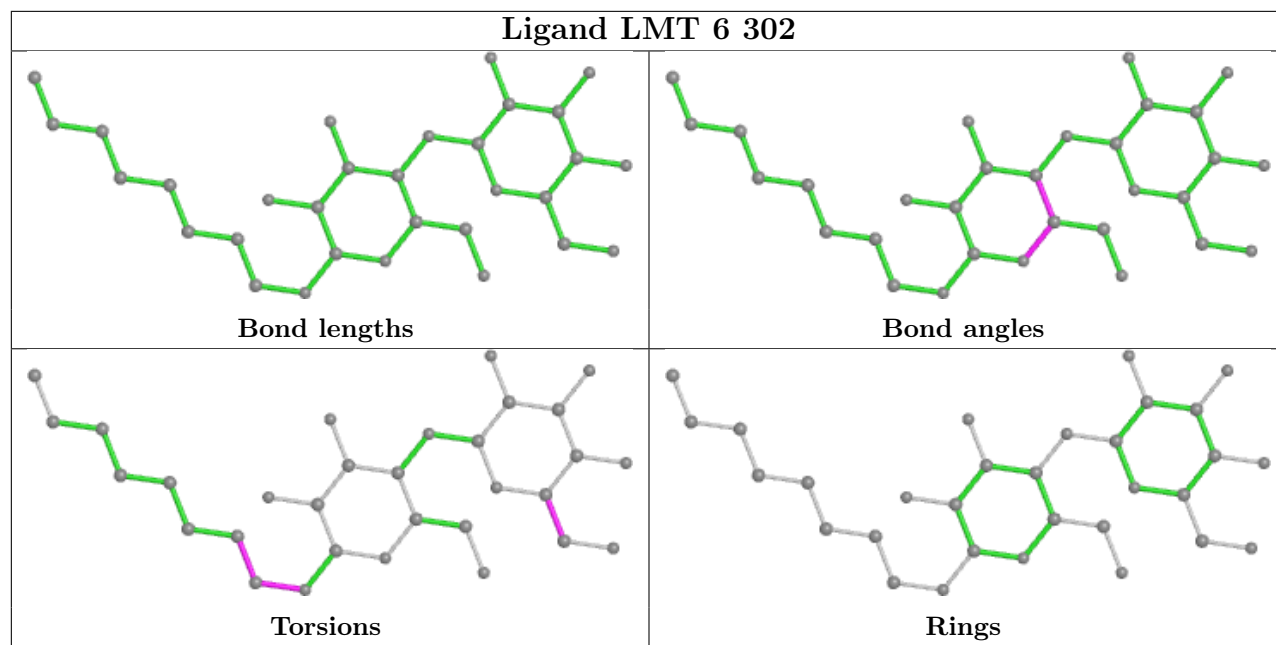
Torsions

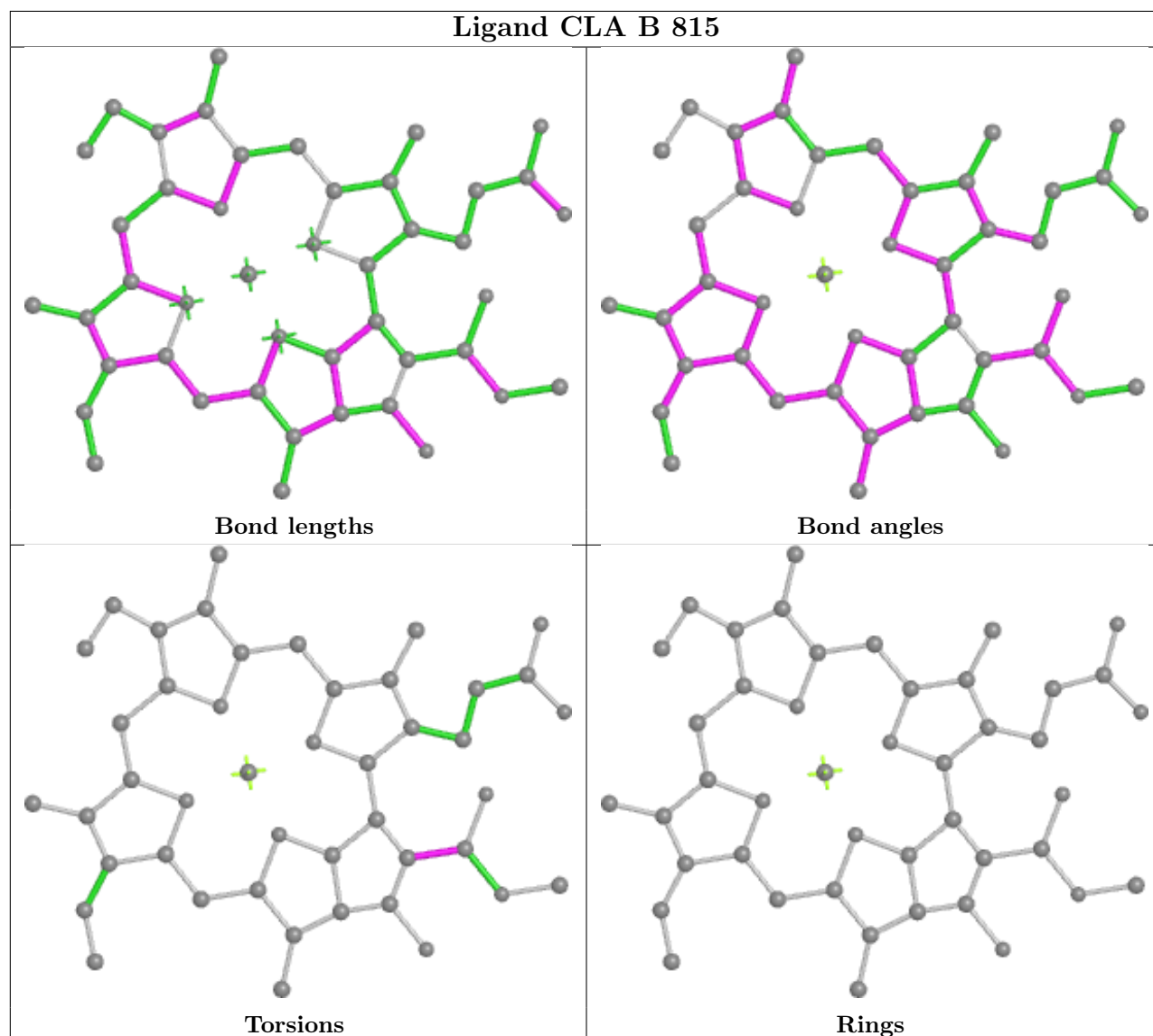
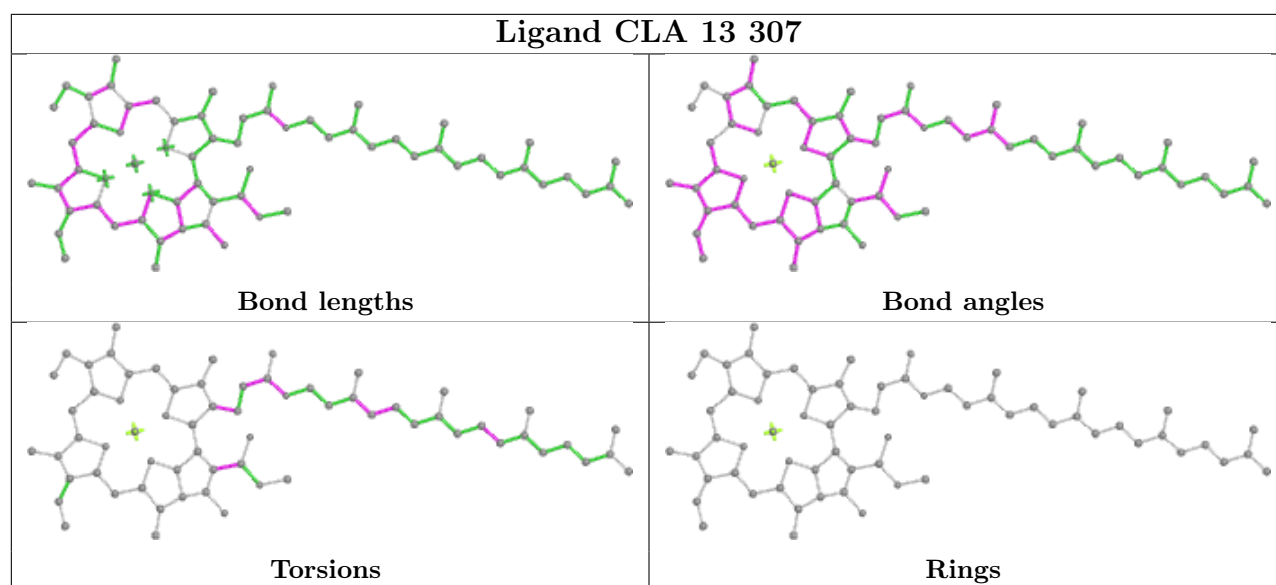


Rings

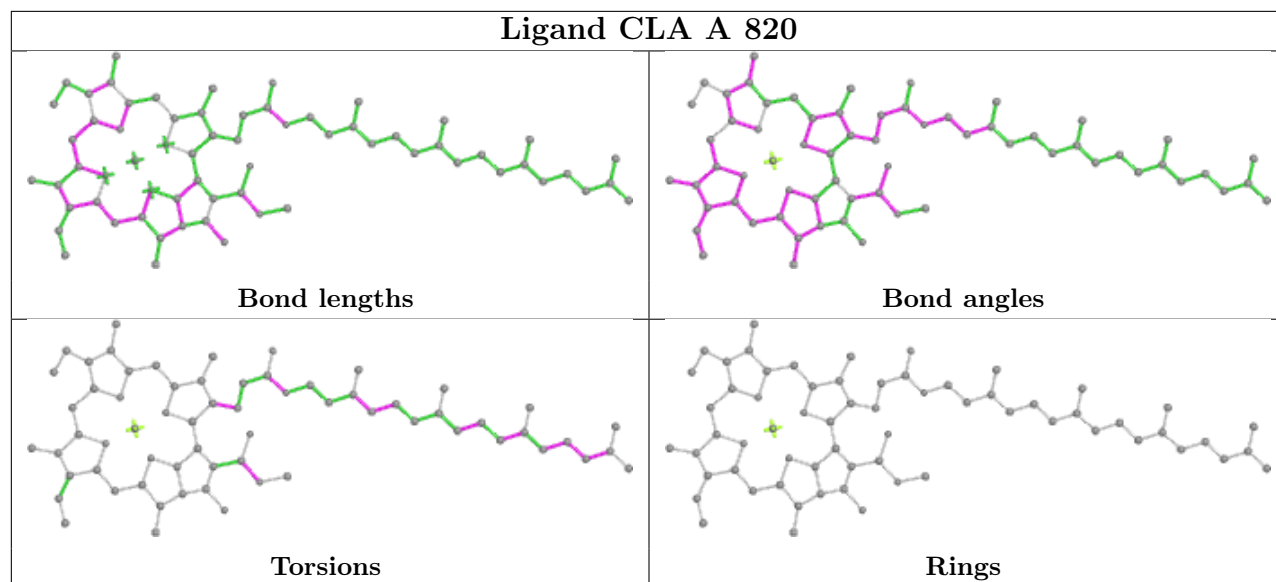


Ligand CLA 4 302**Ligand CLA A 822**

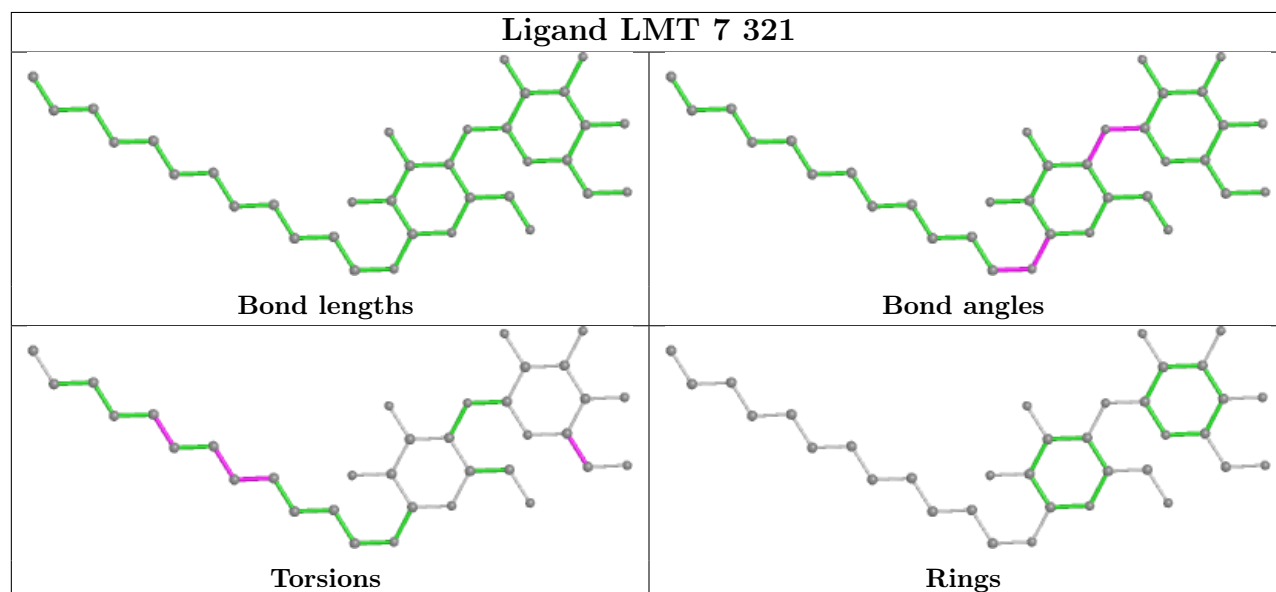




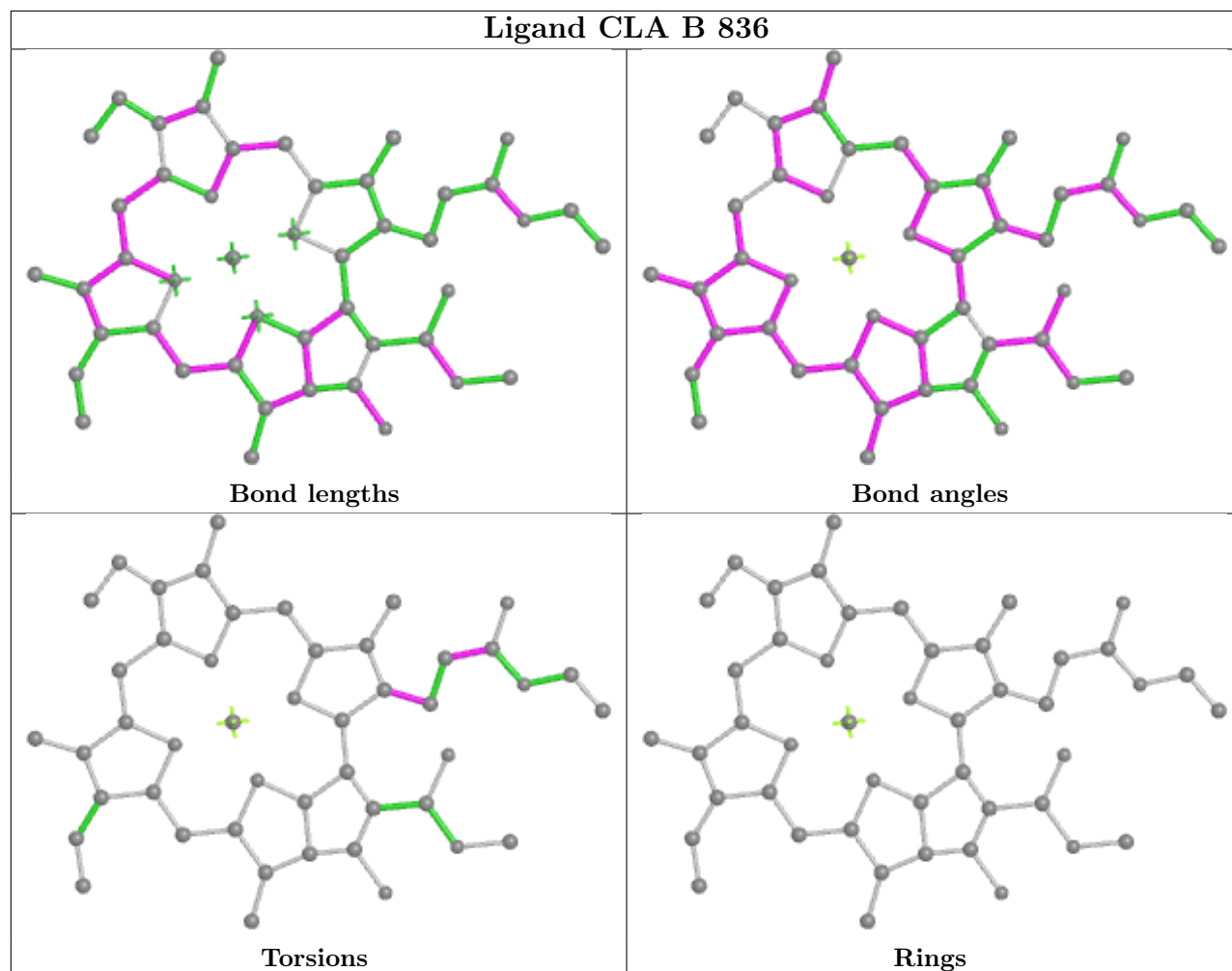
Ligand CLA A 820



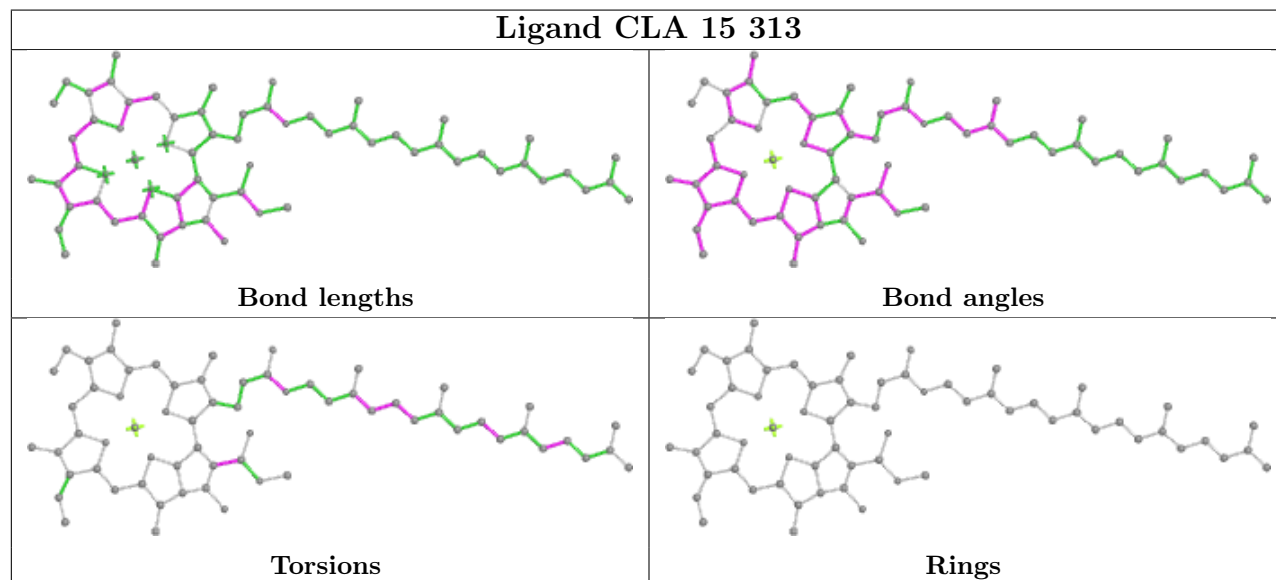
Ligand LMT 7 321

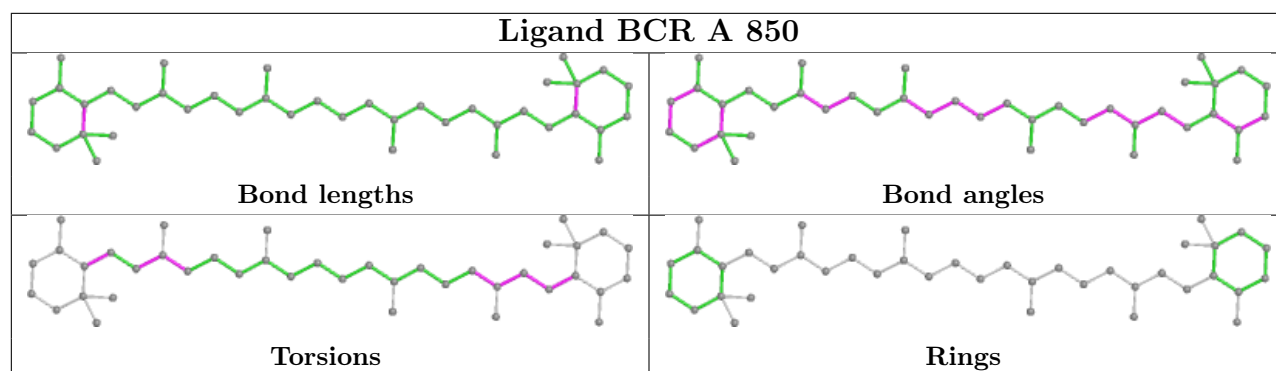
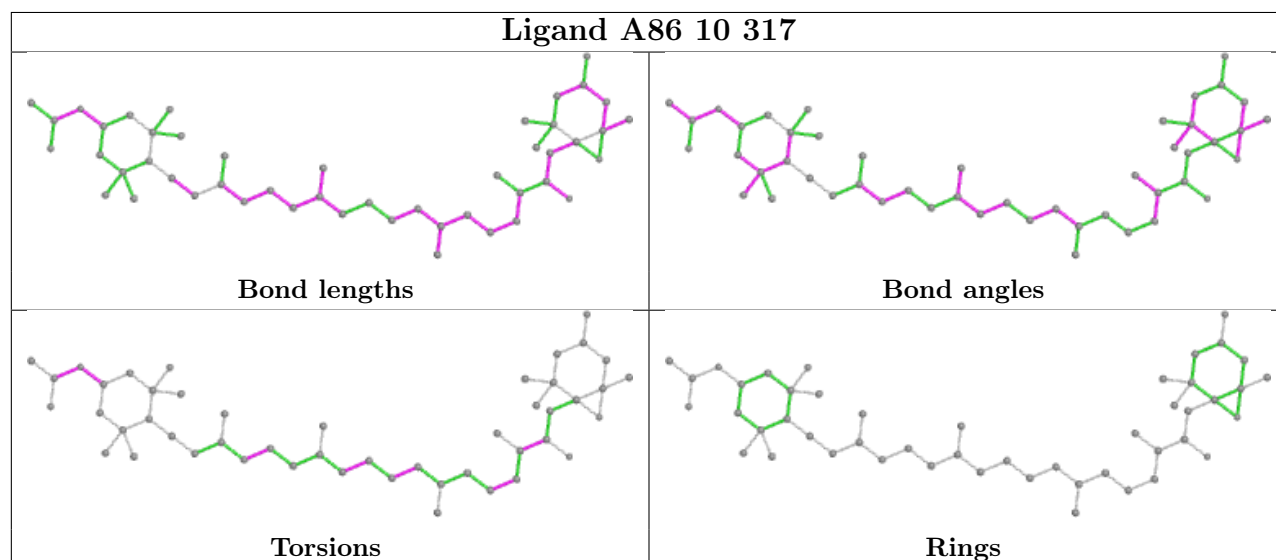
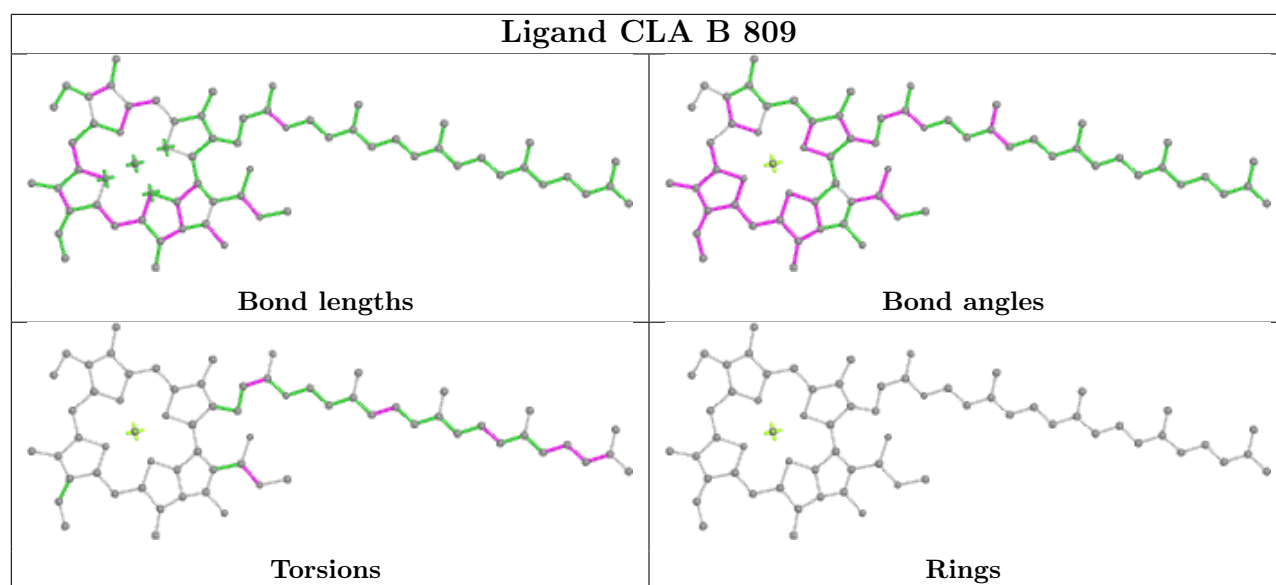


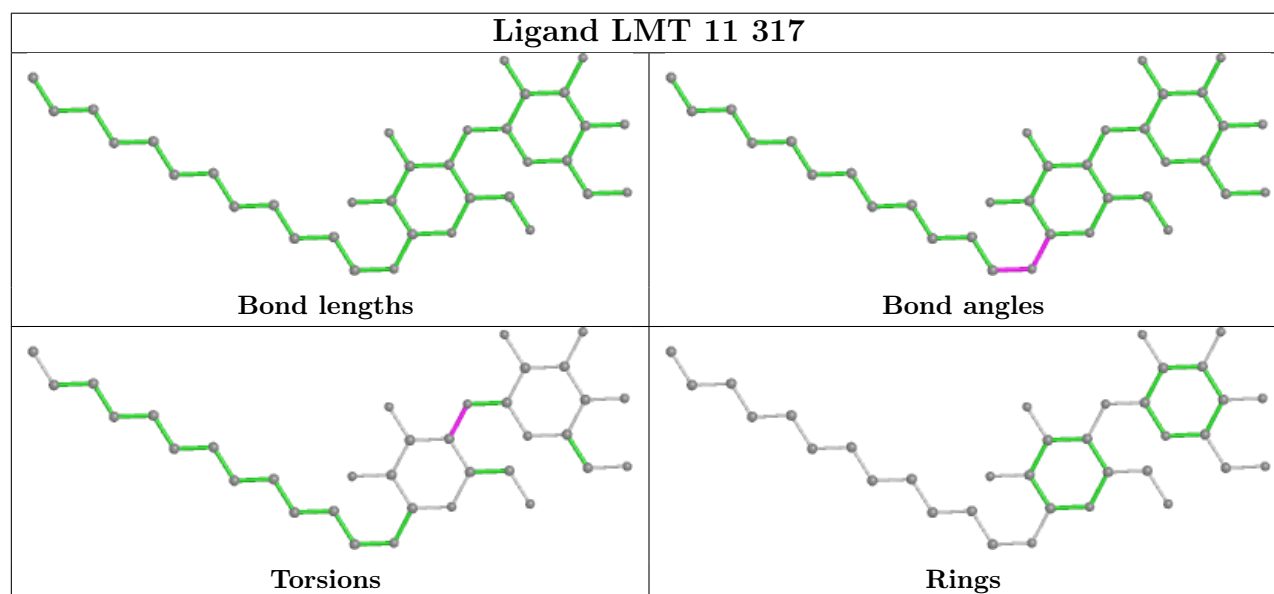
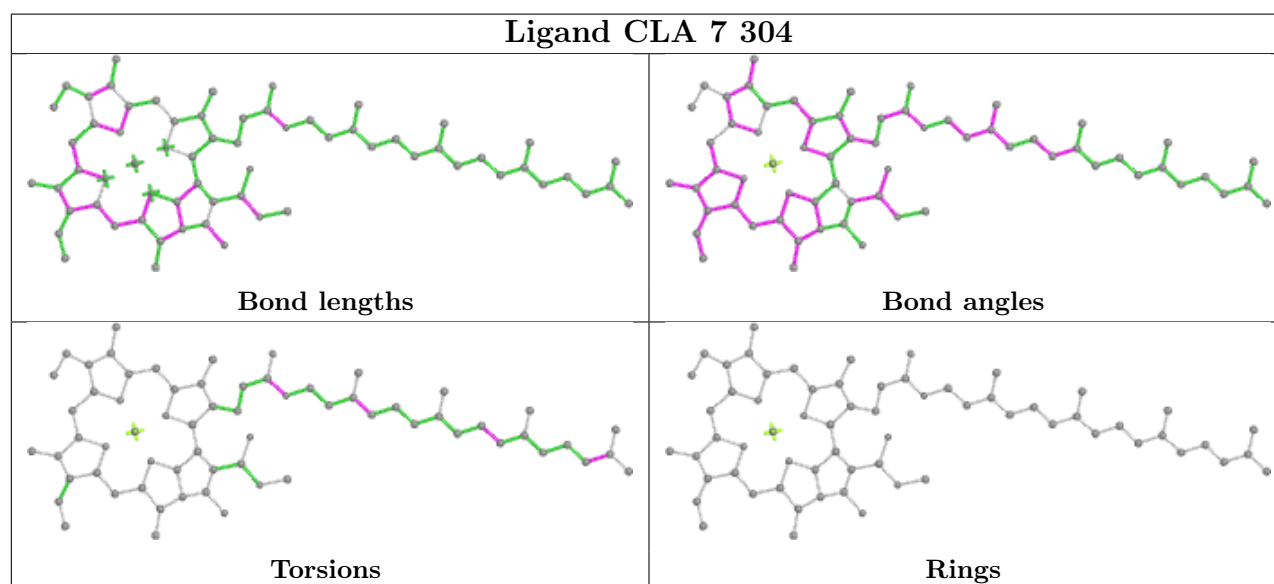
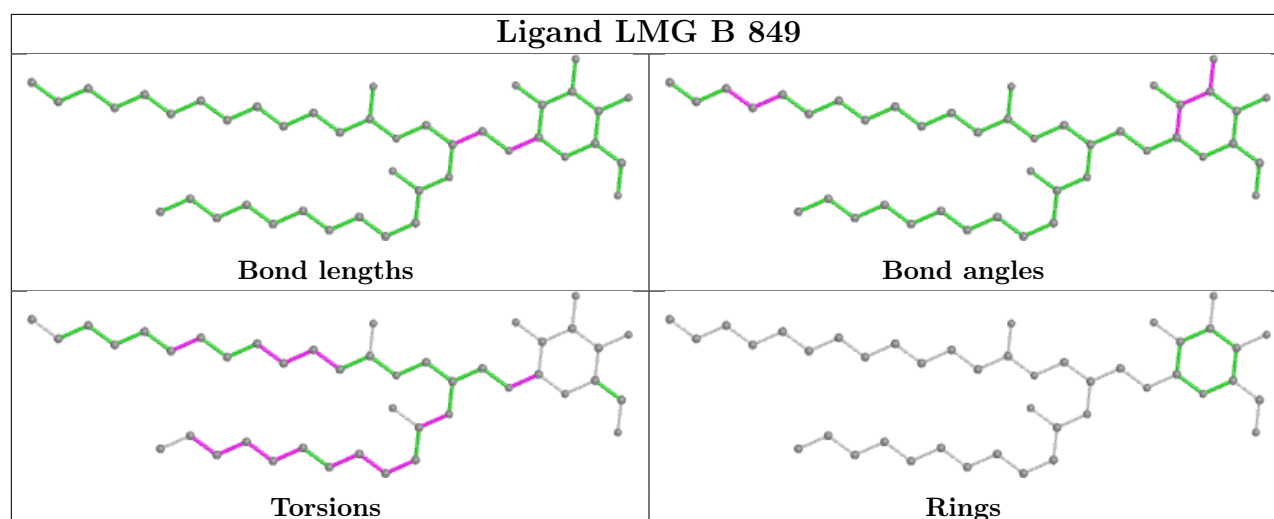
Ligand CLA B 836

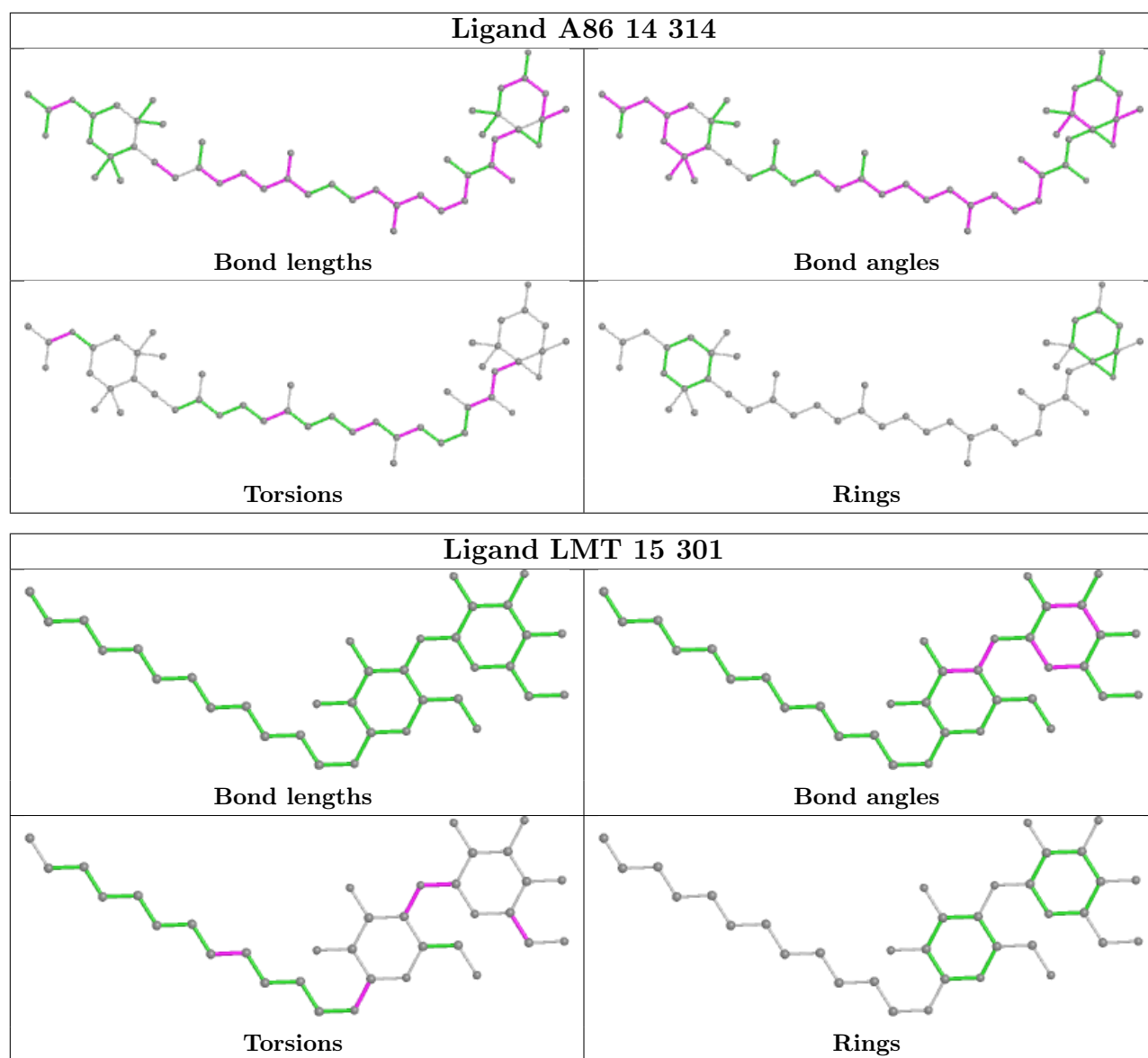


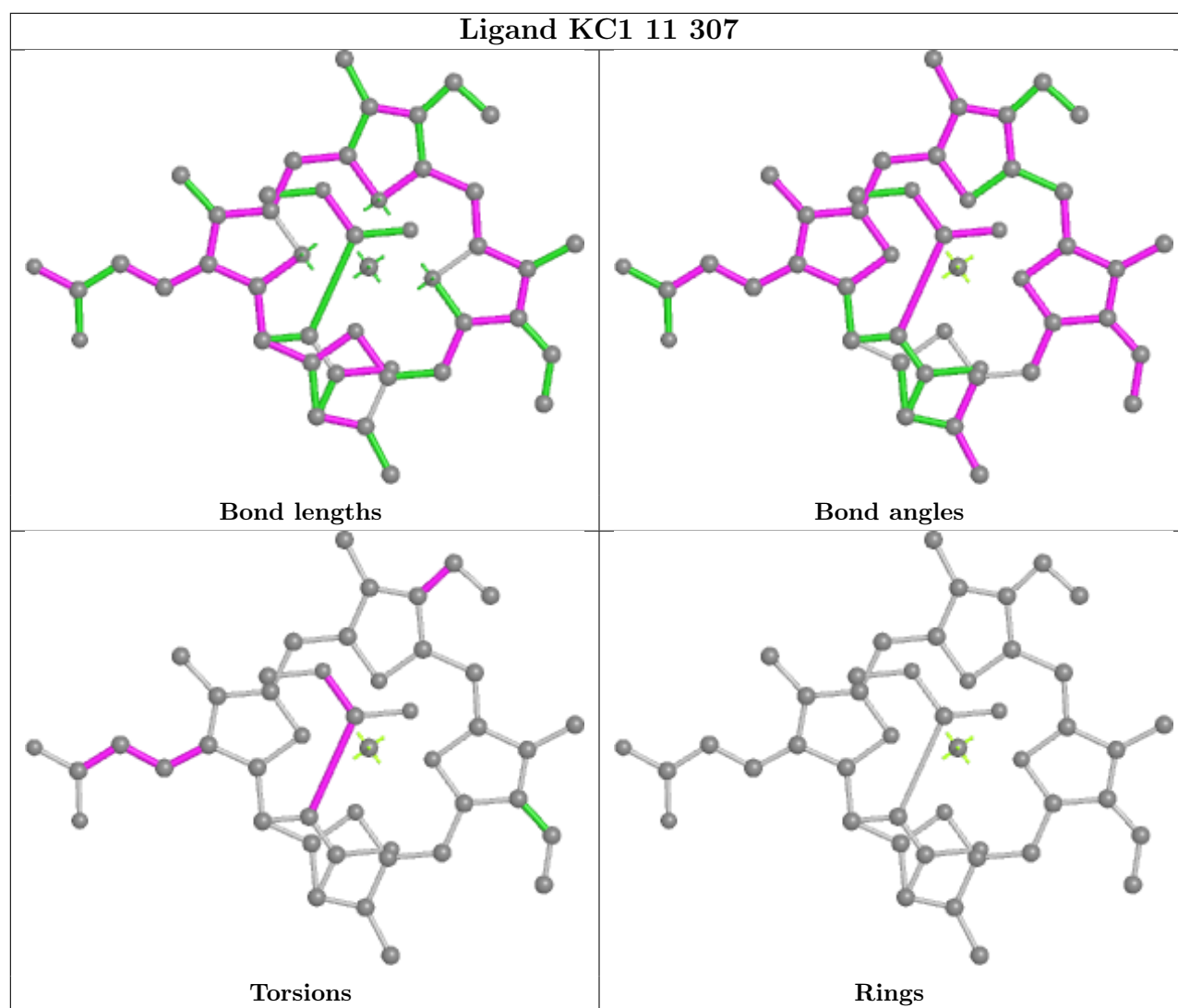
Ligand CLA 15 313

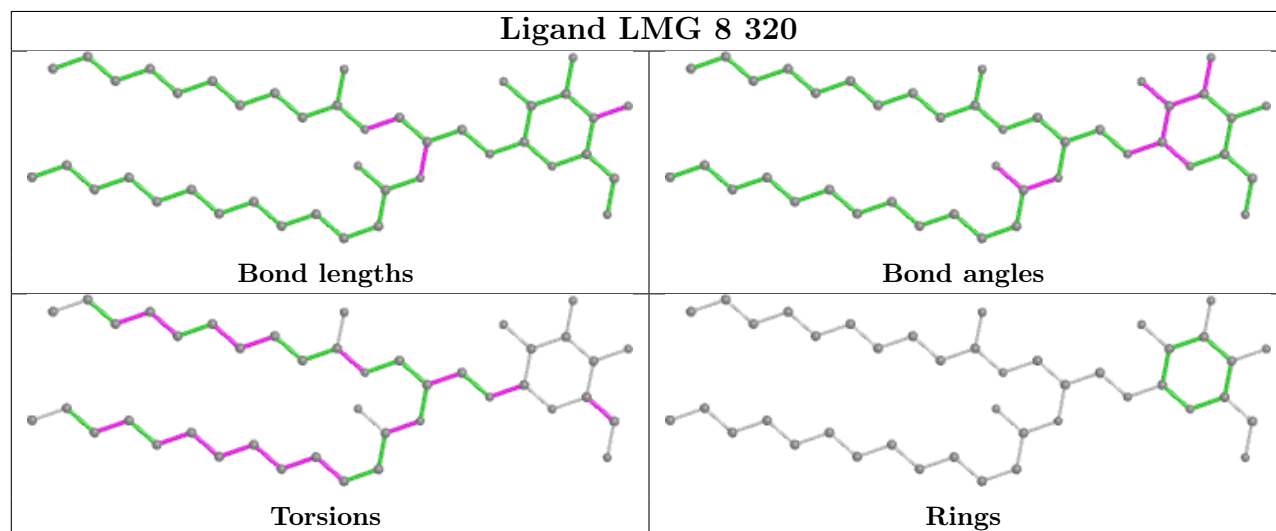
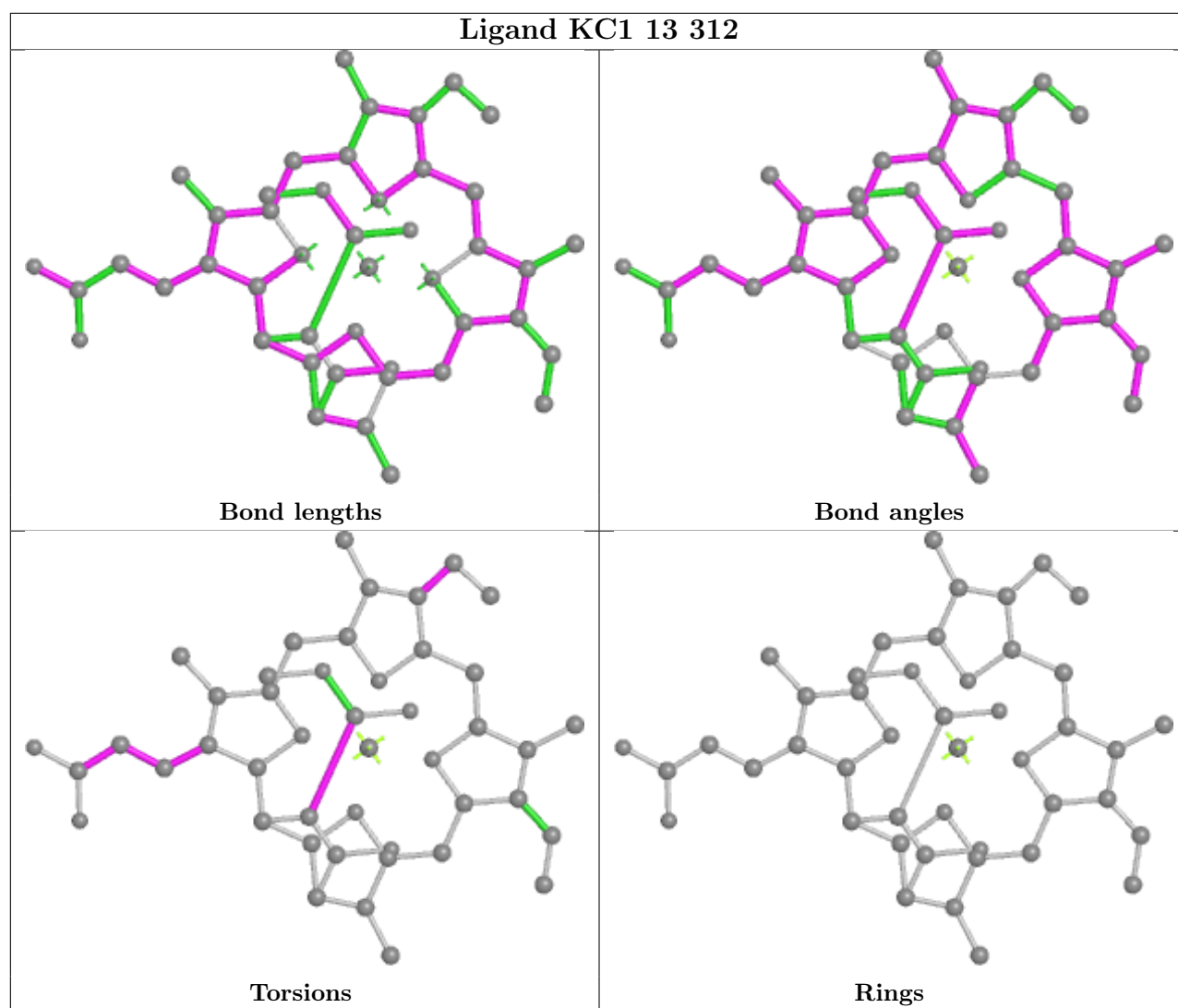


