



Full wwPDB EM Validation Report ⓘ

Mar 31, 2025 – 04:16 PM JST

PDB ID : 6L4T / pdb_00006l4t
EMDB ID : EMD-0834
Title : Structure of the peripheral FCPI from diatom
Authors : Nagao, R.; Kato, K.; Miyazaki, N.; Akita, F.; Shen, J.R.
Deposited on : 2019-10-21
Resolution : 2.60 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

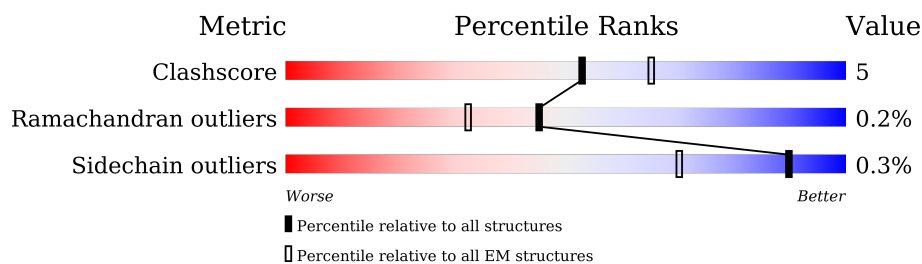
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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	6	208	72% 12% 16%
2	7	296	59% 36%
3	8	270	69% 10% 21%
4	10	207	77% 18%
5	11	229	77% 6% 17%
6	12	204	79% 6% 15%
7	13	244	52% 9% 39%
8	14	249	74% 10% 16%
9	15	281	62% 12% 25%

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Mol	Chain	Length	Quality of chain
10	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
11	CLA	10	304	X	-	-	-
11	CLA	10	305	X	-	-	-
11	CLA	10	307	X	-	-	-
11	CLA	10	308	X	-	-	-
11	CLA	10	309	X	-	-	-
11	CLA	11	305	X	-	-	-
11	CLA	11	307	X	-	-	-
11	CLA	11	309	X	-	-	-
11	CLA	12	303	X	-	-	-
11	CLA	12	304	X	-	-	-
11	CLA	12	306	X	-	-	-
11	CLA	12	307	X	-	-	-
11	CLA	12	308	X	-	-	-
11	CLA	12	312	X	-	-	-
11	CLA	12	321	X	-	-	-
11	CLA	13	302	X	-	-	-
11	CLA	13	307	X	-	-	-
11	CLA	13	309	X	-	-	-
11	CLA	14	302	X	-	-	-
11	CLA	14	303	X	-	-	-
11	CLA	14	304	X	-	-	-
11	CLA	14	305	X	-	-	-
11	CLA	14	309	X	-	-	-
11	CLA	14	310	X	-	-	-
11	CLA	14	313	X	-	-	-
11	CLA	15	303	X	-	-	-
11	CLA	15	304	X	-	-	-
11	CLA	15	305	X	-	-	-
11	CLA	15	306	X	-	-	-
11	CLA	15	307	X	-	-	-
11	CLA	15	308	X	-	-	-
11	CLA	15	309	X	-	-	-
11	CLA	15	310	X	-	-	-
11	CLA	15	311	X	-	-	-
11	CLA	15	312	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	16	302	X	-	-	-
11	CLA	16	303	X	-	-	-
11	CLA	16	305	X	-	-	-
11	CLA	16	306	X	-	-	-
11	CLA	16	307	X	-	-	-
11	CLA	16	308	X	-	-	-
11	CLA	16	310	X	-	-	-
11	CLA	6	301	X	-	-	-
11	CLA	6	302	X	-	-	-
11	CLA	6	303	X	-	-	-
11	CLA	6	304	X	-	-	-
11	CLA	6	306	X	-	-	-
11	CLA	6	307	X	-	-	-
11	CLA	6	312	X	-	-	-
11	CLA	6	313	X	-	-	-
11	CLA	6	314	X	-	-	-
11	CLA	7	302	X	-	-	-
11	CLA	7	303	X	-	-	-
11	CLA	7	304	X	-	-	-
11	CLA	7	305	X	-	-	-
11	CLA	7	308	X	-	-	-
11	CLA	7	309	X	-	-	-
11	CLA	7	310	X	-	-	-
11	CLA	8	301	X	-	-	-
11	CLA	8	302	X	-	-	-
11	CLA	8	303	X	-	-	-
11	CLA	8	304	X	-	-	-
11	CLA	8	308	X	-	-	-

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 23863 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 Fucoxanthin chlorophyll a/c-binding protein Lhcr12.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	6	174	Total	C	N	O	S	0	0
			1354	884	216	246	8		

- Molecule 2 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr10.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	7	188	Total	C	N	O	S	0	0
			1416	894	240	266	16		

- Molecule 3 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	8	213	Total	C	N	O	S	0	0
			1660	1075	274	302	9		

- Molecule 4 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	10	169	Total	C	N	O	S	0	0
			1302	849	212	233	8		

- Molecule 5 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq13.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	11	191	Total	C	N	O	S	0	0
			1479	958	243	270	8		

- Molecule 6 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	12	173	Total	C	N	O	S	0	0
			1274	814	209	243	8		

- Molecule 7 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq11.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	13	150	Total	C	N	O	S	0	0
			1148	736	203	204	5		

- Molecule 8 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	14	208	Total	C	N	O	S	0	0
			1609	1049	262	292	6		

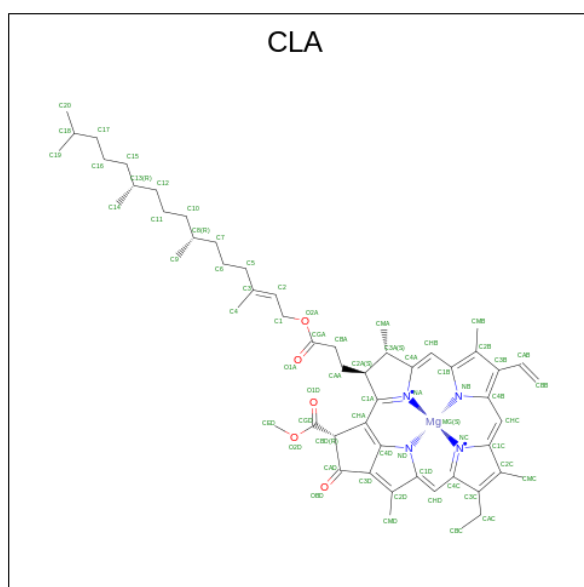
- Molecule 9 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	15	211	Total	C	N	O	S	0	0
			1654	1077	273	298	6		

- Molecule 10 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	16	174	Total	C	N	O	S	0	0
			1313	846	217	242	8		

- Molecule 11 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
11	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
11	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
11	8	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
11	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	8	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
11	10	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	10	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	10	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	10	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	10	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	10	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	11	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	11	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	11	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	11	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	11	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	12	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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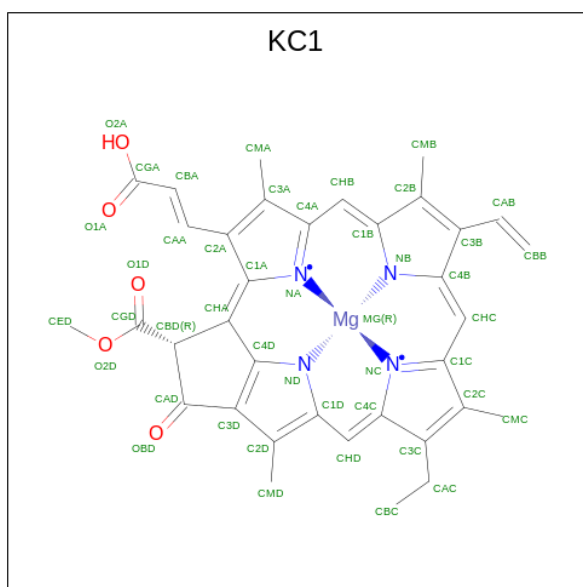
Mol	Chain	Residues	Atoms					AltConf
11	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	13	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	13	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	13	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
11	13	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
11	14	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	14	1	Total 57	C 47	Mg 1	N 4	O 5	0
11	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
11	14	1	Total 50	C 40	Mg 1	N 4	O 5	0
11	14	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
11	14	1	Total 50	C 40	Mg 1	N 4	O 5	0
11	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
11	14	1	Total 46	C 36	Mg 1	N 4	O 5	0
11	15	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	15	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
11	15	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	15	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
11	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	15	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	15	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	16	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	16	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	16	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	16	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
11	16	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
11	16	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
11	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 12 is Chlorophyll c1 (CCD ID: KC1) (formula: $C_{35}H_{30}MgN_4O_5$).



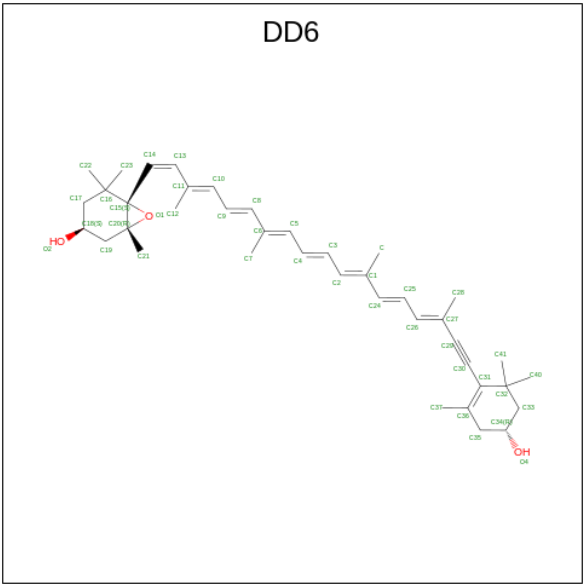
Mol	Chain	Residues	Atoms					AltConf
12	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	10	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
12	10	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	10	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 13 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).



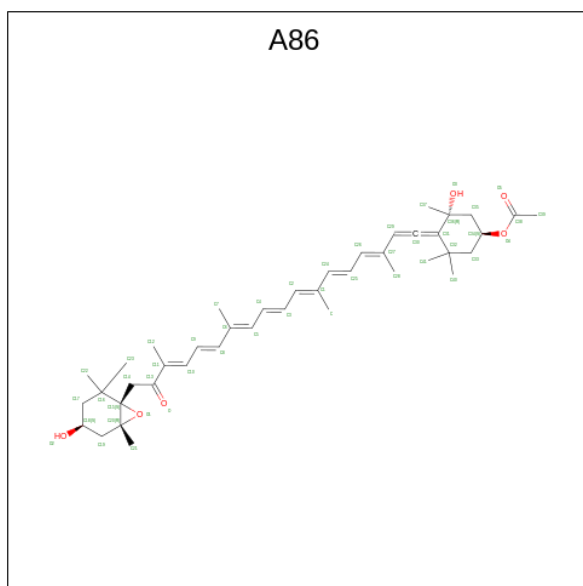
Mol	Chain	Residues	Atoms			AltConf
13	6	1	Total	C	O	0
			43	40	3	
13	6	1	Total	C	O	0
			43	40	3	
13	6	1	Total	C	O	0
			43	40	3	
13	7	1	Total	C	O	0
			43	40	3	
13	7	1	Total	C	O	0
			43	40	3	
13	7	1	Total	C	O	0
			43	40	3	
13	7	1	Total	C	O	0
			43	40	3	
13	8	1	Total	C	O	0
			43	40	3	
13	8	1	Total	C	O	0
			43	40	3	
13	10	1	Total	C	O	0
			43	40	3	
13	10	1	Total	C	O	0
			43	40	3	
13	11	1	Total	C	O	0
			43	40	3	

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Mol	Chain	Residues	Atoms			AltConf
13	12	1	Total	C	O	0
			43	40	3	
13	12	1	Total	C	O	0
			43	40	3	
13	13	1	Total	C	O	0
			43	40	3	
13	15	1	Total	C	O	0
			43	40	3	
13	15	1	Total	C	O	0
			43	40	3	
13	16	1	Total	C	O	0
			43	40	3	

- Molecule 14 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
14	6	1	Total	C	O	0
			48	42	6	
14	7	1	Total	C	O	0
			48	42	6	
14	7	1	Total	C	O	0
			48	42	6	
14	7	1	Total	C	O	0
			48	42	6	
14	8	1	Total	C	O	0
			48	42	6	

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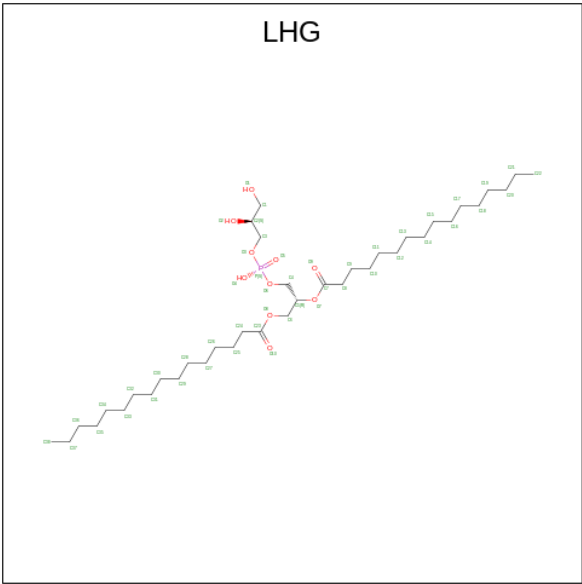
Mol	Chain	Residues	Atoms			AltConf
14	8	1	Total	C	O	0
			48	42	6	
14	10	1	Total	C	O	0
			48	42	6	
14	10	1	Total	C	O	0
			48	42	6	
14	10	1	Total	C	O	0
			48	42	6	
14	10	1	Total	C	O	0
			48	42	6	
14	10	1	Total	C	O	0
			48	42	6	
14	11	1	Total	C	O	0
			48	42	6	
14	11	1	Total	C	O	0
			48	42	6	
14	11	1	Total	C	O	0
			48	42	6	
14	11	1	Total	C	O	0
			48	42	6	
14	12	1	Total	C	O	0
			48	42	6	
14	12	1	Total	C	O	0
			48	42	6	
14	13	1	Total	C	O	0
			45	40	5	
14	13	1	Total	C	O	0
			48	42	6	
14	14	1	Total	C	O	0
			48	42	6	
14	14	1	Total	C	O	0
			48	42	6	
14	14	1	Total	C	O	0
			48	42	6	
14	14	1	Total	C	O	0
			48	42	6	
14	14	1	Total	C	O	0
			48	42	6	
14	14	1	Total	C	O	0
			48	42	6	

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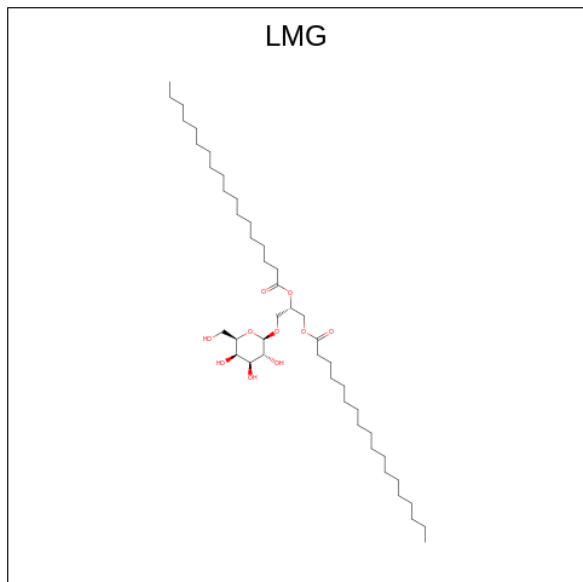
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
14	14	1	48	42	6	0
14	14	1	48	42	6	0
14	15	1	48	42	6	0
14	15	1	48	42	6	0
14	15	1	48	42	6	0
14	15	1	48	42	6	0
14	15	1	48	42	6	0
14	15	1	48	42	6	0
14	16	1	48	42	6	0
14	16	1	48	42	6	0

- Molecule 15 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



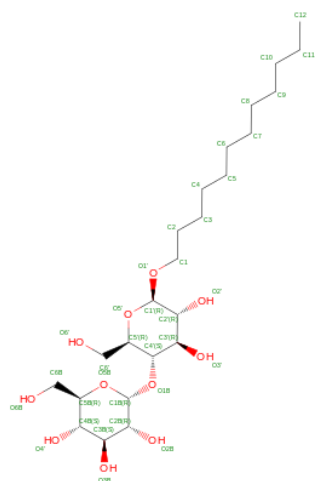
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
15	6	1	27	16	10	1	0

- Molecule 16 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
16	7	1	Total	C	O	0
			37	27	10	
16	8	1	Total	C	O	0
			37	27	10	
16	8	1	Total	C	O	0
			42	32	10	
16	8	1	Total	C	O	0
			29	19	10	
16	14	1	Total	C	O	0
			38	28	10	

- Molecule 17 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



- Molecule 18 is water.

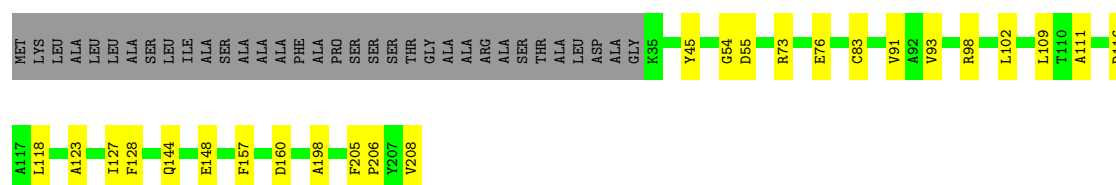
Mol	Chain	Residues	Atoms		AltConf
18	6	2	Total 2	O 2	0
18	7	2	Total 2	O 2	0
18	8	4	Total 4	O 4	0
18	10	1	Total 1	O 1	0
18	11	1	Total 1	O 1	0
18	12	2	Total 2	O 2	0

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.

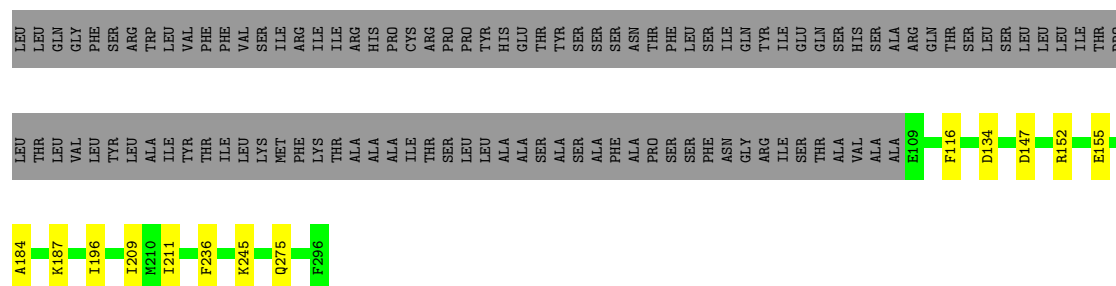
- Molecule 1: Fucoxanthin chlorophyll a/c-binding protein Lhcr12

Chain 6: 



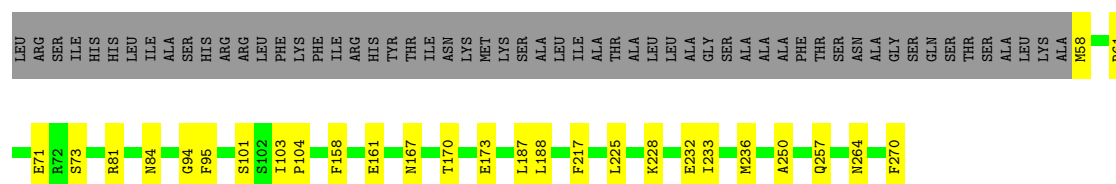
- Molecule 2: Fucoxanthin chlorophyll a/c-binding protein Lhcr10

Chain 7: 




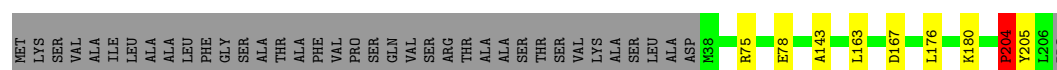
- Molecule 3: Fucoxanthin chlorophyll a/c-binding protein Lhcr4

Chain 8: 




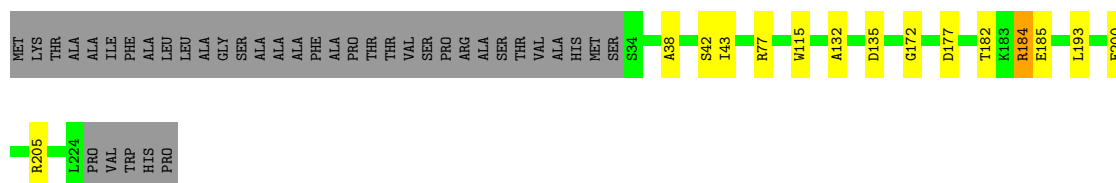
- Molecule 4: Fucoxanthin chlorophyll a/c-binding protein Lhcr3

Chain 10: 




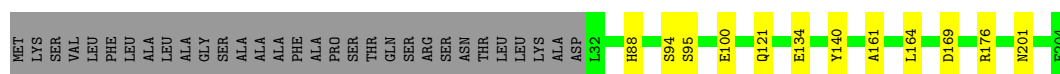
- Molecule 5: Fucoxanthin chlorophyll a/c-binding protein Lhcq13

Chain 11:  77% 6% 17%



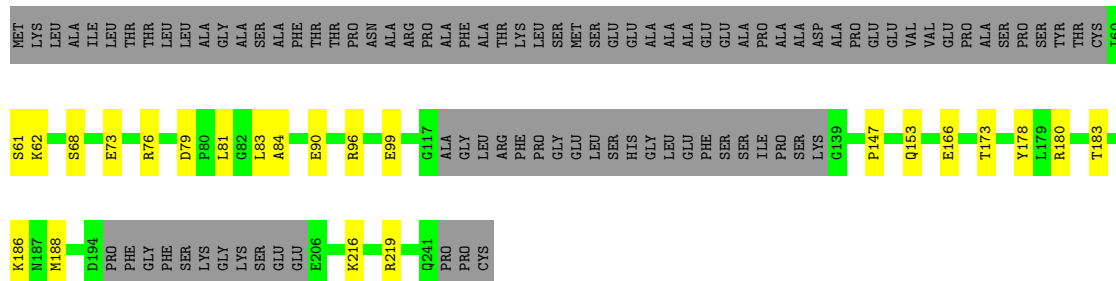
- Molecule 6: Fucoxanthin chlorophyll a/c-binding protein Lhcq3

Chain 12:  79% 6% 15%




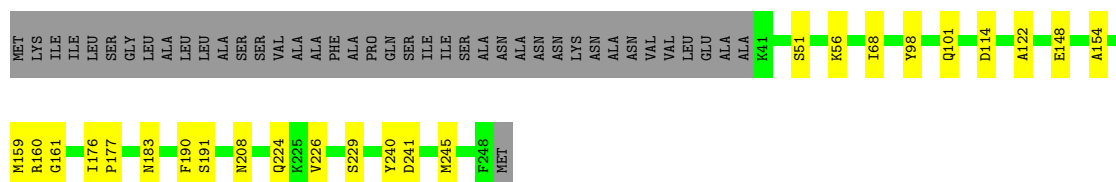
- Molecule 7: Fucoxanthin chlorophyll a/c-binding protein Lhcq11

Chain 13:  52% 9% 39%



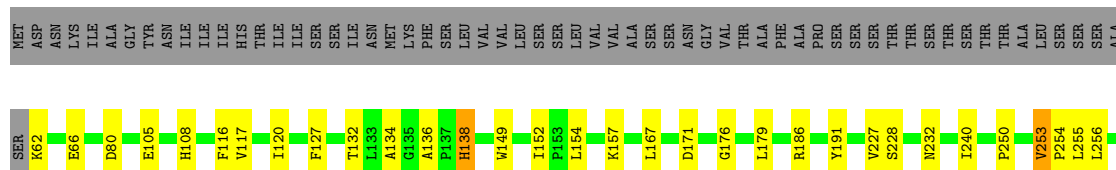
- Molecule 8: Fucoxanthin chlorophyll a/c-binding protein Lhcq10

Chain 14:  74% 10% 16%



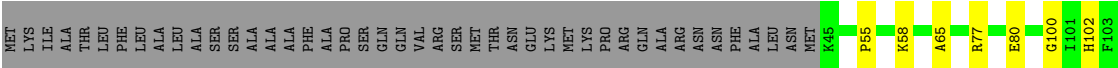
- Molecule 9: Fucoxanthin chlorophyll a/c-binding protein Lhcq8

Chain 15:  62% 12% 25%





● Molecule 10: 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DD6, A86, LMT, CLA, KC1, LMG, 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	6	0.37	1/1391 (0.1%)	0.48	0/1886
2	7	0.34	0/1445	0.46	0/1952
3	8	0.38	0/1706	0.49	0/2310
4	10	0.35	0/1344	0.52	0/1824
5	11	0.33	0/1522	0.49	0/2070
6	12	0.35	0/1305	0.51	1/1776 (0.1%)
7	13	0.30	0/1177	0.51	0/1592
8	14	0.32	0/1660	0.60	2/2255 (0.1%)
9	15	0.33	0/1705	0.68	3/2319 (0.1%)
10	16	0.31	0/1347	0.59	2/1833 (0.1%)
All	All	0.34	1/14602 (0.0%)	0.54	8/19817 (0.0%)

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	10	0	1
8	14	0	2
9	15	0	3
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	6	83	CYS	CB-SG	-5.02	1.73	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	16	169	ASP	CB-CG-OD1	10.03	127.32	118.30
9	15	152	ILE	C-N-CD	-5.65	108.17	120.60
8	14	241	ASP	CB-CG-OD1	5.59	123.33	118.30
6	12	176	ARG	NE-CZ-NH2	-5.51	117.55	120.30
8	14	122	ALA	C-N-CA	5.21	133.24	122.30
10	16	168	ILE	C-N-CA	5.16	134.61	121.70
9	15	265	GLY	N-CA-C	5.10	125.86	113.10
9	15	152	ILE	C-N-CA	5.08	143.34	122.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	10	204	PRO	Peptide
8	14	154	ALA	Peptide
8	14	161	GLY	Peptide
9	15	136	ALA	Peptide
9	15	264	SER	Peptide
9	15	268	MET	Peptide

5.2 Too-close contacts [i](#)

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	6	1354	0	1328	17	0
2	7	1416	0	1379	11	0
3	8	1660	0	1625	20	0
4	10	1302	0	1274	6	0
5	11	1479	0	1452	10	0
6	12	1274	0	1267	7	0
7	13	1148	0	1130	16	0
8	14	1609	0	1568	17	0
9	15	1654	0	1613	21	0
10	16	1313	0	1310	20	0
11	10	435	0	465	9	0
11	11	315	0	337	6	0
11	12	566	0	604	13	0
11	13	350	0	354	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	14	468	0	400	9	0
11	15	685	0	589	17	0
11	16	478	0	429	16	0
11	6	620	0	658	14	0
11	7	566	0	609	14	0
11	8	420	0	427	14	0
12	10	135	0	0	0	0
12	11	180	0	0	0	0
12	12	180	0	0	0	0
12	13	270	0	0	1	0
12	14	135	0	0	0	0
12	16	90	0	0	1	0
12	6	180	0	0	0	0
12	7	90	0	0	0	0
12	8	315	0	0	1	0
13	10	86	0	0	1	0
13	11	43	0	0	1	0
13	12	86	0	0	0	0
13	13	43	0	0	1	0
13	15	86	0	0	0	0
13	16	43	0	0	0	0
13	6	129	0	0	4	0
13	7	172	0	0	1	0
13	8	86	0	0	0	0
14	10	240	0	0	0	0
14	11	192	0	0	1	0
14	12	96	0	0	0	0
14	13	93	0	0	0	0
14	14	432	0	0	2	0
14	15	288	0	0	0	0
14	16	96	0	0	0	0
14	6	48	0	0	0	0
14	7	144	0	0	1	0
14	8	96	0	0	1	0
15	6	27	0	24	0	0
16	14	38	0	46	1	0
16	7	37	0	44	1	0
16	8	108	0	123	2	0
17	11	70	0	92	2	0
17	12	175	0	230	6	0
17	15	35	0	46	0	0
17	16	35	0	46	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	7	35	0	46	0	0
17	8	105	0	138	1	0
18	10	1	0	0	0	0
18	11	1	0	0	0	0
18	12	2	0	0	0	0
18	6	2	0	0	0	0
18	7	2	0	0	0	0
18	8	4	0	0	0	0
All	All	23863	0	19653	223	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 5.

All (223) 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)
8:14:101:GLN:OE1	11:14:303:CLA:NA	2.01	0.94
9:15:105:GLU:OE1	11:15:302:CLA:NB	2.22	0.72
7:13:73:GLU:OE1	11:13:307:CLA:NC	2.23	0.71
1:6:127:ILE:HB	11:6:311:CLA:HBC1	1.77	0.66
9:15:127:PHE:O	9:15:138:HIS:NE2	2.33	0.62
8:14:224:GLN:HB3	8:14:240:TYR:HB3	1.81	0.61
11:16:302:CLA:H202	11:16:302:CLA:HBB1	1.81	0.61
4:10:75:ARG:NH2	4:10:78:GLU:OE1	2.34	0.60
10:16:55:PRO:HB3	11:16:307:CLA:HBB1	1.82	0.60
8:14:245:MET:HG3	11:14:312:CLA:HBB1	1.84	0.59
11:7:308:CLA:H52	7:13:83:LEU:HD22	1.83	0.59
1:6:73:ARG:NH2	1:6:76:GLU:OE1	2.35	0.59
7:13:84:ALA:HB2	11:13:301:CLA:HBA1	1.83	0.59
8:14:101:GLN:OE1	11:14:303:CLA:C1A	2.50	0.59
5:11:77:ARG:NH2	5:11:200:GLU:OE1	2.37	0.58
8:14:98:TYR:OH	8:14:224:GLN:NE2	2.36	0.56
7:13:153:GLN:HB3	11:13:304:CLA:HMA3	1.88	0.56
10:16:135:GLN:OE1	12:16:304:KC1:ND	2.39	0.56
8:14:208:ASN:ND2	11:14:307:CLA:O1D	2.39	0.55
3:8:58:MET:SD	3:8:58:MET:N	2.80	0.55
9:15:191:TYR:HB2	11:15:308:CLA:HMD1	1.89	0.55
3:8:84:ASN:ND2	3:8:101:SER:O	2.40	0.54
11:12:304:CLA:H193	11:12:312:CLA:H172	1.90	0.54
10:16:185:GLU:OE1	11:16:306:CLA:NA	2.40	0.54
7:13:183:THR:HB	7:13:186:LYS:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:15:80:ASP:HB3	11:15:302:CLA:HBA2	1.89	0.54
9:15:232:ASN:ND2	11:15:309:CLA:OBD	2.41	0.54
3:8:236:MET:HE1	11:8:305:CLA:H43	1.90	0.53
16:8:320:LMG:HC8	16:8:323:LMG:H292	1.90	0.53
8:14:159:MET:O	8:14:160:ARG:NH2	2.41	0.53
1:6:118:LEU:HB3	1:6:123:ALA:HB3	1.88	0.53
6:12:88:HIS:NE2	6:12:100:GLU:OE1	2.42	0.53
9:15:154:LEU:HA	9:15:157:LYS:HE3	1.91	0.53
3:8:187:LEU:HG	11:8:303:CLA:H12	1.91	0.52
5:11:184:ARG:HD3	5:11:185:GLU:HG2	1.92	0.52
3:8:270:PHE:HA	11:8:308:CLA:HED2	1.90	0.52
1:6:98:ARG:NH2	1:6:109:LEU:O	2.42	0.52
9:15:253:VAL:HG23	9:15:254:PRO:HD3	1.92	0.52
8:14:226:VAL:HG13	8:14:229:SER:HB2	1.91	0.52
10:16:80:GLU:OE1	11:16:301:CLA:NA	2.42	0.52
3:8:264:ASN:ND2	3:8:270:PHE:O	2.43	0.52
9:15:171:ASP:OD1	9:15:186:ARG:NH1	2.43	0.52
1:6:144:GLN:HA	1:6:148:GLU:HB2	1.92	0.51
6:12:94:SER:OG	6:12:95:SER:N	2.44	0.51
8:14:114:ASP:OD2	8:14:114:ASP:N	2.43	0.51
10:16:65:ALA:HB2	11:16:301:CLA:HBA1	1.93	0.51
3:8:161:GLU:O	3:8:167:ASN:ND2	2.44	0.51
3:8:71:GLU:OE1	3:8:81:ARG:NH2	2.43	0.51
2:7:147:ASP:N	2:7:147:ASP:OD1	2.44	0.50
3:8:257:GLN:NE2	14:8:315:A86:O2	2.44	0.50
11:12:308:CLA:HMC2	17:12:319:LMT:H121	1.94	0.50
1:6:198:ALA:HA	1:6:208:VAL:HA	1.94	0.50
10:16:172:THR:HG22	10:16:174:ASN:H	1.75	0.50
11:10:304:CLA:HED3	11:10:304:CLA:H2	1.94	0.49
7:13:173:THR:OG1	7:13:188:MET:SD	2.64	0.49
8:14:148:GLU:OE1	11:14:305:CLA:NA	2.46	0.49
1:6:98:ARG:HB3	1:6:102:LEU:HD13	1.93	0.49
5:11:42:SER:OG	5:11:43:ILE:N	2.45	0.49
11:10:303:CLA:H143	11:10:304:CLA:H202	1.94	0.49
11:12:303:CLA:H93	11:12:306:CLA:H51	1.95	0.49
11:10:305:CLA:H202	11:10:308:CLA:HMD2	1.94	0.49
11:7:303:CLA:H12	11:7:303:CLA:HED3	1.94	0.49
8:14:101:GLN:OE1	11:14:303:CLA:C4A	2.61	0.48
1:6:157:PHE:HB2	11:6:306:CLA:HMD1	1.95	0.48
2:7:245:LYS:NZ	7:13:90:GLU:OE2	2.46	0.48
4:10:163:LEU:HD13	11:10:308:CLA:H42	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:11:132:ALA:HB3	5:11:135:ASP:HB2	1.95	0.48
8:14:68:ILE:O	14:14:317:A86:O2	2.32	0.48
11:7:305:CLA:HBB1	11:7:305:CLA:HHC	1.95	0.48
11:7:310:CLA:H13	11:12:303:CLA:H191	1.94	0.48
7:13:68:SER:O	7:13:96:ARG:NH2	2.47	0.48
5:11:205:ARG:NH2	11:11:303:CLA:O1D	2.47	0.48
6:12:161:ALA:HA	6:12:164:LEU:HB3	1.95	0.48
7:13:147:PRO:HD2	11:13:304:CLA:HAB	1.95	0.48
14:11:314:A86:O3	17:11:316:LMT:O6'	2.32	0.48
11:7:306:CLA:H151	11:13:302:CLA:H8	1.96	0.48
17:8:324:LMT:H5B	17:8:324:LMT:H6E	1.95	0.48
3:8:228:LYS:HB3	3:8:232:GLU:HG3	1.94	0.47
11:10:304:CLA:HBB1	11:10:307:CLA:H162	1.96	0.47
7:13:99:GLU:OE2	7:13:219:ARG:NE	2.38	0.47
11:15:307:CLA:HBB1	11:15:307:CLA:HHC	1.96	0.47
11:6:311:CLA:H41	11:6:311:CLA:H62	1.59	0.47
6:12:169:ASP:HB2	11:12:308:CLA:HED2	1.96	0.47
7:13:61:SER:OG	7:13:62:LYS:N	2.47	0.47
11:6:301:CLA:H202	2:7:209:ILE:HD13	1.95	0.47
11:11:303:CLA:H41	11:11:303:CLA:H61	1.61	0.47
11:13:301:CLA:H71	11:13:302:CLA:HMA1	1.96	0.47
10:16:122:LEU:HD11	10:16:200:VAL:HG12	1.97	0.47
11:10:303:CLA:H192	11:10:307:CLA:H203	1.97	0.47
11:14:307:CLA:HBB2	11:15:313:CLA:H93	1.97	0.46
9:15:132:THR:HG23	9:15:134:ALA:H	1.80	0.46
10:16:187:ASN:HA	10:16:190:ARG:HD2	1.96	0.46
2:7:116:PHE:HB3	3:8:217:PHE:HA	1.97	0.46
17:12:319:LMT:H111	11:16:310:CLA:HMB3	1.98	0.46
10:16:77:ARG:HG3	10:16:160:LEU:HD21	1.98	0.46
1:6:128:PHE:HB2	11:6:311:CLA:HAC1	1.98	0.46
11:15:302:CLA:H62	11:15:302:CLA:H41	1.75	0.46
8:14:183:ASN:O	14:14:320:A86:O2	2.35	0.45
11:6:304:CLA:HAB	11:6:304:CLA:H191	1.97	0.45
11:8:303:CLA:H42	16:8:321:LMG:H152	1.98	0.45
9:15:228:SER:O	9:15:232:ASN:ND2	2.42	0.45
1:6:116:ASP:OD1	13:6:318:DD6:O2	2.35	0.45
11:12:321:CLA:HBB1	11:12:321:CLA:HHC	1.98	0.45
11:6:313:CLA:H2	11:6:313:CLA:H61	1.71	0.45
11:7:308:CLA:H52	11:7:308:CLA:H8	1.65	0.45
11:8:302:CLA:HBB1	11:8:302:CLA:HMB1	1.99	0.45
11:11:303:CLA:H162	11:11:303:CLA:H122	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:15:167:LEU:HD23	11:15:313:CLA:H43	1.99	0.45
3:8:73:SER:OG	3:8:94:GLY:O	2.31	0.45
9:15:179:LEU:HD23	9:15:186:ARG:HD2	1.98	0.45
1:6:206:PRO:O	13:6:315:DD6:O2	2.34	0.45
17:12:301:LMT:H62	17:12:322:LMT:H51	1.98	0.45
10:16:77:ARG:NH2	11:16:301:CLA:O1D	2.45	0.45
10:16:188:ASN:ND2	11:16:307:CLA:OBD	2.49	0.45
16:7:319:LMG:H121	12:8:313:KC1:C1C	2.47	0.45
5:11:182:THR:HA	5:11:193:LEU:HD11	1.99	0.45
11:16:303:CLA:H41	11:16:303:CLA:H61	1.73	0.45
11:7:308:CLA:H203	11:12:310:CLA:H8	1.99	0.45
9:15:116:PHE:HA	9:15:240:ILE:HD13	1.99	0.45
9:15:227:VAL:HG13	11:15:309:CLA:HED2	1.97	0.45
11:7:308:CLA:H162	7:13:81:LEU:HD11	1.98	0.44
7:13:79:ASP:OD2	13:13:314:DD6:O4	2.35	0.44
9:15:62:LYS:NZ	9:15:66:GLU:OE2	2.47	0.44
11:8:303:CLA:H8	11:12:303:CLA:H202	1.99	0.44
5:11:115:TRP:O	17:11:316:LMT:O6'	2.28	0.44
11:15:303:CLA:HBB1	11:15:303:CLA:HHC	1.98	0.44
10:16:108:SER:OG	10:16:109:SER:N	2.51	0.44
5:11:77:ARG:NH1	5:11:172:GLY:O	2.50	0.44
10:16:104:PRO:HA	10:16:105:GLY:HA2	1.67	0.44
11:16:301:CLA:HBA2	11:16:301:CLA:H3A	1.77	0.44
1:6:111:ALA:O	13:6:316:DD6:O2	2.35	0.44
11:6:304:CLA:H162	11:6:304:CLA:H121	1.83	0.44
2:7:187:LYS:HD3	2:7:187:LYS:HA	1.77	0.44
10:16:187:ASN:HA	10:16:190:ARG:HB2	1.99	0.44
2:7:134:ASP:OD1	14:7:314:A86:O2	2.34	0.44
3:8:61:ARG:HH22	4:10:143:ALA:HB1	1.83	0.44
4:10:167:ASP:OD1	4:10:167:ASP:N	2.49	0.44
7:13:73:GLU:OE2	7:13:216:LYS:NZ	2.48	0.44
8:14:190:PHE:HA	8:14:191:SER:HA	1.72	0.44
5:11:38:ALA:HB3	11:11:303:CLA:HED1	1.98	0.44
2:7:236:PHE:HB2	11:7:306:CLA:HMD1	2.00	0.44
11:11:308:CLA:H91	11:11:308:CLA:H111	1.87	0.44
7:13:166:GLU:OE2	7:13:178:TYR:OH	2.36	0.44
9:15:149:TRP:NE1	9:15:266:GLN:O	2.49	0.44
11:6:306:CLA:H92	11:6:306:CLA:H62	1.83	0.44
1:6:93:VAL:O	1:6:98:ARG:NH1	2.38	0.43
11:8:301:CLA:HBA2	11:8:301:CLA:H3A	1.73	0.43
6:12:201:ASN:ND2	17:12:320:LMT:O2'	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:13:303:CLA:H203	11:13:303:CLA:H161	1.87	0.43
8:14:51:SER:HB2	8:14:208:ASN:HD21	1.83	0.43
3:8:225:LEU:HD13	3:8:233:ILE:HG12	1.99	0.43
9:15:117:VAL:HA	9:15:120:ILE:HG12	2.01	0.43
2:7:211:ILE:HG21	11:7:305:CLA:HMC3	2.01	0.43
7:13:180:ARG:NE	12:13:310:KC1:O2A	2.46	0.43
11:16:301:CLA:H142	11:16:301:CLA:H112	1.85	0.43
11:16:301:CLA:H143	11:16:301:CLA:H161	1.88	0.43
2:7:152:ARG:NH2	2:7:155:GLU:OE1	2.50	0.43
2:7:275:GLN:NE2	13:7:313:DD6:O4	2.52	0.43
3:8:158:PHE:HE1	11:8:303:CLA:HBA2	1.84	0.43
10:16:186:LEU:O	10:16:190:ARG:N	2.52	0.43
11:6:313:CLA:H8	11:6:313:CLA:H52	1.72	0.42
10:16:58:LYS:HE2	10:16:58:LYS:HB3	1.79	0.42
11:12:304:CLA:H143	11:12:304:CLA:H112	1.82	0.42
11:12:302:CLA:H61	11:12:302:CLA:H41	1.78	0.42
11:7:306:CLA:H142	11:7:306:CLA:H111	1.83	0.42
4:10:204:PRO:O	13:10:313:DD6:O2	2.36	0.42
9:15:255:LEU:HA	9:15:256:LEU:HA	1.77	0.42
11:6:302:CLA:H202	11:6:302:CLA:H162	1.92	0.42
11:8:302:CLA:H41	11:8:302:CLA:H61	1.70	0.42
17:12:319:LMT:H5B	17:12:319:LMT:H6E	2.01	0.42
17:12:320:LMT:H91	17:12:320:LMT:H62	1.85	0.42
11:14:302:CLA:H3A	11:14:302:CLA:HBA2	1.86	0.42
10:16:106:MET:HA	10:16:112:SER:HA	2.00	0.42
11:7:309:CLA:H41	11:7:309:CLA:H62	1.87	0.42
11:8:305:CLA:H93	11:8:305:CLA:H61	1.79	0.42
3:8:250:ALA:HA	11:8:308:CLA:HBB1	2.01	0.42
11:8:303:CLA:H41	11:8:303:CLA:H62	1.84	0.42
11:14:302:CLA:H41	11:14:302:CLA:H62	1.63	0.42
9:15:105:GLU:HA	9:15:108:HIS:HB2	2.00	0.42
11:15:303:CLA:H72	11:15:303:CLA:H111	1.82	0.42
1:6:91:VAL:HB	1:6:205:PHE:HE1	1.84	0.41
2:7:184:ALA:HB2	2:7:196:ILE:HD11	2.02	0.41
11:7:302:CLA:H12	11:7:302:CLA:H52	1.82	0.41
6:12:121:GLN:HG2	11:12:310:CLA:HHC	2.02	0.41
11:15:302:CLA:H93	11:15:302:CLA:H61	1.85	0.41
3:8:95:PHE:HE1	11:8:309:CLA:HBC3	1.84	0.41
11:13:307:CLA:H142	11:13:307:CLA:H111	1.88	0.41
11:6:306:CLA:H91	11:6:306:CLA:H112	1.86	0.41
3:8:170:THR:OG1	3:8:173:GLU:OE1	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:10:305:CLA:H8	11:10:308:CLA:H202	2.01	0.41
11:10:309:CLA:H61	11:10:309:CLA:H41	1.69	0.41
11:15:302:CLA:H102	11:15:303:CLA:H61	2.01	0.41
11:15:304:CLA:H152	11:15:304:CLA:H111	1.57	0.41
11:13:307:CLA:HBB1	11:13:307:CLA:HHC	2.02	0.41
10:16:164:VAL:HG23	11:16:310:CLA:HED2	2.01	0.41
10:16:100:GLY:O	10:16:102:HIS:ND1	2.51	0.41
11:16:303:CLA:H121	11:16:303:CLA:H8	1.79	0.41
11:7:310:CLA:H122	11:7:310:CLA:H162	1.63	0.41
11:15:313:CLA:HMA2	11:15:313:CLA:H2	2.03	0.41
1:6:54:GLY:H	1:6:73:ARG:NH1	2.19	0.41
3:8:103:ILE:HA	3:8:104:PRO:HD3	1.91	0.41
5:11:177:ASP:OD1	13:11:312:DD6:O4	2.38	0.41
6:12:134:GLU:OE1	6:12:140:TYR:OH	2.26	0.41
11:12:308:CLA:H62	11:12:308:CLA:H41	1.83	0.41
11:15:313:CLA:H61	11:15:313:CLA:H41	1.73	0.41
1:6:160:ASP:OD1	13:6:315:DD6:O4	2.39	0.41
11:6:301:CLA:H3A	11:6:301:CLA:HBA2	1.66	0.41
16:14:322:LMG:H112	16:14:322:LMG:H141	1.93	0.41
9:15:80:ASP:OD1	9:15:80:ASP:N	2.54	0.41
11:16:303:CLA:HMC1	11:16:303:CLA:H192	2.03	0.41
3:8:188:LEU:HD12	3:8:188:LEU:HA	1.95	0.41
11:11:307:CLA:H122	11:11:307:CLA:H162	1.65	0.41
10:16:80:GLU:OE1	11:16:301:CLA:C4A	2.69	0.41
11:6:303:CLA:H3A	11:6:303:CLA:HBA2	1.79	0.40
8:14:56:LYS:NZ	9:15:176:GLY:O	2.51	0.40
11:15:307:CLA:H3A	11:15:312:CLA:HMC2	2.02	0.40
11:8:304:CLA:H61	11:8:304:CLA:H41	1.71	0.40
4:10:176:LEU:HG	4:10:180:LYS:HE2	2.03	0.40
8:14:176:ILE:HA	8:14:177:PRO:HD3	1.88	0.40
11:13:307:CLA:H62	11:13:307:CLA:H41	1.76	0.40
1:6:45:TYR:OH	1:6:55:ASP:OD2	2.36	0.40
11:10:303:CLA:HBA2	11:10:303:CLA:H3A	1.77	0.40
11:12:306:CLA:H112	11:12:306:CLA:H72	1.76	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	6	172/208 (83%)	170 (99%)	2 (1%)	0	100	100
2	7	186/296 (63%)	178 (96%)	8 (4%)	0	100	100
3	8	211/270 (78%)	205 (97%)	6 (3%)	0	100	100
4	10	167/207 (81%)	152 (91%)	13 (8%)	2 (1%)	11	24
5	11	189/229 (82%)	171 (90%)	18 (10%)	0	100	100
6	12	171/204 (84%)	160 (94%)	11 (6%)	0	100	100
7	13	144/244 (59%)	136 (94%)	8 (6%)	0	100	100
8	14	206/249 (83%)	177 (86%)	29 (14%)	0	100	100
9	15	209/281 (74%)	173 (83%)	35 (17%)	1 (0%)	25	47
10	16	172/218 (79%)	156 (91%)	16 (9%)	0	100	100
All	All	1827/2406 (76%)	1678 (92%)	146 (8%)	3 (0%)	45	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	15	250	PRO
4	10	205	TYR
4	10	204	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	6	140/160 (88%)	140 (100%)	0	100	100
2	7	143/236 (61%)	143 (100%)	0	100	100
3	8	171/215 (80%)	171 (100%)	0	100	100
4	10	133/161 (83%)	133 (100%)	0	100	100
5	11	154/181 (85%)	153 (99%)	1 (1%)	84	94
6	12	136/159 (86%)	136 (100%)	0	100	100
7	13	112/184 (61%)	111 (99%)	1 (1%)	75	90
8	14	166/196 (85%)	166 (100%)	0	100	100
9	15	171/231 (74%)	168 (98%)	3 (2%)	54	77
10	16	139/174 (80%)	139 (100%)	0	100	100
All	All	1465/1897 (77%)	1460 (100%)	5 (0%)	90	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	11	184	ARG
7	13	76	ARG
9	15	138	HIS
9	15	253	VAL
9	15	271	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	7	189	GLN
3	8	167	ASN
4	10	201	HIS
8	14	82	GLN
8	14	183	ASN
8	14	209	ASN
9	15	200	ASN
10	16	177	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

192 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$
12	KC1	14	311	8	48,53,53	3.43	24 (50%)	55,89,89	3.80	30 (54%)
16	LMG	14	322	-	38,38,55	0.97	3 (7%)	46,46,63	1.20	3 (6%)
17	LMT	12	301	-	36,36,36	0.39	0	47,47,47	0.79	0
11	CLA	11	307	5	65,73,73	2.00	15 (23%)	76,113,113	2.68	27 (35%)
14	A86	14	321	-	44,50,50	4.17	23 (52%)	51,76,76	8.40	16 (31%)
17	LMT	12	322	-	36,36,36	0.43	0	47,47,47	0.87	1 (2%)
12	KC1	8	314	18,12	48,53,53	3.39	25 (52%)	55,89,89	3.71	29 (52%)
12	KC1	6	310	1	48,53,53	3.40	23 (47%)	55,89,89	3.76	30 (54%)
13	DD6	6	315	-	39,45,45	6.65	24 (61%)	52,67,67	6.62	27 (51%)
14	A86	12	316	-	44,50,50	4.02	23 (52%)	51,76,76	8.31	17 (33%)
17	LMT	8	324	-	36,36,36	0.40	0	47,47,47	0.70	0
11	CLA	6	302	1	65,73,73	2.03	17 (26%)	76,113,113	2.64	28 (36%)
14	A86	8	318	-	44,50,50	3.96	24 (54%)	51,76,76	10.85	22 (43%)
13	DD6	10	314	-	39,45,45	6.63	23 (58%)	52,67,67	6.73	29 (55%)
11	CLA	11	308	5	65,73,73	2.00	15 (23%)	76,113,113	2.73	29 (38%)
11	CLA	12	308	18	65,73,73	2.00	18 (27%)	76,113,113	2.62	25 (32%)
11	CLA	15	311	14	45,53,73	2.48	16 (35%)	52,89,113	3.16	24 (46%)
12	KC1	16	311	10	48,53,53	3.47	25 (52%)	55,89,89	3.71	26 (47%)
17	LMT	12	320	-	36,36,36	0.35	0	47,47,47	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	6	312	1	45,53,73	2.49	17 (37%)	52,89,113	3.11	23 (44%)
13	DD6	7	317	-	39,45,45	6.75	21 (53%)	52,67,67	6.90	28 (53%)
14	A86	7	315	-	44,50,50	3.75	22 (50%)	51,76,76	7.73	24 (47%)
11	CLA	8	309	3	47,55,73	2.35	16 (34%)	54,91,113	3.04	24 (44%)
11	CLA	15	303	9,14,11	60,68,73	2.09	17 (28%)	70,107,113	2.87	28 (40%)
14	A86	15	321	9	44,50,50	4.09	23 (52%)	51,76,76	8.65	19 (37%)
11	CLA	16	308	10	45,53,73	2.46	17 (37%)	52,89,113	3.23	24 (46%)
11	CLA	13	307	7	65,73,73	2.06	18 (27%)	76,113,113	2.67	28 (36%)
11	CLA	7	309	2	65,73,73	2.01	16 (24%)	76,113,113	2.65	26 (34%)
13	DD6	10	313	-	39,45,45	6.76	23 (58%)	52,67,67	7.06	28 (53%)
11	CLA	6	304	1	65,73,73	2.04	17 (26%)	76,113,113	2.66	27 (35%)
13	DD6	12	315	11	39,45,45	6.61	23 (58%)	52,67,67	6.92	26 (50%)
14	A86	7	318	-	44,50,50	4.01	23 (52%)	51,76,76	7.94	25 (49%)
11	CLA	15	306	-	45,53,73	2.46	17 (37%)	52,89,113	3.29	24 (46%)
14	A86	14	301	8	44,50,50	4.06	23 (52%)	51,76,76	8.05	19 (37%)
11	CLA	12	306	6	65,73,73	1.97	16 (24%)	76,113,113	2.59	26 (34%)
14	A86	10	301	4	44,50,50	3.84	23 (52%)	51,76,76	7.25	24 (47%)
17	LMT	8	322	-	36,36,36	0.37	0	47,47,47	0.71	0
12	KC1	10	310	4	48,53,53	3.44	24 (50%)	55,89,89	3.94	30 (54%)
12	KC1	12	313	6	48,53,53	3.42	23 (47%)	55,89,89	4.51	28 (50%)
12	KC1	6	305	1	48,53,53	3.39	24 (50%)	55,89,89	3.82	27 (49%)
11	CLA	16	303	10	65,73,73	2.00	16 (24%)	76,113,113	2.85	28 (36%)
11	CLA	7	310	2	65,73,73	1.98	16 (24%)	76,113,113	2.60	26 (34%)
11	CLA	12	307	6	46,54,73	2.32	16 (34%)	53,90,113	3.21	26 (49%)
12	KC1	6	309	1	48,53,53	3.42	24 (50%)	55,89,89	3.79	30 (54%)
13	DD6	6	318	-	39,45,45	6.55	23 (58%)	52,67,67	6.75	28 (53%)
14	A86	11	314	-	44,50,50	4.00	22 (50%)	51,76,76	7.45	23 (45%)
14	A86	14	319	11	44,50,50	4.08	23 (52%)	51,76,76	8.28	17 (33%)
11	CLA	8	308	3	55,63,73	2.16	15 (27%)	64,101,113	2.91	26 (40%)
11	CLA	15	313	9	65,73,73	2.05	17 (26%)	76,113,113	2.73	28 (36%)
16	LMG	8	321	-	42,42,55	0.93	2 (4%)	50,50,63	1.33	4 (8%)
12	KC1	11	311	-	48,53,53	3.41	24 (50%)	55,89,89	3.55	29 (52%)
12	KC1	8	306	18	48,53,53	3.35	22 (45%)	55,89,89	3.71	33 (60%)
11	CLA	11	309	5	65,73,73	2.07	17 (26%)	76,113,113	2.64	26 (34%)
17	LMT	15	301	-	36,36,36	0.44	0	47,47,47	1.04	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	DD6	12	317	-	39,45,45	6.69	22 (56%)	52,67,67	7.11	28 (53%)
13	DD6	15	319	11	39,45,45	6.77	22 (56%)	52,67,67	6.93	30 (57%)
14	A86	14	320	-	44,50,50	4.12	23 (52%)	51,76,76	7.23	21 (41%)
12	KC1	8	313	3	48,53,53	3.34	22 (45%)	55,89,89	3.88	30 (54%)
11	CLA	14	303	8	57,65,73	2.19	16 (28%)	66,103,113	2.86	29 (43%)
12	KC1	6	308	1	48,53,53	3.37	23 (47%)	55,89,89	3.98	28 (50%)
12	KC1	11	310	5	48,53,53	3.45	26 (54%)	55,89,89	3.82	29 (52%)
14	A86	15	316	11	44,50,50	4.09	23 (52%)	51,76,76	7.82	17 (33%)
12	KC1	7	307	18	48,53,53	3.41	22 (45%)	55,89,89	3.70	28 (50%)
11	CLA	14	305	8	50,58,73	2.31	16 (32%)	58,95,113	3.03	27 (46%)
17	LMT	8	319	-	36,36,36	0.39	0	47,47,47	0.85	1 (2%)
13	DD6	11	312	-	39,45,45	6.71	23 (58%)	52,67,67	7.00	29 (55%)
17	LMT	16	315	-	36,36,36	0.41	0	47,47,47	0.64	0
11	CLA	6	303	18	65,73,73	2.01	17 (26%)	76,113,113	2.72	27 (35%)
12	KC1	11	306	5	48,53,53	3.46	26 (54%)	55,89,89	3.84	29 (52%)
11	CLA	16	310	10	45,53,73	2.45	19 (42%)	52,89,113	3.17	26 (50%)
11	CLA	13	302	7	65,73,73	2.02	17 (26%)	76,113,113	2.62	28 (36%)
12	KC1	12	305	6	48,53,53	3.41	24 (50%)	55,89,89	3.79	27 (49%)
11	CLA	7	308	2	65,73,73	1.92	17 (26%)	76,113,113	2.67	24 (31%)
11	CLA	13	303	-	65,73,73	2.07	16 (24%)	76,113,113	2.77	29 (38%)
12	KC1	14	308	8,11	48,53,53	3.44	25 (52%)	55,89,89	3.77	29 (52%)
13	DD6	15	318	-	39,45,45	6.74	21 (53%)	52,67,67	6.97	31 (59%)
11	CLA	14	302	8	65,73,73	2.03	17 (26%)	76,113,113	2.74	31 (40%)
11	CLA	10	305	18	65,73,73	1.99	16 (24%)	76,113,113	2.78	27 (35%)
11	CLA	10	309	4	65,73,73	2.03	18 (27%)	76,113,113	2.65	27 (35%)
11	CLA	15	309	9	65,73,73	2.09	16 (24%)	76,113,113	2.70	25 (32%)
11	CLA	8	301	3	65,73,73	2.00	17 (26%)	76,113,113	2.75	27 (35%)
11	CLA	16	301	10	65,73,73	1.98	16 (24%)	76,113,113	2.74	28 (36%)
11	CLA	7	305	2	65,73,73	1.99	17 (26%)	76,113,113	2.61	27 (35%)
13	DD6	6	316	-	39,45,45	6.69	23 (58%)	52,67,67	6.50	30 (57%)
11	CLA	12	303	6	65,73,73	2.06	18 (27%)	76,113,113	2.63	27 (35%)
14	A86	14	316	-	44,50,50	3.99	23 (52%)	51,76,76	8.18	17 (33%)
14	A86	14	317	-	44,50,50	4.03	23 (52%)	51,76,76	8.74	18 (35%)
14	A86	8	315	-	44,50,50	3.65	22 (50%)	51,76,76	8.21	21 (41%)
11	CLA	14	304	8	45,53,73	2.46	16 (35%)	52,89,113	3.18	23 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	15	312	9	45,53,73	2.46	16 (35%)	52,89,113	3.32	28 (53%)
12	KC1	13	312	7	48,53,53	3.52	27 (56%)	55,89,89	3.78	29 (52%)
12	KC1	7	312	-	48,53,53	3.36	22 (45%)	55,89,89	3.81	29 (52%)
11	CLA	15	305	9,14	45,53,73	2.46	17 (37%)	52,89,113	3.16	26 (50%)
12	KC1	12	311	6	48,53,53	3.43	24 (50%)	55,89,89	3.93	31 (56%)
13	DD6	7	316	-	39,45,45	6.72	21 (53%)	52,67,67	6.71	29 (55%)
11	CLA	12	302	6	65,73,73	1.97	17 (26%)	76,113,113	2.82	30 (39%)
11	CLA	8	303	18	65,73,73	1.97	15 (23%)	76,113,113	2.64	27 (35%)
12	KC1	12	309	6	48,53,53	3.40	23 (47%)	55,89,89	3.73	31 (56%)
12	KC1	8	311	18	48,53,53	3.37	23 (47%)	55,89,89	3.79	29 (52%)
11	CLA	14	309	8	45,53,73	2.50	16 (35%)	52,89,113	3.09	24 (46%)
11	CLA	6	311	1	65,73,73	1.96	15 (23%)	76,113,113	2.76	28 (36%)
11	CLA	16	309	10	45,53,73	2.47	17 (37%)	52,89,113	3.26	24 (46%)
14	A86	15	317	11	44,50,50	4.15	23 (52%)	51,76,76	8.46	15 (29%)
12	KC1	13	306	7	48,53,53	3.40	24 (50%)	55,89,89	3.76	30 (54%)
14	A86	13	313	7	41,47,50	4.23	22 (53%)	49,72,76	8.48	14 (28%)
11	CLA	14	310	-	50,58,73	2.32	16 (32%)	58,95,113	3.10	26 (44%)
11	CLA	8	302	3	65,73,73	2.03	17 (26%)	76,113,113	2.78	25 (32%)
13	DD6	16	313	-	39,45,45	6.74	20 (51%)	52,67,67	7.14	30 (57%)
11	CLA	7	302	2	65,73,73	1.95	15 (23%)	76,113,113	2.71	30 (39%)
12	KC1	10	306	4	48,53,53	3.34	25 (52%)	55,89,89	3.95	32 (58%)
14	A86	11	313	-	44,50,50	3.99	23 (52%)	51,76,76	8.39	18 (35%)
14	A86	6	317	-	44,50,50	4.01	24 (54%)	51,76,76	7.16	21 (41%)
13	DD6	8	317	-	39,45,45	6.63	22 (56%)	52,67,67	6.94	29 (55%)
14	A86	14	318	-	44,50,50	4.09	23 (52%)	51,76,76	8.48	17 (33%)
11	CLA	12	321	8,6	65,73,73	2.02	17 (26%)	76,113,113	2.62	27 (35%)
11	CLA	10	304	4	65,73,73	2.02	18 (27%)	76,113,113	2.65	26 (34%)
16	LMG	7	319	-	37,37,55	0.98	3 (8%)	45,45,63	1.27	4 (8%)
12	KC1	13	311	7	48,53,53	3.47	26 (54%)	55,89,89	3.53	28 (50%)
17	LMT	11	316	-	36,36,36	0.40	0	47,47,47	1.00	5 (10%)
11	CLA	13	309	-	45,53,73	2.49	17 (37%)	52,89,113	3.13	26 (50%)
11	CLA	14	312	8,14	45,53,73	2.46	17 (37%)	52,89,113	3.15	24 (46%)
11	CLA	13	301	7	65,73,73	1.97	18 (27%)	76,113,113	2.75	30 (39%)
11	CLA	7	303	2	65,73,73	1.96	16 (24%)	76,113,113	2.70	28 (36%)
12	KC1	10	312	4	48,53,53	3.42	24 (50%)	55,89,89	3.91	29 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	7	304	18,2	65,73,73	2.12	18 (27%)	76,113,113	2.82	28 (36%)
14	A86	10	317	-	44,50,50	4.17	23 (52%)	51,76,76	8.20	17 (33%)
14	A86	11	315	-	44,50,50	3.94	23 (52%)	51,76,76	8.40	18 (35%)
11	CLA	10	311	-	45,53,73	2.45	17 (37%)	52,89,113	3.16	22 (42%)
12	KC1	8	307	3	48,53,53	3.32	22 (45%)	55,89,89	3.85	30 (54%)
11	CLA	15	308	9,11	45,53,73	2.42	16 (35%)	52,89,113	3.13	27 (51%)
11	CLA	16	302	10	65,73,73	1.98	18 (27%)	76,113,113	2.68	27 (35%)
11	CLA	16	307	-	46,54,73	2.42	17 (36%)	53,90,113	3.11	24 (45%)
14	A86	13	315	-	44,50,50	4.17	23 (52%)	51,76,76	8.46	19 (37%)
14	A86	15	322	11	44,50,50	4.26	23 (52%)	51,76,76	8.45	22 (43%)
13	DD6	7	301	-	39,45,45	6.75	22 (56%)	52,67,67	6.70	28 (53%)
11	CLA	15	304	9,11,13	65,73,73	2.06	17 (26%)	76,113,113	2.74	27 (35%)
12	KC1	11	304	5	48,53,53	3.39	25 (52%)	55,89,89	3.82	30 (54%)
14	A86	14	314	-	44,50,50	4.08	23 (52%)	51,76,76	8.24	22 (43%)
17	LMT	12	318	-	36,36,36	0.40	0	47,47,47	0.79	1 (2%)
11	CLA	10	303	4	65,73,73	2.00	16 (24%)	76,113,113	2.69	27 (35%)
13	DD6	13	314	-	39,45,45	6.72	22 (56%)	52,67,67	7.10	32 (61%)
17	LMT	12	319	-	36,36,36	0.37	0	47,47,47	0.80	0
11	CLA	13	304	7	45,53,73	2.50	16 (35%)	52,89,113	3.20	25 (48%)
16	LMG	8	323	16	29,29,55	1.14	2 (6%)	37,37,63	1.27	5 (13%)
14	A86	10	302	-	44,50,50	4.08	23 (52%)	51,76,76	8.60	20 (39%)
11	CLA	8	305	3	65,73,73	1.99	18 (27%)	76,113,113	4.73	30 (39%)
11	CLA	6	307	15	65,73,73	2.02	17 (26%)	76,113,113	2.58	28 (36%)
14	A86	14	315	8	44,50,50	3.95	23 (52%)	51,76,76	8.88	21 (41%)
11	CLA	7	311	2	46,54,73	2.42	17 (36%)	53,90,113	3.10	24 (45%)
17	LMT	7	320	-	36,36,36	0.30	0	47,47,47	0.71	1 (2%)
11	CLA	10	307	4	65,73,73	1.96	18 (27%)	76,113,113	2.64	29 (38%)
14	A86	12	314	-	44,50,50	3.95	23 (52%)	51,76,76	8.15	19 (37%)
11	CLA	6	306	1	65,73,73	2.01	16 (24%)	76,113,113	2.72	32 (42%)
11	CLA	15	310	9	45,53,73	2.52	16 (35%)	52,89,113	3.21	24 (46%)
11	CLA	12	310	18	65,73,73	1.98	18 (27%)	76,113,113	2.72	25 (32%)
11	CLA	14	307	12	65,73,73	2.06	17 (26%)	76,113,113	2.79	24 (31%)
11	CLA	6	301	1	65,73,73	1.97	15 (23%)	76,113,113	2.70	28 (36%)
11	CLA	11	303	5	65,73,73	2.01	16 (24%)	76,113,113	2.72	25 (32%)
15	LHG	6	319	11	26,26,48	0.91	1 (3%)	29,32,54	1.39	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	15	307	9	50,58,73	2.29	18 (36%)	58,95,113	2.99	26 (44%)
11	CLA	12	304	6,13	65,73,73	2.03	18 (27%)	76,113,113	2.88	29 (38%)
11	CLA	6	313	18	55,63,73	2.19	17 (30%)	64,101,113	2.83	25 (39%)
12	KC1	13	310	7	48,53,53	3.45	24 (50%)	55,89,89	3.77	29 (52%)
12	KC1	16	304	10	48,53,53	3.48	24 (50%)	55,89,89	3.57	27 (49%)
11	CLA	11	305	18	55,63,73	2.20	16 (29%)	64,101,113	3.03	27 (42%)
13	DD6	7	313	-	39,45,45	6.57	22 (56%)	52,67,67	7.25	29 (55%)
14	A86	15	315	9	44,50,50	4.30	23 (52%)	51,76,76	8.24	27 (52%)
11	CLA	6	314	-	65,73,73	2.08	17 (26%)	76,113,113	2.64	27 (35%)
11	CLA	7	306	2	65,73,73	1.98	15 (23%)	76,113,113	2.75	26 (34%)
11	CLA	8	304	3	58,66,73	2.07	15 (25%)	67,104,113	2.99	31 (46%)
11	CLA	15	302	9,11	65,73,73	2.05	16 (24%)	76,113,113	2.94	29 (38%)
14	A86	15	320	-	44,50,50	4.24	24 (54%)	51,76,76	8.22	19 (37%)
11	CLA	16	305	10	50,58,73	2.26	17 (34%)	58,95,113	3.00	27 (46%)
12	KC1	14	306	8	48,53,53	3.43	24 (50%)	55,89,89	3.86	30 (54%)
12	KC1	13	305	7	48,53,53	3.44	26 (54%)	55,89,89	3.76	29 (52%)
13	DD6	8	316	-	39,45,45	6.55	22 (56%)	52,67,67	6.81	30 (57%)
14	A86	7	314	-	44,50,50	3.85	23 (52%)	51,76,76	7.93	18 (35%)
11	CLA	14	313	8	46,54,73	2.42	16 (34%)	53,90,113	3.25	26 (49%)
16	LMG	8	320	16,3	37,37,55	0.98	1 (2%)	45,45,63	1.24	4 (8%)
14	A86	11	301	-	44,50,50	3.98	23 (52%)	51,76,76	8.34	19 (37%)
14	A86	16	314	-	44,50,50	4.10	24 (54%)	51,76,76	8.52	21 (41%)
12	KC1	13	308	7	48,53,53	3.45	25 (52%)	55,89,89	3.87	29 (52%)
14	A86	10	316	-	44,50,50	3.92	23 (52%)	51,76,76	7.96	23 (45%)
11	CLA	16	306	10	52,60,73	2.26	18 (34%)	60,97,113	2.95	28 (46%)
17	LMT	11	302	-	36,36,36	0.32	0	47,47,47	0.79	2 (4%)
11	CLA	10	308	4	65,73,73	2.00	15 (23%)	76,113,113	2.73	29 (38%)
11	CLA	12	312	6	65,73,73	2.01	18 (27%)	76,113,113	2.70	27 (35%)
11	CLA	15	314	9,11	45,53,73	2.40	17 (37%)	52,89,113	3.32	23 (44%)
12	KC1	8	310	3	48,53,53	3.31	22 (45%)	55,89,89	3.78	28 (50%)
14	A86	16	312	10	44,50,50	4.02	24 (54%)	51,76,76	8.20	22 (43%)
12	KC1	8	312	12	48,53,53	3.40	24 (50%)	55,89,89	3.39	28 (50%)
14	A86	10	315	-	44,50,50	4.12	22 (50%)	51,76,76	8.21	18 (35%)

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
12	KC1	14	311	8	-	5/15/71/71	-
16	LMG	14	322	-	-	14/33/53/70	0/1/1/1
17	LMT	12	301	-	-	3/21/61/61	0/2/2/2
11	CLA	11	307	5	1/1/15/20	10/37/115/115	-
14	A86	14	321	-	-	15/34/90/90	0/3/3/3
17	LMT	12	322	-	-	1/21/61/61	0/2/2/2
12	KC1	8	314	18,12	-	6/15/71/71	-
12	KC1	6	310	1	-	6/15/71/71	-
13	DD6	6	315	-	-	10/26/80/80	0/3/3/3
14	A86	12	316	-	-	14/34/90/90	0/3/3/3
17	LMT	8	324	-	-	5/21/61/61	0/2/2/2
11	CLA	6	302	1	1/1/15/20	4/37/115/115	-
14	A86	8	318	-	-	14/34/90/90	0/3/3/3
13	DD6	10	314	-	-	9/26/80/80	0/3/3/3
11	CLA	11	308	5	-	15/37/115/115	-
11	CLA	12	308	18	1/1/15/20	9/37/115/115	-
11	CLA	15	311	14	1/1/11/20	8/13/91/115	-
12	KC1	16	311	10	-	6/15/71/71	-
17	LMT	12	320	-	-	1/21/61/61	0/2/2/2
11	CLA	6	312	1	1/1/11/20	4/13/91/115	-
13	DD6	7	317	-	-	15/26/80/80	0/3/3/3
14	A86	7	315	-	-	9/34/90/90	0/3/3/3
11	CLA	8	309	3	-	3/16/94/115	-
11	CLA	15	303	9,14,11	1/1/14/20	9/31/109/115	-
14	A86	15	321	9	-	13/34/90/90	0/3/3/3
11	CLA	16	308	10	1/1/11/20	6/13/91/115	-
11	CLA	13	307	7	1/1/15/20	10/37/115/115	-
11	CLA	7	309	2	1/1/15/20	14/37/115/115	-
13	DD6	10	313	-	-	10/26/80/80	0/3/3/3
11	CLA	6	304	1	1/1/15/20	18/37/115/115	-
13	DD6	12	315	11	-	9/26/80/80	0/3/3/3
14	A86	7	318	-	-	9/34/90/90	0/3/3/3
11	CLA	15	306	-	1/1/11/20	6/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	A86	14	301	8	-	8/34/90/90	0/3/3/3
11	CLA	12	306	6	1/1/15/20	6/37/115/115	-
14	A86	10	301	4	-	9/34/90/90	0/3/3/3
17	LMT	8	322	-	-	1/21/61/61	0/2/2/2
12	KC1	10	310	4	-	8/15/71/71	-
12	KC1	12	313	6	-	7/15/71/71	-
12	KC1	6	305	1	-	6/15/71/71	-
11	CLA	16	303	10	1/1/15/20	19/37/115/115	-
11	CLA	7	310	2	1/1/15/20	12/37/115/115	-
11	CLA	12	307	6	1/1/11/20	7/15/93/115	-
12	KC1	6	309	1	-	5/15/71/71	-
13	DD6	6	318	-	-	9/26/80/80	0/3/3/3
14	A86	11	314	-	-	18/34/90/90	0/3/3/3
14	A86	14	319	11	-	11/34/90/90	0/3/3/3
11	CLA	8	308	3	1/1/13/20	10/25/103/115	-
11	CLA	15	313	9	-	11/37/115/115	-
16	LMG	8	321	-	-	22/37/57/70	0/1/1/1
12	KC1	11	311	-	-	9/15/71/71	-
12	KC1	8	306	18	-	5/15/71/71	-
11	CLA	11	309	5	1/1/15/20	15/37/115/115	-
17	LMT	15	301	-	-	7/21/61/61	0/2/2/2
13	DD6	12	317	-	-	12/26/80/80	0/3/3/3
13	DD6	15	319	11	-	13/26/80/80	0/3/3/3
14	A86	14	320	-	-	9/34/90/90	0/3/3/3
12	KC1	8	313	3	-	8/15/71/71	-
11	CLA	14	303	8	1/1/13/20	7/28/106/115	-
12	KC1	6	308	1	-	8/15/71/71	-
12	KC1	11	310	5	-	6/15/71/71	-
14	A86	15	316	11	-	14/34/90/90	0/3/3/3
12	KC1	7	307	18	-	7/15/71/71	-
11	CLA	14	305	8	1/1/12/20	2/19/97/115	-
17	LMT	8	319	-	-	10/21/61/61	0/2/2/2
13	DD6	11	312	-	-	11/26/80/80	0/3/3/3
17	LMT	16	315	-	-	5/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	6	303	18	1/1/15/20	7/37/115/115	-
12	KC1	11	306	5	-	10/15/71/71	-
11	CLA	16	310	10	1/1/11/20	7/13/91/115	-
11	CLA	13	302	7	1/1/15/20	11/37/115/115	-
12	KC1	12	305	6	-	7/15/71/71	-
11	CLA	7	308	2	1/1/15/20	8/37/115/115	-
11	CLA	13	303	-	-	16/37/115/115	-
12	KC1	14	308	8,11	-	9/15/71/71	-
13	DD6	15	318	-	-	13/26/80/80	0/3/3/3
11	CLA	14	302	8	1/1/15/20	14/37/115/115	-
11	CLA	10	305	18	1/1/15/20	8/37/115/115	-
11	CLA	10	309	4	1/1/15/20	12/37/115/115	-
11	CLA	15	309	9	1/1/15/20	10/37/115/115	-
11	CLA	8	301	3	1/1/15/20	15/37/115/115	-
11	CLA	16	301	10	-	13/37/115/115	-
11	CLA	7	305	2	1/1/15/20	6/37/115/115	-
13	DD6	6	316	-	-	11/26/80/80	0/3/3/3
11	CLA	12	303	6	1/1/15/20	7/37/115/115	-
14	A86	14	316	-	-	12/34/90/90	0/3/3/3
14	A86	14	317	-	-	15/34/90/90	0/3/3/3
14	A86	8	315	-	-	7/34/90/90	0/3/3/3
11	CLA	14	304	8	1/1/11/20	4/13/91/115	-
11	CLA	15	312	9	1/1/11/20	5/13/91/115	-
12	KC1	13	312	7	-	7/15/71/71	-
12	KC1	7	312	-	-	4/15/71/71	-
11	CLA	15	305	9,14	1/1/11/20	8/13/91/115	-
12	KC1	12	311	6	-	6/15/71/71	-
13	DD6	7	316	-	-	10/26/80/80	0/3/3/3
11	CLA	12	302	6	-	14/37/115/115	-
11	CLA	8	303	18	1/1/15/20	10/37/115/115	-
12	KC1	12	309	6	-	7/15/71/71	-
12	KC1	8	311	18	-	8/15/71/71	-
11	CLA	14	309	8	1/1/11/20	3/13/91/115	-
11	CLA	6	311	1	-	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	16	309	10	-	4/13/91/115	-
14	A86	15	317	11	-	16/34/90/90	0/3/3/3
12	KC1	13	306	7	-	11/15/71/71	-
14	A86	13	313	7	-	11/30/86/90	0/3/3/3
11	CLA	14	310	-	1/1/12/20	5/19/97/115	-
11	CLA	8	302	3	1/1/15/20	6/37/115/115	-
13	DD6	16	313	-	-	13/26/80/80	0/3/3/3
11	CLA	7	302	2	1/1/15/20	13/37/115/115	-
12	KC1	10	306	4	-	8/15/71/71	-
14	A86	11	313	-	-	13/34/90/90	0/3/3/3
14	A86	6	317	-	-	8/34/90/90	0/3/3/3
13	DD6	8	317	-	-	11/26/80/80	0/3/3/3
14	A86	14	318	-	-	17/34/90/90	0/3/3/3
11	CLA	12	321	8,6	1/1/15/20	4/37/115/115	-
11	CLA	10	304	4	1/1/15/20	2/37/115/115	-
16	LMG	7	319	-	-	12/32/52/70	0/1/1/1
12	KC1	13	311	7	-	6/15/71/71	-
17	LMT	11	316	-	-	1/21/61/61	0/2/2/2
11	CLA	13	309	-	1/1/11/20	6/13/91/115	-
11	CLA	14	312	8,14	-	7/13/91/115	-
11	CLA	13	301	7	-	16/37/115/115	-
11	CLA	7	303	2	1/1/15/20	6/37/115/115	-
12	KC1	10	312	4	-	5/15/71/71	-
11	CLA	7	304	18,2	1/1/15/20	8/37/115/115	-
14	A86	10	317	-	-	10/34/90/90	0/3/3/3
14	A86	11	315	-	-	15/34/90/90	0/3/3/3
11	CLA	10	311	-	-	7/13/91/115	-
12	KC1	8	307	3	-	8/15/71/71	-
11	CLA	15	308	9,11	1/1/11/20	6/13/91/115	-
11	CLA	16	302	10	1/1/15/20	9/37/115/115	-
11	CLA	16	307	-	1/1/11/20	7/15/93/115	-
14	A86	13	315	-	-	16/34/90/90	0/3/3/3
14	A86	15	322	11	-	15/34/90/90	0/3/3/3
13	DD6	7	301	-	-	11/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	15	304	9,11,13	1/1/15/20	21/37/115/115	-
12	KC1	11	304	5	-	7/15/71/71	-
14	A86	14	314	-	-	13/34/90/90	0/3/3/3
17	LMT	12	318	-	-	1/21/61/61	0/2/2/2
11	CLA	10	303	4	-	12/37/115/115	-
13	DD6	13	314	-	-	13/26/80/80	0/3/3/3
17	LMT	12	319	-	-	0/21/61/61	0/2/2/2
11	CLA	13	304	7	-	6/13/91/115	-
16	LMG	8	323	16	-	5/24/44/70	0/1/1/1
14	A86	10	302	-	-	13/34/90/90	0/3/3/3
11	CLA	8	305	3	-	13/37/115/115	-
11	CLA	6	307	15	1/1/15/20	10/37/115/115	-
14	A86	14	315	8	-	11/34/90/90	0/3/3/3
11	CLA	7	311	2	-	6/15/93/115	-
17	LMT	7	320	-	-	4/21/61/61	0/2/2/2
11	CLA	10	307	4	1/1/15/20	11/37/115/115	-
14	A86	12	314	-	-	12/34/90/90	0/3/3/3
11	CLA	6	306	1	1/1/15/20	12/37/115/115	-
11	CLA	15	310	9	1/1/11/20	6/13/91/115	-
11	CLA	12	310	18	-	9/37/115/115	-
11	CLA	14	307	12	-	9/37/115/115	-
11	CLA	6	301	1	1/1/15/20	12/37/115/115	-
11	CLA	11	303	5	-	10/37/115/115	-
15	LHG	6	319	11	-	13/31/31/53	-
11	CLA	12	304	6,13	1/1/15/20	14/37/115/115	-
11	CLA	6	313	18	1/1/13/20	5/25/103/115	-
11	CLA	15	307	9	1/1/12/20	7/19/97/115	-
12	KC1	13	310	7	-	5/15/71/71	-
12	KC1	16	304	10	-	8/15/71/71	-
11	CLA	11	305	18	1/1/13/20	8/25/103/115	-
13	DD6	7	313	-	-	11/26/80/80	0/3/3/3
14	A86	15	315	9	-	9/34/90/90	0/3/3/3
11	CLA	6	314	-	1/1/15/20	6/37/115/115	-
11	CLA	7	306	2	-	21/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	8	304	3	1/1/13/20	11/29/107/115	-
11	CLA	15	302	9,11	-	15/37/115/115	-
14	A86	15	320	-	-	15/34/90/90	0/3/3/3
11	CLA	16	305	10	1/1/12/20	3/19/97/115	-
12	KC1	14	306	8	-	7/15/71/71	-
12	KC1	13	305	7	-	10/15/71/71	-
13	DD6	8	316	-	-	11/26/80/80	0/3/3/3
14	A86	7	314	-	-	16/34/90/90	0/3/3/3
11	CLA	14	313	8	1/1/11/20	4/15/93/115	-
16	LMG	8	320	16,3	-	17/32/52/70	0/1/1/1
14	A86	11	301	-	-	12/34/90/90	0/3/3/3
14	A86	16	314	-	-	11/34/90/90	0/3/3/3
12	KC1	13	308	7	-	10/15/71/71	-
14	A86	10	316	-	-	11/34/90/90	0/3/3/3
11	CLA	16	306	10	1/1/12/20	13/22/100/115	-
17	LMT	11	302	-	-	0/21/61/61	0/2/2/2
11	CLA	10	308	4	1/1/15/20	10/37/115/115	-
11	CLA	12	312	6	1/1/15/20	12/37/115/115	-
11	CLA	15	314	9,11	-	4/13/91/115	-
12	KC1	8	310	3	-	7/15/71/71	-
14	A86	16	312	10	-	12/34/90/90	0/3/3/3
12	KC1	8	312	12	-	7/15/71/71	-
14	A86	10	315	-	-	15/34/90/90	0/3/3/3