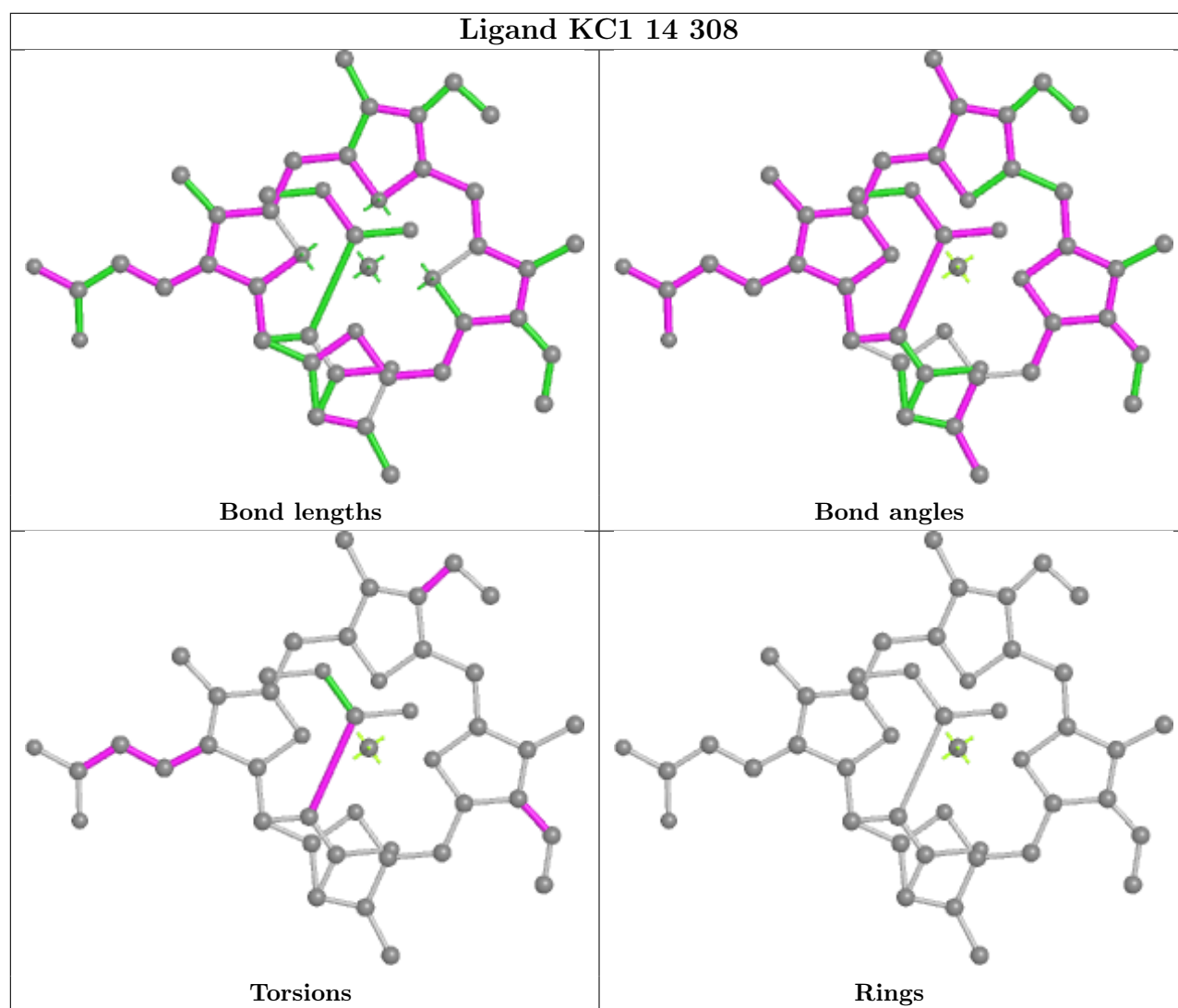


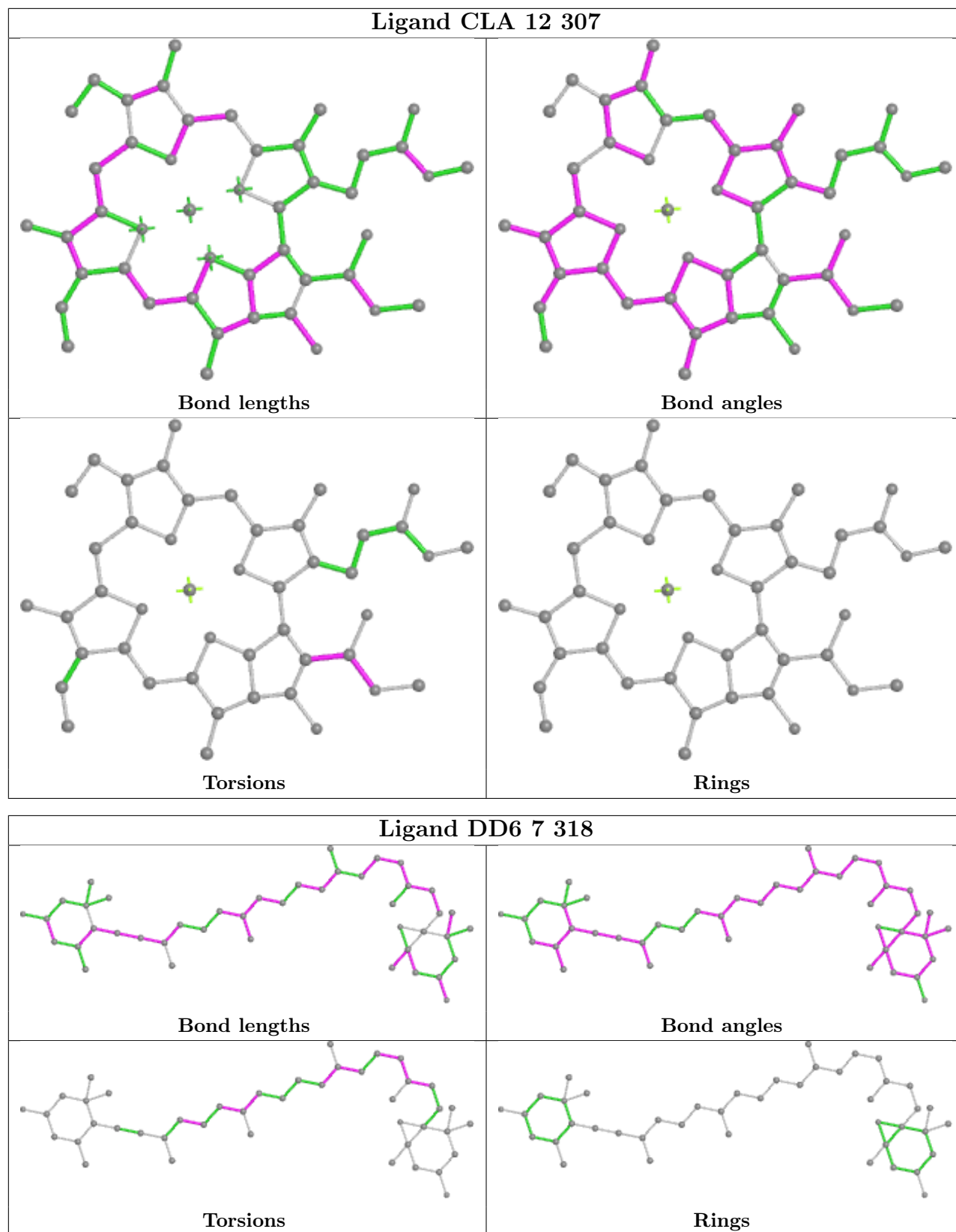


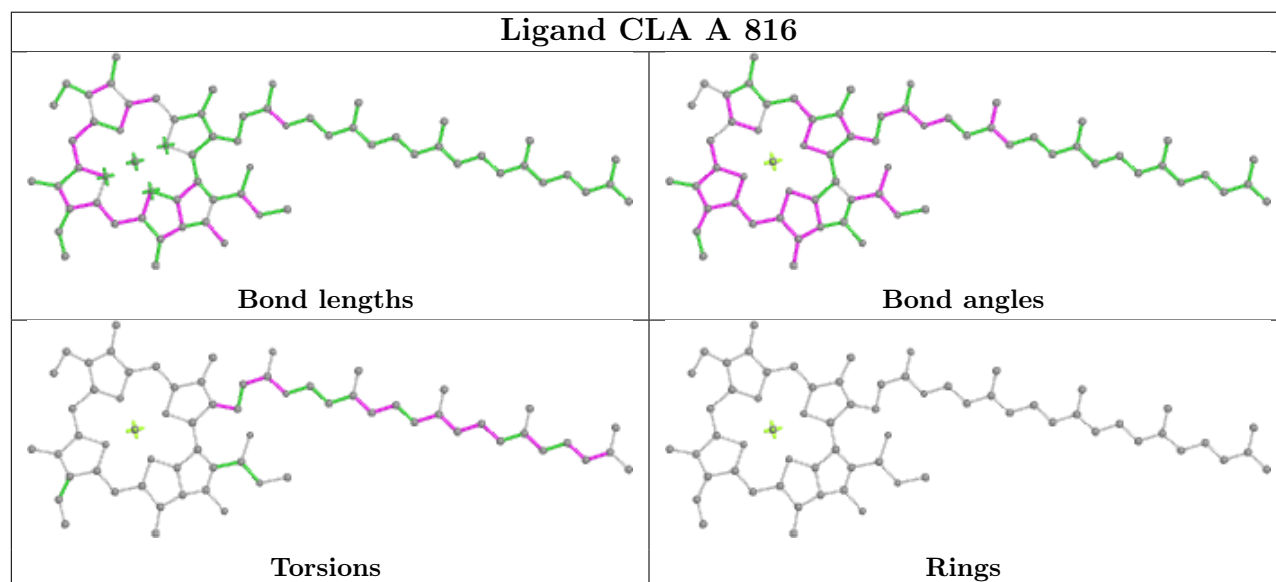
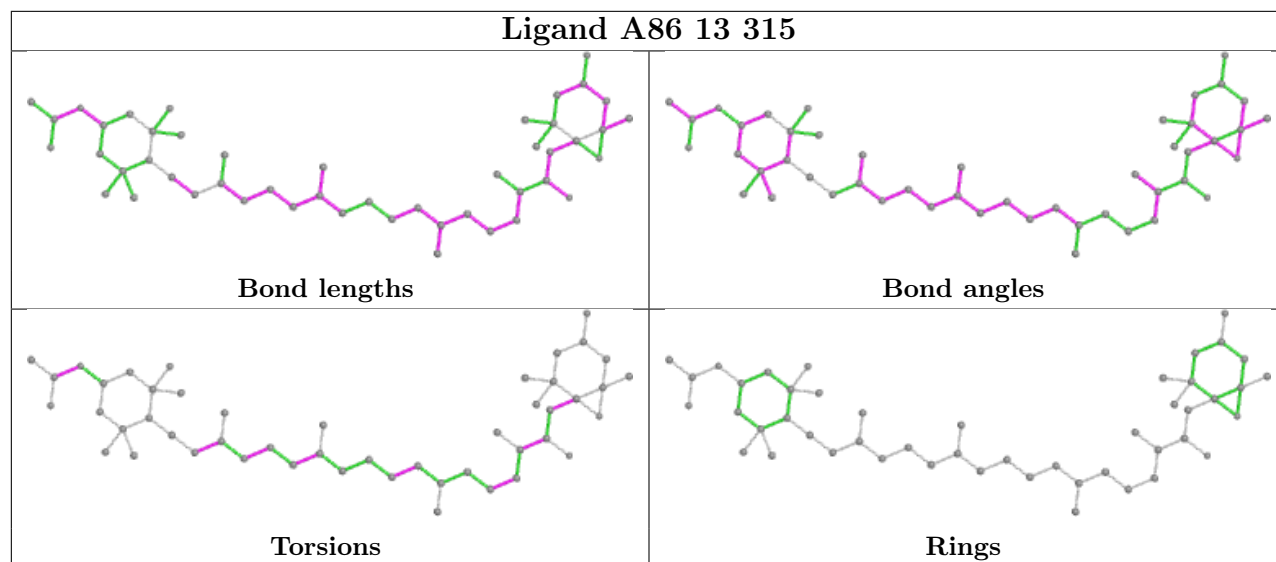
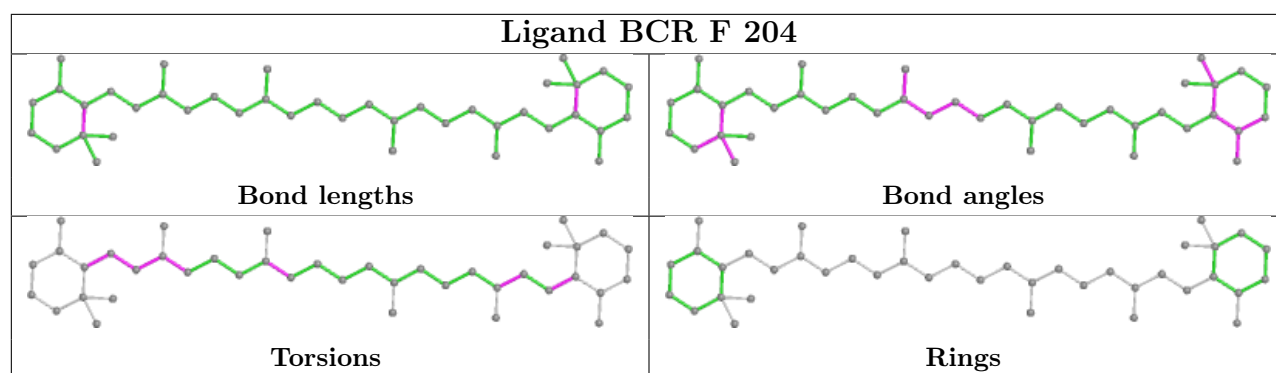


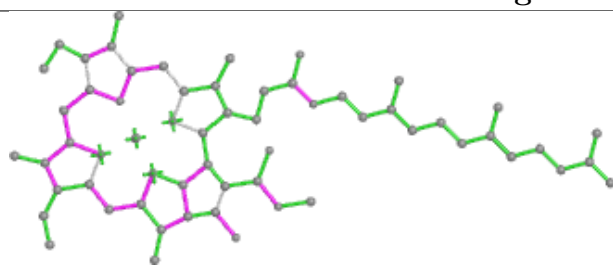
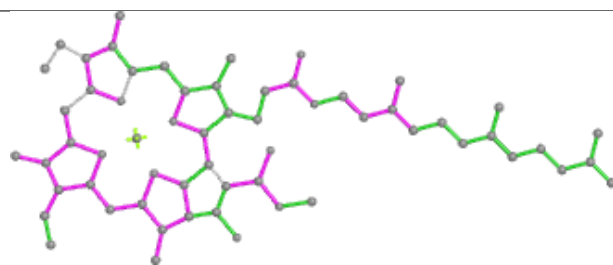
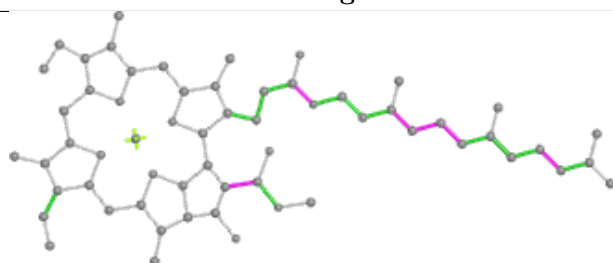
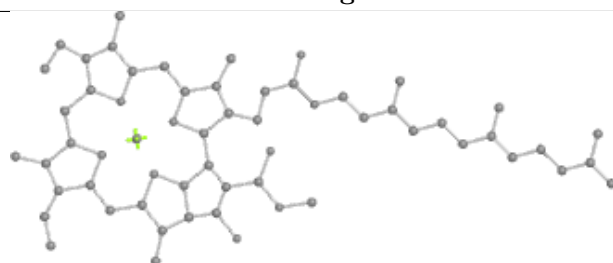
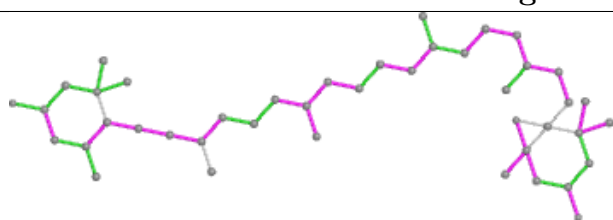
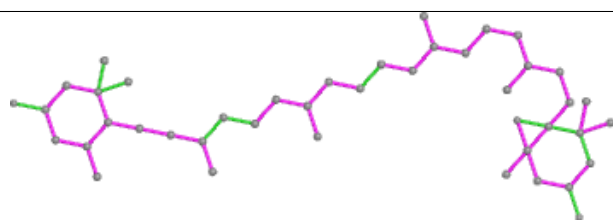
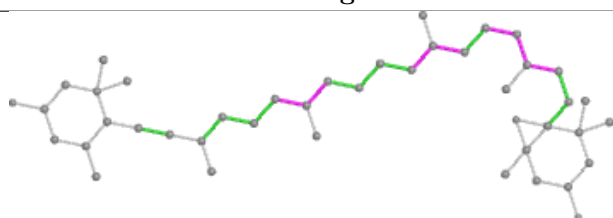
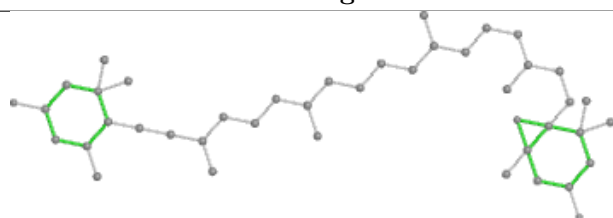




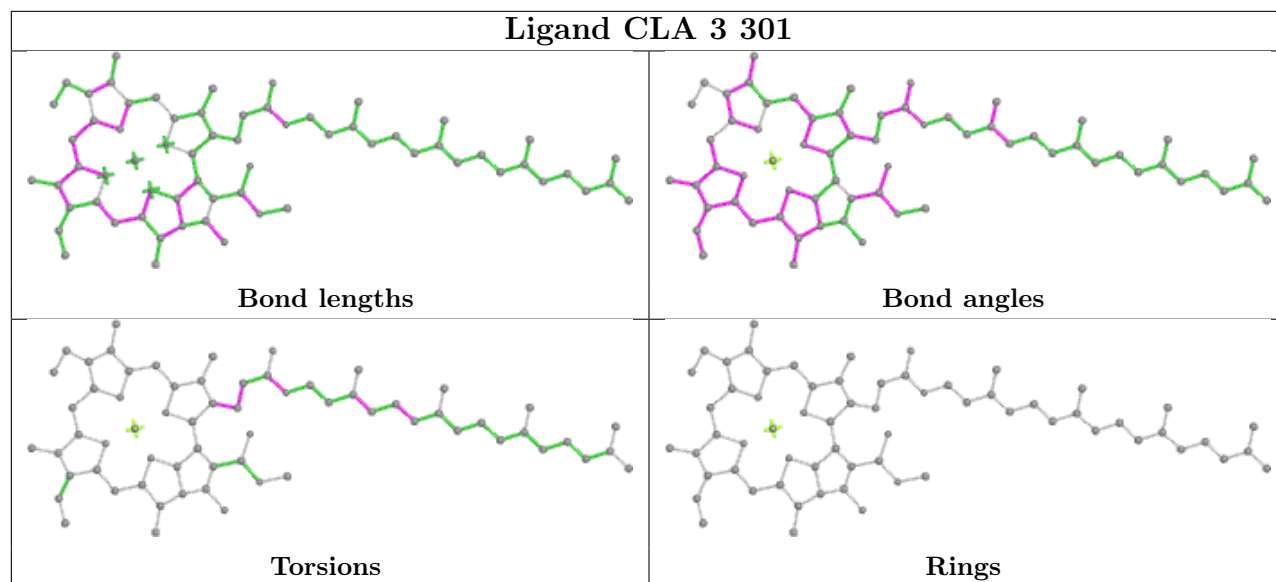




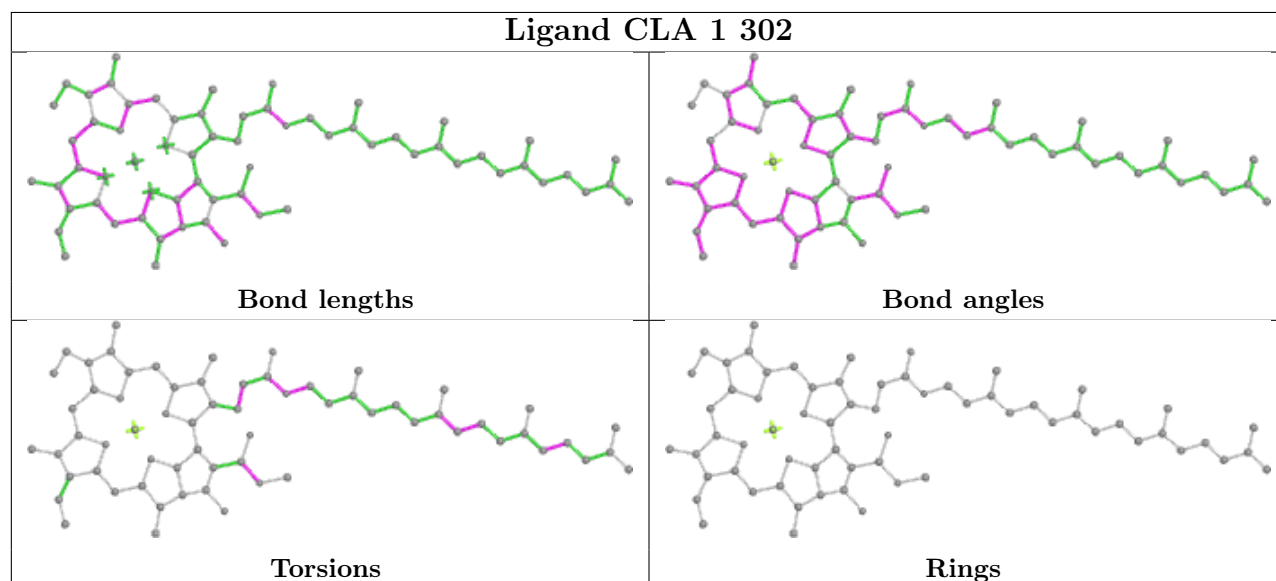


Ligand CLA B 834**Bond lengths****Bond angles****Torsions****Rings****Ligand DD6 6 319****Bond lengths****Bond angles****Torsions****Rings**

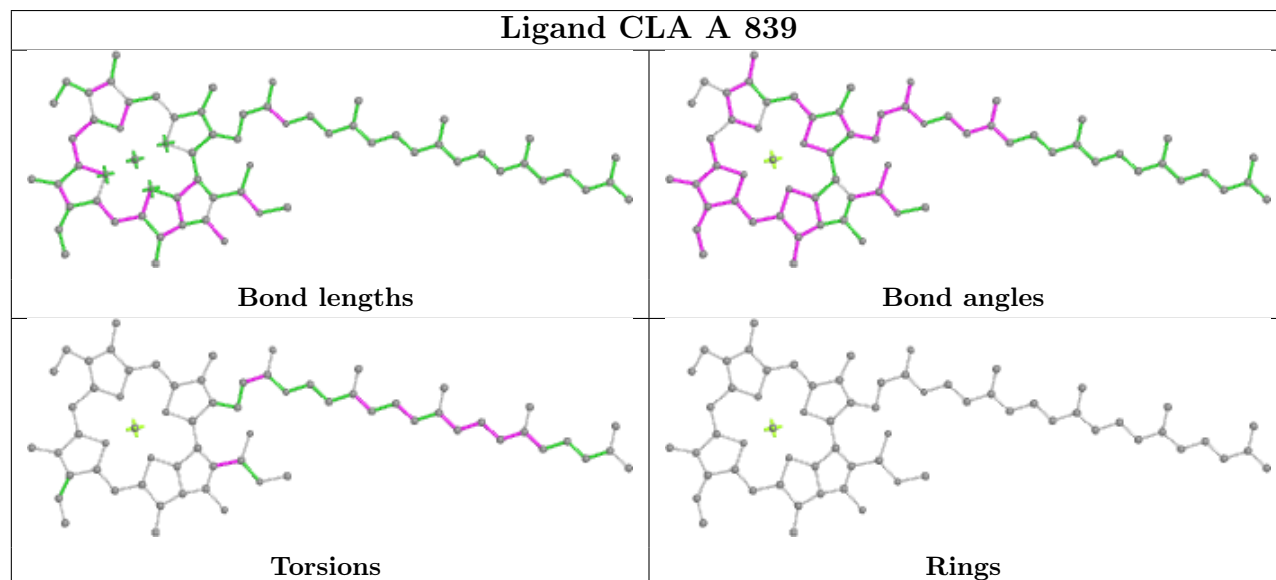
Ligand CLA 3 301

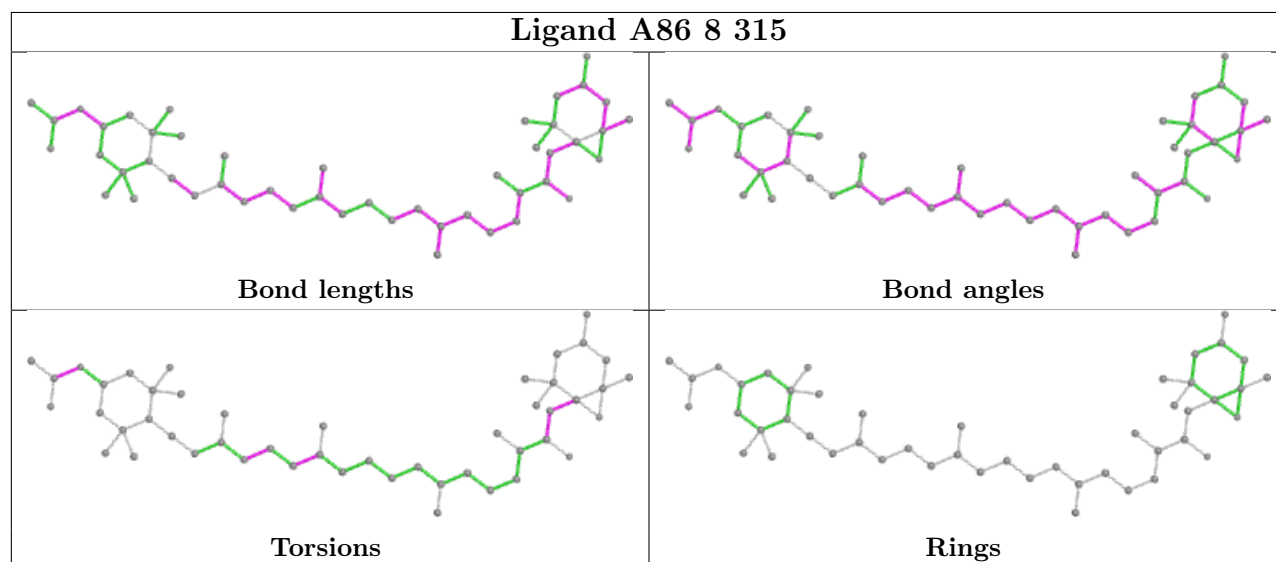
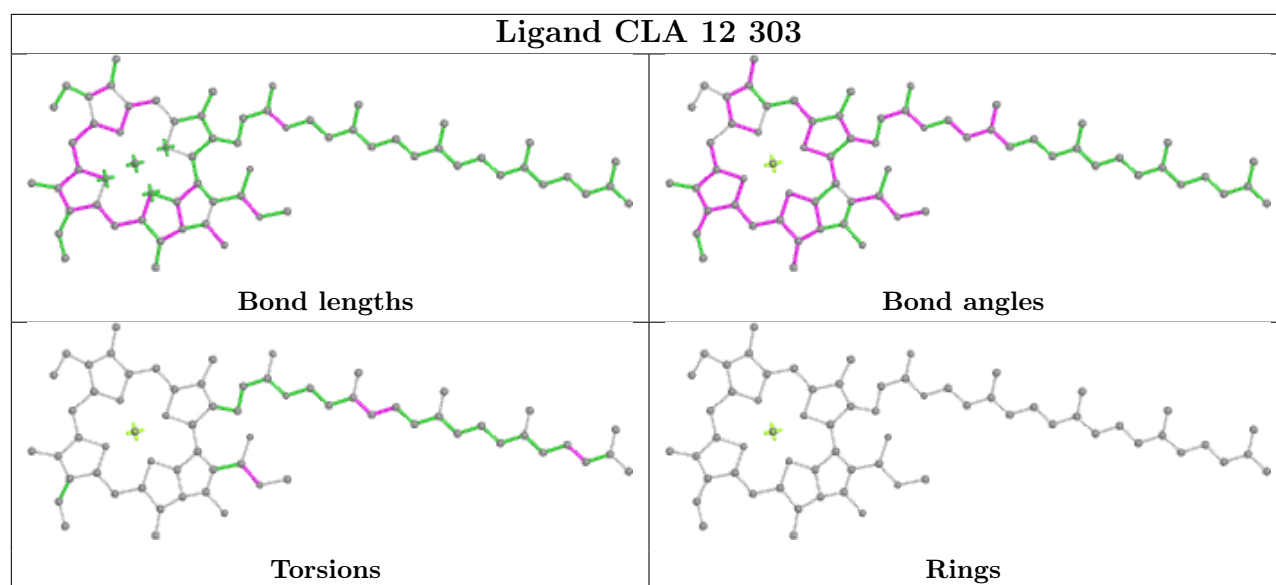


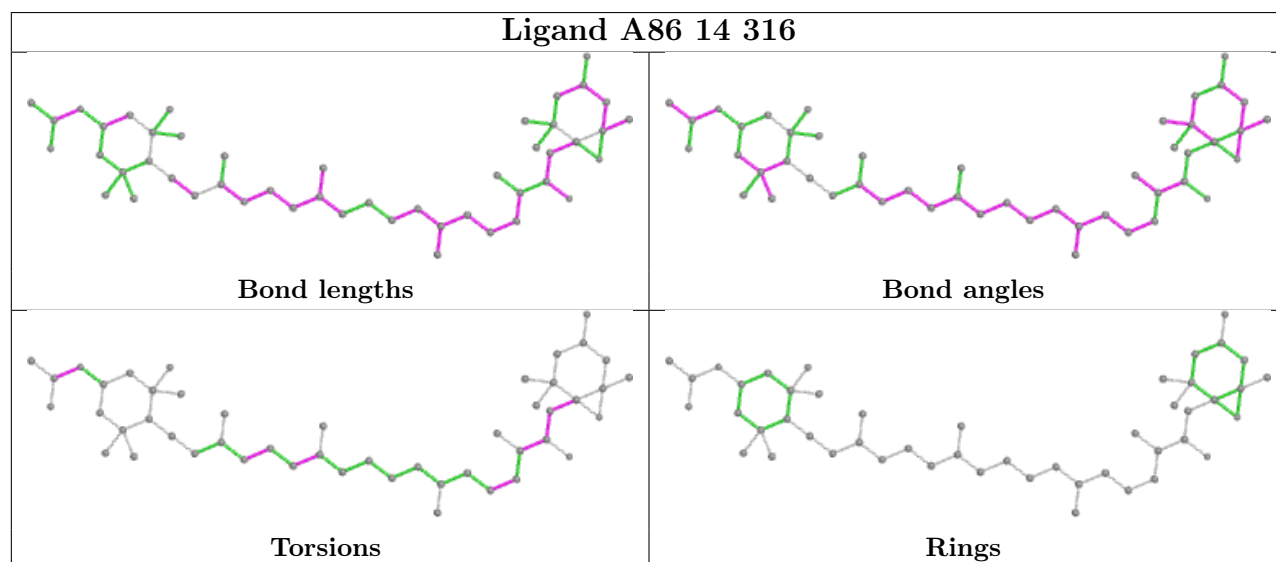
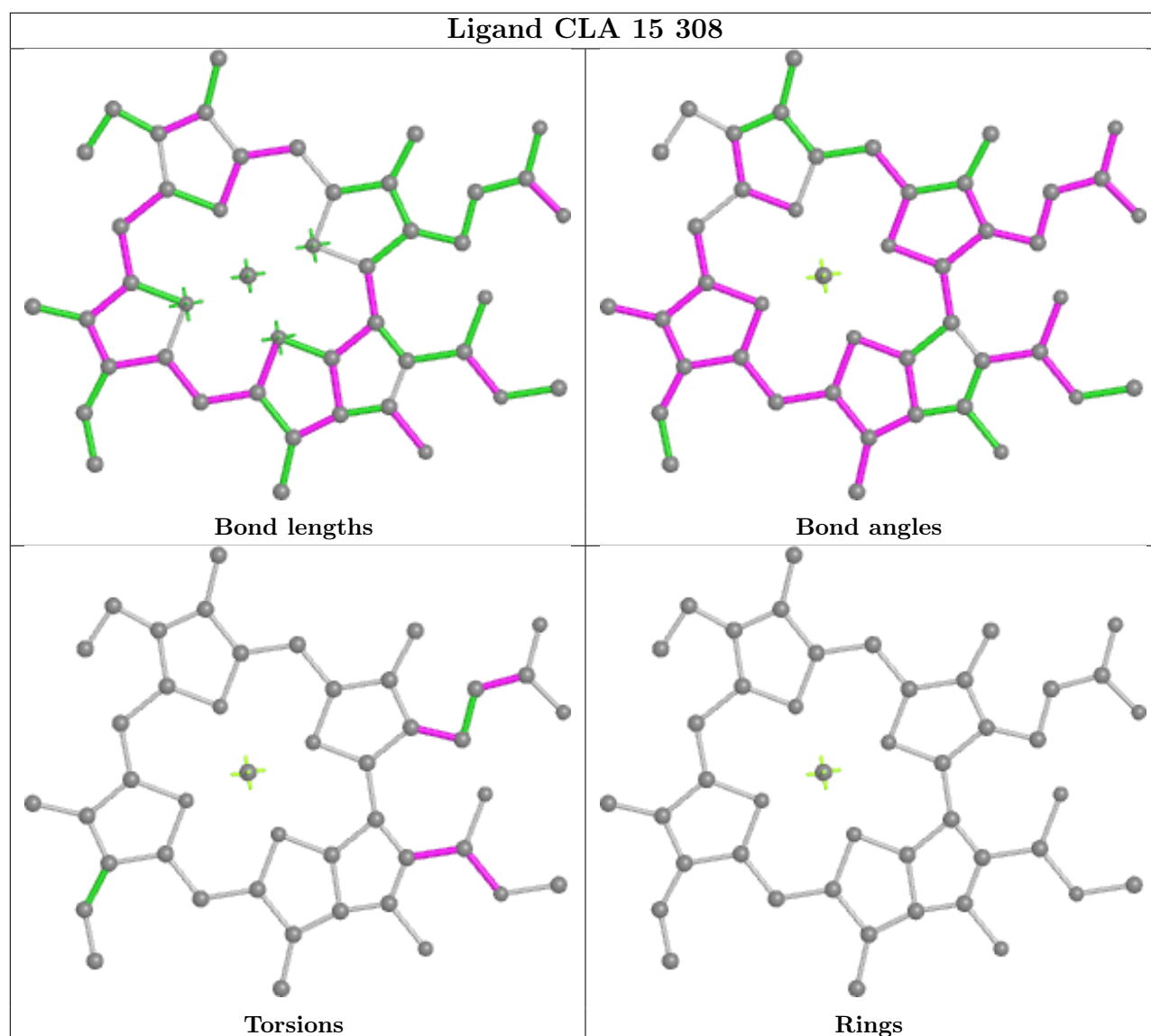
Ligand CLA 1 302



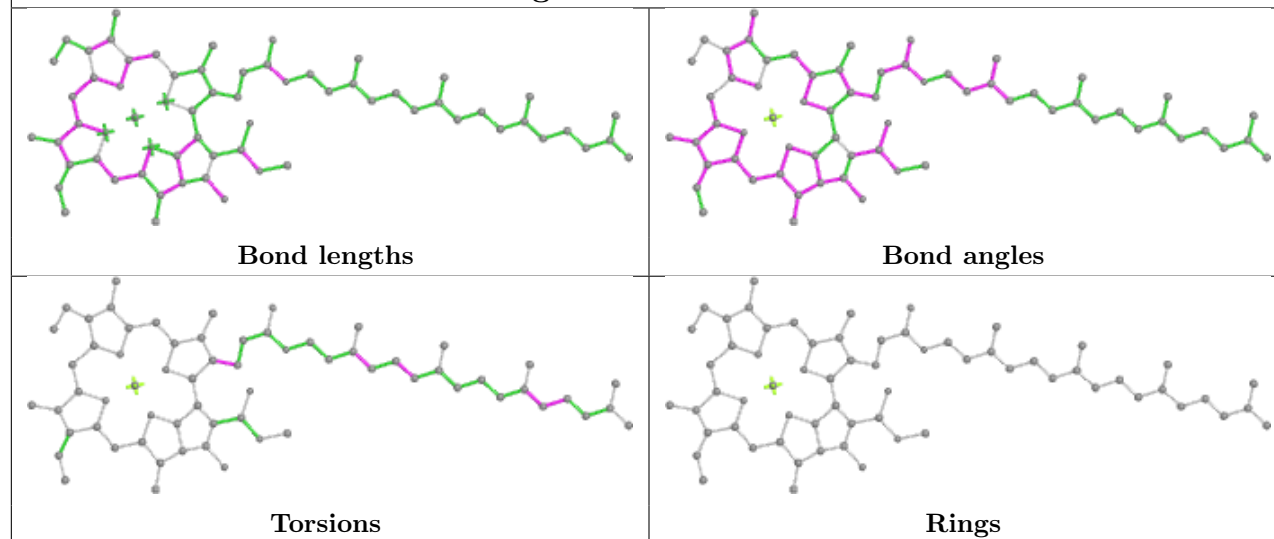
Ligand CLA A 839



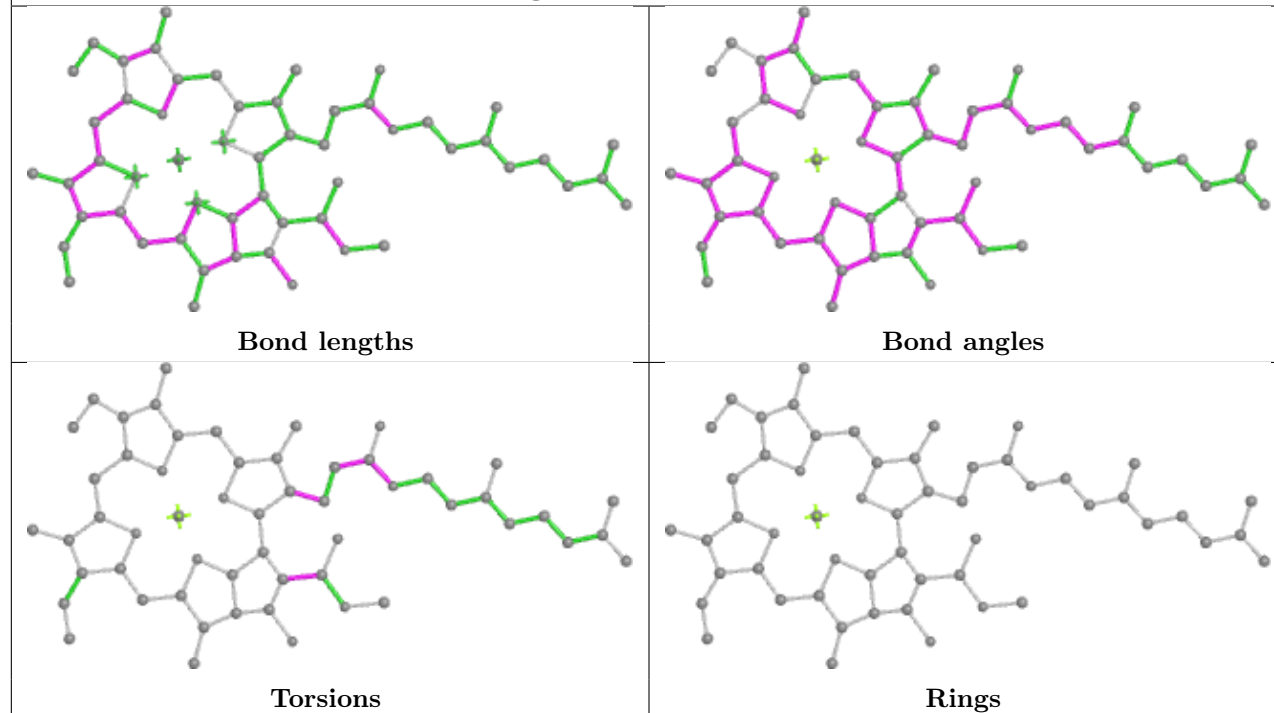




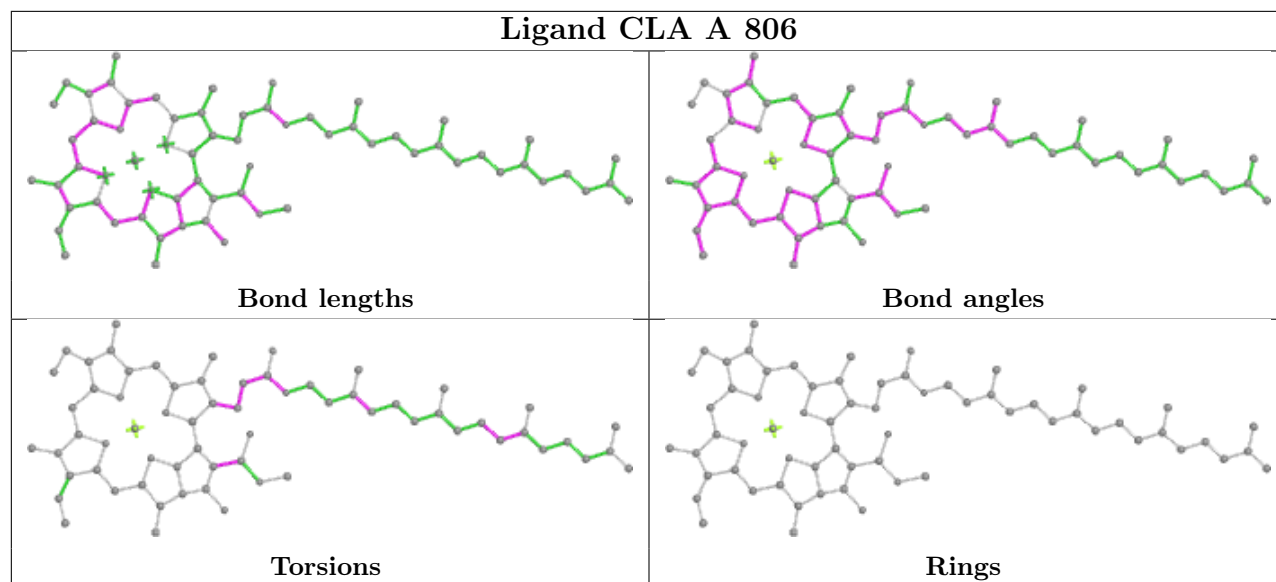
Ligand CLA B 825



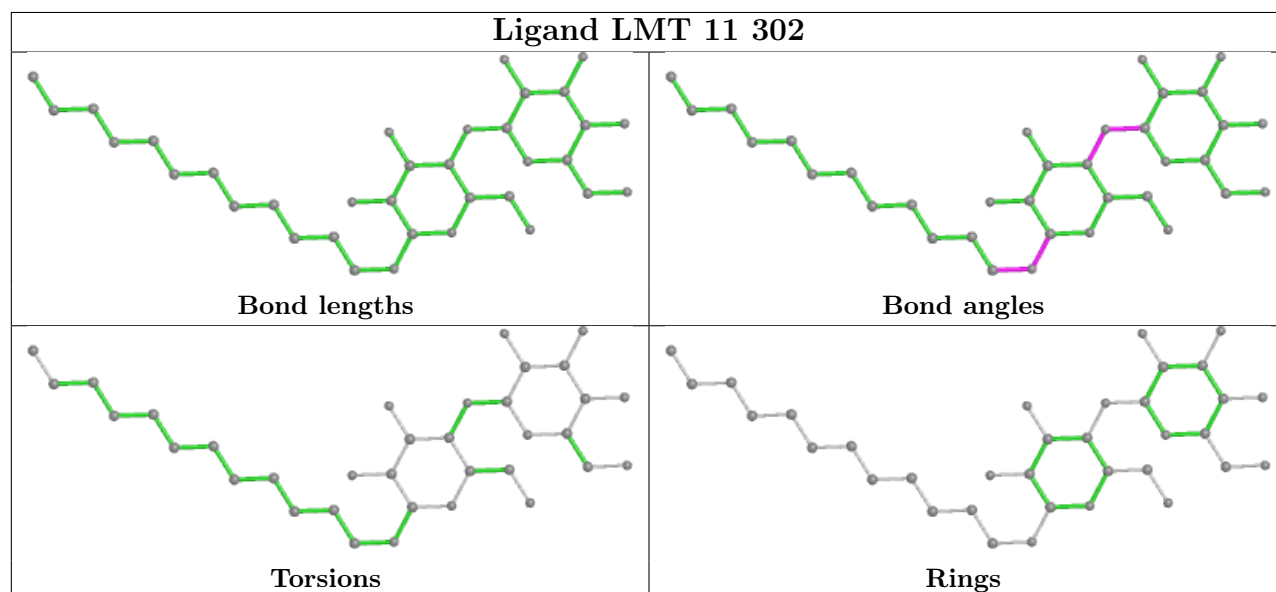
Ligand CLA 11 306



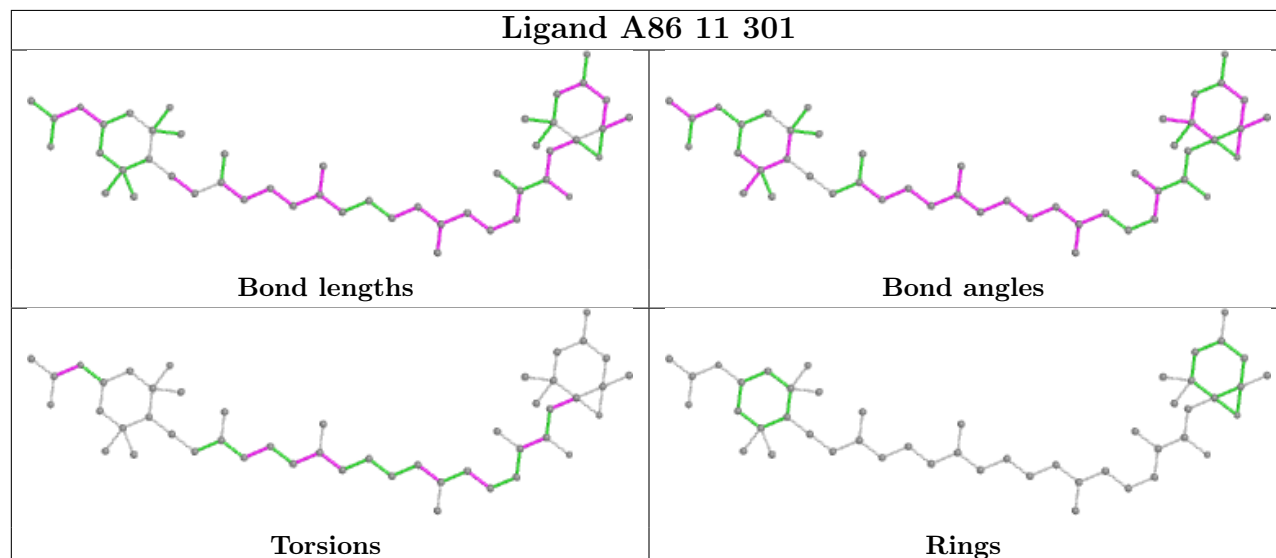
Ligand CLA A 806



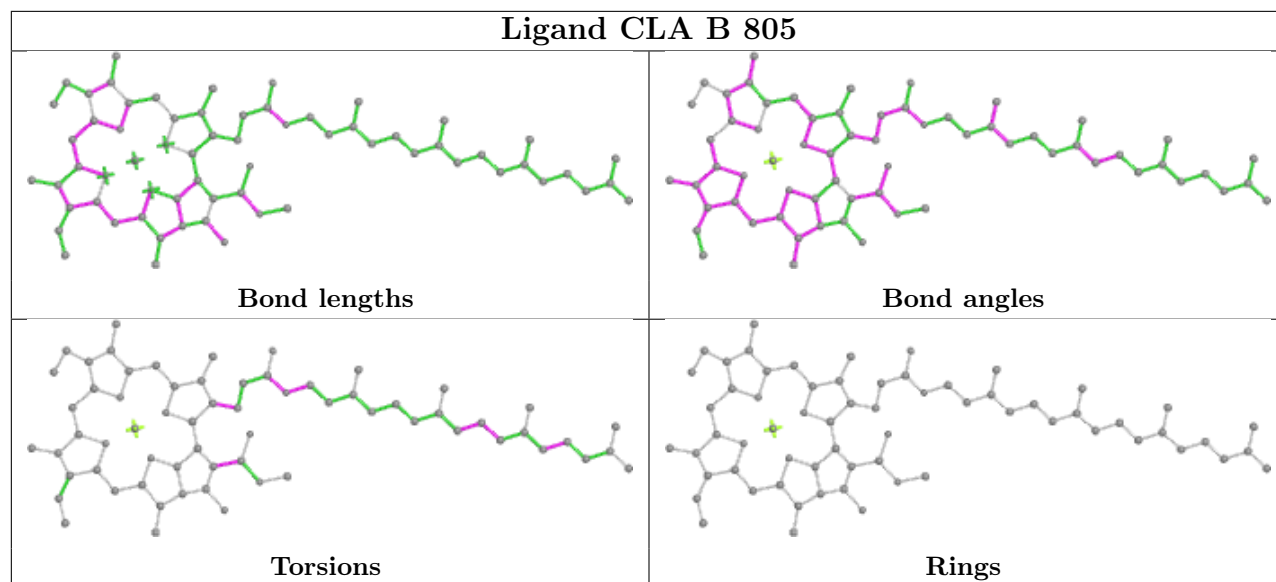
Ligand LMT 11 302



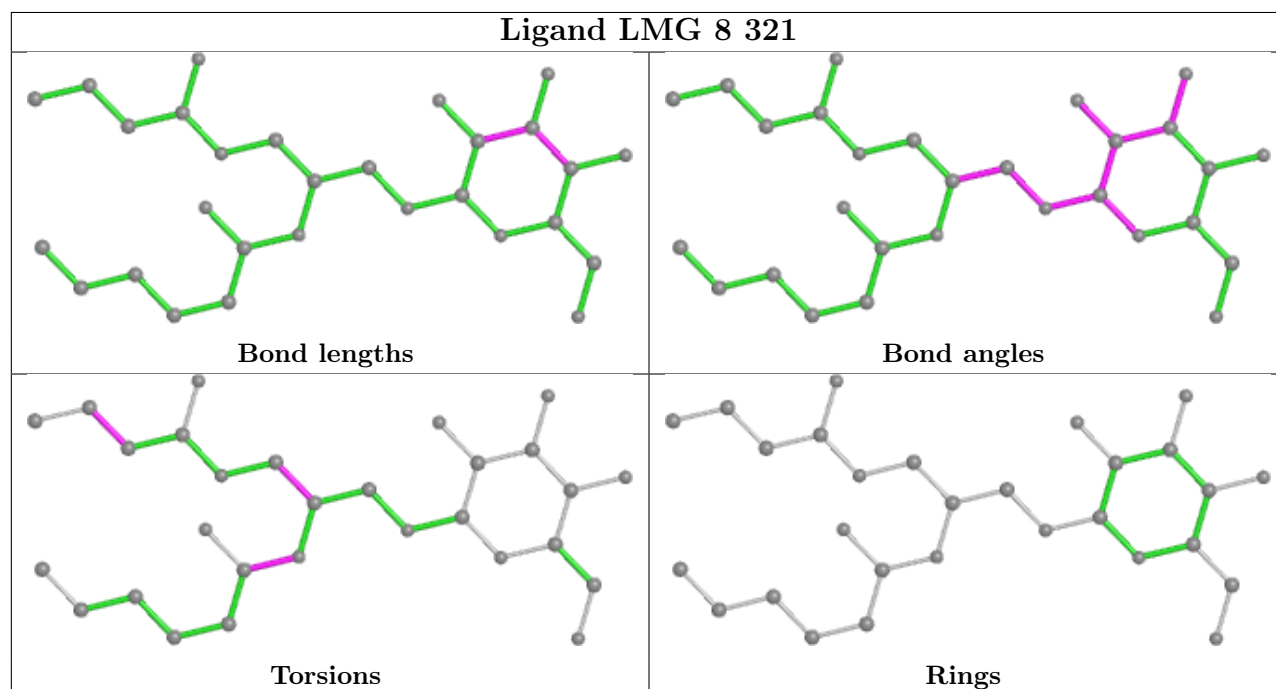
Ligand A86 11 301

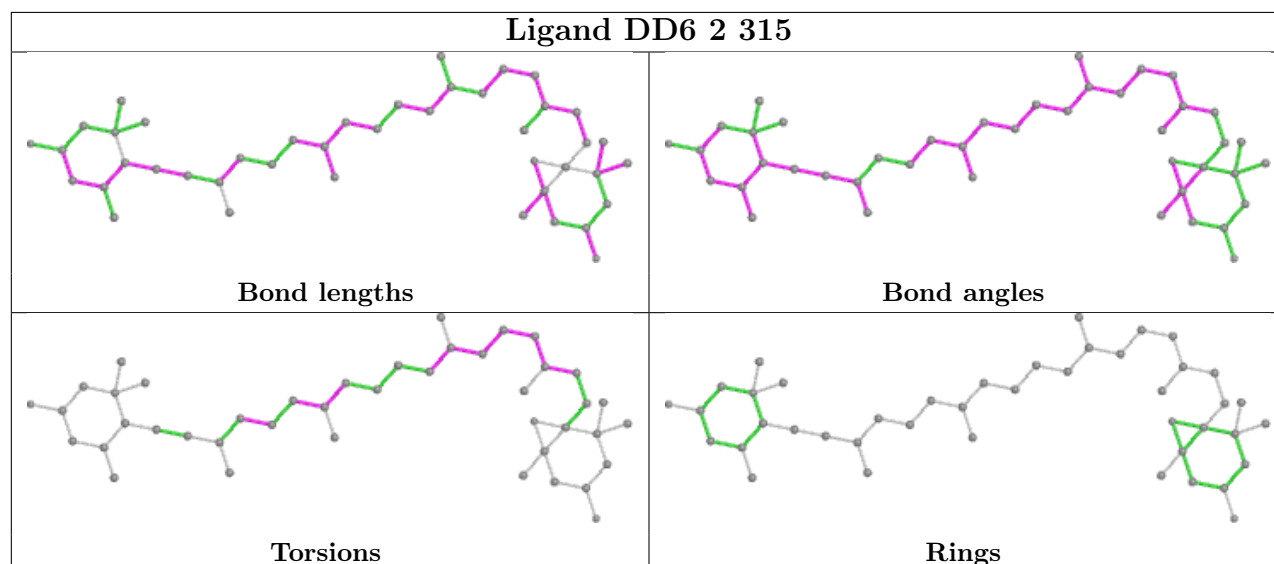
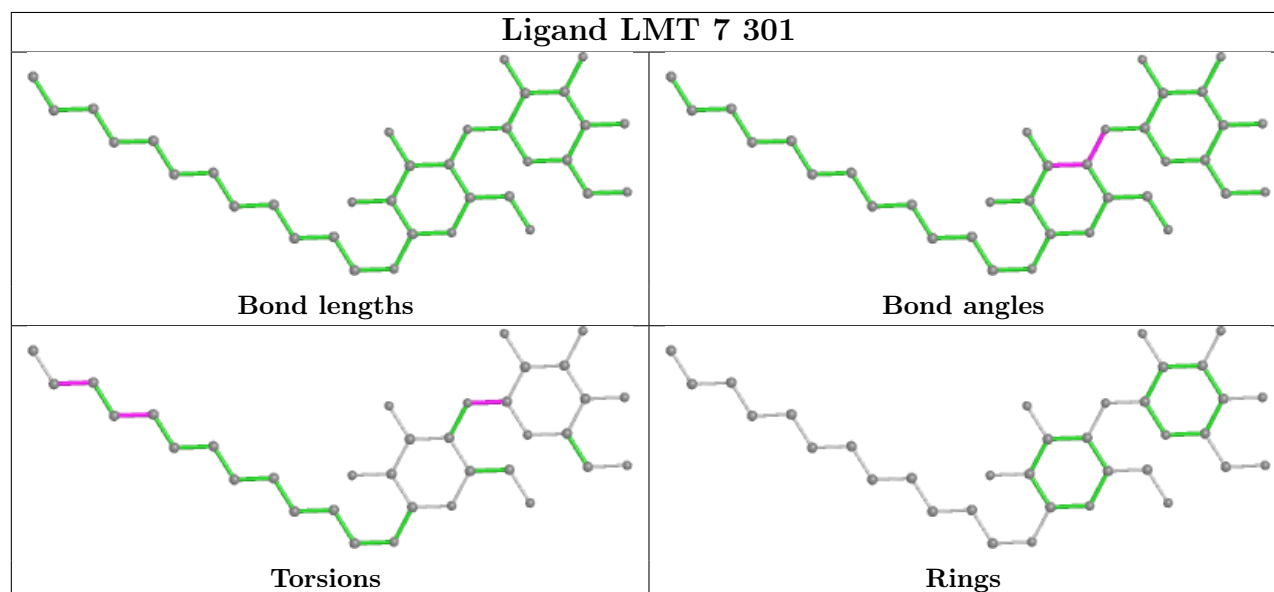
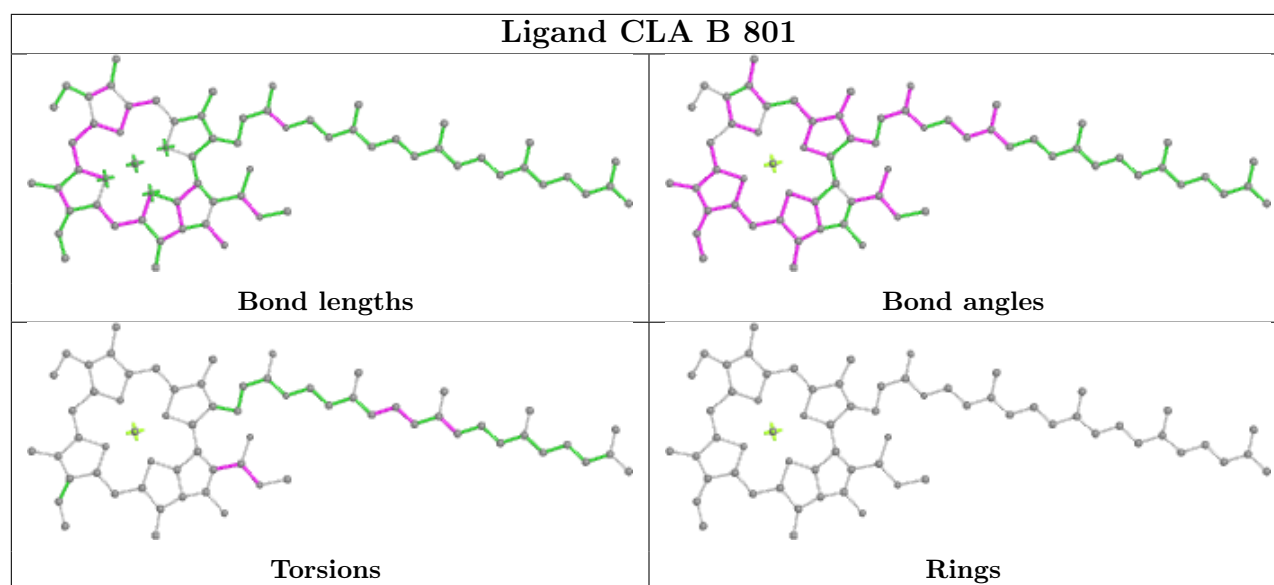


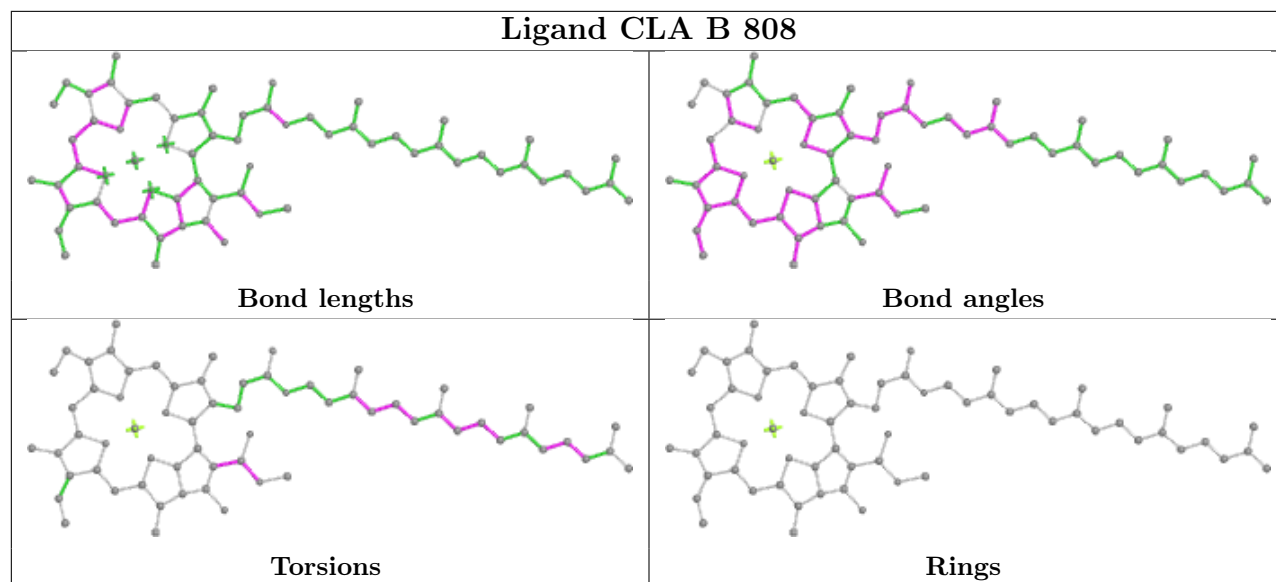
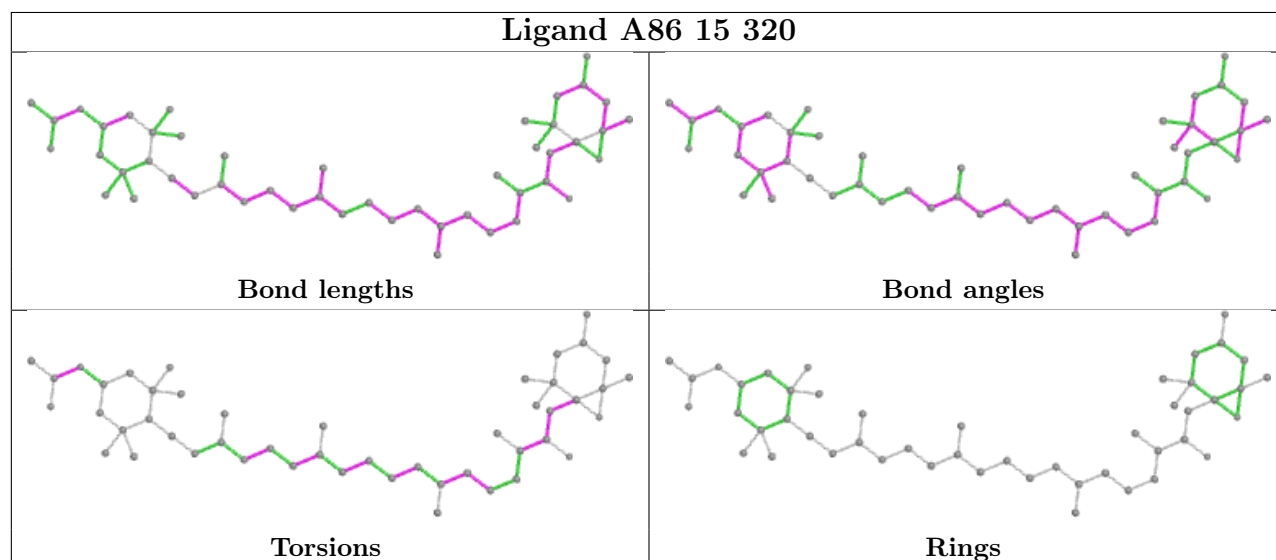
Ligand CLA B 805



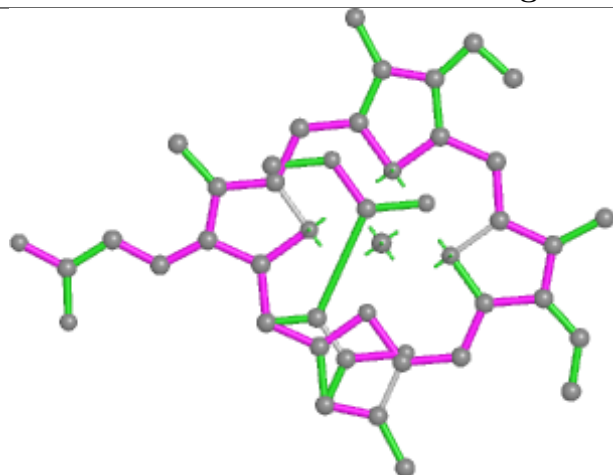
Ligand LMG 8 321



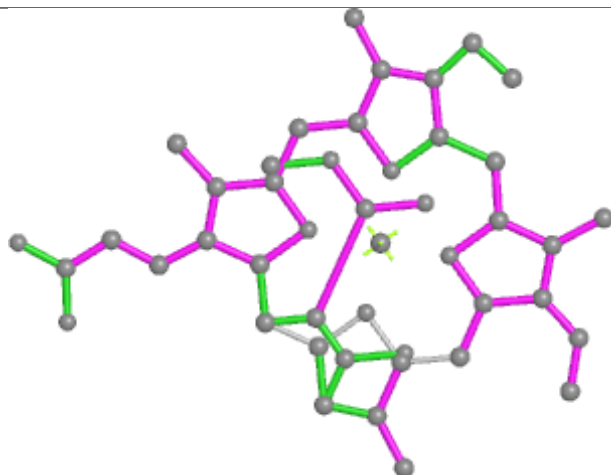


Ligand CLA B 808**Ligand A86 15 320**

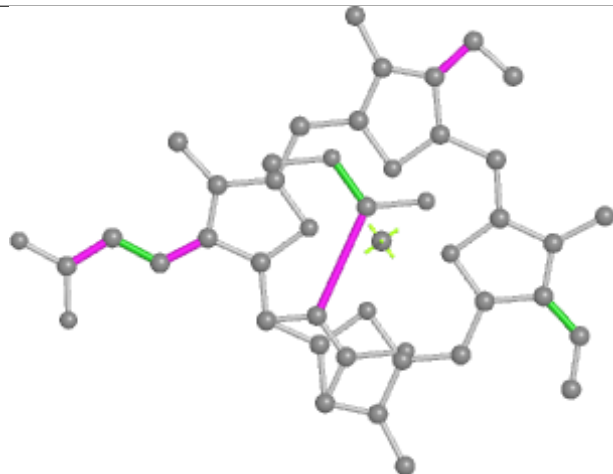
Ligand KC1 2 306



Bond lengths



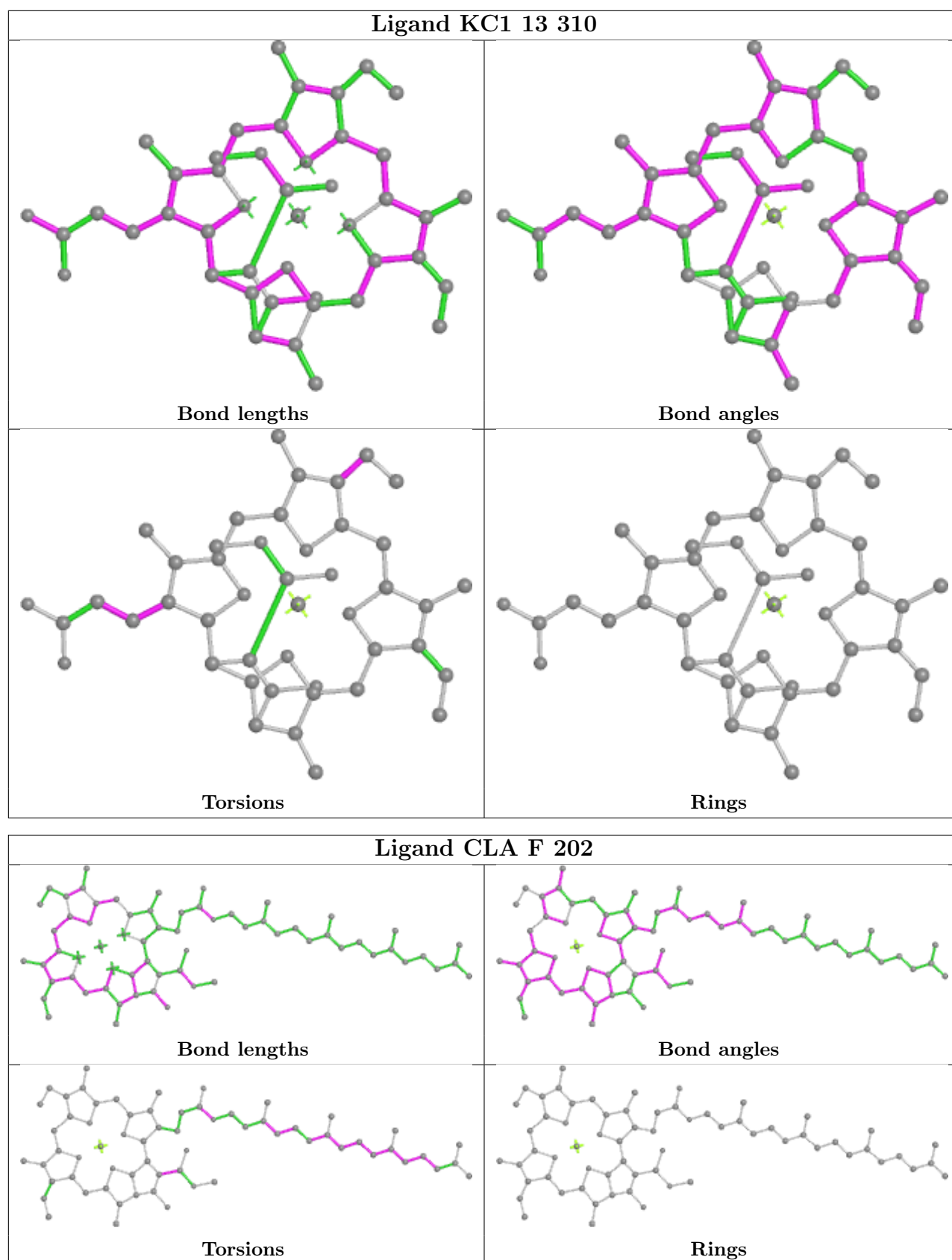
Bond angles



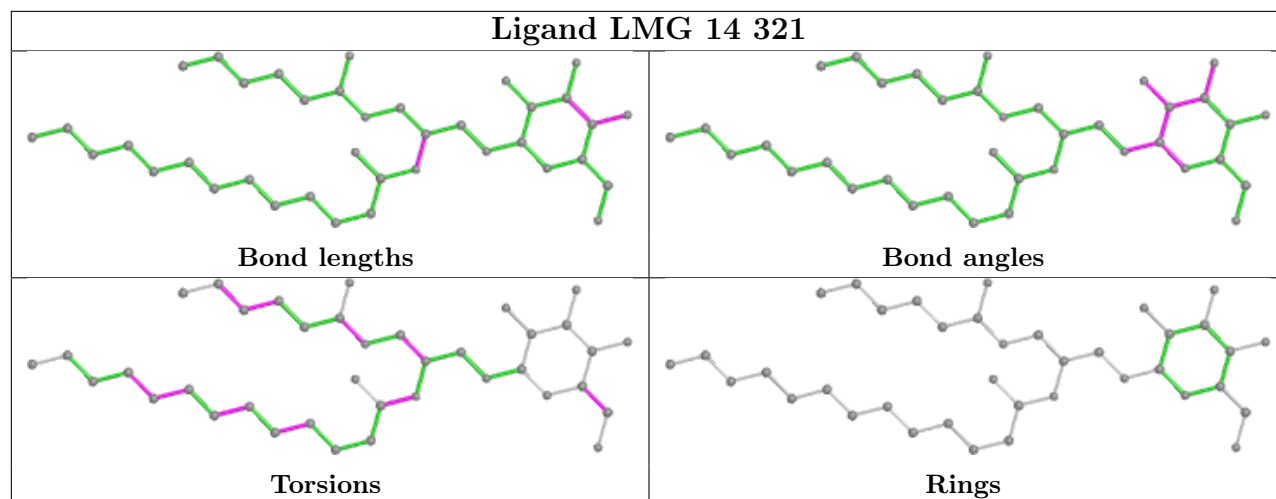
Torsions



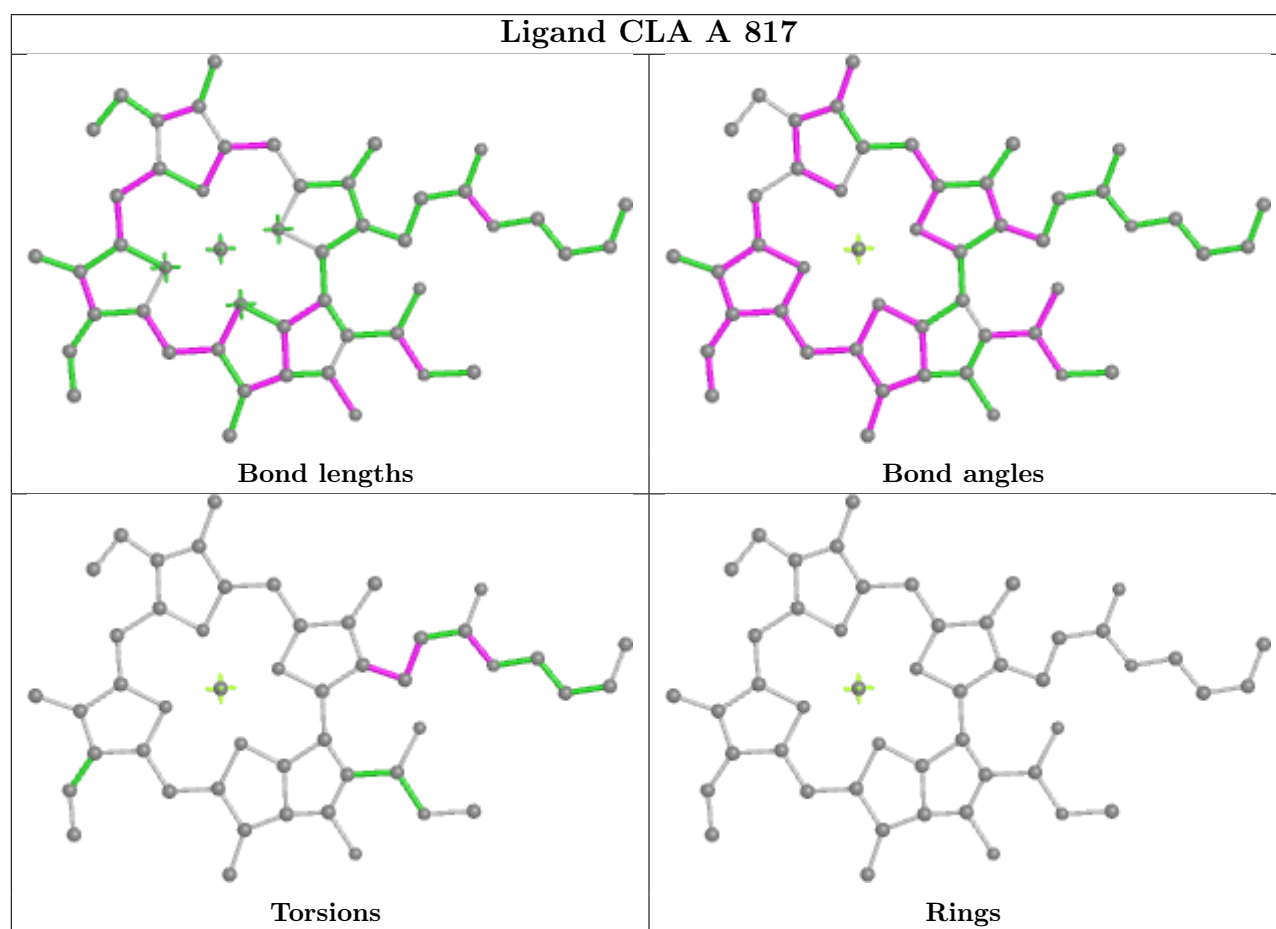
Rings



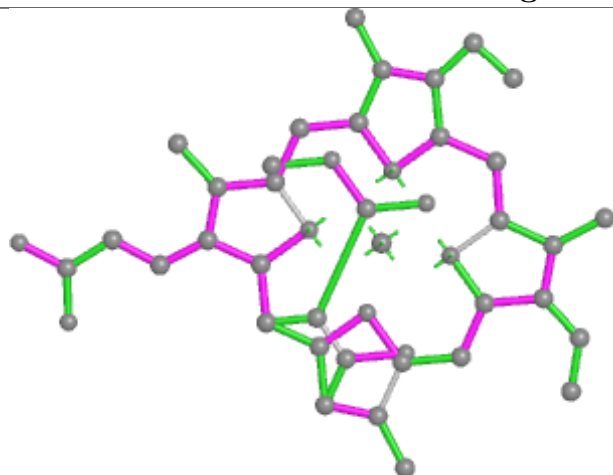
Ligand LMG 14 321



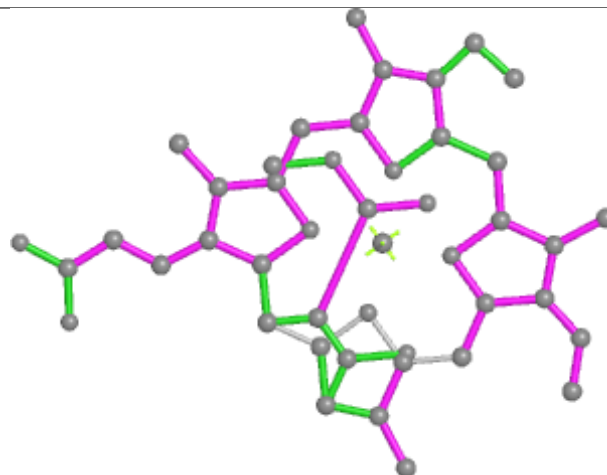
Ligand CLA A 817



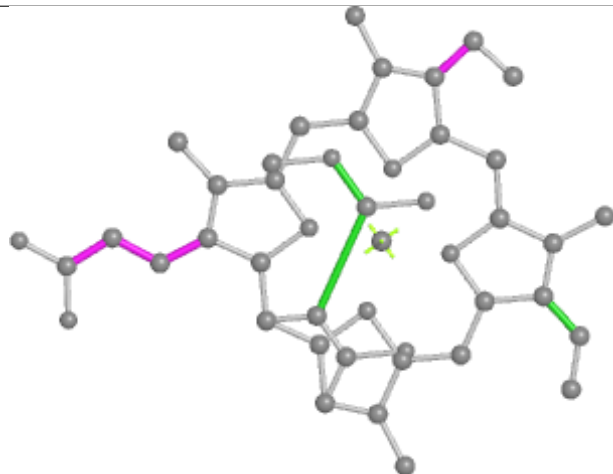
Ligand KC1 9 304



Bond lengths



Bond angles

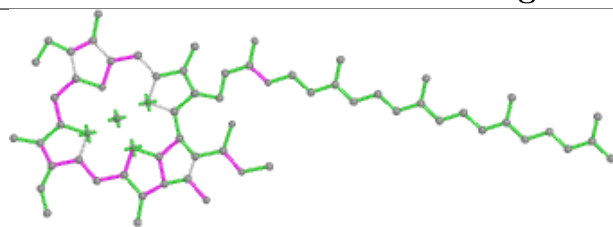


Torsions

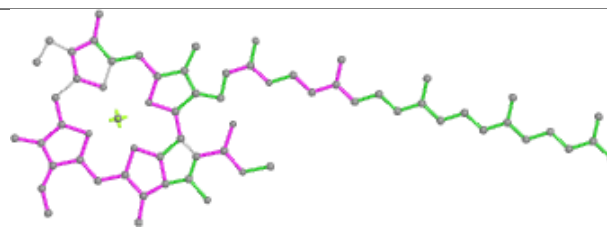


Rings

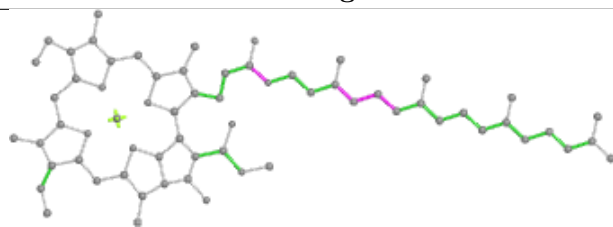
Ligand CLA 2 310



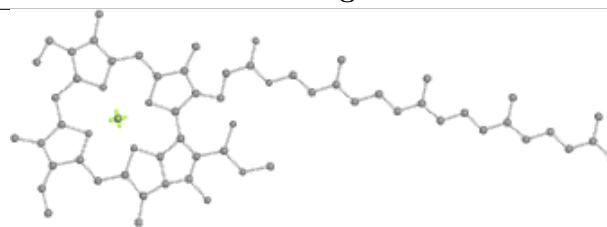
Bond lengths



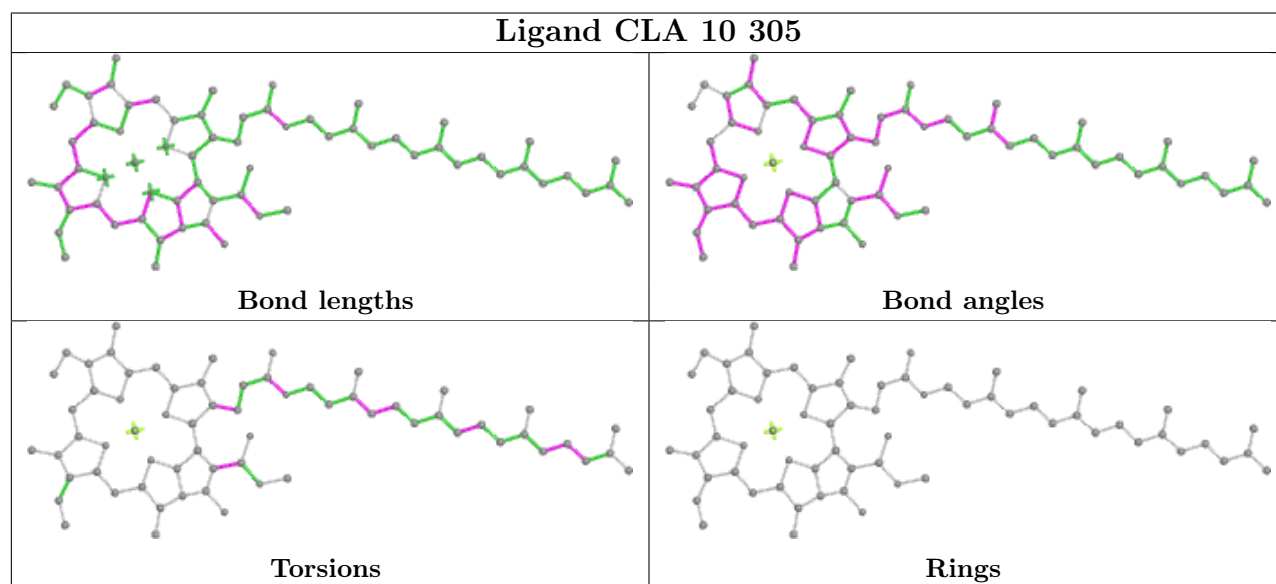
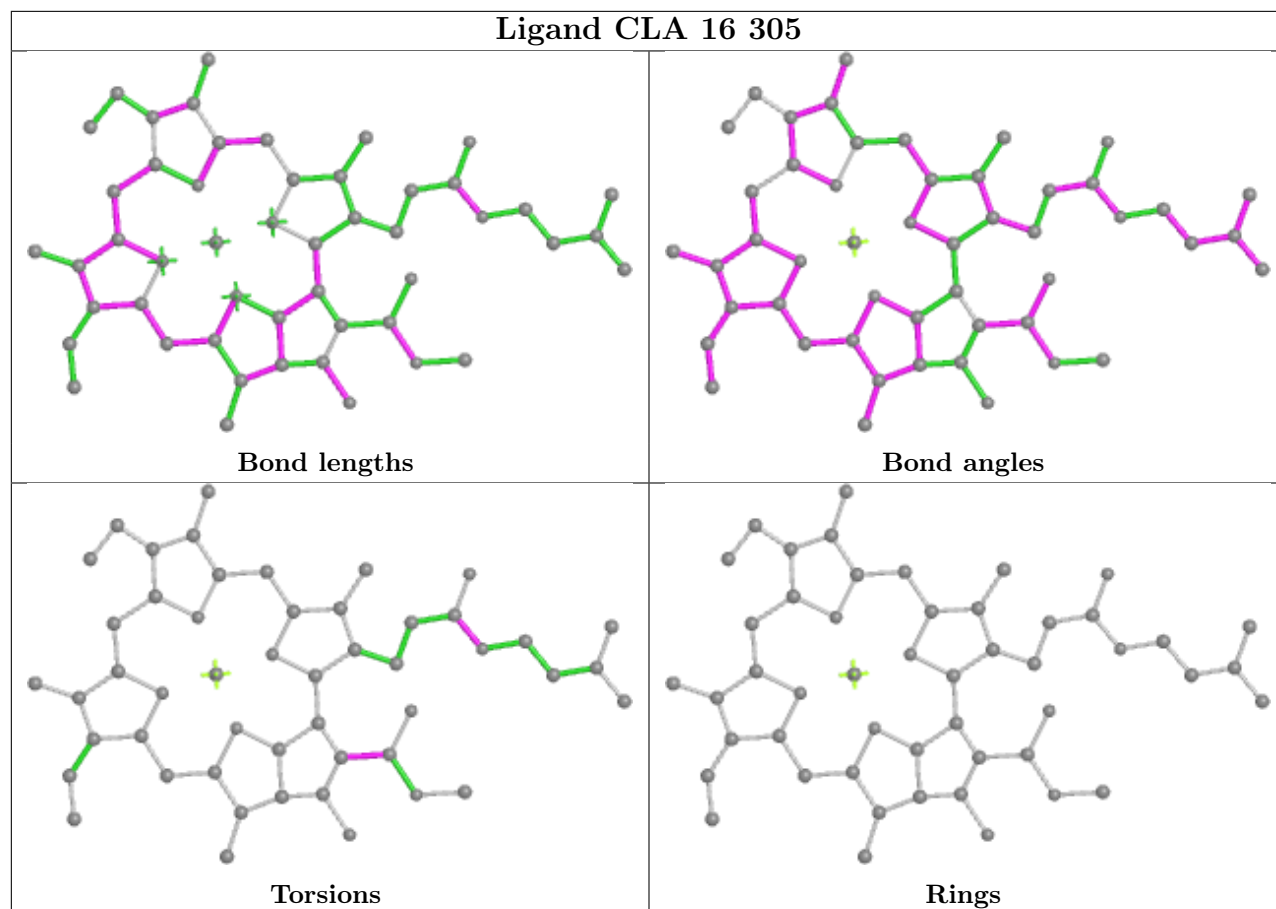
Bond angles



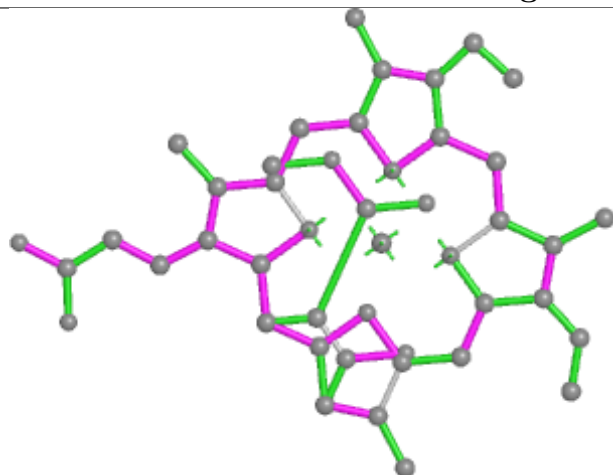
Torsions



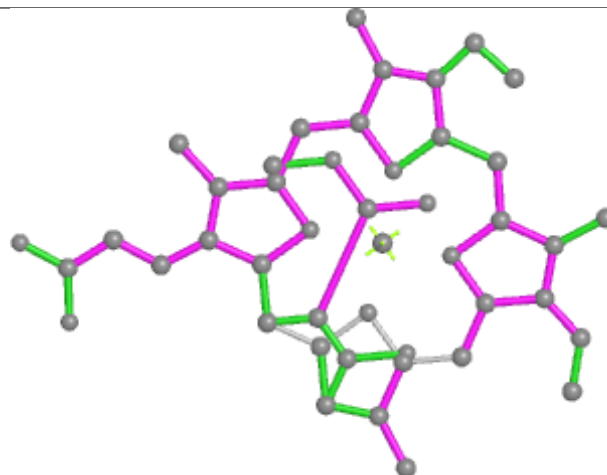
Rings



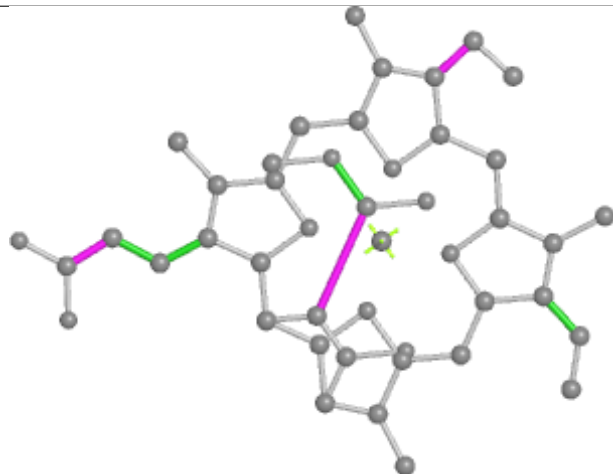
Ligand KC1 8 310



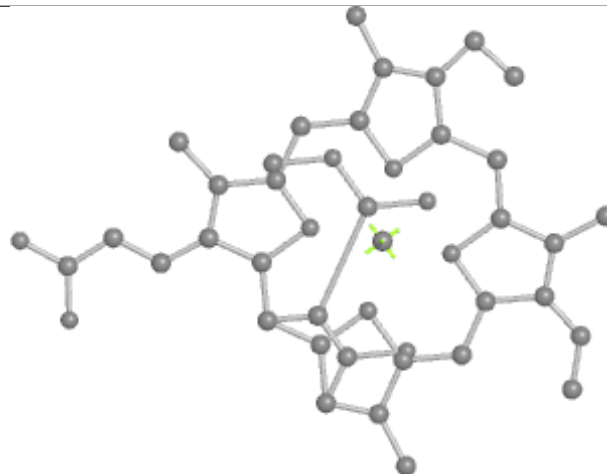
Bond lengths



Bond angles

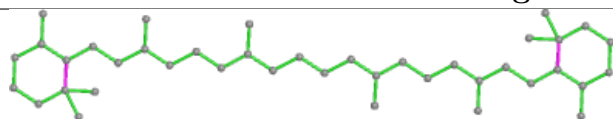


Torsions

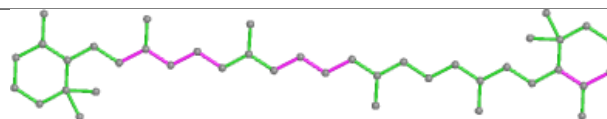


Rings

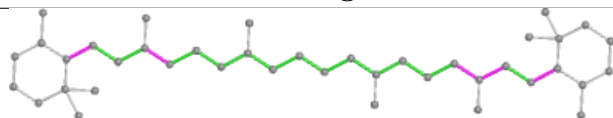
Ligand BCR B 846



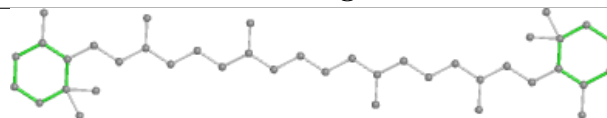
Bond lengths



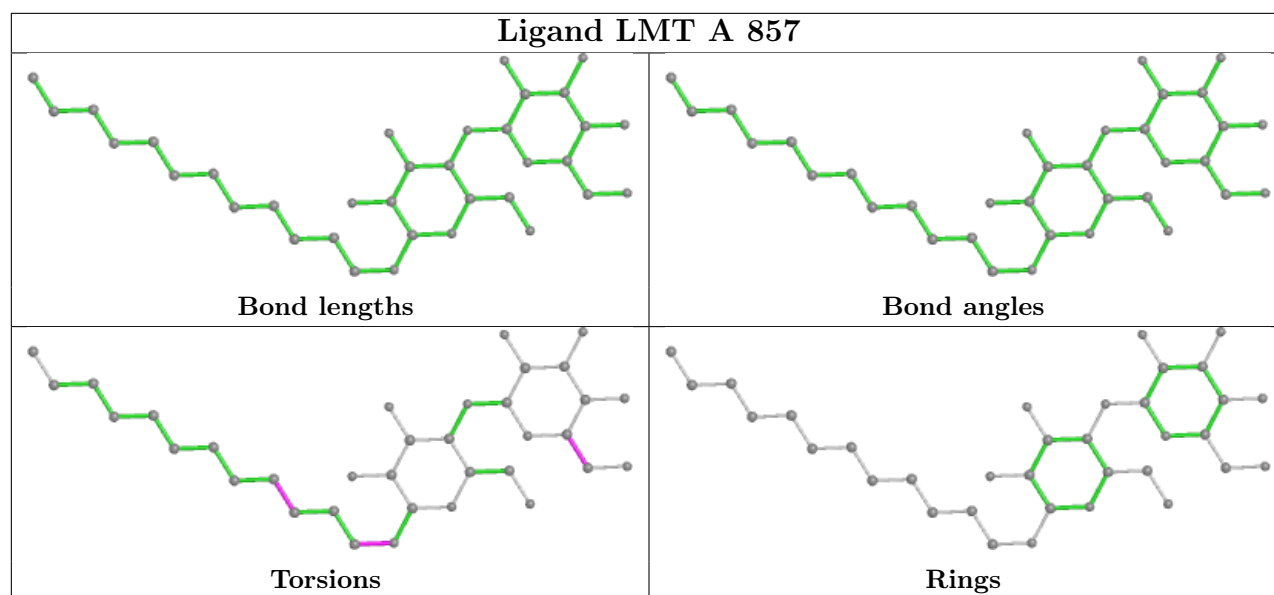
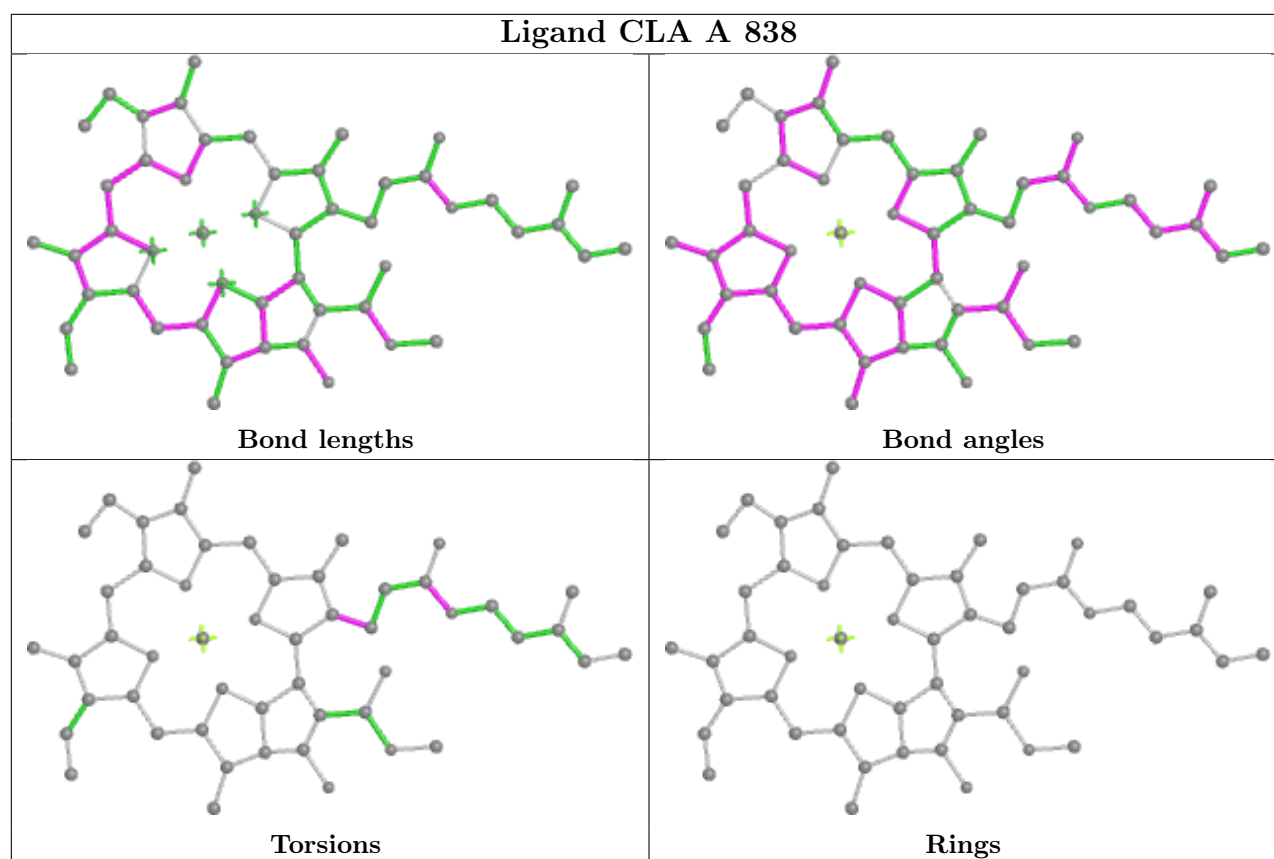
Bond angles