All (3477) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	11	312	DD6	C10-C11	26.03	1.70	1.35
13	10	313	DD6	C10-C11	25.96	1.70	1.35
13	7	317	DD6	C10-C11	25.86	1.70	1.35
13	15	318	DD6	C10-C11	25.75	1.69	1.35
13	10	314	DD6	C10-C11	25.68	1.69	1.35
13	15	319	DD6	C10-C11	25.62	1.69	1.35
13	12	317	DD6	C10-C11	25.58	1.69	1.35
13	13	314	DD6	C10-C11	25.57	1.69	1.35
13	7	301	DD6	C10-C11	25.53	1.69	1.35
13	7	316	DD6	C10-C11	25.50	1.69	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	16	313	DD6	C10-C11	25.39	1.69	1.35
13	6	315	DD6	C10-C11	25.26	1.69	1.35
13	12	315	DD6	C10-C11	25.22	1.69	1.35
13	8	317	DD6	C10-C11	24.99	1.68	1.35
13	6	318	DD6	C10-C11	24.90	1.68	1.35
13	6	316	DD6	C10-C11	24.88	1.68	1.35
13	7	313	DD6	C10-C11	24.85	1.68	1.35
13	8	316	DD6	C10-C11	24.78	1.68	1.35
13	6	316	DD6	C5-C6	18.43	1.60	1.35
13	7	316	DD6	C5-C6	17.75	1.59	1.35
13	10	313	DD6	C5-C6	17.64	1.59	1.35
13	16	313	DD6	C5-C6	17.63	1.59	1.35
13	7	317	DD6	C5-C6	17.57	1.59	1.35
13	13	314	DD6	C5-C6	17.57	1.59	1.35
13	12	317	DD6	C5-C6	17.44	1.58	1.35
13	7	301	DD6	C5-C6	17.40	1.58	1.35
13	8	316	DD6	C5-C6	17.39	1.58	1.35
13	6	315	DD6	C5-C6	17.34	1.58	1.35
13	10	314	DD6	C5-C6	17.27	1.58	1.35
13	15	318	DD6	C5-C6	17.16	1.58	1.35
13	15	319	DD6	C5-C6	17.13	1.58	1.35
13	11	312	DD6	C5-C6	17.07	1.58	1.35
13	8	317	DD6	C5-C6	17.05	1.58	1.35
13	7	313	DD6	C5-C6	16.97	1.58	1.35
13	6	318	DD6	C5-C6	16.96	1.58	1.35
13	12	315	DD6	C5-C6	16.94	1.58	1.35
14	15	322	A86	C14-C13	15.11	1.69	1.51
14	10	317	A86	C14-C13	14.83	1.69	1.51
14	15	315	A86	C14-C13	14.63	1.68	1.51
14	16	314	A86	C14-C13	14.49	1.68	1.51
14	15	320	A86	C14-C13	14.37	1.68	1.51
14	14	320	A86	C14-C13	14.21	1.68	1.51
14	15	321	A86	C14-C13	14.21	1.68	1.51
14	10	315	A86	C14-C13	14.18	1.68	1.51
14	11	314	A86	C14-C13	14.15	1.68	1.51
14	7	318	A86	C14-C13	14.11	1.68	1.51
14	14	301	A86	C14-C13	14.10	1.68	1.51
14	13	315	A86	C14-C13	14.09	1.68	1.51
13	15	319	DD6	C36-C31	14.05	1.50	1.34
13	8	317	DD6	C36-C31	13.94	1.50	1.34
14	14	318	A86	C14-C13	13.92	1.68	1.51
14	15	317	A86	C14-C13	13.90	1.68	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	14	321	A86	C14-C13	13.86	1.68	1.51
14	11	313	A86	C14-C13	13.78	1.67	1.51
14	15	316	A86	C14-C13	13.78	1.67	1.51
14	10	316	A86	C14-C13	13.73	1.67	1.51
14	14	316	A86	C14-C13	13.69	1.67	1.51
14	14	319	A86	C14-C13	13.68	1.67	1.51
14	14	315	A86	C14-C13	13.62	1.67	1.51
13	13	314	DD6	C36-C31	13.61	1.50	1.34
13	6	318	DD6	C36-C31	13.61	1.50	1.34
14	10	302	A86	C14-C13	13.61	1.67	1.51
13	7	301	DD6	C36-C31	13.59	1.50	1.34
14	12	314	A86	C14-C13	13.57	1.67	1.51
14	8	318	A86	C14-C13	13.57	1.67	1.51
13	6	316	DD6	C36-C31	13.55	1.50	1.34
14	14	314	A86	C14-C13	13.55	1.67	1.51
14	14	317	A86	C14-C13	13.55	1.67	1.51
13	7	316	DD6	C36-C31	13.54	1.50	1.34
13	7	317	DD6	C36-C31	13.49	1.50	1.34
14	12	316	A86	C14-C13	13.49	1.67	1.51
13	16	313	DD6	C36-C31	13.48	1.49	1.34
14	16	312	A86	C14-C13	13.47	1.67	1.51
14	13	313	A86	C14-C13	13.45	1.67	1.51
14	10	301	A86	C14-C13	13.44	1.67	1.51
14	11	315	A86	C14-C13	13.37	1.67	1.51
14	7	315	A86	C14-C13	13.28	1.67	1.51
14	6	317	A86	C14-C13	13.26	1.67	1.51
14	7	314	A86	C14-C13	13.25	1.67	1.51
14	11	301	A86	C14-C13	13.24	1.67	1.51
13	15	318	DD6	C36-C31	13.21	1.49	1.34
13	7	313	DD6	C36-C31	13.18	1.49	1.34
13	11	312	DD6	C36-C31	13.17	1.49	1.34
13	10	313	DD6	C36-C31	13.17	1.49	1.34
13	12	315	DD6	C36-C31	13.16	1.49	1.34
13	8	316	DD6	C36-C31	13.13	1.49	1.34
13	12	317	DD6	C36-C31	13.02	1.49	1.34
13	6	315	DD6	C36-C31	13.01	1.49	1.34
13	10	314	DD6	C36-C31	12.91	1.49	1.34
14	8	315	A86	C14-C13	12.35	1.66	1.51
12	13	312	KC1	C1D-ND	10.13	1.44	1.35
12	13	311	KC1	C1D-ND	10.04	1.44	1.35
12	16	304	KC1	C1D-ND	9.96	1.44	1.35
12	11	306	KC1	C1D-ND	9.87	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	12	313	KC1	C1D-ND	9.86	1.44	1.35
12	14	311	KC1	C1D-ND	9.75	1.43	1.35
12	13	308	KC1	C1D-ND	9.71	1.43	1.35
12	10	310	KC1	C1D-ND	9.70	1.43	1.35
12	6	309	KC1	C1D-ND	9.66	1.43	1.35
12	16	311	KC1	C1D-ND	9.65	1.43	1.35
12	14	308	KC1	C1D-ND	9.63	1.43	1.35
12	11	304	KC1	C1D-ND	9.62	1.43	1.35
12	11	311	KC1	C1D-ND	9.59	1.43	1.35
12	11	310	KC1	C1D-ND	9.58	1.43	1.35
12	13	306	KC1	C1D-ND	9.57	1.43	1.35
12	13	310	KC1	C1D-ND	9.55	1.43	1.35
12	12	309	KC1	C1D-ND	9.55	1.43	1.35
12	10	306	KC1	C1D-ND	9.54	1.43	1.35
12	12	305	KC1	C1D-ND	9.51	1.43	1.35
12	13	305	KC1	C1D-ND	9.51	1.43	1.35
12	6	310	KC1	C1D-ND	9.51	1.43	1.35
12	7	307	KC1	C1D-ND	9.49	1.43	1.35
12	10	312	KC1	C1D-ND	9.46	1.43	1.35
12	12	311	KC1	C1D-ND	9.45	1.43	1.35
12	8	314	KC1	C1D-ND	9.41	1.43	1.35
12	8	312	KC1	C1D-ND	9.37	1.43	1.35
12	6	308	KC1	C1D-ND	9.36	1.43	1.35
12	7	312	KC1	C1D-ND	9.36	1.43	1.35
14	15	320	A86	C30-C29	9.30	1.47	1.32
14	15	317	A86	C30-C29	9.29	1.47	1.32
14	15	322	A86	C30-C29	9.26	1.47	1.32
12	8	310	KC1	C1D-ND	9.26	1.43	1.35
12	14	306	KC1	C1D-ND	9.25	1.43	1.35
12	8	307	KC1	C1D-ND	9.21	1.43	1.35
14	15	315	A86	C30-C29	9.21	1.47	1.32
14	13	313	A86	C30-C29	9.21	1.47	1.32
12	8	306	KC1	C1D-ND	9.19	1.43	1.35
14	14	321	A86	C30-C29	9.18	1.47	1.32
14	10	317	A86	C30-C29	9.14	1.47	1.32
14	10	302	A86	C30-C29	9.13	1.47	1.32
14	10	315	A86	C30-C29	9.13	1.47	1.32
14	6	317	A86	C30-C29	9.12	1.47	1.32
14	13	315	A86	C30-C29	9.12	1.47	1.32
12	8	313	KC1	C1D-ND	9.10	1.43	1.35
12	6	305	KC1	C1D-ND	9.09	1.43	1.35
14	14	317	A86	C30-C29	9.08	1.47	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	8	311	KC1	C1D-ND	9.06	1.43	1.35
14	14	320	A86	C30-C29	9.03	1.47	1.32
14	12	316	A86	C30-C29	9.00	1.47	1.32
14	16	312	A86	C30-C29	8.97	1.46	1.32
14	14	316	A86	C30-C29	8.96	1.46	1.32
14	14	318	A86	C30-C29	8.95	1.46	1.32
14	7	318	A86	C30-C29	8.94	1.46	1.32
13	12	315	DD6	C23-C16	8.94	1.71	1.53
14	14	314	A86	C30-C29	8.93	1.46	1.32
13	15	319	DD6	C23-C16	8.90	1.71	1.53
14	14	301	A86	C30-C29	8.89	1.46	1.32
14	15	316	A86	C30-C29	8.84	1.46	1.32
14	15	321	A86	C30-C29	8.74	1.46	1.32
14	11	315	A86	C30-C29	8.73	1.46	1.32
14	16	314	A86	C30-C29	8.71	1.46	1.32
14	11	301	A86	C30-C29	8.68	1.46	1.32
14	14	319	A86	C30-C29	8.67	1.46	1.32
13	10	313	DD6	C23-C16	8.67	1.70	1.53
14	11	314	A86	C30-C29	8.66	1.46	1.32
14	8	318	A86	C30-C29	8.63	1.46	1.32
13	8	317	DD6	C13-C11	-8.57	1.27	1.45
14	11	313	A86	C30-C29	8.56	1.46	1.32
13	15	318	DD6	C23-C16	8.56	1.70	1.53
14	10	316	A86	C30-C29	8.55	1.46	1.32
14	10	301	A86	C30-C29	8.52	1.46	1.32
14	12	314	A86	C30-C29	8.50	1.46	1.32
13	16	313	DD6	C13-C11	-8.48	1.27	1.45
14	14	315	A86	C30-C29	8.47	1.46	1.32
13	12	315	DD6	C13-C11	-8.47	1.27	1.45
13	7	317	DD6	C13-C11	-8.45	1.27	1.45
13	12	317	DD6	C13-C11	-8.42	1.27	1.45
13	15	319	DD6	C13-C11	-8.41	1.27	1.45
13	7	316	DD6	C13-C11	-8.39	1.27	1.45
13	6	315	DD6	C13-C11	-8.34	1.28	1.45
13	6	315	DD6	C23-C16	8.30	1.70	1.53
13	11	312	DD6	C23-C16	8.30	1.70	1.53
13	12	317	DD6	C19-C20	8.29	1.63	1.52
13	13	314	DD6	C23-C16	8.29	1.70	1.53
13	15	318	DD6	C13-C11	-8.28	1.28	1.45
13	6	318	DD6	C13-C11	-8.25	1.28	1.45
13	10	313	DD6	C13-C11	-8.25	1.28	1.45
13	7	301	DD6	C2-C1	8.24	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	7	317	DD6	C23-C16	8.23	1.69	1.53
13	15	318	DD6	C2-C1	8.23	1.46	1.35
14	8	315	A86	C30-C29	8.22	1.45	1.32
13	10	314	DD6	C13-C11	-8.20	1.28	1.45
14	7	315	A86	C30-C29	8.20	1.45	1.32
13	8	317	DD6	C23-C16	8.19	1.69	1.53
13	11	312	DD6	C13-C11	-8.19	1.28	1.45
13	13	314	DD6	C19-C20	8.17	1.63	1.52
13	7	316	DD6	C23-C16	8.15	1.69	1.53
13	11	312	DD6	C19-C20	8.14	1.63	1.52
13	7	313	DD6	C23-C16	8.13	1.69	1.53
13	6	316	DD6	C2-C1	8.11	1.46	1.35
13	7	313	DD6	C13-C11	-8.11	1.28	1.45
13	7	301	DD6	C19-C20	8.07	1.63	1.52
14	7	314	A86	C30-C29	8.04	1.45	1.32
13	6	316	DD6	C13-C11	-8.02	1.28	1.45
13	6	315	DD6	C19-C20	8.02	1.63	1.52
13	12	317	DD6	C23-C16	8.01	1.69	1.53
13	6	318	DD6	C23-C16	8.01	1.69	1.53
13	7	313	DD6	C19-C20	7.99	1.63	1.52
13	10	313	DD6	C2-C1	7.99	1.46	1.35
13	13	314	DD6	C2-C1	7.96	1.46	1.35
14	10	302	A86	C8-C6	7.95	1.63	1.45
13	8	316	DD6	C23-C16	7.92	1.69	1.53
13	13	314	DD6	C13-C11	-7.91	1.28	1.45
13	11	312	DD6	C2-C1	7.89	1.46	1.35
13	7	301	DD6	C13-C11	-7.89	1.29	1.45
13	6	315	DD6	C2-C1	7.89	1.46	1.35
13	7	317	DD6	C19-C20	7.89	1.63	1.52
13	16	313	DD6	C2-C1	7.88	1.46	1.35
14	13	313	A86	C4-C5	7.87	1.67	1.43
13	12	317	DD6	C2-C1	7.86	1.46	1.35
14	15	315	A86	C4-C5	7.83	1.67	1.43
13	10	313	DD6	C19-C20	7.83	1.63	1.52
14	14	314	A86	C4-C5	7.81	1.67	1.43
13	16	313	DD6	C21-C20	-7.77	1.39	1.51
13	7	316	DD6	C19-C20	7.76	1.63	1.52
13	7	301	DD6	C23-C16	7.74	1.68	1.53
14	11	301	A86	C8-C6	7.74	1.62	1.45
12	16	311	KC1	C2A-C3A	7.73	1.52	1.37
13	11	312	DD6	C9-C10	7.72	1.67	1.43
13	10	314	DD6	C2-C1	7.72	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	11	311	KC1	C2A-C3A	7.71	1.52	1.37
13	10	314	DD6	C19-C20	7.70	1.63	1.52
13	10	314	DD6	C23-C16	7.69	1.68	1.53
14	15	315	A86	C8-C6	7.69	1.62	1.45
13	12	317	DD6	C9-C10	7.68	1.67	1.43
14	15	322	A86	C4-C5	7.68	1.67	1.43
14	14	320	A86	C4-C5	7.67	1.67	1.43
13	7	317	DD6	C2-C1	7.67	1.45	1.35
14	8	318	A86	C4-C5	7.66	1.67	1.43
14	15	320	A86	C4-C5	7.65	1.67	1.43
13	6	316	DD6	C19-C20	7.65	1.63	1.52
14	15	320	A86	C8-C6	7.64	1.62	1.45
13	8	317	DD6	C2-C1	7.64	1.45	1.35
13	16	313	DD6	C19-C20	7.63	1.62	1.52
13	15	319	DD6	C2-C1	7.62	1.45	1.35
13	7	316	DD6	C2-C1	7.62	1.45	1.35
13	15	318	DD6	C19-C20	7.62	1.62	1.52
13	7	301	DD6	C9-C10	7.61	1.67	1.43
13	16	313	DD6	C9-C10	7.61	1.67	1.43
13	7	313	DD6	C2-C1	7.60	1.45	1.35
14	13	315	A86	C4-C5	7.60	1.67	1.43
13	8	316	DD6	C13-C11	-7.60	1.29	1.45
13	8	316	DD6	C2-C1	7.60	1.45	1.35
13	6	316	DD6	C9-C10	7.58	1.66	1.43
13	15	319	DD6	C19-C20	7.58	1.62	1.52
13	7	316	DD6	C9-C10	7.57	1.66	1.43
13	13	314	DD6	C9-C10	7.57	1.66	1.43
14	14	319	A86	C4-C5	7.57	1.66	1.43
14	15	317	A86	C4-C5	7.57	1.66	1.43
14	15	316	A86	C4-C5	7.56	1.66	1.43
12	8	314	KC1	C2A-C3A	7.56	1.52	1.37
13	6	316	DD6	C23-C16	7.55	1.68	1.53
13	7	317	DD6	C9-C10	7.54	1.66	1.43
14	14	321	A86	C4-C5	7.53	1.66	1.43
12	14	308	KC1	C2A-C3A	7.53	1.52	1.37
12	13	310	KC1	C2A-C3A	7.53	1.52	1.37
14	16	312	A86	C4-C5	7.52	1.66	1.43
13	15	318	DD6	C9-C10	7.51	1.66	1.43
14	10	315	A86	C4-C5	7.50	1.66	1.43
13	10	313	DD6	C9-C10	7.50	1.66	1.43
14	10	317	A86	C4-C5	7.49	1.66	1.43
13	15	319	DD6	C9-C10	7.49	1.66	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	14	318	A86	C4-C5	7.49	1.66	1.43
14	14	314	A86	C8-C6	7.48	1.62	1.45
14	13	315	A86	C8-C6	7.48	1.62	1.45
13	6	315	DD6	C9-C10	7.48	1.66	1.43
14	14	317	A86	C4-C5	7.48	1.66	1.43
13	16	313	DD6	C23-C16	7.46	1.68	1.53
13	12	315	DD6	C9-C10	7.46	1.66	1.43
14	13	313	A86	C8-C6	7.46	1.62	1.45
13	8	317	DD6	C19-C20	7.45	1.62	1.52
12	8	306	KC1	C2A-C3A	7.45	1.52	1.37
12	14	311	KC1	C2A-C3A	7.45	1.52	1.37
14	12	316	A86	C4-C5	7.45	1.66	1.43
12	16	304	KC1	C2A-C3A	7.44	1.52	1.37
14	14	321	A86	C8-C6	7.44	1.61	1.45
13	10	314	DD6	C9-C10	7.42	1.66	1.43
13	8	316	DD6	C9-C10	7.42	1.66	1.43
14	10	302	A86	C4-C5	7.40	1.66	1.43
14	6	317	A86	C4-C5	7.40	1.66	1.43
14	16	314	A86	C19-C20	7.40	1.62	1.52
14	15	322	A86	C8-C6	7.39	1.61	1.45
13	12	315	DD6	C2-C1	7.39	1.45	1.35
14	14	319	A86	C8-C6	7.39	1.61	1.45
14	11	313	A86	C4-C5	7.38	1.66	1.43
13	6	318	DD6	C9-C10	7.37	1.66	1.43
14	12	314	A86	C4-C5	7.37	1.66	1.43
14	14	301	A86	C4-C5	7.37	1.66	1.43
12	7	307	KC1	C2A-C3A	7.36	1.52	1.37
13	8	317	DD6	C9-C10	7.36	1.66	1.43
14	14	315	A86	C4-C5	7.35	1.66	1.43
14	15	317	A86	C8-C6	7.35	1.61	1.45
14	14	320	A86	C8-C6	7.35	1.61	1.45
12	12	309	KC1	C2A-C3A	7.35	1.52	1.37
12	13	312	KC1	C2A-C3A	7.34	1.52	1.37
14	16	314	A86	C4-C5	7.31	1.66	1.43
14	15	321	A86	C19-C20	7.30	1.62	1.52
14	15	321	A86	C4-C5	7.30	1.66	1.43
14	14	316	A86	C4-C5	7.29	1.66	1.43
12	12	305	KC1	C2A-C3A	7.29	1.52	1.37
14	10	315	A86	C8-C6	7.29	1.61	1.45
12	11	310	KC1	C2A-C3A	7.28	1.52	1.37
14	11	314	A86	C4-C5	7.26	1.65	1.43
12	13	308	KC1	C2A-C3A	7.26	1.52	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	13	315	A86	C19-C20	7.25	1.62	1.52
12	14	306	KC1	C2A-C3A	7.25	1.52	1.37
13	7	313	DD6	C9-C10	7.25	1.65	1.43
14	11	315	A86	C4-C5	7.25	1.65	1.43
12	11	306	KC1	C2A-C3A	7.24	1.51	1.37
14	11	301	A86	C4-C5	7.24	1.65	1.43
14	10	317	A86	C8-C6	7.22	1.61	1.45
14	7	314	A86	C4-C5	7.22	1.65	1.43
14	7	318	A86	C8-C6	7.22	1.61	1.45
14	14	321	A86	C19-C20	7.21	1.62	1.52
13	6	318	DD6	C2-C1	7.21	1.45	1.35
14	15	316	A86	C8-C6	7.19	1.61	1.45
14	12	316	A86	C8-C6	7.19	1.61	1.45
14	14	318	A86	C8-C6	7.19	1.61	1.45
14	7	318	A86	C4-C5	7.19	1.65	1.43
14	14	318	A86	C19-C20	7.18	1.62	1.52
14	10	316	A86	C4-C5	7.17	1.65	1.43
14	16	314	A86	C8-C6	7.17	1.61	1.45
12	12	311	KC1	C2A-C3A	7.17	1.51	1.37
14	14	319	A86	C19-C20	7.15	1.62	1.52
14	6	317	A86	C8-C6	7.15	1.61	1.45
13	7	301	DD6	C24-C1	7.15	1.61	1.45
14	14	317	A86	C8-C6	7.14	1.61	1.45
12	8	312	KC1	C2A-C3A	7.13	1.51	1.37
14	16	312	A86	C8-C6	7.13	1.61	1.45
14	13	313	A86	C19-C20	7.12	1.62	1.52
12	10	310	KC1	C2A-C3A	7.10	1.51	1.37
13	6	318	DD6	C19-C20	7.10	1.62	1.52
12	8	311	KC1	C2A-C3A	7.09	1.51	1.37
14	15	321	A86	C8-C6	7.09	1.61	1.45
14	13	313	A86	C25-C26	7.09	1.65	1.43
14	11	313	A86	C8-C6	7.08	1.61	1.45
14	10	317	A86	C19-C20	7.07	1.62	1.52
14	14	301	A86	C8-C6	7.06	1.61	1.45
12	6	308	KC1	C2A-C3A	7.05	1.51	1.37
12	13	311	KC1	C2A-C3A	7.05	1.51	1.37
12	6	309	KC1	C2A-C3A	7.04	1.51	1.37
14	15	320	A86	C19-C20	7.04	1.62	1.52
12	8	310	KC1	C2A-C3A	7.03	1.51	1.37
13	15	319	DD6	C24-C1	7.02	1.61	1.45
13	12	317	DD6	C24-C1	7.01	1.61	1.45
14	14	315	A86	C19-C20	7.00	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	11	313	A86	C19-C20	6.99	1.62	1.52
14	15	317	A86	C19-C20	6.99	1.62	1.52
12	6	305	KC1	C2A-C3A	6.99	1.51	1.37
12	6	310	KC1	C2A-C3A	6.99	1.51	1.37
13	7	316	DD6	C24-C1	6.99	1.61	1.45
12	13	305	KC1	C2A-C3A	6.99	1.51	1.37
13	12	315	DD6	C21-C20	-6.98	1.40	1.51
14	14	315	A86	C8-C6	6.98	1.60	1.45
14	15	322	A86	C19-C20	6.98	1.62	1.52
14	15	317	A86	C25-C26	6.97	1.65	1.43
14	14	314	A86	C19-C20	6.97	1.62	1.52
14	10	301	A86	C4-C5	6.97	1.65	1.43
14	15	320	A86	C25-C26	6.97	1.65	1.43
14	14	316	A86	C8-C6	6.96	1.60	1.45
14	11	314	A86	C8-C6	6.96	1.60	1.45
14	14	321	A86	C25-C26	6.96	1.65	1.43
13	6	316	DD6	C24-C1	6.96	1.60	1.45
14	10	316	A86	C8-C6	6.96	1.60	1.45
13	8	316	DD6	C19-C20	6.94	1.61	1.52
13	8	316	DD6	C21-C20	-6.94	1.41	1.51
14	15	316	A86	C25-C26	6.94	1.64	1.43
13	8	317	DD6	C24-C1	6.94	1.60	1.45
13	15	318	DD6	C24-C1	6.93	1.60	1.45
14	10	302	A86	C25-C26	6.93	1.64	1.43
13	7	301	DD6	C21-C20	-6.92	1.41	1.51
12	7	312	KC1	C2A-C3A	6.91	1.51	1.37
12	10	312	KC1	C2A-C3A	6.91	1.51	1.37
13	6	315	DD6	C24-C1	6.90	1.60	1.45
14	11	314	A86	C19-C20	6.90	1.61	1.52
13	15	318	DD6	C30-C29	6.90	1.40	1.20
12	13	305	KC1	CBA-CAA	6.89	1.53	1.33
14	7	315	A86	C4-C5	6.89	1.64	1.43
14	11	315	A86	C8-C6	6.89	1.60	1.45
13	15	319	DD6	C30-C29	6.89	1.40	1.20
13	16	313	DD6	C24-C1	6.89	1.60	1.45
12	12	311	KC1	CBA-CAA	6.89	1.53	1.33
12	11	304	KC1	C2A-C3A	6.88	1.51	1.37
13	12	315	DD6	C24-C1	6.88	1.60	1.45
12	13	306	KC1	C2A-C3A	6.87	1.51	1.37
13	12	315	DD6	C19-C20	6.86	1.61	1.52
13	6	318	DD6	C24-C1	6.86	1.60	1.45
14	6	317	A86	C25-C26	6.86	1.64	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	7	313	DD6	C24-C1	6.85	1.60	1.45
14	10	315	A86	C25-C26	6.85	1.64	1.43
14	16	312	A86	C19-C20	6.85	1.61	1.52
14	12	316	A86	C25-C26	6.85	1.64	1.43
14	15	316	A86	C19-C20	6.84	1.61	1.52
13	8	316	DD6	C24-C1	6.83	1.60	1.45
14	12	314	A86	C8-C6	6.83	1.60	1.45
14	13	315	A86	C25-C26	6.83	1.64	1.43
14	15	315	A86	C25-C26	6.83	1.64	1.43
14	15	321	A86	C25-C26	6.82	1.64	1.43
14	8	315	A86	C4-C5	6.82	1.64	1.43
14	14	317	A86	C25-C26	6.82	1.64	1.43
13	7	317	DD6	C24-C1	6.82	1.60	1.45
14	14	317	A86	C19-C20	6.81	1.61	1.52
14	10	317	A86	C25-C26	6.81	1.64	1.43
14	8	318	A86	C19-C20	6.80	1.61	1.52
14	15	315	A86	C19-C20	6.80	1.61	1.52
14	15	322	A86	C25-C26	6.79	1.64	1.43
14	11	301	A86	C19-C20	6.79	1.61	1.52
14	11	315	A86	C19-C20	6.78	1.61	1.52
14	10	315	A86	C19-C20	6.78	1.61	1.52
13	10	313	DD6	C24-C1	6.78	1.60	1.45
14	7	314	A86	C8-C6	6.77	1.60	1.45
13	7	301	DD6	C30-C29	6.77	1.40	1.20
13	7	317	DD6	C30-C29	6.77	1.40	1.20
14	8	318	A86	C8-C6	6.77	1.60	1.45
12	8	307	KC1	C2A-C3A	6.76	1.51	1.37
12	10	306	KC1	C2A-C3A	6.76	1.51	1.37
13	16	313	DD6	C30-C29	6.76	1.40	1.20
14	14	320	A86	C25-C26	6.75	1.64	1.43
14	14	301	A86	C19-C20	6.74	1.61	1.52
13	8	317	DD6	C30-C29	6.74	1.39	1.20
14	14	318	A86	C25-C26	6.74	1.64	1.43
13	13	314	DD6	C30-C29	6.73	1.39	1.20
14	11	315	A86	C25-C26	6.72	1.64	1.43
12	8	311	KC1	CBA-CAA	6.72	1.53	1.33
13	13	314	DD6	C24-C1	6.71	1.60	1.45
14	14	301	A86	C25-C26	6.70	1.64	1.43
13	11	312	DD6	C24-C1	6.70	1.60	1.45
12	14	308	KC1	CBA-CAA	6.69	1.53	1.33
12	8	313	KC1	C2A-C3A	6.69	1.50	1.37
14	14	319	A86	C25-C26	6.68	1.64	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	11	310	KC1	CBA-CAA	6.67	1.53	1.33
14	14	316	A86	C25-C26	6.67	1.64	1.43
14	7	318	A86	C25-C26	6.67	1.64	1.43
13	7	316	DD6	C30-C29	6.67	1.39	1.20
12	12	313	KC1	C2A-C3A	6.67	1.50	1.37
12	13	306	KC1	CBA-CAA	6.67	1.53	1.33
12	12	305	KC1	CBA-CAA	6.66	1.53	1.33
13	10	314	DD6	C24-C1	6.66	1.60	1.45
14	12	316	A86	C19-C20	6.66	1.61	1.52
12	13	310	KC1	CBA-CAA	6.65	1.53	1.33
13	6	316	DD6	C30-C29	6.65	1.39	1.20
12	6	305	KC1	CBA-CAA	6.65	1.53	1.33
14	12	314	A86	C19-C20	6.65	1.61	1.52
14	14	314	A86	C25-C26	6.64	1.64	1.43
14	16	312	A86	C25-C26	6.64	1.64	1.43
12	11	311	KC1	CBA-CAA	6.64	1.53	1.33
13	10	313	DD6	C30-C29	6.64	1.39	1.20
12	14	306	KC1	CBA-CAA	6.61	1.53	1.33
12	8	312	KC1	CBA-CAA	6.61	1.53	1.33
12	16	304	KC1	CBA-CAA	6.61	1.53	1.33
14	7	314	A86	C25-C26	6.60	1.63	1.43
14	11	314	A86	C25-C26	6.60	1.63	1.43
12	6	308	KC1	CBA-CAA	6.59	1.53	1.33
12	7	312	KC1	CBA-CAA	6.59	1.53	1.33
14	11	313	A86	C25-C26	6.59	1.63	1.43
12	13	311	KC1	CBA-CAA	6.59	1.53	1.33
13	8	316	DD6	C30-C29	6.59	1.39	1.20
14	10	301	A86	C8-C6	6.58	1.60	1.45
14	10	316	A86	C19-C20	6.58	1.61	1.52
12	11	306	KC1	CBA-CAA	6.57	1.52	1.33
12	10	312	KC1	CBA-CAA	6.57	1.52	1.33
14	16	314	A86	C25-C26	6.56	1.63	1.43
12	13	308	KC1	CBA-CAA	6.55	1.52	1.33
13	7	313	DD6	C30-C29	6.55	1.39	1.20
14	10	316	A86	C25-C26	6.54	1.63	1.43
14	14	315	A86	C25-C26	6.54	1.63	1.43
14	12	314	A86	C25-C26	6.54	1.63	1.43
13	11	312	DD6	C30-C29	6.54	1.39	1.20
12	8	307	KC1	CBA-CAA	6.54	1.52	1.33
14	10	301	A86	C25-C26	6.53	1.63	1.43
12	12	309	KC1	CBA-CAA	6.52	1.52	1.33
13	12	317	DD6	C30-C29	6.52	1.39	1.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	14	311	KC1	CBA-CAA	6.52	1.52	1.33
12	6	309	KC1	CBA-CAA	6.52	1.52	1.33
13	7	316	DD6	C21-C20	-6.51	1.41	1.51
12	10	306	KC1	CBA-CAA	6.51	1.52	1.33
11	15	310	CLA	C3B-C2B	6.50	1.49	1.40
12	16	311	KC1	CBA-CAA	6.49	1.52	1.33
13	6	318	DD6	C30-C29	6.49	1.39	1.20
13	10	314	DD6	C30-C29	6.49	1.39	1.20
11	12	303	CLA	C3B-C2B	6.49	1.49	1.40
13	6	315	DD6	C30-C29	6.48	1.39	1.20
13	7	317	DD6	C21-C20	-6.48	1.41	1.51
13	12	315	DD6	C30-C29	6.48	1.39	1.20
14	14	316	A86	C19-C20	6.48	1.61	1.52
12	12	313	KC1	CBA-CAA	6.48	1.52	1.33
14	8	318	A86	C25-C26	6.47	1.63	1.43
12	10	310	KC1	CBA-CAA	6.47	1.52	1.33
14	7	315	A86	C8-C6	6.47	1.59	1.45
13	6	316	DD6	C21-C20	-6.47	1.41	1.51
14	11	301	A86	C25-C26	6.46	1.63	1.43
12	13	312	KC1	CBA-CAA	6.46	1.52	1.33
12	7	307	KC1	CBA-CAA	6.45	1.52	1.33
14	10	302	A86	C19-C20	6.44	1.61	1.52
12	8	313	KC1	CBA-CAA	6.43	1.52	1.33
13	7	313	DD6	C21-C20	-6.41	1.41	1.51
12	8	310	KC1	CBA-CAA	6.40	1.52	1.33
12	11	304	KC1	CBA-CAA	6.40	1.52	1.33
13	10	314	DD6	C21-C20	-6.36	1.41	1.51
11	8	302	CLA	C3B-C2B	6.34	1.49	1.40
13	15	318	DD6	C21-C20	-6.34	1.41	1.51
14	8	315	A86	C8-C6	6.33	1.59	1.45
13	15	318	DD6	C30-C31	6.33	1.55	1.42
13	15	319	DD6	C21-C20	-6.33	1.41	1.51
14	7	315	A86	C19-C20	6.33	1.61	1.52
13	16	313	DD6	C13-C14	6.31	1.46	1.32
11	8	305	CLA	C3B-C2B	6.29	1.49	1.40
12	8	306	KC1	CBA-CAA	6.29	1.52	1.33
14	14	320	A86	C19-C20	6.28	1.61	1.52
13	7	313	DD6	C13-C14	6.27	1.46	1.32
12	6	310	KC1	CBA-CAA	6.27	1.52	1.33
12	8	314	KC1	CBA-CAA	6.27	1.52	1.33
11	8	301	CLA	C3B-C2B	6.27	1.49	1.40
13	6	315	DD6	C21-C20	-6.26	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	7	318	A86	C19-C20	6.26	1.61	1.52
11	7	304	CLA	OBD-CAD	6.26	1.33	1.22
14	8	315	A86	C25-C26	6.25	1.62	1.43
13	8	317	DD6	C21-C20	-6.24	1.42	1.51
14	7	315	A86	C25-C26	6.23	1.62	1.43
12	12	313	KC1	C4A-C3A	6.22	1.56	1.44
14	8	315	A86	C19-C20	6.21	1.60	1.52
13	11	312	DD6	C21-C20	-6.20	1.42	1.51
13	15	319	DD6	C30-C31	6.18	1.55	1.42
13	8	316	DD6	C13-C14	6.16	1.46	1.32
11	7	304	CLA	C3B-C2B	6.11	1.48	1.40
13	6	318	DD6	C21-C20	-6.10	1.42	1.51
13	7	301	DD6	C30-C31	6.10	1.55	1.42
13	16	313	DD6	C30-C31	6.09	1.55	1.42
13	10	313	DD6	C21-C20	-6.05	1.42	1.51
13	8	317	DD6	C30-C31	6.04	1.55	1.42
14	7	314	A86	C19-C20	6.04	1.60	1.52
11	6	302	CLA	C3B-C2B	6.04	1.48	1.40
13	13	314	DD6	C13-C14	6.03	1.45	1.32
11	15	309	CLA	C3B-C2B	6.03	1.48	1.40
13	10	313	DD6	C13-C14	5.98	1.45	1.32
12	13	305	KC1	O2A-CGA	5.98	1.45	1.30
11	15	306	CLA	C3B-C2B	5.97	1.48	1.40
12	8	310	KC1	O2A-CGA	5.97	1.45	1.30
13	13	314	DD6	C30-C31	5.97	1.55	1.42
13	10	313	DD6	C30-C31	5.95	1.54	1.42
12	6	305	KC1	O2A-CGA	5.95	1.45	1.30
12	8	313	KC1	O2A-CGA	5.94	1.45	1.30
11	13	307	CLA	C3B-C2B	5.94	1.48	1.40
12	16	311	KC1	O2A-CGA	5.93	1.45	1.30
11	12	304	CLA	C3B-C2B	5.93	1.48	1.40
12	12	311	KC1	O2A-CGA	5.93	1.45	1.30
12	10	306	KC1	O2A-CGA	5.93	1.45	1.30
12	14	311	KC1	O2A-CGA	5.92	1.45	1.30
12	6	308	KC1	O2A-CGA	5.91	1.45	1.30
12	8	311	KC1	O2A-CGA	5.91	1.45	1.30
13	12	317	DD6	C21-C20	-5.91	1.42	1.51
14	10	301	A86	C19-C20	5.90	1.60	1.52
12	13	312	KC1	O2A-CGA	5.90	1.45	1.30
12	10	312	KC1	O2A-CGA	5.90	1.45	1.30
13	7	317	DD6	C30-C31	5.90	1.54	1.42
11	14	307	CLA	C3B-C2B	5.90	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	12	305	KC1	O2A-CGA	5.90	1.45	1.30
11	11	309	CLA	C3B-C2B	5.89	1.48	1.40
12	10	310	KC1	O2A-CGA	5.89	1.45	1.30
12	13	308	KC1	O2A-CGA	5.89	1.45	1.30
12	11	310	KC1	O2A-CGA	5.88	1.45	1.30
12	16	304	KC1	O2A-CGA	5.87	1.45	1.30
12	11	306	KC1	O2A-CGA	5.87	1.45	1.30
11	10	303	CLA	C3B-C2B	5.87	1.48	1.40
12	11	304	KC1	O2A-CGA	5.86	1.45	1.30
11	10	304	CLA	C3B-C2B	5.86	1.48	1.40
12	14	308	KC1	O2A-CGA	5.86	1.45	1.30
13	6	316	DD6	C30-C31	5.86	1.54	1.42
12	13	306	KC1	O2A-CGA	5.85	1.45	1.30
12	13	310	KC1	O2A-CGA	5.85	1.45	1.30
12	6	310	KC1	O2A-CGA	5.84	1.45	1.30
12	14	306	KC1	O2A-CGA	5.84	1.45	1.30
13	15	318	DD6	C13-C14	5.84	1.45	1.32
12	8	306	KC1	O2A-CGA	5.84	1.45	1.30
13	6	318	DD6	C30-C31	5.83	1.54	1.42
11	14	313	CLA	C3B-C2B	5.83	1.48	1.40
13	13	314	DD6	C21-C20	-5.82	1.42	1.51
13	7	316	DD6	C30-C31	5.82	1.54	1.42
11	15	311	CLA	C3B-C2B	5.82	1.48	1.40
12	13	311	KC1	O2A-CGA	5.82	1.45	1.30
11	13	304	CLA	C3B-C2B	5.81	1.48	1.40
11	6	314	CLA	C3B-C2B	5.81	1.48	1.40
12	8	307	KC1	O2A-CGA	5.80	1.45	1.30
13	12	317	DD6	C13-C14	5.79	1.45	1.32
12	7	307	KC1	O2A-CGA	5.79	1.45	1.30
11	6	312	CLA	C3B-C2B	5.79	1.48	1.40
11	16	307	CLA	C3B-C2B	5.79	1.48	1.40
12	7	312	KC1	O2A-CGA	5.78	1.45	1.30
11	14	309	CLA	C3B-C2B	5.78	1.48	1.40
11	16	309	CLA	C3B-C2B	5.78	1.48	1.40
11	12	308	CLA	C3B-C2B	5.77	1.48	1.40
13	8	316	DD6	C30-C31	5.76	1.54	1.42
12	12	309	KC1	O2A-CGA	5.74	1.45	1.30
13	15	319	DD6	C13-C14	5.74	1.45	1.32
13	12	315	DD6	C30-C31	5.74	1.54	1.42
11	7	305	CLA	C3B-C2B	5.73	1.48	1.40
11	12	302	CLA	C3B-C2B	5.73	1.48	1.40
11	7	311	CLA	C3B-C2B	5.73	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	12	313	KC1	O2A-CGA	5.73	1.45	1.30
12	6	309	KC1	O2A-CGA	5.72	1.45	1.30
11	10	311	CLA	C3B-C2B	5.72	1.48	1.40
12	8	312	KC1	O2A-CGA	5.72	1.45	1.30
11	14	304	CLA	C3B-C2B	5.72	1.48	1.40
11	16	310	CLA	C3B-C2B	5.72	1.48	1.40
11	11	308	CLA	C3B-C2B	5.70	1.48	1.40
11	13	309	CLA	C3B-C2B	5.70	1.48	1.40
11	6	307	CLA	C3B-C2B	5.70	1.48	1.40
14	6	317	A86	C19-C20	5.70	1.60	1.52
11	15	307	CLA	C3B-C2B	5.69	1.48	1.40
12	11	311	KC1	O2A-CGA	5.69	1.45	1.30
11	13	302	CLA	C3B-C2B	5.68	1.48	1.40
11	16	306	CLA	C3B-C2B	5.68	1.48	1.40
11	16	308	CLA	C3B-C2B	5.68	1.48	1.40
11	14	310	CLA	C3B-C2B	5.67	1.48	1.40
11	12	312	CLA	C3B-C2B	5.67	1.48	1.40
11	6	306	CLA	C3B-C2B	5.66	1.48	1.40
11	13	303	CLA	C3B-C2B	5.66	1.48	1.40
12	10	312	KC1	C3B-C2B	5.66	1.48	1.37
12	11	310	KC1	C3B-C2B	5.64	1.48	1.37
11	14	312	CLA	C3B-C2B	5.64	1.48	1.40
13	7	301	DD6	C13-C14	5.63	1.44	1.32
11	11	303	CLA	C3B-C2B	5.63	1.48	1.40
13	7	316	DD6	C13-C14	5.63	1.44	1.32
13	7	317	DD6	C13-C14	5.62	1.44	1.32
13	11	312	DD6	C30-C31	5.62	1.54	1.42
11	6	303	CLA	C3B-C2B	5.62	1.48	1.40
13	6	315	DD6	C30-C31	5.62	1.54	1.42
13	12	317	DD6	C30-C31	5.61	1.54	1.42
12	8	314	KC1	O2A-CGA	5.61	1.45	1.30
11	6	304	CLA	C3B-C2B	5.60	1.48	1.40
13	6	316	DD6	C13-C14	5.60	1.44	1.32
13	10	314	DD6	C30-C31	5.60	1.54	1.42
11	12	321	CLA	C3B-C2B	5.60	1.48	1.40
12	14	308	KC1	C3C-C2C	5.60	1.48	1.36
11	16	305	CLA	C3B-C2B	5.59	1.48	1.40
11	10	309	CLA	C3B-C2B	5.58	1.48	1.40
12	13	312	KC1	C3B-C2B	5.58	1.48	1.37
11	14	303	CLA	C3B-C2B	5.57	1.48	1.40
12	10	310	KC1	C3D-C2D	5.56	1.49	1.39
14	13	313	A86	C26-C27	5.56	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	15	313	CLA	C3B-C2B	5.56	1.48	1.40
11	12	307	CLA	C3B-C2B	5.56	1.48	1.40
11	15	304	CLA	C3B-C2B	5.56	1.48	1.40
11	15	305	CLA	C3B-C2B	5.55	1.48	1.40
14	15	315	A86	C2-C1	5.55	1.43	1.35
12	13	311	KC1	C3D-C2D	5.54	1.49	1.39
11	16	302	CLA	C3B-C2B	5.54	1.48	1.40
11	6	313	CLA	C3B-C2B	5.52	1.48	1.40
12	14	306	KC1	C3D-C2D	5.52	1.49	1.39
11	7	302	CLA	C3B-C2B	5.52	1.48	1.40
13	10	314	DD6	C13-C14	5.51	1.44	1.32
11	15	304	CLA	C3C-C2C	5.50	1.48	1.36
12	13	305	KC1	C3D-C2D	5.49	1.49	1.39
12	13	312	KC1	C3D-C2D	5.49	1.49	1.39
12	13	308	KC1	C3B-C2B	5.48	1.48	1.37
11	15	314	CLA	C3B-C2B	5.47	1.48	1.40
11	12	310	CLA	C3B-C2B	5.47	1.48	1.40
12	13	310	KC1	C3D-C2D	5.46	1.49	1.39
11	14	302	CLA	C3B-C2B	5.46	1.47	1.40
11	8	309	CLA	C3B-C2B	5.46	1.47	1.40
11	15	303	CLA	C3B-C2B	5.46	1.47	1.40
13	7	313	DD6	C30-C31	5.45	1.53	1.42
12	16	304	KC1	C3C-C2C	5.45	1.48	1.36
12	16	311	KC1	C3C-C2C	5.45	1.48	1.36
12	10	312	KC1	C3D-C2D	5.45	1.49	1.39
12	13	308	KC1	C3D-C2D	5.45	1.49	1.39
12	11	310	KC1	C3D-C2D	5.45	1.49	1.39
12	14	308	KC1	C3D-C2D	5.44	1.49	1.39
12	12	305	KC1	C3B-C2B	5.43	1.48	1.37
11	7	309	CLA	C3B-C2B	5.43	1.47	1.40
12	11	304	KC1	C3B-C2B	5.42	1.48	1.37
12	11	306	KC1	C3B-C2B	5.42	1.48	1.37
11	14	305	CLA	C3B-C2B	5.41	1.47	1.40
11	12	306	CLA	C3B-C2B	5.41	1.47	1.40
11	16	303	CLA	C3B-C2B	5.41	1.47	1.40
12	6	305	KC1	C3B-C2B	5.41	1.48	1.37
13	6	315	DD6	C13-C14	5.40	1.44	1.32
11	10	307	CLA	C3B-C2B	5.40	1.47	1.40
12	6	305	KC1	C3D-C2D	5.39	1.49	1.39
12	12	309	KC1	C3B-C2B	5.39	1.48	1.37
11	7	306	CLA	C3B-C2B	5.38	1.47	1.40
12	11	306	KC1	C3D-C2D	5.38	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	11	307	CLA	C3C-C2C	5.38	1.48	1.36
12	13	306	KC1	C3B-C2B	5.38	1.48	1.37
12	14	308	KC1	C3B-C2B	5.38	1.48	1.37
12	8	312	KC1	C3B-C2B	5.37	1.48	1.37
11	8	303	CLA	C3B-C2B	5.37	1.47	1.40
12	12	311	KC1	C3D-C2D	5.37	1.49	1.39
12	16	304	KC1	C3B-C2B	5.37	1.48	1.37
12	6	308	KC1	C3D-C2D	5.37	1.49	1.39
14	10	302	A86	C9-C8	5.37	1.48	1.34
12	12	311	KC1	C3B-C2B	5.37	1.48	1.37
11	11	305	CLA	C3B-C2B	5.36	1.47	1.40
12	13	305	KC1	C3B-C2B	5.36	1.48	1.37
11	15	309	CLA	C3C-C2C	5.36	1.48	1.36
12	13	310	KC1	C3B-C2B	5.35	1.48	1.37
12	6	309	KC1	C3D-C2D	5.35	1.49	1.39
11	13	304	CLA	C3C-C2C	5.34	1.48	1.36
12	6	310	KC1	C3B-C2B	5.34	1.48	1.37
12	7	307	KC1	C3D-C2D	5.34	1.49	1.39
12	8	310	KC1	C3D-C2D	5.34	1.49	1.39
12	6	310	KC1	C3D-C2D	5.33	1.49	1.39
11	15	309	CLA	C1D-ND	5.33	1.44	1.37
11	15	302	CLA	C3B-C2B	5.32	1.47	1.40
11	7	309	CLA	C3C-C2C	5.32	1.48	1.36
11	15	311	CLA	C3C-C2C	5.32	1.48	1.36
12	12	305	KC1	C3D-C2D	5.32	1.49	1.39
12	6	309	KC1	C3B-C2B	5.32	1.48	1.37
11	6	304	CLA	C3C-C2C	5.31	1.48	1.36
11	16	309	CLA	C3C-C2C	5.31	1.48	1.36
13	11	312	DD6	C13-C14	5.31	1.44	1.32
14	15	315	A86	C26-C27	5.31	1.42	1.35
11	13	303	CLA	C3C-C2C	5.31	1.48	1.36
11	15	308	CLA	C3C-C2C	5.30	1.48	1.36
14	15	315	A86	C9-C8	5.30	1.48	1.34
13	6	318	DD6	C13-C14	5.30	1.44	1.32
12	10	310	KC1	C3C-C2C	5.30	1.48	1.36
11	16	301	CLA	C3B-C2B	5.30	1.47	1.40
11	15	310	CLA	C3C-C2C	5.30	1.48	1.36
12	13	308	KC1	C3C-C2C	5.30	1.48	1.36
11	15	312	CLA	C3B-C2B	5.30	1.47	1.40
11	16	303	CLA	C3C-C2C	5.30	1.48	1.36
12	7	307	KC1	C3C-C2C	5.30	1.48	1.36
12	16	311	KC1	C3B-C2B	5.29	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	15	306	CLA	C3C-C2C	5.29	1.48	1.36
12	8	311	KC1	C3C-C2C	5.29	1.48	1.36
11	16	308	CLA	C3C-C2C	5.29	1.48	1.36
11	14	312	CLA	C3C-C2C	5.29	1.48	1.36
12	8	314	KC1	C3D-C2D	5.28	1.48	1.39
11	13	304	CLA	C1D-ND	5.28	1.44	1.37
11	13	309	CLA	O2D-CGD	5.28	1.46	1.33
12	8	314	KC1	C3B-C2B	5.28	1.48	1.37
12	16	304	KC1	C3D-C2D	5.28	1.48	1.39
11	6	303	CLA	C3C-C2C	5.27	1.47	1.36
11	8	302	CLA	C3C-C2C	5.27	1.47	1.36
11	15	312	CLA	C1D-ND	5.27	1.44	1.37
11	6	314	CLA	C1D-ND	5.27	1.44	1.37
11	14	309	CLA	C3C-C2C	5.27	1.47	1.36
11	14	307	CLA	C3C-C2C	5.27	1.47	1.36
12	13	306	KC1	C3D-C2D	5.26	1.48	1.39
11	14	310	CLA	C3C-C2C	5.26	1.47	1.36
11	14	313	CLA	C3C-C2C	5.26	1.47	1.36
11	7	303	CLA	C3B-C2B	5.26	1.47	1.40
11	11	309	CLA	C3C-C2C	5.25	1.47	1.36
11	15	311	CLA	C1D-ND	5.25	1.44	1.37
12	16	311	KC1	C3D-C2D	5.25	1.48	1.39
12	13	312	KC1	O2D-CGD	5.25	1.46	1.33
11	10	309	CLA	C3C-C2C	5.24	1.47	1.36
12	16	304	KC1	CHD-C4C	5.24	1.48	1.35
11	6	312	CLA	C3C-C2C	5.24	1.47	1.36
11	15	312	CLA	C3C-C2C	5.24	1.47	1.36
11	6	312	CLA	C1D-ND	5.24	1.44	1.37
11	16	310	CLA	O2D-CGD	5.24	1.46	1.33
11	7	311	CLA	C3C-C2C	5.24	1.47	1.36
11	16	307	CLA	C3C-C2C	5.24	1.47	1.36
11	15	313	CLA	C3C-C2C	5.24	1.47	1.36
11	15	302	CLA	CHC-C1C	5.24	1.48	1.35
12	11	304	KC1	C3D-C2D	5.24	1.48	1.39
11	8	304	CLA	C3B-C2B	5.24	1.47	1.40
12	6	308	KC1	C3B-C2B	5.24	1.47	1.37
12	8	313	KC1	C3D-C2D	5.24	1.48	1.39
11	13	309	CLA	C3C-C2C	5.23	1.47	1.36
12	11	306	KC1	C3C-C2C	5.23	1.47	1.36
12	13	312	KC1	CHD-C4C	5.23	1.48	1.35
12	7	312	KC1	C3D-C2D	5.23	1.48	1.39
11	7	310	CLA	C3B-C2B	5.23	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	13	305	KC1	C3C-C2C	5.23	1.47	1.36
11	15	303	CLA	C3C-C2C	5.23	1.47	1.36
12	8	313	KC1	C3B-C2B	5.23	1.47	1.37
12	13	306	KC1	O2D-CGD	5.22	1.45	1.33
11	8	308	CLA	C3B-C2B	5.22	1.47	1.40
12	13	312	KC1	C3C-C2C	5.22	1.47	1.36
11	6	314	CLA	C3C-C2C	5.21	1.47	1.36
11	6	307	CLA	C3C-C2C	5.21	1.47	1.36
12	10	310	KC1	C3B-C2B	5.21	1.47	1.37
11	15	302	CLA	C3C-C2C	5.21	1.47	1.36
12	8	307	KC1	C3D-C2D	5.20	1.48	1.39
11	15	305	CLA	C3C-C2C	5.20	1.47	1.36
11	12	310	CLA	C3C-C2C	5.20	1.47	1.36
12	8	314	KC1	C3C-C2C	5.20	1.47	1.36
11	12	307	CLA	CHC-C1C	5.20	1.48	1.35
11	10	308	CLA	C3B-C2B	5.20	1.47	1.40
12	12	309	KC1	C3D-C2D	5.20	1.48	1.39
11	12	304	CLA	C3C-C2C	5.20	1.47	1.36
13	12	315	DD6	C13-C14	5.19	1.43	1.32
11	12	308	CLA	C3C-C2C	5.19	1.47	1.36
12	8	312	KC1	C3C-C2C	5.19	1.47	1.36
11	10	305	CLA	C3C-C2C	5.19	1.47	1.36
11	15	311	CLA	O2D-CGD	5.19	1.45	1.33
11	11	305	CLA	C3C-C2C	5.19	1.47	1.36
11	7	302	CLA	CHC-C1C	5.18	1.48	1.35
11	14	309	CLA	C1D-ND	5.18	1.44	1.37
11	14	305	CLA	C3C-C2C	5.18	1.47	1.36
11	11	309	CLA	C1D-ND	5.18	1.44	1.37
11	11	307	CLA	C3B-C2B	5.18	1.47	1.40
14	15	320	A86	C26-C27	5.18	1.42	1.35
12	7	307	KC1	C3B-C2B	5.18	1.47	1.37
11	11	305	CLA	CHC-C1C	5.18	1.48	1.35
11	15	307	CLA	C3C-C2C	5.17	1.47	1.36
12	13	311	KC1	C3C-C2C	5.17	1.47	1.36
12	11	310	KC1	C3C-C2C	5.17	1.47	1.36
12	13	311	KC1	CHD-C4C	5.17	1.48	1.35
11	14	304	CLA	C3C-C2C	5.17	1.47	1.36
11	15	309	CLA	CHC-C1C	5.17	1.48	1.35
11	12	303	CLA	C3C-C2C	5.17	1.47	1.36
11	10	309	CLA	O2D-CGD	5.17	1.45	1.33
12	11	311	KC1	C3B-C2B	5.17	1.47	1.37
12	14	306	KC1	CHD-C4C	5.17	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	14	304	CLA	O2D-CGD	5.16	1.45	1.33
11	6	314	CLA	O2D-CGD	5.16	1.45	1.33
11	11	303	CLA	CHC-C1C	5.16	1.48	1.35
11	10	308	CLA	CHC-C1C	5.16	1.48	1.35
11	10	311	CLA	C3C-C2C	5.16	1.47	1.36
12	6	308	KC1	C3C-C2C	5.16	1.47	1.36
11	16	309	CLA	C1D-ND	5.16	1.44	1.37
11	13	309	CLA	C1D-ND	5.16	1.44	1.37
11	13	304	CLA	O2D-CGD	5.16	1.45	1.33
11	7	311	CLA	C1D-ND	5.16	1.44	1.37
12	13	310	KC1	C3C-C2C	5.15	1.47	1.36
12	11	311	KC1	CHD-C4C	5.15	1.48	1.35
11	13	302	CLA	C3C-C2C	5.15	1.47	1.36
12	13	308	KC1	CHD-C4C	5.15	1.48	1.35
11	10	305	CLA	C3B-C2B	5.15	1.47	1.40
11	15	310	CLA	O2D-CGD	5.15	1.45	1.33
11	6	313	CLA	C3C-C2C	5.14	1.47	1.36
12	8	307	KC1	C3C-C2C	5.14	1.47	1.36
11	15	310	CLA	C1D-ND	5.14	1.44	1.37
11	14	303	CLA	C3C-C2C	5.14	1.47	1.36
11	15	308	CLA	CHC-C1C	5.14	1.48	1.35
12	13	311	KC1	O2D-CGD	5.14	1.45	1.33
11	8	309	CLA	C3C-C2C	5.14	1.47	1.36
12	12	309	KC1	C3C-C2C	5.13	1.47	1.36
11	13	303	CLA	C1D-ND	5.13	1.44	1.37
11	15	304	CLA	C1D-ND	5.13	1.44	1.37
12	12	313	KC1	C3B-C2B	5.13	1.47	1.37
11	14	309	CLA	O2D-CGD	5.13	1.45	1.33
12	11	304	KC1	C3C-C2C	5.13	1.47	1.36
11	7	306	CLA	CHC-C1C	5.13	1.48	1.35
11	12	321	CLA	C3C-C2C	5.13	1.47	1.36
11	14	302	CLA	CHC-C1C	5.13	1.48	1.35
12	13	311	KC1	C3B-C2B	5.13	1.47	1.37
12	8	312	KC1	C3D-C2D	5.12	1.48	1.39
12	13	308	KC1	O2D-CGD	5.12	1.45	1.33
11	12	312	CLA	C3C-C2C	5.12	1.47	1.36
11	16	306	CLA	C3C-C2C	5.12	1.47	1.36
11	10	307	CLA	C3C-C2C	5.12	1.47	1.36
12	6	310	KC1	C3C-C2C	5.12	1.47	1.36
11	15	304	CLA	O2D-CGD	5.12	1.45	1.33
12	14	306	KC1	C3B-C2B	5.12	1.47	1.37
12	10	306	KC1	C3B-C2B	5.11	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	11	301	A86	C9-C8	5.11	1.47	1.34
11	7	311	CLA	O2D-CGD	5.11	1.45	1.33
11	14	302	CLA	O2D-CGD	5.11	1.45	1.33
11	8	308	CLA	C3C-C2C	5.11	1.47	1.36
12	16	311	KC1	CHD-C4C	5.11	1.48	1.35
11	16	306	CLA	O2D-CGD	5.11	1.45	1.33
11	15	306	CLA	C1D-ND	5.11	1.44	1.37
11	14	307	CLA	O2D-CGD	5.11	1.45	1.33
11	10	304	CLA	C3C-C2C	5.11	1.47	1.36
11	6	311	CLA	O2D-CGD	5.11	1.45	1.33
11	16	302	CLA	O2D-CGD	5.11	1.45	1.33
11	16	310	CLA	C3C-C2C	5.11	1.47	1.36
12	14	311	KC1	O2D-CGD	5.10	1.45	1.33
11	13	307	CLA	C3C-C2C	5.10	1.47	1.36
12	8	313	KC1	C1A-NA	-5.10	1.28	1.38
11	16	308	CLA	C1D-ND	5.10	1.44	1.37
12	8	306	KC1	C3D-C2D	5.10	1.48	1.39