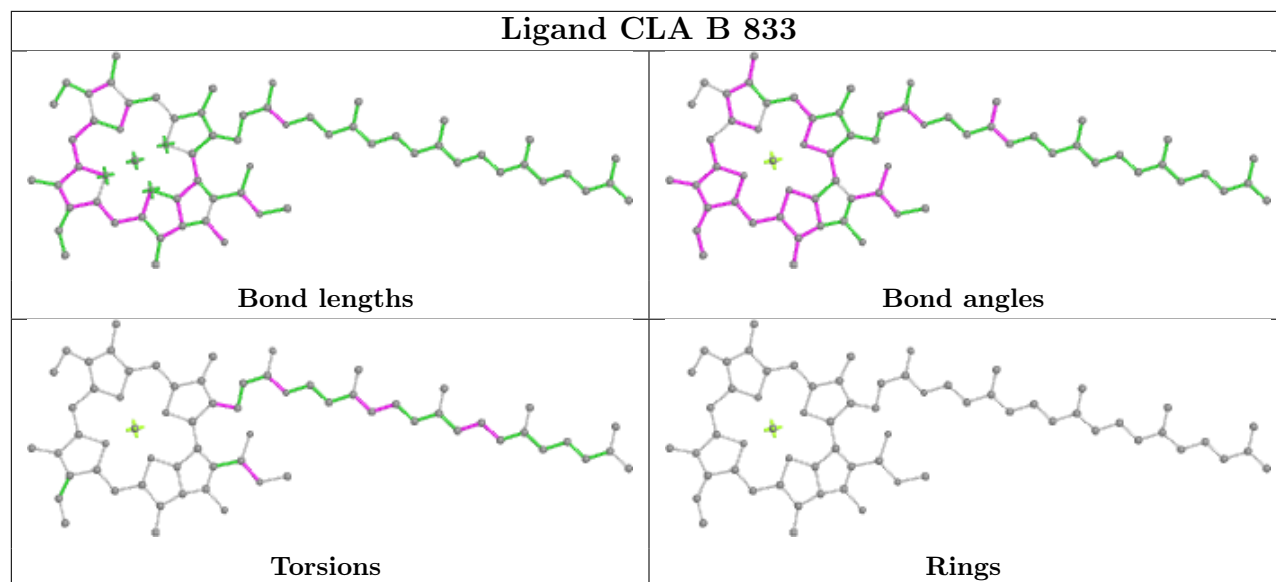
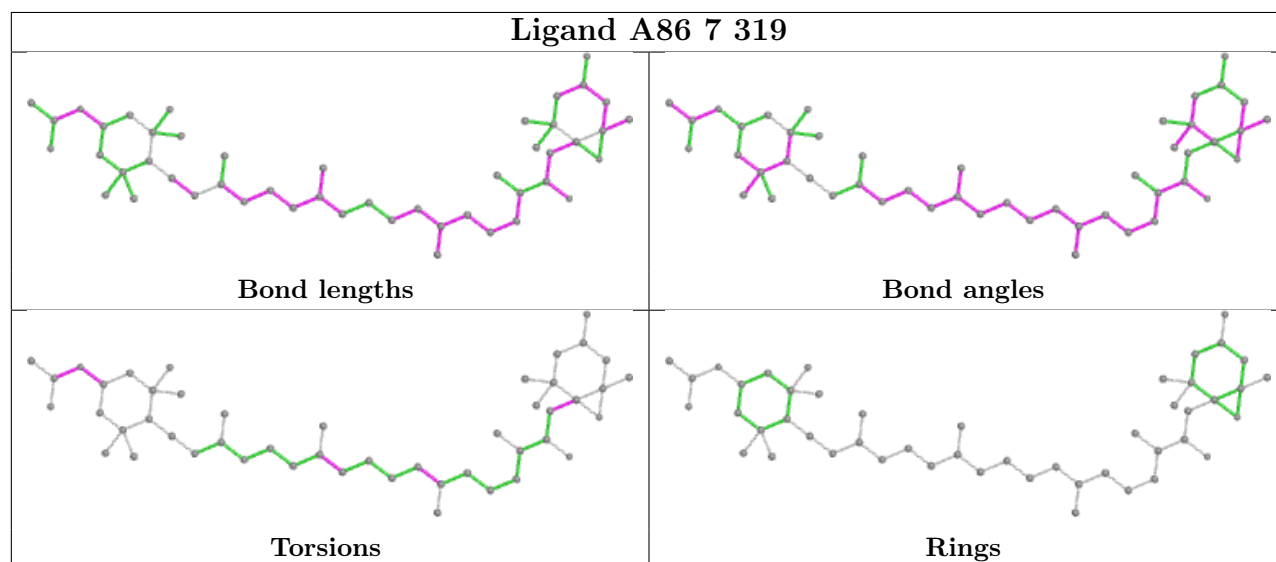


Torsions

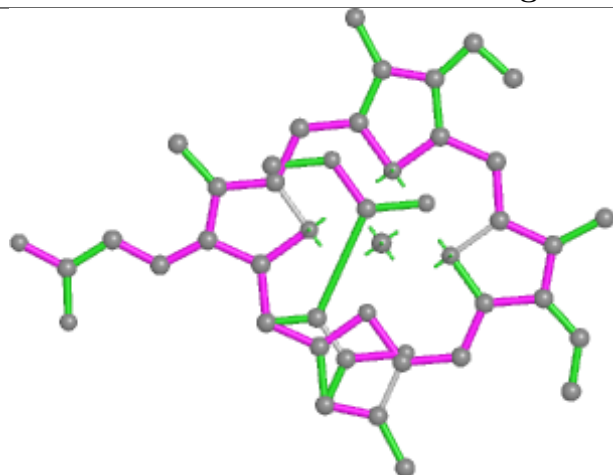


Rings

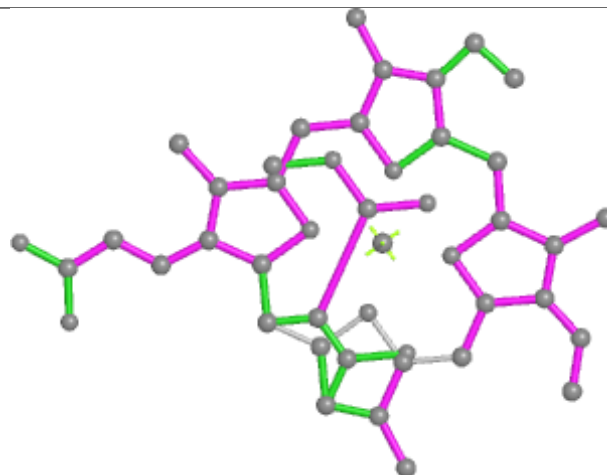


Ligand CLA B 833**Ligand A86 7 319**

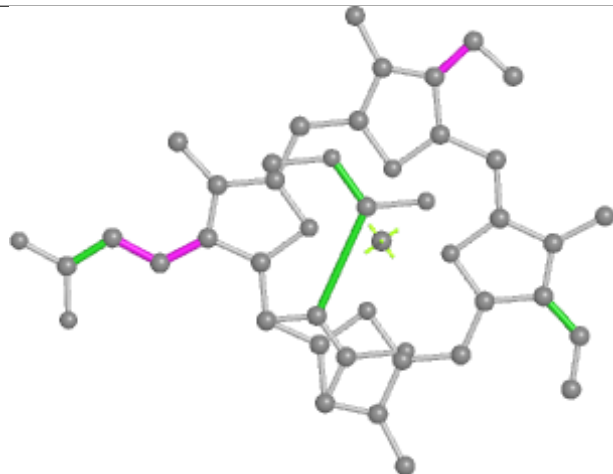
Ligand KC1 4 310



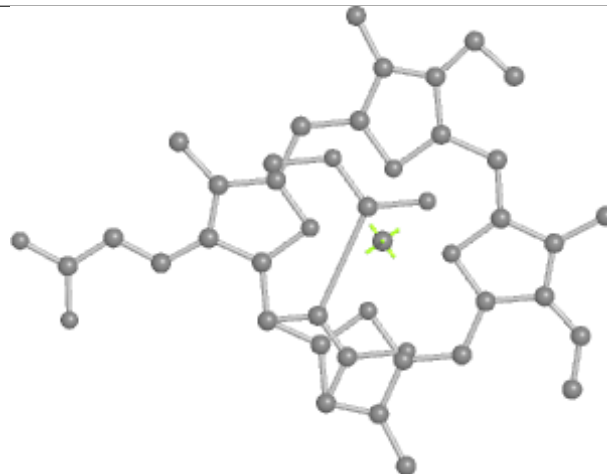
Bond lengths



Bond angles

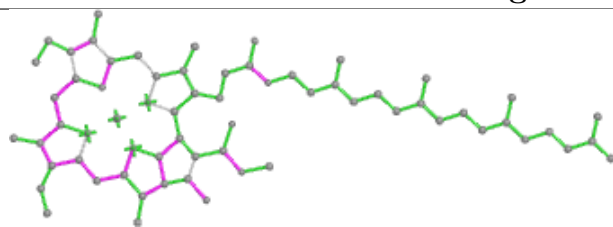


Torsions

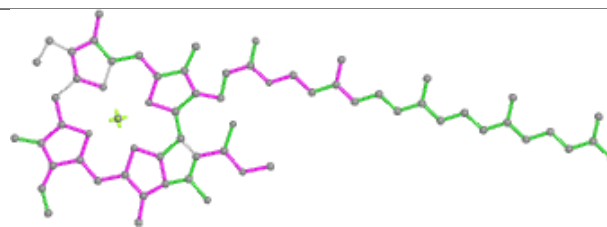


Rings

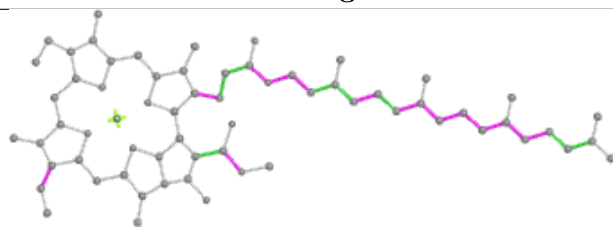
Ligand CLA 15 304



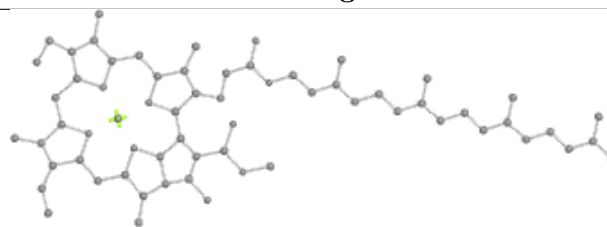
Bond lengths



Bond angles

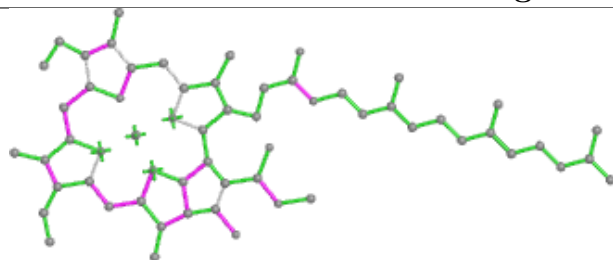


Torsions

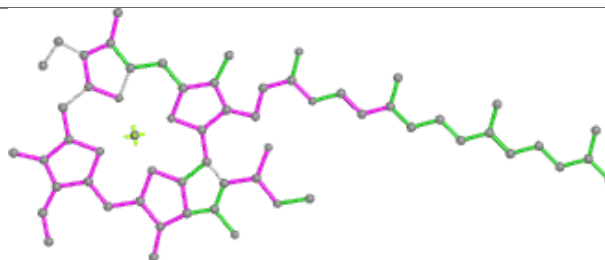


Rings

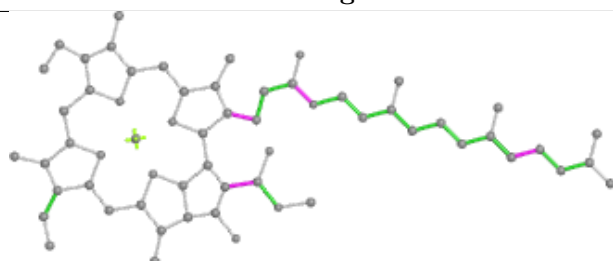
Ligand CLA B 818



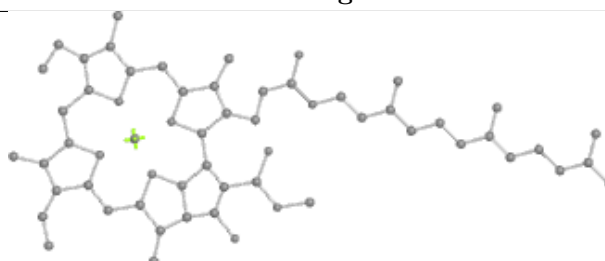
Bond lengths



Bond angles

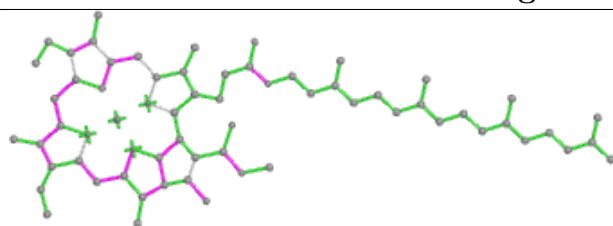


Torsions

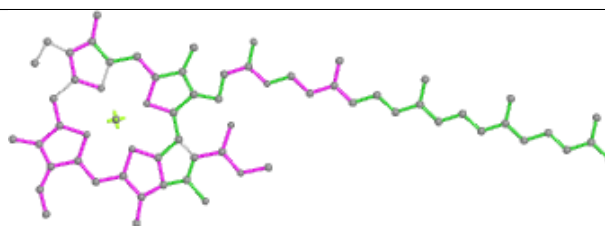


Rings

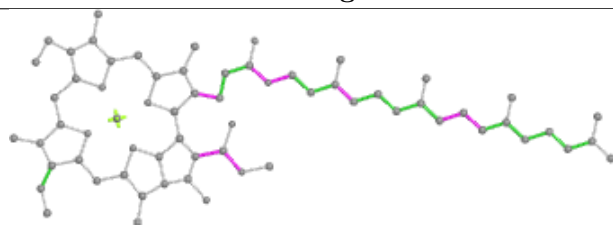
Ligand CLA 1 304



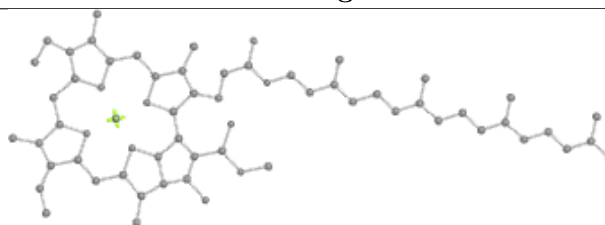
Bond lengths



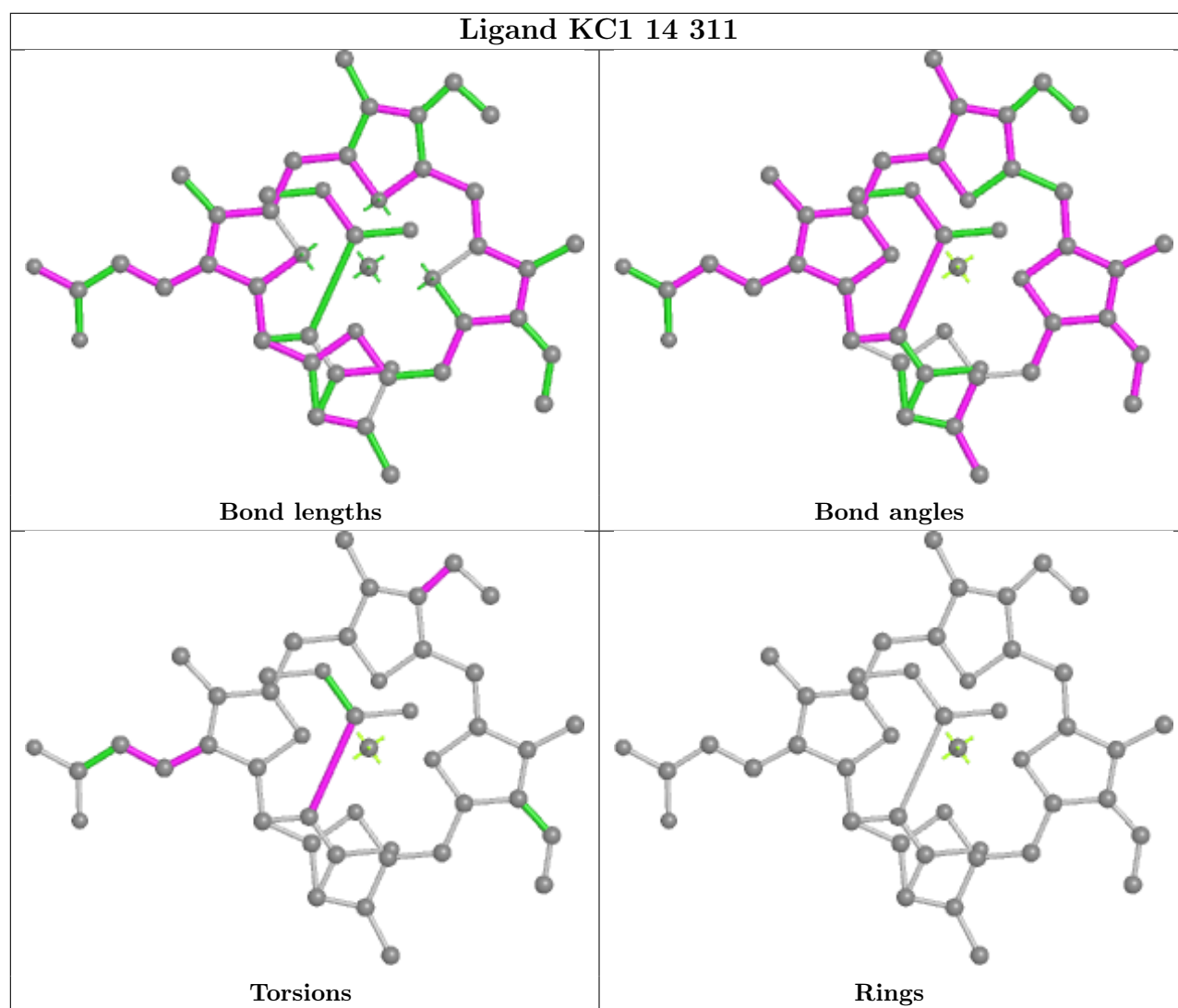
Bond angles



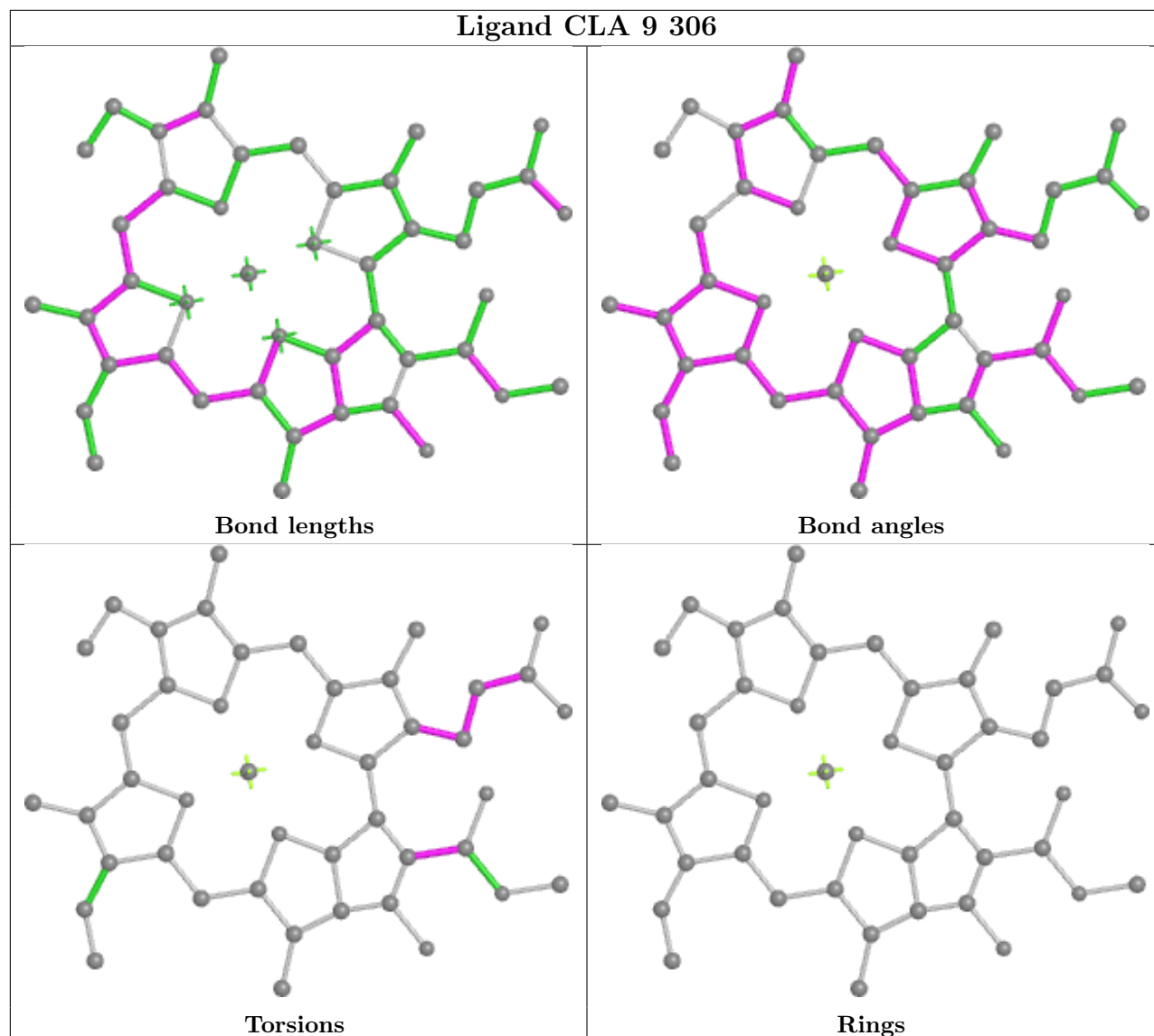
Torsions



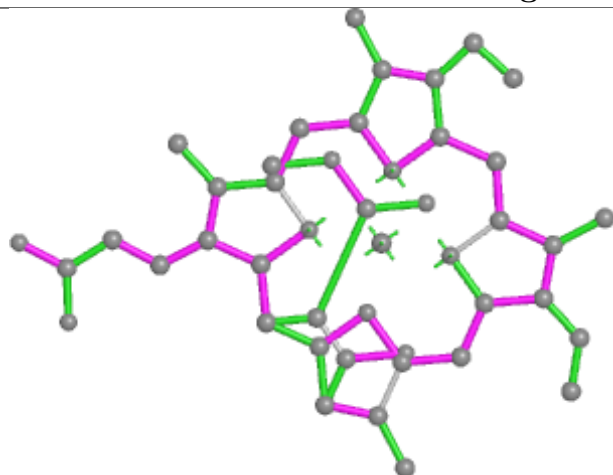
Rings



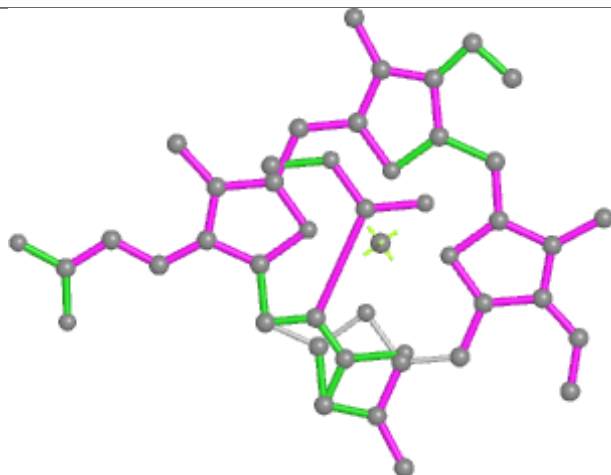
Ligand CLA 9 306



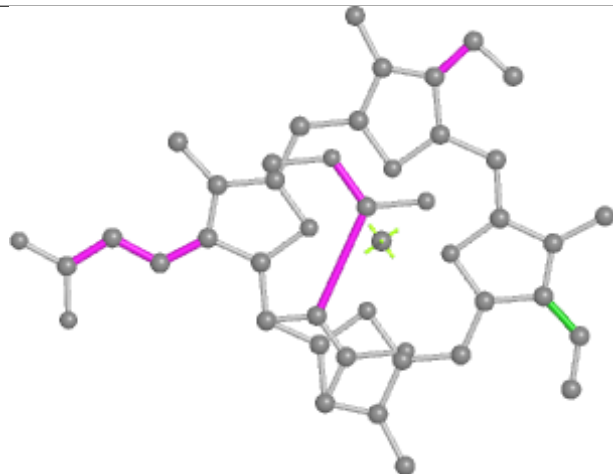
Ligand KC1 5 306



Bond lengths



Bond angles

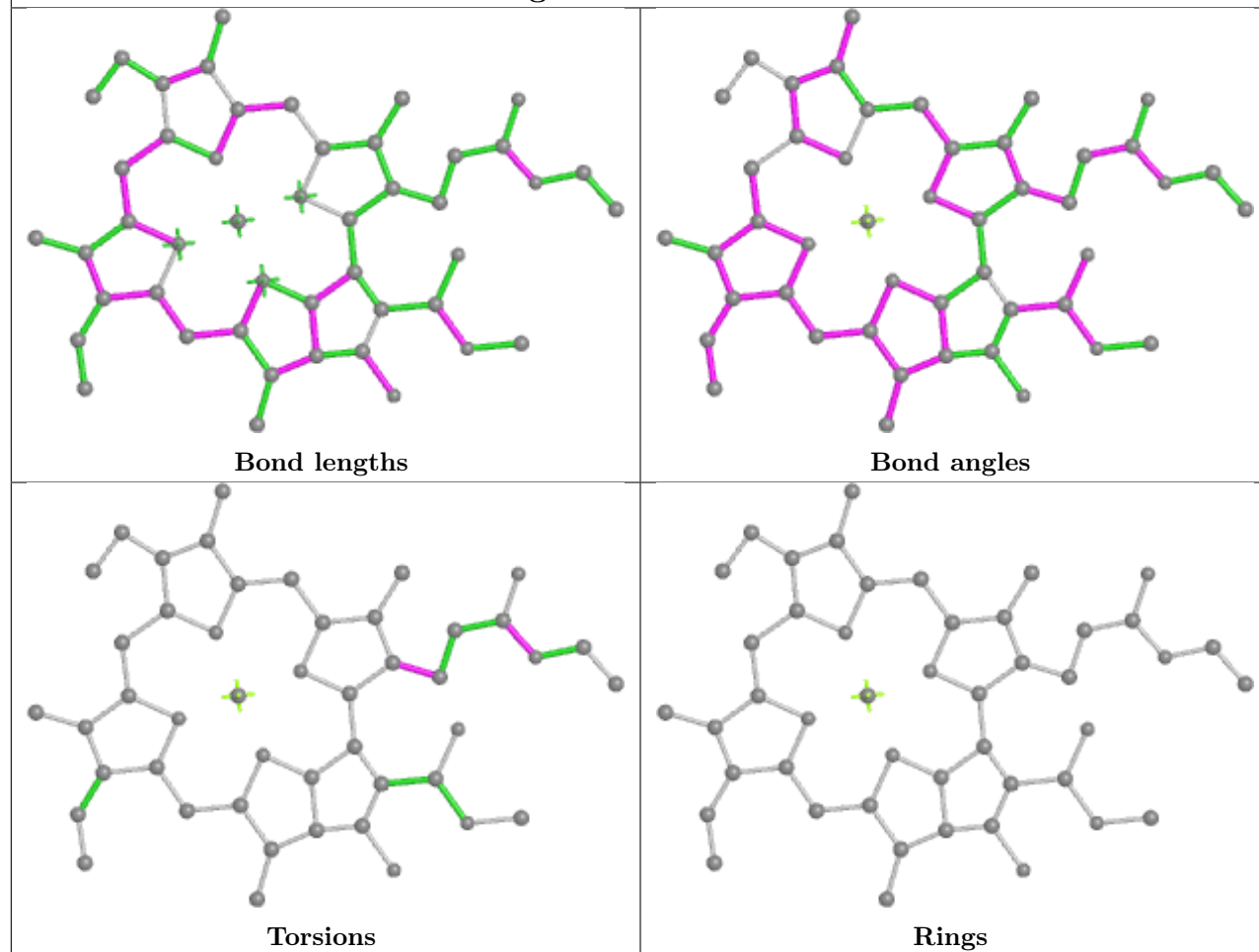


Torsions

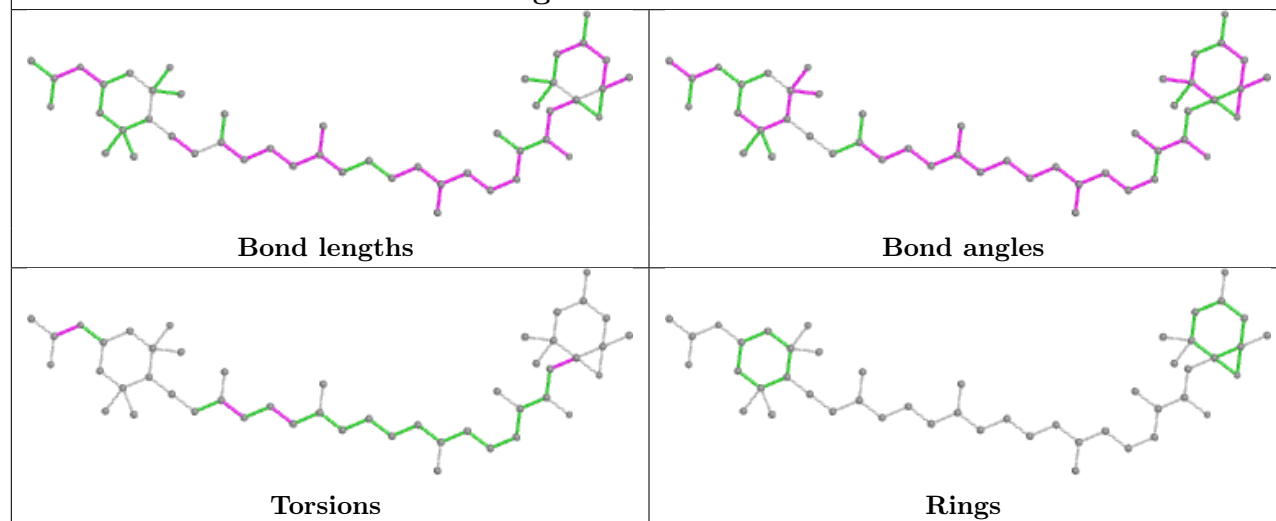


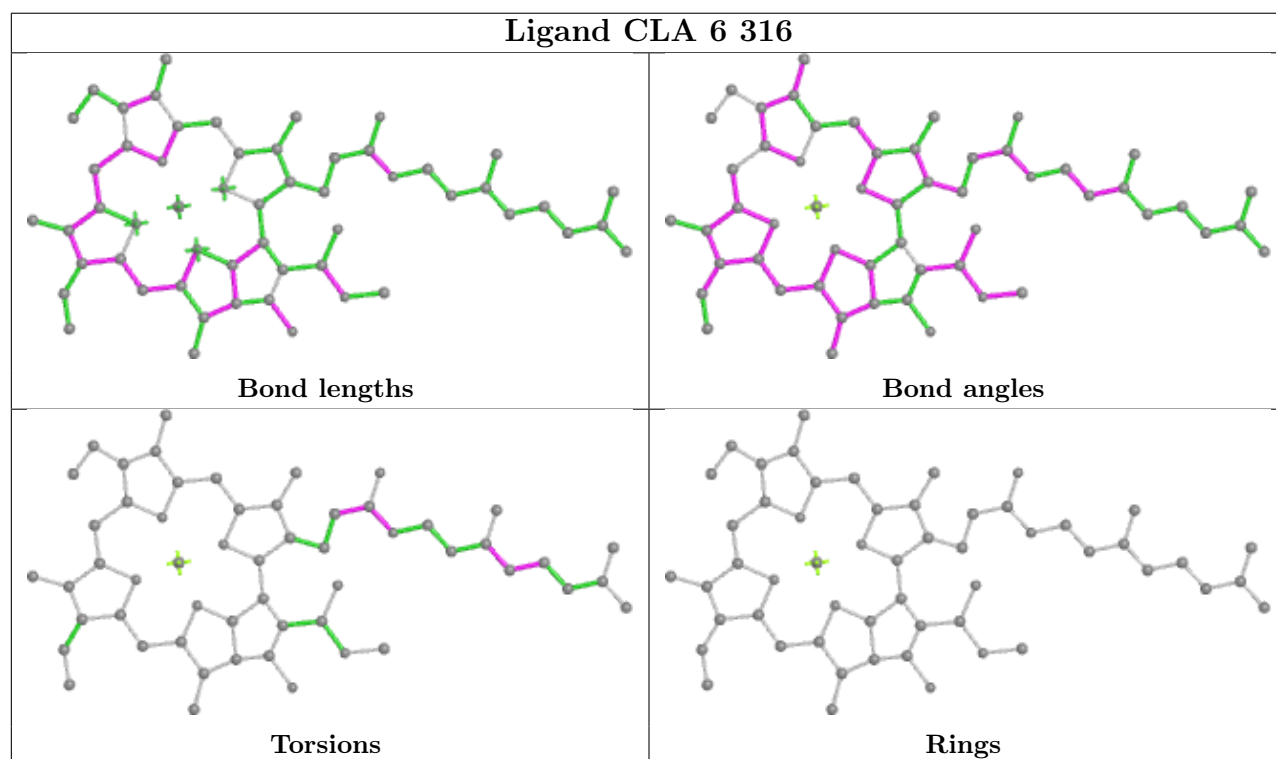
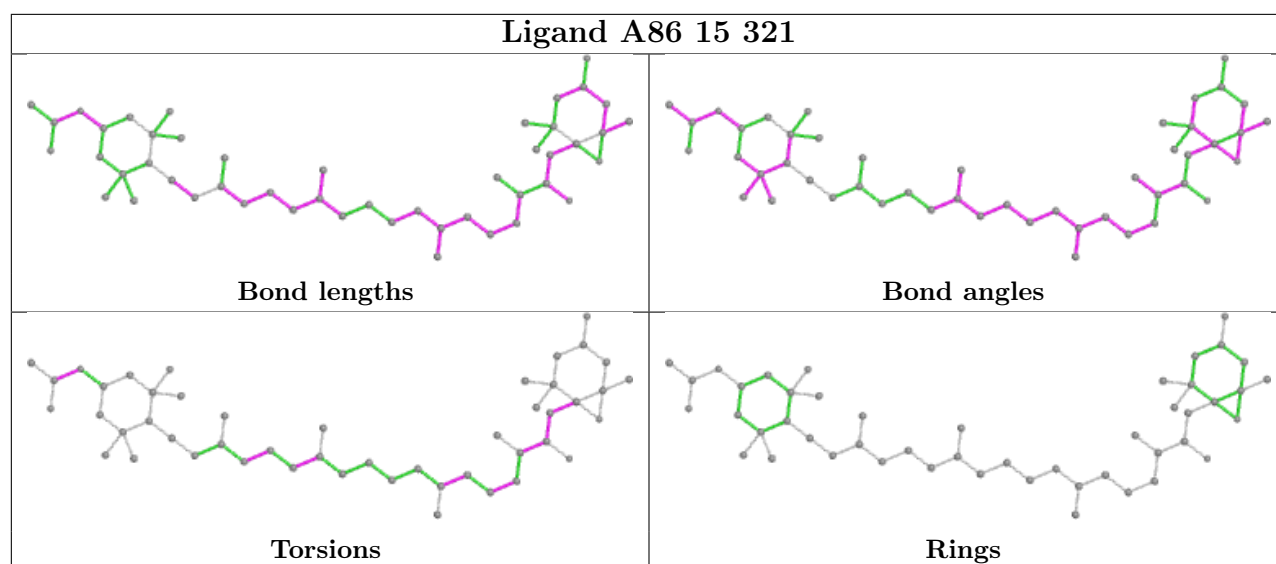
Rings

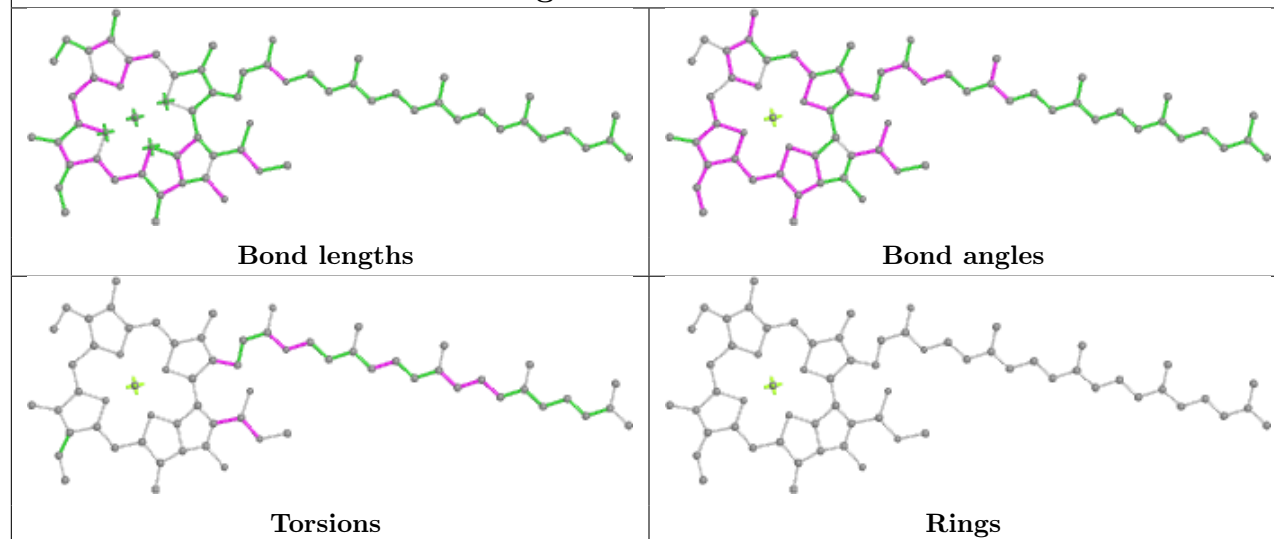
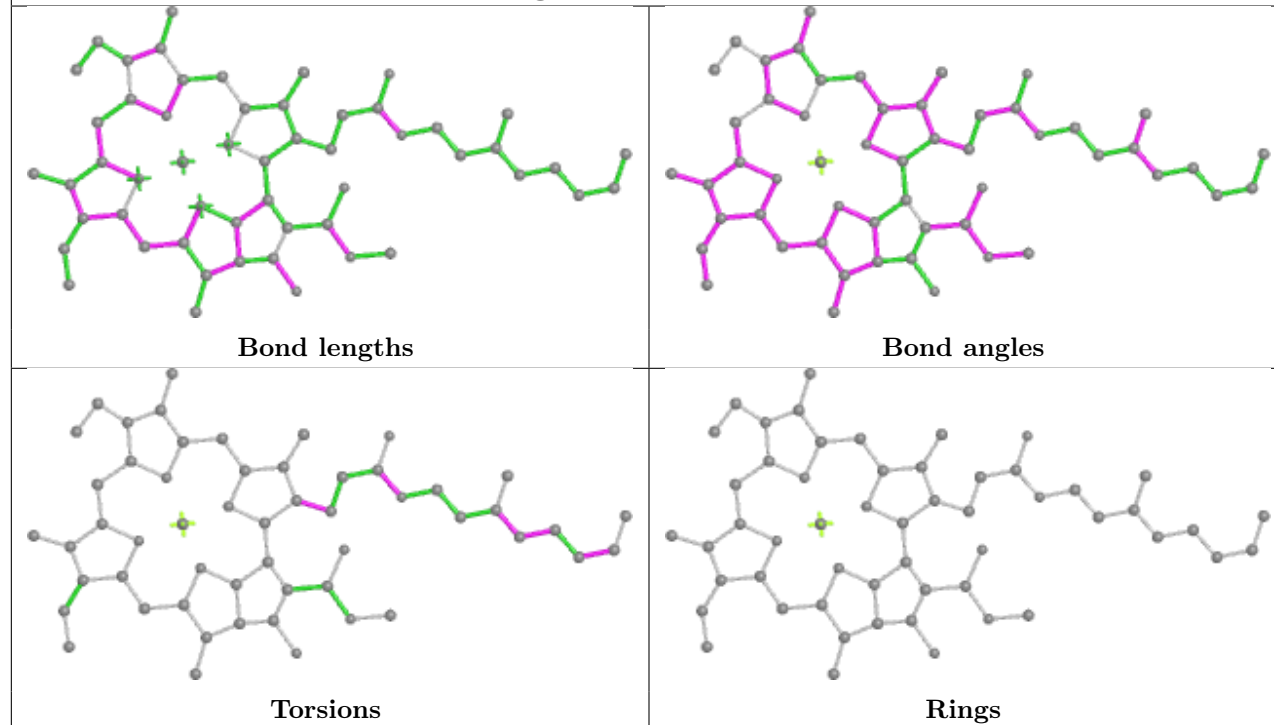
Ligand CLA 8 309

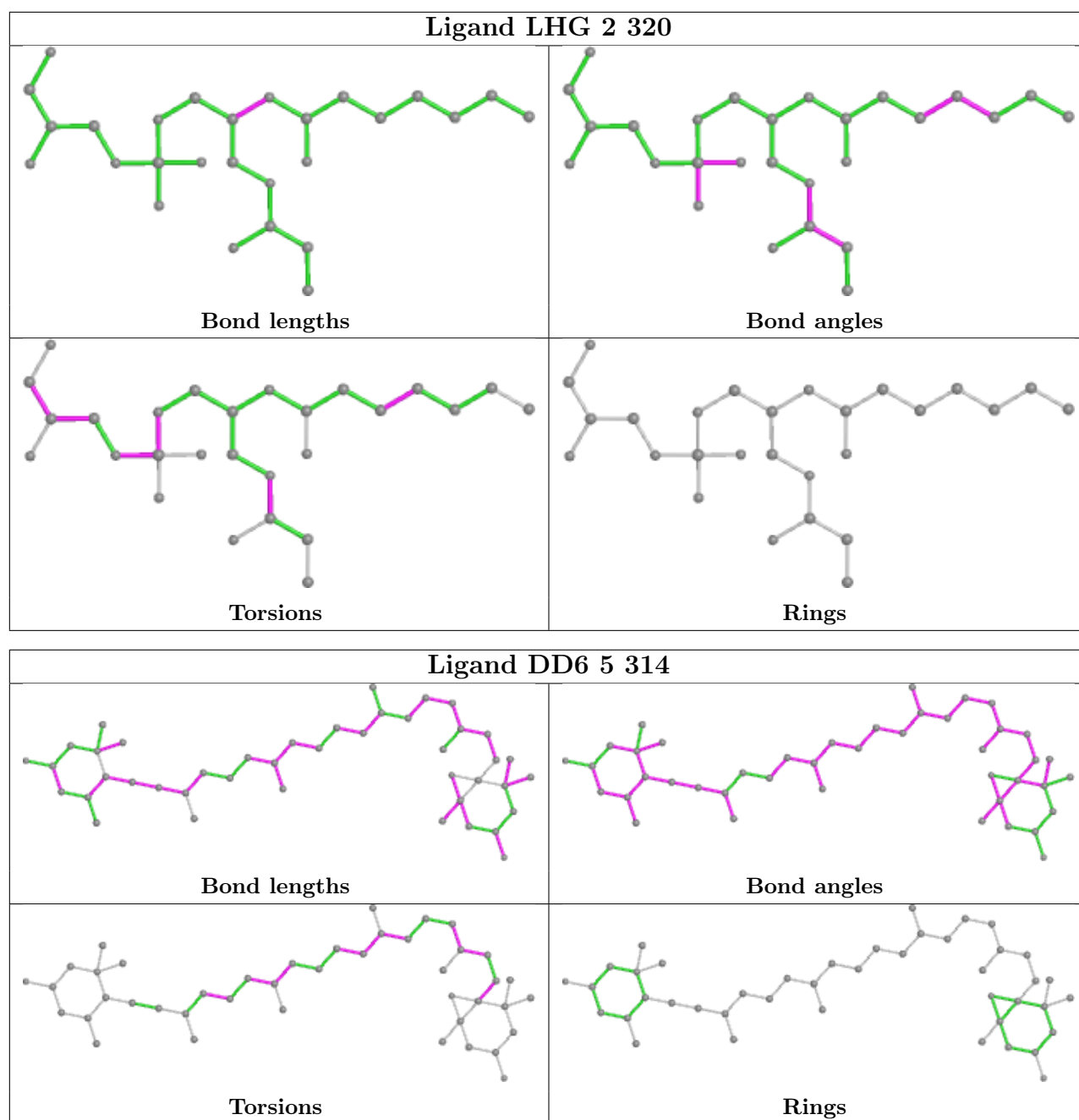


Ligand A86 10 301

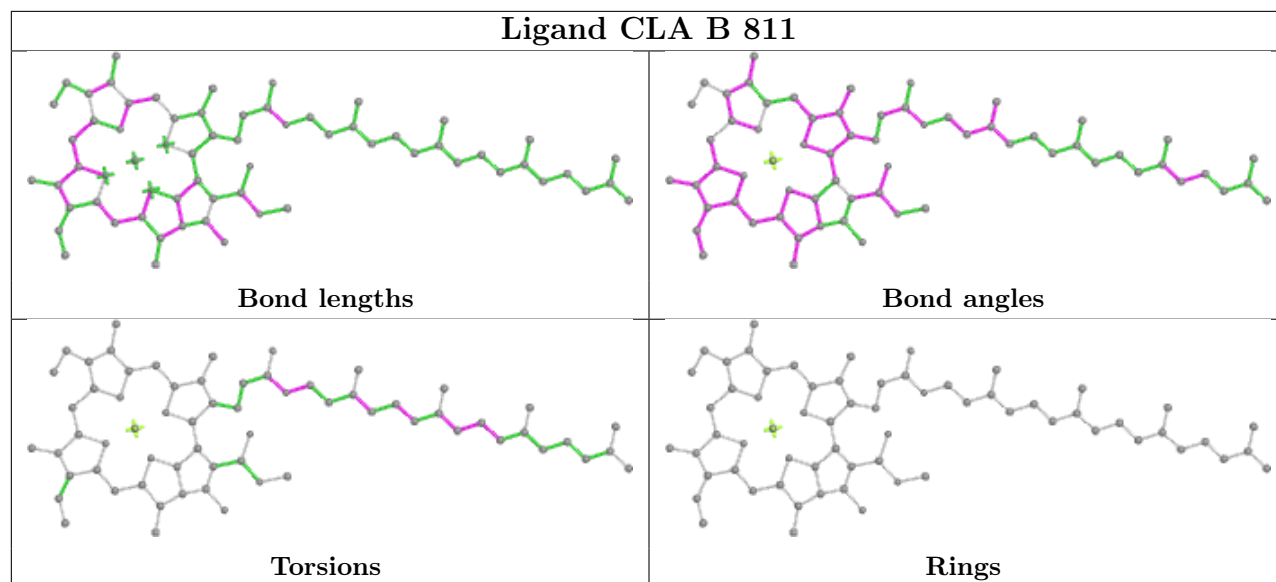




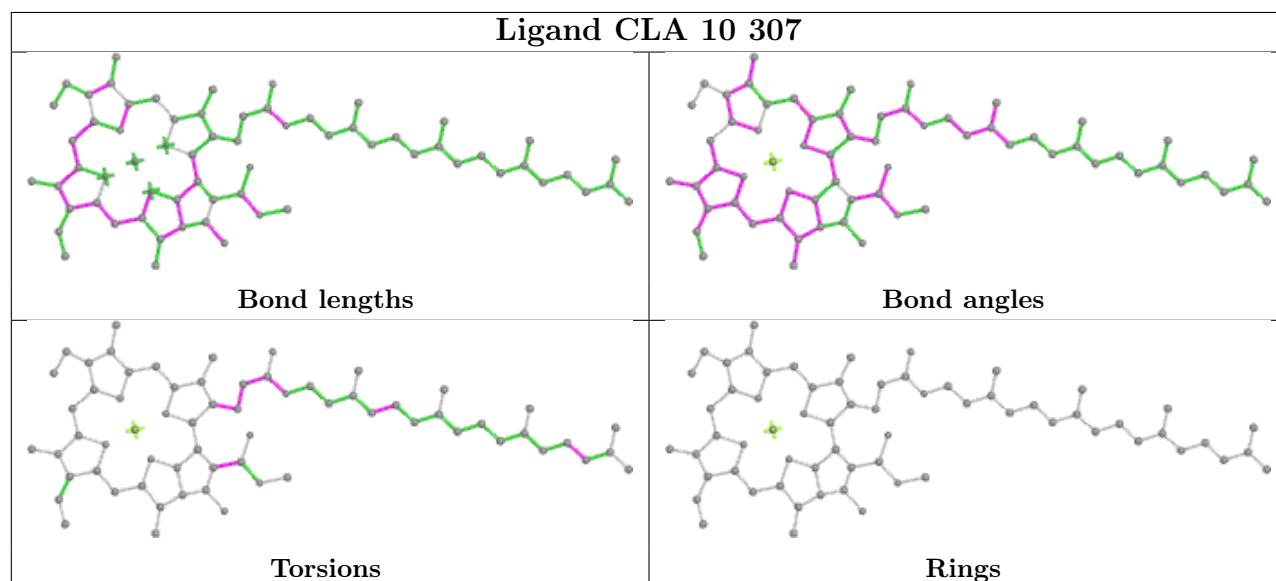
Ligand CLA 5 311**Ligand CLA A 836**



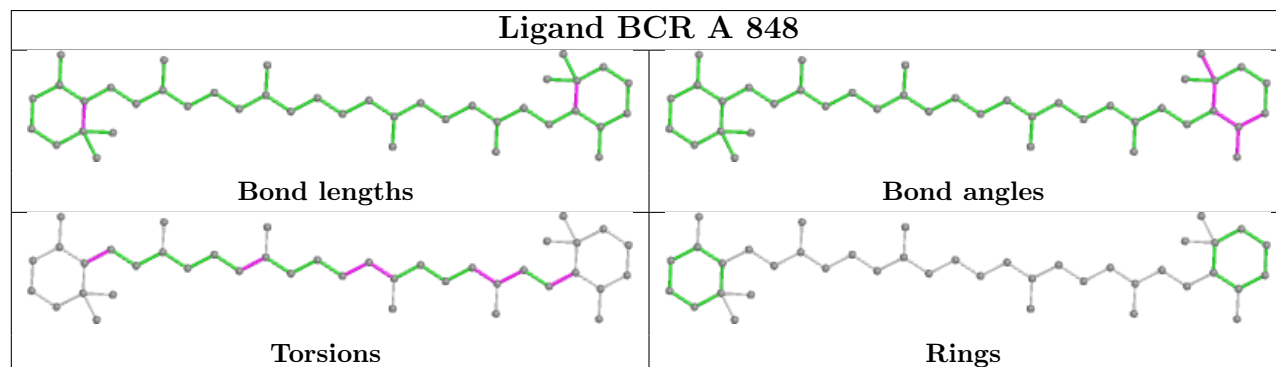
Ligand CLA B 811

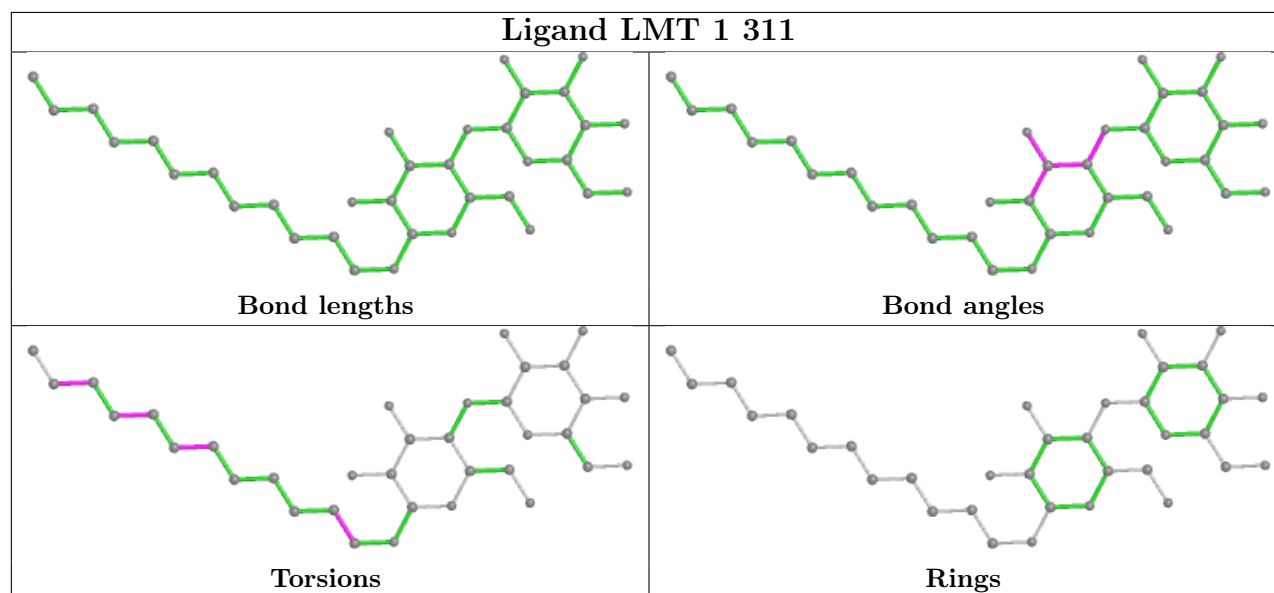
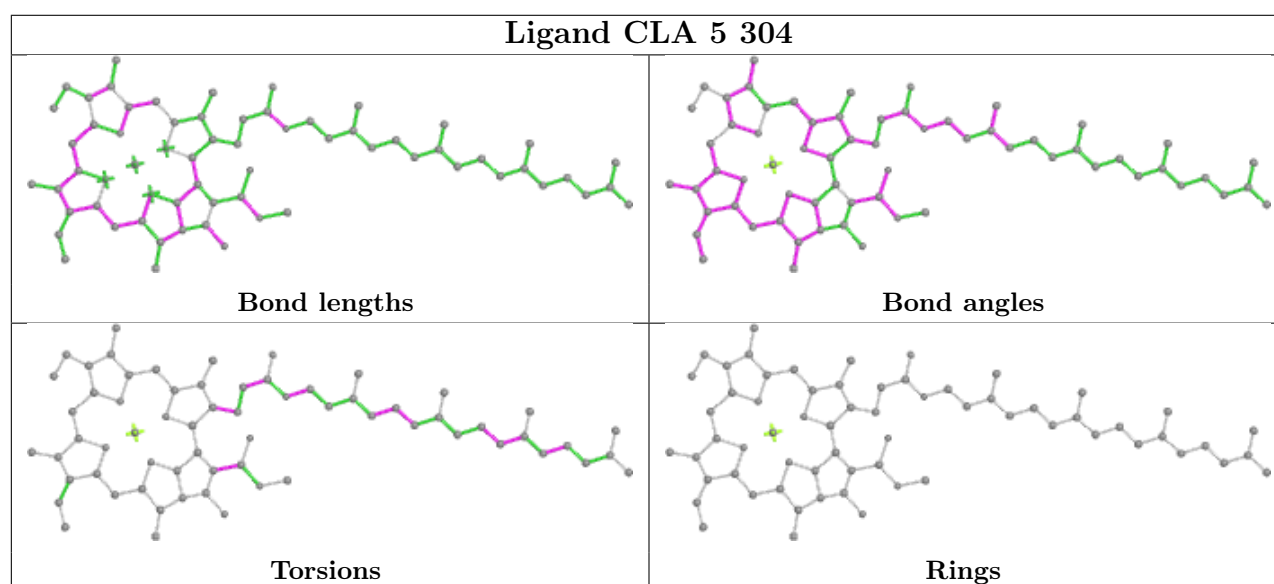
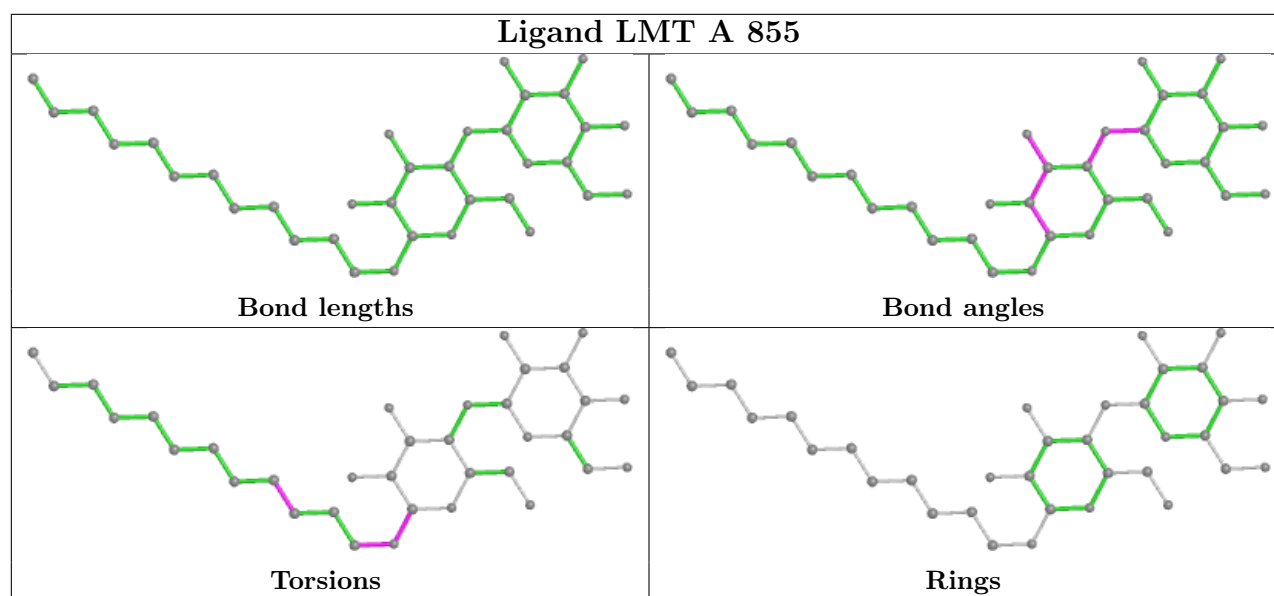


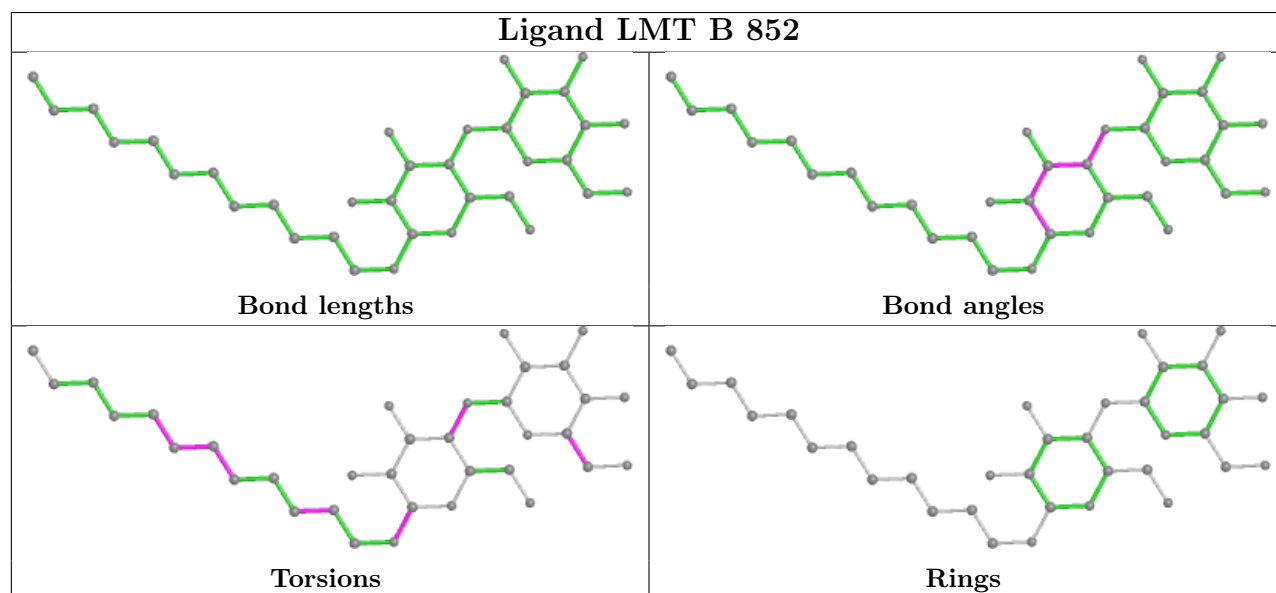
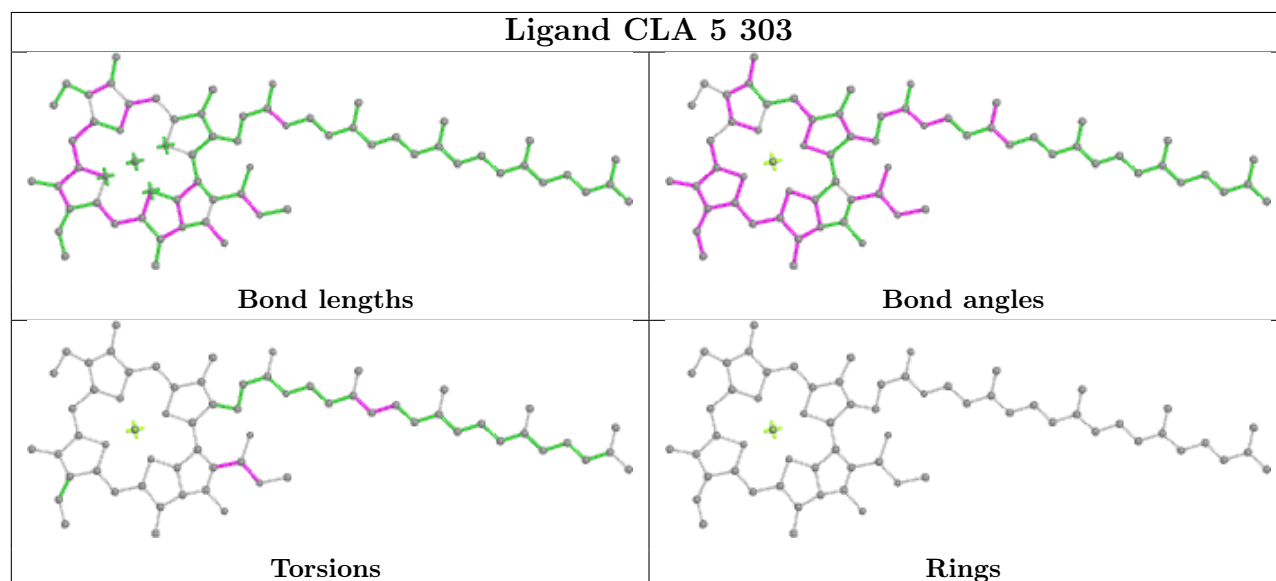
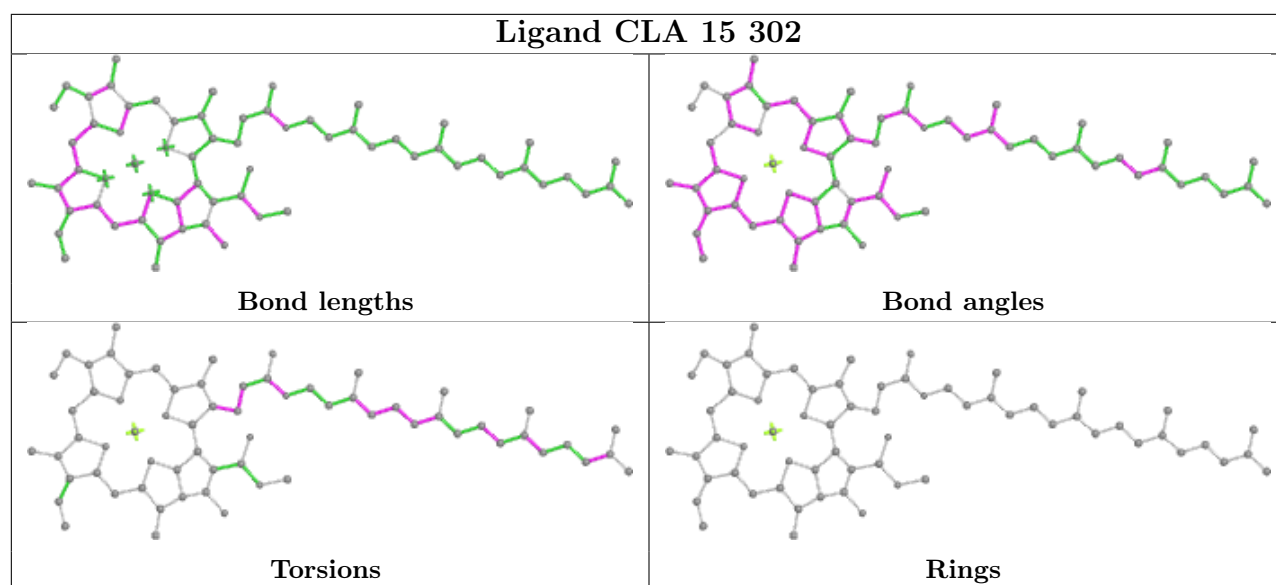
Ligand CLA 10 307



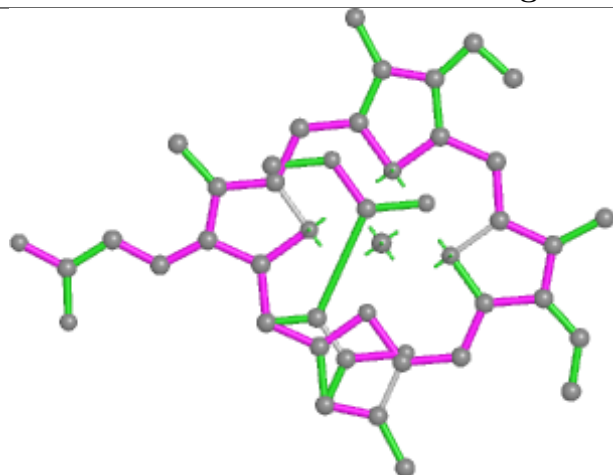
Ligand BCR A 848



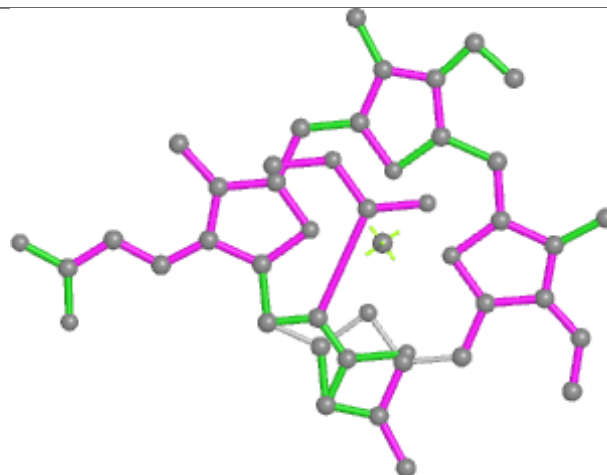




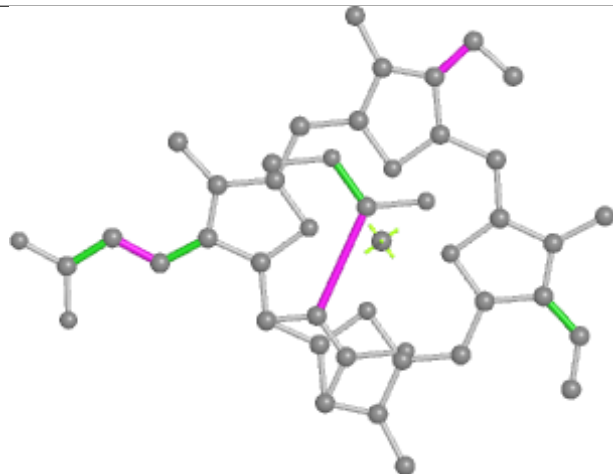
Ligand KC1 1 308



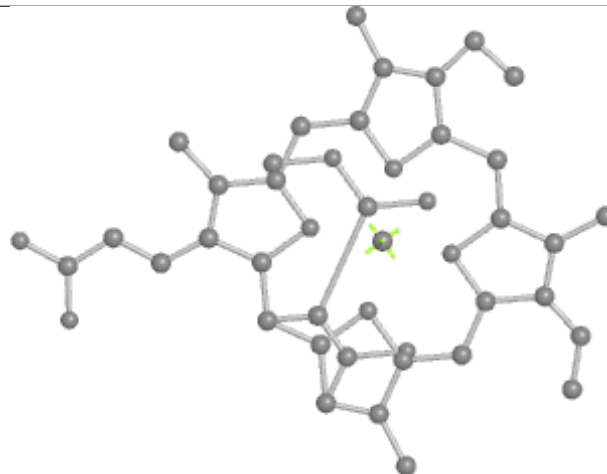
Bond lengths



Bond angles

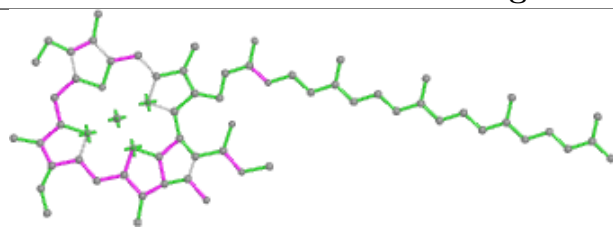


Torsions

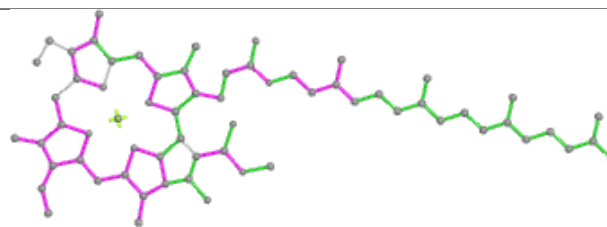


Rings

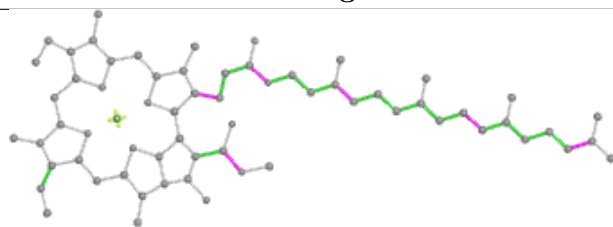
Ligand CLA 15 309



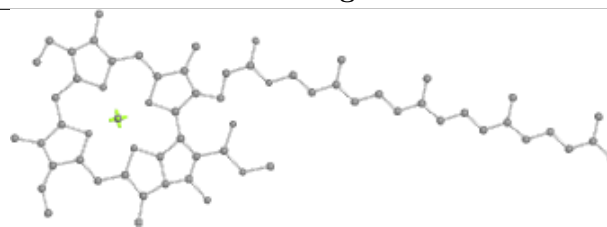
Bond lengths



Bond angles

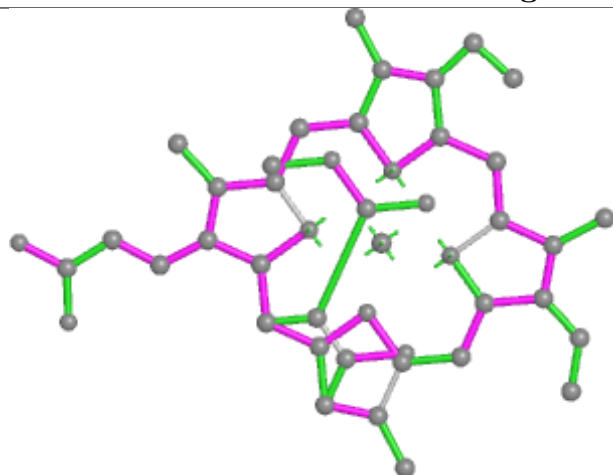


Torsions

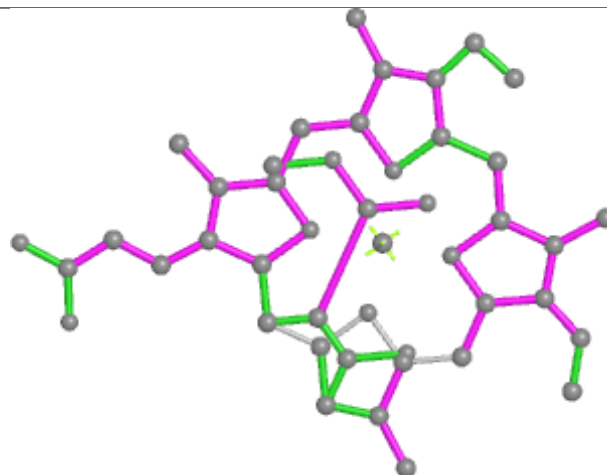


Rings

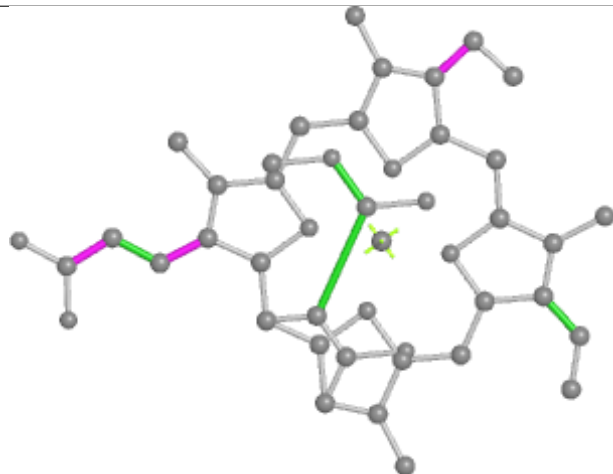
Ligand KC1 5 305



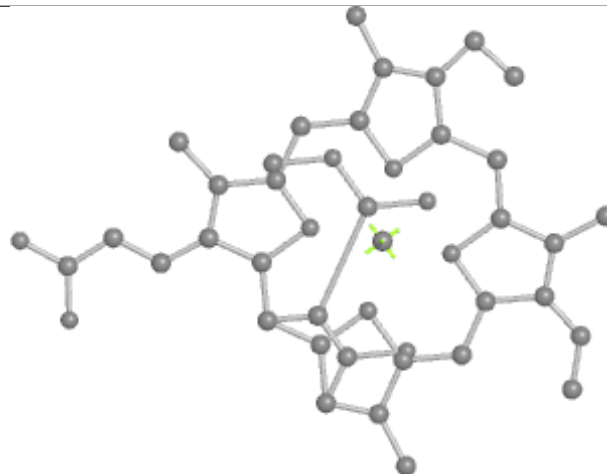
Bond lengths



Bond angles

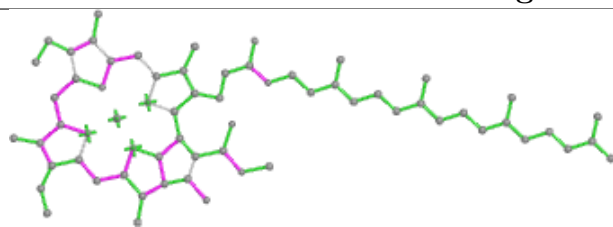


Torsions

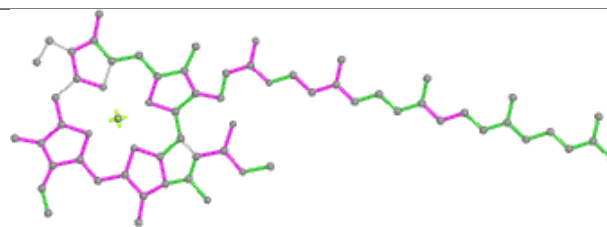


Rings

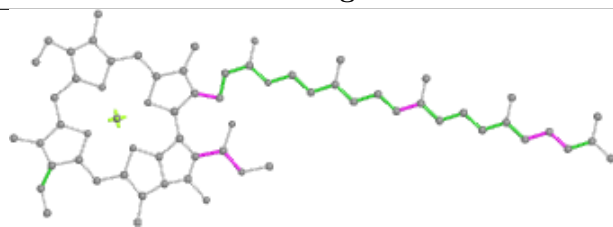
Ligand CLA F 201



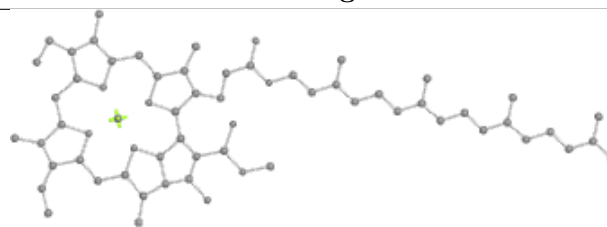
Bond lengths



Bond angles

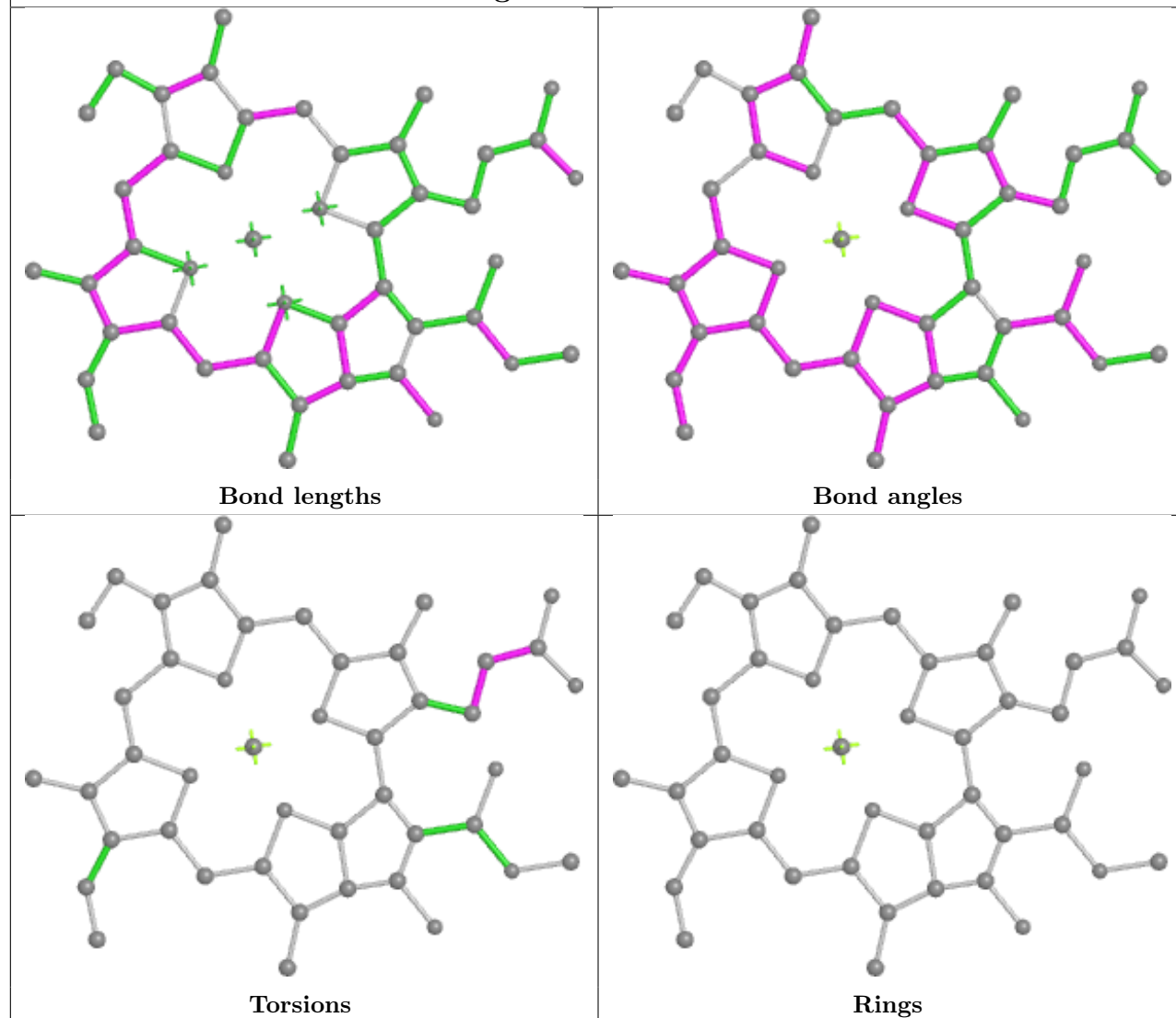


Torsions

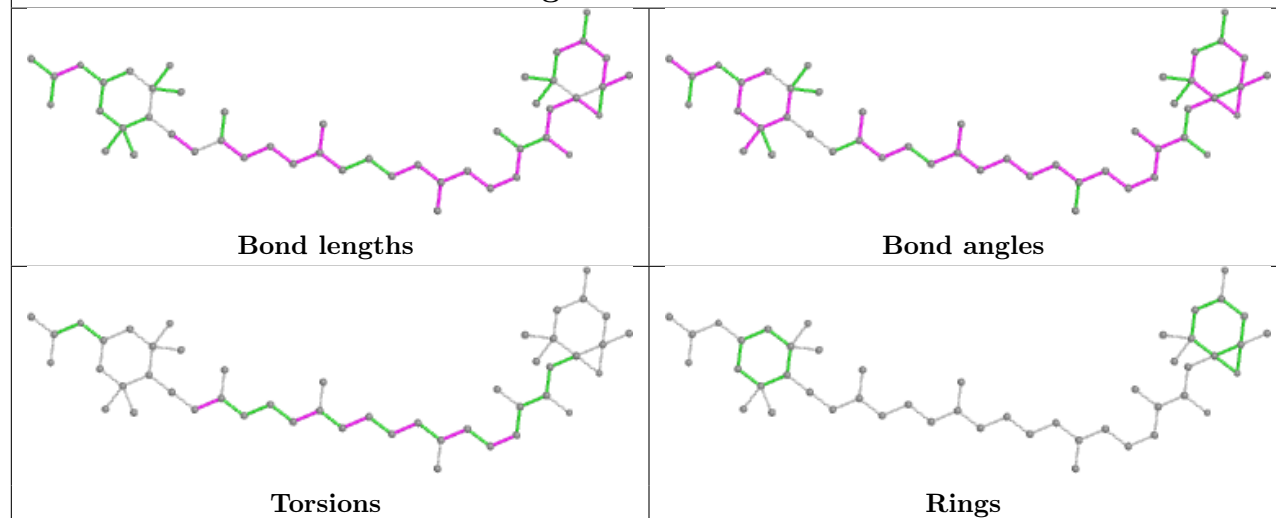


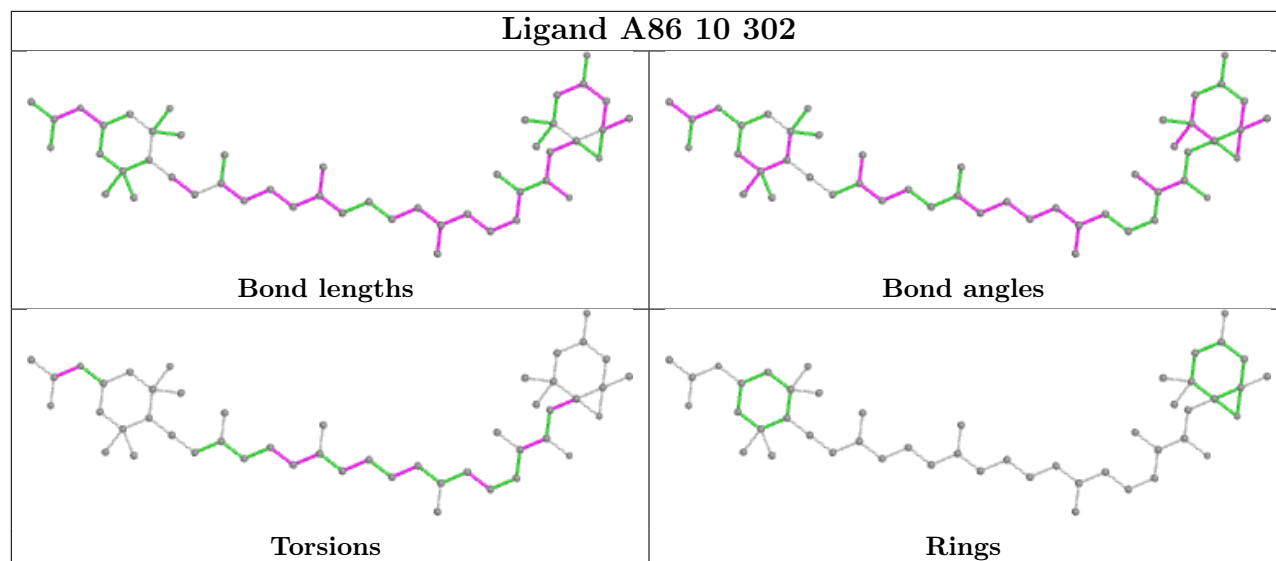
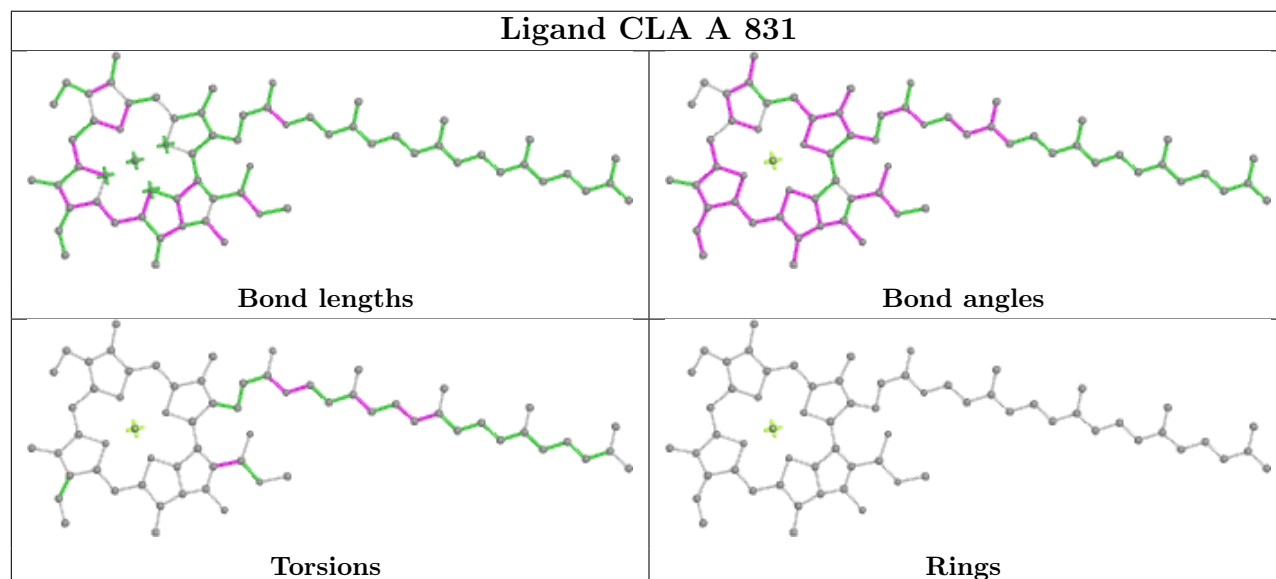
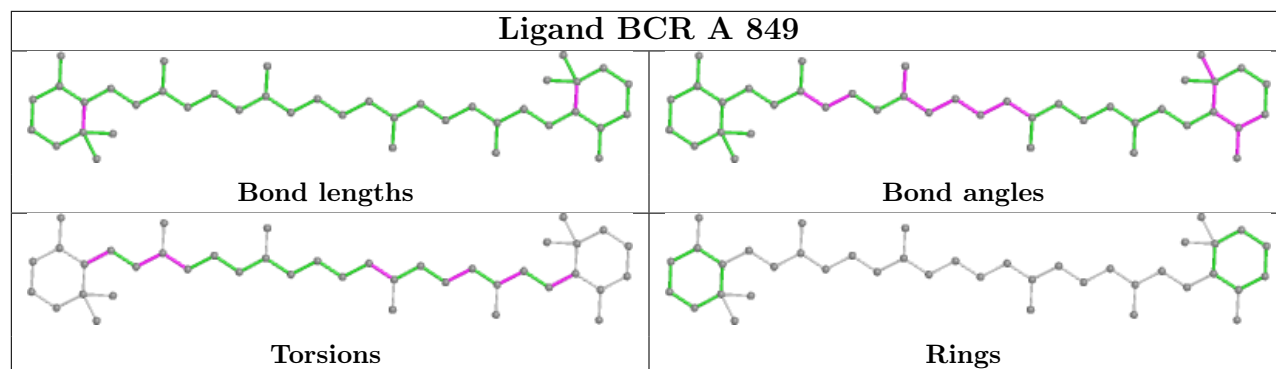
Rings