11	7	303	CLA	C3C-C2C	5.10	1.47	1.36
13	7	301	DD6	C3-C2	5.10	1.59	1.43
11	15	314	CLA	C3C-C2C	5.10	1.47	1.36
11	16	307	CLA	O2D-CGD	5.09	1.45	1.33
12	14	311	KC1	C3B-C2B	5.09	1.47	1.37
12	11	306	KC1	CHD-C4C	5.09	1.48	1.35
11	6	304	CLA	CHC-C1C	5.09	1.48	1.35
12	13	305	KC1	CHD-C4C	5.09	1.48	1.35
11	13	307	CLA	O2D-CGD	5.09	1.45	1.33
11	15	305	CLA	O2D-CGD	5.09	1.45	1.33
12	12	305	KC1	C3C-C2C	5.09	1.47	1.36
11	15	312	CLA	O2D-CGD	5.09	1.45	1.33
11	16	303	CLA	CHC-C1C	5.09	1.48	1.35
12	6	309	KC1	C3C-C2C	5.08	1.47	1.36
12	11	306	KC1	O2D-CGD	5.08	1.45	1.33
11	16	308	CLA	O2D-CGD	5.08	1.45	1.33
12	8	311	KC1	C3B-C2B	5.08	1.47	1.37
11	13	302	CLA	O2D-CGD	5.08	1.45	1.33
13	6	316	DD6	C3-C2	5.08	1.59	1.43
12	14	311	KC1	C3C-C2C	5.08	1.47	1.36
11	15	313	CLA	O2D-CGD	5.08	1.45	1.33
11	14	312	CLA	CHC-C1C	5.08	1.48	1.35
11	15	302	CLA	C1D-ND	5.08	1.44	1.37
12	12	311	KC1	C3C-C2C	5.08	1.47	1.36
11	11	303	CLA	C3C-C2C	5.08	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	7	312	KC1	C1A-NA	-5.08	1.28	1.38
11	15	303	CLA	O2D-CGD	5.08	1.45	1.33
11	6	303	CLA	CHC-C1C	5.08	1.48	1.35
11	15	313	CLA	C1D-ND	5.07	1.44	1.37
12	10	306	KC1	CHD-C4C	5.07	1.48	1.35
11	6	302	CLA	C3C-C2C	5.07	1.47	1.36
12	10	312	KC1	CHD-C4C	5.07	1.48	1.35
12	11	304	KC1	O2D-CGD	5.07	1.45	1.33
13	15	319	DD6	C3-C2	5.07	1.59	1.43
11	7	305	CLA	C3C-C2C	5.07	1.47	1.36
13	15	318	DD6	C3-C2	5.07	1.59	1.43
11	13	303	CLA	O2D-CGD	5.07	1.45	1.33
11	10	311	CLA	O2D-CGD	5.06	1.45	1.33
12	10	310	KC1	O2D-CGD	5.06	1.45	1.33
12	8	312	KC1	O2D-CGD	5.06	1.45	1.33
12	6	305	KC1	C3C-C2C	5.06	1.47	1.36
13	16	313	DD6	C3-C2	5.06	1.59	1.43
13	8	317	DD6	C13-C14	5.06	1.43	1.32
12	8	311	KC1	CHD-C4C	5.06	1.47	1.35
12	11	304	KC1	CHD-C4C	5.06	1.47	1.35
11	14	303	CLA	C1D-ND	5.06	1.44	1.37
11	12	321	CLA	O2D-CGD	5.06	1.45	1.33
11	6	312	CLA	O2D-CGD	5.06	1.45	1.33
12	11	311	KC1	C3D-C2D	5.05	1.48	1.39
11	12	306	CLA	C3C-C2C	5.05	1.47	1.36
14	10	315	A86	C9-C8	5.05	1.47	1.34
11	14	312	CLA	C1D-ND	5.05	1.44	1.37
12	11	310	KC1	CHD-C4C	5.05	1.47	1.35
12	10	312	KC1	C3C-C2C	5.05	1.47	1.36
12	10	310	KC1	CHD-C4C	5.05	1.47	1.35
12	8	313	KC1	C3C-C2C	5.05	1.47	1.36
11	16	309	CLA	O2D-CGD	5.05	1.45	1.33
11	8	303	CLA	C3C-C2C	5.05	1.47	1.36
12	12	311	KC1	CHD-C4C	5.05	1.47	1.35
13	6	315	DD6	C3-C2	5.05	1.59	1.43
11	7	304	CLA	C3C-C2C	5.05	1.47	1.36
12	7	312	KC1	C3B-C2B	5.05	1.47	1.37
12	14	311	KC1	C3D-C2D	5.05	1.48	1.39
13	13	314	DD6	C3-C2	5.05	1.59	1.43
11	10	311	CLA	C1D-ND	5.04	1.44	1.37
12	12	309	KC1	CHD-C4C	5.04	1.47	1.35
12	7	312	KC1	CHD-C4C	5.04	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	15	316	A86	C26-C27	5.04	1.42	1.35
11	15	309	CLA	O2D-CGD	5.04	1.45	1.33
11	12	303	CLA	O2D-CGD	5.04	1.45	1.33
11	7	306	CLA	O2D-CGD	5.04	1.45	1.33
12	8	314	KC1	CHD-C4C	5.04	1.47	1.35
11	14	310	CLA	C1D-ND	5.04	1.44	1.37
13	12	317	DD6	C3-C2	5.04	1.59	1.43
12	7	307	KC1	CHD-C4C	5.04	1.47	1.35
12	10	312	KC1	O2D-CGD	5.04	1.45	1.33
11	16	305	CLA	C3C-C2C	5.04	1.47	1.36
11	7	303	CLA	O2D-CGD	5.03	1.45	1.33
12	8	310	KC1	C1A-NA	-5.03	1.28	1.38
12	6	310	KC1	C1A-NA	-5.03	1.28	1.38
11	14	303	CLA	CHC-C1C	5.03	1.47	1.35
11	10	304	CLA	O2D-CGD	5.03	1.45	1.33
12	13	310	KC1	O2D-CGD	5.03	1.45	1.33
11	13	303	CLA	CHC-C1C	5.03	1.47	1.35
12	7	312	KC1	C3C-C2C	5.02	1.47	1.36
11	14	313	CLA	CHC-C1C	5.02	1.47	1.35
13	10	314	DD6	C3-C2	5.02	1.59	1.43
11	14	302	CLA	C3C-C2C	5.02	1.47	1.36
11	14	307	CLA	CHC-C1C	5.02	1.47	1.35
12	11	310	KC1	O2D-CGD	5.02	1.45	1.33
11	14	310	CLA	CHC-C1C	5.02	1.47	1.35
11	12	310	CLA	O2D-CGD	5.02	1.45	1.33
12	8	310	KC1	O2D-CGD	5.02	1.45	1.33
12	11	311	KC1	C3C-C2C	5.02	1.47	1.36
12	16	304	KC1	O2D-CGD	5.02	1.45	1.33
11	11	307	CLA	CHC-C1C	5.02	1.47	1.35
14	15	322	A86	C26-C27	5.02	1.42	1.35
12	13	310	KC1	CHD-C4C	5.02	1.47	1.35
11	15	304	CLA	CHC-C1C	5.01	1.47	1.35
12	8	307	KC1	CHD-C4C	5.01	1.47	1.35
11	7	308	CLA	C3B-C2B	5.01	1.47	1.40
12	10	312	KC1	C1A-NA	-5.01	1.28	1.38
11	16	301	CLA	CHC-C1C	5.01	1.47	1.35
12	8	306	KC1	C3C-C2C	5.01	1.47	1.36
14	15	320	A86	C9-C8	5.01	1.47	1.34
13	10	313	DD6	C3-C2	5.01	1.59	1.43
11	14	310	CLA	O2D-CGD	5.01	1.45	1.33
12	6	308	KC1	CHD-C4C	5.01	1.47	1.35
11	12	307	CLA	O2D-CGD	5.01	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	14	302	CLA	C1D-ND	5.01	1.43	1.37
12	8	310	KC1	C3B-C2B	5.01	1.47	1.37
12	10	310	KC1	C1A-NA	-5.01	1.28	1.38
12	14	308	KC1	CHD-C4C	5.01	1.47	1.35
12	14	306	KC1	C3C-C2C	5.00	1.47	1.36
11	6	304	CLA	O2D-CGD	5.00	1.45	1.33
12	8	312	KC1	CHD-C4C	5.00	1.47	1.35
11	15	310	CLA	CHC-C1C	5.00	1.47	1.35
12	8	313	KC1	O2D-CGD	5.00	1.45	1.33
12	6	308	KC1	C1A-NA	-5.00	1.28	1.38
11	15	312	CLA	CHC-C1C	5.00	1.47	1.35
12	8	306	KC1	C3B-C2B	5.00	1.47	1.37
11	12	321	CLA	C1D-ND	5.00	1.43	1.37
12	10	306	KC1	C3C-C2C	5.00	1.47	1.36
14	15	322	A86	C9-C8	4.99	1.47	1.34
12	8	307	KC1	C1A-NA	-4.99	1.28	1.38
11	16	307	CLA	C1D-ND	4.99	1.43	1.37
11	7	302	CLA	C3C-C2C	4.99	1.47	1.36
11	10	308	CLA	O2D-CGD	4.99	1.45	1.33
11	10	308	CLA	C3C-C2C	4.99	1.47	1.36
11	13	301	CLA	C3B-C2B	4.98	1.47	1.40
11	11	309	CLA	O2D-CGD	4.98	1.45	1.33
14	13	315	A86	C9-C8	4.98	1.47	1.34
11	6	302	CLA	O2D-CGD	4.98	1.45	1.33
11	14	312	CLA	O2D-CGD	4.98	1.45	1.33
11	7	308	CLA	C3C-C2C	4.98	1.47	1.36
11	6	307	CLA	O2D-CGD	4.98	1.45	1.33
11	8	301	CLA	C3C-C2C	4.98	1.47	1.36
11	16	302	CLA	C3C-C2C	4.98	1.47	1.36
12	14	311	KC1	CHD-C4C	4.97	1.47	1.35
11	8	305	CLA	C3C-C2C	4.97	1.47	1.36
11	15	305	CLA	C1D-ND	4.97	1.43	1.37
11	15	305	CLA	CHC-C1C	4.97	1.47	1.35
11	11	308	CLA	CHC-C1C	4.97	1.47	1.35
11	8	308	CLA	CHC-C1C	4.97	1.47	1.35
11	14	304	CLA	C1D-ND	4.97	1.43	1.37
11	16	301	CLA	C1D-ND	4.97	1.43	1.37
11	6	313	CLA	O2D-CGD	4.97	1.45	1.33
11	6	314	CLA	CHC-C1C	4.97	1.47	1.35
12	6	310	KC1	CHD-C4C	4.97	1.47	1.35
11	7	310	CLA	C3C-C2C	4.97	1.47	1.36
13	11	312	DD6	C3-C2	4.96	1.58	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	6	301	CLA	C3C-C2C	4.96	1.47	1.36
11	14	305	CLA	O2D-CGD	4.96	1.45	1.33
11	14	313	CLA	C1D-ND	4.96	1.43	1.37
12	11	304	KC1	C1A-NA	-4.96	1.28	1.38
12	8	311	KC1	O2D-CGD	4.96	1.45	1.33
11	13	301	CLA	CHC-C1C	4.96	1.47	1.35
11	6	306	CLA	O2D-CGD	4.96	1.45	1.33
11	6	311	CLA	C3B-C2B	4.96	1.47	1.40
11	12	310	CLA	CHC-C1C	4.96	1.47	1.35
11	15	308	CLA	C3B-C2B	4.96	1.47	1.40
11	14	305	CLA	CHC-C1C	4.96	1.47	1.35
11	11	305	CLA	O2D-CGD	4.96	1.45	1.33
11	14	303	CLA	O2D-CGD	4.95	1.45	1.33
14	14	320	A86	C9-C8	4.95	1.47	1.34
11	15	313	CLA	CHC-C1C	4.95	1.47	1.35
12	12	311	KC1	O2D-CGD	4.95	1.45	1.33
12	10	306	KC1	C3D-C2D	4.95	1.48	1.39
11	16	301	CLA	C3C-C2C	4.94	1.47	1.36
11	14	304	CLA	CHC-C1C	4.94	1.47	1.35
11	13	304	CLA	CHC-C1C	4.94	1.47	1.35
11	10	307	CLA	CHC-C1C	4.94	1.47	1.35
12	12	313	KC1	O2D-CGD	4.94	1.45	1.33
11	13	307	CLA	C1D-ND	4.94	1.43	1.37
11	12	308	CLA	O2D-CGD	4.94	1.45	1.33
14	15	317	A86	C26-C27	4.94	1.42	1.35
12	12	305	KC1	O2D-CGD	4.94	1.45	1.33
12	14	308	KC1	O2D-CGD	4.93	1.45	1.33
11	11	309	CLA	CHC-C1C	4.93	1.47	1.35
12	8	306	KC1	CHD-C4C	4.93	1.47	1.35
11	16	301	CLA	O2D-CGD	4.93	1.45	1.33
12	16	311	KC1	O2D-CGD	4.93	1.45	1.33
11	10	309	CLA	CHC-C1C	4.93	1.47	1.35
12	11	311	KC1	O2D-CGD	4.93	1.45	1.33
11	8	302	CLA	CHC-C1C	4.93	1.47	1.35
11	6	303	CLA	O2D-CGD	4.93	1.45	1.33
11	15	314	CLA	C1D-ND	4.93	1.43	1.37
12	6	309	KC1	CHD-C4C	4.93	1.47	1.35
13	7	316	DD6	C3-C2	4.92	1.58	1.43
12	8	311	KC1	C3D-C2D	4.92	1.48	1.39
11	13	301	CLA	C1D-ND	4.92	1.43	1.37
11	16	308	CLA	CHC-C1C	4.92	1.47	1.35
11	16	306	CLA	CHC-C1C	4.92	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	16	303	CLA	O2D-CGD	4.91	1.45	1.33
11	10	309	CLA	C1D-ND	4.91	1.43	1.37
11	15	303	CLA	CHC-C1C	4.91	1.47	1.35
11	15	303	CLA	C1D-ND	4.91	1.43	1.37
11	8	305	CLA	O2D-CGD	4.91	1.45	1.33
11	6	306	CLA	C3C-C2C	4.91	1.47	1.36
11	12	302	CLA	C3C-C2C	4.91	1.47	1.36
12	13	306	KC1	CHD-C4C	4.91	1.47	1.35
11	12	304	CLA	CHC-C1C	4.91	1.47	1.35
12	13	306	KC1	C3C-C2C	4.90	1.47	1.36
14	6	317	A86	C26-C27	4.90	1.42	1.35
11	16	309	CLA	CHC-C1C	4.90	1.47	1.35
11	14	313	CLA	O2D-CGD	4.90	1.45	1.33
11	16	307	CLA	CHC-C1C	4.90	1.47	1.35
12	6	309	KC1	CHC-C4B	4.90	1.47	1.38
11	6	312	CLA	CHC-C1C	4.90	1.47	1.35
12	6	309	KC1	O2D-CGD	4.90	1.45	1.33
11	7	304	CLA	CHC-C1C	4.90	1.47	1.35
11	10	305	CLA	CHC-C1C	4.90	1.47	1.35
11	11	308	CLA	O2D-CGD	4.90	1.45	1.33
11	8	304	CLA	C3C-C2C	4.90	1.47	1.36
11	6	301	CLA	CHC-C1C	4.90	1.47	1.35
14	14	320	A86	C26-C27	4.90	1.42	1.35
14	14	321	A86	C9-C8	4.89	1.47	1.34
11	11	308	CLA	C3C-C2C	4.89	1.47	1.36
13	7	317	DD6	C3-C2	4.89	1.58	1.43
14	14	319	A86	C9-C8	4.89	1.47	1.34
11	13	301	CLA	C3C-C2C	4.89	1.47	1.36
11	11	307	CLA	C1D-ND	4.89	1.43	1.37
11	14	309	CLA	CHC-C1C	4.89	1.47	1.35
14	12	316	A86	C9-C8	4.89	1.47	1.34
13	7	313	DD6	C3-C2	4.88	1.58	1.43
12	13	306	KC1	C1A-NA	-4.88	1.28	1.38
11	15	306	CLA	O2D-CGD	4.88	1.45	1.33
11	6	306	CLA	CHC-C1C	4.88	1.47	1.35
11	15	302	CLA	O2D-CGD	4.88	1.45	1.33
12	6	310	KC1	O2D-CGD	4.88	1.45	1.33
11	6	311	CLA	C3C-C2C	4.88	1.47	1.36
11	8	305	CLA	CHC-C1C	4.87	1.47	1.35
11	15	311	CLA	CHC-C1C	4.87	1.47	1.35
14	14	321	A86	C26-C27	4.87	1.42	1.35
13	6	318	DD6	C3-C2	4.87	1.58	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	7	309	CLA	C1D-ND	4.87	1.43	1.37
14	10	317	A86	C9-C8	4.87	1.47	1.34
12	14	306	KC1	O2D-CGD	4.87	1.45	1.33
11	12	304	CLA	O2D-CGD	4.86	1.45	1.33
13	8	317	DD6	C3-C2	4.86	1.58	1.43
11	12	312	CLA	O2D-CGD	4.86	1.45	1.33
13	12	315	DD6	C3-C2	4.86	1.58	1.43
11	15	307	CLA	O2D-CGD	4.86	1.45	1.33
11	10	303	CLA	C3C-C2C	4.86	1.47	1.36
12	6	305	KC1	CHD-C4C	4.86	1.47	1.35
11	10	311	CLA	CHC-C1C	4.86	1.47	1.35
14	13	313	A86	C9-C8	4.86	1.47	1.34
11	10	303	CLA	O2D-CGD	4.86	1.45	1.33
14	13	315	A86	C26-C27	4.86	1.42	1.35
11	6	304	CLA	C1D-ND	4.86	1.43	1.37
11	7	310	CLA	O2D-CGD	4.86	1.45	1.33
12	12	305	KC1	CHD-C4C	4.85	1.47	1.35
11	11	303	CLA	C1D-ND	4.85	1.43	1.37
12	12	313	KC1	C3C-C2C	4.85	1.47	1.36
11	13	301	CLA	O2D-CGD	4.85	1.45	1.33
11	11	303	CLA	O2D-CGD	4.85	1.45	1.33
14	16	312	A86	C9-C8	4.85	1.47	1.34
11	13	309	CLA	CHC-C1C	4.85	1.47	1.35
11	12	308	CLA	CHC-C1C	4.85	1.47	1.35
11	8	304	CLA	CHC-C1C	4.85	1.47	1.35
11	15	314	CLA	CHC-C1C	4.85	1.47	1.35
11	8	308	CLA	O2D-CGD	4.85	1.45	1.33
12	8	313	KC1	CHD-C4C	4.85	1.47	1.35
12	6	308	KC1	O2D-CGD	4.84	1.45	1.33
11	10	308	CLA	C1D-ND	4.84	1.43	1.37
11	16	302	CLA	CHC-C1C	4.84	1.47	1.35
14	14	314	A86	C9-C8	4.84	1.47	1.34
14	15	317	A86	C9-C8	4.83	1.47	1.34
11	15	307	CLA	C1D-ND	4.83	1.43	1.37
14	6	317	A86	C9-C8	4.83	1.47	1.34
11	10	305	CLA	O2D-CGD	4.83	1.45	1.33
11	13	302	CLA	CHC-C1C	4.83	1.47	1.35
11	10	304	CLA	CHC-C1C	4.83	1.47	1.35
11	12	306	CLA	O2D-CGD	4.83	1.45	1.33
12	8	306	KC1	O2D-CGD	4.82	1.45	1.33
11	7	309	CLA	CHC-C1C	4.82	1.47	1.35
12	6	309	KC1	C1A-NA	-4.82	1.28	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	6	307	CLA	C1D-ND	4.82	1.43	1.37
11	8	309	CLA	O2D-CGD	4.82	1.45	1.33
12	11	306	KC1	C1A-NA	-4.82	1.28	1.38
11	16	310	CLA	CHC-C1C	4.82	1.47	1.35
11	8	303	CLA	O2D-CGD	4.81	1.44	1.33
14	12	316	A86	C26-C27	4.81	1.42	1.35
11	13	302	CLA	C1D-ND	4.81	1.43	1.37
11	14	305	CLA	C1D-ND	4.81	1.43	1.37
14	7	318	A86	C26-C27	4.81	1.42	1.35
12	7	307	KC1	C1A-NA	-4.81	1.28	1.38
12	7	312	KC1	O2D-CGD	4.81	1.44	1.33
11	15	308	CLA	O2D-CGD	4.80	1.44	1.33
11	7	306	CLA	C3C-C2C	4.80	1.46	1.36
13	8	316	DD6	C3-C2	4.80	1.58	1.43
12	8	307	KC1	C3B-C2B	4.80	1.47	1.37
14	7	314	A86	C17-C18	-4.80	1.45	1.52
14	10	315	A86	C26-C27	4.80	1.42	1.35
12	11	310	KC1	C1A-NA	-4.80	1.28	1.38
12	14	306	KC1	C1A-NA	-4.80	1.28	1.38
11	6	302	CLA	CHC-C1C	4.80	1.47	1.35
14	10	301	A86	C17-C18	-4.80	1.45	1.52
11	12	312	CLA	CHC-C1C	4.80	1.47	1.35
11	12	321	CLA	CHC-C1C	4.79	1.47	1.35
11	16	305	CLA	O2D-CGD	4.79	1.44	1.33
12	8	307	KC1	O2D-CGD	4.79	1.44	1.33
11	15	306	CLA	CHC-C1C	4.79	1.47	1.35
14	14	301	A86	C9-C8	4.79	1.46	1.34
12	8	311	KC1	C1A-NA	-4.79	1.28	1.38
11	7	308	CLA	O2D-CGD	4.79	1.44	1.33
12	13	310	KC1	CHC-C4B	4.79	1.47	1.38
12	12	305	KC1	C1A-NA	-4.79	1.28	1.38
12	13	312	KC1	OBD-CAD	4.78	1.29	1.22
11	13	307	CLA	CHC-C1C	4.78	1.47	1.35
11	12	303	CLA	CHC-C1C	4.78	1.47	1.35
14	8	315	A86	C17-C18	-4.78	1.45	1.52
12	14	306	KC1	CHC-C4B	4.78	1.47	1.38
11	16	310	CLA	C1D-ND	4.78	1.43	1.37
14	13	313	A86	C2-C1	4.77	1.42	1.35
11	8	304	CLA	O2D-CGD	4.77	1.44	1.33
11	6	311	CLA	C1D-ND	4.77	1.43	1.37
14	15	321	A86	C9-C8	4.77	1.46	1.34
12	12	309	KC1	O2D-CGD	4.77	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	6	305	KC1	CHC-C4B	4.77	1.47	1.38
14	10	302	A86	C26-C27	4.76	1.42	1.35
12	8	310	KC1	CHD-C4C	4.76	1.47	1.35
11	8	302	CLA	O2D-CGD	4.76	1.44	1.33
12	13	311	KC1	CHB-C1B	4.76	1.47	1.38
11	7	311	CLA	CHC-C1C	4.76	1.47	1.35
11	7	304	CLA	C1D-ND	4.76	1.43	1.37
12	13	308	KC1	C1A-NA	-4.75	1.28	1.38
12	7	307	KC1	O2D-CGD	4.75	1.44	1.33
14	7	318	A86	C9-C8	4.75	1.46	1.34
14	10	315	A86	O4-C38	4.75	1.45	1.35
11	6	307	CLA	CHC-C1C	4.75	1.47	1.35
11	16	305	CLA	CHC-C1C	4.75	1.47	1.35
11	6	311	CLA	CHC-C1C	4.75	1.47	1.35
12	6	305	KC1	O2D-CGD	4.74	1.44	1.33
14	15	321	A86	C26-C27	4.74	1.42	1.35
12	8	306	KC1	C1A-NA	-4.74	1.28	1.38
11	7	305	CLA	O2D-CGD	4.74	1.44	1.33
14	15	316	A86	C9-C8	4.74	1.46	1.34
11	6	303	CLA	C1D-ND	4.74	1.43	1.37
11	10	305	CLA	C1D-ND	4.73	1.43	1.37
14	8	318	A86	C17-C18	-4.73	1.45	1.52
12	12	313	KC1	CHD-C4C	4.73	1.47	1.35
11	7	309	CLA	O2D-CGD	4.73	1.44	1.33
14	16	314	A86	C9-C8	4.73	1.46	1.34
12	8	312	KC1	C1A-NA	-4.73	1.28	1.38
14	11	314	A86	C9-C8	4.72	1.46	1.34
11	7	304	CLA	O2D-CGD	4.72	1.44	1.33
11	11	305	CLA	C1D-ND	4.72	1.43	1.37
12	13	306	KC1	CHC-C4B	4.71	1.47	1.38
11	6	313	CLA	CHC-C1C	4.71	1.47	1.35
11	7	310	CLA	C1D-ND	4.71	1.43	1.37
12	10	306	KC1	C1A-NA	-4.70	1.28	1.38
12	16	304	KC1	C1A-NA	-4.70	1.28	1.38
12	8	312	KC1	CHB-C1B	4.70	1.47	1.38
14	14	318	A86	C9-C8	4.70	1.46	1.34
14	16	312	A86	C17-C18	-4.70	1.45	1.52
14	11	313	A86	C9-C8	4.70	1.46	1.34
11	12	302	CLA	CHC-C1C	4.70	1.47	1.35
11	7	306	CLA	C1D-ND	4.70	1.43	1.37
11	6	301	CLA	C3B-C2B	4.69	1.46	1.40
14	14	318	A86	C26-C27	4.69	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	7	310	CLA	CHC-C1C	4.69	1.47	1.35
14	10	316	A86	C9-C8	4.69	1.46	1.34
12	8	312	KC1	CHC-C4B	4.69	1.47	1.38
11	12	312	CLA	C1D-ND	4.69	1.43	1.37
11	10	304	CLA	C1D-ND	4.68	1.43	1.37
11	7	305	CLA	CHC-C1C	4.68	1.47	1.35
12	13	312	KC1	CHC-C4B	4.68	1.47	1.38
11	8	308	CLA	C1D-ND	4.68	1.43	1.37
11	6	301	CLA	C1D-ND	4.68	1.43	1.37
14	15	315	A86	C17-C18	-4.68	1.45	1.52
14	14	316	A86	C9-C8	4.68	1.46	1.34
14	12	314	A86	C17-C18	-4.67	1.45	1.52
14	15	320	A86	C2-C1	4.67	1.42	1.35
12	10	306	KC1	O2D-CGD	4.67	1.44	1.33
11	16	305	CLA	C1D-ND	4.67	1.43	1.37
11	10	303	CLA	CHC-C1C	4.67	1.46	1.35
14	11	301	A86	C17-C18	-4.67	1.45	1.52
11	7	303	CLA	CHC-C1C	4.66	1.46	1.35
11	8	301	CLA	O2D-CGD	4.66	1.44	1.33
12	12	311	KC1	C1A-NA	-4.66	1.28	1.38
14	14	315	A86	C9-C8	4.66	1.46	1.34
11	12	303	CLA	C1D-ND	4.66	1.43	1.37
12	13	305	KC1	CHC-C4B	4.66	1.47	1.38
14	12	314	A86	C9-C8	4.65	1.46	1.34
11	8	309	CLA	CHC-C1C	4.65	1.46	1.35
12	8	313	KC1	CHC-C4B	4.65	1.47	1.38
11	11	307	CLA	O2D-CGD	4.65	1.44	1.33
14	14	314	A86	C2-C1	4.65	1.41	1.35
12	6	305	KC1	C1A-NA	-4.65	1.28	1.38
14	14	317	A86	C9-C8	4.65	1.46	1.34
11	12	304	CLA	C1D-ND	4.65	1.43	1.37
11	8	301	CLA	CHC-C1C	4.65	1.46	1.35
12	13	305	KC1	O2D-CGD	4.65	1.44	1.33
11	15	314	CLA	O2D-CGD	4.64	1.44	1.33
12	12	309	KC1	C1A-NA	-4.64	1.29	1.38
14	11	315	A86	C26-C27	4.64	1.41	1.35
11	14	307	CLA	C1D-ND	4.63	1.43	1.37
14	14	321	A86	C2-C1	4.63	1.41	1.35
12	14	308	KC1	OBD-CAD	4.63	1.28	1.22
11	15	307	CLA	CHC-C1C	4.62	1.46	1.35
11	10	303	CLA	C1D-ND	4.62	1.43	1.37
11	7	302	CLA	O2D-CGD	4.62	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	16	303	CLA	C1D-ND	4.62	1.43	1.37
12	11	306	KC1	CHC-C4B	4.62	1.47	1.38
11	12	306	CLA	CHC-C1C	4.62	1.46	1.35
14	14	301	A86	C26-C27	4.62	1.41	1.35
11	16	302	CLA	C1D-ND	4.62	1.43	1.37
12	13	310	KC1	C1A-NA	-4.62	1.29	1.38
12	11	304	KC1	CHC-C4B	4.62	1.47	1.38
14	10	315	A86	C2-C1	4.61	1.41	1.35
12	16	311	KC1	C1A-NA	-4.60	1.29	1.38
11	8	305	CLA	C1D-ND	4.60	1.43	1.37
12	16	311	KC1	CHC-C4B	4.59	1.47	1.38
14	13	315	A86	C2-C1	4.59	1.41	1.35
11	8	303	CLA	CHC-C1C	4.59	1.46	1.35
12	8	314	KC1	O2D-CGD	4.59	1.44	1.33
11	7	308	CLA	CHC-C1C	4.59	1.46	1.35
11	8	309	CLA	C1D-ND	4.58	1.43	1.37
14	14	315	A86	C17-C18	-4.58	1.45	1.52
11	6	301	CLA	O2D-CGD	4.58	1.44	1.33
11	6	306	CLA	C1D-ND	4.58	1.43	1.37
14	7	314	A86	C9-C8	4.58	1.46	1.34
12	13	305	KC1	C1A-NA	-4.57	1.29	1.38
14	14	317	A86	C26-C27	4.57	1.41	1.35
12	13	308	KC1	CHC-C4B	4.57	1.47	1.38
12	6	310	KC1	CHC-C4B	4.56	1.47	1.38
12	13	311	KC1	CHC-C4B	4.56	1.47	1.38
14	14	319	A86	C26-C27	4.56	1.41	1.35
11	10	307	CLA	O2D-CGD	4.56	1.44	1.33
11	12	310	CLA	C1D-ND	4.56	1.43	1.37
12	13	311	KC1	C1A-NA	-4.55	1.29	1.38
12	10	312	KC1	CHC-C4B	4.55	1.47	1.38
12	13	312	KC1	C1A-NA	-4.55	1.29	1.38
12	8	310	KC1	C3C-C2C	4.54	1.46	1.36
12	14	311	KC1	CHC-C4B	4.54	1.47	1.38
12	8	314	KC1	C1A-NA	-4.54	1.29	1.38
14	8	318	A86	C9-C8	4.53	1.46	1.34
14	15	317	A86	C17-C18	-4.53	1.45	1.52
14	14	316	A86	C17-C18	-4.53	1.45	1.52
11	14	309	CLA	CHD-C1D	4.53	1.47	1.38
11	15	308	CLA	C1D-ND	4.53	1.43	1.37
14	11	315	A86	C9-C8	4.53	1.46	1.34
12	14	308	KC1	C1A-NA	-4.53	1.29	1.38
12	11	310	KC1	CHC-C4B	4.52	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	10	317	A86	C26-C27	4.52	1.41	1.35
11	15	308	CLA	O2A-CGA	4.52	1.45	1.30
11	15	306	CLA	O2A-CGA	4.52	1.45	1.30
11	14	309	CLA	O2A-CGA	4.52	1.45	1.30
12	11	304	KC1	CHB-C1B	4.52	1.47	1.38
12	12	311	KC1	CHC-C4B	4.51	1.47	1.38
11	14	304	CLA	O2A-CGA	4.51	1.45	1.30
12	13	312	KC1	CHB-C1B	4.51	1.47	1.38
12	13	311	KC1	OBD-CAD	4.51	1.28	1.22
12	14	308	KC1	CHC-C4B	4.51	1.47	1.38
14	15	316	A86	C2-C1	4.50	1.41	1.35
12	8	314	KC1	CHC-C4B	4.50	1.47	1.38
14	15	322	A86	C2-C1	4.50	1.41	1.35
12	12	313	KC1	CHC-C4B	4.50	1.47	1.38
14	10	316	A86	C17-C18	-4.49	1.45	1.52
14	15	315	A86	C5-C6	4.49	1.41	1.35
11	6	302	CLA	C1D-ND	4.49	1.43	1.37
12	10	306	KC1	CHC-C4B	4.49	1.47	1.38
11	16	310	CLA	O2A-CGA	4.49	1.45	1.30
11	12	302	CLA	O2D-CGD	4.49	1.44	1.33
12	7	312	KC1	OBD-CAD	4.49	1.28	1.22
12	10	312	KC1	OBD-CAD	4.49	1.28	1.22
12	7	307	KC1	CHC-C4B	4.49	1.47	1.38
12	6	310	KC1	CHB-C1B	4.49	1.47	1.38
11	6	312	CLA	O2A-CGA	4.49	1.45	1.30
11	12	308	CLA	C1D-ND	4.49	1.43	1.37
12	14	306	KC1	OBD-CAD	4.49	1.28	1.22
11	7	308	CLA	C1D-ND	4.48	1.43	1.37
12	16	311	KC1	OBD-CAD	4.48	1.28	1.22
14	14	314	A86	C26-C27	4.48	1.41	1.35
11	16	309	CLA	O2A-CGA	4.48	1.45	1.30
12	13	306	KC1	CHB-C1B	4.48	1.47	1.38
11	14	312	CLA	O2A-CGA	4.48	1.45	1.30
11	10	311	CLA	O2A-CGA	4.48	1.45	1.30
14	14	320	A86	O4-C38	4.48	1.45	1.35
11	15	305	CLA	O2A-CGA	4.48	1.45	1.30
11	13	304	CLA	O2A-CGA	4.47	1.45	1.30
12	12	305	KC1	CHC-C4B	4.47	1.47	1.38
11	13	309	CLA	O2A-CGA	4.47	1.45	1.30
14	14	316	A86	C26-C27	4.47	1.41	1.35
11	8	302	CLA	C1D-ND	4.47	1.43	1.37
11	15	314	CLA	O2A-CGA	4.46	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	12	313	KC1	C3D-C2D	4.46	1.47	1.39
14	15	315	A86	C10-C11	4.46	1.47	1.34
11	12	307	CLA	C3C-C2C	4.46	1.46	1.36
12	16	304	KC1	CHC-C4B	4.46	1.47	1.38
11	15	310	CLA	O2A-CGA	4.46	1.45	1.30
11	15	311	CLA	O2A-CGA	4.46	1.45	1.30
11	15	312	CLA	O2A-CGA	4.46	1.45	1.30
14	14	319	A86	C2-C1	4.46	1.41	1.35
11	16	308	CLA	O2A-CGA	4.46	1.45	1.30
12	6	309	KC1	OBD-CAD	4.46	1.28	1.22
12	12	313	KC1	OBD-CAD	4.46	1.28	1.22
12	11	311	KC1	C1A-NA	-4.45	1.29	1.38
11	7	305	CLA	C1D-ND	4.45	1.43	1.37
12	8	312	KC1	OBD-CAD	4.45	1.28	1.22
14	12	316	A86	C17-C18	-4.45	1.45	1.52
11	6	312	CLA	CHD-C1D	4.45	1.47	1.38
14	6	317	A86	O4-C38	4.45	1.45	1.35
14	15	322	A86	C7-C6	4.45	1.60	1.50
12	16	304	KC1	OBD-CAD	4.44	1.28	1.22
11	11	305	CLA	O2A-CGA	4.44	1.46	1.33
14	14	301	A86	O4-C38	4.44	1.45	1.35
12	12	305	KC1	OBD-CAD	4.44	1.28	1.22
12	14	311	KC1	OBD-CAD	4.43	1.28	1.22
11	16	303	CLA	O2A-CGA	4.43	1.46	1.33
14	7	315	A86	C17-C18	-4.43	1.45	1.52
11	15	302	CLA	O2A-CGA	4.43	1.46	1.33
11	12	302	CLA	C1D-ND	4.43	1.43	1.37
12	14	311	KC1	CHB-C1B	4.43	1.47	1.38
12	12	311	KC1	OBD-CAD	4.42	1.28	1.22
12	11	310	KC1	OBD-CAD	4.42	1.28	1.22
12	8	306	KC1	CHC-C4B	4.42	1.47	1.38
11	12	306	CLA	C1D-ND	4.42	1.43	1.37
12	8	311	KC1	OBD-CAD	4.42	1.28	1.22
12	8	307	KC1	CHC-C4B	4.41	1.47	1.38
11	11	309	CLA	CHD-C1D	4.41	1.47	1.38
14	14	317	A86	C17-C18	-4.41	1.46	1.52
12	13	310	KC1	OBD-CAD	4.41	1.28	1.22
14	10	301	A86	C9-C8	4.41	1.45	1.34
11	15	312	CLA	CHD-C1D	4.40	1.46	1.38
11	7	303	CLA	C1D-ND	4.40	1.43	1.37
14	11	314	A86	O4-C38	4.40	1.45	1.35
11	13	309	CLA	CHD-C1D	4.40	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	7	312	KC1	CHC-C4B	4.40	1.46	1.38
12	11	311	KC1	CHC-C4B	4.39	1.46	1.38
12	10	310	KC1	CHC-C4B	4.39	1.46	1.38
14	10	317	A86	O4-C38	4.39	1.45	1.35
14	10	301	A86	O4-C38	4.39	1.45	1.35
14	7	315	A86	C9-C8	4.39	1.45	1.34
12	12	305	KC1	CHB-C1B	4.39	1.46	1.38
14	14	319	A86	O4-C38	4.39	1.45	1.35
14	15	320	A86	O4-C38	4.39	1.45	1.35
14	14	320	A86	C7-C6	4.39	1.60	1.50
12	12	309	KC1	CHC-C4B	4.39	1.46	1.38
11	7	302	CLA	O2A-CGA	4.39	1.46	1.33
14	11	301	A86	C7-C6	4.39	1.59	1.50
11	14	307	CLA	O2A-CGA	4.39	1.46	1.33
12	7	307	KC1	OBD-CAD	4.39	1.28	1.22
12	11	306	KC1	OBD-CAD	4.38	1.28	1.22
12	12	313	KC1	C1A-CHA	4.38	1.52	1.40
12	8	307	KC1	CHB-C1B	4.38	1.46	1.38
14	7	314	A86	C26-C27	4.37	1.41	1.35
12	11	310	KC1	CHB-C1B	4.37	1.46	1.38
14	15	315	A86	O4-C38	4.37	1.45	1.35
11	6	314	CLA	CHD-C1D	4.37	1.46	1.38
14	16	312	A86	C7-C6	4.37	1.59	1.50
11	15	311	CLA	CHD-C1D	4.37	1.46	1.38
12	13	305	KC1	C4D-ND	4.37	1.39	1.35
11	14	303	CLA	CHD-C1D	4.37	1.46	1.38
11	15	304	CLA	O2A-CGA	4.37	1.46	1.33
12	14	311	KC1	C1A-NA	-4.37	1.29	1.38
11	13	303	CLA	O2A-CGA	4.37	1.46	1.33
11	13	304	CLA	CHD-C1D	4.37	1.46	1.38
12	13	305	KC1	CHB-C1B	4.37	1.46	1.38
14	10	302	A86	O4-C38	4.37	1.45	1.35
12	8	306	KC1	OBD-CAD	4.37	1.28	1.22
11	13	303	CLA	CHD-C1D	4.36	1.46	1.38
11	15	309	CLA	CHD-C1D	4.36	1.46	1.38
11	6	314	CLA	O2A-CGA	4.36	1.46	1.33
12	7	307	KC1	CHB-C1B	4.36	1.46	1.38
14	14	316	A86	O4-C38	4.35	1.45	1.35
14	11	315	A86	O4-C38	4.35	1.45	1.35
11	6	303	CLA	O2A-CGA	4.35	1.46	1.33
12	11	311	KC1	OBD-CAD	4.35	1.28	1.22
14	11	315	A86	C17-C18	-4.35	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	6	310	KC1	OBD-CAD	4.35	1.28	1.22
14	10	302	A86	C7-C6	4.35	1.59	1.50
11	14	305	CLA	CHD-C1D	4.35	1.46	1.38
12	12	309	KC1	OBD-CAD	4.35	1.28	1.22
12	13	312	KC1	C4D-ND	4.35	1.39	1.35
11	6	313	CLA	C1D-ND	4.34	1.43	1.37
14	11	314	A86	C19-C18	4.34	1.58	1.52
14	15	317	A86	C2-C1	4.34	1.41	1.35
12	8	311	KC1	CHC-C4B	4.34	1.46	1.38
14	16	312	A86	O4-C38	4.34	1.45	1.35
12	10	310	KC1	OBD-CAD	4.34	1.28	1.22
14	16	312	A86	C26-C27	4.34	1.41	1.35
12	13	308	KC1	OBD-CAD	4.34	1.28	1.22
11	8	304	CLA	C1D-ND	4.34	1.43	1.37
12	14	308	KC1	CHB-C1B	4.34	1.46	1.38
14	15	322	A86	O4-C38	4.33	1.45	1.35
11	15	303	CLA	O2A-CGA	4.33	1.46	1.33
14	14	318	A86	O4-C38	4.33	1.45	1.35
11	16	307	CLA	CHD-C1D	4.32	1.46	1.38
11	14	312	CLA	CHD-C1D	4.32	1.46	1.38
14	14	321	A86	O4-C38	4.32	1.45	1.35
11	12	321	CLA	O2A-CGA	4.32	1.46	1.33
14	13	315	A86	C10-C11	4.31	1.47	1.34
14	11	314	A86	C26-C27	4.31	1.41	1.35
11	15	313	CLA	CHD-C1D	4.31	1.46	1.38
14	15	317	A86	O4-C38	4.31	1.44	1.35
11	6	302	CLA	O2A-CGA	4.31	1.45	1.33
11	10	307	CLA	C1D-ND	4.31	1.43	1.37
14	15	320	A86	C7-C6	4.30	1.59	1.50
11	10	305	CLA	O2A-CGA	4.30	1.45	1.33
11	16	309	CLA	CHD-C1D	4.30	1.46	1.38
11	6	313	CLA	O2A-CGA	4.30	1.45	1.33
14	14	319	A86	C7-C6	4.30	1.59	1.50
12	6	309	KC1	CHB-C1B	4.30	1.46	1.38
12	10	306	KC1	CHB-C1B	4.30	1.46	1.38
12	13	310	KC1	CHB-C1B	4.29	1.46	1.38
11	12	303	CLA	O2A-CGA	4.29	1.45	1.33
14	15	321	A86	C7-C6	4.29	1.59	1.50
14	13	315	A86	O4-C38	4.29	1.44	1.35
11	11	307	CLA	O2A-CGA	4.29	1.45	1.33
11	7	306	CLA	O2A-CGA	4.29	1.45	1.33
11	15	309	CLA	O2A-CGA	4.29	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	13	307	CLA	O2A-CGA	4.29	1.45	1.33
12	16	304	KC1	CHB-C1B	4.29	1.46	1.38
14	13	313	A86	C17-C18	-4.28	1.46	1.52
14	14	314	A86	O4-C38	4.28	1.44	1.35
11	14	304	CLA	CHD-C1D	4.28	1.46	1.38
14	14	317	A86	O4-C38	4.28	1.44	1.35
11	6	301	CLA	O2A-CGA	4.28	1.45	1.33
11	10	303	CLA	O2A-CGA	4.28	1.45	1.33
11	7	304	CLA	O2A-CGA	4.28	1.45	1.33
11	12	312	CLA	O2A-CGA	4.27	1.45	1.33
11	13	307	CLA	CHD-C1D	4.27	1.46	1.38
14	16	314	A86	O4-C38	4.27	1.44	1.35
14	15	317	A86	C7-C6	4.27	1.59	1.50
14	10	317	A86	C7-C6	4.27	1.59	1.50
12	11	306	KC1	CHB-C1B	4.27	1.46	1.38
14	14	320	A86	C2-C1	4.27	1.41	1.35
11	15	310	CLA	CHD-C1D	4.26	1.46	1.38
12	13	308	KC1	CHB-C1B	4.26	1.46	1.38
11	14	305	CLA	O2A-CGA	4.26	1.45	1.33
14	14	315	A86	C7-C6	4.26	1.59	1.50
14	14	301	A86	C17-C18	-4.26	1.46	1.52
14	6	317	A86	C2-C1	4.26	1.41	1.35
11	7	311	CLA	CHD-C1D	4.26	1.46	1.38
11	10	309	CLA	O2A-CGA	4.26	1.45	1.33
12	8	310	KC1	CHB-C1B	4.26	1.46	1.38
14	14	318	A86	C17-C18	-4.26	1.46	1.52
11	6	304	CLA	CHD-C1D	4.26	1.46	1.38
11	16	306	CLA	C1D-ND	4.25	1.43	1.37
12	6	308	KC1	CHB-C1B	4.25	1.46	1.38
14	14	317	A86	C7-C6	4.25	1.59	1.50
11	12	321	CLA	CHD-C1D	4.25	1.46	1.38
14	15	321	A86	O4-C38	4.25	1.44	1.35
11	16	306	CLA	O2A-CGA	4.25	1.45	1.33
11	15	307	CLA	O2A-CGA	4.25	1.45	1.33
12	8	311	KC1	CHB-C1B	4.24	1.46	1.38
11	11	308	CLA	C1D-ND	4.24	1.43	1.37
12	8	313	KC1	OBD-CAD	4.24	1.28	1.22
11	11	303	CLA	O2A-CGA	4.24	1.45	1.33
12	14	311	KC1	C4D-ND	4.24	1.39	1.35
14	7	318	A86	O4-C38	4.24	1.44	1.35
14	12	314	A86	O4-C38	4.24	1.44	1.35
14	14	321	A86	C7-C6	4.24	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	15	304	CLA	CHD-C1D	4.24	1.46	1.38
14	15	320	A86	C5-C6	4.24	1.41	1.35
14	12	316	A86	C2-C1	4.24	1.41	1.35
12	11	311	KC1	CHB-C1B	4.24	1.46	1.38
11	14	310	CLA	O2A-CGA	4.24	1.45	1.33
11	14	302	CLA	O2A-CGA	4.23	1.45	1.33
11	16	308	CLA	CHD-C1D	4.23	1.46	1.38
11	8	304	CLA	O2A-CGA	4.23	1.45	1.33
11	15	302	CLA	CHD-C1D	4.23	1.46	1.38
11	15	313	CLA	O2A-CGA	4.23	1.45	1.33
12	12	313	KC1	C4D-ND	4.23	1.39	1.35
14	16	314	A86	C17-C18	-4.22	1.46	1.52
11	15	305	CLA	CHD-C1D	4.22	1.46	1.38
14	13	315	A86	C17-C18	-4.22	1.46	1.52
11	6	313	CLA	CHD-C1D	4.22	1.46	1.38
11	6	311	CLA	O2A-CGA	4.22	1.45	1.33
12	7	307	KC1	C1B-NB	-4.22	1.32	1.37
11	7	309	CLA	O2A-CGA	4.22	1.45	1.33
11	8	303	CLA	O2A-CGA	4.22	1.45	1.33
11	12	304	CLA	O2A-CGA	4.21	1.45	1.33
14	16	314	A86	C19-C18	4.21	1.58	1.52
12	6	308	KC1	CHC-C4B	4.21	1.46	1.38
11	14	303	CLA	O2A-CGA	4.21	1.45	1.33
11	15	306	CLA	CHD-C1D	4.21	1.46	1.38
14	6	317	A86	C17-C18	-4.21	1.46	1.52
12	8	306	KC1	CHB-C1B	4.21	1.46	1.38
11	10	311	CLA	CHD-C1D	4.21	1.46	1.38
14	8	315	A86	O4-C38	4.21	1.44	1.35
14	16	314	A86	C26-C27	4.21	1.41	1.35
14	14	301	A86	C7-C6	4.21	1.59	1.50
11	14	302	CLA	CHD-C1D	4.21	1.46	1.38
12	8	306	KC1	C1B-NB	-4.20	1.32	1.37
14	14	319	A86	C17-C18	-4.20	1.46	1.52
14	15	316	A86	C7-C6	4.20	1.59	1.50
14	14	317	A86	C2-C1	4.20	1.41	1.35
14	10	317	A86	C2-C1	4.20	1.41	1.35
11	8	309	CLA	O2A-CGA	4.20	1.45	1.33
11	12	307	CLA	C1D-ND	4.19	1.42	1.37
11	6	301	CLA	CHD-C1D	4.19	1.46	1.38
14	11	313	A86	O4-C38	4.19	1.44	1.35
14	14	321	A86	C17-C18	-4.19	1.46	1.52
14	15	320	A86	C10-C11	4.19	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	14	306	KC1	CHB-C1B	4.19	1.46	1.38
11	14	310	CLA	CHD-C1D	4.19	1.46	1.38
14	15	321	A86	C17-C18	-4.19	1.46	1.52
14	12	316	A86	O4-C38	4.18	1.44	1.35
12	13	311	KC1	C4D-ND	4.18	1.38	1.35
12	8	314	KC1	C1B-NB	-4.18	1.32	1.37
12	6	305	KC1	CHB-C1B	4.18	1.46	1.38
14	11	301	A86	C26-C27	4.18	1.41	1.35
14	11	313	A86	C26-C27	4.18	1.41	1.35
14	11	301	A86	O4-C38	4.18	1.44	1.35
11	14	313	CLA	CHD-C1D	4.18	1.46	1.38
14	10	301	A86	C7-C6	4.17	1.59	1.50
14	10	315	A86	C7-C6	4.17	1.59	1.50
11	10	305	CLA	CHD-C1D	4.17	1.46	1.38
11	8	309	CLA	CHD-C1D	4.17	1.46	1.38
11	13	302	CLA	CHD-C1D	4.17	1.46	1.38
12	13	305	KC1	OBD-CAD	4.17	1.28	1.22
11	11	309	CLA	O2A-CGA	4.17	1.45	1.33
14	14	316	A86	C7-C6	4.17	1.59	1.50
11	12	308	CLA	O2A-CGA	4.17	1.45	1.33
11	7	304	CLA	CHD-C1D	4.17	1.46	1.38
14	14	315	A86	O4-C38	4.16	1.44	1.35
11	15	303	CLA	CHD-C1D	4.16	1.46	1.38
12	8	307	KC1	OBD-CAD	4.16	1.28	1.22
12	10	310	KC1	C1B-NB	-4.16	1.32	1.37
12	8	313	KC1	CHB-C1B	4.16	1.46	1.38
11	7	309	CLA	CHD-C1D	4.16	1.46	1.38
14	8	315	A86	C9-C8	4.16	1.45	1.34
11	12	312	CLA	CHD-C1D	4.16	1.46	1.38
11	10	307	CLA	O2A-CGA	4.15	1.45	1.33
11	11	307	CLA	CHD-C1D	4.15	1.46	1.38
11	8	308	CLA	O2A-CGA	4.15	1.45	1.33
14	14	320	A86	C5-C6	4.15	1.41	1.35
14	14	318	A86	C2-C1	4.15	1.41	1.35
12	8	310	KC1	CHC-C4B	4.15	1.46	1.38
11	10	304	CLA	O2A-CGA	4.15	1.45	1.33
11	12	304	CLA	CHD-C1D	4.15	1.46	1.38
11	6	307	CLA	O2A-CGA	4.15	1.45	1.33
14	10	316	A86	O4-C38	4.15	1.44	1.35
11	11	308	CLA	CHD-C1D	4.14	1.46	1.38
14	15	316	A86	O4-C38	4.14	1.44	1.35
11	13	302	CLA	O2A-CGA	4.14	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	7	315	A86	C7-C6	4.14	1.59	1.50
14	14	318	A86	C7-C6	4.14	1.59	1.50
14	14	301	A86	C21-C20	4.14	1.58	1.51
14	13	315	A86	C7-C6	4.14	1.59	1.50
11	15	307	CLA	CHD-C1D	4.14	1.46	1.38
14	11	315	A86	C7-C6	4.14	1.59	1.50
14	12	314	A86	C26-C27	4.14	1.41	1.35
11	16	310	CLA	CHD-C1D	4.14	1.46	1.38
11	12	310	CLA	O2A-CGA	4.13	1.45	1.33
11	15	312	CLA	CHD-C4C	4.13	1.48	1.39
12	6	305	KC1	C1A-CHA	4.13	1.51	1.40
11	7	310	CLA	CHD-C1D	4.13	1.46	1.38
12	10	312	KC1	C1B-NB	-4.13	1.32	1.37
11	7	311	CLA	O2A-CGA	4.13	1.46	1.33
12	10	310	KC1	C4D-ND	4.13	1.38	1.35
11	16	301	CLA	O2A-CGA	4.12	1.45	1.33
11	11	305	CLA	CHD-C1D	4.12	1.46	1.38
14	16	312	A86	C10-C11	4.12	1.46	1.34
11	6	302	CLA	CHD-C1D	4.12	1.46	1.38
14	11	313	A86	C2-C1	4.12	1.41	1.35
14	14	321	A86	C21-C20	4.12	1.58	1.51
14	11	313	A86	C7-C6	4.12	1.59	1.50
14	11	314	A86	C7-C6	4.12	1.59	1.50
11	13	301	CLA	O2A-CGA	4.12	1.45	1.33
11	6	304	CLA	O2A-CGA	4.12	1.45	1.33
11	12	302	CLA	O2A-CGA	4.11	1.45	1.33
12	16	304	KC1	C4D-ND	4.11	1.38	1.35
14	14	319	A86	C10-C11	4.11	1.46	1.34
14	14	316	A86	C2-C1	4.11	1.41	1.35
12	12	313	KC1	C1A-NA	-4.11	1.30	1.38
12	13	305	KC1	C1A-CHA	4.11	1.51	1.40
11	13	303	CLA	CHD-C4C	4.11	1.48	1.39
14	6	317	A86	C7-C6	4.11	1.59	1.50
11	8	302	CLA	O2A-CGA	4.11	1.45	1.33
14	14	314	A86	C5-C6	4.10	1.41	1.35
12	16	311	KC1	C4D-ND	4.10	1.38	1.35
14	14	318	A86	C21-C20	4.10	1.58	1.51
11	7	310	CLA	O2A-CGA	4.10	1.45	1.33
11	16	302	CLA	O2A-CGA	4.10	1.45	1.33
12	14	306	KC1	C4D-ND	4.10	1.38	1.35
14	7	318	A86	C7-C6	4.09	1.59	1.50
11	6	307	CLA	CHD-C1D	4.09	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	10	309	CLA	CHD-C1D	4.09	1.46	1.38
14	15	321	A86	C2-C1	4.09	1.41	1.35
11	12	303	CLA	CHD-C1D	4.09	1.46	1.38
12	10	312	KC1	CHB-C1B	4.09	1.46	1.38
14	16	314	A86	C7-C6	4.09	1.59	1.50
14	14	301	A86	C2-C1	4.08	1.41	1.35
11	10	308	CLA	CHD-C1D	4.08	1.46	1.38
11	16	305	CLA	O2A-CGA	4.08	1.45	1.33
11	11	303	CLA	CHD-C1D	4.08	1.46	1.38
12	11	306	KC1	C4D-ND	4.08	1.38	1.35
12	8	311	KC1	C1B-NB	-4.08	1.32	1.37
14	12	316	A86	C7-C6	4.08	1.59	1.50
12	7	307	KC1	C4D-ND	4.08	1.38	1.35
11	14	309	CLA	CHD-C4C	4.08	1.48	1.39
11	11	308	CLA	O2A-CGA	4.08	1.45	1.33
12	11	311	KC1	C1A-CHA	4.07	1.51	1.40
12	13	308	KC1	C4D-ND	4.07	1.38	1.35
11	6	306	CLA	CHD-C1D	4.07	1.46	1.38
12	6	305	KC1	OBD-CAD	4.07	1.28	1.22
14	15	322	A86	C10-C11	4.07	1.46	1.34
11	8	308	CLA	CHD-C1D	4.07	1.46	1.38
14	10	317	A86	C10-C11	4.07	1.46	1.34
12	13	310	KC1	C4D-ND	4.07	1.38	1.35
12	12	309	KC1	C1A-CHA	4.07	1.51	1.40
12	16	311	KC1	C1B-NB	-4.07	1.32	1.37
11	16	307	CLA	O2A-CGA	4.06	1.45	1.33
11	6	311	CLA	CHD-C1D	4.06	1.46	1.38
12	12	311	KC1	CHB-C1B	4.06	1.46	1.38
14	8	318	A86	O4-C38	4.06	1.44	1.35
14	12	314	A86	C2-C1	4.06	1.41	1.35
12	7	312	KC1	CHB-C1B	4.06	1.46	1.38
11	12	306	CLA	O2A-CGA	4.06	1.45	1.33
14	15	316	A86	C19-C18	4.06	1.58	1.52
11	12	306	CLA	CHD-C1D	4.05	1.46	1.38
14	15	315	A86	C7-C6	4.05	1.59	1.50
12	13	306	KC1	OBD-CAD	4.05	1.28	1.22
14	12	314	A86	C21-C20	4.05	1.58	1.51
14	13	315	A86	C21-C20	4.05	1.58	1.51
14	8	318	A86	C7-C6	4.04	1.59	1.50
11	14	302	CLA	CHD-C4C	4.04	1.48	1.39
14	7	314	A86	C2-C1	4.04	1.41	1.35
11	6	303	CLA	CHD-C1D	4.04	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	10	303	CLA	CHD-C1D	4.04	1.46	1.38
14	7	315	A86	O4-C38	4.04	1.44	1.35
11	13	309	CLA	CHD-C4C	4.04	1.48	1.39
14	14	314	A86	C9-C10	4.04	1.56	1.43
11	7	303	CLA	O2A-CGA	4.04	1.45	1.33
12	12	313	KC1	C1B-NB	-4.04	1.32	1.37
12	12	311	KC1	C1B-NB	-4.03	1.32	1.37
14	14	319	A86	C21-C20	4.03	1.58	1.51
11	6	312	CLA	CHD-C4C	4.03	1.48	1.39
11	14	303	CLA	CHD-C4C	4.03	1.48	1.39
14	7	314	A86	C7-C6	4.03	1.59	1.50
11	15	302	CLA	CHD-C4C	4.03	1.48	1.39
11	11	305	CLA	CHD-C4C	4.03	1.48	1.39
11	10	308	CLA	O2A-CGA	4.02	1.45	1.33
12	16	311	KC1	C1A-CHA	4.02	1.51	1.40
11	14	307	CLA	CHD-C1D	4.02	1.46	1.38
11	15	309	CLA	CHD-C4C	4.02	1.48	1.39
14	7	318	A86	C2-C1	4.02	1.41	1.35
14	13	315	A86	C9-C10	4.02	1.55	1.43
14	10	302	A86	C17-C18	-4.02	1.46	1.52
11	16	306	CLA	CHD-C1D	4.01	1.46	1.38
11	10	304	CLA	CHD-C1D	4.01	1.46	1.38
12	10	306	KC1	OBD-CAD	4.01	1.27	1.22
11	15	308	CLA	CHD-C1D	4.01	1.46	1.38
14	8	318	A86	C21-C20	4.01	1.58	1.51
14	14	320	A86	C21-C20	4.01	1.58	1.51
14	13	313	A86	C10-C11	4.01	1.46	1.34
12	14	311	KC1	C1A-CHA	4.01	1.51	1.40
11	8	303	CLA	C1D-ND	4.01	1.42	1.37
11	8	301	CLA	O2A-CGA	4.01	1.45	1.33
14	10	316	A86	C7-C6	4.00	1.59	1.50
11	16	305	CLA	CHD-C1D	4.00	1.46	1.38
11	8	305	CLA	O2A-CGA	4.00	1.45	1.33
14	14	319	A86	C9-C10	4.00	1.55	1.43
12	8	306	KC1	C4D-ND	4.00	1.38	1.35
11	16	308	CLA	CHD-C4C	4.00	1.48	1.39
12	12	305	KC1	C1A-CHA	4.00	1.51	1.40
14	14	314	A86	C10-C11	4.00	1.46	1.34
14	11	313	A86	C21-C20	4.00	1.58	1.51
14	15	316	A86	C21-C20	3.99	1.58	1.51
11	14	313	CLA	O2A-CGA	3.99	1.45	1.33
12	10	306	KC1	C4D-ND	3.99	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	7	308	CLA	O2A-CGA	3.99	1.45	1.33
14	16	312	A86	C21-C20	3.99	1.58	1.51
12	6	308	KC1	C1B-NB	-3.99	1.32	1.37
12	11	310	KC1	C4D-ND	3.99	1.38	1.35
12	8	314	KC1	CHB-C1B	3.99	1.46	1.38
11	8	303	CLA	CHD-C1D	3.99	1.46	1.38
11	15	314	CLA	CHD-C1D	3.98	1.46	1.38
12	13	312	KC1	C1A-CHA	3.98	1.51	1.40
11	7	305	CLA	O2A-CGA	3.98	1.45	1.33
14	14	320	A86	C10-C11	3.98	1.46	1.34
14	15	321	A86	C21-C20	3.98	1.58	1.51
14	11	301	A86	C21-C20	3.98	1.58	1.51
11	7	305	CLA	CHD-C1D	3.98	1.46	1.38
12	6	305	KC1	C4D-ND	3.98	1.38	1.35
11	16	302	CLA	CHD-C1D	3.98	1.46	1.38
12	8	313	KC1	C1B-NB	-3.98	1.32	1.37
12	12	311	KC1	C4D-ND	3.97	1.38	1.35
14	14	315	A86	C2-C1	3.97	1.41	1.35
11	14	304	CLA	CHD-C4C	3.97	1.48	1.39
11	8	304	CLA	CHD-C1D	3.97	1.46	1.38
11	13	304	CLA	CHD-C4C	3.97	1.48	1.39
11	6	314	CLA	CHD-C4C	3.97	1.48	1.39
14	14	314	A86	C21-C20	3.97	1.58	1.51
12	14	308	KC1	C1A-CHA	3.97	1.51	1.40
11	14	312	CLA	CHD-C4C	3.96	1.48	1.39
12	12	311	KC1	C1A-CHA	3.96	1.51	1.40
11	7	311	CLA	CHD-C4C	3.96	1.48	1.39
14	13	313	A86	C5-C6	3.96	1.41	1.35
11	15	304	CLA	CHD-C4C	3.96	1.48	1.39
14	10	317	A86	C19-C18	3.95	1.58	1.52
12	6	305	KC1	C1B-NB	-3.95	1.32	1.37
11	14	313	CLA	CHD-C4C	3.95	1.48	1.39
14	15	315	A86	C9-C10	3.95	1.55	1.43
11	15	308	CLA	CHD-C4C	3.95	1.48	1.39
14	14	314	A86	C7-C6	3.95	1.59	1.50
12	10	310	KC1	CHB-C1B	3.95	1.46	1.38
14	14	321	A86	C10-C11	3.95	1.46	1.34
12	12	309	KC1	C1B-NB	-3.95	1.32	1.37
14	15	317	A86	C5-C6	3.95	1.41	1.35
11	11	309	CLA	CHD-C4C	3.95	1.48	1.39
11	6	304	CLA	CHD-C4C	3.95	1.48	1.39
14	7	318	A86	C17-C18	-3.94	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	6	310	KC1	C4D-ND	3.94	1.38	1.35
11	15	310	CLA	CHD-C4C	3.94	1.48	1.39
12	8	314	KC1	C1A-CHA	3.94	1.51	1.40
14	14	316	A86	C21-C20	3.94	1.58	1.51
14	14	319	A86	C5-C6	3.94	1.41	1.35
12	8	310	KC1	OBD-CAD	3.94	1.27	1.22
11	15	305	CLA	CHD-C4C	3.93	1.48	1.39
11	6	306	CLA	O2A-CGA	3.93	1.44	1.33
11	16	309	CLA	CHD-C4C	3.93	1.48	1.39
12	14	306	KC1	C1B-NB	-3.93	1.32	1.37
14	11	301	A86	C10-C11	3.93	1.46	1.34
11	12	307	CLA	CHD-C1D	3.93	1.46	1.38
12	6	309	KC1	C4D-ND	3.93	1.38	1.35
12	8	310	KC1	C1B-NB	-3.93	1.33	1.37
14	15	317	A86	C21-C20	3.93	1.58	1.51
14	7	318	A86	C10-C11	3.92	1.46	1.34
14	15	320	A86	C21-C20	3.92	1.58	1.51
12	11	306	KC1	C1A-CHA	3.92	1.51	1.40
12	7	312	KC1	C1B-NB	-3.92	1.33	1.37
11	10	308	CLA	CHD-C4C	3.92	1.48	1.39
11	15	303	CLA	CHD-C4C	3.92	1.48	1.39
11	12	308	CLA	CHD-C1D	3.92	1.46	1.38
12	7	307	KC1	C1A-CHA	3.92	1.51	1.40
14	14	321	A86	C5-C6	3.92	1.41	1.35
12	11	311	KC1	C1B-NB	-3.92	1.33	1.37
11	6	313	CLA	CHD-C4C	3.92	1.48	1.39
12	8	311	KC1	C1A-CHA	3.92	1.51	1.40
14	7	315	A86	C21-C20	3.91	1.58	1.51
14	8	315	A86	C7-C6	3.91	1.59	1.50
14	15	322	A86	C9-C10	3.91	1.55	1.43
14	14	315	A86	C26-C27	3.91	1.41	1.35
12	13	310	KC1	C1A-CHA	3.91	1.51	1.40
14	15	317	A86	C10-C11	3.90	1.45	1.34
14	10	302	A86	C21-C20	3.90	1.57	1.51
11	7	309	CLA	CHD-C4C	3.90	1.48	1.39
11	11	308	CLA	CHD-C4C	3.90	1.48	1.39
12	12	309	KC1	CHB-C1B	3.90	1.46	1.38
14	15	316	A86	C10-C11	3.90	1.45	1.34
14	14	314	A86	C19-C18	3.90	1.57	1.52
12	6	309	KC1	C1B-NB	-3.90	1.33	1.37
11	11	307	CLA	CHD-C4C	3.90	1.48	1.39
14	14	320	A86	C17-C18	-3.89	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	14	307	CLA	CHD-C4C	3.89	1.48	1.39
14	15	320	A86	C9-C10	3.89	1.55	1.43
11	12	307	CLA	O2A-CGA	3.89	1.45	1.33
14	12	314	A86	C7-C6	3.89	1.58	1.50
14	11	315	A86	C21-C20	3.89	1.57	1.51
11	7	303	CLA	CHD-C1D	3.89	1.45	1.38
14	14	320	A86	C9-C10	3.89	1.55	1.43
11	8	301	CLA	C1D-ND	3.89	1.42	1.37
14	10	316	A86	C26-C27	3.89	1.40	1.35
11	13	301	CLA	CHD-C1D	3.89	1.45	1.38
14	14	321	A86	C9-C10	3.89	1.55	1.43
12	6	308	KC1	OBD-CAD	3.89	1.27	1.22
11	15	306	CLA	CHD-C4C	3.88	1.48	1.39
14	15	320	A86	C19-C18	3.88	1.57	1.52
14	11	314	A86	C21-C20	3.88	1.57	1.51
11	6	301	CLA	CHD-C4C	3.88	1.48	1.39
11	12	304	CLA	CHD-C4C	3.88	1.48	1.39
14	10	317	A86	C9-C10	3.88	1.55	1.43
11	15	311	CLA	CHD-C4C	3.88	1.48	1.39
11	14	310	CLA	CHD-C4C	3.88	1.48	1.39
14	11	301	A86	C9-C10	3.88	1.55	1.43
14	13	313	A86	C7-C6	3.88	1.58	1.50
11	14	305	CLA	CHD-C4C	3.88	1.48	1.39
14	16	314	A86	C2-C1	3.88	1.40	1.35
11	10	309	CLA	CHD-C4C	3.88	1.48	1.39
11	10	311	CLA	CHD-C4C	3.88	1.48	1.39
14	15	322	A86	C5-C6	3.87	1.40	1.35
14	13	313	A86	C21-C20	3.87	1.57	1.51
12	6	310	KC1	C1B-NB	-3.87	1.33	1.37
11	12	321	CLA	CHD-C4C	3.87	1.48	1.39
14	12	314	A86	C9-C10	3.87	1.55	1.43
12	8	310	KC1	C1A-CHA	3.87	1.51	1.40
12	12	309	KC1	C4D-ND	3.87	1.38	1.35
12	16	304	KC1	C1A-CHA	3.87	1.51	1.40
11	15	314	CLA	CHD-C4C	3.87	1.48	1.39
12	8	314	KC1	C4D-ND	3.87	1.38	1.35
11	12	310	CLA	CHD-C1D	3.87	1.45	1.38
11	15	313	CLA	CHD-C4C	3.87	1.48	1.39
14	10	315	A86	C10-C11	3.87	1.45	1.34
11	10	305	CLA	CHD-C4C	3.87	1.48	1.39
11	7	308	CLA	CHD-C1D	3.86	1.45	1.38
14	6	317	A86	C5-C6	3.86	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	8	312	KC1	C4D-ND	3.86	1.38	1.35
14	7	318	A86	C9-C10	3.86	1.55	1.43
12	13	306	KC1	C1B-NB	-3.86	1.33	1.37
14	8	318	A86	C26-C27	3.86	1.40	1.35
14	10	315	A86	C9-C10	3.85	1.55	1.43
14	15	316	A86	C5-C6	3.85	1.40	1.35
12	13	310	KC1	CHC-C1C	3.85	1.48	1.39
12	6	309	KC1	C1A-CHA	3.85	1.50	1.40
12	8	313	KC1	C1A-CHA	3.84	1.50	1.40
14	10	301	A86	C26-C27	3.84	1.40	1.35
14	7	314	A86	O4-C38	3.84	1.43	1.35
12	13	306	KC1	CHC-C1C	3.84	1.48	1.39
11	16	307	CLA	CHD-C4C	3.84	1.48	1.39
11	7	304	CLA	CHD-C4C	3.84	1.48	1.39
12	8	313	KC1	CHC-C1C	3.84	1.48	1.39
12	14	306	KC1	CHC-C1C	3.83	1.48	1.39
11	7	303	CLA	CHD-C4C	3.83	1.48	1.39
14	14	315	A86	C21-C20	3.83	1.57	1.51
12	11	306	KC1	C1B-NB	-3.83	1.33	1.37
12	11	311	KC1	C4D-ND	3.83	1.38	1.35
11	13	302	CLA	CHD-C4C	3.83	1.48	1.39
11	11	303	CLA	CHD-C4C	3.83	1.48	1.39
12	10	312	KC1	C4D-ND	3.82	1.38	1.35
12	10	306	KC1	C1A-CHA	3.82	1.50	1.40
12	12	313	KC1	CHB-C1B	3.82	1.45	1.38
11	6	302	CLA	CHD-C4C	3.82	1.48	1.39
12	8	307	KC1	C4D-ND	3.82	1.38	1.35
12	11	304	KC1	C1B-NB	-3.82	1.33	1.37
14	16	314	A86	C9-C10	3.82	1.55	1.43
12	11	304	KC1	OBD-CAD	3.82	1.27	1.22
14	7	314	A86	C21-C20	3.82	1.57	1.51
11	13	307	CLA	CHD-C4C	3.82	1.47	1.39
14	8	315	A86	C21-C20	3.81	1.57	1.51
11	6	307	CLA	CHD-C4C	3.81	1.47	1.39
12	8	306	KC1	C1A-CHA	3.81	1.50	1.40
14	6	317	A86	C10-C11	3.81	1.45	1.34
14	15	317	A86	C9-C10	3.81	1.55	1.43
12	6	310	KC1	C1A-CHA	3.81	1.50	1.40
11	6	314	CLA	C3D-C2D	3.81	1.49	1.39
11	7	306	CLA	CHD-C1D	3.81	1.45	1.38
14	10	316	A86	C21-C20	3.80	1.57	1.51
12	8	310	KC1	C4B-NB	-3.80	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	12	312	CLA	CHD-C4C	3.80	1.47	1.39
12	12	305	KC1	C1B-NB	-3.80	1.33	1.37
12	13	311	KC1	C1B-NB	-3.80	1.33	1.37
11	6	311	CLA	CHD-C4C	3.80	1.47	1.39
14	11	314	A86	C10-C11	3.80	1.45	1.34
11	16	301	CLA	CHD-C1D	3.80	1.45	1.38
14	11	301	A86	C2-C1	3.79	1.40	1.35
11	6	303	CLA	CHD-C4C	3.79	1.47	1.39
14	16	312	A86	C9-C10	3.79	1.55	1.43
11	15	310	CLA	C3D-C2D	3.79	1.49	1.39
14	6	317	A86	C9-C10	3.79	1.55	1.43
11	6	312	CLA	C3D-C2D	3.79	1.49	1.39
14	14	317	A86	C21-C20	3.79	1.57	1.51
12	8	307	KC1	C1B-NB	-3.79	1.33	1.37
14	12	314	A86	C10-C11	3.79	1.45	1.34
11	14	309	CLA	C3D-C2D	3.79	1.49	1.39
11	13	303	CLA	C3D-C2D	3.78	1.49	1.39
11	8	308	CLA	CHD-C4C	3.78	1.47	1.39
14	13	313	A86	C9-C10	3.78	1.55	1.43
12	8	312	KC1	C1A-CHA	3.78	1.50	1.40
14	15	316	A86	C9-C10	3.78	1.55	1.43
14	10	315	A86	C21-C20	3.78	1.57	1.51
11	13	309	CLA	C3D-C2D	3.78	1.49	1.39
11	15	308	CLA	C3D-C2D	3.78	1.49	1.39
14	14	301	A86	C10-C11	3.78	1.45	1.34
11	16	302	CLA	CHD-C4C	3.78	1.47	1.39
11	8	309	CLA	C3D-C2D	3.78	1.49	1.39
12	11	310	KC1	C1B-NB	-3.78	1.33	1.37
12	13	308	KC1	C1A-CHA	3.78	1.50	1.40
12	13	311	KC1	C1A-CHA	3.78	1.50	1.40
14	11	313	A86	C17-C18	-3.77	1.46	1.52
11	15	314	CLA	OBD-CAD	3.77	1.29	1.22
14	10	301	A86	C21-C20	3.77	1.57	1.51
11	6	306	CLA	CHD-C4C	3.77	1.47	1.39
12	14	306	KC1	C1A-CHA	3.77	1.50	1.40
12	7	312	KC1	C4D-ND	3.77	1.38	1.35
12	13	306	KC1	C4D-ND	3.77	1.38	1.35
11	13	302	CLA	C3D-C2D	3.77	1.49	1.39
14	10	302	A86	C9-C10	3.76	1.55	1.43
11	16	303	CLA	CHD-C1D	3.76	1.45	1.38
11	7	306	CLA	CHD-C4C	3.76	1.47	1.39
12	6	305	KC1	CHC-C1C	3.76	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	10	310	KC1	C1A-CHA	3.76	1.50	1.40
11	13	301	CLA	CHD-C4C	3.76	1.47	1.39
12	7	312	KC1	C1A-CHA	3.75	1.50	1.40
14	14	318	A86	C9-C10	3.75	1.55	1.43
14	11	315	A86	C2-C1	3.75	1.40	1.35
11	8	302	CLA	CHD-C1D	3.75	1.45	1.38
11	8	302	CLA	CHD-C4C	3.75	1.47	1.39
11	16	303	CLA	CHD-C4C	3.75	1.47	1.39
11	15	311	CLA	OBD-CAD	3.75	1.28	1.22
12	11	306	KC1	CHC-C1C	3.75	1.47	1.39
11	11	309	CLA	C3D-C2D	3.75	1.49	1.39
12	10	306	KC1	C1B-NB	-3.75	1.33	1.37
11	15	307	CLA	C3D-C2D	3.75	1.49	1.39
12	16	304	KC1	C1B-NB	-3.75	1.33	1.37
14	12	316	A86	C9-C10	3.75	1.55	1.43
14	16	314	A86	C21-C20	3.75	1.57	1.51
12	12	305	KC1	C4D-ND	3.75	1.38	1.35
14	12	316	A86	C10-C11	3.75	1.45	1.34
11	14	312	CLA	C3D-C2D	3.75	1.49	1.39
14	10	302	A86	C19-C18	3.74	1.57	1.52
11	15	313	CLA	C3D-C2D	3.74	1.49	1.39
14	16	312	A86	C5-C6	3.74	1.40	1.35
14	13	315	A86	C5-C6	3.74	1.40	1.35
11	14	305	CLA	C3D-C2D	3.74	1.49	1.39
11	12	303	CLA	C3D-C2D	3.74	1.49	1.39
11	13	304	CLA	C3D-C2D	3.74	1.49	1.39
12	16	311	KC1	CHB-C1B	3.73	1.45	1.38
11	14	309	CLA	OBD-CAD	3.73	1.28	1.22
11	15	307	CLA	CHD-C4C	3.73	1.47	1.39
12	8	311	KC1	CHC-C1C	3.73	1.47	1.39
14	14	318	A86	C10-C11	3.73	1.45	1.34
11	6	306	CLA	C3D-C2D	3.73	1.49	1.39
11	8	309	CLA	CHD-C4C	3.73	1.47	1.39
12	11	310	KC1	C1A-CHA	3.73	1.50	1.40
12	10	312	KC1	C1A-CHA	3.73	1.50	1.40
11	7	310	CLA	CHD-C4C	3.73	1.47	1.39
11	12	308	CLA	CHD-C4C	3.73	1.47	1.39
11	16	306	CLA	CHD-C4C	3.73	1.47	1.39
11	15	309	CLA	OBD-CAD	3.73	1.28	1.22
14	15	321	A86	C10-C11	3.73	1.45	1.34
11	10	304	CLA	CHD-C4C	3.73	1.47	1.39
11	10	307	CLA	CHD-C4C	3.73	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	15	308	CLA	OBD-CAD	3.73	1.28	1.22
11	13	303	CLA	OBD-CAD	3.72	1.28	1.22
12	11	304	KC1	C4D-ND	3.72	1.38	1.35
14	16	312	A86	C2-C1	3.72	1.40	1.35
14	15	321	A86	C9-C10	3.72	1.55	1.43
11	14	303	CLA	C3D-C2D	3.72	1.49	1.39
11	14	304	CLA	C3D-C2D	3.72	1.49	1.39
11	11	305	CLA	C3D-C2D	3.72	1.49	1.39
11	12	304	CLA	C3D-C2D	3.72	1.49	1.39
11	16	309	CLA	C3D-C2D	3.72	1.49	1.39
12	7	312	KC1	CHC-C1C	3.71	1.47	1.39
11	8	301	CLA	C3D-C2D	3.71	1.49	1.39
11	6	307	CLA	C3D-C2D	3.71	1.49	1.39
11	16	308	CLA	OBD-CAD	3.71	1.28	1.22
11	15	305	CLA	C3D-C2D	3.71	1.49	1.39
14	11	313	A86	C10-C11	3.71	1.45	1.34
12	8	314	KC1	OBD-CAD	3.71	1.27	1.22
11	14	304	CLA	OBD-CAD	3.71	1.28	1.22
11	13	304	CLA	OBD-CAD	3.71	1.28	1.22
12	6	308	KC1	C4D-ND	3.70	1.38	1.35
14	8	318	A86	C9-C10	3.70	1.54	1.43
11	13	309	CLA	OBD-CAD	3.70	1.28	1.22
11	15	310	CLA	OBD-CAD	3.70	1.28	1.22
12	14	311	KC1	CHC-C1C	3.70	1.47	1.39
11	15	306	CLA	C3D-C2D	3.70	1.49	1.39
14	8	318	A86	C5-C6	3.70	1.40	1.35
11	16	310	CLA	CHD-C4C	3.70	1.47	1.39
12	11	310	KC1	CHC-C1C	3.70	1.47	1.39
14	15	315	A86	C21-C20	3.70	1.57	1.51
11	15	304	CLA	C3D-C2D	3.69	1.49	1.39
12	8	312	KC1	CHC-C1C	3.69	1.47	1.39
14	15	321	A86	C5-C6	3.69	1.40	1.35
11	16	305	CLA	C3D-C2D	3.69	1.49	1.39
11	8	303	CLA	CHD-C4C	3.69	1.47	1.39
11	16	309	CLA	OBD-CAD	3.69	1.28	1.22
12	13	308	KC1	C1B-NB	-3.69	1.33	1.37
11	6	312	CLA	OBD-CAD	3.68	1.28	1.22
11	13	307	CLA	C3D-C2D	3.68	1.49	1.39
11	14	313	CLA	C3D-C2D	3.68	1.49	1.39
11	12	321	CLA	C3D-C2D	3.68	1.49	1.39
11	15	311	CLA	C3D-C2D	3.68	1.49	1.39
14	14	315	A86	C9-C10	3.68	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	10	311	CLA	C3D-C2D	3.68	1.49	1.39
11	15	303	CLA	C3D-C2D	3.68	1.49	1.39
14	14	318	A86	C5-C6	3.68	1.40	1.35
11	8	303	CLA	C3D-C2D	3.68	1.49	1.39
14	12	316	A86	C21-C20	3.68	1.57	1.51
12	13	305	KC1	C1B-NB	-3.68	1.33	1.37
11	7	302	CLA	C1D-ND	3.68	1.42	1.37
12	14	311	KC1	C1B-NB	-3.68	1.33	1.37
14	14	317	A86	C9-C10	3.68	1.54	1.43
11	12	302	CLA	CHD-C1D	3.68	1.45	1.38
11	7	310	CLA	C3D-C2D	3.67	1.49	1.39
11	12	306	CLA	CHD-C4C	3.67	1.47	1.39
14	14	317	A86	C5-C6	3.67	1.40	1.35
11	10	303	CLA	C3D-C2D	3.67	1.49	1.39
11	15	302	CLA	C3D-C2D	3.67	1.49	1.39
11	15	306	CLA	OBD-CAD	3.67	1.28	1.22
11	10	307	CLA	CHD-C1D	3.67	1.45	1.38
11	14	313	CLA	OBD-CAD	3.67	1.28	1.22
14	10	315	A86	C19-C18	3.67	1.57	1.52
12	13	312	KC1	CHC-C1C	3.67	1.47	1.39
11	7	305	CLA	C3D-C2D	3.67	1.49	1.39
12	16	311	KC1	CHC-C1C	3.67	1.47	1.39
11	15	309	CLA	C3D-C2D	3.67	1.49	1.39
11	12	312	CLA	C3D-C2D	3.66	1.49	1.39
11	10	304	CLA	C3D-C2D	3.66	1.49	1.39
14	10	302	A86	C10-C11	3.66	1.45	1.34
12	6	309	KC1	CHC-C1C	3.66	1.47	1.39
14	10	316	A86	C2-C1	3.66	1.40	1.35
11	12	303	CLA	CHD-C4C	3.66	1.47	1.39
11	12	310	CLA	CHD-C4C	3.66	1.47	1.39
12	11	304	KC1	C1A-CHA	3.66	1.50	1.40
11	16	307	CLA	C3D-C2D	3.65	1.49	1.39
14	16	314	A86	C10-C11	3.65	1.45	1.34
11	13	307	CLA	OBD-CAD	3.65	1.28	1.22
14	11	313	A86	C9-C10	3.65	1.54	1.43
12	12	309	KC1	CHC-C1C	3.65	1.47	1.39
14	14	301	A86	C9-C10	3.65	1.54	1.43
13	15	319	DD6	C35-C34	3.65	1.58	1.52
12	10	312	KC1	CHC-C1C	3.64	1.47	1.39
11	11	308	CLA	OBD-CAD	3.64	1.28	1.22
11	8	304	CLA	C3D-C2D	3.64	1.49	1.39
11	8	301	CLA	CHD-C1D	3.64	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	16	301	CLA	C3D-C2D	3.64	1.49	1.39
11	6	302	CLA	C3D-C2D	3.64	1.49	1.39
14	10	302	A86	C2-C1	3.64	1.40	1.35
11	14	307	CLA	C3D-C2D	3.64	1.49	1.39
14	11	314	A86	C2-C1	3.64	1.40	1.35
14	14	316	A86	C9-C10	3.64	1.54	1.43
11	12	307	CLA	C3D-C2D	3.64	1.49	1.39
11	14	303	CLA	OBD-CAD	3.64	1.28	1.22
12	8	307	KC1	C1A-CHA	3.64	1.50	1.40
11	16	305	CLA	CHD-C4C	3.64	1.47	1.39
11	15	305	CLA	OBD-CAD	3.64	1.28	1.22
14	15	322	A86	C21-C20	3.64	1.57	1.51
14	15	322	A86	C19-C18	3.64	1.57	1.52
14	10	317	A86	C5-C6	3.64	1.40	1.35
12	8	311	KC1	C4D-ND	3.64	1.38	1.35
12	8	314	KC1	CHC-C1C	3.63	1.47	1.39
11	16	307	CLA	OBD-CAD	3.63	1.28	1.22
11	12	307	CLA	CHD-C4C	3.63	1.47	1.39
12	8	307	KC1	CHC-C1C	3.63	1.47	1.39
14	11	314	A86	C9-C10	3.63	1.54	1.43
11	15	313	CLA	OBD-CAD	3.63	1.28	1.22
12	14	308	KC1	C1B-NB	-3.63	1.33	1.37
12	13	308	KC1	CHC-C1C	3.63	1.47	1.39
11	6	301	CLA	C3D-C2D	3.63	1.49	1.39
12	16	304	KC1	CHC-C1C	3.63	1.47	1.39
11	16	301	CLA	CHD-C4C	3.63	1.47	1.39
11	7	305	CLA	CHD-C4C	3.63	1.47	1.39
11	12	306	CLA	C3D-C2D	3.62	1.49	1.39
11	14	310	CLA	OBD-CAD	3.62	1.28	1.22
12	13	306	KC1	C1A-CHA	3.62	1.50	1.40
14	14	315	A86	C10-C11	3.62	1.45	1.34
12	6	310	KC1	CHC-C1C	3.62	1.47	1.39
12	13	305	KC1	CHC-C1C	3.62	1.47	1.39
11	7	302	CLA	C3D-C2D	3.62	1.49	1.39
11	7	311	CLA	C3D-C2D	3.61	1.49	1.39
11	10	307	CLA	C3D-C2D	3.61	1.49	1.39
11	14	312	CLA	OBD-CAD	3.61	1.28	1.22
11	7	311	CLA	OBD-CAD	3.61	1.28	1.22
14	10	316	A86	C9-C10	3.61	1.54	1.43
11	10	305	CLA	C3D-C2D	3.61	1.49	1.39
11	16	303	CLA	C3D-C2D	3.61	1.49	1.39
11	14	307	CLA	OBD-CAD	3.60	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	10	303	CLA	CHD-C4C	3.60	1.47	1.39
11	15	302	CLA	OBD-CAD	3.60	1.28	1.22
14	12	314	A86	C5-C6	3.60	1.40	1.35
11	6	314	CLA	OBD-CAD	3.60	1.28	1.22
11	7	303	CLA	C3D-C2D	3.60	1.48	1.39
14	10	315	A86	C17-C18	-3.60	1.47	1.52
11	14	305	CLA	OBD-CAD	3.59	1.28	1.22
11	10	308	CLA	C3D-C2D	3.59	1.48	1.39
11	11	309	CLA	OBD-CAD	3.59	1.28	1.22
11	12	308	CLA	OBD-CAD	3.59	1.28	1.22
11	10	309	CLA	C3D-C2D	3.59	1.48	1.39
14	8	318	A86	C2-C1	3.59	1.40	1.35
14	10	316	A86	C10-C11	3.58	1.45	1.34
14	14	316	A86	C10-C11	3.58	1.45	1.34
14	7	314	A86	C9-C10	3.58	1.54	1.43
14	14	301	A86	C5-C6	3.58	1.40	1.35
11	16	308	CLA	C3D-C2D	3.57	1.48	1.39
11	6	311	CLA	OBD-CAD	3.57	1.28	1.22
11	15	314	CLA	C3D-C2D	3.57	1.48	1.39
11	10	311	CLA	OBD-CAD	3.57	1.28	1.22
11	13	301	CLA	C3D-C2D	3.57	1.48	1.39
11	8	308	CLA	C3D-C2D	3.57	1.48	1.39
11	10	309	CLA	OBD-CAD	3.57	1.28	1.22
11	11	307	CLA	C3D-C2D	3.57	1.48	1.39
11	13	301	CLA	OBD-CAD	3.57	1.28	1.22
11	6	303	CLA	C3D-C2D	3.57	1.48	1.39
14	14	315	A86	C5-C6	3.57	1.40	1.35
11	8	304	CLA	CHD-C4C	3.57	1.47	1.39
14	13	313	A86	C19-C18	3.57	1.57	1.52
14	11	315	A86	C9-C10	3.56	1.54	1.43
11	15	304	CLA	OBD-CAD	3.56	1.28	1.22
12	6	308	KC1	C1A-CHA	3.56	1.50	1.40
14	11	315	A86	C10-C11	3.56	1.44	1.34
14	14	319	A86	C19-C18	3.56	1.57	1.52
11	8	309	CLA	OBD-CAD	3.56	1.28	1.22
14	7	314	A86	C10-C11	3.56	1.44	1.34
11	16	302	CLA	C3D-C2D	3.55	1.48	1.39
13	15	318	DD6	C35-C34	3.55	1.58	1.52
11	14	302	CLA	OBD-CAD	3.54	1.28	1.22
11	7	302	CLA	CHD-C4C	3.54	1.47	1.39
11	16	306	CLA	C3D-C2D	3.54	1.48	1.39
11	7	308	CLA	CHD-C4C	3.54	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	15	312	CLA	OBD-CAD	3.54	1.28	1.22
12	13	310	KC1	C1B-NB	-3.54	1.33	1.37
12	10	312	KC1	C4B-NB	-3.53	1.33	1.37
11	8	305	CLA	CHD-C4C	3.53	1.47	1.39
14	14	321	A86	C19-C18	3.53	1.57	1.52
14	11	313	A86	C19-C18	3.53	1.57	1.52
12	14	308	KC1	CHC-C1C	3.53	1.47	1.39
12	13	311	KC1	CHC-C1C	3.53	1.47	1.39
11	7	308	CLA	C3D-C2D	3.52	1.48	1.39
14	7	318	A86	C21-C20	3.52	1.57	1.51
14	10	317	A86	C21-C20	3.52	1.57	1.51
14	14	317	A86	C10-C11	3.51	1.44	1.34
11	7	309	CLA	C3D-C2D	3.51	1.48	1.39
12	10	310	KC1	CHC-C1C	3.51	1.47	1.39
14	11	313	A86	C5-C6	3.51	1.40	1.35
11	14	310	CLA	C3D-C2D	3.51	1.48	1.39
11	6	313	CLA	C3D-C2D	3.50	1.48	1.39
14	13	315	A86	C19-C18	3.50	1.57	1.52
11	15	312	CLA	C3D-C2D	3.50	1.48	1.39
11	6	304	CLA	OBD-CAD	3.50	1.28	1.22
11	12	310	CLA	C3D-C2D	3.50	1.48	1.39
11	16	301	CLA	OBD-CAD	3.50	1.28	1.22
12	11	304	KC1	CHC-C1C	3.49	1.47	1.39
12	10	306	KC1	CHC-C1C	3.49	1.47	1.39
12	12	311	KC1	CHC-C1C	3.49	1.47	1.39
14	15	322	A86	C17-C18	-3.49	1.47	1.52
14	7	315	A86	C9-C10	3.49	1.54	1.43
14	6	317	A86	C21-C20	3.49	1.57	1.51
11	14	302	CLA	C3D-C2D	3.49	1.48	1.39
11	8	301	CLA	CHD-C4C	3.49	1.47	1.39
14	14	314	A86	C17-C18	-3.49	1.47	1.52
12	7	312	KC1	C4B-NB	-3.49	1.33	1.37
11	6	311	CLA	C3D-C2D	3.49	1.48	1.39
11	10	308	CLA	OBD-CAD	3.49	1.28	1.22
11	6	313	CLA	OBD-CAD	3.48	1.28	1.22
11	16	305	CLA	OBD-CAD	3.48	1.28	1.22
11	8	305	CLA	CHD-C1D	3.48	1.45	1.38
11	16	310	CLA	C3D-C2D	3.48	1.48	1.39
11	6	306	CLA	OBD-CAD	3.48	1.28	1.22
12	11	311	KC1	CHC-C1C	3.48	1.47	1.39
12	8	311	KC1	C4B-NB	-3.48	1.33	1.37
11	12	302	CLA	C3D-C2D	3.48	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	15	316	A86	C17-C18	-3.47	1.47	1.52
11	12	308	CLA	C3D-C2D	3.47	1.48	1.39
11	15	307	CLA	OBD-CAD	3.47	1.28	1.22
12	8	313	KC1	C4D-ND	3.47	1.38	1.35
11	6	304	CLA	C3D-C2D	3.47	1.48	1.39
12	7	307	KC1	CHC-C1C	3.47	1.47	1.39
14	7	315	A86	C10-C11	3.47	1.44	1.34
11	12	312	CLA	OBD-CAD	3.46	1.28	1.22
11	11	303	CLA	C3D-C2D	3.46	1.48	1.39
14	10	317	A86	C17-C18	-3.46	1.47	1.52
13	12	317	DD6	O2-C18	3.46	1.53	1.43
11	7	306	CLA	C3D-C2D	3.46	1.48	1.39
11	11	303	CLA	OBD-CAD	3.45	1.28	1.22
14	14	315	A86	C19-C18	3.45	1.57	1.52
12	6	308	KC1	C4B-NB	-3.45	1.33	1.37
11	11	308	CLA	C3D-C2D	3.45	1.48	1.39
12	8	310	KC1	CHC-C1C	3.44	1.47	1.39
12	12	305	KC1	CHC-C1C	3.44	1.47	1.39
11	8	308	CLA	OBD-CAD	3.44	1.28	1.22
13	11	312	DD6	O2-C18	3.44	1.53	1.43
14	12	316	A86	C5-C6	3.44	1.40	1.35
11	6	307	CLA	OBD-CAD	3.43	1.28	1.22
14	14	318	A86	C19-C18	3.43	1.57	1.52
12	12	309	KC1	C4B-NB	-3.43	1.33	1.37
12	8	306	KC1	CHC-C1C	3.42	1.47	1.39
11	8	302	CLA	C3D-C2D	3.42	1.48	1.39
11	7	309	CLA	OBD-CAD	3.41	1.28	1.22
14	10	301	A86	C2-C1	3.41	1.40	1.35
11	12	302	CLA	CHD-C4C	3.41	1.47	1.39
14	11	314	A86	C5-C6	3.41	1.40	1.35
12	8	314	KC1	C4B-NB	-3.41	1.33	1.37
12	13	312	KC1	C1B-NB	-3.41	1.33	1.37
14	15	320	A86	C17-C18	-3.41	1.47	1.52
11	16	303	CLA	OBD-CAD	3.41	1.28	1.22
14	8	315	A86	C26-C27	3.40	1.40	1.35
12	12	313	KC1	CHC-C1C	3.40	1.47	1.39
12	6	308	KC1	CHC-C1C	3.40	1.47	1.39
14	12	314	A86	C19-C18	3.40	1.57	1.52
14	11	314	A86	C17-C18	-3.39	1.47	1.52
14	10	302	A86	C5-C6	3.39	1.40	1.35
11	6	301	CLA	OBD-CAD	3.39	1.28	1.22
13	15	318	DD6	C-C1	3.39	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	13	314	DD6	O2-C18	3.38	1.53	1.43
11	7	306	CLA	OBD-CAD	3.37	1.28	1.22
12	7	307	KC1	C4B-NB	-3.37	1.33	1.37
11	7	305	CLA	OBD-CAD	3.37	1.28	1.22
11	12	306	CLA	OBD-CAD	3.37	1.28	1.22
11	7	302	CLA	CHD-C1D	3.37	1.44	1.38
14	15	317	A86	C19-C18	3.37	1.57	1.52
12	6	310	KC1	C4B-NB	-3.37	1.33	1.37
12	8	312	KC1	C1B-NB	-3.37	1.33	1.37
14	14	316	A86	C5-C6	3.37	1.40	1.35
14	15	321	A86	C19-C18	3.36	1.57	1.52
14	15	320	A86	C25-C24	3.36	1.43	1.34
14	11	315	A86	C5-C6	3.36	1.40	1.35
14	14	320	A86	C19-C18	3.36	1.57	1.52
11	7	302	CLA	OBD-CAD	3.36	1.28	1.22
14	16	314	A86	C5-C6	3.35	1.40	1.35
12	11	310	KC1	C4B-NB	-3.35	1.33	1.37
13	7	316	DD6	O2-C18	3.35	1.53	1.43
14	10	301	A86	C9-C10	3.34	1.53	1.43
11	10	303	CLA	OBD-CAD	3.34	1.28	1.22
11	8	305	CLA	C3D-C2D	3.34	1.48	1.39
13	7	317	DD6	O2-C18	3.33	1.53	1.43
12	12	313	KC1	C4B-NB	-3.33	1.33	1.37
11	8	303	CLA	OBD-CAD	3.33	1.28	1.22
13	15	319	DD6	O2-C18	3.33	1.53	1.43
11	7	304	CLA	C3D-C2D	3.33	1.48	1.39
11	12	304	CLA	OBD-CAD	3.33	1.28	1.22
12	11	311	KC1	C4B-NB	-3.32	1.33	1.37
11	12	302	CLA	OBD-CAD	3.32	1.28	1.22
11	11	305	CLA	OBD-CAD	3.32	1.28	1.22
13	15	318	DD6	O2-C18	3.31	1.53	1.43
14	8	318	A86	C10-C11	3.31	1.44	1.34
12	16	311	KC1	C4B-NB	-3.30	1.33	1.37
11	11	307	CLA	OBD-CAD	3.30	1.28	1.22
14	8	318	A86	C19-C18	3.30	1.57	1.52
11	13	302	CLA	OBD-CAD	3.30	1.28	1.22
11	7	310	CLA	OBD-CAD	3.30	1.28	1.22
11	8	301	CLA	OBD-CAD	3.29	1.28	1.22
12	12	305	KC1	C4B-NB	-3.29	1.33	1.37
13	7	313	DD6	O2-C18	3.29	1.53	1.43
13	10	313	DD6	O2-C18	3.29	1.53	1.43
13	10	314	DD6	O2-C18	3.28	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	7	301	DD6	C-C1	3.28	1.57	1.50
14	7	318	A86	C5-C6	3.28	1.40	1.35
12	11	304	KC1	C4B-NB	-3.28	1.33	1.37
12	16	304	KC1	C4B-NB	-3.28	1.33	1.37
14	10	315	A86	C5-C6	3.28	1.40	1.35
14	15	322	A86	C25-C24	3.27	1.43	1.34
13	15	319	DD6	C-C1	3.27	1.57	1.50
13	7	301	DD6	O2-C18	3.27	1.53	1.43
13	6	316	DD6	O2-C18	3.26	1.53	1.43
14	10	301	A86	C10-C11	3.26	1.44	1.34
14	14	321	A86	C25-C24	3.25	1.42	1.34
14	15	322	A86	C14-C15	3.25	1.59	1.52
12	8	307	KC1	C4B-NB	-3.24	1.33	1.37
14	6	317	A86	C19-C18	3.24	1.57	1.52
14	10	302	A86	C25-C24	3.24	1.42	1.34
14	7	315	A86	C26-C27	3.24	1.40	1.35
14	10	316	A86	C5-C6	3.24	1.40	1.35
12	8	313	KC1	C4B-NB	-3.23	1.33	1.37
14	15	317	A86	C25-C24	3.22	1.42	1.34
11	10	304	CLA	OBD-CAD	3.22	1.28	1.22
12	11	306	KC1	C4B-NB	-3.22	1.33	1.37
12	13	310	KC1	C4B-NB	-3.21	1.33	1.37
13	6	315	DD6	O2-C18	3.20	1.52	1.43
12	13	311	KC1	C4A-C3A	3.20	1.50	1.44
13	16	313	DD6	O2-C18	3.19	1.52	1.43
14	7	315	A86	C2-C1	3.19	1.40	1.35
11	12	321	CLA	OBD-CAD	3.19	1.28	1.22
14	12	316	A86	C25-C24	3.18	1.42	1.34
14	8	315	A86	C9-C10	3.18	1.53	1.43
14	14	301	A86	C19-C18	3.18	1.56	1.52
13	8	317	DD6	O2-C18	3.17	1.52	1.43
11	8	301	CLA	C4B-NB	-3.17	1.32	1.35
11	6	302	CLA	OBD-CAD	3.17	1.27	1.22
13	6	318	DD6	O2-C18	3.17	1.52	1.43
13	16	313	DD6	C-C1	3.16	1.57	1.50
14	14	320	A86	C25-C24	3.16	1.42	1.34
13	7	316	DD6	C-C1	3.16	1.57	1.50
13	6	318	DD6	C35-C34	3.16	1.57	1.52
14	14	317	A86	C19-C18	3.16	1.56	1.52
13	12	315	DD6	O2-C18	3.16	1.52	1.43
14	16	312	A86	C19-C18	3.15	1.56	1.52
13	7	317	DD6	C-C1	3.15	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	8	303	CLA	C1B-NB	-3.15	1.32	1.35
14	10	301	A86	C19-C18	3.15	1.56	1.52
11	10	305	CLA	OBD-CAD	3.15	1.27	1.22
14	8	315	A86	C10-C11	3.15	1.43	1.34
13	12	317	DD6	C-C1	3.15	1.57	1.50
11	16	310	CLA	OBD-CAD	3.14	1.27	1.22
13	7	301	DD6	C35-C34	3.14	1.57	1.52
13	7	317	DD6	C35-C34	3.14	1.57	1.52
14	13	315	A86	C25-C24	3.14	1.42	1.34
14	15	316	A86	C25-C24	3.13	1.42	1.34
11	12	307	CLA	C1B-NB	-3.13	1.32	1.35
13	8	316	DD6	O2-C18	3.13	1.52	1.43
12	12	311	KC1	C4B-NB	-3.13	1.33	1.37
11	8	304	CLA	OBD-CAD	3.13	1.27	1.22
12	14	308	KC1	C4D-ND	3.13	1.38	1.35
14	15	315	A86	C25-C24	3.11	1.42	1.34
12	6	305	KC1	C4B-NB	-3.11	1.34	1.37
14	7	318	A86	C19-C18	3.11	1.56	1.52
14	7	314	A86	C5-C6	3.10	1.39	1.35
11	12	310	CLA	OBD-CAD	3.10	1.27	1.22
14	6	317	A86	C25-C24	3.10	1.42	1.34
14	14	314	A86	C25-C24	3.10	1.42	1.34
14	14	318	A86	C25-C24	3.09	1.42	1.34
11	6	313	CLA	C1B-NB	-3.09	1.32	1.35
11	6	303	CLA	OBD-CAD	3.09	1.27	1.22
14	11	301	A86	C5-C6	3.09	1.39	1.35
14	10	317	A86	C25-C24	3.09	1.42	1.34
14	13	313	A86	C25-C24	3.09	1.42	1.34
13	11	312	DD6	C-C1	3.09	1.57	1.50
13	10	313	DD6	C9-C8	3.09	1.42	1.34
14	8	315	A86	C2-C1	3.09	1.39	1.35
12	8	312	KC1	C4B-NB	-3.08	1.34	1.37
11	15	303	CLA	OBD-CAD	3.08	1.27	1.22
12	10	310	KC1	C4B-NB	-3.08	1.34	1.37
13	7	313	DD6	C-C1	3.07	1.57	1.50
12	10	306	KC1	C4B-NB	-3.07	1.34	1.37
14	7	318	A86	C25-C24	3.07	1.42	1.34
11	16	306	CLA	OBD-CAD	3.07	1.27	1.22
13	8	316	DD6	C-C1	3.06	1.57	1.50
14	10	315	A86	C25-C24	3.06	1.42	1.34
13	13	314	DD6	C9-C8	3.06	1.42	1.34
12	13	308	KC1	C4B-NB	-3.05	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	12	315	DD6	C-C1	3.05	1.57	1.50
14	11	301	A86	C19-C18	3.04	1.56	1.52
12	13	306	KC1	C4B-NB	-3.04	1.34	1.37
12	8	310	KC1	C4D-ND	3.04	1.37	1.35
14	14	319	A86	C25-C24	3.04	1.42	1.34
11	6	306	CLA	C1B-NB	-3.03	1.32	1.35
13	7	313	DD6	C26-C27	-3.03	1.30	1.37
11	16	306	CLA	C1B-NB	-3.03	1.32	1.35
11	7	310	CLA	C1B-NB	-3.02	1.32	1.35
14	14	316	A86	C25-C24	3.01	1.42	1.34
12	14	311	KC1	C4B-NB	-3.01	1.34	1.37
13	11	312	DD6	C9-C8	3.01	1.42	1.34
14	15	315	A86	C24-C1	3.01	1.52	1.45
14	11	315	A86	C25-C24	3.01	1.42	1.34
13	6	316	DD6	C-C1	3.01	1.57	1.50
13	6	316	DD6	C9-C8	3.00	1.42	1.34
14	16	312	A86	C25-C24	3.00	1.42	1.34
11	12	307	CLA	OBD-CAD	3.00	1.27	1.22
13	7	301	DD6	C9-C8	3.00	1.42	1.34
14	15	321	A86	C25-C24	3.00	1.42	1.34
13	6	315	DD6	C-C1	3.00	1.57	1.50
13	8	317	DD6	C-C1	3.00	1.57	1.50
14	8	318	A86	O-C13	-3.00	1.17	1.23
13	12	317	DD6	C35-C34	3.00	1.57	1.52
13	16	313	DD6	C9-C8	2.99	1.42	1.34
13	10	314	DD6	C-C1	2.99	1.57	1.50
14	14	301	A86	C25-C24	2.98	1.42	1.34
14	10	317	A86	C14-C15	2.98	1.58	1.52
13	12	317	DD6	C9-C8	2.98	1.42	1.34
14	11	315	A86	C19-C18	2.97	1.56	1.52
14	15	315	A86	C19-C18	2.97	1.56	1.52
12	8	306	KC1	C4B-NB	-2.96	1.34	1.37
13	11	312	DD6	C35-C34	2.96	1.57	1.52
13	10	313	DD6	C-C1	2.96	1.57	1.50
12	10	310	KC1	CHB-C4A	-2.95	1.32	1.39
13	6	318	DD6	C-C1	2.95	1.57	1.50
11	10	307	CLA	OBD-CAD	2.95	1.27	1.22
14	15	315	A86	C14-C15	2.94	1.58	1.52
13	6	315	DD6	C35-C34	2.94	1.57	1.52
13	7	316	DD6	C9-C8	2.94	1.42	1.34
14	11	313	A86	C25-C24	2.94	1.42	1.34
12	6	309	KC1	C4B-NB	-2.93	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	8	302	CLA	C1B-NB	-2.93	1.32	1.35
11	12	303	CLA	C1B-NB	-2.93	1.32	1.35
13	7	313	DD6	C35-C34	2.93	1.57	1.52
13	8	317	DD6	C35-C34	2.93	1.57	1.52
14	16	314	A86	C14-C15	2.93	1.58	1.52
14	14	317	A86	C25-C24	2.92	1.42	1.34
12	14	306	KC1	C4C-C3C	2.92	1.50	1.45
14	8	315	A86	C19-C18	2.91	1.56	1.52
12	10	312	KC1	CHB-C4A	-2.91	1.32	1.39
13	15	318	DD6	C9-C8	2.91	1.42	1.34
11	8	309	CLA	C1B-NB	-2.90	1.32	1.35
13	13	314	DD6	C-C1	2.90	1.56	1.50
12	13	305	KC1	C4B-NB	-2.90	1.34	1.37
11	11	308	CLA	C1B-NB	-2.90	1.32	1.35
14	14	321	A86	C24-C1	2.90	1.52	1.45
13	6	315	DD6	C9-C8	2.89	1.42	1.34
13	15	319	DD6	C9-C8	2.89	1.42	1.34
13	13	314	DD6	C35-C34	2.89	1.57	1.52
11	7	308	CLA	OBD-CAD	2.89	1.27	1.22
11	16	302	CLA	OBD-CAD	2.88	1.27	1.22
13	10	314	DD6	C9-C8	2.88	1.42	1.34
14	15	320	A86	C24-C1	2.88	1.52	1.45
11	8	302	CLA	OBD-CAD	2.88	1.27	1.22
12	8	312	KC1	C4A-C3A	2.87	1.50	1.44
14	10	301	A86	C25-C24	2.87	1.42	1.34
12	8	314	KC1	C2A-C1A	2.87	1.53	1.44
14	11	314	A86	C25-C24	2.87	1.42	1.34
14	16	314	A86	C25-C24	2.87	1.42	1.34
11	6	301	CLA	C1B-NB	-2.86	1.32	1.35
12	13	312	KC1	C4B-NB	-2.86	1.34	1.37
13	7	316	DD6	C35-C34	2.86	1.57	1.52
13	8	316	DD6	C9-C8	2.85	1.41	1.34
14	15	322	A86	C24-C1	2.85	1.52	1.45
12	14	308	KC1	C4C-C3C	2.85	1.50	1.45
13	11	312	DD6	C26-C27	-2.85	1.31	1.37
12	12	309	KC1	CHB-C4A	-2.84	1.32	1.39
11	8	305	CLA	C3D-C4D	-2.84	1.37	1.44
14	6	317	A86	C24-C1	2.84	1.52	1.45
14	13	315	A86	C-C1	2.84	1.56	1.50
13	16	313	DD6	C35-C34	2.83	1.57	1.52
13	7	316	DD6	C26-C27	-2.83	1.31	1.37
12	13	305	KC1	CAA-C2A	2.83	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	7	305	CLA	C1B-NB	-2.83	1.32	1.35
14	11	301	A86	C25-C24	2.82	1.41	1.34
11	10	303	CLA	C1B-NB	-2.82	1.32	1.35
12	7	312	KC1	CHB-C4A	-2.82	1.32	1.39
14	10	316	A86	C19-C18	2.82	1.56	1.52
14	7	315	A86	C19-C18	2.81	1.56	1.52
11	6	307	CLA	C1B-NB	-2.81	1.32	1.35
14	12	314	A86	C25-C24	2.80	1.41	1.34
13	12	315	DD6	C9-C8	2.80	1.41	1.34
12	16	311	KC1	CHB-C4A	-2.80	1.32	1.39
11	12	303	CLA	OBD-CAD	2.80	1.27	1.22
11	13	309	CLA	C4D-CHA	2.80	1.48	1.38
11	7	302	CLA	C1B-NB	-2.80	1.32	1.35
11	12	302	CLA	C4B-NB	-2.80	1.32	1.35
11	7	303	CLA	OBD-CAD	2.79	1.27	1.22
12	16	311	KC1	C2A-C1A	2.79	1.53	1.44
12	6	305	KC1	CAA-C2A	2.79	1.55	1.46
14	8	318	A86	C25-C24	2.79	1.41	1.34
11	12	306	CLA	C1B-NB	-2.78	1.32	1.35
14	10	315	A86	C24-C1	2.78	1.51	1.45
12	14	306	KC1	CHB-C4A	-2.78	1.32	1.39
14	15	322	A86	C-C1	2.77	1.56	1.50
14	13	315	A86	C24-C1	2.77	1.51	1.45
12	13	310	KC1	C2A-C1A	2.77	1.53	1.44
14	13	313	A86	C24-C1	2.77	1.51	1.45
14	10	301	A86	O-C13	-2.77	1.17	1.23
14	12	316	A86	C19-C18	2.77	1.56	1.52
12	6	308	KC1	CHB-C4A	-2.76	1.32	1.39
12	6	309	KC1	CHB-C4A	-2.76	1.32	1.39
11	8	301	CLA	C1B-NB	-2.76	1.32	1.35
13	12	317	DD6	C26-C27	-2.76	1.31	1.37
12	8	314	KC1	CHB-C4A	-2.76	1.32	1.39
14	14	321	A86	C-C1	2.76	1.56	1.50
14	14	315	A86	C25-C24	2.76	1.41	1.34
13	8	317	DD6	C9-C8	2.75	1.41	1.34
12	8	313	KC1	CHB-C4A	-2.75	1.32	1.39
14	11	301	A86	O-C13	-2.75	1.17	1.23
14	15	316	A86	C24-C1	2.75	1.51	1.45
14	7	315	A86	C5-C6	2.75	1.39	1.35
14	13	313	A86	C-C1	2.75	1.56	1.50
14	7	314	A86	C25-C24	2.74	1.41	1.34
14	10	316	A86	C25-C24	2.74	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	16	304	KC1	C4A-C3A	2.74	1.49	1.44
14	15	320	A86	C-C1	2.74	1.56	1.50
14	14	320	A86	C-C1	2.74	1.56	1.50
14	7	315	A86	O-C13	-2.73	1.17	1.23
12	12	313	KC1	CAA-C2A	2.73	1.55	1.46
11	15	312	CLA	C1B-NB	-2.73	1.32	1.35
11	10	308	CLA	C1B-NB	-2.73	1.32	1.35
11	12	302	CLA	C1B-NB	-2.72	1.32	1.35
14	14	320	A86	C24-C1	2.72	1.51	1.45
11	14	307	CLA	C4C-C3C	2.72	1.49	1.45
14	14	316	A86	C19-C18	2.71	1.56	1.52
11	8	308	CLA	C1B-NB	-2.71	1.32	1.35
14	7	314	A86	C19-C18	2.71	1.56	1.52
13	10	314	DD6	C26-C27	-2.71	1.31	1.37
14	10	315	A86	C-C1	2.71	1.56	1.50
11	13	307	CLA	C4D-CHA	2.71	1.48	1.38
11	15	306	CLA	C4D-CHA	2.70	1.48	1.38
13	7	313	DD6	C9-C8	2.70	1.41	1.34
14	10	316	A86	C14-C15	2.70	1.58	1.52
14	15	316	A86	C14-C15	2.70	1.58	1.52
14	15	317	A86	C24-C1	2.70	1.51	1.45
11	15	308	CLA	C4D-CHA	2.70	1.48	1.38
12	12	311	KC1	CHB-C4A	-2.70	1.33	1.39
11	8	305	CLA	C4B-NB	-2.70	1.32	1.35
14	7	314	A86	O-C13	-2.70	1.17	1.23
11	8	304	CLA	C1B-NB	-2.69	1.32	1.35
11	7	308	CLA	C1B-NB	-2.69	1.32	1.35
14	10	316	A86	O-C13	-2.69	1.17	1.23
11	13	304	CLA	C4D-CHA	2.69	1.48	1.38
12	6	305	KC1	CHB-C4A	-2.69	1.33	1.39
11	14	303	CLA	C4D-CHA	2.69	1.48	1.38
11	15	303	CLA	C4D-CHA	2.69	1.48	1.38
12	14	308	KC1	C4B-NB	-2.68	1.34	1.37
13	7	317	DD6	C9-C8	2.68	1.41	1.34
14	12	316	A86	C24-C1	2.68	1.51	1.45
12	13	312	KC1	C4A-C3A	2.68	1.49	1.44
14	7	318	A86	C14-C15	2.68	1.58	1.52
14	7	318	A86	O-C13	-2.68	1.17	1.23
11	8	305	CLA	OBD-CAD	2.68	1.27	1.22
11	6	314	CLA	C4D-CHA	2.68	1.47	1.38
12	14	311	KC1	C2A-C1A	2.68	1.52	1.44
13	6	318	DD6	C26-C27	-2.68	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	7	303	CLA	C1B-NB	-2.67	1.32	1.35
11	10	307	CLA	C1B-NB	-2.67	1.32	1.35
14	10	301	A86	C5-C6	2.67	1.39	1.35
14	15	315	A86	C-C1	2.67	1.56	1.50
12	14	306	KC1	C3B-C4B	2.67	1.50	1.46
11	15	311	CLA	C4D-CHA	2.67	1.47	1.38
12	11	311	KC1	C2A-C1A	2.67	1.52	1.44
12	6	305	KC1	C2A-C1A	2.67	1.52	1.44
14	8	315	A86	O-C13	-2.67	1.17	1.23
11	14	309	CLA	C4D-CHA	2.67	1.47	1.38
11	6	312	CLA	C4D-CHA	2.66	1.47	1.38
11	12	321	CLA	C4D-CHA	2.66	1.47	1.38
11	13	307	CLA	C1B-NB	-2.66	1.32	1.35
14	10	301	A86	C-C1	2.66	1.56	1.50
14	7	318	A86	C24-C1	2.66	1.51	1.45
14	15	316	A86	C-C1	2.66	1.56	1.50
14	6	317	A86	O-C13	-2.66	1.17	1.23
12	16	304	KC1	CHB-C4A	-2.66	1.33	1.39
11	8	302	CLA	C4B-NB	-2.66	1.32	1.35
14	15	317	A86	C-C1	2.66	1.56	1.50
14	15	321	A86	C-C1	2.66	1.56	1.50
12	13	308	KC1	CHB-C4A	-2.66	1.33	1.39
11	15	309	CLA	C4D-CHA	2.66	1.47	1.38
13	6	315	DD6	C26-C27	-2.65	1.31	1.37
11	15	305	CLA	C4D-CHA	2.65	1.47	1.38
14	8	318	A86	C-C1	2.65	1.56	1.50
12	12	309	KC1	C2A-C1A	2.65	1.52	1.44
12	13	311	KC1	C2A-C1A	2.65	1.52	1.44
13	7	317	DD6	C26-C27	-2.64	1.31	1.37
12	14	308	KC1	C4A-C3A	2.64	1.49	1.44
12	8	306	KC1	CHB-C4A	-2.64	1.33	1.39
14	14	318	A86	C24-C1	2.64	1.51	1.45
11	6	302	CLA	C1B-NB	-2.64	1.32	1.35
14	15	320	A86	C14-C15	2.64	1.57	1.52
14	14	316	A86	C-C1	2.64	1.56	1.50
11	16	307	CLA	C4D-CHA	2.64	1.47	1.38
14	10	317	A86	C24-C1	2.64	1.51	1.45
13	8	316	DD6	C26-C27	-2.64	1.31	1.37
14	14	318	A86	C-C1	2.63	1.56	1.50
11	15	310	CLA	C4D-CHA	2.63	1.47	1.38
14	10	301	A86	C24-C1	2.63	1.51	1.45
11	14	305	CLA	C4D-CHA	2.63	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	16	314	A86	O-C13	-2.63	1.17	1.23
11	7	309	CLA	C1B-NB	-2.63	1.32	1.35
11	16	310	CLA	C3D-C4D	-2.63	1.38	1.44
11	8	308	CLA	C4D-CHA	2.63	1.47	1.38
14	14	317	A86	O-C13	-2.62	1.17	1.23
12	11	306	KC1	CHB-C4A	-2.62	1.33	1.39
11	6	302	CLA	C3D-C4D	-2.62	1.38	1.44
11	10	303	CLA	C4D-CHA	2.62	1.47	1.38
12	8	311	KC1	CHB-C4A	-2.62	1.33	1.39
16	8	323	LMG	C3-C2	2.62	1.59	1.52
12	11	311	KC1	C4A-C3A	2.62	1.49	1.44
11	10	305	CLA	C3D-C4D	-2.62	1.38	1.44
11	16	309	CLA	C4D-CHA	2.62	1.47	1.38
11	16	310	CLA	O1D-CGD	2.62	1.27	1.21
14	6	317	A86	C-C1	2.62	1.56	1.50
14	14	314	A86	O-C13	-2.61	1.17	1.23
12	8	314	KC1	C4A-C3A	2.61	1.49	1.44
11	16	306	CLA	C3D-C4D	-2.61	1.38	1.44
11	11	309	CLA	C4D-CHA	2.61	1.47	1.38
12	14	311	KC1	C4A-C3A	2.61	1.49	1.44
11	13	302	CLA	C4D-CHA	2.61	1.47	1.38
14	14	301	A86	C24-C1	2.61	1.51	1.45
11	16	305	CLA	C4D-CHA	2.61	1.47	1.38
12	16	311	KC1	C4A-C3A	2.61	1.49	1.44
11	15	304	CLA	C4D-CHA	2.61	1.47	1.38
11	12	302	CLA	C1C-NC	-2.61	1.33	1.37
11	14	312	CLA	C4D-CHA	2.61	1.47	1.38
12	7	307	KC1	CHB-C4A	-2.61	1.33	1.39
16	8	321	LMG	O8-C9	-2.60	1.39	1.45
12	14	306	KC1	C4A-C3A	2.60	1.49	1.44
14	7	314	A86	C-C1	2.60	1.56	1.50
12	8	310	KC1	CHB-C4A	-2.60	1.33	1.39
12	13	310	KC1	C4A-C3A	2.60	1.49	1.44
12	11	311	KC1	CHB-C4A	-2.60	1.33	1.39
13	7	301	DD6	C26-C27	-2.60	1.31	1.37
11	6	307	CLA	C4D-CHA	2.60	1.47	1.38
12	13	308	KC1	C4A-C3A	2.60	1.49	1.44
14	13	315	A86	C14-C15	2.60	1.57	1.52
11	8	303	CLA	C3D-C4D	-2.60	1.38	1.44
11	14	310	CLA	C4D-CHA	2.60	1.47	1.38