Ligand CLA 2 313

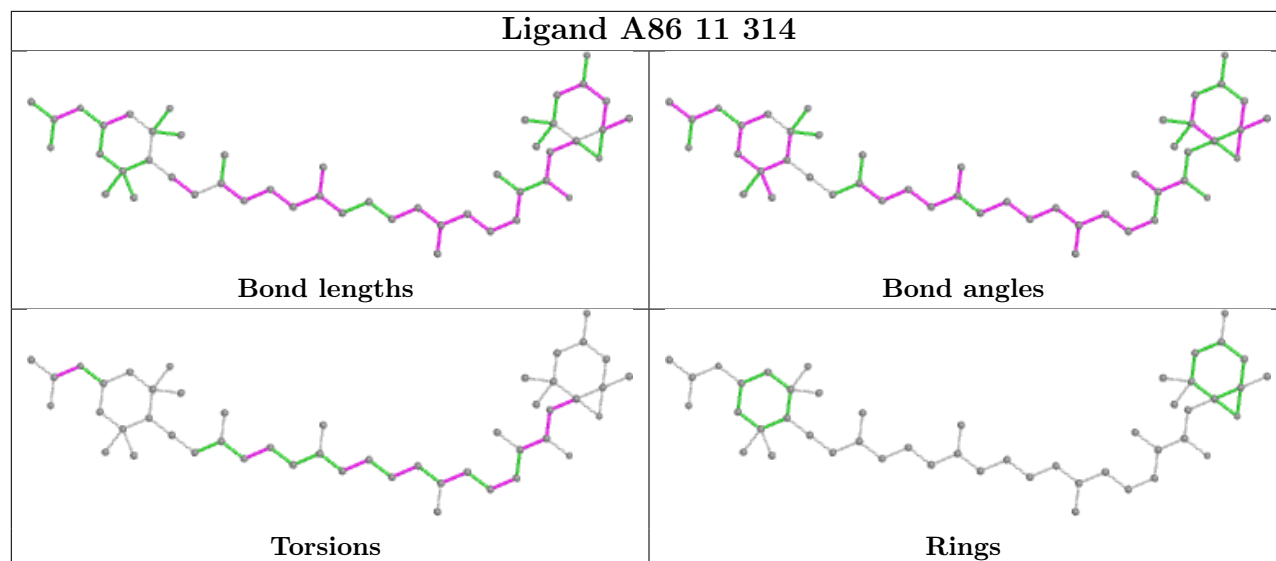


Ligand A86 6 320

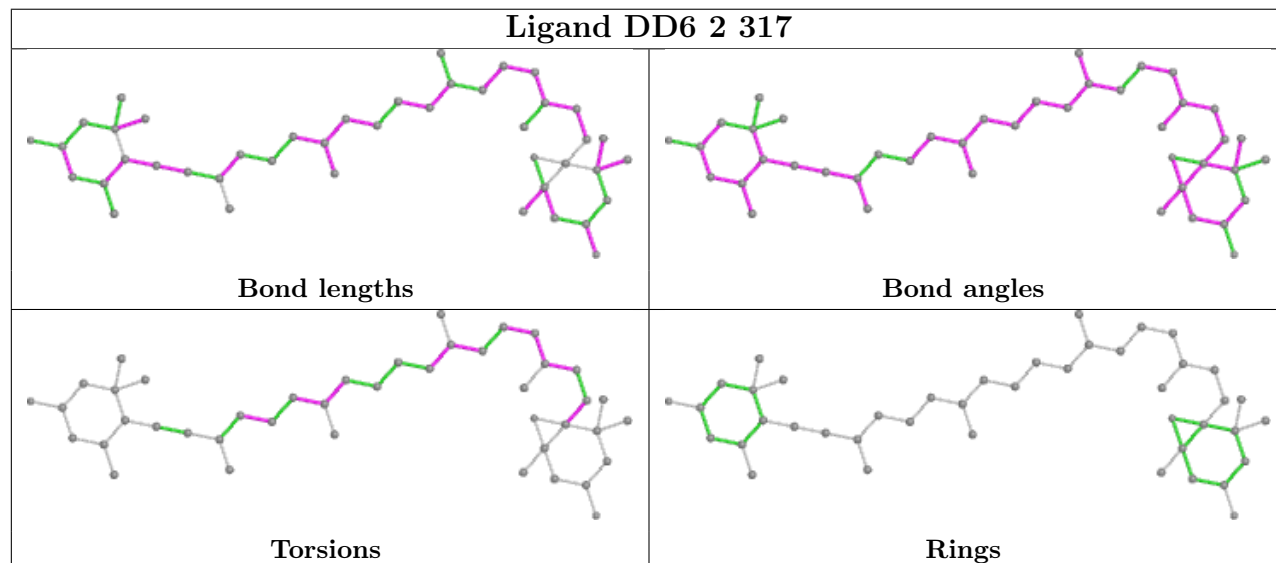


Ligand A86 10 302**Ligand CLA A 831****Ligand BCR A 849**

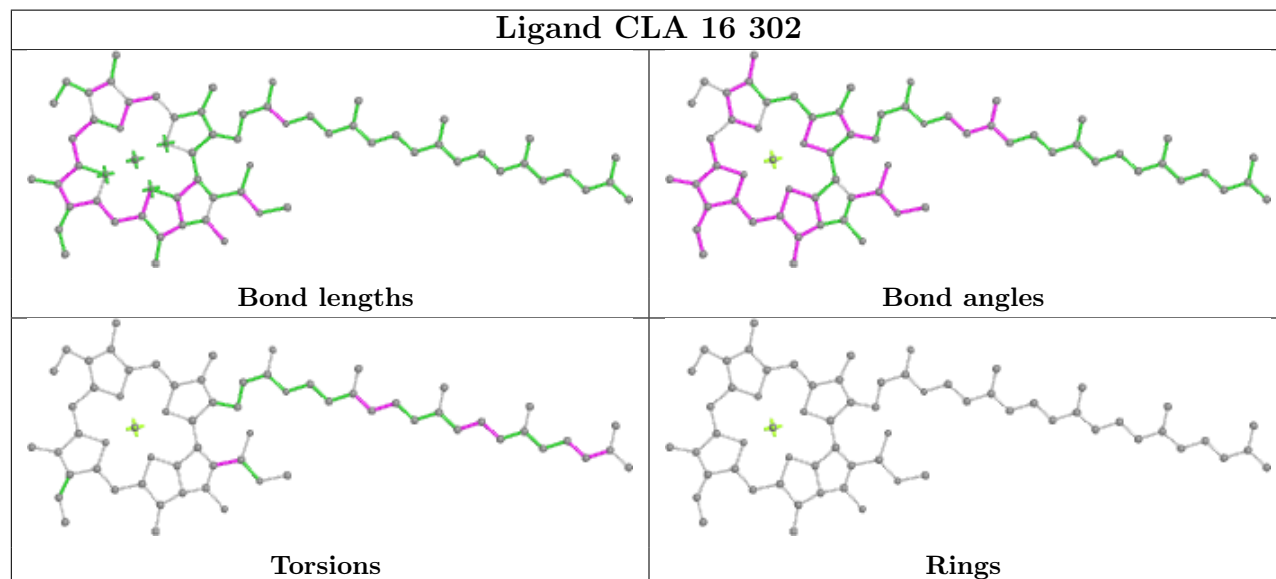
Ligand A86 11 314

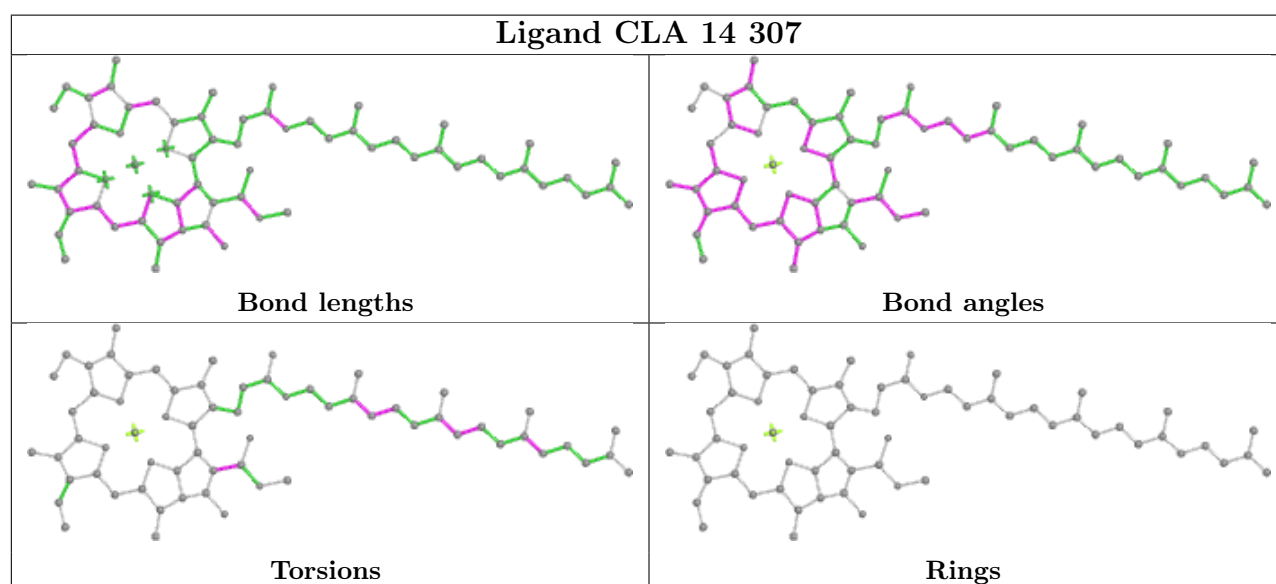
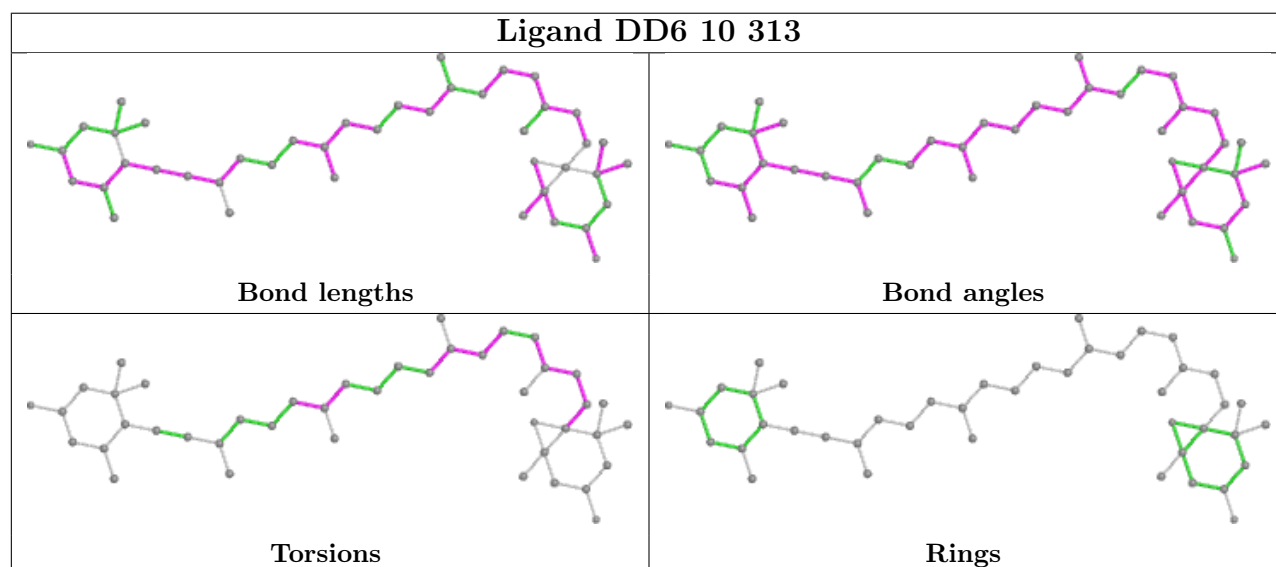
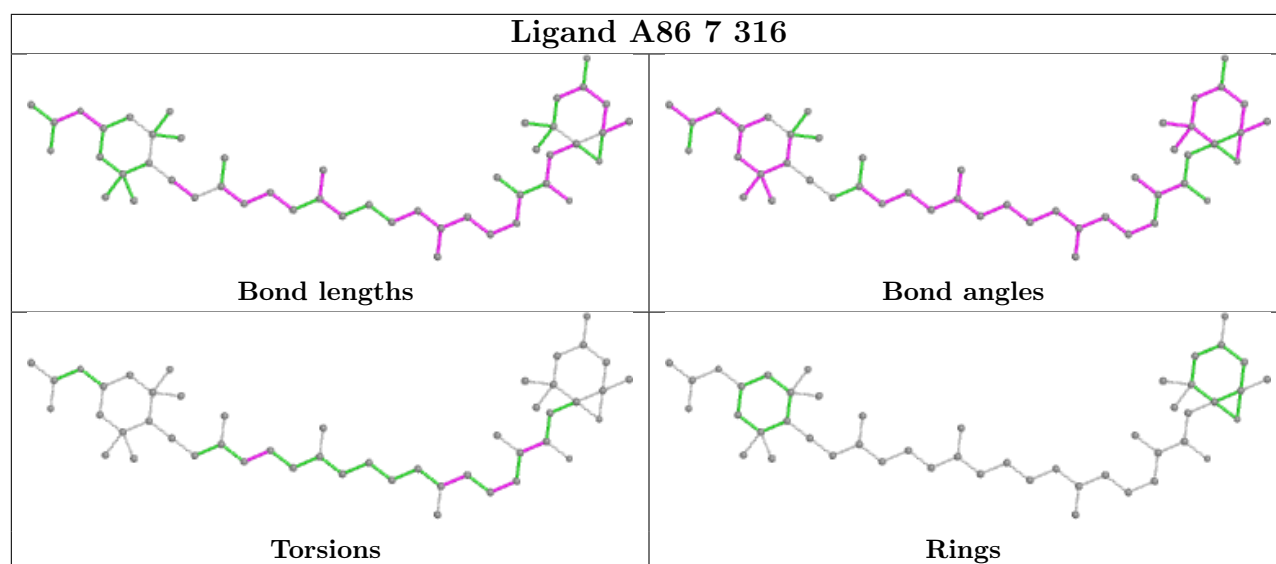


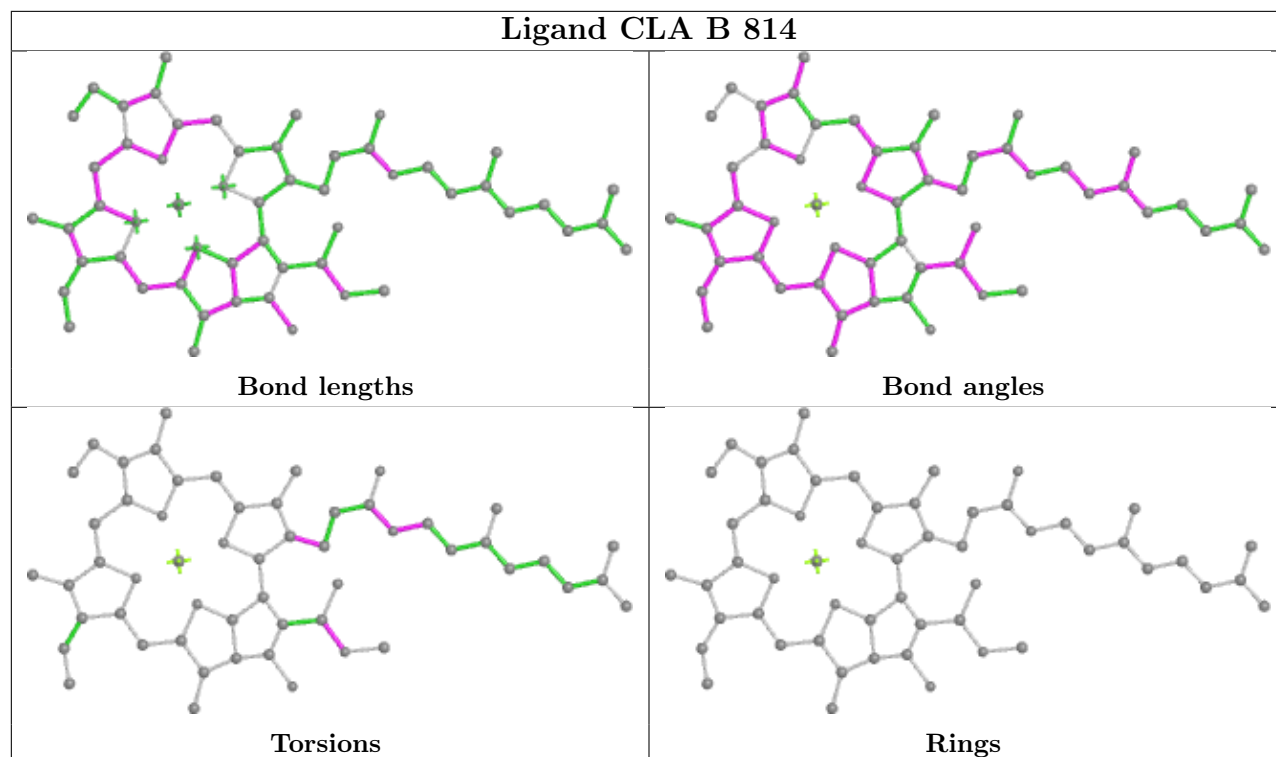
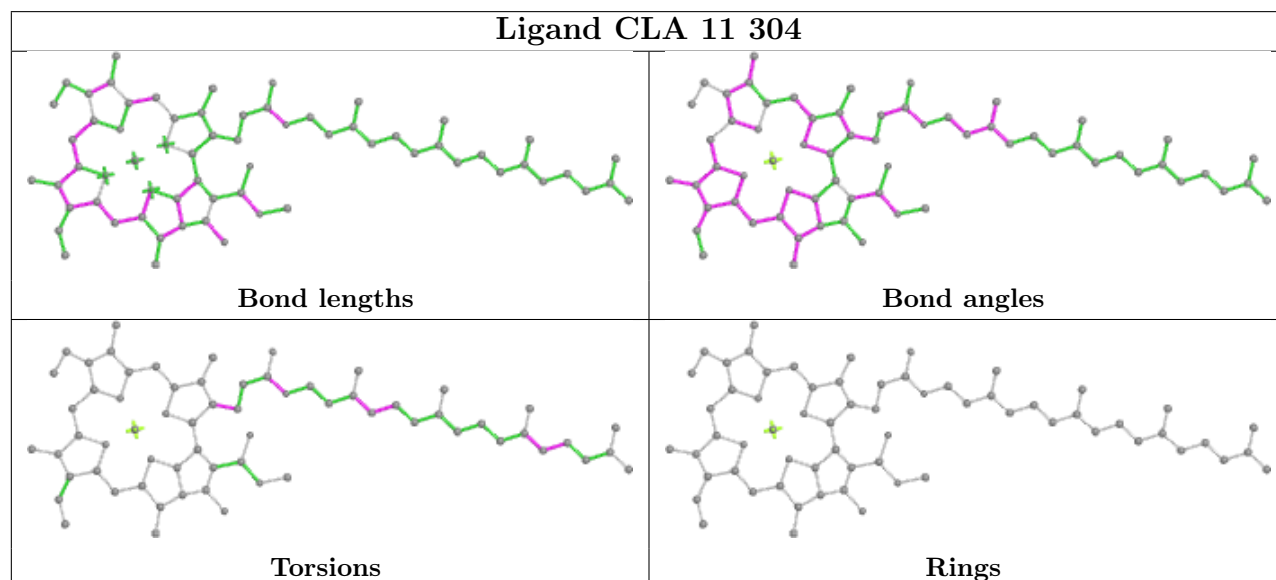
Ligand DD6 2 317

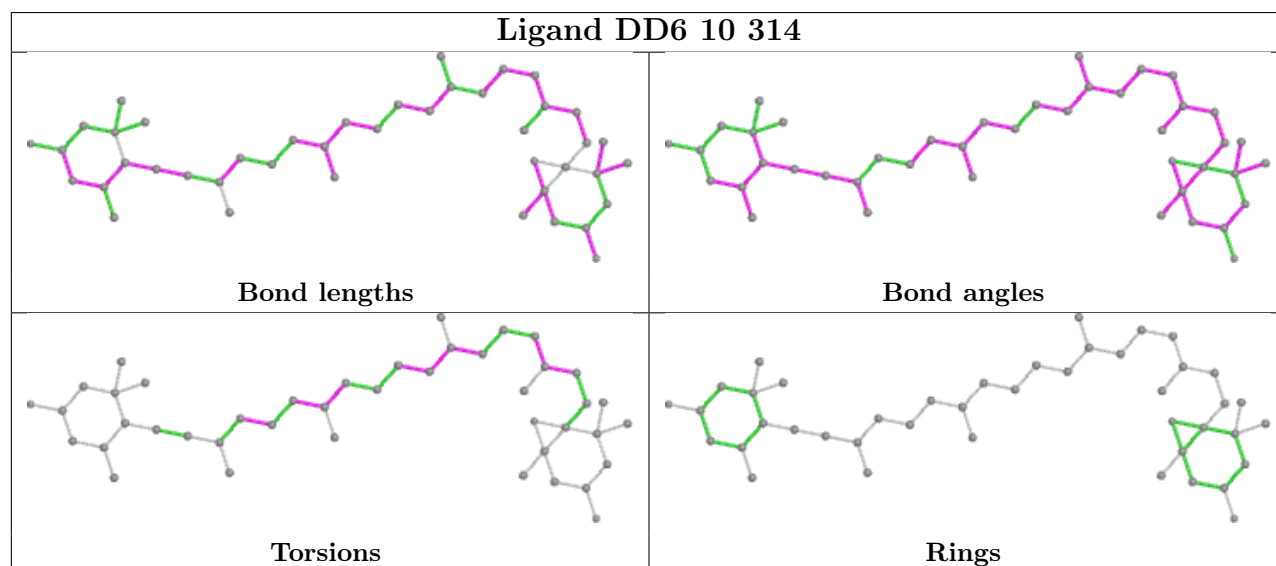
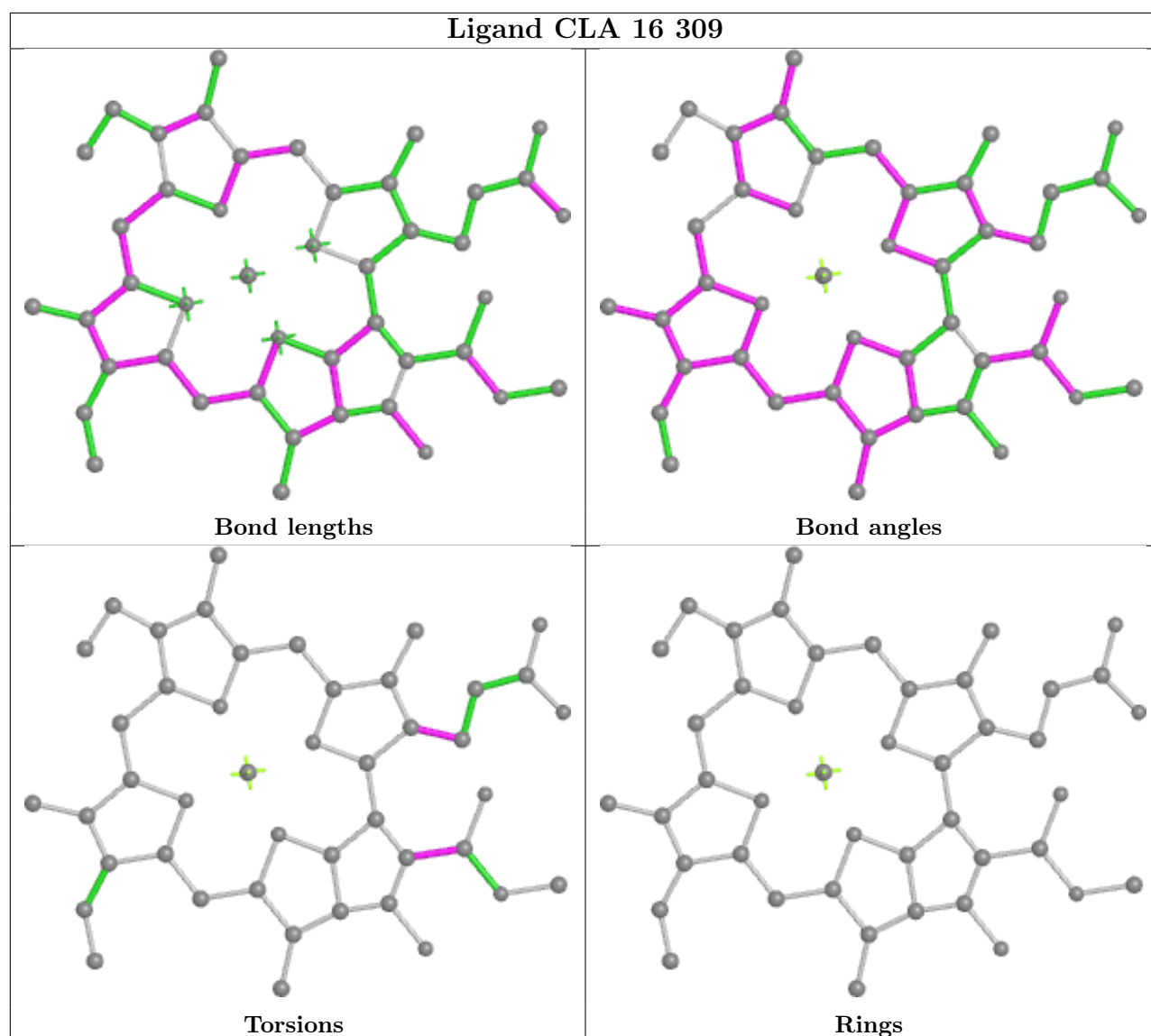


Ligand CLA 16 302

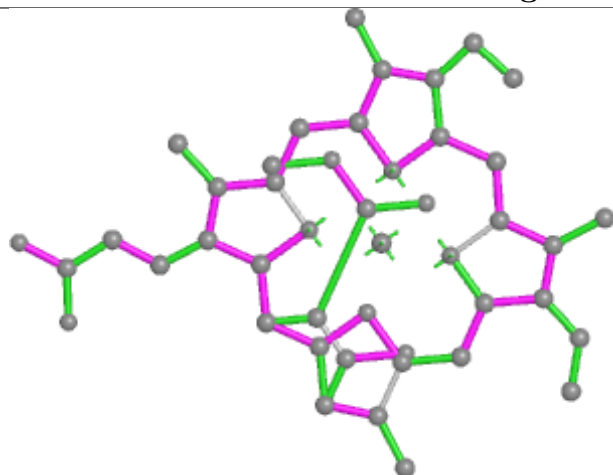




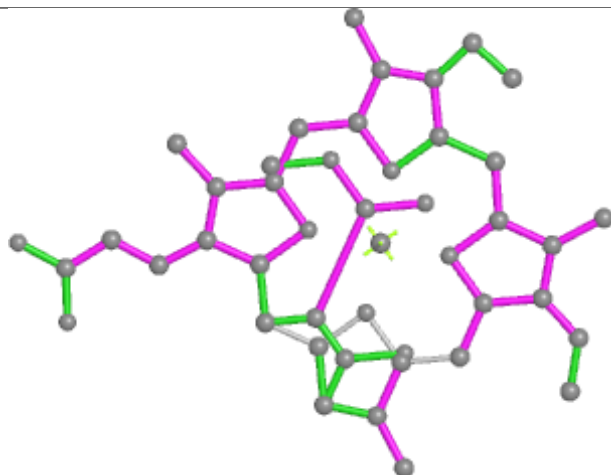
Ligand CLA B 814**Ligand CLA 11 304**



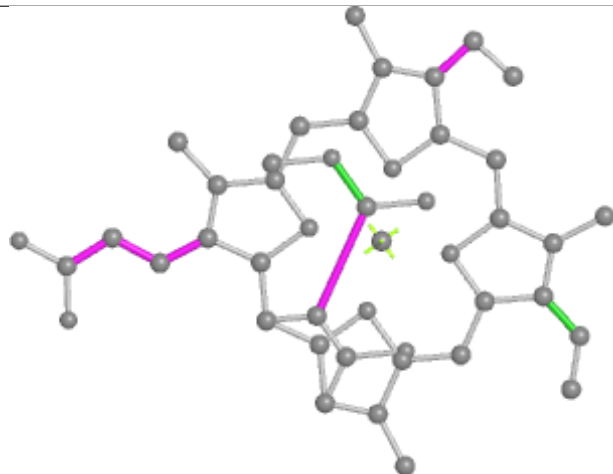
Ligand KC1 3 308



Bond lengths



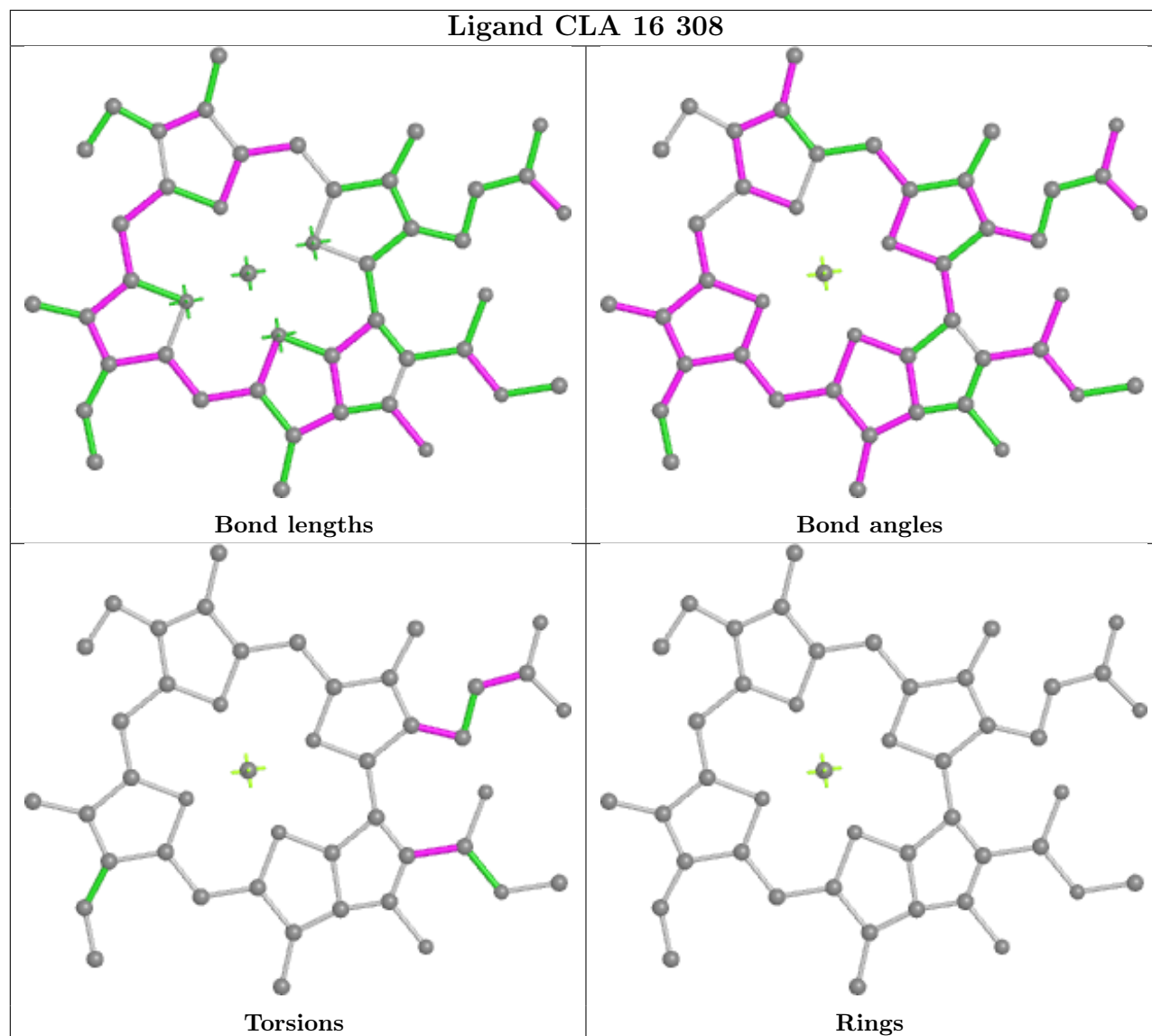
Bond angles

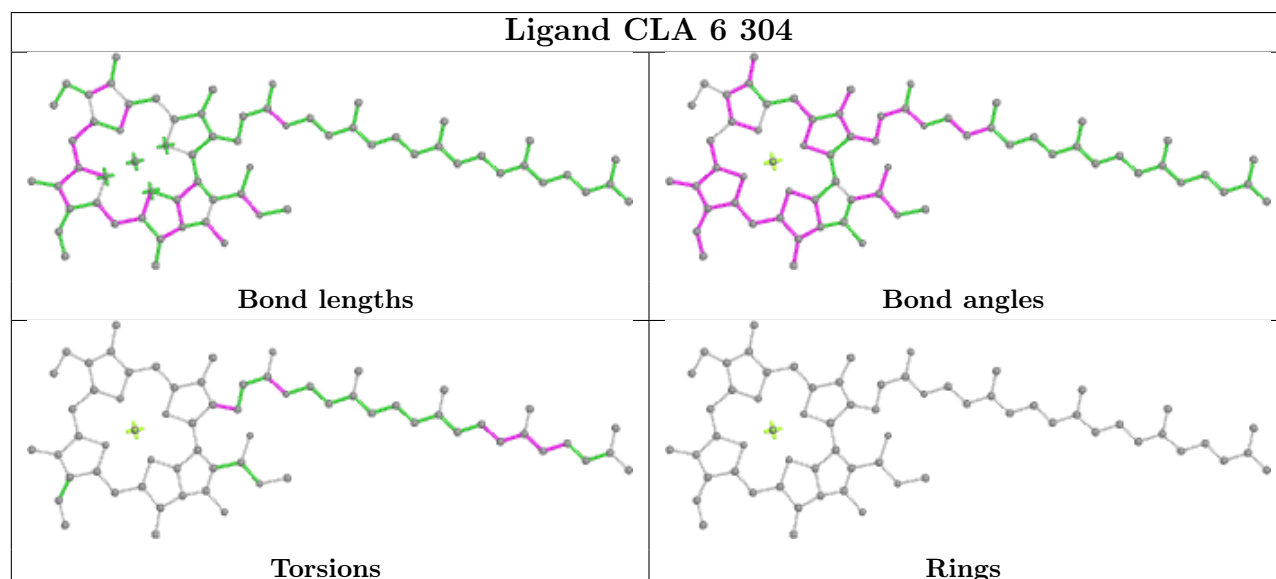
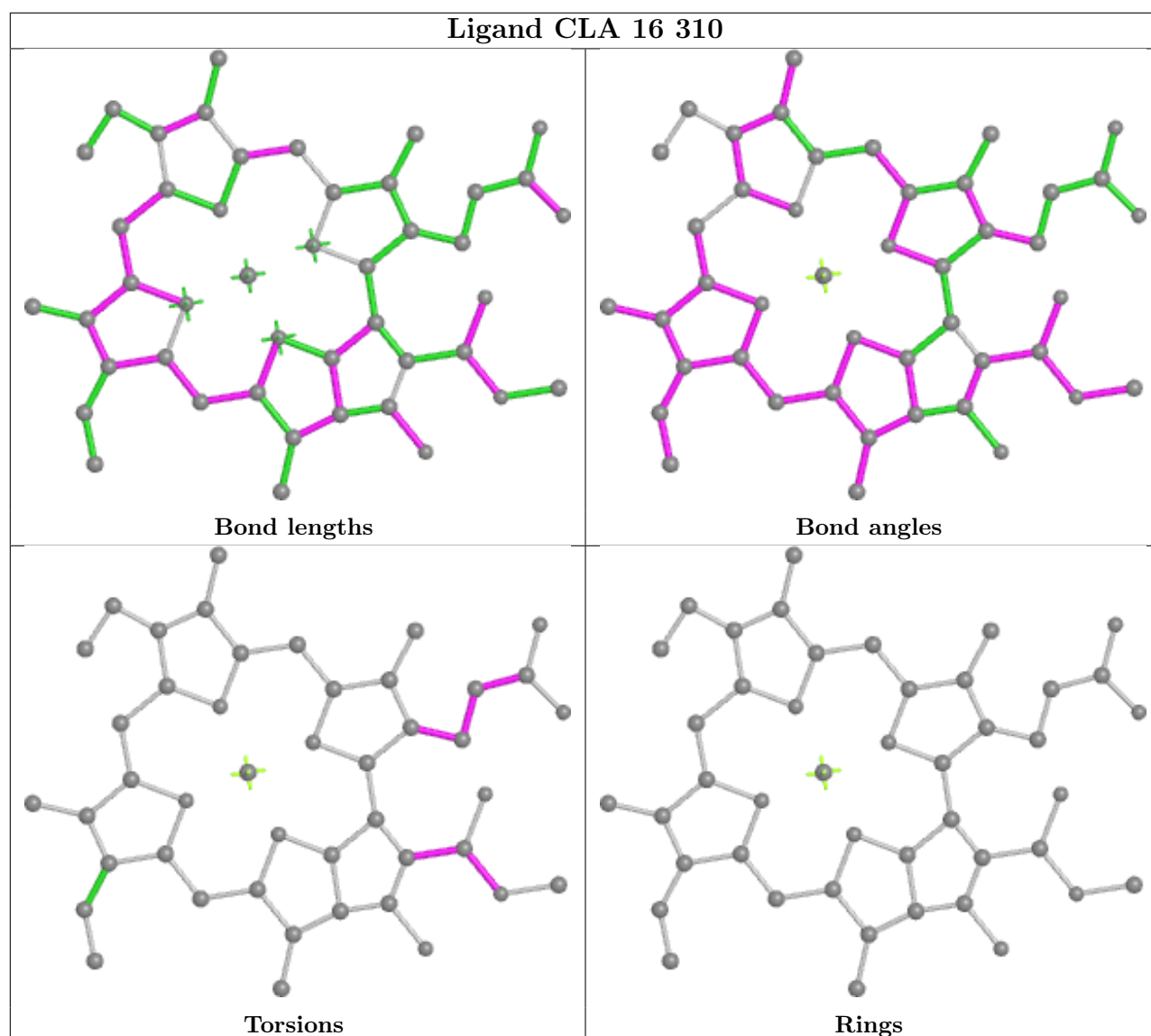