11	15	308	CLA	C4C-C3C	2.59	1.49	1.45
12	14	306	KC1	C4B-NB	-2.59	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	15	313	CLA	C4D-CHA	2.59	1.47	1.38
14	12	316	A86	C-C1	2.59	1.56	1.50
14	16	314	A86	C-C1	2.59	1.56	1.50
13	6	318	DD6	C9-C8	2.59	1.41	1.34
12	13	312	KC1	C2A-C1A	2.59	1.52	1.44
12	11	304	KC1	CHB-C4A	-2.59	1.33	1.39
11	6	311	CLA	C1B-NB	-2.59	1.32	1.35
12	13	306	KC1	C4A-C3A	2.59	1.49	1.44
11	6	313	CLA	C4D-CHA	2.59	1.47	1.38
14	10	316	A86	C-C1	2.59	1.56	1.50
14	15	322	A86	O-C13	-2.59	1.17	1.23
11	12	307	CLA	C3D-C4D	-2.58	1.38	1.44
11	12	303	CLA	C4D-CHA	2.58	1.47	1.38
12	11	310	KC1	C4A-C3A	2.58	1.49	1.44
11	8	301	CLA	C1C-NC	-2.58	1.34	1.37
12	16	304	KC1	C2A-C1A	2.58	1.52	1.44
11	10	307	CLA	C4D-CHA	2.58	1.47	1.38
14	6	317	A86	O1-C15	2.58	1.50	1.45
14	10	302	A86	O-C13	-2.58	1.17	1.23
13	12	315	DD6	C26-C27	-2.58	1.31	1.37
13	10	313	DD6	C35-C34	2.58	1.56	1.52
11	10	304	CLA	C4D-CHA	2.58	1.47	1.38
11	15	307	CLA	C4D-CHA	2.58	1.47	1.38
14	12	316	A86	O-C13	-2.57	1.17	1.23
14	11	301	A86	C-C1	2.57	1.56	1.50
14	8	315	A86	C25-C24	2.57	1.41	1.34
13	8	316	DD6	C35-C34	2.57	1.56	1.52
14	10	302	A86	C14-C15	2.57	1.57	1.52
13	6	316	DD6	C26-C27	-2.57	1.31	1.37
14	14	316	A86	O-C13	-2.57	1.17	1.23
11	6	306	CLA	C4D-CHA	2.57	1.47	1.38
14	14	317	A86	C24-C1	2.57	1.51	1.45
11	16	308	CLA	C4D-CHA	2.57	1.47	1.38
13	12	315	DD6	C35-C34	2.57	1.56	1.52
11	15	312	CLA	C4D-CHA	2.57	1.47	1.38
11	7	306	CLA	C1B-NB	-2.57	1.32	1.35
11	16	301	CLA	C4D-CHA	2.57	1.47	1.38
14	11	313	A86	C14-C15	2.57	1.57	1.52
14	7	315	A86	C25-C24	2.56	1.41	1.34
11	10	304	CLA	C1B-NB	-2.56	1.32	1.35
11	11	308	CLA	C3D-C4D	-2.56	1.38	1.44
11	7	310	CLA	C4D-CHA	2.56	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	11	306	KC1	C4A-C3A	2.56	1.49	1.44
11	13	301	CLA	C4D-CHA	2.56	1.47	1.38
11	12	306	CLA	C4D-CHA	2.56	1.47	1.38
11	8	302	CLA	C3D-C4D	-2.55	1.38	1.44
14	10	302	A86	C24-C1	2.55	1.51	1.45
12	6	310	KC1	CHB-C4A	-2.55	1.33	1.39
13	13	314	DD6	C26-C27	-2.55	1.31	1.37
11	6	311	CLA	C3D-C4D	-2.55	1.38	1.44
11	14	305	CLA	C1B-NB	-2.55	1.32	1.35
11	7	309	CLA	C4D-CHA	2.55	1.47	1.38
11	6	301	CLA	C4D-CHA	2.55	1.47	1.38
12	8	307	KC1	CHB-C4A	-2.55	1.33	1.39
12	13	311	KC1	C4B-NB	-2.55	1.34	1.37
11	13	303	CLA	C4D-CHA	2.55	1.47	1.38
14	7	314	A86	O4-C34	-2.55	1.40	1.46
11	6	304	CLA	C4D-CHA	2.55	1.47	1.38
11	7	303	CLA	C4D-CHA	2.55	1.47	1.38
11	11	307	CLA	C4D-CHA	2.55	1.47	1.38
11	7	305	CLA	C4D-CHA	2.54	1.47	1.38
11	16	302	CLA	C4D-CHA	2.54	1.47	1.38
11	10	311	CLA	C4D-CHA	2.54	1.47	1.38
11	8	309	CLA	C4D-CHA	2.54	1.47	1.38
13	6	316	DD6	C4-C5	2.54	1.51	1.43
12	6	310	KC1	C4A-C3A	2.54	1.49	1.44
14	14	301	A86	C-C1	2.54	1.56	1.50
11	15	305	CLA	C4C-C3C	2.54	1.49	1.45
12	12	305	KC1	C2A-C1A	2.54	1.52	1.44
14	7	315	A86	C-C1	2.54	1.56	1.50
14	14	320	A86	O-C13	-2.54	1.18	1.23
11	13	301	CLA	C1B-NB	-2.53	1.32	1.35
12	13	310	KC1	CHB-C4A	-2.53	1.33	1.39
11	6	302	CLA	C4D-CHA	2.53	1.47	1.38
11	7	308	CLA	C3D-C4D	-2.53	1.38	1.44
13	10	313	DD6	C26-C27	-2.53	1.31	1.37
11	7	311	CLA	C4D-CHA	2.53	1.47	1.38
14	14	319	A86	O-C13	-2.53	1.18	1.23
14	15	321	A86	C14-C15	2.53	1.57	1.52
11	6	303	CLA	C4D-CHA	2.53	1.47	1.38
12	11	306	KC1	C2A-C1A	2.53	1.52	1.44
14	12	314	A86	O-C13	-2.53	1.18	1.23
14	16	312	A86	O-C13	-2.52	1.18	1.23
14	15	321	A86	C24-C1	2.52	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	12	311	KC1	C2A-C1A	2.52	1.52	1.44
11	12	307	CLA	C4B-CHC	2.52	1.48	1.41
11	12	310	CLA	C3D-C4D	-2.52	1.38	1.44
11	7	304	CLA	C1B-NB	-2.52	1.33	1.35
11	15	314	CLA	C4D-CHA	2.52	1.47	1.38
14	11	315	A86	O-C13	-2.51	1.18	1.23
12	12	311	KC1	CAA-C2A	2.51	1.54	1.46
11	6	313	CLA	C3D-C4D	-2.51	1.38	1.44
14	11	314	A86	C-C1	2.51	1.56	1.50
11	16	302	CLA	C3D-C4D	-2.51	1.38	1.44
11	7	302	CLA	C3D-C4D	-2.51	1.38	1.44
11	12	303	CLA	C3D-C4D	-2.51	1.38	1.44
12	12	309	KC1	C4A-C3A	2.51	1.49	1.44
14	10	317	A86	O-C13	-2.51	1.18	1.23
11	7	306	CLA	C3D-C4D	-2.51	1.38	1.44
11	16	308	CLA	C4C-C3C	2.51	1.49	1.45
13	15	318	DD6	C26-C27	-2.51	1.31	1.37
12	13	308	KC1	C2A-C1A	2.51	1.52	1.44
11	14	304	CLA	C4D-CHA	2.50	1.47	1.38
11	6	301	CLA	C3D-C4D	-2.50	1.38	1.44
14	10	317	A86	C-C1	2.50	1.56	1.50
14	14	316	A86	C24-C1	2.50	1.51	1.45
14	14	321	A86	O-C13	-2.50	1.18	1.23
13	10	314	DD6	C35-C34	2.50	1.56	1.52
11	8	309	CLA	C3D-C4D	-2.50	1.38	1.44
12	13	310	KC1	C1C-C2C	2.49	1.49	1.44
12	12	305	KC1	CHB-C4A	-2.49	1.33	1.39
12	10	306	KC1	CHB-C4A	-2.49	1.33	1.39
11	12	308	CLA	C1B-NB	-2.49	1.33	1.35
11	13	309	CLA	C4C-C3C	2.49	1.49	1.45
11	12	304	CLA	C4D-CHA	2.49	1.47	1.38
14	11	314	A86	O-C13	-2.49	1.18	1.23
12	8	311	KC1	CAA-C2A	2.49	1.54	1.46
11	7	310	CLA	C3D-C4D	-2.49	1.38	1.44
11	10	308	CLA	C3D-C4D	-2.49	1.38	1.44
11	7	308	CLA	C4D-CHA	2.49	1.47	1.38
13	6	316	DD6	C22-C16	-2.49	1.49	1.53
11	16	310	CLA	C4D-CHA	2.49	1.47	1.38
11	15	302	CLA	C4B-CHC	2.48	1.47	1.41
11	7	306	CLA	C4D-CHA	2.48	1.47	1.38
14	11	313	A86	O-C13	-2.48	1.18	1.23
11	11	305	CLA	C3D-C4D	-2.48	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	14	318	A86	C14-C15	2.48	1.57	1.52
11	12	303	CLA	C4B-NB	-2.48	1.33	1.35
11	6	306	CLA	C3D-C4D	-2.48	1.38	1.44
12	12	305	KC1	C4A-C3A	2.48	1.49	1.44
14	14	315	A86	O-C13	-2.48	1.18	1.23
12	14	308	KC1	CHB-C4A	-2.48	1.33	1.39
11	12	308	CLA	C4D-CHA	2.48	1.47	1.38
14	14	315	A86	C-C1	2.48	1.56	1.50
12	13	312	KC1	CAA-C2A	2.48	1.54	1.46
13	13	314	DD6	C4-C5	2.47	1.51	1.43
12	11	310	KC1	CHB-C4A	-2.47	1.33	1.39
14	12	314	A86	C-C1	2.47	1.56	1.50
12	16	304	KC1	C4C-C3C	2.47	1.49	1.45
11	10	304	CLA	C3D-C4D	-2.47	1.38	1.44
12	13	306	KC1	CHB-C4A	-2.47	1.33	1.39
12	7	307	KC1	C4A-C3A	2.47	1.49	1.44
12	14	308	KC1	C2A-C1A	2.47	1.52	1.44
11	12	310	CLA	C4D-CHA	2.47	1.47	1.38
14	14	317	A86	C-C1	2.47	1.56	1.50
14	8	318	A86	C14-C15	2.47	1.57	1.52
11	12	312	CLA	C4D-CHA	2.47	1.47	1.38
12	13	305	KC1	CHB-C4A	-2.47	1.33	1.39
13	7	301	DD6	C22-C16	-2.47	1.49	1.53
11	10	305	CLA	C4D-CHA	2.47	1.47	1.38
14	14	318	A86	O-C13	-2.47	1.18	1.23
11	14	302	CLA	C4D-CHA	2.47	1.47	1.38
11	15	302	CLA	C1B-NB	-2.47	1.33	1.35
11	11	303	CLA	C3D-C4D	-2.46	1.38	1.44
13	6	316	DD6	C35-C34	2.46	1.56	1.52
14	15	316	A86	O-C13	-2.46	1.18	1.23
14	14	320	A86	C14-C15	2.46	1.57	1.52
14	14	319	A86	C-C1	2.46	1.56	1.50
14	10	315	A86	C14-C15	2.46	1.57	1.52
13	15	318	DD6	C22-C16	-2.46	1.49	1.53
11	14	307	CLA	C4B-CHC	2.46	1.47	1.41
11	6	311	CLA	C4D-CHA	2.46	1.47	1.38
14	11	314	A86	C24-C1	2.46	1.51	1.45
11	15	302	CLA	C4D-CHA	2.46	1.47	1.38
14	10	302	A86	C-C1	2.46	1.56	1.50
11	12	321	CLA	C1B-NB	-2.46	1.33	1.35
11	12	312	CLA	C3D-C4D	-2.46	1.38	1.44
11	8	303	CLA	C4D-CHA	2.46	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	11	305	CLA	C4D-CHA	2.46	1.47	1.38
11	15	307	CLA	C1B-NB	-2.45	1.33	1.35
13	7	317	DD6	C4-C5	2.45	1.51	1.43
11	7	304	CLA	C4D-CHA	2.45	1.47	1.38
11	8	304	CLA	C4D-CHA	2.45	1.47	1.38
14	15	320	A86	O-C13	-2.45	1.18	1.23
11	14	307	CLA	C4D-CHA	2.45	1.47	1.38
11	8	305	CLA	C1B-NB	-2.45	1.33	1.35
13	16	313	DD6	C26-C27	-2.45	1.31	1.37
14	13	313	A86	O-C13	-2.45	1.18	1.23
11	10	309	CLA	C4D-CHA	2.45	1.47	1.38
12	12	313	KC1	C2A-C1A	2.45	1.52	1.44
11	8	302	CLA	C4D-CHA	2.45	1.47	1.38
11	6	304	CLA	C3D-C4D	-2.45	1.38	1.44
13	16	313	DD6	C4-C5	2.45	1.51	1.43
13	8	317	DD6	C26-C27	-2.45	1.31	1.37
11	8	308	CLA	C3D-C4D	-2.44	1.38	1.44
11	8	305	CLA	C4D-CHA	2.44	1.47	1.38
11	14	309	CLA	C4C-C3C	2.44	1.49	1.45
11	7	303	CLA	C3D-C4D	-2.44	1.38	1.44
11	7	309	CLA	C3D-C4D	-2.44	1.38	1.44
11	12	304	CLA	C3D-C4D	-2.44	1.38	1.44
11	7	305	CLA	C1C-NC	-2.44	1.34	1.37
11	13	304	CLA	C4C-C3C	2.44	1.49	1.45
11	12	307	CLA	C4D-CHA	2.44	1.47	1.38
11	10	308	CLA	C4D-CHA	2.44	1.47	1.38
12	13	312	KC1	CHB-C4A	-2.44	1.33	1.39
14	10	315	A86	O-C13	-2.44	1.18	1.23
14	14	319	A86	C24-C1	2.44	1.51	1.45
12	6	309	KC1	C3B-C4B	2.43	1.50	1.46
12	11	304	KC1	C4A-C3A	2.43	1.49	1.44
13	15	319	DD6	C26-C27	-2.43	1.31	1.37
11	6	312	CLA	C4C-C3C	2.43	1.49	1.45
11	11	303	CLA	C4D-CHA	2.43	1.47	1.38
12	13	305	KC1	C2A-C1A	2.43	1.52	1.44
14	7	315	A86	C14-C15	2.43	1.57	1.52
12	13	311	KC1	C4C-C3C	2.43	1.49	1.45
11	12	304	CLA	C4B-NB	-2.43	1.33	1.35
11	11	307	CLA	C1B-NB	-2.43	1.33	1.35
11	10	308	CLA	C4B-CHC	2.43	1.47	1.41
13	6	315	DD6	C4-C5	2.43	1.51	1.43
11	8	301	CLA	C4D-CHA	2.42	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	11	310	KC1	C2A-C1A	2.42	1.52	1.44
12	6	309	KC1	C4A-C3A	2.42	1.49	1.44
11	14	302	CLA	C3D-C4D	-2.42	1.38	1.44
11	12	302	CLA	C3D-C4D	-2.42	1.38	1.44
12	10	310	KC1	C3B-C4B	2.42	1.50	1.46
11	7	311	CLA	C3D-C4D	-2.42	1.38	1.44
14	7	314	A86	C24-C1	2.42	1.51	1.45
12	14	311	KC1	CHB-C4A	-2.42	1.33	1.39
14	11	315	A86	C24-C1	2.42	1.51	1.45
12	13	306	KC1	C2A-C1A	2.42	1.52	1.44
12	8	312	KC1	CHB-C4A	-2.41	1.33	1.39
11	14	313	CLA	C3D-C4D	-2.41	1.38	1.44
12	6	309	KC1	C2A-C1A	2.41	1.52	1.44
13	11	312	DD6	O1-C20	2.41	1.49	1.46
12	14	306	KC1	C2A-C1A	2.41	1.52	1.44
11	16	306	CLA	C4D-CHA	2.41	1.47	1.38
15	6	319	LHG	O7-C5	-2.41	1.40	1.46
14	11	313	A86	C-C1	2.41	1.55	1.50
11	15	308	CLA	C4B-CHC	2.41	1.47	1.41
11	14	313	CLA	C4D-CHA	2.41	1.47	1.38
11	15	302	CLA	C3D-C4D	-2.41	1.38	1.44
14	14	301	A86	O-C13	-2.41	1.18	1.23
11	12	308	CLA	C4B-CHC	2.41	1.47	1.41
11	7	302	CLA	C4D-CHA	2.41	1.47	1.38
11	10	303	CLA	C4B-NB	-2.41	1.33	1.35
14	10	316	A86	C24-C1	2.41	1.51	1.45
11	12	304	CLA	C1B-NB	-2.41	1.33	1.35
12	8	312	KC1	C2A-C1A	2.41	1.52	1.44
14	7	318	A86	C-C1	2.41	1.55	1.50
13	7	301	DD6	C4-C5	2.40	1.50	1.43
11	8	304	CLA	C3D-C4D	-2.40	1.38	1.44
11	7	302	CLA	C1C-C2C	2.40	1.49	1.44
12	10	310	KC1	C2A-C1A	2.40	1.52	1.44
11	6	304	CLA	C1B-NB	-2.40	1.33	1.35
11	11	305	CLA	C1B-NB	-2.40	1.33	1.35
14	16	314	A86	C24-C1	2.40	1.51	1.45
12	8	306	KC1	C4A-C3A	2.40	1.49	1.44
11	15	313	CLA	C1B-NB	-2.40	1.33	1.35
12	8	310	KC1	C2A-C1A	2.40	1.51	1.44
12	14	311	KC1	C1C-C2C	2.40	1.49	1.44
11	15	311	CLA	C4B-CHC	2.40	1.47	1.41
13	15	319	DD6	C4-C5	2.40	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	15	315	A86	O-C13	-2.40	1.18	1.23
11	15	302	CLA	C1C-C2C	2.39	1.49	1.44
11	16	303	CLA	C3D-C4D	-2.39	1.38	1.44
14	14	314	A86	C24-C1	2.39	1.51	1.45
11	15	310	CLA	C4C-C3C	2.39	1.49	1.45
11	12	306	CLA	C1C-NC	-2.39	1.34	1.37
11	15	309	CLA	C4C-C3C	2.39	1.49	1.45
12	13	305	KC1	C4A-C3A	2.39	1.49	1.44
11	7	305	CLA	C3D-C4D	-2.39	1.38	1.44
13	7	316	DD6	C4-C5	2.39	1.50	1.43
14	14	301	A86	C14-C15	2.39	1.57	1.52
12	10	310	KC1	C4A-C3A	2.38	1.49	1.44
11	8	305	CLA	C1C-NC	-2.38	1.34	1.37
11	16	303	CLA	C4D-CHA	2.38	1.46	1.38
11	15	313	CLA	C4B-CHC	2.38	1.47	1.41
12	7	307	KC1	C2A-C1A	2.38	1.51	1.44
13	15	319	DD6	C35-C36	2.38	1.54	1.51
14	12	314	A86	C24-C1	2.38	1.51	1.45
11	11	303	CLA	C4B-CHC	2.38	1.47	1.41
12	6	308	KC1	C4A-C3A	2.38	1.49	1.44
12	13	311	KC1	CHB-C4A	-2.38	1.33	1.39
11	11	308	CLA	C4D-CHA	2.38	1.46	1.38
11	15	304	CLA	C4C-C3C	2.37	1.49	1.45
11	16	305	CLA	C1B-NB	-2.37	1.33	1.35
12	8	314	KC1	C4D-CHA	2.37	1.48	1.45
11	15	303	CLA	C4B-CHC	2.37	1.47	1.41
14	10	301	A86	C14-C15	2.37	1.57	1.52
12	13	312	KC1	C4C-C3C	2.37	1.49	1.45
11	10	309	CLA	C3D-C4D	-2.37	1.38	1.44
12	6	308	KC1	C2A-C1A	2.37	1.51	1.44
11	15	312	CLA	C3D-C4D	-2.37	1.38	1.44
11	7	302	CLA	C4B-CHC	2.36	1.47	1.41
13	12	317	DD6	C4-C5	2.36	1.50	1.43
14	14	315	A86	C14-C15	2.36	1.57	1.52
11	14	304	CLA	C4C-C3C	2.36	1.49	1.45
11	15	308	CLA	C1C-C2C	2.36	1.49	1.44
11	16	307	CLA	C4C-C3C	2.36	1.49	1.45
13	10	313	DD6	C4-C5	2.36	1.50	1.43
11	7	306	CLA	C4B-CHC	2.36	1.47	1.41
14	15	320	A86	C35-C34	2.36	1.56	1.51
11	14	304	CLA	C4B-CHC	2.36	1.47	1.41
11	13	301	CLA	C3D-C4D	-2.36	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	14	302	CLA	C4B-CHC	2.36	1.47	1.41
11	14	313	CLA	C4B-CHC	2.36	1.47	1.41
12	13	305	KC1	C4D-CHA	2.36	1.48	1.45
11	16	306	CLA	C4C-C3C	2.35	1.49	1.45
11	11	307	CLA	C4B-CHC	2.35	1.47	1.41
12	16	311	KC1	C1C-C2C	2.35	1.49	1.44
13	11	312	DD6	C4-C5	2.35	1.50	1.43
12	6	309	KC1	CAA-C2A	2.35	1.53	1.46
14	11	301	A86	C24-C1	2.35	1.51	1.45
11	10	311	CLA	C3D-C4D	-2.35	1.38	1.44
12	10	310	KC1	C4C-C3C	2.35	1.49	1.45
14	11	301	A86	C14-C15	2.35	1.57	1.52
11	6	313	CLA	C4B-NB	-2.35	1.33	1.35
11	13	307	CLA	C4C-C3C	2.35	1.49	1.45
11	6	303	CLA	C3D-C4D	-2.34	1.38	1.44
11	15	314	CLA	C1C-C2C	2.34	1.49	1.44
12	13	312	KC1	C4D-CHA	2.34	1.48	1.45
11	6	304	CLA	C4B-CHC	2.34	1.47	1.41
11	6	314	CLA	C4B-CHC	2.34	1.47	1.41
14	11	315	A86	C-C1	2.34	1.55	1.50
11	10	309	CLA	C4B-CHC	2.34	1.47	1.41
11	13	303	CLA	C4C-C3C	2.34	1.49	1.45
11	12	306	CLA	C3D-C4D	-2.34	1.38	1.44
11	13	303	CLA	C4B-CHC	2.34	1.47	1.41
11	16	308	CLA	C4B-CHC	2.33	1.47	1.41
11	11	307	CLA	C3D-C4D	-2.33	1.38	1.44
11	16	301	CLA	C4B-CHC	2.33	1.47	1.41
11	11	305	CLA	C4B-CHC	2.33	1.47	1.41
14	14	314	A86	C14-C15	2.33	1.57	1.52
11	8	304	CLA	C1C-NC	-2.33	1.34	1.37
11	13	304	CLA	C1C-C2C	2.33	1.49	1.44
11	15	309	CLA	C4B-CHC	2.33	1.47	1.41
11	12	308	CLA	C3D-C4D	-2.33	1.38	1.44
11	14	304	CLA	C3D-C4D	-2.33	1.38	1.44
14	15	317	A86	C14-C15	2.33	1.57	1.52
12	7	312	KC1	CAA-C2A	2.33	1.53	1.46
11	15	306	CLA	C4C-C3C	2.33	1.49	1.45
11	6	312	CLA	C3D-C4D	-2.33	1.38	1.44
11	16	303	CLA	C4B-CHC	2.33	1.47	1.41
11	16	307	CLA	C4B-CHC	2.32	1.47	1.41
11	14	312	CLA	C4C-C3C	2.32	1.49	1.45
11	16	305	CLA	C1C-NC	-2.32	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	16	311	KC1	C4D-CHA	2.32	1.47	1.45
11	10	303	CLA	C3D-C4D	-2.32	1.38	1.44
11	13	303	CLA	C3D-C4D	-2.32	1.38	1.44
11	13	304	CLA	C4B-CHC	2.32	1.47	1.41
11	8	301	CLA	C3D-C4D	-2.32	1.38	1.44
13	12	315	DD6	O1-C20	2.32	1.49	1.46
11	16	310	CLA	C1B-NB	-2.32	1.33	1.35
14	11	315	A86	C14-C15	2.32	1.57	1.52
11	12	310	CLA	C1C-C2C	2.32	1.49	1.44
11	10	307	CLA	C3D-C4D	-2.31	1.39	1.44
11	13	302	CLA	C3D-C4D	-2.31	1.39	1.44
11	7	311	CLA	C4C-C3C	2.31	1.49	1.45
11	6	313	CLA	C4C-C3C	2.31	1.49	1.45
14	8	315	A86	C5-C6	2.31	1.38	1.35
12	8	310	KC1	C4A-C3A	2.31	1.49	1.44
14	7	315	A86	O4-C34	-2.31	1.40	1.46
13	12	315	DD6	C29-C27	-2.31	1.38	1.42
14	14	321	A86	C14-C15	2.31	1.57	1.52
11	11	309	CLA	C4B-CHC	2.31	1.47	1.41
11	14	307	CLA	C3D-C4D	-2.31	1.39	1.44
11	14	312	CLA	C3D-C4D	-2.31	1.39	1.44
14	15	317	A86	O-C13	-2.31	1.18	1.23
12	8	311	KC1	C4A-C3A	2.30	1.49	1.44
11	16	303	CLA	C1C-C2C	2.30	1.49	1.44
13	6	318	DD6	C29-C27	-2.30	1.38	1.42
14	16	312	A86	C14-C15	2.30	1.57	1.52
11	10	307	CLA	C4B-CHC	2.30	1.47	1.41
11	13	307	CLA	C4B-CHC	2.30	1.47	1.41
14	7	314	A86	C14-C15	2.30	1.57	1.52
11	15	307	CLA	C4B-CHC	2.30	1.47	1.41
11	15	313	CLA	C3D-C4D	-2.30	1.39	1.44
14	8	318	A86	C24-C1	2.30	1.50	1.45
11	14	312	CLA	C4B-CHC	2.30	1.47	1.41
11	16	306	CLA	C4B-CHC	2.30	1.47	1.41
12	8	311	KC1	C2A-C1A	2.30	1.51	1.44
13	8	317	DD6	C22-C16	-2.30	1.49	1.53
13	7	313	DD6	C29-C27	-2.30	1.38	1.42
11	16	301	CLA	C1B-NB	-2.29	1.33	1.35
11	14	309	CLA	C4B-CHC	2.29	1.47	1.41
11	7	308	CLA	C1C-NC	-2.29	1.34	1.37
13	12	317	DD6	C29-C27	-2.29	1.38	1.42
12	10	312	KC1	C4A-C3A	2.29	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	6	302	CLA	C4B-NB	-2.29	1.33	1.35
14	16	312	A86	C24-C1	2.29	1.50	1.45
11	15	314	CLA	C4C-C3C	2.29	1.49	1.45
13	15	318	DD6	C4-C5	2.29	1.50	1.43
11	8	309	CLA	C1C-NC	-2.29	1.34	1.37
11	14	303	CLA	C4B-CHC	2.29	1.47	1.41
14	16	314	A86	C35-C34	2.29	1.55	1.51
12	10	312	KC1	C2A-C1A	2.29	1.51	1.44
11	16	301	CLA	C1C-C2C	2.29	1.49	1.44
13	10	314	DD6	C4-C5	2.29	1.50	1.43
11	14	313	CLA	C1B-CHB	2.28	1.47	1.41
12	13	312	KC1	C1C-C2C	2.28	1.49	1.44
11	11	303	CLA	C1C-C2C	2.28	1.49	1.44
11	13	302	CLA	C4B-CHC	2.28	1.47	1.41
11	15	308	CLA	C1B-NB	-2.28	1.33	1.35
14	15	321	A86	O-C13	-2.28	1.18	1.23
11	10	307	CLA	C1C-C2C	2.28	1.49	1.44
11	11	309	CLA	C3D-C4D	-2.28	1.39	1.44
11	16	307	CLA	C3D-C4D	-2.28	1.39	1.44
11	6	303	CLA	C4B-CHC	2.28	1.47	1.41
11	10	305	CLA	C4B-NB	-2.28	1.33	1.35
11	12	302	CLA	C4D-CHA	2.28	1.46	1.38
12	13	305	KC1	C4C-C3C	2.28	1.49	1.45
11	12	321	CLA	C4B-CHC	2.28	1.47	1.41
12	8	313	KC1	C4A-C3A	2.28	1.49	1.44
11	14	310	CLA	C4B-CHC	2.28	1.47	1.41
11	15	304	CLA	C4B-CHC	2.28	1.47	1.41
11	15	305	CLA	C1C-C2C	2.27	1.49	1.44
11	15	304	CLA	C3D-C4D	-2.27	1.39	1.44
14	11	313	A86	C24-C1	2.27	1.50	1.45
13	10	313	DD6	C22-C16	-2.27	1.49	1.53
12	8	310	KC1	CAA-C2A	2.27	1.53	1.46
11	13	302	CLA	C1B-CHB	2.27	1.47	1.41
11	14	303	CLA	C4C-C3C	2.27	1.48	1.45
11	15	311	CLA	C4C-C3C	2.27	1.48	1.45
11	10	304	CLA	C1B-CHB	2.27	1.47	1.41
13	10	314	DD6	C29-C27	-2.27	1.38	1.42
11	11	309	CLA	C4C-C3C	2.26	1.48	1.45
11	7	304	CLA	C3D-C4D	-2.26	1.39	1.44
11	16	306	CLA	C1C-NC	-2.26	1.34	1.37
13	6	315	DD6	C29-C27	-2.26	1.38	1.42
11	15	313	CLA	C4C-C3C	2.26	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	15	314	CLA	C4B-CHC	2.26	1.47	1.41
13	8	317	DD6	C35-C36	2.26	1.54	1.51
11	12	321	CLA	C3D-C4D	-2.26	1.39	1.44
11	6	314	CLA	C4C-C3C	2.26	1.48	1.45
11	14	305	CLA	C3D-C4D	-2.26	1.39	1.44
11	16	309	CLA	C3D-C4D	-2.26	1.39	1.44
14	14	317	A86	C14-C15	2.26	1.57	1.52
12	8	306	KC1	C3B-C4B	2.26	1.50	1.46
11	6	314	CLA	C3D-C4D	-2.26	1.39	1.44
11	14	303	CLA	C1B-NB	-2.26	1.33	1.35
12	6	309	KC1	C1C-C2C	2.26	1.48	1.44
12	12	311	KC1	C4C-C3C	2.26	1.48	1.45
13	6	318	DD6	C35-C36	2.26	1.54	1.51
11	6	304	CLA	C1C-C2C	2.26	1.48	1.44
12	10	306	KC1	C4C-C3C	2.26	1.48	1.45
11	13	301	CLA	C4B-CHC	2.26	1.47	1.41
11	16	302	CLA	C4B-CHC	2.26	1.47	1.41
12	14	306	KC1	CAA-C2A	2.25	1.53	1.46
11	7	305	CLA	C4B-CHC	2.25	1.47	1.41
13	6	315	DD6	C35-C36	2.25	1.54	1.51
14	13	315	A86	O-C13	-2.25	1.18	1.23
12	10	306	KC1	C4A-C3A	2.25	1.48	1.44
11	15	307	CLA	C3D-C4D	-2.25	1.39	1.44
11	12	312	CLA	C1B-NB	-2.25	1.33	1.35
11	16	309	CLA	C4B-CHC	2.25	1.47	1.41
11	16	309	CLA	C4C-C3C	2.25	1.48	1.45
14	13	313	A86	C14-C15	2.25	1.57	1.52
12	6	305	KC1	C1C-C2C	2.25	1.48	1.44
11	12	321	CLA	C1C-NC	-2.25	1.34	1.37
11	16	307	CLA	C1B-NB	-2.25	1.33	1.35
12	10	306	KC1	CAA-C2A	2.25	1.53	1.46
14	15	321	A86	O4-C34	-2.25	1.41	1.46
11	11	309	CLA	C1B-NB	-2.25	1.33	1.35
12	8	306	KC1	C2A-C1A	2.24	1.51	1.44
11	15	305	CLA	C4B-CHC	2.24	1.47	1.41
14	11	314	A86	C14-C15	2.24	1.57	1.52
11	14	310	CLA	C4C-C3C	2.24	1.48	1.45
11	10	311	CLA	C1B-CHB	2.24	1.47	1.41
11	6	303	CLA	C1B-NB	-2.24	1.33	1.35
11	14	307	CLA	C1C-C2C	2.24	1.48	1.44
14	14	301	A86	C35-C34	2.24	1.55	1.51
14	12	316	A86	C14-C15	2.24	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	15	307	CLA	C1C-NC	-2.24	1.34	1.37
12	10	306	KC1	C2A-C1A	2.24	1.51	1.44
11	14	310	CLA	C3D-C4D	-2.24	1.39	1.44
11	7	310	CLA	C4C-C3C	2.24	1.48	1.45
12	8	307	KC1	C4A-C3A	2.24	1.48	1.44
11	12	310	CLA	C1B-CHB	2.23	1.47	1.41
16	7	319	LMG	O1-C7	-2.23	1.39	1.43
11	16	301	CLA	C3D-C4D	-2.23	1.39	1.44
11	6	307	CLA	C4B-CHC	2.23	1.47	1.41
14	14	319	A86	C14-C15	2.23	1.57	1.52
11	11	305	CLA	C1C-C2C	2.23	1.48	1.44
11	16	302	CLA	C1B-NB	-2.23	1.33	1.35
11	6	312	CLA	C4B-CHC	2.23	1.47	1.41
16	14	322	LMG	C4-C3	2.23	1.58	1.52
11	15	303	CLA	C1C-C2C	2.23	1.48	1.44
14	12	314	A86	C14-C15	2.23	1.57	1.52
11	8	303	CLA	C1C-NC	-2.23	1.34	1.37
12	11	311	KC1	C4C-C3C	2.23	1.48	1.45
11	14	309	CLA	C3D-C4D	-2.23	1.39	1.44
11	15	310	CLA	C4B-CHC	2.23	1.47	1.41
11	7	304	CLA	C1A-CHA	2.23	1.52	1.43
16	7	319	LMG	C4-C5	2.22	1.57	1.53
11	6	304	CLA	C4C-C3C	2.22	1.48	1.45
11	10	305	CLA	C1B-NB	-2.22	1.33	1.35
13	6	315	DD6	C22-C16	-2.22	1.49	1.53
11	10	311	CLA	C4B-CHC	2.22	1.47	1.41
11	15	311	CLA	C1B-CHB	2.22	1.47	1.41
11	16	302	CLA	C1B-CHB	2.22	1.47	1.41
11	10	304	CLA	C4B-NB	-2.22	1.33	1.35
11	8	305	CLA	C4B-CHC	2.22	1.47	1.41
11	16	310	CLA	C4B-CHC	2.22	1.47	1.41
11	10	309	CLA	C1B-NB	-2.22	1.33	1.35
11	14	302	CLA	C1B-NB	-2.22	1.33	1.35
14	11	301	A86	O4-C34	-2.22	1.41	1.46
13	11	312	DD6	C29-C27	-2.22	1.38	1.42
13	10	314	DD6	C22-C16	-2.22	1.49	1.53
11	16	310	CLA	C1B-CHB	2.22	1.47	1.41
12	13	312	KC1	C3B-C4B	2.22	1.50	1.46
11	8	302	CLA	C4B-CHC	2.22	1.47	1.41
14	8	315	A86	O4-C34	-2.22	1.41	1.46
11	14	302	CLA	C1C-C2C	2.21	1.48	1.44
11	13	309	CLA	C4B-CHC	2.21	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	14	304	CLA	C1B-CHB	2.21	1.47	1.41
11	8	308	CLA	C4B-CHC	2.21	1.47	1.41
11	15	307	CLA	C4C-C3C	2.21	1.48	1.45
12	8	314	KC1	C4C-C3C	2.21	1.48	1.45
11	14	307	CLA	C1B-NB	-2.21	1.33	1.35
12	12	311	KC1	C4D-CHA	2.21	1.47	1.45
11	16	310	CLA	C1C-NC	-2.21	1.34	1.37
11	12	312	CLA	C4B-CHC	2.21	1.47	1.41
11	10	303	CLA	C1C-NC	-2.21	1.34	1.37
12	12	313	KC1	C1C-C2C	2.21	1.48	1.44
11	14	310	CLA	C1C-C2C	2.20	1.48	1.44
12	6	305	KC1	C4D-CHA	2.20	1.47	1.45
11	10	304	CLA	C4B-CHC	2.20	1.47	1.41
11	6	303	CLA	C1C-C2C	2.20	1.48	1.44
11	14	303	CLA	C3D-C4D	-2.20	1.39	1.44
11	13	302	CLA	C4C-C3C	2.20	1.48	1.45
11	15	311	CLA	C3D-C4D	-2.20	1.39	1.44
11	15	314	CLA	C3D-C4D	-2.20	1.39	1.44
11	10	311	CLA	C4C-C3C	2.20	1.48	1.45
12	12	309	KC1	C4D-CHA	2.20	1.47	1.45
12	13	306	KC1	CAA-C2A	2.19	1.53	1.46
11	12	308	CLA	C1B-CHB	2.19	1.47	1.41
12	14	308	KC1	C1C-C2C	2.19	1.48	1.44
11	16	305	CLA	C3D-C4D	-2.19	1.39	1.44
11	16	308	CLA	C3D-C4D	-2.19	1.39	1.44
11	15	305	CLA	C1B-NB	-2.19	1.33	1.35
11	8	302	CLA	C1C-C2C	2.19	1.48	1.44
11	11	309	CLA	C1C-C2C	2.19	1.48	1.44
13	8	316	DD6	C29-C27	-2.19	1.38	1.42
11	15	306	CLA	C1B-NB	-2.19	1.33	1.35
11	14	313	CLA	C1C-C2C	2.19	1.48	1.44
11	15	311	CLA	C1C-C2C	2.19	1.48	1.44
13	15	319	DD6	C22-C16	-2.19	1.49	1.53
11	6	314	CLA	C1C-C2C	2.19	1.48	1.44
13	6	318	DD6	O1-C20	2.19	1.49	1.46
14	6	317	A86	C35-C34	2.19	1.55	1.51
11	11	308	CLA	C4B-CHC	2.19	1.47	1.41
12	13	308	KC1	C4C-C3C	2.19	1.48	1.45
11	15	303	CLA	C3D-C4D	-2.19	1.39	1.44
11	7	309	CLA	C1C-C2C	2.19	1.48	1.44
12	16	311	KC1	C4C-C3C	2.18	1.48	1.45
11	12	310	CLA	C4B-CHC	2.18	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	15	310	CLA	C1C-C2C	2.18	1.48	1.44
11	10	311	CLA	C1B-NB	-2.18	1.33	1.35
11	14	303	CLA	C1C-C2C	2.18	1.48	1.44
11	13	309	CLA	C1B-CHB	2.18	1.47	1.41
13	13	314	DD6	O1-C20	2.18	1.49	1.46
13	7	317	DD6	C35-C36	2.18	1.54	1.51
12	8	311	KC1	C4C-C3C	2.18	1.48	1.45
13	7	313	DD6	C4-C5	2.18	1.50	1.43
11	12	308	CLA	C1C-C2C	2.18	1.48	1.44
12	13	311	KC1	C4D-CHA	2.18	1.47	1.45
11	6	306	CLA	C4B-NB	-2.18	1.33	1.35
11	6	312	CLA	C1B-NB	-2.18	1.33	1.35
11	6	311	CLA	C4B-CHC	2.18	1.47	1.41
11	13	304	CLA	C3D-C4D	-2.18	1.39	1.44
11	16	307	CLA	C1B-CHB	2.17	1.47	1.41
11	15	303	CLA	C1B-NB	-2.17	1.33	1.35
12	8	312	KC1	C4C-C3C	2.17	1.48	1.45
11	11	307	CLA	C1C-NC	-2.17	1.34	1.37
11	7	303	CLA	C4B-NB	-2.17	1.33	1.35
11	13	307	CLA	C1C-NC	-2.17	1.34	1.37
11	14	305	CLA	C4B-CHC	2.17	1.47	1.41
11	12	321	CLA	C4C-C3C	2.17	1.48	1.45
11	15	306	CLA	C3D-C4D	-2.17	1.39	1.44
14	11	315	A86	O4-C34	-2.17	1.41	1.46
11	16	307	CLA	C1C-C2C	2.17	1.48	1.44
11	8	309	CLA	C4C-C3C	2.17	1.48	1.45
11	6	301	CLA	C4B-CHC	2.17	1.47	1.41
11	15	302	CLA	C4C-C3C	2.17	1.48	1.45
11	7	308	CLA	C4B-CHC	2.17	1.47	1.41
11	16	306	CLA	C1C-C2C	2.17	1.48	1.44
11	6	306	CLA	C4B-CHC	2.16	1.47	1.41
12	13	308	KC1	C1C-C2C	2.16	1.48	1.44
14	6	317	A86	C14-C15	2.16	1.57	1.52
12	11	306	KC1	C4C-C3C	2.16	1.48	1.45
11	16	309	CLA	C1C-C2C	2.16	1.48	1.44
11	15	310	CLA	C3D-C4D	-2.16	1.39	1.44
14	12	314	A86	O4-C34	-2.16	1.41	1.46
14	14	315	A86	O4-C34	-2.16	1.41	1.46
11	15	305	CLA	C1B-CHB	2.16	1.47	1.41
11	13	302	CLA	C1C-C2C	2.16	1.48	1.44
11	16	305	CLA	C4B-CHC	2.16	1.47	1.41
11	8	308	CLA	C1C-C2C	2.16	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	13	302	CLA	C1B-NB	-2.16	1.33	1.35
13	8	317	DD6	C4-C5	2.16	1.50	1.43
11	15	309	CLA	C3D-C4D	-2.16	1.39	1.44
11	13	303	CLA	C1C-C2C	2.16	1.48	1.44
12	11	310	KC1	C1C-C2C	2.16	1.48	1.44
11	15	305	CLA	C3D-C4D	-2.16	1.39	1.44
14	11	313	A86	O4-C34	-2.16	1.41	1.46
11	10	309	CLA	C4C-C3C	2.16	1.48	1.45
12	10	312	KC1	CAA-C2A	2.16	1.53	1.46
11	14	309	CLA	C1B-CHB	2.15	1.47	1.41
11	6	307	CLA	C3D-C4D	-2.15	1.39	1.44
11	10	305	CLA	C1B-CHB	2.15	1.47	1.41
11	15	306	CLA	C4B-CHC	2.15	1.47	1.41
13	8	316	DD6	C22-C16	-2.15	1.49	1.53
13	12	315	DD6	C22-C16	-2.15	1.49	1.53
11	13	307	CLA	C3D-C4D	-2.15	1.39	1.44
12	16	304	KC1	C1D-CHD	2.15	1.47	1.41
11	15	309	CLA	C1C-C2C	2.15	1.48	1.44
11	15	303	CLA	C4C-C3C	2.15	1.48	1.45
12	12	309	KC1	C4C-C3C	2.15	1.48	1.45
12	6	305	KC1	C4A-C3A	2.15	1.48	1.44
12	8	312	KC1	C1C-C2C	2.15	1.48	1.44
11	10	307	CLA	C4B-NB	-2.15	1.33	1.35
11	11	305	CLA	C4C-C3C	2.15	1.48	1.45
11	12	302	CLA	C1C-C2C	2.15	1.48	1.44
11	16	309	CLA	C1B-CHB	2.15	1.47	1.41
11	12	303	CLA	C1C-NC	-2.15	1.34	1.37
12	12	311	KC1	C3B-C4B	2.14	1.49	1.46
13	8	316	DD6	C4-C5	2.14	1.50	1.43
11	14	309	CLA	C1B-NB	-2.14	1.33	1.35
11	12	304	CLA	C4B-CHC	2.14	1.46	1.41
11	12	304	CLA	C1C-NC	-2.14	1.34	1.37
11	15	306	CLA	C1B-CHB	2.14	1.46	1.41
12	11	310	KC1	C4C-C3C	2.14	1.48	1.45
11	6	302	CLA	C4B-CHC	2.14	1.46	1.41
12	6	310	KC1	C1C-C2C	2.14	1.48	1.44
11	13	309	CLA	C3D-C4D	-2.14	1.39	1.44
12	13	311	KC1	C1D-CHD	2.14	1.46	1.41
12	14	311	KC1	C4D-CHA	2.14	1.47	1.45
12	8	312	KC1	CAA-C2A	2.14	1.53	1.46
12	8	313	KC1	C2A-C1A	2.14	1.51	1.44
11	7	311	CLA	C1B-NB	-2.14	1.33	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	8	315	A86	C-C1	2.14	1.55	1.50
12	10	312	KC1	C1C-C2C	2.14	1.48	1.44
12	13	308	KC1	C4D-CHA	2.13	1.47	1.45
12	13	306	KC1	C1C-C2C	2.13	1.48	1.44
11	14	307	CLA	C1B-CHB	2.13	1.46	1.41
12	8	307	KC1	C2A-C1A	2.13	1.51	1.44
16	8	323	LMG	C4-C3	2.13	1.57	1.52
11	15	304	CLA	C1B-NB	-2.13	1.33	1.35
11	12	308	CLA	C1C-NC	-2.13	1.34	1.37
11	7	311	CLA	C4B-CHC	2.13	1.46	1.41
11	7	305	CLA	C4C-C3C	2.13	1.48	1.45
11	13	309	CLA	C1C-C2C	2.13	1.48	1.44
11	15	313	CLA	C1C-C2C	2.13	1.48	1.44
11	16	303	CLA	C1B-NB	-2.13	1.33	1.35
12	11	306	KC1	C1C-C2C	2.13	1.48	1.44
14	8	315	A86	C14-C15	2.13	1.56	1.52
13	12	315	DD6	C4-C5	2.13	1.50	1.43
11	7	311	CLA	C1B-CHB	2.13	1.46	1.41
11	14	302	CLA	C4C-C3C	2.13	1.48	1.45
12	11	304	KC1	C4C-C3C	2.13	1.48	1.45
11	7	311	CLA	C1C-NC	-2.13	1.34	1.37
11	15	304	CLA	C1C-C2C	2.13	1.48	1.44
11	12	303	CLA	C4B-CHC	2.13	1.46	1.41
14	14	315	A86	C24-C1	2.12	1.50	1.45
11	7	304	CLA	C4C-C3C	2.12	1.48	1.45
11	8	309	CLA	C4B-CHC	2.12	1.46	1.41
12	11	310	KC1	CAA-C2A	2.12	1.53	1.46
11	10	308	CLA	C1C-C2C	2.12	1.48	1.44
11	16	310	CLA	C1C-C2C	2.12	1.48	1.44
11	13	307	CLA	C1C-C2C	2.12	1.48	1.44
11	8	302	CLA	C1C-NC	-2.12	1.34	1.37
11	7	303	CLA	C1B-CHB	2.12	1.46	1.41
11	15	310	CLA	C1B-CHB	2.12	1.46	1.41
11	6	307	CLA	C4C-C3C	2.12	1.48	1.45
11	14	313	CLA	C4C-C3C	2.12	1.48	1.45
14	8	318	A86	C35-C34	2.12	1.55	1.51
12	6	310	KC1	C2A-C1A	2.12	1.51	1.44
11	11	308	CLA	C4C-C3C	2.12	1.48	1.45
11	14	312	CLA	C1C-C2C	2.12	1.48	1.44
11	10	311	CLA	C1C-NC	-2.12	1.34	1.37
11	12	312	CLA	C1C-NC	-2.12	1.34	1.37
11	10	305	CLA	C4C-C3C	2.12	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	13	313	A86	C35-C34	2.12	1.55	1.52
12	8	307	KC1	C3D-C4D	-2.11	1.38	1.40
11	14	305	CLA	C1C-C2C	2.11	1.48	1.44
16	8	321	LMG	O1-C7	-2.11	1.39	1.43
13	7	301	DD6	C35-C36	2.11	1.54	1.51
14	7	318	A86	O4-C34	-2.11	1.41	1.46
11	12	306	CLA	C4B-CHC	2.11	1.46	1.41
11	13	303	CLA	C1B-CHB	2.11	1.46	1.41
13	7	316	DD6	C29-C27	-2.11	1.38	1.42
11	10	309	CLA	C1B-CHB	2.11	1.46	1.41
13	12	317	DD6	O1-C20	2.11	1.49	1.46
11	10	309	CLA	C1C-C2C	2.11	1.48	1.44
12	11	304	KC1	CAA-C2A	2.11	1.53	1.46
16	14	322	LMG	O7-C8	-2.11	1.41	1.46
11	6	312	CLA	C1B-CHB	2.11	1.46	1.41
11	13	304	CLA	C1B-CHB	2.11	1.46	1.41
11	10	304	CLA	C1C-C2C	2.11	1.48	1.44
14	14	316	A86	C35-C34	2.11	1.55	1.51
11	12	312	CLA	C4C-C3C	2.11	1.48	1.45
11	16	302	CLA	C1C-NC	-2.11	1.34	1.37
11	6	304	CLA	C1B-CHB	2.10	1.46	1.41
11	15	309	CLA	C1B-CHB	2.10	1.46	1.41
14	10	302	A86	O4-C34	-2.10	1.41	1.46
14	13	315	A86	O4-C34	-2.10	1.41	1.46
11	7	310	CLA	C4B-CHC	2.10	1.46	1.41
11	15	312	CLA	C4B-CHC	2.10	1.46	1.41
12	16	311	KC1	C1D-CHD	2.10	1.46	1.41
13	6	316	DD6	C29-C27	-2.10	1.38	1.42
14	14	314	A86	C-C1	2.10	1.55	1.50
11	16	308	CLA	C1C-C2C	2.10	1.48	1.44
12	7	312	KC1	C2A-C1A	2.10	1.51	1.44
11	12	302	CLA	C4B-CHC	2.10	1.46	1.41
11	15	312	CLA	C4C-C3C	2.10	1.48	1.45
14	10	301	A86	O4-C34	-2.10	1.41	1.46
11	14	304	CLA	C1C-C2C	2.10	1.48	1.44
11	15	308	CLA	C3D-C4D	-2.10	1.39	1.44
11	7	303	CLA	C1C-NC	-2.10	1.34	1.37
11	8	303	CLA	C4C-C3C	2.09	1.48	1.45
12	13	311	KC1	C1C-C2C	2.09	1.48	1.44
12	14	311	KC1	CAA-C2A	2.09	1.53	1.46
11	11	303	CLA	C1B-NB	-2.09	1.33	1.35
11	14	305	CLA	C4C-C3C	2.09	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	8	320	LMG	C7-C8	2.09	1.57	1.50
12	10	306	KC1	C4D-CHA	2.09	1.47	1.45
12	14	308	KC1	C1D-CHD	2.09	1.46	1.41
14	14	314	A86	O4-C34	-2.09	1.41	1.46
11	15	312	CLA	C1C-C2C	2.09	1.48	1.44
12	10	310	KC1	C4D-CHA	2.09	1.47	1.45
12	16	304	KC1	CAA-C2A	2.09	1.53	1.46
11	6	303	CLA	C1B-CHB	2.09	1.46	1.41
11	16	301	CLA	C1B-CHB	2.09	1.46	1.41
14	8	318	A86	O4-C34	-2.09	1.41	1.46
12	13	312	KC1	C1D-CHD	2.08	1.46	1.41
11	12	310	CLA	C1B-NB	-2.08	1.33	1.35
11	7	309	CLA	C4C-C3C	2.08	1.48	1.45
12	13	310	KC1	C4D-CHA	2.08	1.47	1.45
11	6	302	CLA	C4C-C3C	2.08	1.48	1.45
12	13	311	KC1	CAA-C2A	2.08	1.53	1.46
14	15	317	A86	C35-C34	2.08	1.55	1.51
14	14	321	A86	C4-C3	2.08	1.41	1.36
12	11	304	KC1	C2A-C1A	2.08	1.50	1.44
11	6	306	CLA	C4C-C3C	2.08	1.48	1.45
13	6	316	DD6	O1-C20	2.08	1.49	1.46
12	6	310	KC1	C4C-C3C	2.08	1.48	1.45
12	6	308	KC1	C4C-C3C	2.08	1.48	1.45
14	12	316	A86	O4-C34	-2.08	1.41	1.46
14	15	316	A86	O4-C34	-2.08	1.41	1.46
11	8	305	CLA	C1C-C2C	2.08	1.48	1.44
11	11	303	CLA	C1B-CHB	2.07	1.46	1.41
12	13	305	KC1	C1C-C2C	2.07	1.48	1.44
12	13	310	KC1	CAA-C2A	2.07	1.52	1.46
11	15	303	CLA	C1B-CHB	2.07	1.46	1.41
13	6	318	DD6	C4-C5	2.07	1.49	1.43
14	15	320	A86	C4-C3	2.07	1.41	1.36
11	13	301	CLA	C1C-C2C	2.07	1.48	1.44
12	8	314	KC1	CAA-C2A	2.07	1.52	1.46
14	10	316	A86	O4-C34	-2.07	1.41	1.46
13	10	313	DD6	O1-C20	2.07	1.49	1.46
13	13	314	DD6	C35-C36	2.07	1.54	1.51
11	8	301	CLA	C1C-C2C	2.07	1.48	1.44
12	11	304	KC1	C1C-C2C	2.07	1.48	1.44
12	13	308	KC1	CAA-C2A	2.07	1.52	1.46
12	11	311	KC1	C4D-CHA	2.07	1.47	1.45
11	11	309	CLA	C1B-CHB	2.07	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	15	314	CLA	C1B-CHB	2.07	1.46	1.41
11	13	301	CLA	C4C-C3C	2.07	1.48	1.45
11	12	303	CLA	C1C-C2C	2.06	1.48	1.44
12	8	313	KC1	CAA-C2A	2.06	1.52	1.46
12	6	308	KC1	CAA-C2A	2.06	1.52	1.46
11	7	304	CLA	C4B-CHC	2.06	1.46	1.41
14	10	317	A86	O4-C34	-2.06	1.41	1.46
11	8	305	CLA	C1B-CHB	2.06	1.46	1.41
12	14	308	KC1	CAA-C2A	2.06	1.52	1.46
11	12	308	CLA	C4C-C3C	2.06	1.48	1.45
13	11	312	DD6	C35-C36	2.06	1.54	1.51
11	6	301	CLA	C1C-NC	-2.06	1.34	1.37
11	7	304	CLA	C1B-CHB	2.06	1.46	1.41
11	12	303	CLA	C1B-CHB	2.06	1.46	1.41
11	15	313	CLA	C1B-CHB	2.06	1.46	1.41
12	11	304	KC1	C4D-CHA	2.06	1.47	1.45
11	14	312	CLA	C1B-CHB	2.06	1.46	1.41
11	6	307	CLA	C1B-CHB	2.06	1.46	1.41
16	14	322	LMG	C4-C5	2.06	1.57	1.53
11	13	309	CLA	C1A-CHA	2.05	1.51	1.43
12	11	310	KC1	C4D-CHA	2.05	1.47	1.45
12	12	313	KC1	C3B-C4B	2.05	1.49	1.46
11	14	310	CLA	C1B-NB	-2.05	1.33	1.35
11	6	311	CLA	C1C-NC	-2.05	1.34	1.37
12	7	312	KC1	C4A-C3A	2.05	1.48	1.44
11	6	303	CLA	C4C-C3C	2.05	1.48	1.45
11	7	310	CLA	C1B-CHB	2.05	1.46	1.41
12	11	306	KC1	C4D-CHA	2.05	1.47	1.45
11	16	310	CLA	C4B-NB	-2.05	1.33	1.35
14	16	312	A86	C-C1	2.05	1.55	1.50
14	14	320	A86	O4-C34	-2.05	1.41	1.46
11	7	309	CLA	C4B-CHC	2.05	1.46	1.41
11	8	304	CLA	C4B-CHC	2.05	1.46	1.41
11	16	302	CLA	C1C-C2C	2.05	1.48	1.44
11	13	301	CLA	C1B-CHB	2.05	1.46	1.41
12	11	306	KC1	C1D-CHD	2.05	1.46	1.41
14	15	315	A86	O4-C34	-2.05	1.41	1.46
11	12	321	CLA	C1B-CHB	2.05	1.46	1.41
11	16	308	CLA	C1B-CHB	2.05	1.46	1.41
14	14	316	A86	C14-C15	2.04	1.56	1.52
12	10	306	KC1	C1C-C2C	2.04	1.48	1.44
11	15	307	CLA	C1C-C2C	2.04	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	16	312	A86	O4-C34	-2.04	1.41	1.46
11	12	307	CLA	C1C-C2C	2.04	1.48	1.44
12	8	314	KC1	C1D-CHD	2.04	1.46	1.41
11	15	306	CLA	C1C-C2C	2.04	1.48	1.44
11	7	304	CLA	C1C-NC	-2.04	1.34	1.37
11	12	306	CLA	C4C-C3C	2.04	1.48	1.45
12	12	305	KC1	C4C-C3C	2.04	1.48	1.45
11	6	314	CLA	C1B-CHB	2.04	1.46	1.41
11	16	309	CLA	C1B-NB	-2.04	1.33	1.35
11	15	304	CLA	C1C-NC	-2.04	1.34	1.37
14	16	312	A86	C35-C34	2.04	1.55	1.51
11	6	307	CLA	C1C-NC	-2.04	1.34	1.37
14	14	318	A86	C35-C34	2.04	1.55	1.51
11	15	307	CLA	C1B-CHB	2.04	1.46	1.41
12	11	306	KC1	CAA-C2A	2.03	1.52	1.46
12	11	311	KC1	CAA-C2A	2.03	1.52	1.46
11	12	312	CLA	C1C-C2C	2.03	1.48	1.44
13	6	315	DD6	O1-C20	2.03	1.49	1.46
11	6	302	CLA	C1C-C2C	2.03	1.48	1.44
14	14	319	A86	O3-C36	-2.03	1.39	1.43
11	16	305	CLA	C1A-CHA	2.03	1.51	1.43
11	6	312	CLA	C1C-C2C	2.03	1.48	1.44
11	7	308	CLA	C4C-C3C	2.03	1.48	1.45
11	6	313	CLA	C1C-NC	-2.03	1.34	1.37
11	16	305	CLA	C1B-CHB	2.03	1.46	1.41
11	14	302	CLA	C1B-CHB	2.03	1.46	1.41
12	12	305	KC1	CAA-C2A	2.02	1.52	1.46
12	12	305	KC1	C4D-CHA	2.02	1.47	1.45
11	6	314	CLA	C1B-NB	-2.02	1.33	1.35
11	14	312	CLA	C1B-NB	-2.02	1.33	1.35
11	10	304	CLA	C1C-NC	-2.02	1.34	1.37
11	16	302	CLA	C4C-C3C	2.02	1.48	1.45
11	12	312	CLA	C1B-CHB	2.02	1.46	1.41
11	7	305	CLA	C1A-CHA	2.02	1.51	1.43
11	16	303	CLA	C1B-CHB	2.02	1.46	1.41
11	7	308	CLA	C1B-CHB	2.02	1.46	1.41
11	10	307	CLA	C4C-C3C	2.02	1.48	1.45
11	13	301	CLA	C1A-CHA	2.02	1.51	1.43
13	7	313	DD6	C22-C16	-2.02	1.49	1.53
11	6	313	CLA	C4B-CHC	2.02	1.46	1.41
11	15	314	CLA	C4B-NB	-2.02	1.33	1.35
14	14	317	A86	O4-C34	-2.02	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	10	309	CLA	C1C-NC	-2.02	1.34	1.37
16	7	319	LMG	O4-C4	-2.02	1.38	1.43
11	12	307	CLA	C1B-CHB	2.02	1.46	1.41
12	11	310	KC1	C1D-CHD	2.02	1.46	1.41
12	10	312	KC1	C1D-CHD	2.02	1.46	1.41
11	7	306	CLA	C1C-NC	-2.01	1.34	1.37
11	16	306	CLA	C1B-CHB	2.01	1.46	1.41
11	12	310	CLA	C1C-NC	-2.01	1.34	1.37
12	7	307	KC1	CAA-C2A	2.01	1.52	1.46
11	10	307	CLA	C1A-CHA	2.01	1.51	1.43
11	12	304	CLA	C1B-CHB	2.01	1.46	1.41
12	13	305	KC1	C1D-CHD	2.01	1.46	1.41
13	10	314	DD6	O1-C20	2.01	1.49	1.46
14	15	322	A86	C4-C3	2.01	1.41	1.36
11	10	303	CLA	C1A-CHA	2.01	1.51	1.43
11	8	301	CLA	C4B-CHC	2.01	1.46	1.41
11	12	304	CLA	C4C-C3C	2.01	1.48	1.45
13	10	313	DD6	C29-C27	-2.00	1.38	1.42
14	16	314	A86	O4-C34	-2.00	1.41	1.46
12	13	306	KC1	C3B-C4B	2.00	1.49	1.46
11	13	307	CLA	C1A-CHA	2.00	1.51	1.43
11	12	310	CLA	C4C-C3C	2.00	1.48	1.45
11	16	308	CLA	C1B-NB	-2.00	1.33	1.35

All (4528) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	14	315	A86	O1-C20-C19	58.19	157.09	113.38
14	14	317	A86	O1-C20-C19	57.22	156.37	113.38
14	15	321	A86	O1-C20-C19	57.11	156.29	113.38
14	8	318	A86	O1-C20-C19	56.82	156.07	113.38
14	16	314	A86	O1-C20-C19	56.19	155.59	113.38
14	14	318	A86	O1-C20-C19	55.93	155.40	113.38
14	15	317	A86	O1-C20-C19	55.82	155.31	113.38
14	10	302	A86	O1-C20-C19	55.62	155.16	113.38
14	14	321	A86	O1-C20-C19	55.47	155.05	113.38
14	11	315	A86	O1-C20-C19	55.41	155.00	113.38
14	15	322	A86	O1-C20-C19	55.02	154.71	113.38
14	13	315	A86	O1-C20-C19	54.96	154.67	113.38
14	12	316	A86	O1-C20-C19	54.71	154.48	113.38
14	13	313	A86	O1-C20-C19	54.68	154.46	113.38
14	11	313	A86	O1-C20-C19	54.59	154.39	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	11	301	A86	O1-C20-C19	54.29	154.17	113.38
14	14	319	A86	O1-C20-C19	54.19	154.09	113.38
14	15	320	A86	O1-C20-C19	54.10	154.02	113.38
14	10	315	A86	O1-C20-C19	54.05	153.98	113.38
14	10	317	A86	O1-C20-C19	53.96	153.92	113.38
14	8	315	A86	O1-C20-C19	53.81	153.81	113.38
14	14	316	A86	O1-C20-C19	53.67	153.70	113.38
14	12	314	A86	O1-C20-C19	53.66	153.69	113.38
14	14	314	A86	O1-C20-C19	52.94	153.15	113.38
14	14	301	A86	O1-C20-C19	52.18	152.58	113.38
14	16	312	A86	O1-C20-C19	52.17	152.57	113.38
14	15	315	A86	O1-C20-C19	51.61	152.15	113.38
14	15	316	A86	O1-C20-C19	51.37	151.97	113.38
14	10	316	A86	O1-C20-C19	51.35	151.96	113.38
14	7	314	A86	O1-C20-C19	51.06	151.74	113.38
14	7	318	A86	O1-C20-C19	50.35	151.20	113.38
14	7	315	A86	O1-C20-C19	50.04	150.97	113.38
14	11	314	A86	O1-C20-C19	47.63	149.16	113.38
14	14	320	A86	O1-C20-C19	44.99	147.18	113.38
14	10	301	A86	O1-C20-C19	44.23	146.61	113.38
14	6	317	A86	O1-C20-C19	43.81	146.29	113.38
14	8	318	A86	C-C1-C2	-33.41	76.12	122.92
13	7	313	DD6	O1-C20-C19	31.54	137.08	113.38
13	8	317	DD6	O1-C20-C19	31.10	136.75	113.38
13	13	314	DD6	O1-C20-C19	30.74	136.47	113.38
13	12	317	DD6	O1-C20-C19	30.57	136.35	113.38
13	16	313	DD6	O1-C20-C19	30.53	136.32	113.38
13	15	318	DD6	O1-C20-C19	30.49	136.29	113.38
13	12	315	DD6	O1-C20-C19	30.41	136.23	113.38
13	10	313	DD6	O1-C20-C19	29.94	135.87	113.38
13	11	312	DD6	O1-C20-C19	29.87	135.82	113.38
13	8	316	DD6	O1-C20-C19	29.53	135.56	113.38
13	7	301	DD6	O1-C20-C19	28.79	135.01	113.38
13	6	316	DD6	O1-C20-C19	28.47	134.77	113.38
13	7	317	DD6	O1-C20-C19	28.35	134.68	113.38
13	15	319	DD6	O1-C20-C19	27.73	134.21	113.38
13	6	318	DD6	O1-C20-C19	27.59	134.11	113.38
13	10	314	DD6	O1-C20-C19	27.35	133.93	113.38
13	6	315	DD6	O1-C20-C19	27.16	133.78	113.38
13	7	316	DD6	O1-C20-C19	26.76	133.48	113.38
14	8	318	A86	C-C1-C24	-26.33	76.60	118.08
14	8	318	A86	C24-C1-C2	22.00	152.69	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	8	305	CLA	C4-C3-C5	-21.13	79.73	115.27
12	12	313	KC1	C2A-C3A-C4A	-20.42	91.34	106.49
11	8	305	CLA	C5-C3-C2	18.97	159.51	121.12
13	7	313	DD6	C28-C27-C29	18.21	152.90	116.84
13	7	316	DD6	C28-C27-C29	17.73	151.95	116.84
13	11	312	DD6	C28-C27-C29	17.25	151.00	116.84
13	8	316	DD6	C28-C27-C29	17.24	150.99	116.84
13	10	314	DD6	C28-C27-C29	17.24	150.98	116.84
13	7	317	DD6	C28-C27-C29	17.22	150.94	116.84
13	12	317	DD6	C28-C27-C29	17.11	150.72	116.84
11	8	305	CLA	C4-C3-C2	-17.08	79.87	123.68
13	6	315	DD6	C28-C27-C29	17.03	150.58	116.84
13	6	316	DD6	C28-C27-C29	16.87	150.26	116.84
13	6	318	DD6	C28-C27-C29	16.78	150.07	116.84
13	13	314	DD6	C28-C27-C29	16.68	149.87	116.84
13	16	313	DD6	C28-C27-C29	16.59	149.70	116.84
13	10	313	DD6	C28-C27-C29	16.47	149.45	116.84
13	15	318	DD6	C28-C27-C29	16.42	149.35	116.84
13	12	315	DD6	C28-C27-C29	16.13	148.78	116.84
13	15	319	DD6	C28-C27-C29	16.12	148.76	116.84
13	8	317	DD6	C28-C27-C29	16.11	148.74	116.84
13	7	301	DD6	C28-C27-C29	16.09	148.71	116.84
13	15	319	DD6	C29-C30-C31	-15.82	135.37	175.43
13	11	312	DD6	C29-C30-C31	-15.41	136.41	175.43
13	12	317	DD6	C29-C30-C31	-15.36	136.55	175.43
13	12	315	DD6	C29-C30-C31	-15.02	137.41	175.43
13	7	313	DD6	C29-C30-C31	-14.62	138.41	175.43
13	8	317	DD6	C29-C30-C31	-14.57	138.53	175.43
13	6	318	DD6	C29-C30-C31	-14.56	138.56	175.43
13	15	318	DD6	C29-C30-C31	-14.51	138.69	175.43
13	10	313	DD6	C29-C30-C31	-14.40	138.96	175.43
13	13	314	DD6	C29-C30-C31	-14.40	138.97	175.43
13	6	315	DD6	C29-C30-C31	-14.36	139.07	175.43
13	16	313	DD6	C29-C30-C31	-14.32	139.16	175.43
13	10	314	DD6	C29-C30-C31	-14.22	139.41	175.43
13	7	301	DD6	C29-C30-C31	-14.01	139.95	175.43
13	7	317	DD6	C29-C30-C31	-13.95	140.12	175.43
13	8	316	DD6	C29-C30-C31	-13.79	140.52	175.43
13	8	316	DD6	C12-C11-C10	-13.69	103.74	122.92
13	6	316	DD6	C29-C30-C31	-13.39	141.52	175.43
13	16	313	DD6	C37-C36-C31	-13.37	106.17	124.35
14	6	317	A86	O1-C15-C14	-13.30	86.52	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	7	316	DD6	C37-C36-C31	-13.24	106.35	124.35
13	12	315	DD6	C37-C36-C31	-12.96	106.74	124.35
13	10	313	DD6	C37-C36-C31	-12.95	106.76	124.35
13	8	317	DD6	C37-C36-C31	-12.90	106.83	124.35
13	7	316	DD6	C29-C30-C31	-12.79	143.05	175.43
13	6	318	DD6	C37-C36-C31	-12.76	107.01	124.35
13	13	314	DD6	C12-C11-C10	-12.66	105.18	122.92
13	11	312	DD6	C37-C36-C31	-12.60	107.22	124.35
14	11	315	A86	C21-C20-C19	-12.60	100.10	114.28
13	10	313	DD6	C12-C11-C10	-12.59	105.29	122.92
14	15	321	A86	C21-C20-C19	-12.58	100.12	114.28
14	12	316	A86	C21-C20-C19	-12.56	100.15	114.28
14	16	314	A86	O1-C20-C21	-12.48	100.10	115.06
13	10	314	DD6	C37-C36-C31	-12.47	107.40	124.35
12	12	313	KC1	CMA-C3A-C4A	-12.44	106.09	125.04
13	12	317	DD6	C37-C36-C31	-12.38	107.52	124.35
14	15	322	A86	C21-C20-C19	-12.29	100.45	114.28
12	10	306	KC1	CMA-C3A-C4A	-12.19	106.47	125.04
13	7	313	DD6	C13-C11-C10	-12.19	100.24	118.94
14	14	315	A86	C21-C20-C19	-12.15	100.61	114.28
13	8	316	DD6	C37-C36-C31	-12.10	107.91	124.35
14	11	313	A86	C21-C20-C19	-12.10	100.67	114.28
14	10	316	A86	C21-C20-C19	-12.08	100.69	114.28
13	7	317	DD6	C9-C10-C11	-12.01	110.18	127.31
14	10	301	A86	C17-C16-C15	11.94	121.35	109.16
14	14	316	A86	C21-C20-C19	-11.90	100.89	114.28
13	7	301	DD6	C37-C36-C31	-11.89	108.19	124.35
13	6	318	DD6	C9-C10-C11	-11.88	110.35	127.31
13	7	316	DD6	C9-C10-C11	-11.85	110.40	127.31
14	8	318	A86	O1-C20-C21	-11.80	100.91	115.06
12	12	311	KC1	CMA-C3A-C4A	-11.69	107.23	125.04
12	8	307	KC1	CMA-C3A-C4A	-11.68	107.26	125.04
13	13	314	DD6	C37-C36-C31	-11.67	108.49	124.35
12	8	311	KC1	CMA-C3A-C4A	-11.58	107.41	125.04
12	6	308	KC1	CMA-C3A-C4A	-11.55	107.45	125.04
14	14	314	A86	C21-C20-C19	-11.49	101.36	114.28
12	16	311	KC1	C2A-C3A-C4A	-11.49	97.96	106.49
14	7	318	A86	C17-C16-C15	11.46	120.85	109.16
14	14	317	A86	C21-C20-C19	-11.44	101.41	114.28
13	7	317	DD6	C37-C36-C31	-11.41	108.84	124.35
13	6	316	DD6	C12-C11-C10	-11.41	106.94	122.92
14	16	312	A86	C4-C5-C6	-11.40	111.04	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	10	313	DD6	C9-C10-C11	-11.38	111.06	127.31
14	14	318	A86	C21-C20-C19	-11.37	101.49	114.28
14	15	315	A86	C21-C20-C19	-11.33	101.53	114.28
12	12	309	KC1	C2A-C3A-C4A	-11.33	98.08	106.49
13	7	313	DD6	C12-C11-C10	-11.27	107.13	122.92
14	10	317	A86	C21-C20-C19	-11.26	101.61	114.28
12	6	305	KC1	CMA-C3A-C4A	-11.24	107.92	125.04
14	10	315	A86	C21-C20-C19	-11.23	101.65	114.28
12	10	312	KC1	CMA-C3A-C4A	-11.22	107.95	125.04
14	15	320	A86	C21-C20-C19	-11.21	101.67	114.28
13	10	314	DD6	C13-C11-C10	-11.20	101.75	118.94
12	8	313	KC1	CMA-C3A-C4A	-11.19	108.00	125.04
14	14	301	A86	C33-C32-C31	11.19	120.08	109.21
13	6	315	DD6	C37-C36-C31	-11.18	109.16	124.35
13	15	318	DD6	C37-C36-C31	-11.17	109.17	124.35
14	14	317	A86	O1-C20-C21	-11.16	101.68	115.06
12	11	304	KC1	CMA-C3A-C4A	-11.13	108.08	125.04
13	7	313	DD6	C37-C36-C31	-11.13	109.22	124.35
14	15	317	A86	O1-C20-C21	-11.11	101.74	115.06
13	11	312	DD6	C9-C10-C11	-11.09	111.48	127.31
13	15	319	DD6	C-C1-C2	-11.09	107.39	122.92
13	7	316	DD6	C3-C2-C1	-11.09	111.49	127.31
14	14	321	A86	O1-C20-C21	-11.02	101.85	115.06
14	14	315	A86	O1-C20-C21	-11.01	101.87	115.06
14	13	315	A86	C21-C20-C19	-10.97	101.94	114.28
14	14	319	A86	C21-C20-C19	-10.91	102.00	114.28
13	12	317	DD6	C12-C11-C10	-10.90	107.65	122.92
13	6	316	DD6	C37-C36-C31	-10.90	109.54	124.35
12	6	309	KC1	CMA-C3A-C4A	-10.86	108.50	125.04
14	14	320	A86	C17-C16-C15	10.83	120.21	109.16
13	13	314	DD6	C13-C11-C10	-10.78	102.40	118.94
14	8	315	A86	C21-C20-C19	-10.78	102.15	114.28
13	7	316	DD6	C12-C11-C10	-10.78	107.82	122.92
14	10	301	A86	C25-C26-C27	-10.76	111.95	127.31
13	15	319	DD6	C3-C2-C1	-10.75	111.97	127.31
14	10	302	A86	C21-C20-C19	-10.75	102.19	114.28
12	8	310	KC1	CMA-C3A-C4A	-10.74	108.68	125.04
13	11	312	DD6	C4-C5-C6	-10.73	111.99	127.31
12	13	308	KC1	CMA-C3A-C4A	-10.73	108.70	125.04
12	11	310	KC1	CMA-C3A-C4A	-10.72	108.71	125.04
13	16	313	DD6	C12-C11-C10	-10.71	107.92	122.92
14	13	313	A86	O1-C20-C21	-10.70	102.24	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	11	301	A86	C21-C20-C19	-10.70	102.25	114.28
14	14	321	A86	C21-C20-C19	-10.69	102.25	114.28
14	14	318	A86	O1-C20-C21	-10.69	102.24	115.06
14	10	302	A86	O1-C20-C21	-10.66	102.28	115.06
14	16	312	A86	C21-C20-C19	-10.65	102.30	114.28
12	11	306	KC1	CMA-C3A-C4A	-10.64	108.83	125.04
14	15	317	A86	C21-C20-C19	-10.63	102.32	114.28
13	7	301	DD6	C9-C10-C11	-10.61	112.17	127.31
13	15	319	DD6	C9-C10-C11	-10.61	112.17	127.31
14	8	318	A86	C21-C20-C19	-10.60	102.35	114.28
14	13	313	A86	C21-C20-C19	-10.59	102.37	114.28
13	7	317	DD6	C12-C11-C10	-10.58	108.10	122.92
13	6	318	DD6	C12-C11-C10	-10.57	108.11	122.92
14	13	315	A86	O1-C20-C21	-10.57	102.39	115.06
12	13	310	KC1	CMA-C3A-C4A	-10.57	108.95	125.04
12	12	305	KC1	CMA-C3A-C4A	-10.57	108.95	125.04
12	10	310	KC1	CMA-C3A-C4A	-10.56	108.96	125.04
12	13	312	KC1	CMA-C3A-C4A	-10.52	109.01	125.04
13	8	317	DD6	C12-C11-C10	-10.51	108.20	122.92
13	8	317	DD6	C13-C11-C10	-10.50	102.83	118.94
12	7	312	KC1	CMA-C3A-C4A	-10.49	109.07	125.04
13	6	315	DD6	C3-C2-C1	-10.47	112.36	127.31
12	10	310	KC1	C2A-C3A-C4A	-10.47	98.72	106.49
13	16	313	DD6	C13-C11-C10	-10.46	102.89	118.94
13	12	317	DD6	C3-C2-C1	-10.41	112.46	127.31
14	11	301	A86	O1-C20-C21	-10.40	102.59	115.06
14	7	314	A86	C21-C20-C19	-10.39	102.60	114.28
12	6	310	KC1	CMA-C3A-C4A	-10.37	109.25	125.04
13	15	319	DD6	C12-C11-C10	-10.36	108.41	122.92
13	15	318	DD6	C4-C5-C6	-10.36	112.53	127.31
12	14	311	KC1	CMA-C3A-C4A	-10.35	109.27	125.04
12	13	305	KC1	CMA-C3A-C4A	-10.34	109.29	125.04
14	14	314	A86	C33-C32-C31	10.34	119.26	109.21
14	12	314	A86	C21-C20-C19	-10.33	102.65	114.28
14	15	321	A86	O1-C20-C21	-10.30	102.71	115.06
12	8	313	KC1	C2A-C3A-C4A	-10.28	98.86	106.49
14	14	319	A86	O1-C20-C21	-10.28	102.74	115.06
13	6	315	DD6	C4-C5-C6	-10.25	112.68	127.31
13	10	314	DD6	C4-C5-C6	-10.23	112.72	127.31
11	14	307	CLA	C1D-ND-C4D	-10.20	99.09	106.33
14	11	314	A86	C33-C32-C31	10.19	119.11	109.21
14	15	315	A86	C3-C2-C1	-10.18	112.78	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	13	315	A86	C33-C32-C31	10.17	119.10	109.21
13	6	315	DD6	C9-C10-C11	-10.17	112.80	127.31
11	16	303	CLA	C1D-ND-C4D	-10.16	99.12	106.33
12	11	306	KC1	C2A-C3A-C4A	-10.14	98.97	106.49
13	7	313	DD6	C3-C2-C1	-10.12	112.87	127.31
12	8	306	KC1	CMA-C3A-C4A	-10.10	109.66	125.04
14	12	314	A86	O1-C20-C21	-10.09	102.96	115.06
12	7	307	KC1	CMA-C3A-C4A	-10.08	109.68	125.04
13	6	315	DD6	C12-C11-C10	-10.08	108.81	122.92
12	6	310	KC1	C2A-C3A-C4A	-10.07	99.02	106.49
14	14	301	A86	C21-C20-C19	-10.06	102.97	114.28
11	15	302	CLA	C1D-ND-C4D	-10.04	99.20	106.33
13	10	313	DD6	C3-C2-C1	-10.02	113.01	127.31
12	14	308	KC1	C2A-C3A-C4A	-10.02	99.05	106.49
13	12	317	DD6	C9-C10-C11	-10.01	113.02	127.31
14	7	314	A86	C17-C16-C15	10.01	119.37	109.16
13	11	312	DD6	C7-C6-C5	-9.99	108.93	122.92
13	10	313	DD6	C8-C6-C5	-9.92	103.71	118.94
14	14	301	A86	O1-C20-C21	-9.92	103.17	115.06
13	15	319	DD6	C4-C5-C6	-9.91	113.17	127.31
12	13	306	KC1	CMA-C3A-C4A	-9.89	109.97	125.04
12	14	311	KC1	C2A-C3A-C4A	-9.88	99.16	106.49
11	15	314	CLA	C1D-ND-C4D	-9.87	99.32	106.33
13	15	319	DD6	C37-C36-C31	-9.86	110.95	124.35
12	13	308	KC1	C2A-C3A-C4A	-9.86	99.17	106.49
11	11	303	CLA	C1D-ND-C4D	-9.83	99.35	106.33
12	7	307	KC1	C2A-C3A-C4A	-9.80	99.22	106.49
14	7	318	A86	C21-C20-C19	-9.79	103.26	114.28
13	15	318	DD6	C9-C10-C11	-9.79	113.33	127.31
12	13	305	KC1	C2A-C3A-C4A	-9.78	99.23	106.49
14	6	317	A86	C17-C16-C15	9.77	119.13	109.16
13	6	316	DD6	C9-C10-C11	-9.75	113.40	127.31
14	7	315	A86	C21-C20-C19	-9.75	103.32	114.28
11	7	306	CLA	C1D-ND-C4D	-9.74	99.41	106.33
12	14	306	KC1	CMA-C3A-C4A	-9.73	110.22	125.04
14	8	315	A86	O1-C20-C21	-9.73	103.39	115.06
14	15	316	A86	C21-C20-C19	-9.73	103.34	114.28
14	10	315	A86	O1-C20-C21	-9.73	103.40	115.06
14	10	317	A86	O1-C20-C21	-9.70	103.43	115.06
12	11	310	KC1	C2A-C3A-C4A	-9.70	99.29	106.49
14	14	315	A86	C4-C5-C6	-9.70	113.47	127.31
13	16	313	DD6	C3-C2-C1	-9.70	113.47	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	11	312	DD6	C3-C2-C1	-9.69	113.48	127.31
12	6	308	KC1	C2A-C3A-C4A	-9.67	99.31	106.49
11	7	304	CLA	C1D-ND-C4D	-9.67	99.47	106.33
13	7	317	DD6	C-C1-C2	-9.66	109.39	122.92
12	14	308	KC1	CMA-C3A-C4A	-9.66	110.33	125.04
14	15	316	A86	O1-C20-C21	-9.66	103.48	115.06
12	10	312	KC1	C2A-C3A-C4A	-9.66	99.32	106.49
14	15	320	A86	O1-C20-C21	-9.65	103.49	115.06
13	15	319	DD6	C7-C6-C5	-9.61	109.47	122.92
14	15	322	A86	O1-C20-C21	-9.59	103.56	115.06
11	10	308	CLA	C1D-ND-C4D	-9.59	99.52	106.33
13	12	315	DD6	C12-C11-C10	-9.58	109.51	122.92
12	14	306	KC1	C2A-C3A-C4A	-9.57	99.39	106.49
12	12	305	KC1	C2A-C3A-C4A	-9.57	99.39	106.49
14	14	314	A86	C4-C5-C6	-9.56	113.66	127.31
13	15	318	DD6	C12-C11-C10	-9.55	109.54	122.92
13	7	301	DD6	C4-C5-C6	-9.54	113.69	127.31
13	13	314	DD6	C3-C2-C1	-9.54	113.69	127.31
11	15	309	CLA	C1D-ND-C4D	-9.54	99.56	106.33
13	7	317	DD6	C3-C2-C1	-9.53	113.71	127.31
13	8	316	DD6	C4-C5-C6	-9.53	113.71	127.31
13	10	313	DD6	C7-C6-C5	-9.52	109.58	122.92
11	13	303	CLA	C1D-ND-C4D	-9.52	99.57	106.33
14	11	313	A86	O1-C20-C21	-9.50	103.68	115.06
13	6	318	DD6	C4-C5-C6	-9.49	113.76	127.31
11	7	302	CLA	C1D-ND-C4D	-9.49	99.60	106.33
13	16	313	DD6	C-C1-C2	-9.49	109.63	122.92
11	16	301	CLA	C1D-ND-C4D	-9.48	99.60	106.33
14	16	314	A86	C21-C20-C19	-9.47	103.62	114.28
12	13	310	KC1	C2A-C3A-C4A	-9.46	99.47	106.49
13	15	318	DD6	C7-C6-C5	-9.44	109.70	122.92
11	10	309	CLA	C1D-ND-C4D	-9.41	99.65	106.33
11	12	302	CLA	C1D-ND-C4D	-9.41	99.65	106.33
11	8	305	CLA	C1D-ND-C4D	-9.40	99.66	106.33
13	12	315	DD6	C4-C5-C6	-9.40	113.89	127.31
11	12	310	CLA	C1D-ND-C4D	-9.39	99.67	106.33
12	7	312	KC1	C2A-C3A-C4A	-9.38	99.53	106.49
11	14	313	CLA	C1D-ND-C4D	-9.38	99.67	106.33
13	7	301	DD6	C12-C11-C10	-9.38	109.79	122.92
13	12	317	DD6	C-C1-C2	-9.37	109.79	122.92
13	8	317	DD6	C8-C6-C5	-9.37	104.56	118.94
11	11	308	CLA	C1D-ND-C4D	-9.36	99.68	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	13	312	KC1	C2A-C3A-C4A	-9.34	99.55	106.49
14	11	314	A86	C21-C20-C19	-9.34	103.78	114.28
13	13	314	DD6	C4-C5-C6	-9.33	114.00	127.31
11	14	310	CLA	C1D-ND-C4D	-9.33	99.71	106.33
14	14	317	A86	C33-C32-C31	9.32	118.27	109.21
13	7	317	DD6	C4-C5-C6	-9.32	114.02	127.31
11	6	303	CLA	C1D-ND-C4D	-9.31	99.72	106.33
12	11	304	KC1	C2A-C3A-C4A	-9.30	99.58	106.49
11	15	304	CLA	C1D-ND-C4D	-9.30	99.73	106.33
12	8	310	KC1	C2A-C3A-C4A	-9.30	99.59	106.49
14	16	312	A86	O1-C20-C21	-9.29	103.93	115.06
14	7	315	A86	O1-C20-C21	-9.29	103.93	115.06
12	6	309	KC1	C2A-C3A-C4A	-9.28	99.60	106.49
14	10	301	A86	C21-C20-C19	-9.27	103.85	114.28
13	7	301	DD6	C7-C6-C5	-9.26	109.95	122.92
14	11	315	A86	O1-C20-C21	-9.25	103.97	115.06
13	13	314	DD6	C7-C6-C5	-9.25	109.97	122.92
11	8	301	CLA	C1D-ND-C4D	-9.25	99.77	106.33
11	6	311	CLA	C1D-ND-C4D	-9.25	99.77	106.33
13	6	318	DD6	C3-C2-C1	-9.24	114.12	127.31
11	13	301	CLA	C1D-ND-C4D	-9.24	99.77	106.33
11	11	305	CLA	C1D-ND-C4D	-9.24	99.77	106.33
11	16	309	CLA	C1D-ND-C4D	-9.24	99.77	106.33
13	12	317	DD6	C7-C6-C5	-9.24	109.98	122.92
12	6	305	KC1	C2A-C3A-C4A	-9.23	99.64	106.49
12	8	306	KC1	C2A-C3A-C4A	-9.20	99.66	106.49
14	12	316	A86	O1-C20-C21	-9.19	104.05	115.06
12	8	314	KC1	C2A-C3A-C4A	-9.18	99.68	106.49
11	10	311	CLA	C1D-ND-C4D	-9.17	99.82	106.33
13	16	313	DD6	C7-C6-C5	-9.15	110.11	122.92
11	11	307	CLA	C1D-ND-C4D	-9.14	99.84	106.33
12	8	307	KC1	C2A-C3A-C4A	-9.13	99.71	106.49
11	10	305	CLA	C1D-ND-C4D	-9.13	99.85	106.33
12	16	304	KC1	C2A-C3A-C4A	-9.11	99.72	106.49
11	15	313	CLA	C1D-ND-C4D	-9.11	99.86	106.33
12	13	311	KC1	C2A-C3A-C4A	-9.10	99.73	106.49
11	12	307	CLA	C1D-ND-C4D	-9.08	99.89	106.33
11	14	302	CLA	C1D-ND-C4D	-9.07	99.89	106.33
13	12	315	DD6	C-C1-C2	-9.06	110.23	122.92
11	16	308	CLA	C1D-ND-C4D	-9.06	99.90	106.33
14	13	313	A86	C4-C5-C6	-9.05	114.40	127.31
11	14	304	CLA	C1D-ND-C4D	-9.04	99.91	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	15	311	CLA	C1D-ND-C4D	-9.03	99.92	106.33
11	8	302	CLA	C1D-ND-C4D	-9.03	99.92	106.33
11	13	304	CLA	C1D-ND-C4D	-9.02	99.93	106.33
13	10	314	DD6	C12-C11-C10	-9.01	110.30	122.92
14	14	316	A86	O1-C20-C21	-9.01	104.26	115.06
11	14	312	CLA	C1D-ND-C4D	-9.01	99.94	106.33
11	12	312	CLA	C1D-ND-C4D	-9.01	99.94	106.33
11	15	303	CLA	C1D-ND-C4D	-8.99	99.95	106.33
14	7	318	A86	C33-C32-C31	8.99	117.95	109.21
13	7	316	DD6	C-C1-C2	-8.98	110.34	122.92
11	12	308	CLA	C1D-ND-C4D	-8.98	99.96	106.33
11	12	304	CLA	C1D-ND-C4D	-8.97	99.96	106.33
11	16	307	CLA	C1D-ND-C4D	-8.95	99.98	106.33
11	7	308	CLA	C1D-ND-C4D	-8.95	99.98	106.33
13	10	313	DD6	C-C1-C2	-8.94	110.39	122.92
12	10	306	KC1	CMA-C3A-C2A	-8.94	106.42	128.30
14	14	320	A86	C21-C20-C19	-8.93	104.23	114.28
12	12	313	KC1	C2B-C1B-NB	8.93	116.68	110.10
11	16	303	CLA	C2D-C1D-ND	8.93	116.68	110.10
13	8	317	DD6	C4-C5-C6	-8.91	114.60	127.31
13	7	301	DD6	C3-C2-C1	-8.90	114.61	127.31
11	8	305	CLA	C2D-C1D-ND	8.90	116.66	110.10
11	15	306	CLA	C1D-ND-C4D	-8.89	100.02	106.33
11	15	310	CLA	C1D-ND-C4D	-8.89	100.02	106.33
13	6	316	DD6	C3-C2-C1	-8.89	114.62	127.31
14	7	318	A86	O1-C20-C21	-8.88	104.42	115.06
12	11	311	KC1	C2A-C3A-C4A	-8.87	99.90	106.49
11	10	303	CLA	C1D-ND-C4D	-8.87	100.04	106.33
11	7	309	CLA	C1D-ND-C4D	-8.86	100.04	106.33
13	12	315	DD6	C9-C10-C11	-8.86	114.67	127.31
11	14	303	CLA	C1D-ND-C4D	-8.85	100.05	106.33
11	8	304	CLA	C1D-ND-C4D	-8.85	100.05	106.33
14	7	314	A86	O1-C20-C21	-8.85	104.46	115.06
11	8	301	CLA	C2D-C1D-ND	8.84	116.62	110.10
13	7	301	DD6	C-C1-C2	-8.83	110.55	122.92
12	8	307	KC1	CMA-C3A-C2A	-8.83	106.69	128.30
14	15	315	A86	C25-C26-C27	-8.83	114.71	127.31
11	15	305	CLA	C1D-ND-C4D	-8.82	100.07	106.33
13	11	312	DD6	C12-C11-C10	-8.82	110.57	122.92
11	16	302	CLA	C1D-ND-C4D	-8.82	100.07	106.33
11	12	321	CLA	C1D-ND-C4D	-8.82	100.07	106.33
13	10	314	DD6	C3-C2-C1	-8.82	114.73	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	7	302	CLA	C2D-C1D-ND	8.80	116.59	110.10
11	14	307	CLA	C2D-C1D-ND	8.80	116.59	110.10
11	8	309	CLA	C1D-ND-C4D	-8.80	100.09	106.33
13	12	315	DD6	C7-C6-C5	-8.79	110.60	122.92
11	6	304	CLA	C1D-ND-C4D	-8.79	100.09	106.33
11	11	309	CLA	C1D-ND-C4D	-8.79	100.09	106.33
11	7	311	CLA	C1D-ND-C4D	-8.78	100.10	106.33
11	7	303	CLA	C1D-ND-C4D	-8.77	100.11	106.33
14	14	314	A86	O1-C20-C21	-8.77	104.55	115.06
14	14	319	A86	C33-C32-C31	8.76	117.73	109.21
13	12	315	DD6	C13-C11-C10	-8.75	105.52	118.94
11	8	308	CLA	C1D-ND-C4D	-8.74	100.13	106.33
11	8	303	CLA	C1D-ND-C4D	-8.74	100.13	106.33
11	16	310	CLA	C1D-ND-C4D	-8.73	100.14	106.33
13	6	318	DD6	C-C1-C2	-8.72	110.71	122.92
11	6	314	CLA	C1D-ND-C4D	-8.71	100.15	106.33
12	16	311	KC1	CMA-C3A-C4A	-8.70	111.79	125.04
14	11	313	A86	C4-C5-C6	-8.69	114.90	127.31
11	16	301	CLA	C2D-C1D-ND	8.69	116.51	110.10
11	7	306	CLA	C2D-C1D-ND	8.67	116.50	110.10
12	8	311	KC1	C2A-C3A-C4A	-8.67	100.06	106.49
11	6	301	CLA	C1D-ND-C4D	-8.66	100.18	106.33
11	6	312	CLA	C1D-ND-C4D	-8.65	100.19	106.33
11	16	305	CLA	C1D-ND-C4D	-8.65	100.19	106.33
14	11	313	A86	C17-C16-C15	8.65	117.98	109.16
11	15	307	CLA	C1D-ND-C4D	-8.65	100.19	106.33
11	10	304	CLA	C1D-ND-C4D	-8.64	100.19	106.33
13	13	314	DD6	C-C1-C2	-8.64	110.82	122.92
13	6	318	DD6	C8-C6-C5	-8.64	105.69	118.94
14	15	322	A86	C17-C16-C15	8.64	117.97	109.16
11	14	305	CLA	C1D-ND-C4D	-8.63	100.21	106.33
14	15	315	A86	O1-C20-C21	-8.62	104.73	115.06
11	15	314	CLA	C2D-C1D-ND	8.61	116.45	110.10
13	7	313	DD6	C8-C6-C5	-8.60	105.74	118.94
11	12	302	CLA	C2D-C1D-ND	8.59	116.44	110.10
11	13	302	CLA	C1D-ND-C4D	-8.59	100.23	106.33
11	16	306	CLA	C1D-ND-C4D	-8.59	100.23	106.33
12	13	306	KC1	CMA-C3A-C2A	-8.59	107.28	128.30
13	8	316	DD6	C3-C2-C1	-8.58	115.07	127.31
14	15	315	A86	C17-C16-C15	8.57	117.90	109.16
11	10	307	CLA	C1D-ND-C4D	-8.56	100.26	106.33
13	6	318	DD6	C7-C6-C5	-8.55	110.95	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	12	309	KC1	C2B-C1B-NB	8.53	116.39	110.10
13	6	315	DD6	C7-C6-C5	-8.53	110.98	122.92
14	14	320	A86	C33-C32-C31	8.51	117.48	109.21
11	10	307	CLA	C2D-C1D-ND	8.51	116.37	110.10
11	15	312	CLA	C1D-ND-C4D	-8.50	100.30	106.33
12	12	311	KC1	C2A-C3A-C4A	-8.49	100.18	106.49
11	7	310	CLA	C1D-ND-C4D	-8.48	100.31	106.33
13	11	312	DD6	C-C1-C2	-8.47	111.06	122.92
11	12	306	CLA	C1D-ND-C4D	-8.46	100.33	106.33
13	16	313	DD6	C8-C6-C5	-8.44	105.98	118.94
12	13	306	KC1	C2A-C3A-C4A	-8.44	100.23	106.49
11	7	305	CLA	C1D-ND-C4D	-8.43	100.34	106.33
13	15	319	DD6	C32-C31-C36	-8.43	110.73	122.63
11	15	308	CLA	C1D-ND-C4D	-8.41	100.36	106.33
13	8	317	DD6	C7-C6-C5	-8.41	111.14	122.92
11	13	307	CLA	C1D-ND-C4D	-8.40	100.37	106.33
13	10	314	DD6	C7-C6-C5	-8.38	111.19	122.92
14	14	315	A86	C33-C32-C31	8.36	117.33	109.21
11	6	306	CLA	C1D-ND-C4D	-8.35	100.40	106.33
11	6	302	CLA	C1D-ND-C4D	-8.35	100.41	106.33
13	7	317	DD6	C7-C6-C5	-8.34	111.23	122.92
14	10	316	A86	C33-C32-C31	8.34	117.31	109.21
12	10	306	KC1	C2A-C3A-C4A	-8.32	100.31	106.49
11	14	309	CLA	C1D-ND-C4D	-8.32	100.42	106.33
13	12	315	DD6	C3-C2-C1	-8.32	115.44	127.31
11	8	302	CLA	C2D-C1D-ND	8.31	116.23	110.10
13	8	316	DD6	C7-C6-C5	-8.31	111.28	122.92
13	10	313	DD6	C13-C11-C10	-8.31	106.19	118.94
12	12	311	KC1	CMA-C3A-C2A	-8.31	107.96	128.30
11	6	307	CLA	C1D-ND-C4D	-8.31	100.44	106.33
11	10	303	CLA	C2D-C1D-ND	8.30	116.22	110.10
11	15	302	CLA	C2D-C1D-ND	8.30	116.22	110.10
13	6	316	DD6	C-C1-C2	-8.29	111.31	122.92
13	6	315	DD6	C-C1-C2	-8.28	111.33	122.92
14	14	319	A86	C4-C5-C6	-8.27	115.50	127.31
11	7	308	CLA	C2D-C1D-ND	8.26	116.19	110.10
14	11	314	A86	O1-C20-C21	-8.25	105.17	115.06
11	13	309	CLA	C1D-ND-C4D	-8.23	100.49	106.33
13	10	314	DD6	C-C1-C2	-8.23	111.39	122.92
12	8	312	KC1	C2A-C3A-C4A	-8.22	100.39	106.49
14	14	318	A86	C4-C5-C6	-8.22	115.58	127.31
12	6	305	KC1	CMA-C3A-C2A	-8.22	108.19	128.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	6	303	CLA	C2D-C1D-ND	8.20	116.15	110.10
11	11	303	CLA	C2D-C1D-ND	8.20	116.15	110.10
14	7	314	A86	C33-C32-C31	8.19	117.17	109.21
14	7	315	A86	C17-C16-C15	8.18	117.51	109.16
11	12	303	CLA	C1D-ND-C4D	-8.17	100.53	106.33
11	7	303	CLA	C2D-C1D-ND	8.15	116.11	110.10
11	6	313	CLA	C1D-ND-C4D	-8.15	100.55	106.33
13	7	313	DD6	C4-C5-C6	-8.14	115.69	127.31
11	13	301	CLA	C2D-C1D-ND	8.11	116.08	110.10
11	12	310	CLA	C2D-C1D-ND	8.11	116.08	110.10
11	10	308	CLA	C2D-C1D-ND	8.10	116.08	110.10
11	10	309	CLA	C2D-C1D-ND	8.10	116.07	110.10
13	8	317	DD6	C3-C2-C1	-8.09	115.76	127.31
14	15	321	A86	C33-C32-C31	8.06	117.05	109.21
13	8	316	DD6	C8-C6-C5	-8.06	106.57	118.94
13	16	313	DD6	C4-C5-C6	-8.05	115.82	127.31
13	12	317	DD6	C8-C6-C5	-8.05	106.58	118.94
13	12	317	DD6	C4-C5-C6	-8.04	115.84	127.31
11	8	304	CLA	C2D-C1D-ND	8.03	116.02	110.10
11	15	309	CLA	C2D-C1D-ND	8.03	116.02	110.10
14	14	317	A86	C4-C5-C6	-8.03	115.85	127.31
12	13	311	KC1	CMA-C3A-C2A	-8.02	108.67	128.30
11	15	304	CLA	C2D-C1D-ND	8.01	116.01	110.10
12	13	305	KC1	CMA-C3A-C2A	-8.00	108.72	128.30
11	15	303	CLA	C2D-C1D-ND	8.00	116.00	110.10
12	11	304	KC1	CMA-C3A-C2A	-8.00	108.73	128.30
11	15	308	CLA	C2D-C1D-ND	7.98	115.99	110.10
14	10	302	A86	C25-C26-C27	-7.98	115.93	127.31
12	12	311	KC1	C2B-C1B-NB	7.96	115.97	110.10
14	15	317	A86	C4-C5-C6	-7.95	115.96	127.31
11	16	305	CLA	C2D-C1D-ND	7.94	115.96	110.10
11	10	311	CLA	C2D-C1D-ND	7.94	115.95	110.10
11	15	313	CLA	C2D-C1D-ND	7.93	115.95	110.10
11	12	307	CLA	C2D-C1D-ND	7.93	115.95	110.10
13	12	315	DD6	C8-C6-C5	-7.93	106.78	118.94
12	8	314	KC1	C2B-C1B-NB	7.93	115.94	110.10
11	16	309	CLA	C2D-C1D-ND	7.92	115.94	110.10
12	7	312	KC1	CMA-C3A-C2A	-7.91	108.94	128.30
11	13	303	CLA	C2D-C1D-ND	7.90	115.93	110.10
13	7	316	DD6	C7-C6-C5	-7.90	111.86	122.92
12	8	310	KC1	CMA-C3A-C2A	-7.90	108.96	128.30
11	12	312	CLA	C2D-C1D-ND	7.90	115.92	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	15	318	DD6	C3-C2-C1	-7.89	116.04	127.31
11	7	304	CLA	C2D-C1D-ND	7.89	115.92	110.10
11	14	310	CLA	C2D-C1D-ND	7.89	115.92	110.10
11	16	302	CLA	C2D-C1D-ND	7.87	115.90	110.10
11	12	308	CLA	C2D-C1D-ND	7.86	115.90	110.10
11	15	310	CLA	C2D-C1D-ND	7.85	115.89	110.10
11	11	307	CLA	C2D-C1D-ND	7.85	115.89	110.10
11	15	306	CLA	C2D-C1D-ND	7.84	115.88	110.10
11	15	311	CLA	C2D-C1D-ND	7.83	115.87	110.10
11	14	312	CLA	C2D-C1D-ND	7.82	115.87	110.10
11	7	305	CLA	C2D-C1D-ND	7.82	115.87	110.10
12	10	310	KC1	C2B-C1B-NB	7.82	115.87	110.10
12	16	311	KC1	C2B-C1B-NB	7.82	115.86	110.10
14	10	302	A86	C17-C16-C15	7.82	117.14	109.16
11	11	305	CLA	C2D-C1D-ND	7.81	115.86	110.10
11	12	321	CLA	C2D-C1D-ND	7.80	115.85	110.10
11	16	308	CLA	C2D-C1D-ND	7.80	115.85	110.10
12	10	312	KC1	C2B-C1B-NB	7.80	115.85	110.10
14	10	317	A86	C17-C16-C15	7.79	117.11	109.16
13	15	318	DD6	C32-C31-C36	-7.79	111.64	122.63
14	10	316	A86	C4-C5-C6	-7.78	116.21	127.31
12	8	314	KC1	O2D-CGD-CBD	7.78	125.09	111.27
12	8	313	KC1	CMA-C3A-C2A	-7.77	109.27	128.30
13	8	317	DD6	C9-C10-C11	-7.77	116.22	127.31
12	7	312	KC1	C2B-C1B-NB	7.76	115.83	110.10
11	13	302	CLA	C2D-C1D-ND	7.76	115.82	110.10
12	6	308	KC1	CMA-C3A-C2A	-7.76	109.31	128.30
11	12	304	CLA	C2D-C1D-ND	7.76	115.82	110.10
11	13	304	CLA	C2D-C1D-ND	7.75	115.81	110.10
11	14	304	CLA	C2D-C1D-ND	7.73	115.80	110.10
11	15	305	CLA	C2D-C1D-ND	7.72	115.80	110.10
13	7	316	DD6	C4-C5-C6	-7.72	116.29	127.31
11	10	304	CLA	C2D-C1D-ND	7.72	115.79	110.10
11	12	304	CLA	CAA-C2A-C3A	-7.71	91.66	112.78
11	8	308	CLA	C2D-C1D-ND	7.71	115.79	110.10
12	8	311	KC1	CMA-C3A-C2A	-7.71	109.43	128.30
11	14	313	CLA	C2D-C1D-ND	7.71	115.78	110.10
12	13	312	KC1	CMA-C3A-C2A	-7.71	109.43	128.30
11	15	312	CLA	CMD-C2D-C1D	7.71	138.30	124.71
13	7	313	DD6	C15-C14-C13	7.70	142.27	125.99
12	8	313	KC1	C2B-C1B-NB	7.69	115.77	110.10
14	10	315	A86	C17-C16-C15	7.69	117.01	109.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	6	317	A86	C21-C20-C19	-7.69	105.63	114.28
14	7	315	A86	C33-C32-C31	7.69	116.68	109.21
12	10	312	KC1	CMA-C3A-C2A	-7.68	109.50	128.30
12	11	306	KC1	C2B-C1B-NB	7.67	115.76	110.10
11	15	307	CLA	C2D-C1D-ND	7.67	115.76	110.10
14	10	316	A86	O1-C20-C21	-7.66	105.88	115.06
14	12	314	A86	C4-C5-C6	-7.66	116.38	127.31
11	6	307	CLA	C2D-C1D-ND	7.66	115.75	110.10
14	14	318	A86	C33-C32-C31	7.63	116.63	109.21
12	16	304	KC1	C2B-C1B-NB	7.63	115.73	110.10
11	7	310	CLA	C2D-C1D-ND	7.62	115.72	110.10
11	11	309	CLA	C2D-C1D-ND	7.62	115.72	110.10
14	16	312	A86	C17-C16-C15	7.61	116.93	109.16
13	16	313	DD6	C15-C14-C13	7.61	142.08	125.99
13	7	313	DD6	C7-C6-C5	-7.60	112.27	122.92
12	14	308	KC1	C2B-C1B-NB	7.60	115.70	110.10
12	13	308	KC1	C2B-C1B-NB	7.59	115.70	110.10
11	7	304	CLA	CMD-C2D-C1D	7.59	138.10	124.71
11	6	311	CLA	C2D-C1D-ND	7.59	115.70	110.10
11	6	314	CLA	C2D-C1D-ND	7.59	115.70	110.10
11	14	305	CLA	C2D-C1D-ND	7.59	115.69	110.10
13	8	317	DD6	C-C1-C2	-7.58	112.30	122.92
11	12	306	CLA	C2D-C1D-ND	7.58	115.69	110.10
11	14	303	CLA	C2D-C1D-ND	7.58	115.69	110.10
11	13	307	CLA	C2D-C1D-ND	7.57	115.69	110.10
11	6	301	CLA	C2D-C1D-ND	7.57	115.68	110.10
13	7	313	DD6	C9-C10-C11	-7.56	116.52	127.31
11	10	305	CLA	C2D-C1D-ND	7.56	115.68	110.10
11	11	308	CLA	C2D-C1D-ND	7.56	115.67	110.10
11	8	309	CLA	C2D-C1D-ND	7.53	115.65	110.10
14	15	320	A86	C17-C16-C15	7.53	116.85	109.16
13	8	316	DD6	C9-C10-C11	-7.53	116.57	127.31
12	13	306	KC1	C1A-C2A-C3A	-7.52	101.14	107.11
13	13	314	DD6	C7-C6-C8	-7.51	106.25	118.08
11	16	307	CLA	C2D-C1D-ND	7.51	115.64	110.10
14	14	320	A86	C25-C26-C27	-7.50	116.60	127.31
13	15	318	DD6	C-C1-C2	-7.50	112.42	122.92
13	7	313	DD6	C14-C13-C11	7.49	137.16	125.53
11	7	309	CLA	C2D-C1D-ND	7.48	115.62	110.10
12	6	309	KC1	CMA-C3A-C2A	-7.48	110.00	128.30
11	7	311	CLA	C2D-C1D-ND	7.48	115.61	110.10
12	6	305	KC1	C2B-C1B-NB	7.47	115.61	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	8	303	CLA	C2D-C1D-ND	7.46	115.60	110.10
11	6	306	CLA	C2D-C1D-ND	7.43	115.58	110.10
11	14	302	CLA	C2D-C1D-ND	7.43	115.58	110.10
11	12	303	CLA	C2D-C1D-ND	7.43	115.58	110.10
11	16	310	CLA	C2D-C1D-ND	7.43	115.58	110.10
14	10	302	A86	C4-C5-C6	-7.42	116.72	127.31
13	6	318	DD6	C13-C11-C10	-7.42	107.55	118.94
14	12	316	A86	C33-C32-C31	7.42	116.42	109.21
13	7	317	DD6	C7-C6-C8	-7.42	106.39	118.08
12	12	311	KC1	C1A-C2A-C3A	-7.41	101.23	107.11
12	12	305	KC1	CMA-C3A-C2A	-7.40	110.19	128.30
13	15	319	DD6	C8-C6-C5	-7.39	107.59	118.94
12	8	311	KC1	C2B-C1B-NB	7.39	115.55	110.10
12	12	309	KC1	CMA-C3A-C4A	-7.39	113.78	125.04
12	6	308	KC1	C2B-C1B-NB	7.38	115.55	110.10
11	13	309	CLA	C2D-C1D-ND	7.38	115.54	110.10
12	12	305	KC1	C2B-C1B-NB	7.37	115.54	110.10
12	6	310	KC1	CMA-C3A-C2A	-7.37	110.26	128.30
11	6	302	CLA	C2D-C1D-ND	7.37	115.53	110.10
12	12	309	KC1	CHB-C4A-C3A	-7.37	113.47	124.98
14	11	315	A86	C33-C32-C31	7.36	116.36	109.21
13	8	316	DD6	C-C1-C2	-7.35	112.62	122.92
12	8	312	KC1	C1A-C2A-C3A	-7.35	101.28	107.11
12	10	310	KC1	C3A-C4A-NA	7.35	118.59	110.57
12	11	310	KC1	C2B-C1B-NB	7.35	115.52	110.10
12	14	306	KC1	C2B-C1B-NB	7.33	115.51	110.10
12	16	311	KC1	C3A-C4A-NA	7.32	118.57	110.57
13	15	318	DD6	C8-C6-C5	-7.32	107.71	118.94
12	11	310	KC1	CMA-C3A-C2A	-7.31	110.41	128.30
11	6	312	CLA	C2D-C1D-ND	7.31	115.49	110.10
12	11	311	KC1	CMA-C3A-C4A	-7.30	113.92	125.04
11	14	302	CLA	CMD-C2D-C1D	7.30	137.58	124.71
12	13	308	KC1	CMA-C3A-C2A	-7.28	110.47	128.30
14	14	314	A86	C17-C16-C15	7.26	116.57	109.16
13	7	313	DD6	C32-C31-C36	-7.24	112.41	122.63
14	16	312	A86	C3-C2-C1	-7.23	116.99	127.31
11	6	304	CLA	C2D-C1D-ND	7.23	115.43	110.10
14	16	312	A86	C33-C32-C31	7.22	116.22	109.21
13	7	317	DD6	C32-C31-C36	-7.21	112.45	122.63
12	16	311	KC1	CHB-C4A-C3A	-7.21	113.71	124.98
14	7	314	A86	C3-C2-C1	-7.20	117.03	127.31
12	12	311	KC1	CHB-C4A-C3A	-7.19	113.74	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	7	317	DD6	C12-C11-C13	-7.19	106.75	118.08
12	6	309	KC1	C2B-C1B-NB	7.17	115.39	110.10
12	13	305	KC1	C2B-C1B-NB	7.17	115.39	110.10
14	15	315	A86	C33-C32-C31	7.17	116.18	109.21
12	11	311	KC1	C1A-C2A-C3A	-7.17	101.42	107.11
12	13	312	KC1	C2B-C1B-NB	7.16	115.38	110.10
11	14	310	CLA	CMD-C2D-C1D	7.16	137.33	124.71
14	13	313	A86	C33-C32-C31	7.14	116.16	109.21
14	10	315	A86	C33-C32-C31	7.12	116.13	109.21
12	8	314	KC1	C1A-C2A-C3A	-7.11	101.47	107.11
14	10	302	A86	C33-C32-C31	7.11	116.12	109.21
12	10	306	KC1	C2B-C1B-NB	7.11	115.34	110.10
12	12	309	KC1	C3A-C4A-NA	7.10	118.32	110.57
12	10	310	KC1	CHB-C4A-C3A	-7.09	113.90	124.98
12	8	306	KC1	C2B-C1B-NB	7.09	115.33	110.10
14	14	316	A86	C33-C32-C31	7.08	116.09	109.21
12	16	304	KC1	C1A-C2A-C3A	-7.08	101.50	107.11
11	6	313	CLA	C2D-C1D-ND	7.07	115.31	110.10
12	11	306	KC1	CMA-C3A-C2A	-7.07	111.00	128.30
14	11	301	A86	C33-C32-C31	7.06	116.08	109.21
12	11	311	KC1	C2B-C1B-NB	7.06	115.31	110.10
11	14	309	CLA	C2D-C1D-ND	7.06	115.31	110.10
11	15	314	CLA	CMD-C2D-C1D	7.05	137.14	124.71
11	16	308	CLA	CMD-C2D-C1D	7.04	137.12	124.71
12	8	314	KC1	CHB-C4A-C3A	-7.04	113.98	124.98
11	15	306	CLA	O2D-CGD-CBD	7.03	123.75	111.27
12	14	311	KC1	CMA-C3A-C2A	-7.01	111.13	128.30
13	7	301	DD6	C32-C31-C36	-7.01	112.73	122.63
11	7	304	CLA	O2D-CGD-CBD	7.01	123.73	111.27
13	7	317	DD6	C24-C1-C2	-7.01	108.18	118.94
13	10	314	DD6	C8-C6-C5	-7.01	108.18	118.94
13	13	314	DD6	C9-C10-C11	-7.01	117.30	127.31
11	15	302	CLA	CHD-C1D-ND	-7.01	118.02	124.45
14	7	318	A86	C25-C26-C27	-7.00	117.32	127.31
13	15	319	DD6	C13-C11-C10	-7.00	108.21	118.94
11	16	306	CLA	C2D-C1D-ND	7.00	115.26	110.10
11	6	311	CLA	CMD-C2D-C1D	6.98	137.01	124.71
13	10	314	DD6	C9-C10-C11	-6.97	117.37	127.31
14	14	321	A86	C4-C5-C6	-6.96	117.37	127.31
12	6	305	KC1	CHB-C4A-C3A	-6.96	114.11	124.98
11	7	311	CLA	CMD-C2D-C1D	6.96	136.97	124.71
12	10	310	KC1	CMA-C3A-C2A	-6.95	111.30	128.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	8	306	KC1	C1A-C2A-C3A	-6.94	101.60	107.11
12	13	310	KC1	CMA-C3A-C2A	-6.94	111.31	128.30
11	8	302	CLA	CMD-C2D-C1D	6.94	136.94	124.71
14	15	316	A86	C17-C16-C15	6.94	116.24	109.16
12	10	306	KC1	C1A-C2A-C3A	-6.94	101.61	107.11
12	6	310	KC1	C2B-C1B-NB	6.92	115.21	110.10
12	8	312	KC1	CMA-C3A-C2A	-6.92	111.35	128.30
11	14	307	CLA	CHD-C1D-ND	-6.92	118.09	124.45
12	6	308	KC1	C3A-C4A-NA	6.91	118.12	110.57
11	15	302	CLA	CMD-C2D-C1D	6.91	136.90	124.71
12	14	311	KC1	C2B-C1B-NB	6.91	115.20	110.10
14	8	315	A86	C17-C16-C15	6.91	116.21	109.16
14	6	317	A86	C25-C26-C27	-6.90	117.46	127.31
12	13	310	KC1	C2B-C1B-NB	6.90	115.19	110.10
12	11	304	KC1	C2B-C1B-NB	6.90	115.19	110.10
12	13	305	KC1	CHB-C4A-C3A	-6.90	114.20	124.98
12	7	307	KC1	C2B-C1B-NB	6.90	115.19	110.10
11	15	309	CLA	CMD-C2D-C1D	6.90	136.87	124.71
14	15	317	A86	C17-C16-C15	6.90	116.20	109.16
12	7	312	KC1	CHB-C4A-C3A	-6.89	114.22	124.98
14	15	316	A86	C33-C32-C31	6.88	115.90	109.21
12	6	305	KC1	C3A-C4A-NA	6.88	118.08	110.57
14	15	315	A86	C24-C1-C2	6.88	129.49	118.94
13	8	317	DD6	C24-C1-C2	-6.87	108.39	118.94
13	7	316	DD6	C8-C6-C5	-6.87	108.40	118.94
13	7	313	DD6	C-C1-C2	-6.87	113.30	122.92
12	11	306	KC1	CHB-C4A-C3A	-6.87	114.25	124.98
14	14	320	A86	O1-C20-C21	-6.86	106.84	115.06
13	12	317	DD6	C12-C11-C13	-6.85	107.28	118.08
14	12	314	A86	C33-C32-C31	6.85	115.87	109.21
12	14	311	KC1	CHB-C4A-C3A	-6.85	114.28	124.98
12	6	308	KC1	C1A-C2A-C3A	-6.84	101.68	107.11
12	14	311	KC1	C3A-C4A-NA	6.84	118.04	110.57
13	6	316	DD6	C7-C6-C5	-6.84	113.35	122.92
13	12	317	DD6	C32-C31-C36	-6.83	112.98	122.63
12	6	308	KC1	CHB-C4A-C3A	-6.83	114.31	124.98
11	11	307	CLA	CMD-C2D-C1D	6.82	136.73	124.71
11	6	304	CLA	CMD-C2D-C1D	6.81	136.71	124.71
11	7	309	CLA	CMD-C2D-C1D	6.81	136.71	124.71
11	16	310	CLA	CMD-C2D-C1D	6.81	136.71	124.71
11	14	304	CLA	CMD-C2D-C1D	6.80	136.71	124.71
12	11	306	KC1	C3A-C4A-NA	6.80	118.00	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	13	308	KC1	C3A-C4A-NA	6.80	117.99	110.57
11	14	313	CLA	CMD-C2D-C1D	6.80	136.69	124.71
12	14	306	KC1	CMA-C3A-C2A	-6.79	111.69	128.30
13	15	318	DD6	C13-C11-C10	-6.78	108.54	118.94
12	13	308	KC1	CHB-C4A-C3A	-6.78	114.39	124.98
12	8	311	KC1	C1A-C2A-C3A	-6.78	101.73	107.11
14	11	314	A86	C4-C5-C6	-6.77	117.65	127.31
12	8	313	KC1	CHB-C4A-C3A	-6.76	114.42	124.98
14	12	314	A86	C17-C16-C15	6.75	116.05	109.16
12	8	313	KC1	C3A-C4A-NA	6.75	117.94	110.57
12	10	312	KC1	C3A-C4A-NA	6.75	117.94	110.57
11	15	312	CLA	C2D-C1D-ND	6.75	115.08	110.10
11	15	314	CLA	CHD-C1D-ND	-6.75	118.25	124.45
12	6	305	KC1	C1A-C2A-C3A	-6.74	101.76	107.11
11	13	304	CLA	CMD-C2D-C1D	6.73	136.58	124.71
12	14	308	KC1	CHB-C4A-C3A	-6.73	114.47	124.98
13	11	312	DD6	C24-C1-C2	-6.73	108.62	118.94
12	14	306	KC1	C1A-C2A-C3A	-6.73	101.77	107.11
13	12	315	DD6	C24-C1-C2	-6.73	108.62	118.94
11	15	311	CLA	CMD-C2D-C1D	6.73	136.57	124.71
12	8	307	KC1	C2B-C1B-NB	6.72	115.05	110.10
12	16	304	KC1	CMA-C3A-C4A	-6.72	114.81	125.04
13	11	312	DD6	C32-C31-C36	-6.71	113.16	122.63
11	13	303	CLA	CMD-C2D-C1D	6.70	136.53	124.71
13	6	316	DD6	C4-C5-C6	-6.70	117.75	127.31
12	8	307	KC1	C1A-C2A-C3A	-6.70	101.80	107.11
12	16	304	KC1	CHB-C4A-C3A	-6.69	114.53	124.98
11	6	301	CLA	CMD-C2D-C1D	6.69	136.50	124.71
14	15	317	A86	C36-C31-C32	-6.69	113.06	119.70
12	10	312	KC1	CHB-C4A-C3A	-6.69	114.53	124.98
11	13	309	CLA	CMD-C2D-C1D	6.69	136.50	124.71
12	11	311	KC1	CHB-C4A-C3A	-6.68	114.54	124.98
11	10	308	CLA	CMD-C2D-C1D	6.68	136.49	124.71
13	12	317	DD6	C13-C11-C10	-6.68	108.69	118.94
11	14	309	CLA	CMD-C2D-C1D	6.68	136.48	124.71
11	6	313	CLA	CMD-C2D-C1D	6.67	136.47	124.71
12	14	306	KC1	C3A-C4A-NA	6.67	117.85	110.57
11	15	304	CLA	CMD-C2D-C1D	6.67	136.46	124.71
11	7	306	CLA	CMD-C2D-C1D	6.67	136.46	124.71
13	10	313	DD6	C-C1-C24	-6.66	107.58	118.08
12	13	310	KC1	CHB-C4A-C3A	-6.65	114.59	124.98
12	14	308	KC1	C3A-C4A-NA	6.65	117.83	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	12	313	KC1	C3B-C2B-C1B	-6.65	100.73	107.08
11	16	309	CLA	CMD-C2D-C1D	6.64	136.42	124.71
12	6	309	KC1	C1A-C2A-C3A	-6.64	101.84	107.11
12	13	310	KC1	C1A-C2A-C3A	-6.64	101.84	107.11
12	13	312	KC1	CHB-C4A-C3A	-6.64	114.61	124.98
12	11	310	KC1	C3A-C4A-NA	6.64	117.82	110.57
12	8	310	KC1	C2B-C1B-NB	6.63	114.99	110.10