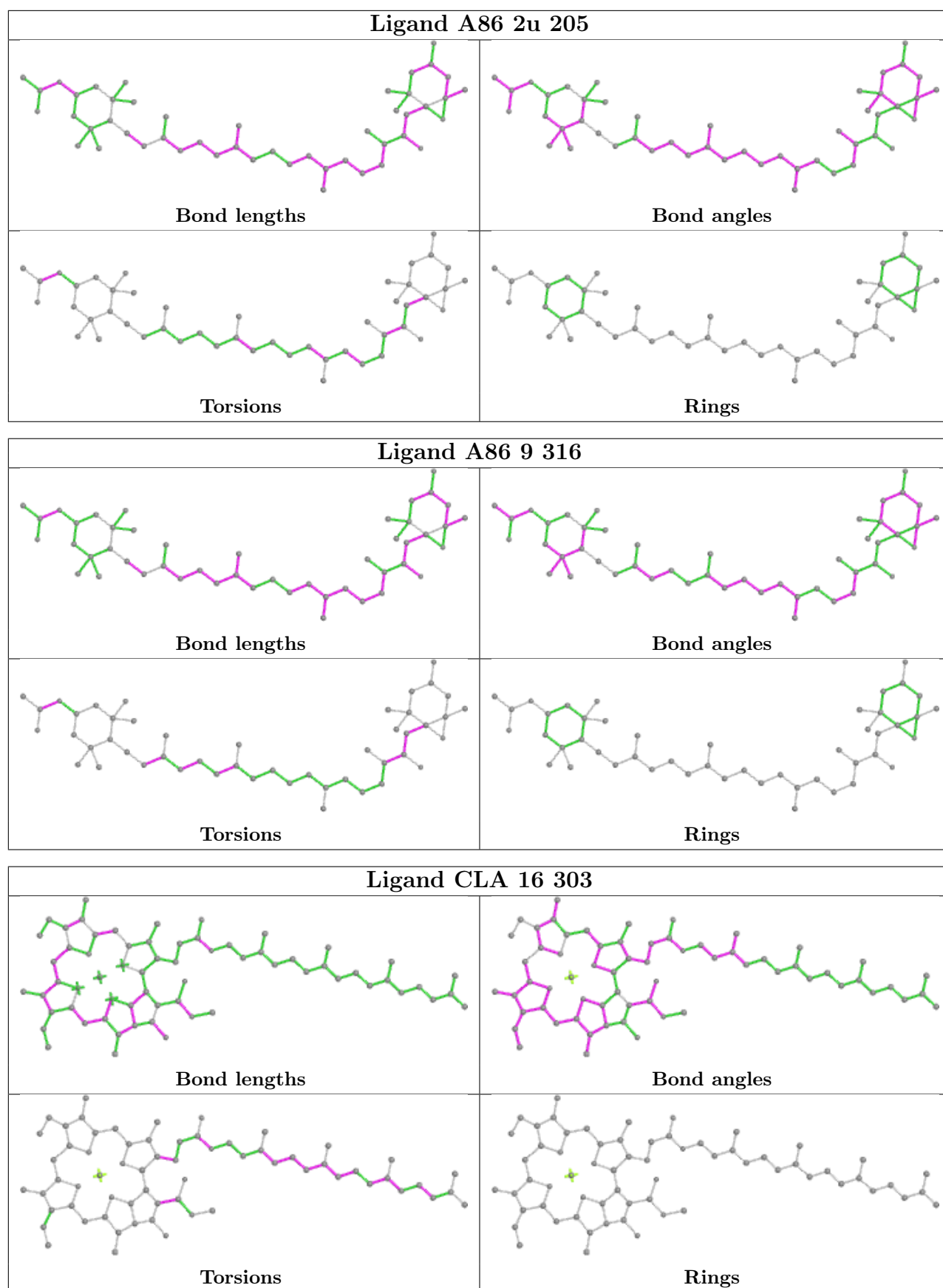
Torsions



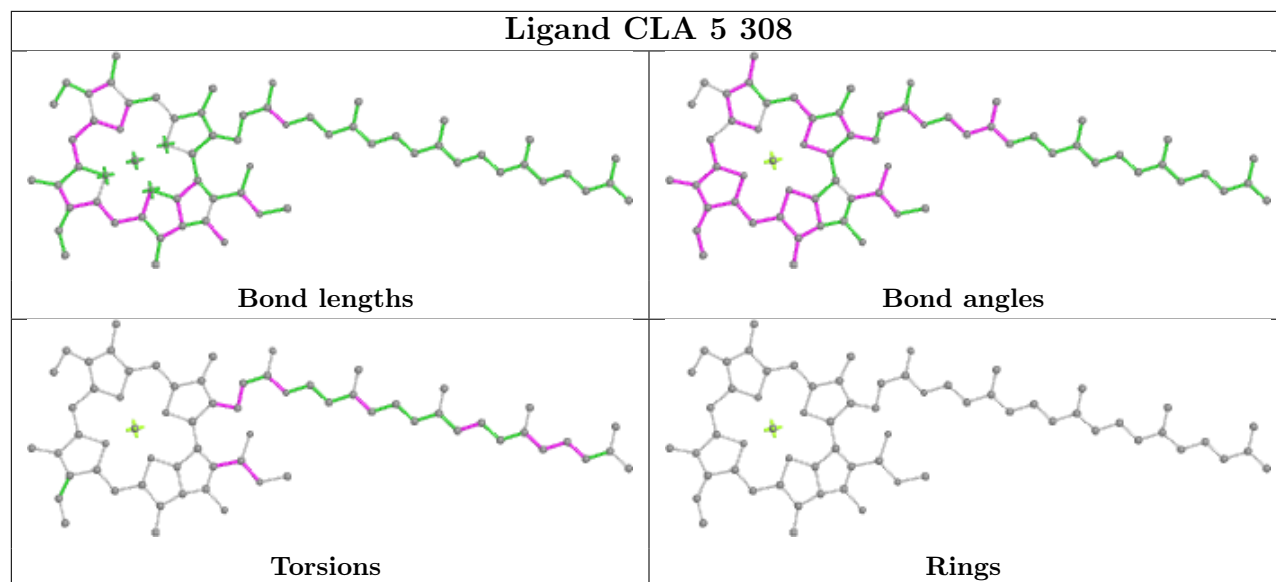
Rings



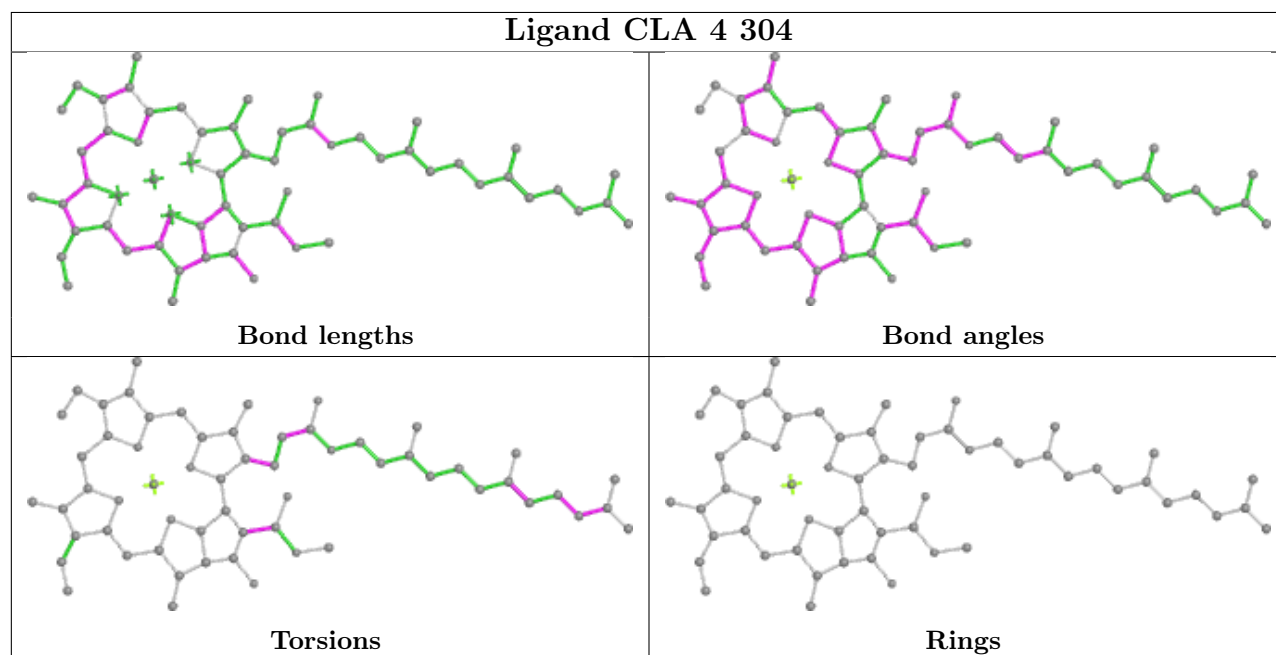




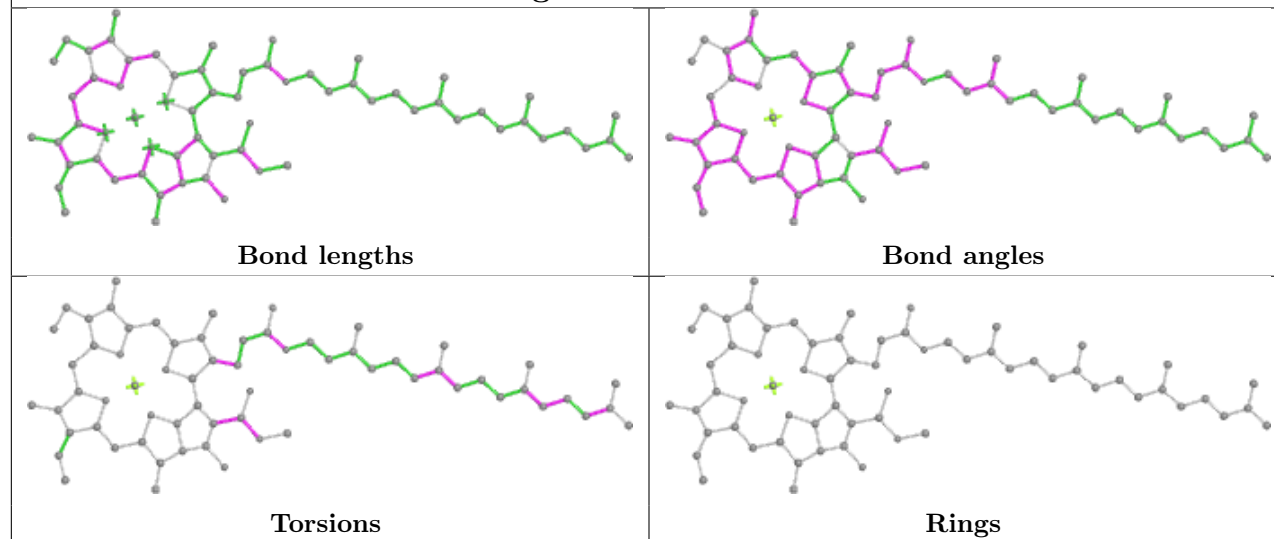
Ligand CLA 5 308



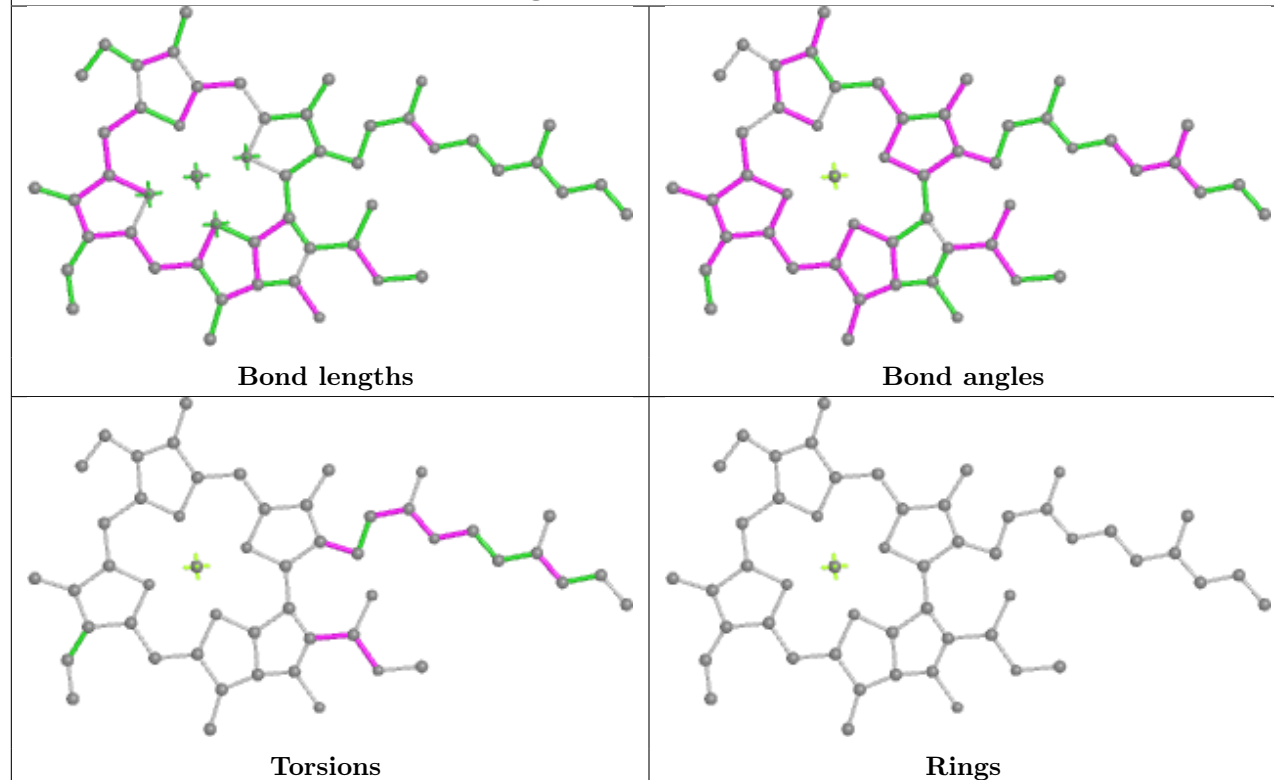
Ligand CLA 4 304



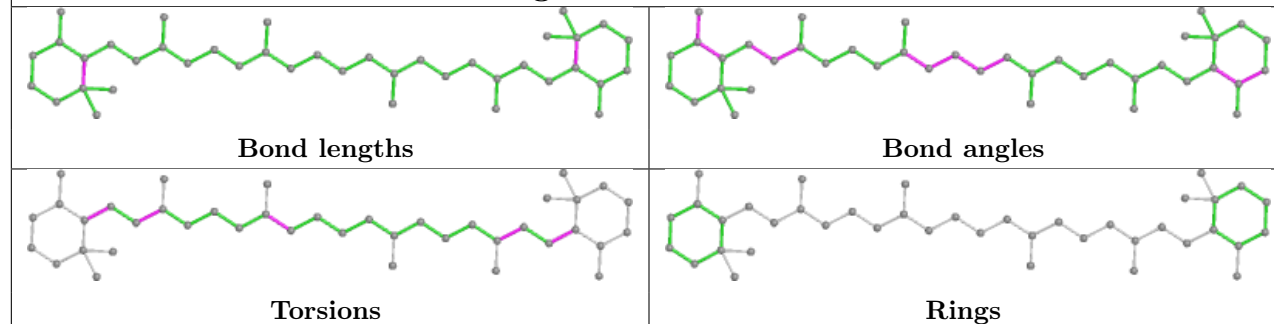
Ligand CLA B 851

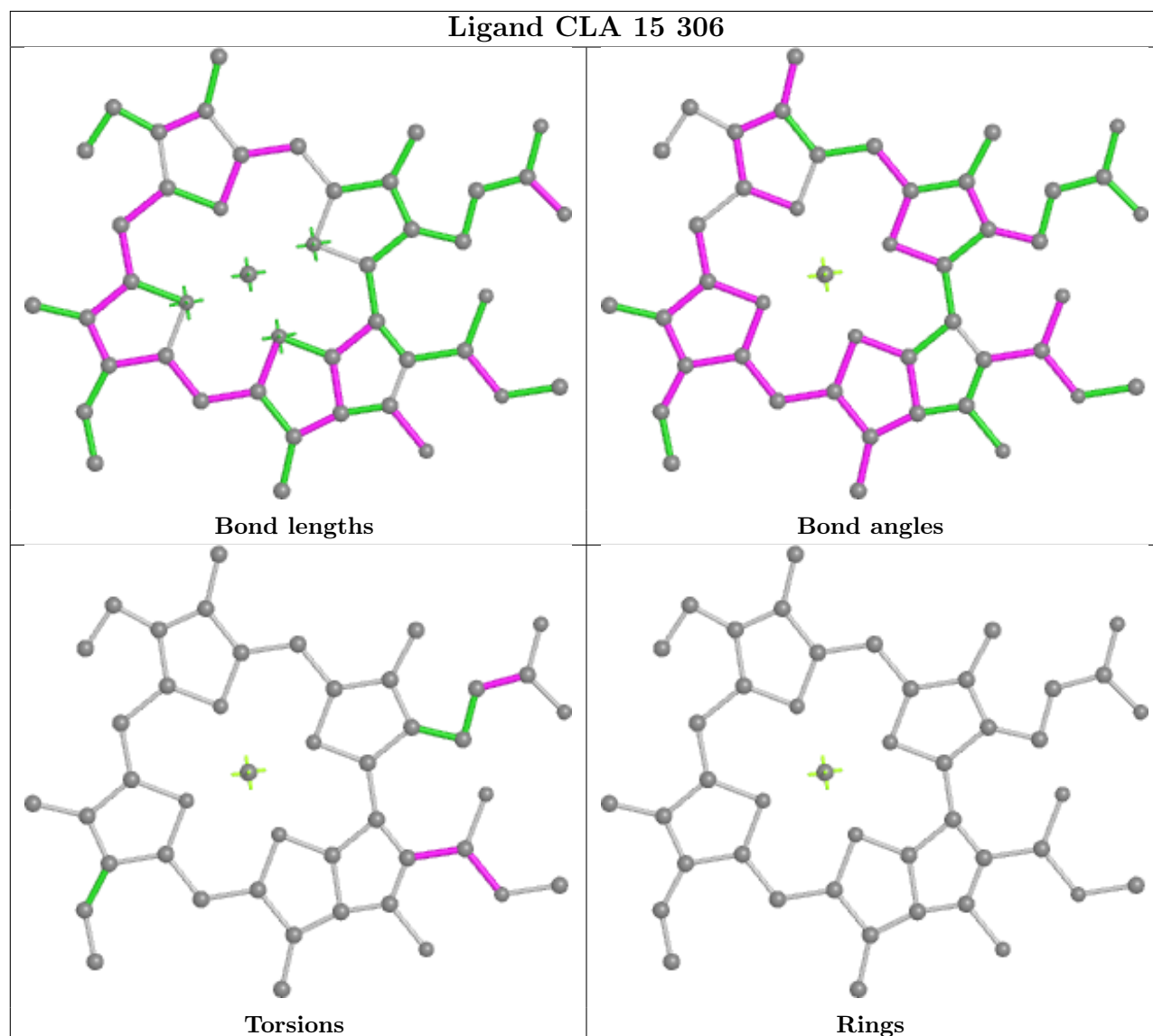
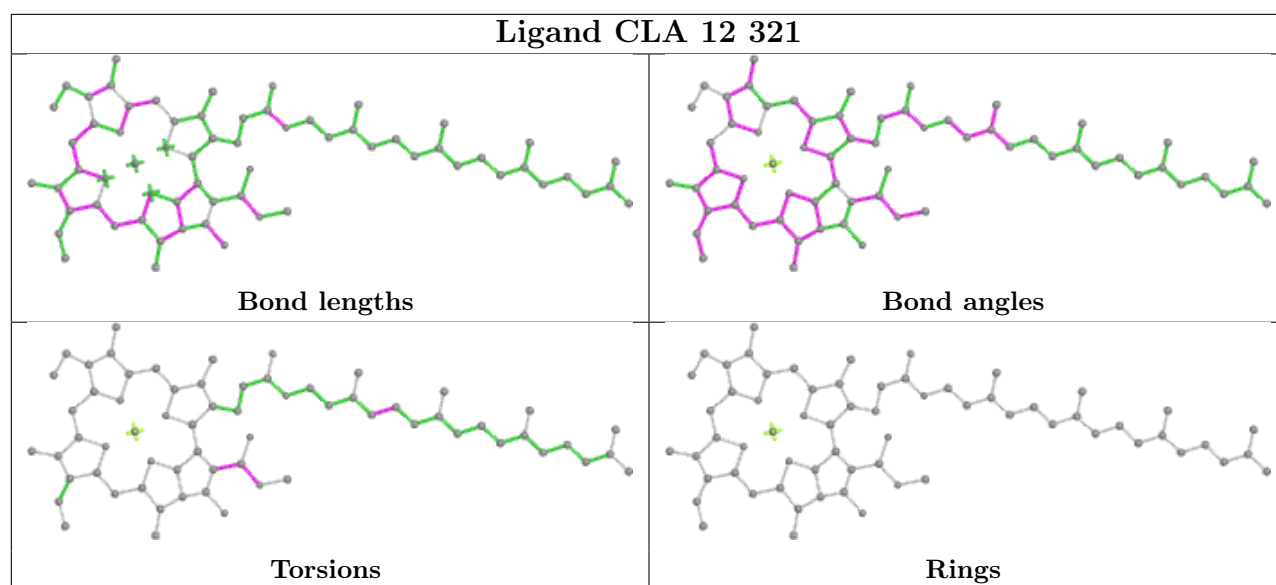


Ligand CLA 16 306

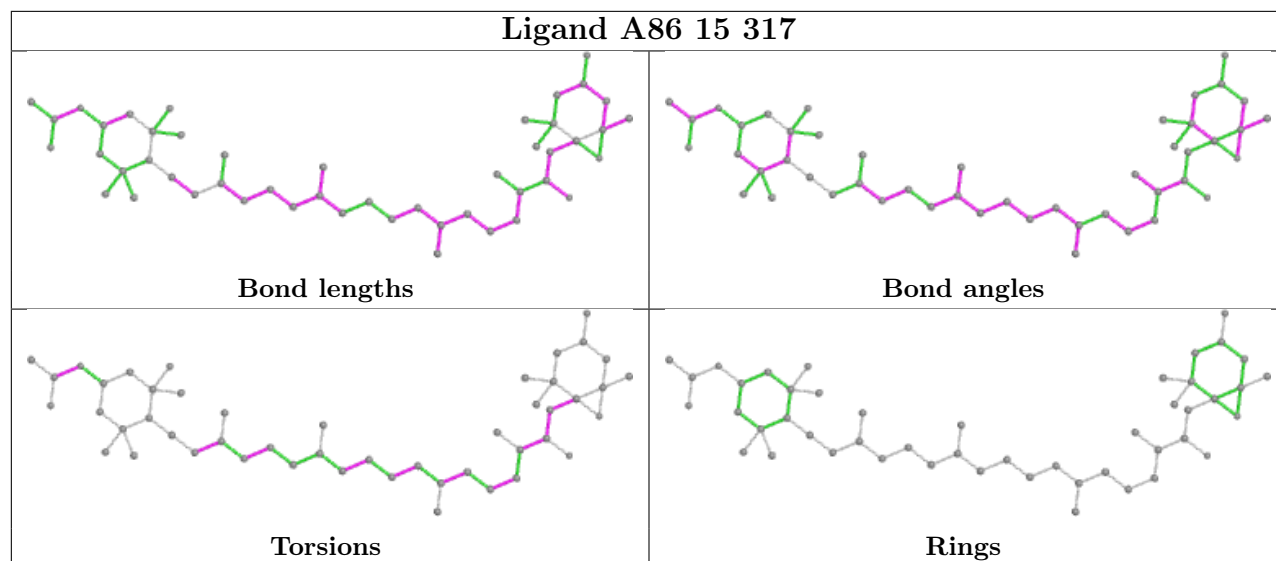


Ligand BCR L 205

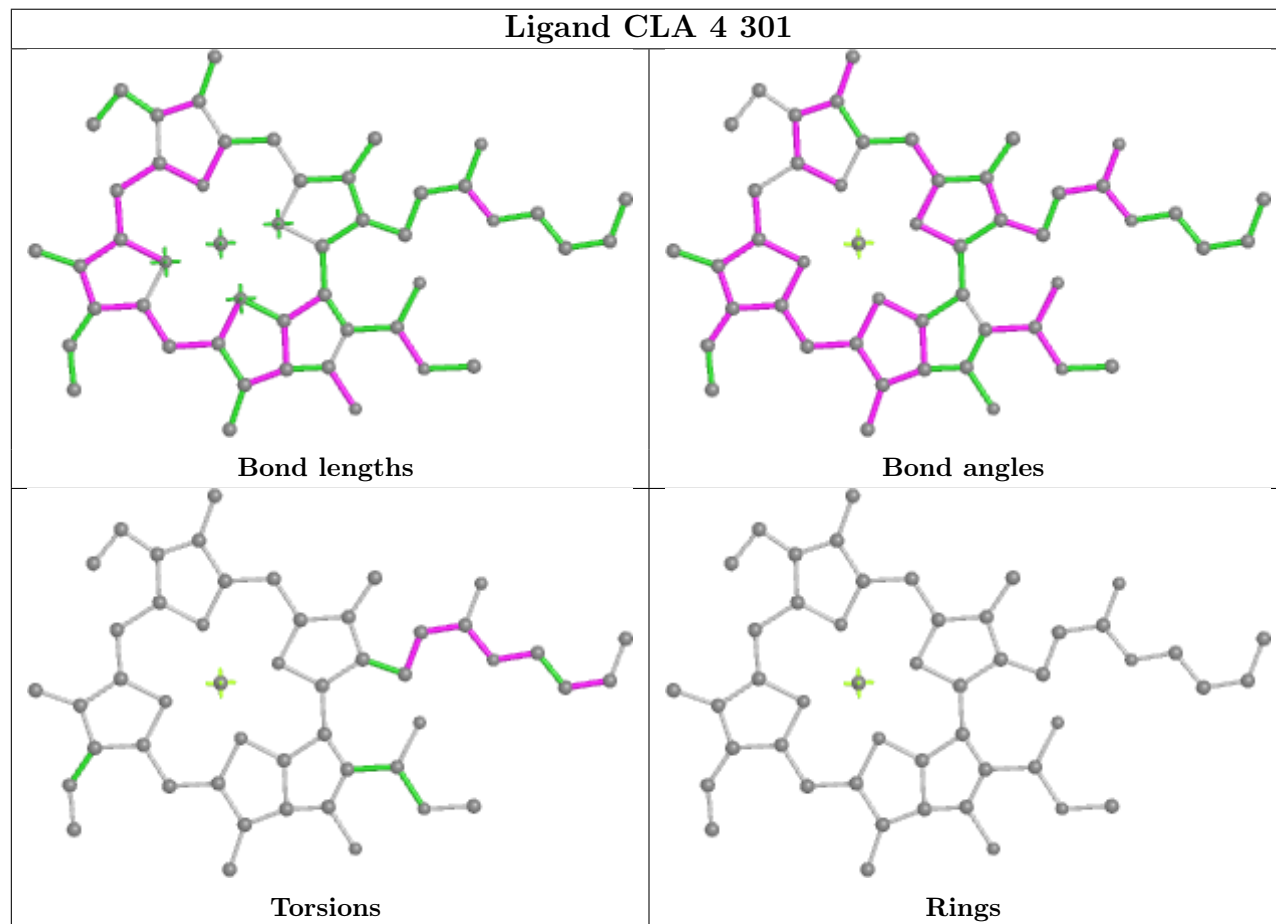




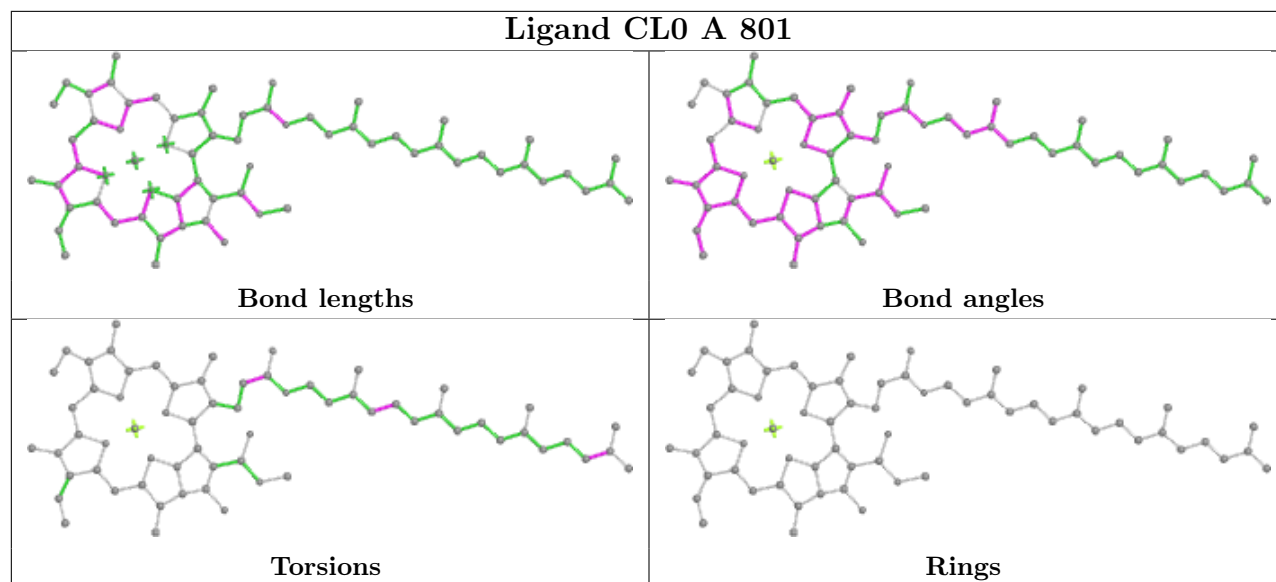
Ligand A86 15 317



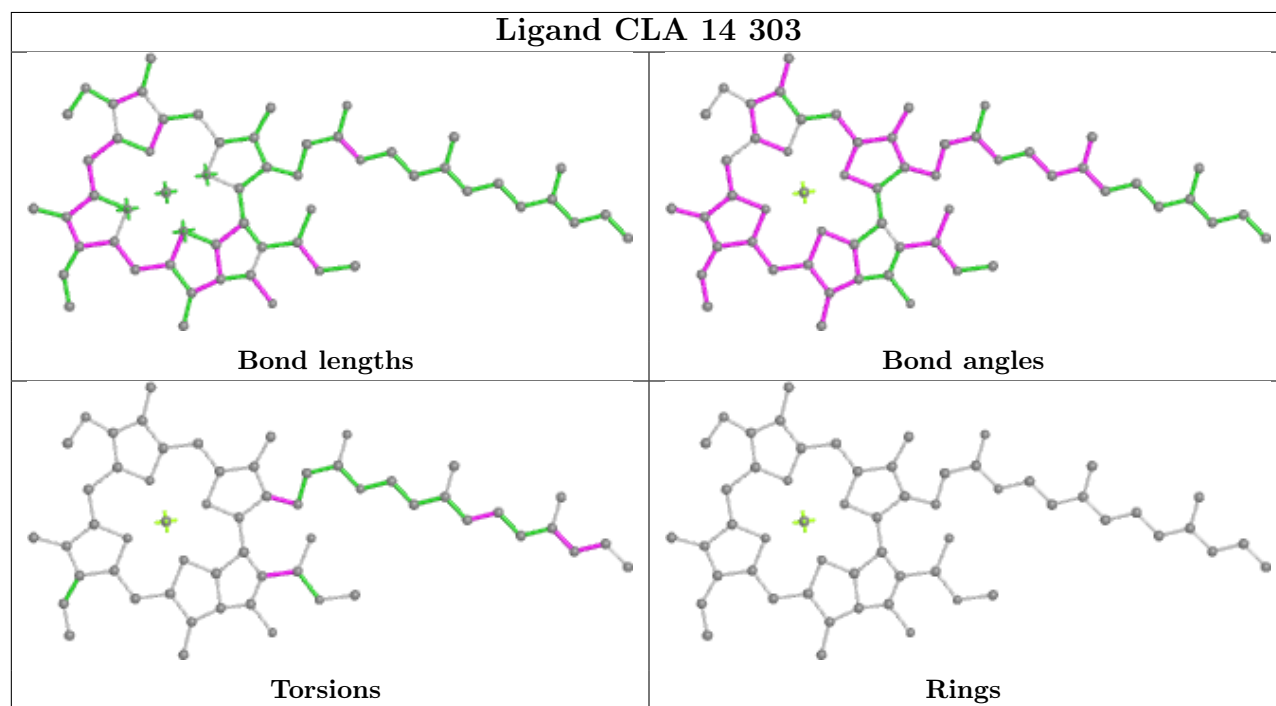
Ligand CLA 4 301

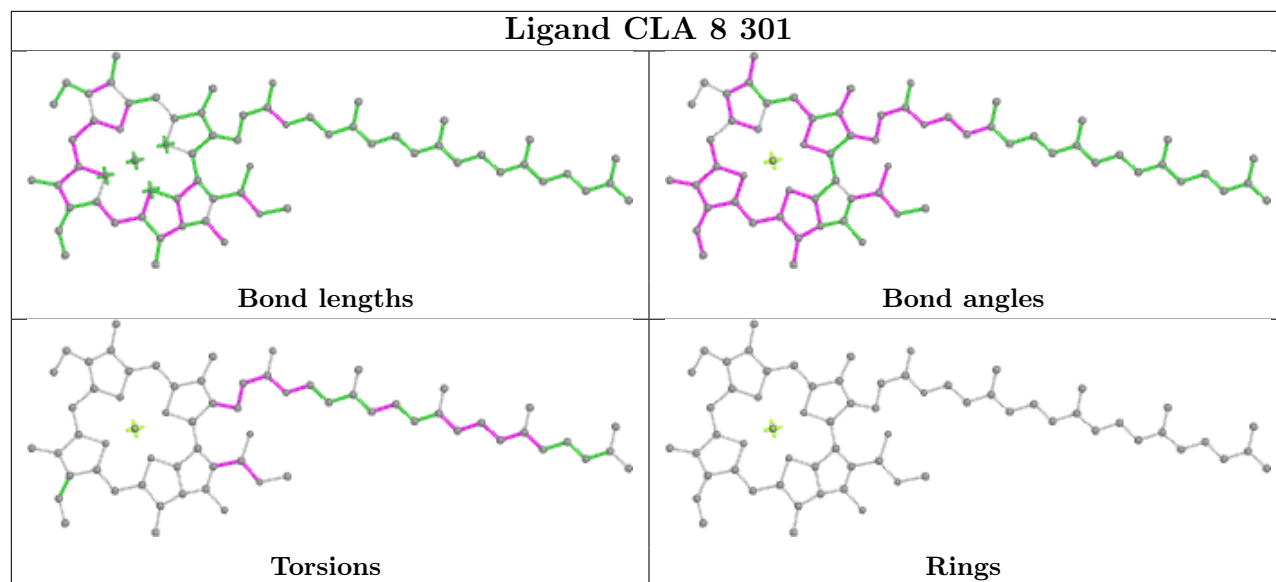
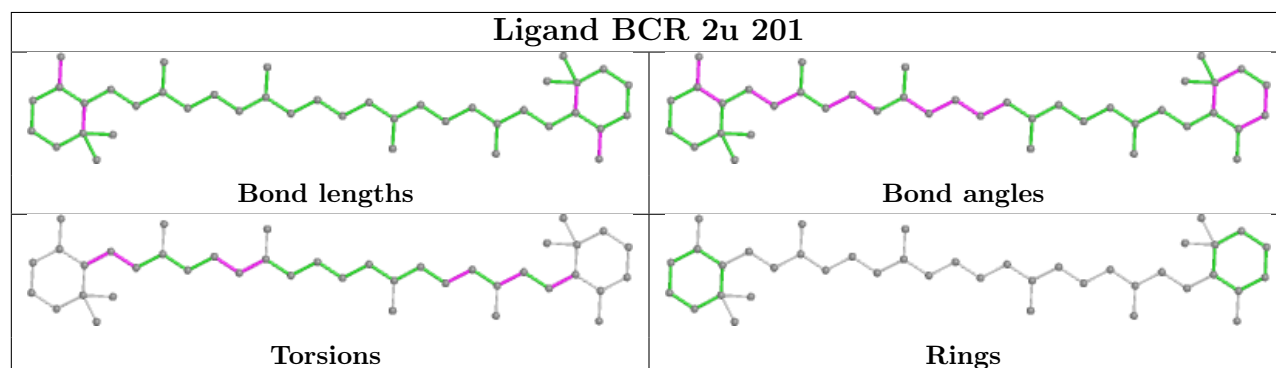
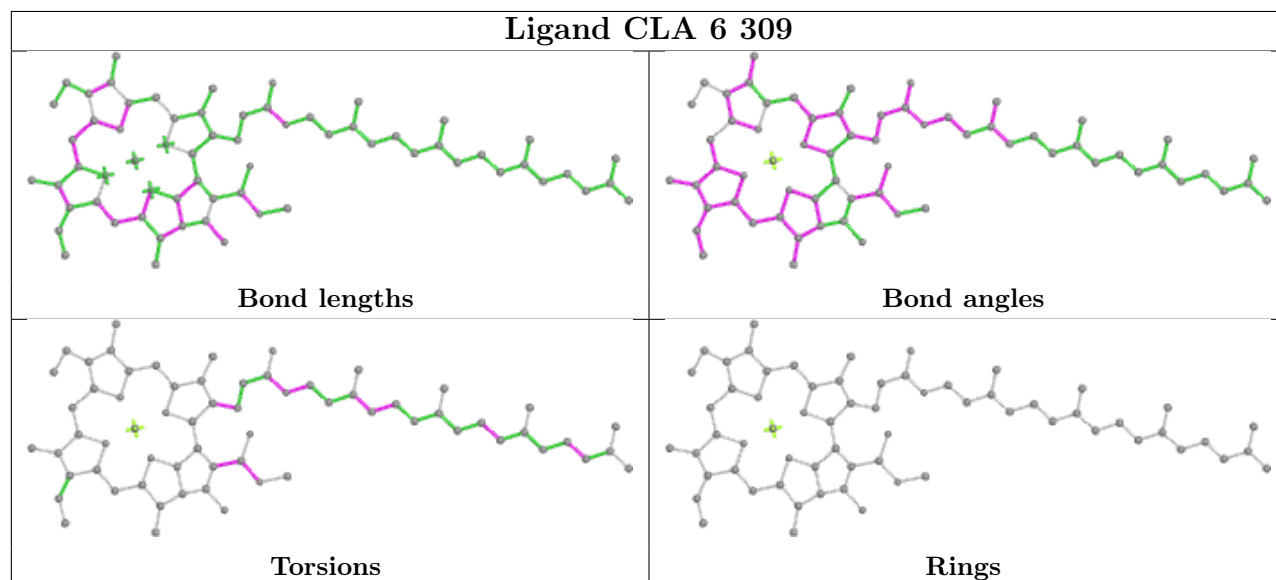


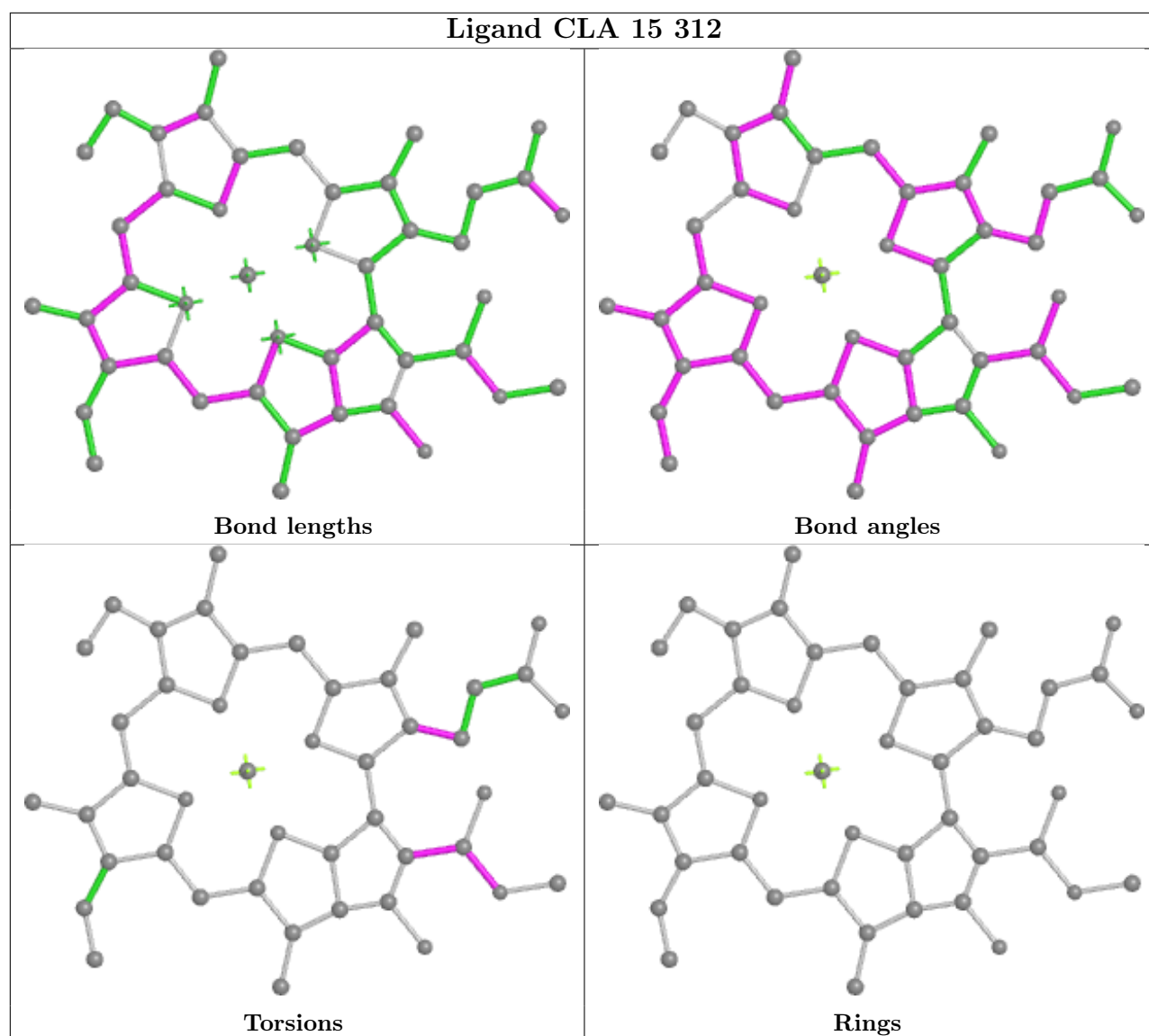
Ligand CL0 A 801



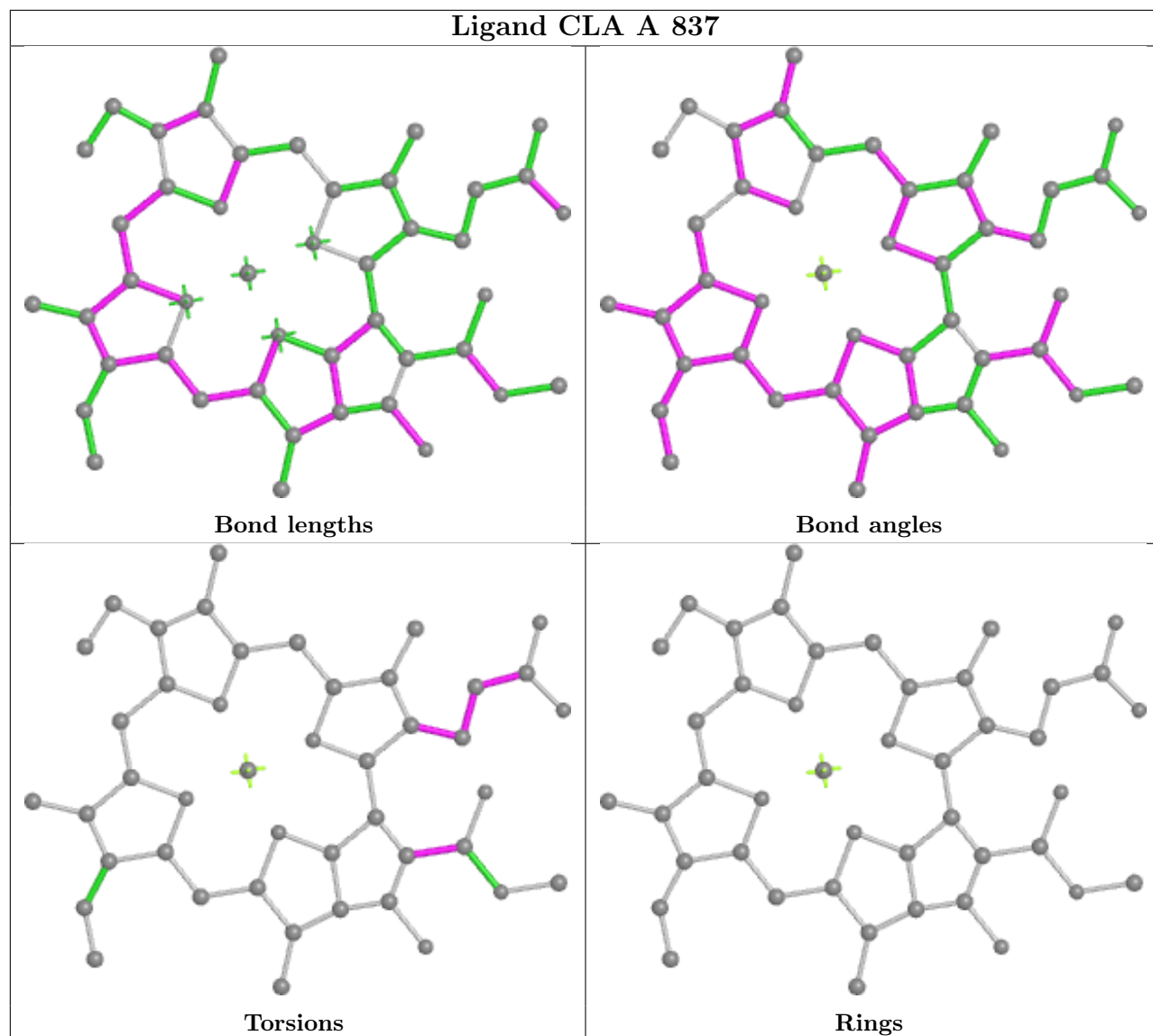
Ligand CLA 14 303



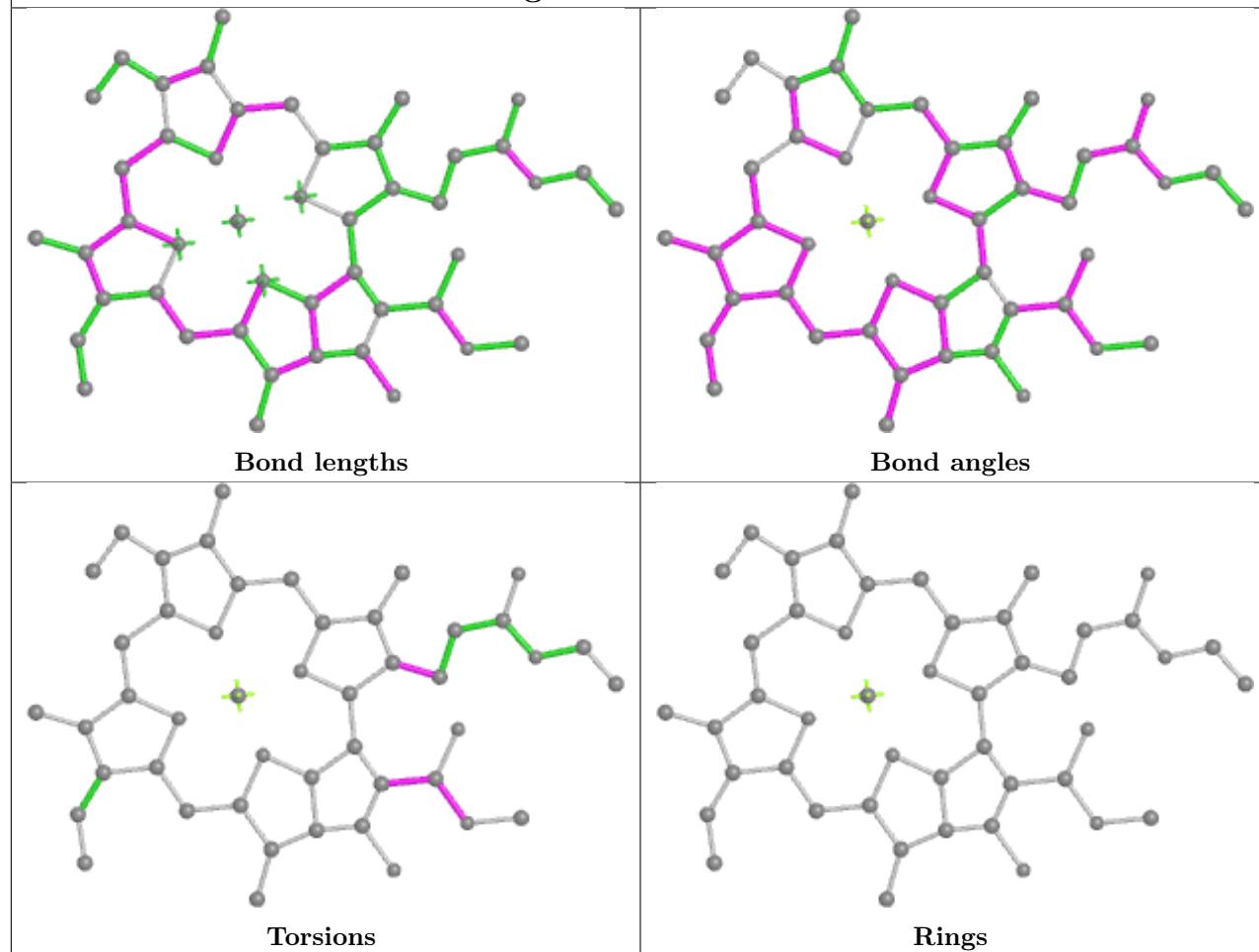
Ligand CLA 8 301**Ligand BCR 2u 201****Ligand CLA 6 309**



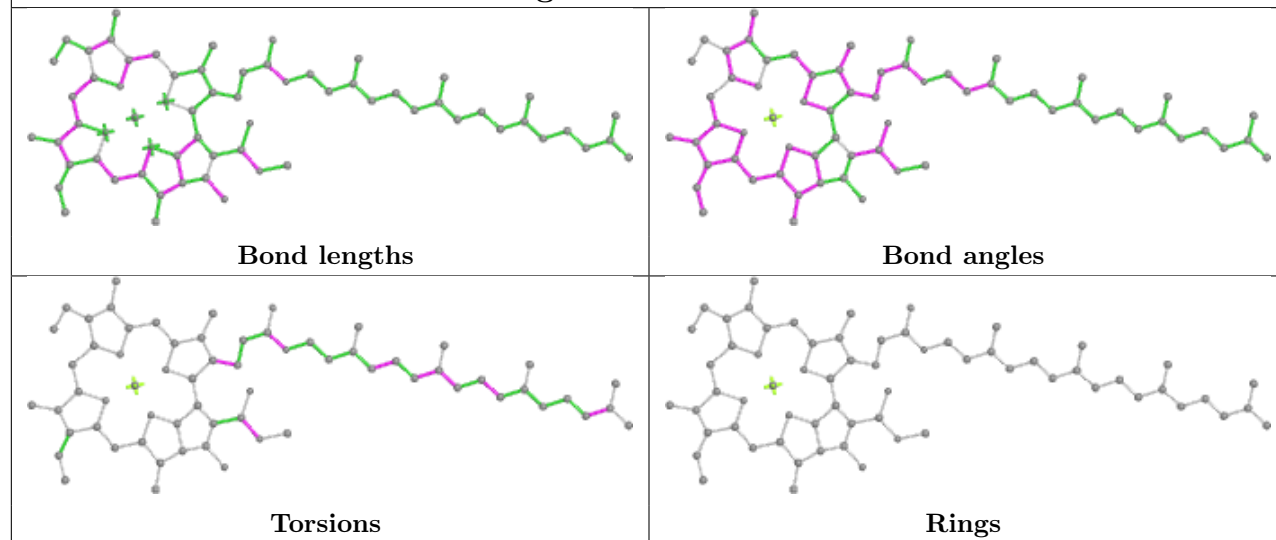
Ligand CLA A 837



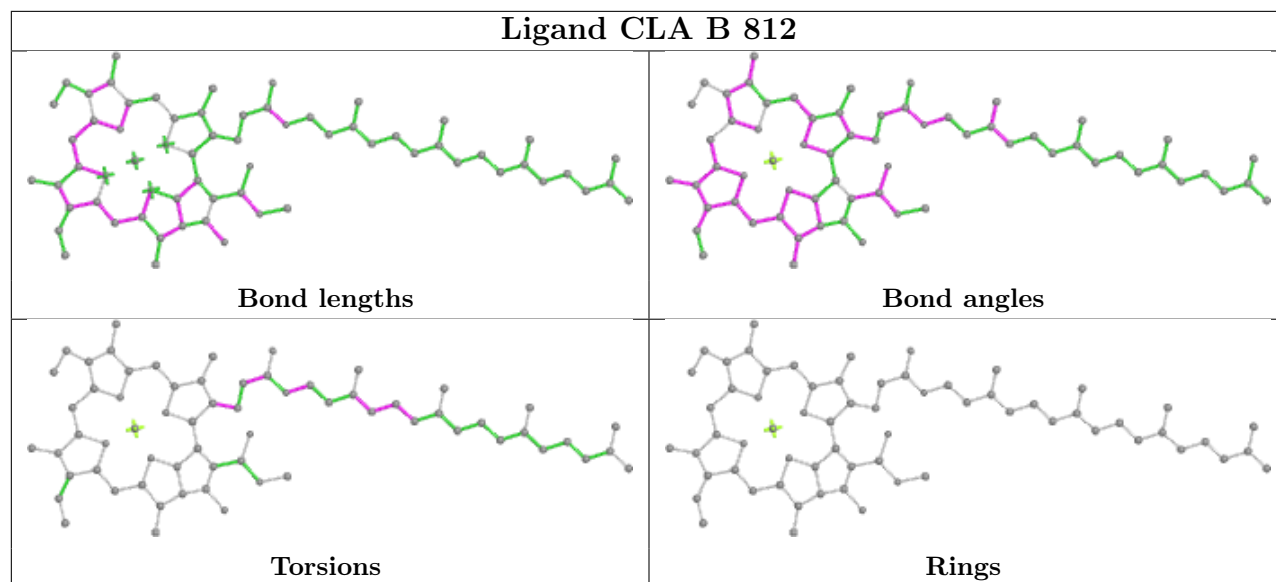
Ligand CLA A 840



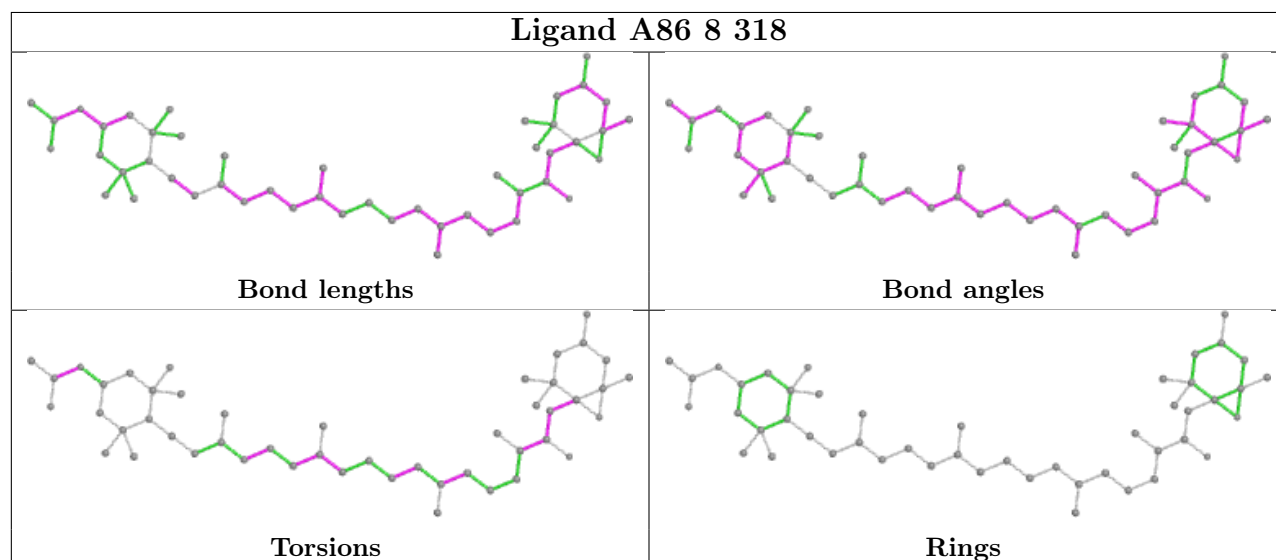
Ligand CLA 5 302



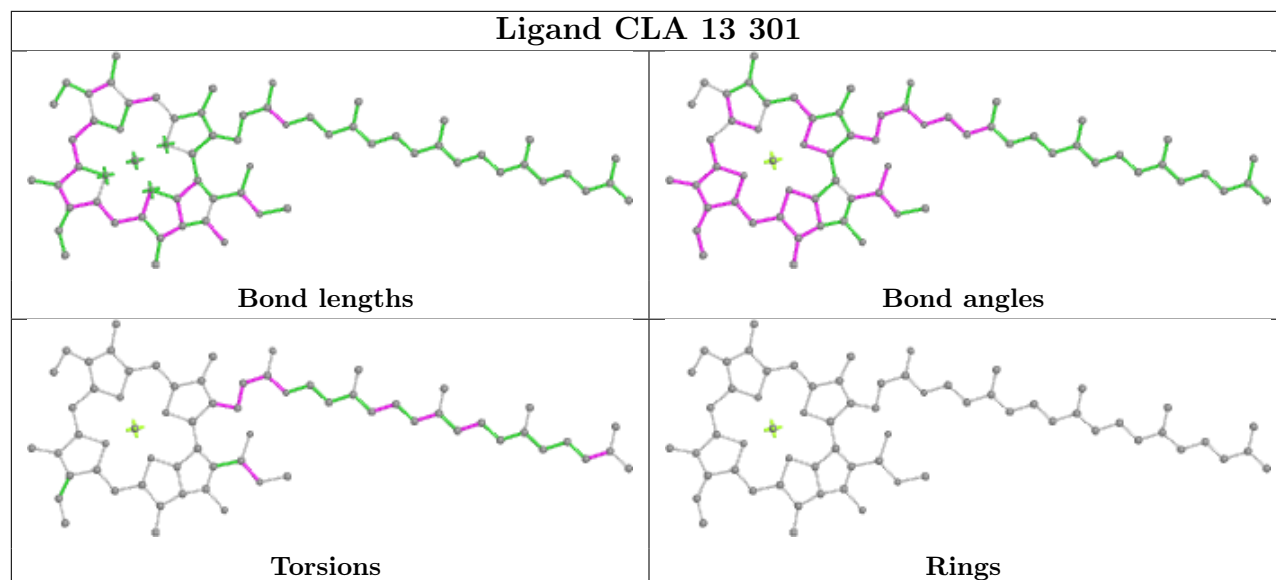
Ligand CLA B 812

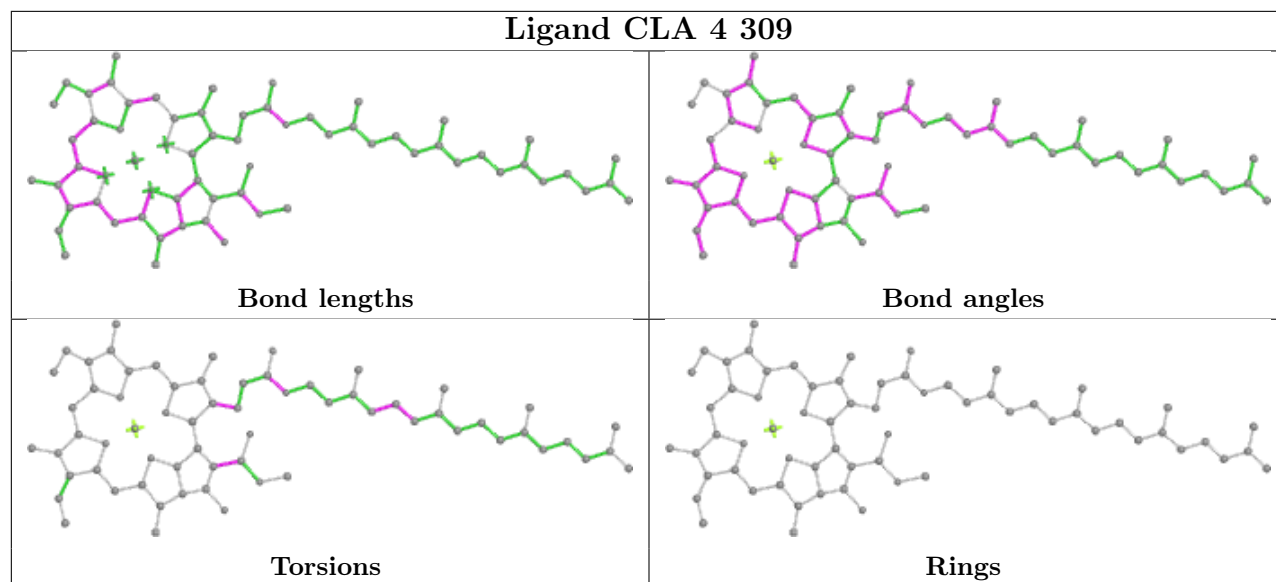
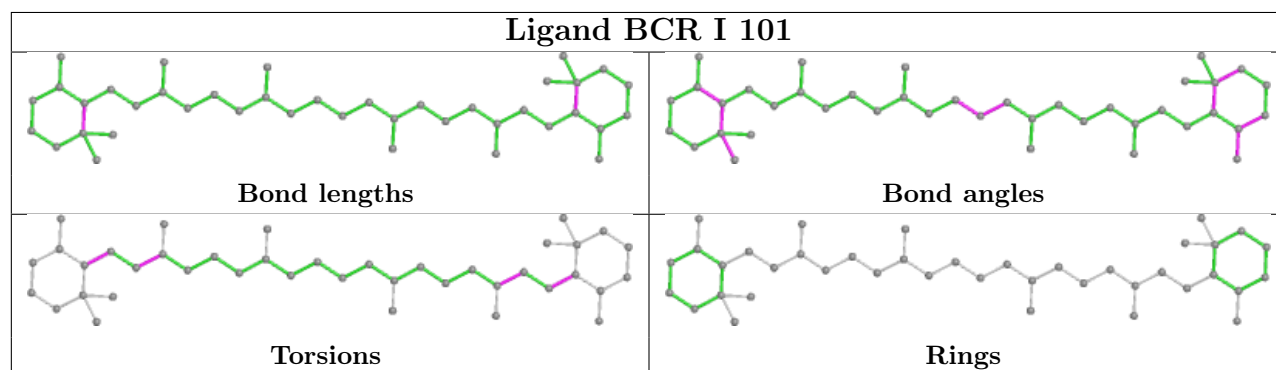
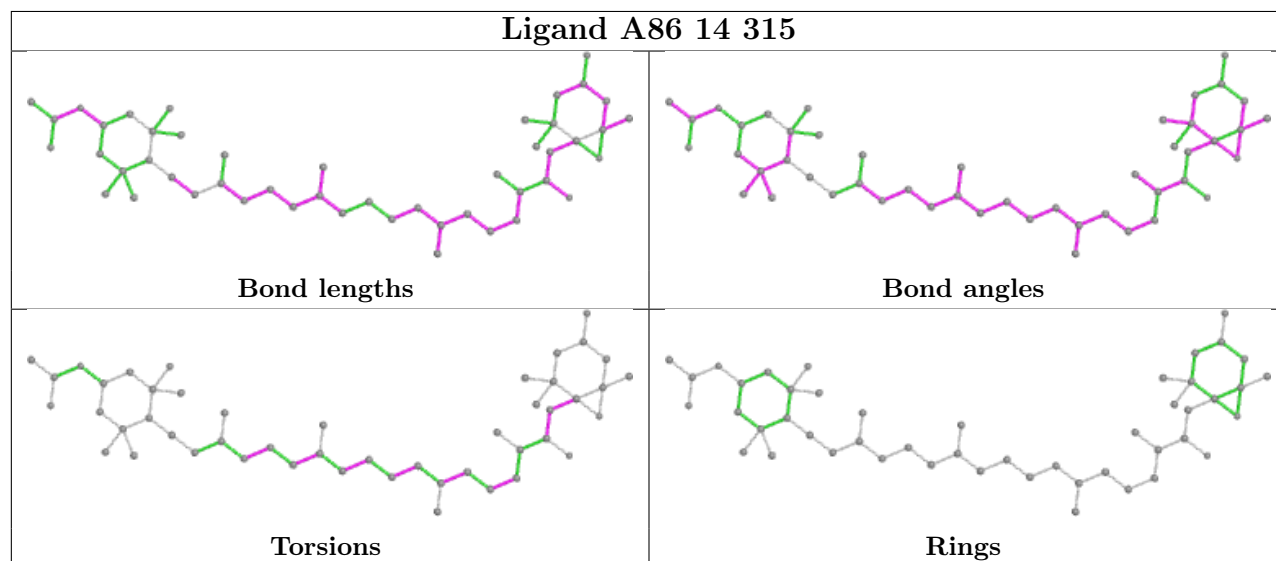


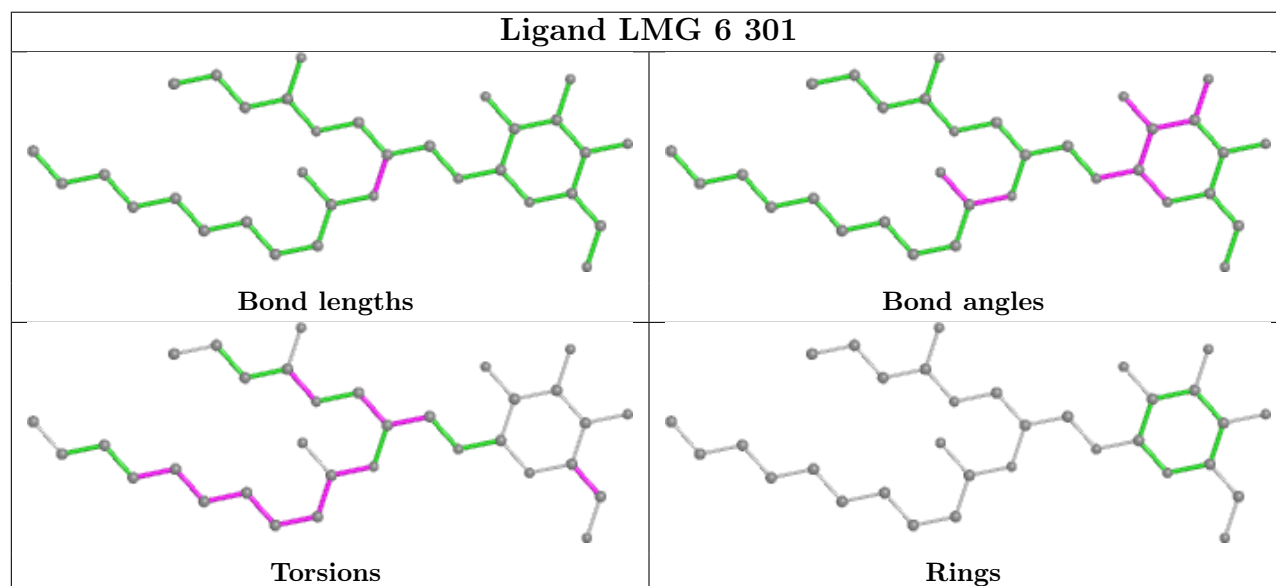
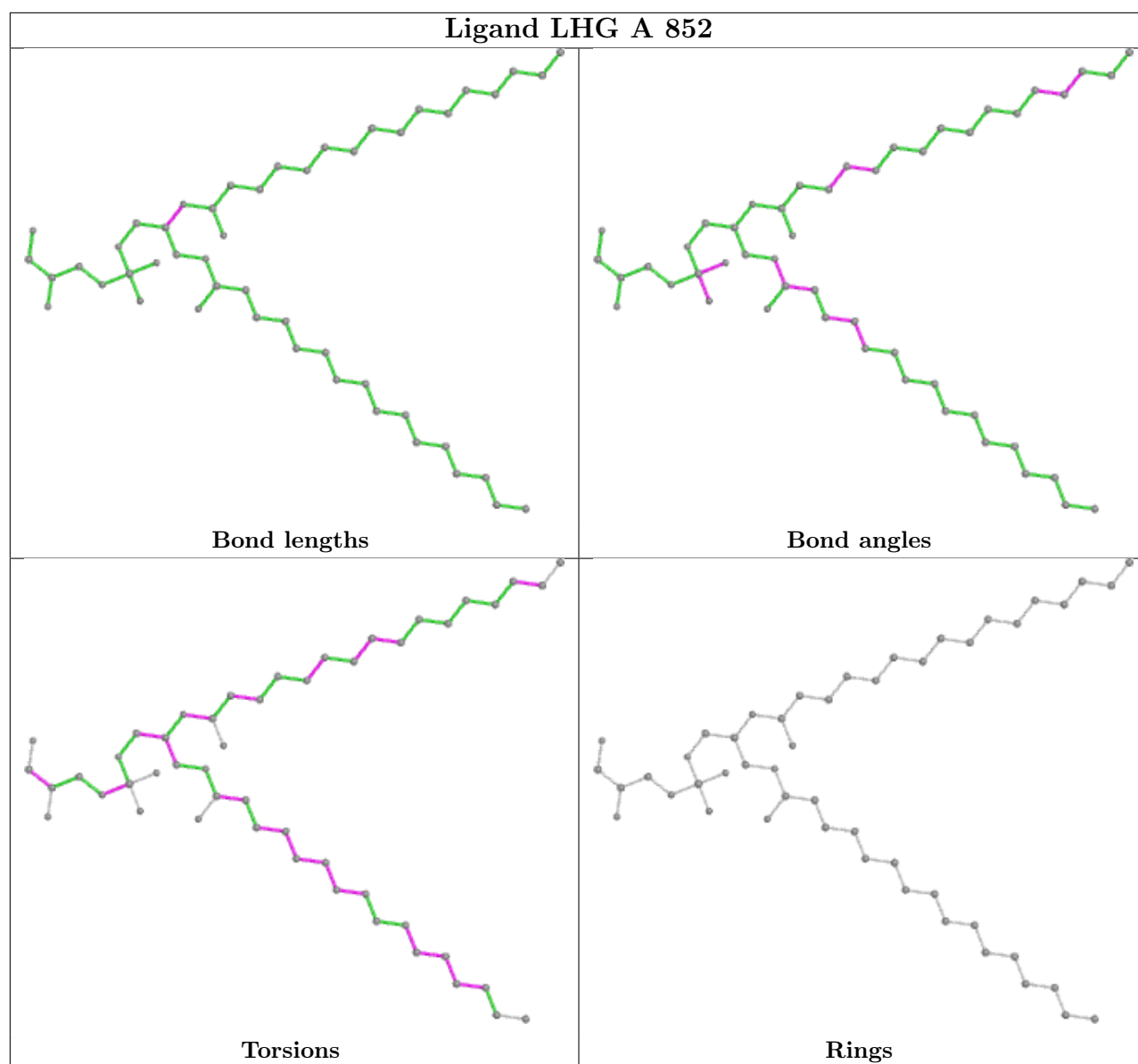
Ligand A86 8 318



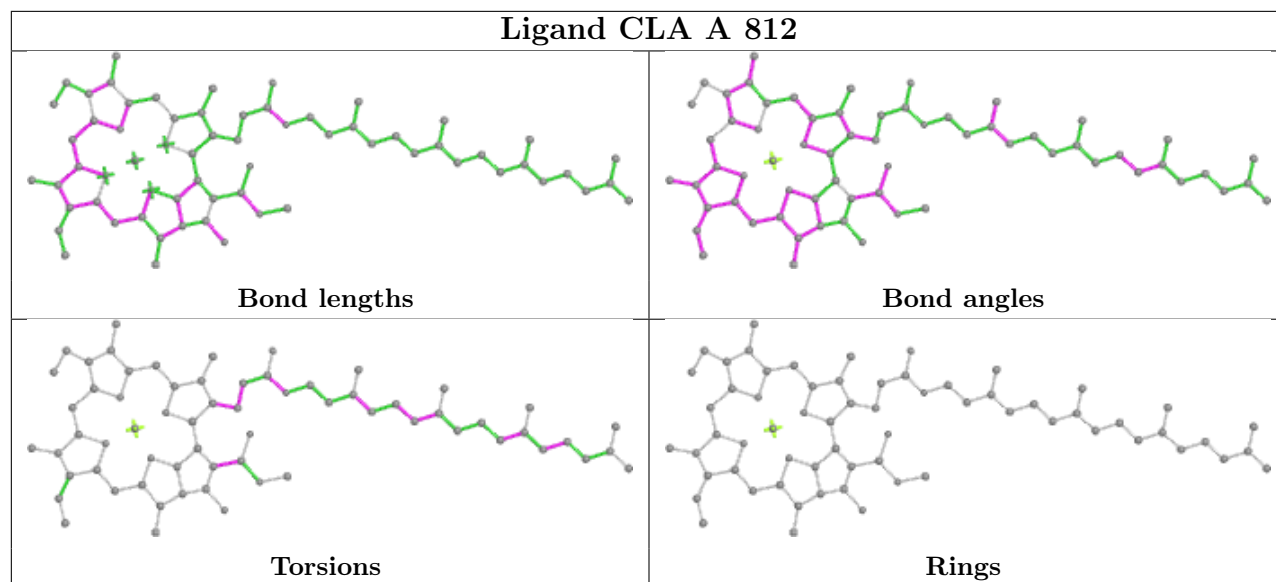
Ligand CLA 13 301



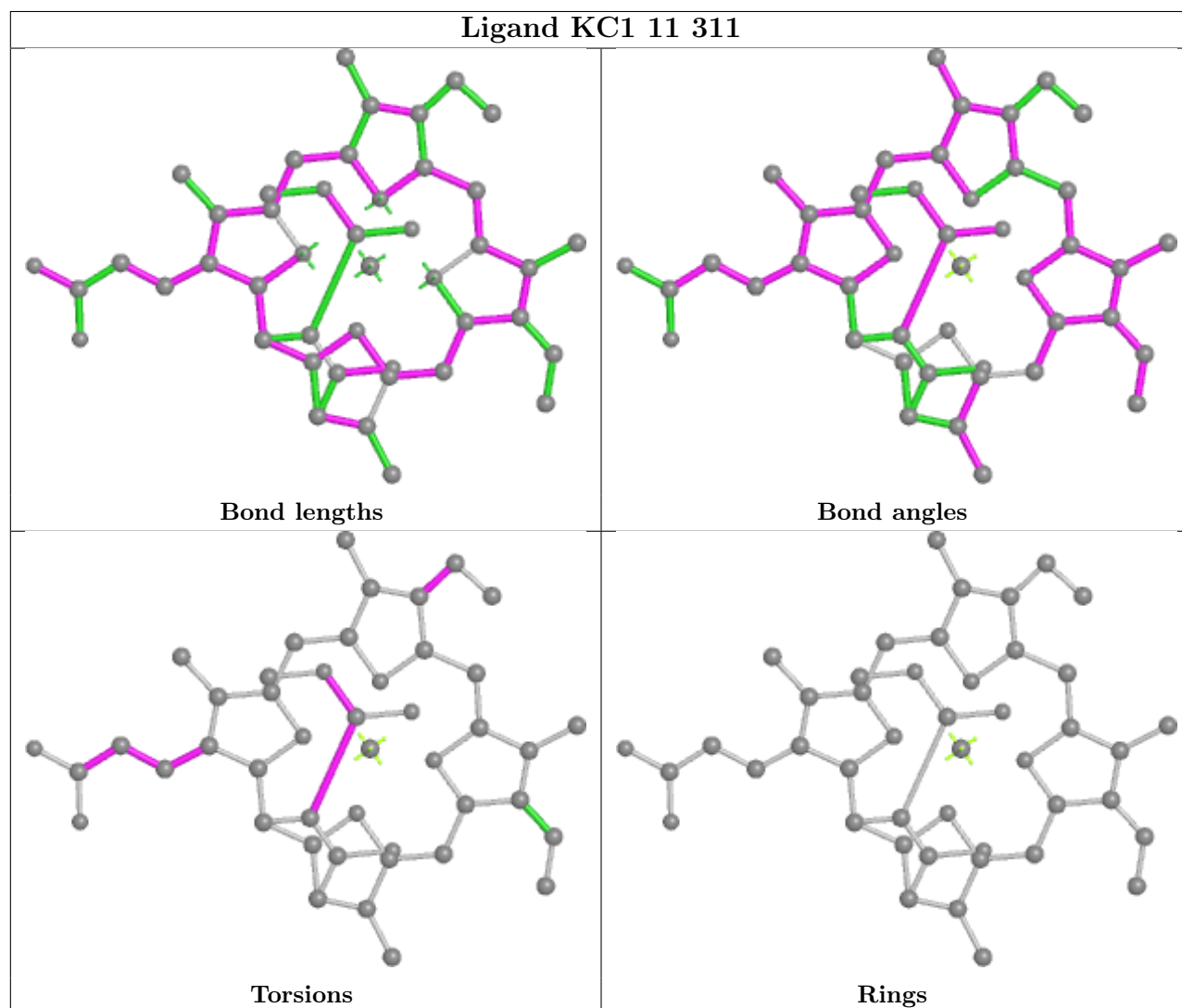
Ligand CLA 4 309**Ligand BCR I 101****Ligand A86 14 315**

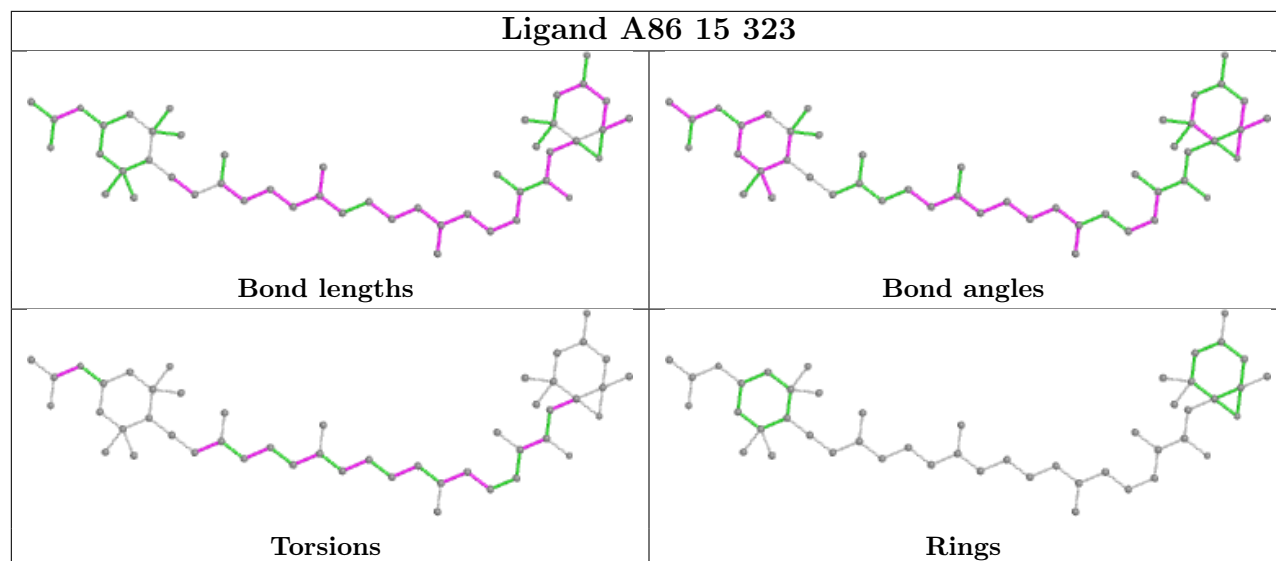
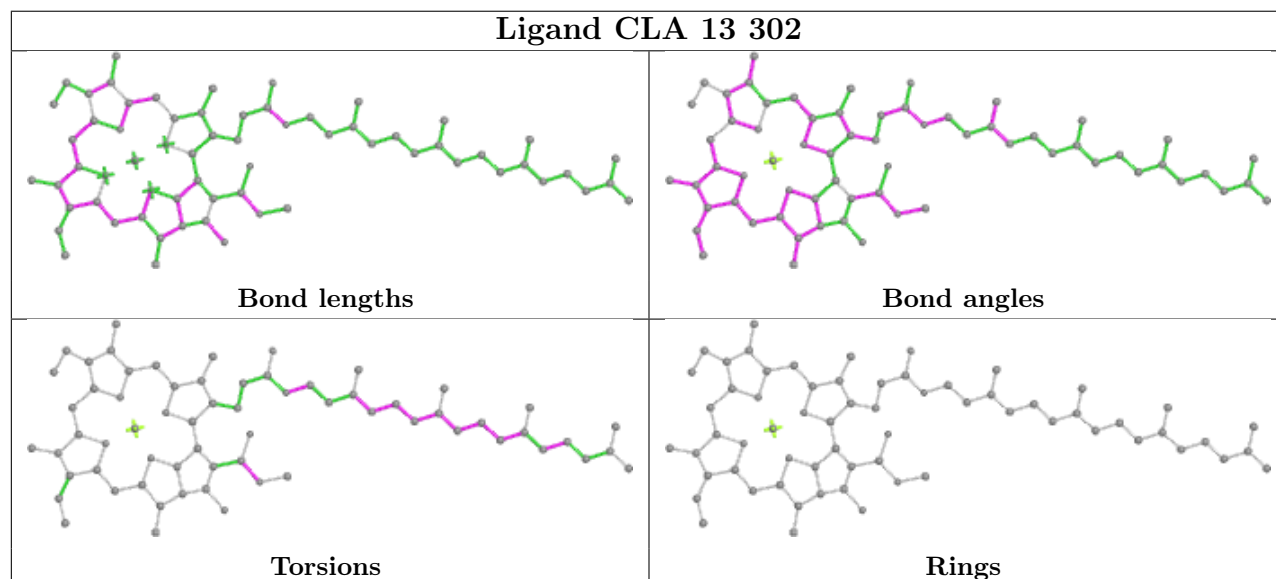
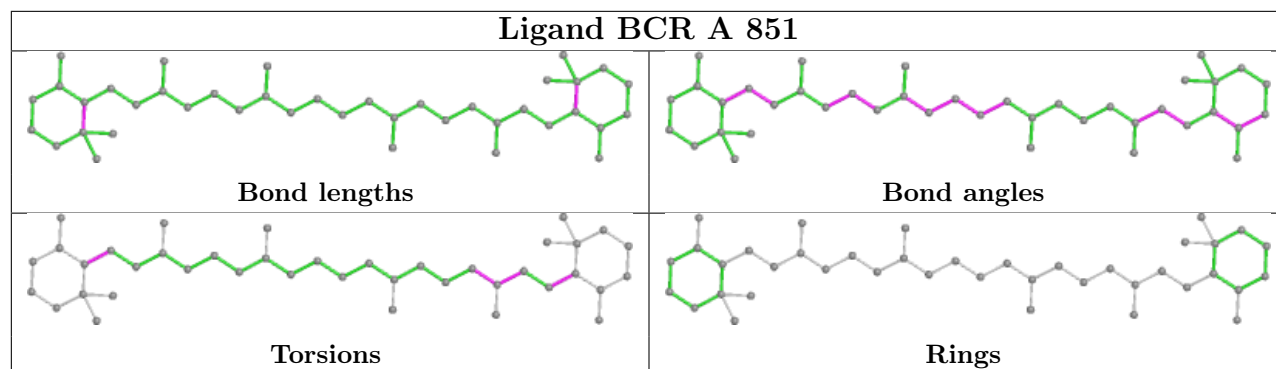


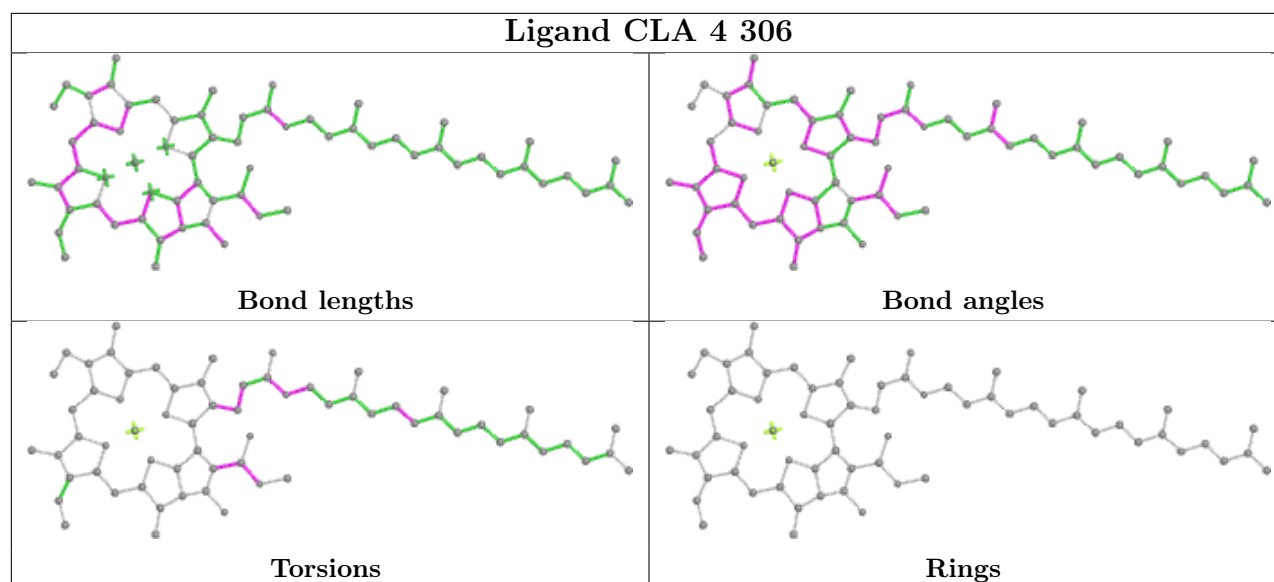
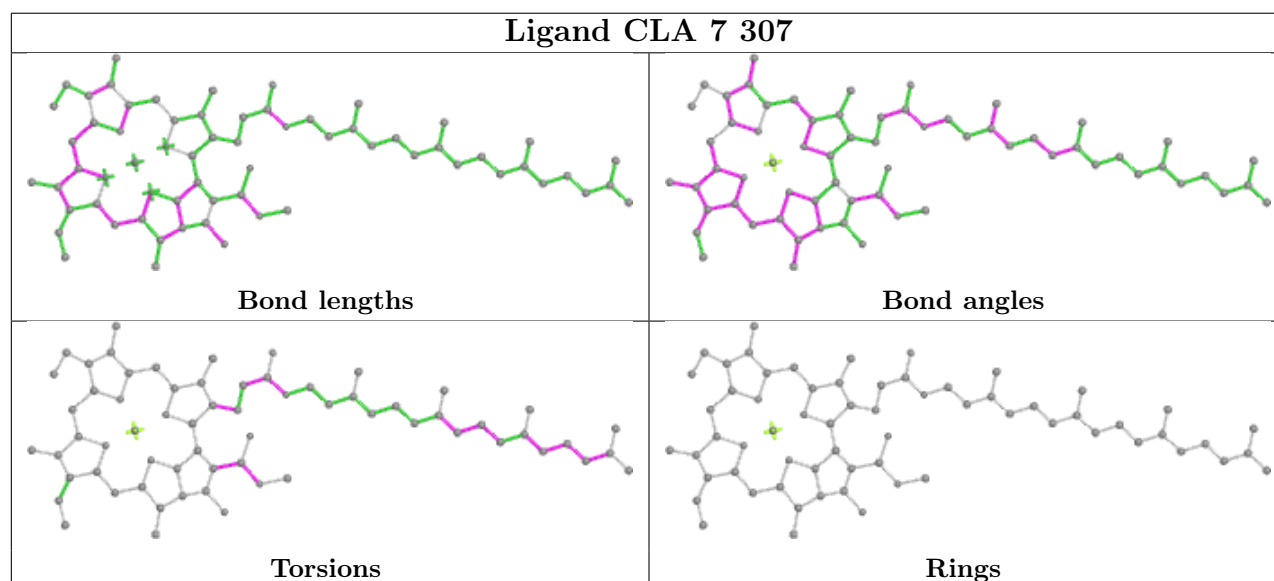
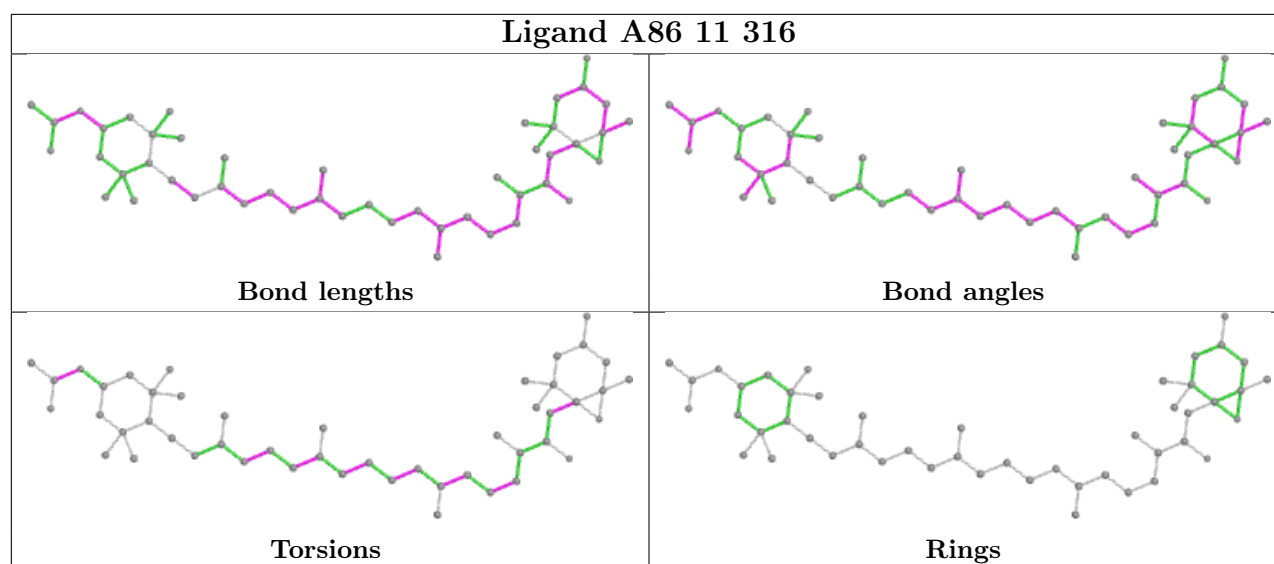
Ligand CLA A 812

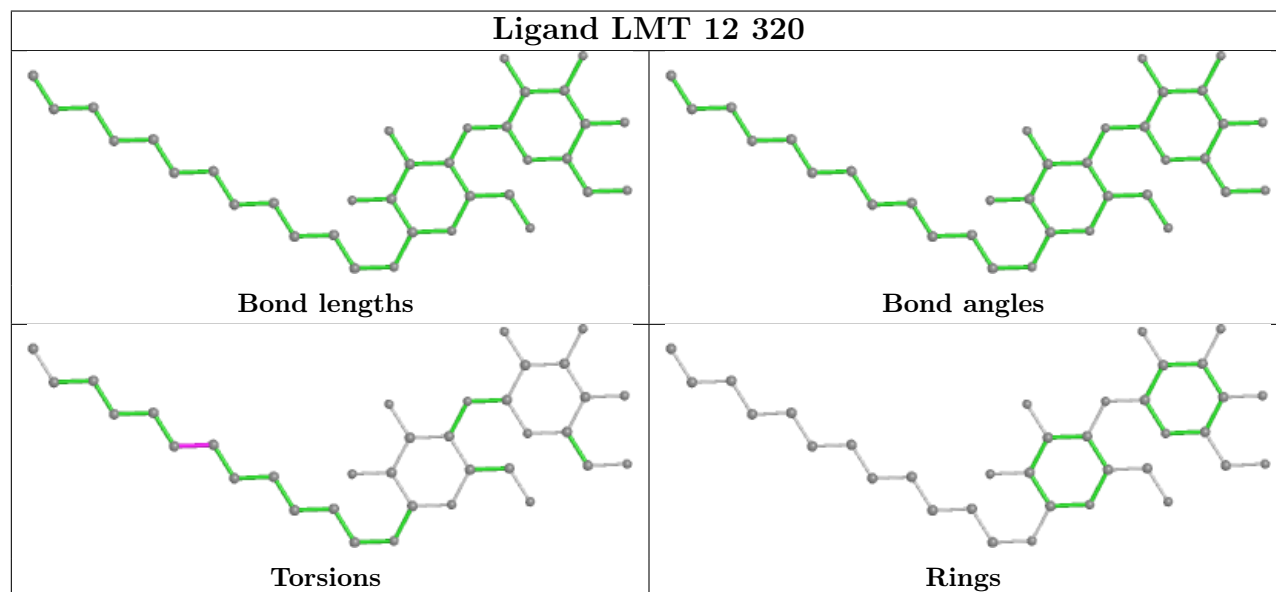
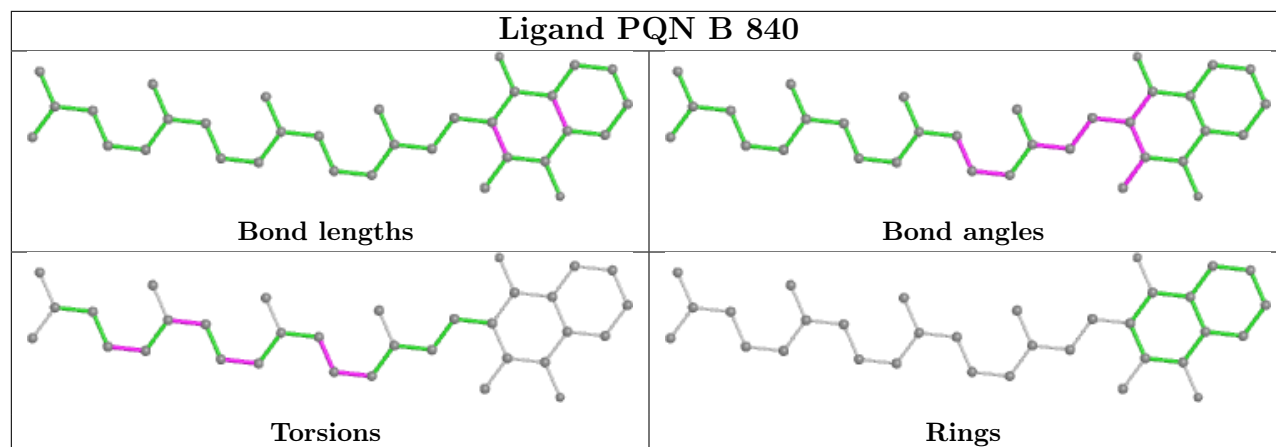


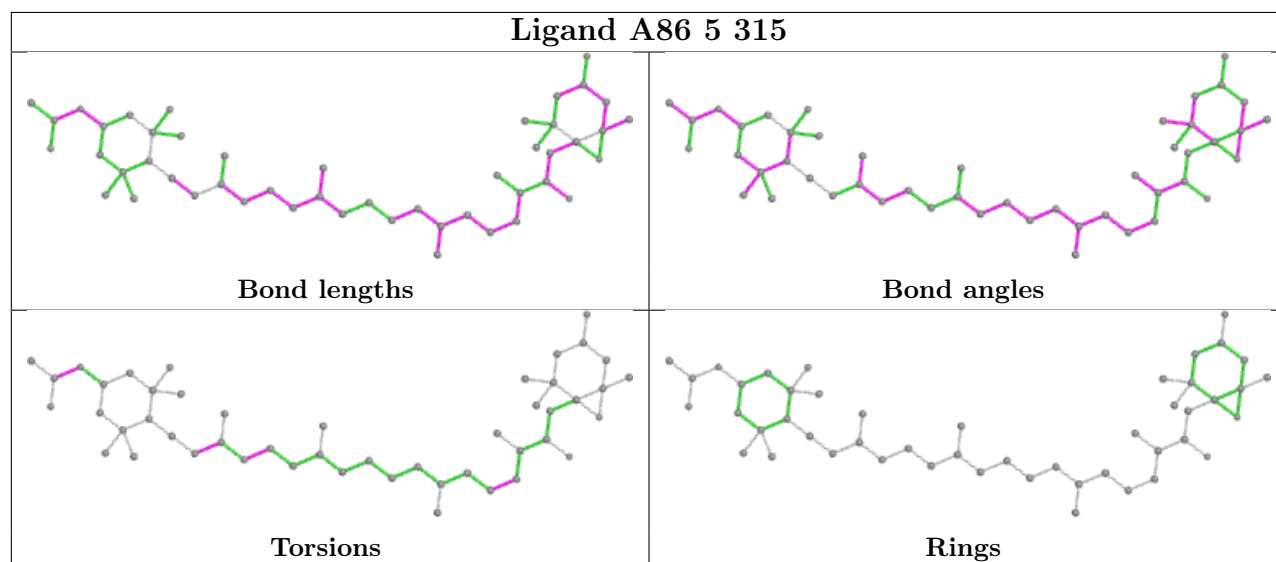
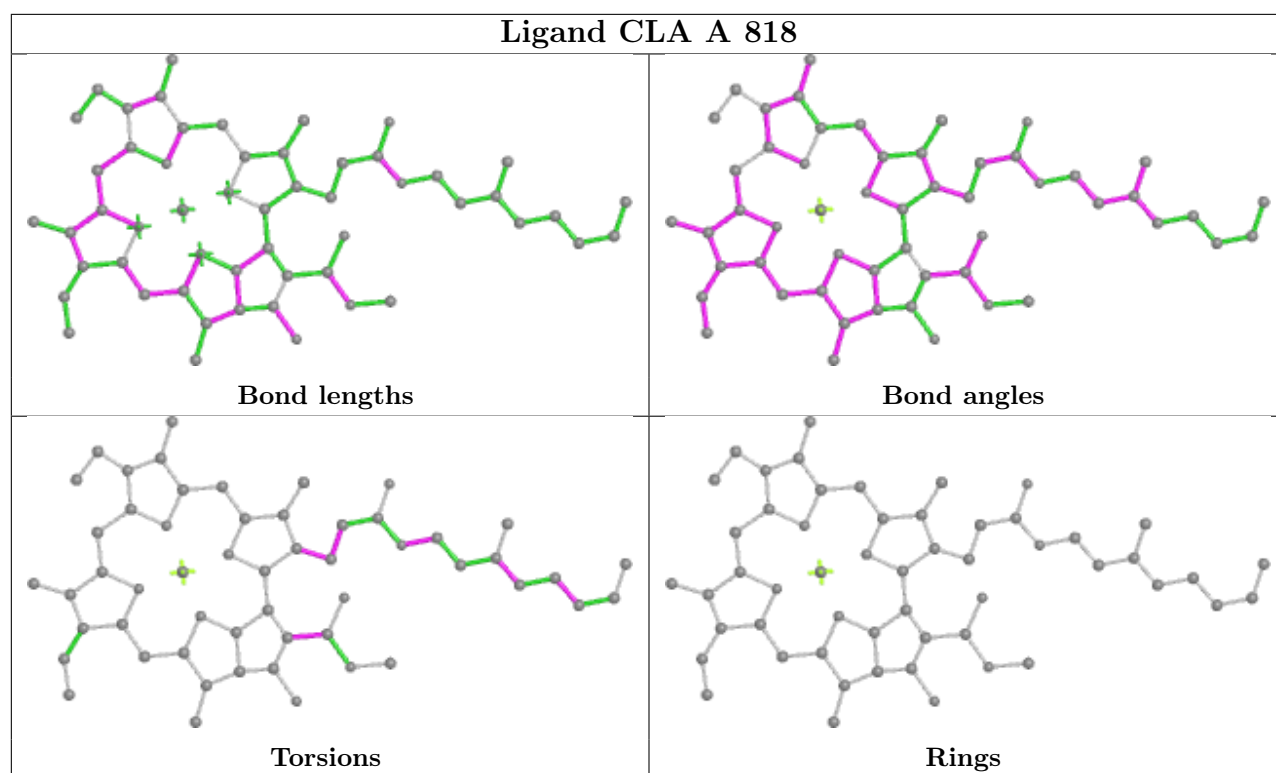
Ligand KC1 11 311

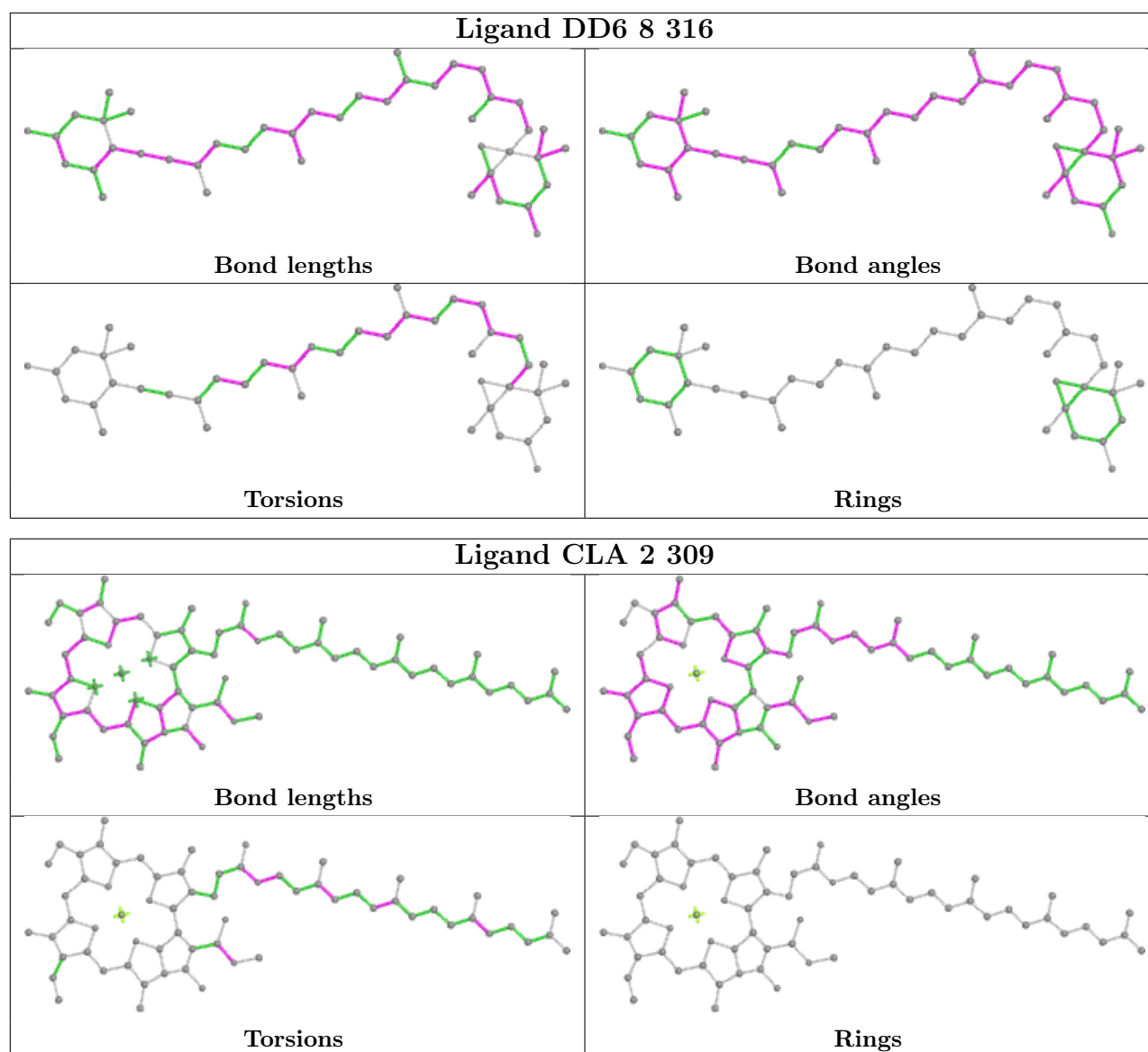


Ligand A86 15 323**Ligand CLA 13 302****Ligand BCR A 851**









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 ⓘ

This section contains visualisations of the EMDB entry EMD-0835. 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 ⓘ

This section was not generated.

6.2 Central slices ⓘ

This section was not generated.

6.3 Largest variance slices ⓘ

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

This section was not generated.

6.5 Orthogonal surface views ⓘ

This section was not generated.

6.6 Mask visualisation ⓘ

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

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

9 Map-model fit

This section was not generated.