12	13	310	KC1	C3A-C4A-NA	6.63	117.81	110.57
11	14	312	CLA	CMD-C2D-C1D	6.63	136.39	124.71
11	8	304	CLA	CAA-C2A-C3A	-6.62	94.64	112.78
12	12	309	KC1	C3B-C2B-C1B	-6.62	100.76	107.08
13	11	312	DD6	C12-C11-C13	-6.61	107.66	118.08
12	7	307	KC1	CHB-C4A-C3A	-6.61	114.65	124.98
11	12	312	CLA	CMD-C2D-C1D	6.61	136.35	124.71
14	14	321	A86	C33-C32-C31	6.60	115.62	109.21
12	11	304	KC1	C1A-C2A-C3A	-6.59	101.88	107.11
12	7	312	KC1	C1A-C2A-C3A	-6.59	101.88	107.11
12	11	310	KC1	CHB-C4A-C3A	-6.58	114.69	124.98
14	14	316	A86	C17-C16-C15	6.58	115.88	109.16
11	15	303	CLA	CMD-C2D-C1D	6.58	136.30	124.71
11	10	309	CLA	CMD-C2D-C1D	6.58	136.30	124.71
14	16	314	A86	C33-C32-C31	6.57	115.60	109.21
11	15	313	CLA	CMD-C2D-C1D	6.57	136.30	124.71
14	11	301	A86	C3-C2-C1	-6.57	117.93	127.31
12	7	307	KC1	C3A-C4A-NA	6.57	117.75	110.57
12	10	312	KC1	C1A-C2A-C3A	-6.57	101.90	107.11
13	13	314	DD6	C14-C13-C11	6.57	135.72	125.53
11	15	310	CLA	CMD-C2D-C1D	6.56	136.28	124.71
13	6	315	DD6	C12-C11-C13	-6.56	107.74	118.08
11	10	305	CLA	CMD-C2D-C1D	6.56	136.27	124.71
11	14	303	CLA	CMD-C2D-C1D	6.55	136.26	124.71
11	11	305	CLA	CMD-C2D-C1D	6.55	136.25	124.71
11	13	301	CLA	CMD-C2D-C1D	6.54	136.25	124.71
12	13	311	KC1	C1A-C2A-C3A	-6.54	101.92	107.11
12	8	314	KC1	C3A-C4A-NA	6.53	117.71	110.57
12	6	309	KC1	CHB-C4A-C3A	-6.53	114.77	124.98
11	8	308	CLA	CMD-C2D-C1D	6.53	136.23	124.71
12	8	314	KC1	CMA-C3A-C4A	-6.53	115.09	125.04
12	12	305	KC1	CHB-C4A-C3A	-6.53	114.77	124.98
12	8	306	KC1	CHB-C4A-C3A	-6.53	114.77	124.98
11	6	312	CLA	CMD-C2D-C1D	6.53	136.22	124.71
14	13	315	A86	C3-C2-C1	-6.53	117.99	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	10	306	KC1	O2D-CGD-CBD	6.53	122.87	111.27
12	8	310	KC1	CHB-C4A-C3A	-6.53	114.78	124.98
13	13	314	DD6	C-C1-C24	-6.53	107.80	118.08
11	10	311	CLA	CMD-C2D-C1D	6.52	136.20	124.71
14	6	317	A86	O1-C20-C21	-6.52	107.25	115.06
11	15	312	CLA	CHD-C1D-ND	-6.51	118.47	124.45
14	15	322	A86	C25-C26-C27	-6.51	118.02	127.31
13	6	318	DD6	C24-C1-C2	-6.50	108.96	118.94
11	11	303	CLA	CMD-C2D-C1D	6.50	136.17	124.71
12	13	312	KC1	C1A-C2A-C3A	-6.50	101.95	107.11
12	11	310	KC1	C1A-C2A-C3A	-6.50	101.96	107.11
11	14	310	CLA	CHD-C1D-ND	-6.50	118.48	124.45
11	15	305	CLA	CMD-C2D-C1D	6.49	136.16	124.71
12	13	306	KC1	C2B-C1B-NB	6.49	114.89	110.10
13	7	301	DD6	C8-C6-C5	-6.49	108.99	118.94
11	8	305	CLA	CMD-C2D-C1D	6.48	136.14	124.71
11	15	309	CLA	CHD-C1D-ND	-6.48	118.50	124.45
12	12	313	KC1	CMD-C2D-C1D	6.48	138.42	128.46
11	16	301	CLA	CHD-C4C-C3C	-6.48	115.32	124.84
11	13	309	CLA	C2C-C1C-NC	6.47	116.03	109.97
12	13	305	KC1	C3A-C4A-NA	6.47	117.64	110.57
12	14	306	KC1	CHB-C4A-C3A	-6.46	114.89	124.98
12	7	312	KC1	C3B-C2B-C1B	-6.46	100.91	107.08
13	7	301	DD6	C13-C11-C10	-6.45	109.04	118.94
12	6	309	KC1	C3A-C4A-NA	6.45	117.61	110.57
12	12	311	KC1	C3A-C4A-NA	6.45	117.61	110.57
12	13	312	KC1	C3A-C4A-NA	6.45	117.61	110.57
13	10	314	DD6	C-C1-C24	-6.45	107.92	118.08
12	10	306	KC1	CHB-C4A-C3A	-6.45	114.91	124.98
11	7	308	CLA	CMD-C2D-C1D	6.44	136.07	124.71
12	6	310	KC1	CHB-C4A-C3A	-6.44	114.92	124.98
11	16	302	CLA	CMD-C2D-C1D	6.44	136.06	124.71
11	10	308	CLA	CHD-C1D-ND	-6.43	118.54	124.45
12	8	310	KC1	C1A-C2A-C3A	-6.42	102.01	107.11
12	8	311	KC1	CHB-C4A-C3A	-6.42	114.95	124.98
11	6	303	CLA	CMD-C2D-C1D	6.42	136.02	124.71
11	11	309	CLA	CMD-C2D-C1D	6.40	136.00	124.71
13	8	316	DD6	C32-C31-C36	-6.40	113.60	122.63
12	12	305	KC1	C3A-C4A-NA	6.40	117.56	110.57
11	13	307	CLA	CMD-C2D-C1D	6.40	135.99	124.71
11	14	305	CLA	CMD-C2D-C1D	6.40	135.99	124.71
12	12	313	KC1	C3A-C4A-NA	6.39	117.55	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	14	307	CLA	CMD-C2D-C1D	6.39	135.98	124.71
11	11	308	CLA	CMD-C2D-C1D	6.39	135.97	124.71
12	8	307	KC1	CHB-C4A-C3A	-6.39	115.00	124.98
11	6	314	CLA	CMD-C2D-C1D	6.38	135.96	124.71
11	12	321	CLA	CMD-C2D-C1D	6.38	135.96	124.71
12	14	308	KC1	CMA-C3A-C2A	-6.37	112.71	128.30
14	13	315	A86	C4-C5-C6	-6.37	118.23	127.31
11	6	302	CLA	CMD-C2D-C1D	6.36	135.92	124.71
11	11	305	CLA	CHD-C1D-ND	-6.36	118.61	124.45
13	7	316	DD6	C12-C11-C13	-6.36	108.06	118.08
13	16	313	DD6	C9-C10-C11	-6.35	118.24	127.31
11	6	307	CLA	CMD-C2D-C1D	6.35	135.91	124.71
11	16	307	CLA	CMD-C2D-C1D	6.35	135.91	124.71
11	12	304	CLA	CMD-C2D-C1D	6.35	135.90	124.71
11	15	302	CLA	O2D-CGD-CBD	6.35	122.55	111.27
12	6	310	KC1	C3A-C4A-NA	6.35	117.50	110.57
12	8	313	KC1	C3B-C2B-C1B	-6.33	101.03	107.08
11	14	305	CLA	CHD-C1D-ND	-6.32	118.64	124.45
11	16	303	CLA	CHD-C1D-ND	-6.32	118.64	124.45
12	13	308	KC1	C1A-C2A-C3A	-6.32	102.10	107.11
12	14	308	KC1	C3C-C4C-NC	6.32	115.82	109.88
14	15	315	A86	C3-C4-C5	-6.31	110.54	123.47
11	16	301	CLA	CMD-C2D-C1D	6.31	135.84	124.71
12	7	312	KC1	C3A-C4A-NA	6.31	117.46	110.57
11	15	306	CLA	CMD-C2D-C1D	6.31	135.83	124.71
11	12	302	CLA	CHD-C4C-C3C	-6.30	115.58	124.84
11	10	304	CLA	CMD-C2D-C1D	6.30	135.81	124.71
11	14	313	CLA	CHD-C1D-ND	-6.30	118.67	124.45
12	7	307	KC1	CMA-C3A-C2A	-6.30	112.89	128.30
11	16	303	CLA	CMD-C2D-C1D	6.29	135.80	124.71
12	7	307	KC1	C1A-C2A-C3A	-6.29	102.12	107.11
11	8	302	CLA	CHD-C1D-ND	-6.29	118.68	124.45
11	7	303	CLA	CMD-C2D-C1D	6.28	135.79	124.71
14	6	317	A86	C33-C32-C31	6.28	115.32	109.21
11	15	304	CLA	CHD-C1D-ND	-6.28	118.68	124.45
14	13	315	A86	C25-C26-C27	-6.27	118.36	127.31
13	6	315	DD6	C32-C31-C36	-6.26	113.79	122.63
14	15	320	A86	C4-C5-C6	-6.26	118.37	127.31
12	14	306	KC1	CAC-C3C-C4C	6.26	132.93	124.81
14	10	301	A86	C4-C5-C6	-6.26	118.38	127.31
12	16	304	KC1	C3A-C4A-NA	6.26	117.41	110.57
13	8	316	DD6	C24-C1-C2	-6.25	109.35	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	11	313	A86	C33-C32-C31	6.25	115.29	109.21
12	11	304	KC1	CHB-C4A-C3A	-6.25	115.21	124.98
11	14	304	CLA	CHD-C1D-ND	-6.25	118.71	124.45
11	10	305	CLA	CHD-C1D-ND	-6.24	118.72	124.45
11	13	303	CLA	CHD-C1D-ND	-6.24	118.72	124.45
11	15	307	CLA	C2C-C1C-NC	6.24	115.82	109.97
11	7	306	CLA	CHD-C1D-ND	-6.24	118.72	124.45
12	12	305	KC1	C1A-C2A-C3A	-6.23	102.17	107.11
12	13	310	KC1	C3C-C4C-NC	6.23	115.74	109.88
12	8	306	KC1	C3A-C4A-NA	6.23	117.37	110.57
12	8	307	KC1	C3A-C4A-NA	6.22	117.37	110.57
12	16	311	KC1	C3B-C2B-C1B	-6.22	101.13	107.08
11	15	306	CLA	C2C-C1C-NC	6.22	115.80	109.97
11	11	308	CLA	CHD-C1D-ND	-6.22	118.74	124.45
11	12	304	CLA	CHD-C1D-ND	-6.21	118.75	124.45
13	10	314	DD6	C32-C31-C36	-6.21	113.86	122.63
12	11	304	KC1	C3A-C4A-NA	6.21	117.35	110.57
12	8	310	KC1	C3A-C4A-NA	6.21	117.35	110.57
11	7	304	CLA	CHD-C1D-ND	-6.19	118.76	124.45
12	8	314	KC1	C3B-C2B-C1B	-6.19	101.16	107.08
11	11	307	CLA	CHD-C1D-ND	-6.17	118.79	124.45
12	14	306	KC1	O2D-CGD-CBD	6.16	122.22	111.27
12	10	310	KC1	C1A-C2A-C3A	-6.16	102.22	107.11
11	16	308	CLA	CHD-C1D-ND	-6.16	118.80	124.45
11	14	302	CLA	CHD-C1D-ND	-6.15	118.80	124.45
12	13	306	KC1	CHB-C4A-C3A	-6.15	115.38	124.98
11	7	309	CLA	CHD-C1D-ND	-6.14	118.81	124.45
13	15	319	DD6	C12-C11-C13	-6.14	108.40	118.08
13	10	313	DD6	C32-C31-C36	-6.13	113.98	122.63
12	11	311	KC1	C3A-C4A-NA	6.13	117.26	110.57
11	15	303	CLA	CHD-C1D-ND	-6.12	118.83	124.45
11	12	302	CLA	CMD-C2D-C1D	6.12	135.50	124.71
13	13	314	DD6	C32-C31-C36	-6.12	113.99	122.63
11	8	305	CLA	CHD-C4C-C3C	-6.12	115.85	124.84
12	8	312	KC1	C2B-C1B-NB	6.12	114.61	110.10
13	12	317	DD6	C24-C1-C2	-6.11	109.56	118.94
14	11	315	A86	O4-C38-C39	6.11	122.33	111.09
11	15	302	CLA	C4A-NA-C1A	-6.11	103.96	106.71
13	6	316	DD6	C-C1-C24	-6.11	108.45	118.08
11	13	302	CLA	CMD-C2D-C1D	6.11	135.48	124.71
12	11	306	KC1	C3B-C2B-C1B	-6.10	101.25	107.08
12	13	311	KC1	CMA-C3A-C4A	-6.09	115.76	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	10	301	A86	O1-C20-C21	-6.09	107.76	115.06
11	12	307	CLA	CHD-C4C-C3C	-6.08	115.90	124.84
14	11	301	A86	C17-C16-C15	6.08	115.37	109.16
14	6	317	A86	C20-C19-C18	-6.08	100.71	112.75
12	13	306	KC1	C3A-C4A-NA	6.08	117.21	110.57
14	10	316	A86	C17-C16-C15	6.08	115.37	109.16
12	13	311	KC1	C3A-C4A-NA	6.07	117.20	110.57
12	6	305	KC1	C3C-C4C-NC	6.07	115.59	109.88
12	14	311	KC1	C1A-C2A-C3A	-6.06	102.30	107.11
11	8	302	CLA	CHD-C4C-C3C	-6.06	115.93	124.84
12	11	310	KC1	C3B-C2B-C1B	-6.05	101.30	107.08
13	11	312	DD6	C-C1-C24	-6.05	108.54	118.08
12	10	312	KC1	C3B-C2B-C1B	-6.05	101.30	107.08
11	11	303	CLA	CHD-C4C-C3C	-6.04	115.96	124.84
14	11	301	A86	C4-C5-C6	-6.04	118.69	127.31
11	8	308	CLA	CHD-C1D-ND	-6.03	118.92	124.45
12	16	304	KC1	C3B-C2B-C1B	-6.03	101.32	107.08
12	8	311	KC1	C3B-C2B-C1B	-6.02	101.32	107.08
11	14	312	CLA	CHD-C1D-ND	-6.02	118.92	124.45
11	12	303	CLA	CMD-C2D-C1D	6.01	135.31	124.71
11	6	303	CLA	CHD-C1D-ND	-6.01	118.93	124.45
11	13	304	CLA	CHD-C1D-ND	-6.01	118.93	124.45
11	12	310	CLA	CMD-C2D-C1D	6.01	135.31	124.71
11	13	301	CLA	CHD-C4C-C3C	-6.01	116.01	124.84
14	10	301	A86	C-C1-C24	6.00	127.53	118.08
11	7	306	CLA	CHD-C4C-C3C	-6.00	116.03	124.84
13	16	313	DD6	C32-C31-C36	-5.99	114.17	122.63
11	7	302	CLA	CHD-C4C-C3C	-5.99	116.03	124.84
12	14	311	KC1	C3C-C4C-NC	5.99	115.52	109.88
11	12	312	CLA	CHD-C1D-ND	-5.98	118.96	124.45
11	10	303	CLA	CHD-C4C-C3C	-5.98	116.06	124.84
11	12	310	CLA	CHD-C4C-C3C	-5.97	116.07	124.84
11	6	311	CLA	CHD-C1D-ND	-5.96	118.97	124.45
12	6	305	KC1	C3B-C2B-C1B	-5.96	101.38	107.08
12	12	305	KC1	C3B-C2B-C1B	-5.96	101.39	107.08
11	7	305	CLA	C2C-C1C-NC	5.96	115.55	109.97
11	16	303	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
11	16	309	CLA	O2D-CGD-CBD	5.96	121.85	111.27
12	14	308	KC1	C1A-C2A-C3A	-5.95	102.39	107.11
14	10	317	A86	C33-C32-C31	5.95	114.99	109.21
12	6	308	KC1	C1A-NA-C4A	-5.95	104.03	106.71
12	13	310	KC1	C3B-C2B-C1B	-5.95	101.40	107.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	11	303	CLA	CHD-C1D-ND	-5.95	118.99	124.45
11	6	306	CLA	CMD-C2D-C1D	5.94	135.18	124.71
11	7	310	CLA	CMD-C2D-C1D	5.94	135.18	124.71
11	16	309	CLA	CHD-C1D-ND	-5.94	119.00	124.45
11	14	313	CLA	CHD-C4C-C3C	-5.94	116.11	124.84
11	15	303	CLA	C2C-C1C-NC	5.93	115.53	109.97
12	13	308	KC1	C3B-C2B-C1B	-5.93	101.41	107.08
11	16	302	CLA	CHD-C4C-C3C	-5.92	116.13	124.84
11	12	308	CLA	CMD-C2D-C1D	5.92	135.15	124.71
13	6	315	DD6	C-C1-C24	-5.92	108.75	118.08
13	16	313	DD6	C24-C1-C2	-5.92	109.86	118.94
13	13	314	DD6	C21-C20-C19	-5.91	107.63	114.28
12	11	306	KC1	C1A-C2A-C3A	-5.91	102.42	107.11
11	8	303	CLA	O2D-CGD-CBD	5.91	121.77	111.27
14	14	320	A86	C20-C19-C18	-5.90	101.08	112.75
14	10	315	A86	C3-C2-C1	-5.90	118.90	127.31
12	10	310	KC1	C1A-NA-C4A	-5.89	104.06	106.71
11	14	309	CLA	C2C-C1C-NC	5.89	115.49	109.97
11	6	301	CLA	CHD-C1D-ND	-5.89	119.04	124.45
13	7	317	DD6	C8-C6-C5	-5.89	109.90	118.94
11	10	303	CLA	CMD-C2D-C1D	5.88	135.08	124.71
11	8	301	CLA	C2C-C1C-NC	5.88	115.48	109.97
11	15	310	CLA	CHD-C1D-ND	-5.88	119.05	124.45
11	10	304	CLA	CHD-C4C-C3C	-5.88	116.19	124.84
14	11	301	A86	C7-C6-C8	5.88	127.34	118.08
11	14	309	CLA	CHD-C1D-ND	-5.88	119.05	124.45
11	10	309	CLA	CHD-C1D-ND	-5.87	119.06	124.45
14	10	301	A86	C4-C3-C2	-5.87	111.45	123.47
12	12	311	KC1	C3B-C2B-C1B	-5.87	101.47	107.08
11	12	303	CLA	CHD-C4C-C3C	-5.87	116.22	124.84
14	10	317	A86	C4-C5-C6	-5.86	118.94	127.31
11	6	313	CLA	CHD-C1D-ND	-5.86	119.07	124.45
11	8	301	CLA	CHD-C4C-C3C	-5.86	116.23	124.84
11	10	308	CLA	CHD-C4C-C3C	-5.86	116.23	124.84
12	8	312	KC1	CHB-C4A-C3A	-5.86	115.83	124.98
11	12	308	CLA	CHD-C4C-C3C	-5.86	116.23	124.84
11	11	308	CLA	O2D-CGD-CBD	5.86	121.68	111.27
11	6	307	CLA	C2C-C1C-NC	5.85	115.46	109.97
11	15	313	CLA	CHD-C1D-ND	-5.85	119.08	124.45
11	8	309	CLA	C2C-C1C-NC	5.85	115.45	109.97
13	16	313	DD6	C-C1-C24	-5.85	108.86	118.08
11	6	302	CLA	CHD-C1D-ND	-5.85	119.08	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	14	303	CLA	CHD-C1D-ND	-5.85	119.08	124.45
11	13	309	CLA	CHD-C1D-ND	-5.85	119.08	124.45
11	10	307	CLA	CMD-C2D-C1D	5.84	135.01	124.71
11	16	305	CLA	CMD-C2D-C1D	5.84	135.01	124.71
12	12	313	KC1	C3C-C4C-NC	5.83	115.37	109.88
11	15	303	CLA	CHD-C4C-C3C	-5.83	116.27	124.84
14	14	317	A86	C41-C32-C31	-5.82	105.26	110.47
11	15	312	CLA	CBA-CAA-C2A	-5.82	96.68	113.86
11	15	312	CLA	O2D-CGD-CBD	5.81	121.60	111.27
12	10	306	KC1	CMD-C2D-C1D	5.81	137.40	128.46
11	14	313	CLA	O2D-CGD-CBD	5.81	121.60	111.27
11	15	307	CLA	CMD-C2D-C1D	5.81	134.95	124.71
11	14	302	CLA	O2D-CGD-CBD	5.81	121.58	111.27
14	6	317	A86	C4-C5-C6	-5.80	119.03	127.31
11	7	303	CLA	CHD-C1D-ND	-5.80	119.13	124.45
11	13	307	CLA	C2C-C1C-NC	5.80	115.40	109.97
11	8	304	CLA	CHD-C4C-C3C	-5.79	116.32	124.84
11	16	310	CLA	CHD-C4C-C3C	-5.79	116.33	124.84
12	10	306	KC1	C3A-C4A-NA	5.79	116.90	110.57
12	8	307	KC1	C3B-C2B-C1B	-5.79	101.55	107.08
11	10	307	CLA	CHD-C4C-C3C	-5.79	116.33	124.84
12	13	311	KC1	C2B-C1B-NB	5.79	114.37	110.10
12	6	310	KC1	C3B-C2B-C1B	-5.79	101.55	107.08
11	16	310	CLA	CHD-C1D-ND	-5.78	119.14	124.45
11	12	307	CLA	C4A-NA-C1A	-5.78	104.11	106.71
12	8	311	KC1	C3A-C4A-NA	5.78	116.88	110.57
11	8	308	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
11	7	308	CLA	C2C-C1C-NC	5.77	115.38	109.97
12	8	312	KC1	CMA-C3A-C4A	-5.77	116.25	125.04
13	13	314	DD6	C24-C1-C2	-5.77	110.09	118.94
14	14	320	A86	C4-C3-C2	-5.77	111.66	123.47
12	13	305	KC1	C3B-C2B-C1B	-5.76	101.57	107.08
11	6	303	CLA	CHD-C4C-C3C	-5.76	116.37	124.84
13	7	317	DD6	C13-C11-C10	-5.76	110.10	118.94
11	6	312	CLA	C2C-C1C-NC	5.75	115.36	109.97
12	8	310	KC1	C3B-C2B-C1B	-5.75	101.58	107.08
12	14	311	KC1	C3B-C2B-C1B	-5.75	101.58	107.08
12	14	308	KC1	C3B-C2B-C1B	-5.75	101.58	107.08
14	10	302	A86	O4-C38-C39	5.75	121.67	111.09
12	13	311	KC1	CHB-C4A-C3A	-5.75	116.00	124.98
11	15	314	CLA	C2C-C1C-NC	5.75	115.36	109.97
13	6	316	DD6	C8-C6-C5	-5.75	110.12	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	10	306	KC1	C3B-C2B-C1B	-5.74	101.59	107.08
11	12	306	CLA	C2C-C1C-NC	5.74	115.35	109.97
11	6	313	CLA	C2C-C1C-NC	5.74	115.35	109.97
14	11	314	A86	C25-C26-C27	-5.74	119.12	127.31
11	16	305	CLA	C2C-C1C-NC	5.73	115.34	109.97
11	16	308	CLA	C2C-C1C-NC	5.73	115.34	109.97
11	12	303	CLA	C2C-C1C-NC	5.73	115.34	109.97
11	13	304	CLA	C2C-C1C-NC	5.73	115.34	109.97
13	7	316	DD6	C13-C11-C10	-5.73	110.16	118.94
11	16	309	CLA	C2C-C1C-NC	5.72	115.33	109.97
13	11	312	DD6	C8-C6-C5	-5.72	110.16	118.94
14	15	322	A86	C4-C3-C2	-5.72	111.76	123.47
12	6	310	KC1	C1A-C2A-C3A	-5.72	102.57	107.11
11	13	302	CLA	CHD-C4C-C3C	-5.72	116.43	124.84
13	12	315	DD6	C12-C11-C13	-5.72	109.07	118.08
11	7	311	CLA	CHD-C1D-ND	-5.72	119.20	124.45
12	8	313	KC1	C3C-C4C-NC	5.71	115.26	109.88
12	11	311	KC1	C3B-C2B-C1B	-5.71	101.62	107.08
11	15	311	CLA	CHD-C1D-ND	-5.71	119.21	124.45
11	15	302	CLA	CHD-C4C-C3C	-5.70	116.45	124.84
12	13	306	KC1	C3C-C4C-NC	5.70	115.25	109.88
11	15	313	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
11	15	305	CLA	CHD-C1D-ND	-5.70	119.21	124.45
11	8	303	CLA	C2C-C1C-NC	5.70	115.31	109.97
11	6	306	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
14	11	314	A86	C17-C16-C15	5.70	114.98	109.16
13	6	316	DD6	C32-C31-C36	-5.70	114.59	122.63
11	16	306	CLA	CMD-C2D-C1D	5.70	134.75	124.71
11	10	311	CLA	CHD-C1D-ND	-5.70	119.22	124.45
12	16	311	KC1	C3C-C4C-NC	5.69	115.24	109.88
14	10	302	A86	C7-C6-C8	5.69	127.05	118.08
11	15	304	CLA	C2C-C1C-NC	5.69	115.30	109.97
13	15	318	DD6	C12-C11-C13	-5.69	109.12	118.08
12	14	306	KC1	C3C-C4C-NC	5.68	115.23	109.88
11	15	305	CLA	O2D-CGD-CBD	5.68	121.37	111.27
11	10	311	CLA	CHD-C4C-C3C	-5.68	116.49	124.84
14	11	301	A86	C25-C26-C27	-5.68	119.20	127.31
11	10	304	CLA	CHD-C1D-ND	-5.68	119.23	124.45
11	15	311	CLA	CHD-C4C-C3C	-5.68	116.49	124.84
11	6	312	CLA	CHD-C1D-ND	-5.68	119.24	124.45
11	7	303	CLA	C2C-C1C-NC	5.67	115.29	109.97
13	7	316	DD6	C32-C31-C36	-5.67	114.63	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	12	312	CLA	CHD-C4C-C3C	-5.67	116.51	124.84
12	12	305	KC1	C3C-C4C-NC	5.67	115.21	109.88
11	7	309	CLA	CHD-C4C-C3C	-5.67	116.51	124.84
12	6	308	KC1	C3C-C4C-NC	5.66	115.21	109.88
11	15	311	CLA	C2C-C1C-NC	5.66	115.28	109.97
12	13	305	KC1	C3C-C4C-NC	5.66	115.20	109.88
13	15	319	DD6	C24-C1-C2	-5.66	110.26	118.94
14	11	313	A86	C41-C32-C31	-5.65	105.41	110.47
14	16	314	A86	C25-C26-C27	-5.65	119.24	127.31
12	8	311	KC1	CMD-C2D-C1D	5.65	137.14	128.46
14	14	319	A86	O4-C38-C39	5.65	121.47	111.09
12	14	308	KC1	O2D-CGD-CBD	5.64	121.30	111.27
11	11	309	CLA	CHD-C1D-ND	-5.64	119.27	124.45
11	6	314	CLA	CHD-C1D-ND	-5.64	119.27	124.45
11	15	308	CLA	O2D-CGD-CBD	5.64	121.29	111.27
13	7	316	DD6	C24-C1-C2	-5.64	110.29	118.94
11	16	305	CLA	CHD-C4C-C3C	-5.63	116.56	124.84
13	15	319	DD6	C7-C6-C8	-5.63	109.20	118.08
12	6	309	KC1	C3C-C4C-NC	5.63	115.18	109.88
12	11	311	KC1	CMD-C2D-C1D	5.63	137.12	128.46
11	15	314	CLA	CHD-C4C-C3C	-5.63	116.57	124.84
14	14	321	A86	C17-C16-C15	5.62	114.90	109.16
13	16	313	DD6	C14-C13-C11	5.62	134.26	125.53
11	7	311	CLA	C2C-C1C-NC	5.62	115.24	109.97
11	7	310	CLA	C2C-C1C-NC	5.62	115.24	109.97
12	8	310	KC1	C3C-C4C-NC	5.62	115.17	109.88
12	8	312	KC1	C3C-C4C-NC	5.61	115.16	109.88
12	8	313	KC1	C1A-C2A-C3A	-5.61	102.66	107.11
12	11	304	KC1	C3B-C2B-C1B	-5.61	101.72	107.08
11	16	301	CLA	CHD-C1D-ND	-5.60	119.31	124.45
14	8	315	A86	O4-C38-C39	5.60	121.40	111.09
11	6	304	CLA	CHD-C4C-C3C	-5.60	116.61	124.84
11	15	310	CLA	C2C-C1C-NC	5.59	115.21	109.97
11	6	314	CLA	CHD-C4C-C3C	-5.59	116.62	124.84
11	13	302	CLA	C2C-C1C-NC	5.59	115.21	109.97
11	13	307	CLA	O2D-CGD-CBD	5.58	121.19	111.27
11	6	306	CLA	O2D-CGD-CBD	5.58	121.19	111.27
11	10	307	CLA	CHD-C1D-ND	-5.58	119.33	124.45
11	6	311	CLA	CHD-C4C-C3C	-5.58	116.64	124.84
12	6	308	KC1	C3B-C2B-C1B	-5.58	101.75	107.08
11	8	304	CLA	CHD-C1D-ND	-5.58	119.33	124.45
11	10	309	CLA	CHD-C4C-C3C	-5.58	116.64	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	15	318	DD6	C24-C1-C2	-5.57	110.39	118.94
11	15	308	CLA	CMD-C2D-C1D	5.57	134.54	124.71
14	13	315	A86	C17-C16-C15	5.57	114.85	109.16
13	12	315	DD6	C21-C20-C19	-5.57	108.01	114.28
11	8	304	CLA	CMD-C2D-C1D	5.57	134.53	124.71
11	16	309	CLA	CHD-C4C-C3C	-5.57	116.65	124.84
13	7	301	DD6	C24-C1-C2	-5.57	110.39	118.94
12	7	307	KC1	C3C-C4C-NC	5.57	115.12	109.88
12	13	312	KC1	C3B-C2B-C1B	-5.57	101.76	107.08
11	14	307	CLA	C2C-C1C-NC	5.56	115.19	109.97
11	7	308	CLA	CHD-C1D-ND	-5.56	119.34	124.45
11	13	304	CLA	CHD-C4C-C3C	-5.56	116.66	124.84
11	14	305	CLA	CHD-C4C-C3C	-5.56	116.66	124.84
11	11	307	CLA	CHD-C4C-C3C	-5.56	116.67	124.84
11	6	306	CLA	CHD-C1D-ND	-5.56	119.35	124.45
11	7	308	CLA	CHD-C4C-C3C	-5.56	116.67	124.84
12	13	305	KC1	C1A-C2A-C3A	-5.55	102.71	107.11
14	14	301	A86	O4-C38-C39	5.55	121.30	111.09
11	15	306	CLA	CHD-C4C-C3C	-5.55	116.68	124.84
13	10	314	DD6	C24-C1-C2	-5.55	110.42	118.94
14	15	316	A86	C3-C2-C1	-5.55	119.39	127.31
11	15	307	CLA	CHD-C4C-C3C	-5.55	116.69	124.84
11	7	305	CLA	CMD-C2D-C1D	5.55	134.49	124.71
11	13	303	CLA	O2D-CGD-CBD	5.55	121.12	111.27
12	8	311	KC1	C3C-C4C-NC	5.54	115.10	109.88
12	11	311	KC1	C3C-C4C-NC	5.54	115.10	109.88
11	11	305	CLA	CAA-C2A-C3A	-5.54	97.60	112.78
13	15	318	DD6	C33-C34-C35	5.54	117.89	110.30
13	7	317	DD6	C-C1-C24	-5.53	109.36	118.08
11	13	302	CLA	CHD-C1D-ND	-5.53	119.37	124.45
11	13	301	CLA	O2D-CGD-CBD	5.53	121.09	111.27
11	8	309	CLA	O2D-CGD-CBD	5.52	121.08	111.27
14	12	316	A86	C3-C2-C1	-5.52	119.43	127.31
11	15	306	CLA	CHD-C1D-ND	-5.52	119.38	124.45
14	10	301	A86	C20-C19-C18	-5.52	101.83	112.75
11	10	303	CLA	C2C-C1C-NC	5.52	115.14	109.97
12	12	313	KC1	O2D-CGD-CBD	5.51	121.06	111.27
11	15	304	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
13	10	313	DD6	C24-C1-C2	-5.51	110.48	118.94
11	13	301	CLA	CHD-C1D-ND	-5.51	119.39	124.45
13	7	301	DD6	C21-C20-C15	-5.51	113.03	122.26
11	14	312	CLA	CHD-C4C-C3C	-5.51	116.75	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	10	316	A86	C25-C26-C27	-5.50	119.45	127.31
11	15	305	CLA	C2C-C1C-NC	5.50	115.13	109.97
11	15	312	CLA	C2C-C1C-NC	5.50	115.13	109.97
14	12	316	A86	C4-C5-C6	-5.50	119.46	127.31
11	14	310	CLA	C2C-C1C-NC	5.50	115.13	109.97
11	10	303	CLA	CHD-C1D-ND	-5.50	119.40	124.45
11	6	307	CLA	CHD-C1D-ND	-5.50	119.40	124.45
11	12	321	CLA	CHD-C1D-ND	-5.49	119.41	124.45
11	14	304	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
12	16	311	KC1	CMD-C2D-C1D	5.49	136.90	128.46
11	14	302	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
11	15	309	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
11	16	307	CLA	CHD-C1D-ND	-5.49	119.41	124.45
11	14	304	CLA	C2C-C1C-NC	5.49	115.11	109.97
11	12	306	CLA	O2D-CGD-CBD	5.48	121.01	111.27
11	11	305	CLA	C4A-NA-C1A	-5.48	104.24	106.71
14	14	320	A86	O4-C38-C39	5.48	121.17	111.09
14	10	317	A86	C3-C2-C1	-5.48	119.49	127.31
11	6	304	CLA	CHD-C1D-ND	-5.48	119.42	124.45
11	15	310	CLA	CHD-C4C-C3C	-5.48	116.79	124.84
11	12	312	CLA	C2C-C1C-NC	5.47	115.10	109.97
14	8	318	A86	C10-C9-C8	-5.47	106.15	123.22
11	7	303	CLA	CHD-C4C-C3C	-5.47	116.81	124.84
11	8	302	CLA	C4A-NA-C1A	-5.47	104.25	106.71
12	8	312	KC1	C3A-C4A-NA	5.46	116.54	110.57
11	14	303	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
11	11	309	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
11	6	302	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
12	8	306	KC1	CMA-C3A-C2A	-5.46	114.93	128.30
11	13	309	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
11	14	310	CLA	CHD-C4C-C3C	-5.46	116.82	124.84
11	12	310	CLA	CHD-C1D-ND	-5.46	119.44	124.45
11	10	304	CLA	C2C-C1C-NC	5.46	115.08	109.97
11	8	309	CLA	CMD-C2D-C1D	5.46	134.33	124.71
12	12	309	KC1	O2D-CGD-CBD	5.45	120.96	111.27
13	12	317	DD6	C21-C20-C19	-5.45	108.14	114.28
11	16	307	CLA	CHD-C4C-C3C	-5.45	116.83	124.84
13	7	313	DD6	C24-C1-C2	-5.45	110.58	118.94
12	8	314	KC1	C3C-C4C-NC	5.45	115.01	109.88
11	12	306	CLA	CMD-C2D-C1D	5.45	134.32	124.71
11	7	305	CLA	CHD-C4C-C3C	-5.45	116.83	124.84
14	10	302	A86	C7-C6-C5	-5.44	115.30	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	11	304	KC1	C3C-C4C-NC	5.44	115.00	109.88
11	6	301	CLA	CHD-C4C-C3C	-5.44	116.84	124.84
11	12	302	CLA	CHD-C1D-ND	-5.44	119.45	124.45
11	6	314	CLA	C2C-C1C-NC	5.44	115.07	109.97
12	8	312	KC1	C3B-C2B-C1B	-5.44	101.88	107.08
12	8	306	KC1	C3C-C4C-NC	5.44	114.99	109.88
11	12	306	CLA	CHD-C4C-C3C	-5.43	116.85	124.84
11	11	305	CLA	CHD-C4C-C3C	-5.43	116.86	124.84
14	14	301	A86	C41-C32-C31	-5.43	105.61	110.47
11	10	305	CLA	C2C-C1C-NC	5.43	115.06	109.97
11	16	310	CLA	C2C-C1C-NC	5.43	115.06	109.97
11	8	305	CLA	CHD-C1D-ND	-5.42	119.47	124.45
14	14	301	A86	C17-C16-C15	5.42	114.69	109.16
11	16	307	CLA	C2C-C1C-NC	5.42	115.05	109.97
11	7	311	CLA	CHD-C4C-C3C	-5.42	116.88	124.84
12	13	308	KC1	O2D-CGD-CBD	5.41	120.89	111.27
12	6	310	KC1	C3C-C4C-NC	5.41	114.97	109.88
11	12	308	CLA	C2C-C1C-NC	5.41	115.04	109.97
11	12	310	CLA	C2C-C1C-NC	5.41	115.04	109.97
11	13	304	CLA	O2D-CGD-CBD	5.40	120.87	111.27
12	13	305	KC1	O2D-CGD-CBD	5.40	120.87	111.27
12	11	310	KC1	C3C-C4C-NC	5.40	114.96	109.88
12	12	311	KC1	O2D-CGD-CBD	5.40	120.86	111.27
11	14	305	CLA	C2C-C1C-NC	5.40	115.03	109.97
11	8	305	CLA	C3D-C2D-C1D	-5.39	98.47	105.83
11	15	307	CLA	CHD-C1D-ND	-5.39	119.50	124.45
12	10	310	KC1	C3C-C4C-NC	5.39	114.95	109.88
11	12	302	CLA	C2C-C1C-NC	5.39	115.02	109.97
12	13	312	KC1	CMD-C2D-C1D	5.39	136.75	128.46
11	10	305	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
12	11	306	KC1	C3C-C4C-NC	5.38	114.94	109.88
11	12	321	CLA	C2C-C1C-NC	5.38	115.01	109.97
11	6	307	CLA	CHD-C4C-C3C	-5.37	116.94	124.84
14	14	319	A86	C17-C16-C15	5.37	114.64	109.16
11	12	307	CLA	CMD-C2D-C1D	5.36	134.16	124.71
13	12	315	DD6	C-C1-C24	-5.36	109.63	118.08
11	7	304	CLA	CHD-C4C-C3C	-5.36	116.97	124.84
12	16	304	KC1	CMD-C2D-C1D	5.35	136.69	128.46
11	6	312	CLA	O2D-CGD-CBD	5.35	120.78	111.27
13	7	316	DD6	C7-C6-C8	-5.35	109.65	118.08
11	15	308	CLA	CHD-C4C-C3C	-5.35	116.98	124.84
11	13	303	CLA	CHD-C4C-C3C	-5.35	116.98	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	11	309	CLA	C2C-C1C-NC	5.35	114.98	109.97
13	16	313	DD6	C12-C11-C13	-5.35	109.65	118.08
11	15	313	CLA	C2C-C1C-NC	5.35	114.98	109.97
13	10	313	DD6	C4-C5-C6	-5.35	119.68	127.31
11	8	303	CLA	CHD-C4C-C3C	-5.34	116.99	124.84
14	14	314	A86	C8-C6-C5	5.34	127.14	118.94
13	15	319	DD6	C-C1-C24	-5.34	109.67	118.08
11	15	312	CLA	CHD-C4C-C3C	-5.34	116.99	124.84
11	12	321	CLA	CHD-C4C-C3C	-5.34	117.00	124.84
14	14	316	A86	C25-C26-C27	-5.34	119.70	127.31
11	16	306	CLA	C4A-NA-C1A	-5.33	104.31	106.71
14	10	302	A86	C36-C31-C32	-5.33	114.40	119.70
12	11	306	KC1	CMD-C2D-C1D	5.33	136.66	128.46
11	16	302	CLA	CHD-C1D-ND	-5.33	119.56	124.45
11	8	309	CLA	CHD-C4C-C3C	-5.32	117.01	124.84
12	6	309	KC1	C3B-C2B-C1B	-5.32	102.00	107.08
13	6	315	DD6	C8-C6-C5	-5.31	110.79	118.94
11	16	308	CLA	CHD-C4C-C3C	-5.31	117.03	124.84
13	7	313	DD6	O1-C20-C21	-5.31	108.69	115.06
11	6	312	CLA	CHD-C4C-C3C	-5.31	117.03	124.84
12	11	304	KC1	CMD-C2D-C1D	5.31	136.62	128.46
13	12	315	DD6	C32-C31-C36	-5.31	115.14	122.63
11	15	308	CLA	C2C-C1C-NC	5.30	114.94	109.97
11	10	305	CLA	O2D-CGD-CBD	5.30	120.69	111.27
11	7	310	CLA	CHD-C1D-ND	-5.30	119.58	124.45
11	7	304	CLA	C2C-C1C-NC	5.30	114.94	109.97
11	7	302	CLA	O2D-CGD-CBD	5.30	120.69	111.27
12	12	309	KC1	CMD-C2D-C1D	5.30	136.61	128.46
11	15	305	CLA	CHD-C4C-C3C	-5.30	117.05	124.84
11	12	304	CLA	O2D-CGD-CBD	5.30	120.69	111.27
11	6	311	CLA	C2C-C1C-NC	5.30	114.93	109.97
13	8	317	DD6	O1-C20-C21	-5.29	108.72	115.06
11	16	307	CLA	O2D-CGD-CBD	5.29	120.67	111.27
12	10	312	KC1	C3C-C4C-NC	5.29	114.86	109.88
14	11	314	A86	O4-C38-C39	5.29	120.82	111.09
11	12	304	CLA	CHD-C4C-C3C	-5.28	117.08	124.84
12	13	308	KC1	C3C-C4C-NC	5.28	114.85	109.88
14	14	316	A86	C4-C5-C6	-5.28	119.78	127.31
12	12	311	KC1	C3C-C4C-NC	5.28	114.84	109.88
12	13	306	KC1	C3B-C2B-C1B	-5.27	102.04	107.08
11	6	301	CLA	C2C-C1C-NC	5.27	114.91	109.97
11	6	302	CLA	C2C-C1C-NC	5.27	114.91	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	15	318	DD6	C-C1-C24	-5.27	109.78	118.08
11	13	307	CLA	CHD-C4C-C3C	-5.27	117.10	124.84
12	12	313	KC1	CHD-C4C-C3C	-5.27	115.44	125.33
12	12	309	KC1	CBA-CAA-C2A	-5.26	105.21	125.27
11	6	303	CLA	O2D-CGD-CBD	5.26	120.62	111.27
12	13	311	KC1	CMD-C2D-C1D	5.26	136.55	128.46
12	7	307	KC1	C3B-C2B-C1B	-5.26	102.06	107.08
13	7	316	DD6	C21-C20-C15	-5.25	113.45	122.26
11	15	308	CLA	CHD-C1D-ND	-5.25	119.63	124.45
11	12	303	CLA	CHD-C1D-ND	-5.24	119.64	124.45
11	7	310	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
11	13	303	CLA	C2C-C1C-NC	5.24	114.88	109.97
11	11	308	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
14	15	321	A86	O4-C38-C39	5.23	120.72	111.09
12	10	306	KC1	C3C-C4C-NC	5.23	114.80	109.88
11	8	303	CLA	CMD-C2D-C1D	5.23	133.93	124.71
12	13	310	KC1	CHD-C4C-C3C	-5.23	115.52	125.33
11	16	306	CLA	CHD-C4C-C3C	-5.22	117.17	124.84
12	10	312	KC1	C1A-NA-C4A	-5.22	104.36	106.71
14	14	321	A86	O4-C38-C39	5.22	120.69	111.09
13	6	315	DD6	C13-C11-C10	-5.21	110.94	118.94
11	16	302	CLA	C2C-C1C-NC	5.21	114.85	109.97
13	6	318	DD6	C7-C6-C8	-5.21	109.87	118.08
11	16	306	CLA	C2C-C1C-NC	5.21	114.85	109.97
11	12	310	CLA	O2D-CGD-CBD	5.21	120.52	111.27
12	13	306	KC1	O2D-CGD-CBD	5.20	120.52	111.27
11	14	312	CLA	C2C-C1C-NC	5.20	114.85	109.97
12	8	313	KC1	CHD-C4C-C3C	-5.20	115.56	125.33
12	6	305	KC1	CHD-C4C-C3C	-5.20	115.56	125.33
11	15	310	CLA	O2D-CGD-CBD	5.20	120.51	111.27
11	16	305	CLA	CHD-C1D-ND	-5.20	119.67	124.45
12	8	312	KC1	CMD-C2D-C1D	5.19	136.45	128.46
11	6	311	CLA	O2D-CGD-CBD	5.19	120.50	111.27
13	12	317	DD6	C7-C6-C8	-5.19	109.90	118.08
14	8	315	A86	C12-C11-C13	5.19	124.74	116.02
12	8	314	KC1	CMD-C2D-C1D	5.19	136.44	128.46
13	10	314	DD6	C7-C6-C8	-5.18	109.91	118.08
11	12	306	CLA	CHD-C1D-ND	-5.18	119.69	124.45
12	16	304	KC1	O2D-CGD-CBD	5.18	120.48	111.27
11	10	309	CLA	C2C-C1C-NC	5.18	114.83	109.97
12	7	312	KC1	CMD-C2D-C1D	5.18	136.43	128.46
12	14	311	KC1	CHD-C4C-C3C	-5.18	115.61	125.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	13	307	CLA	CHD-C1D-ND	-5.18	119.70	124.45
11	14	309	CLA	CHD-C4C-C3C	-5.18	117.23	124.84
13	12	317	DD6	C-C1-C24	-5.18	109.92	118.08
14	15	320	A86	C3-C4-C5	-5.17	112.88	123.47
12	6	309	KC1	CHD-C4C-C3C	-5.17	115.62	125.33
14	13	315	A86	O4-C38-C39	5.17	120.60	111.09
12	14	311	KC1	CMD-C2D-C1D	5.17	136.40	128.46
13	10	313	DD6	C21-C20-C19	-5.16	108.47	114.28
12	16	304	KC1	C3C-C4C-NC	5.16	114.74	109.88
11	8	303	CLA	CHD-C1D-ND	-5.16	119.71	124.45
11	15	303	CLA	C4A-NA-C1A	-5.16	104.39	106.71
14	11	301	A86	O4-C38-C39	5.16	120.58	111.09
11	8	308	CLA	C2C-C1C-NC	5.16	114.80	109.97
11	14	307	CLA	C4A-NA-C1A	-5.16	104.39	106.71
14	8	318	A86	C17-C16-C15	5.15	114.42	109.16
11	8	309	CLA	CHD-C1D-ND	-5.15	119.72	124.45
14	13	313	A86	C8-C6-C5	5.15	126.85	118.94
11	12	321	CLA	C4A-NA-C1A	-5.15	104.39	106.71
13	6	316	DD6	C12-C11-C13	-5.15	109.97	118.08
11	6	313	CLA	CHD-C4C-C3C	-5.15	117.28	124.84
11	12	308	CLA	CHD-C1D-ND	-5.15	119.72	124.45
11	16	305	CLA	O2D-CGD-CBD	5.14	120.40	111.27
11	12	304	CLA	C2C-C1C-NC	5.13	114.78	109.97
11	8	305	CLA	O2D-CGD-CBD	5.13	120.39	111.27
11	16	308	CLA	C4A-NA-C1A	-5.13	104.40	106.71
12	14	306	KC1	C1A-NA-C4A	-5.13	104.40	106.71
11	16	301	CLA	C2C-C1C-NC	5.13	114.78	109.97
12	10	312	KC1	CMD-C2D-C1D	5.13	136.34	128.46
11	10	311	CLA	C2C-C1C-NC	5.13	114.78	109.97
12	13	306	KC1	CHD-C4C-C3C	-5.13	115.70	125.33
12	13	312	KC1	C3C-C4C-NC	5.13	114.70	109.88
14	10	317	A86	O4-C38-C39	5.13	120.52	111.09
14	16	314	A86	C17-C16-C15	5.12	114.38	109.16
14	13	313	A86	C17-C16-C15	5.12	114.38	109.16
11	6	304	CLA	C2C-C1C-NC	5.11	114.76	109.97
11	12	307	CLA	CHD-C1D-ND	-5.11	119.76	124.45
12	8	313	KC1	CMD-C2D-C1D	5.10	136.31	128.46
11	16	302	CLA	C4A-NA-C1A	-5.10	104.41	106.71
12	12	305	KC1	O2D-CGD-CBD	5.10	120.33	111.27
12	8	310	KC1	CHD-C4C-C3C	-5.10	115.76	125.33
12	6	308	KC1	O2D-CGD-CBD	5.10	120.33	111.27
12	12	309	KC1	C3C-C4C-NC	5.09	114.67	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	10	310	KC1	C3B-C2B-C1B	-5.09	102.22	107.08
11	7	309	CLA	C2C-C1C-NC	5.08	114.73	109.97
12	8	307	KC1	CMD-C2D-C1D	5.08	136.27	128.46
12	13	306	KC1	C1A-NA-C4A	-5.08	104.42	106.71
12	8	310	KC1	O2D-CGD-CBD	5.08	120.29	111.27
12	7	312	KC1	C3C-C4C-NC	5.07	114.65	109.88
11	14	303	CLA	C2C-C1C-NC	5.07	114.72	109.97
12	13	310	KC1	O2D-CGD-CBD	5.07	120.28	111.27
14	11	314	A86	C41-C32-C31	-5.07	105.93	110.47
13	6	316	DD6	C24-C1-C2	-5.07	111.16	118.94
12	8	307	KC1	C3C-C4C-NC	5.06	114.64	109.88
14	16	312	A86	C36-C31-C32	-5.06	114.67	119.70
13	6	315	DD6	C24-C1-C2	-5.06	111.17	118.94
12	11	310	KC1	O2D-CGD-CBD	5.06	120.26	111.27
11	6	306	CLA	C2C-C1C-NC	5.06	114.71	109.97
11	8	302	CLA	C2C-C1C-NC	5.06	114.71	109.97
12	12	305	KC1	CMD-C2D-C1D	5.06	136.24	128.46
13	6	315	DD6	C21-C20-C15	-5.05	113.80	122.26
12	8	306	KC1	C3B-C2B-C1B	-5.05	102.25	107.08
12	13	311	KC1	C3C-C4C-NC	5.05	114.63	109.88
11	6	301	CLA	C4A-NA-C1A	-5.05	104.44	106.71
11	8	301	CLA	CHD-C1D-ND	-5.03	119.83	124.45
12	13	312	KC1	O2D-CGD-CBD	5.03	120.20	111.27
11	6	302	CLA	C4A-NA-C1A	-5.03	104.45	106.71
11	15	309	CLA	C2C-C1C-NC	5.03	114.68	109.97
14	11	315	A86	C17-C16-C15	5.03	114.29	109.16
14	14	317	A86	O4-C38-C39	5.02	120.33	111.09
11	8	302	CLA	C3D-C2D-C1D	-5.02	98.97	105.83
12	12	311	KC1	CMD-C2D-C1D	5.02	136.18	128.46
11	10	307	CLA	C2C-C1C-NC	5.02	114.68	109.97
11	14	307	CLA	CAC-C3C-C4C	5.02	131.32	124.81
11	13	301	CLA	C2C-C1C-NC	5.01	114.67	109.97
12	13	311	KC1	C4B-C3B-C2B	-5.01	102.64	106.75
11	15	313	CLA	C4A-NA-C1A	-5.00	104.46	106.71
12	11	306	KC1	O2D-CGD-CBD	4.99	120.14	111.27
12	10	312	KC1	O2D-CGD-CBD	4.99	120.13	111.27
13	10	314	DD6	C21-C20-C15	-4.98	113.91	122.26
12	13	306	KC1	CMD-C2D-C1D	4.98	136.12	128.46
13	11	312	DD6	C7-C6-C8	-4.98	110.23	118.08
13	16	313	DD6	C21-C20-C19	-4.97	108.69	114.28
14	14	318	A86	C41-C32-C31	-4.97	106.02	110.47
14	16	314	A86	O4-C38-C39	4.97	120.24	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	6	311	CLA	C4A-NA-C1A	-4.97	104.47	106.71
11	14	313	CLA	C2C-C1C-NC	4.97	114.63	109.97
11	16	306	CLA	O2D-CGD-CBD	4.97	120.09	111.27
14	10	301	A86	O4-C38-C39	4.96	120.21	111.09
12	11	310	KC1	CMD-C2D-C1D	4.96	136.08	128.46
11	16	301	CLA	C3D-C2D-C1D	-4.95	99.07	105.83
11	11	309	CLA	O2D-CGD-CBD	4.95	120.07	111.27
14	15	316	A86	C41-C32-C31	-4.95	106.05	110.47
14	15	320	A86	O4-C38-C39	4.94	120.19	111.09
14	10	315	A86	O4-C38-C39	4.94	120.18	111.09
12	6	308	KC1	C2C-C1C-NC	4.94	115.96	110.57
11	10	307	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
11	7	306	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
11	16	308	CLA	O2D-CGD-CBD	4.93	120.03	111.27
12	16	311	KC1	C1A-C2A-C3A	-4.93	103.20	107.11
11	16	303	CLA	C3D-C2D-C1D	-4.93	99.11	105.83
14	14	315	A86	O4-C38-C39	4.92	120.15	111.09
14	7	318	A86	O4-C38-C39	4.92	120.15	111.09
12	16	311	KC1	O2D-CGD-CBD	4.92	120.01	111.27
11	7	305	CLA	CHD-C1D-ND	-4.92	119.94	124.45
11	6	303	CLA	C2C-C1C-NC	4.91	114.58	109.97
14	15	315	A86	O4-C38-C39	4.91	120.12	111.09
14	15	316	A86	O4-C38-C39	4.91	120.11	111.09
11	11	307	CLA	C2C-C1C-NC	4.90	114.57	109.97
14	14	314	A86	O4-C38-C39	4.90	120.11	111.09
13	8	317	DD6	C32-C31-C36	-4.90	115.71	122.63
11	7	305	CLA	O2D-CGD-CBD	4.89	119.96	111.27
13	16	313	DD6	C7-C6-C8	-4.89	110.37	118.08
12	13	308	KC1	C1A-NA-C4A	-4.89	104.51	106.71
12	8	306	KC1	CMD-C2D-C1D	4.89	135.97	128.46
14	8	315	A86	C10-C9-C8	-4.88	107.98	123.22
11	7	308	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
14	15	315	A86	C4-C3-C2	4.88	133.48	123.47
11	16	306	CLA	CHD-C1D-ND	-4.88	119.97	124.45
11	12	307	CLA	O2D-CGD-CBD	4.88	119.94	111.27
11	8	305	CLA	C2C-C1C-NC	4.88	114.54	109.97
11	7	302	CLA	CHD-C1D-ND	-4.87	119.98	124.45
11	8	308	CLA	O2D-CGD-CBD	4.87	119.93	111.27
11	7	303	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
13	7	313	DD6	C-C1-C24	-4.87	110.41	118.08
11	14	303	CLA	O2D-CGD-CBD	4.86	119.91	111.27
14	15	322	A86	C36-C31-C32	-4.86	114.87	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	6	309	KC1	CMD-C2D-C1D	4.86	135.94	128.46
12	10	310	KC1	C4B-C3B-C2B	-4.86	102.76	106.75
14	14	301	A86	C3-C2-C1	-4.85	120.39	127.31
11	15	304	CLA	C4A-NA-C1A	-4.85	104.53	106.71
14	10	301	A86	C24-C1-C2	-4.85	111.50	118.94
11	15	314	CLA	C3D-C2D-C1D	-4.85	99.21	105.83
12	11	310	KC1	C1A-NA-C4A	-4.85	104.53	106.71
14	11	315	A86	C3-C2-C1	-4.85	120.39	127.31
14	15	322	A86	O4-C38-C39	4.84	120.00	111.09
11	8	301	CLA	CMD-C2D-C1D	4.84	133.25	124.71
11	6	304	CLA	O2D-CGD-CBD	4.84	119.87	111.27
13	11	312	DD6	C21-C20-C19	-4.83	108.85	114.28
11	10	305	CLA	CAA-C2A-C3A	-4.83	99.55	112.78
11	14	309	CLA	O2D-CGD-CBD	4.83	119.85	111.27
11	14	310	CLA	O2D-CGD-CBD	4.83	119.84	111.27
14	11	315	A86	C4-C5-C6	-4.82	120.42	127.31
11	10	303	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
12	12	305	KC1	CHD-C4C-C3C	-4.82	116.28	125.33
11	7	303	CLA	C4A-NA-C1A	-4.82	104.54	106.71
14	7	315	A86	C3-C2-C1	-4.82	120.43	127.31
13	15	318	DD6	C7-C6-C8	-4.82	110.48	118.08
11	11	308	CLA	C2C-C1C-NC	4.81	114.48	109.97
11	11	307	CLA	O2D-CGD-CBD	4.81	119.82	111.27
12	16	304	KC1	CMA-C3A-C2A	-4.81	116.52	128.30
14	12	316	A86	C17-C16-C15	4.81	114.07	109.16
12	11	311	KC1	O2D-CGD-CBD	4.81	119.81	111.27
11	14	304	CLA	O2D-CGD-CBD	4.81	119.81	111.27
11	7	306	CLA	O2D-CGD-CBD	4.81	119.81	111.27
11	14	312	CLA	C4A-NA-C1A	-4.80	104.55	106.71
12	13	308	KC1	CMD-C2D-C1D	4.80	135.84	128.46
12	7	307	KC1	CHD-C4C-C3C	-4.80	116.31	125.33
12	10	312	KC1	CHD-C4C-C3C	-4.80	116.32	125.33
11	15	302	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
12	12	309	KC1	CMA-C3A-C2A	-4.79	116.56	128.30
12	14	306	KC1	C3B-C2B-C1B	-4.79	102.50	107.08
11	12	303	CLA	C4A-NA-C1A	-4.79	104.55	106.71
11	15	306	CLA	C4A-NA-C1A	-4.79	104.55	106.71
14	14	317	A86	C17-C16-C15	4.79	114.05	109.16
14	15	317	A86	O4-C38-C39	4.79	119.90	111.09
12	8	311	KC1	O2D-CGD-CBD	4.77	119.75	111.27
12	8	307	KC1	CHD-C4C-C3C	-4.77	116.37	125.33
12	11	311	KC1	CHC-C1C-C2C	-4.77	117.53	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	14	316	A86	C3-C2-C1	-4.77	120.51	127.31
11	11	303	CLA	O2D-CGD-CBD	4.76	119.73	111.27
11	6	306	CLA	C4A-NA-C1A	-4.76	104.56	106.71
14	11	313	A86	O4-C38-C39	4.76	119.85	111.09
12	8	313	KC1	C1A-NA-C4A	-4.76	104.57	106.71
11	10	305	CLA	C4A-NA-C1A	-4.76	104.57	106.71
14	10	316	A86	O4-C38-C39	4.76	119.84	111.09
12	6	310	KC1	CMD-C2D-C1D	4.76	135.77	128.46
14	14	318	A86	C17-C16-C15	4.76	114.01	109.16
12	16	304	KC1	CHC-C1C-C2C	-4.75	117.55	124.98
12	11	310	KC1	CHD-C4C-C3C	-4.75	116.42	125.33
11	8	304	CLA	C2C-C1C-NC	4.75	114.42	109.97
14	16	314	A86	C3-C2-C1	-4.75	120.53	127.31
12	13	311	KC1	CHC-C1C-C2C	-4.75	117.57	124.98
13	6	318	DD6	C-C1-C24	-4.74	110.60	118.08
12	6	310	KC1	CHD-C4C-C3C	-4.74	116.43	125.33
11	12	302	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
12	13	311	KC1	O2D-CGD-CBD	4.74	119.69	111.27
14	6	317	A86	O4-C38-C39	4.73	119.80	111.09
12	13	306	KC1	C2A-C1A-NA	4.73	116.99	109.40
11	7	310	CLA	O2D-CGD-CBD	4.73	119.67	111.27
14	15	320	A86	C33-C32-C31	4.73	113.80	109.21
14	8	318	A86	O4-C38-C39	4.73	119.78	111.09
11	12	312	CLA	C3D-C2D-C1D	-4.72	99.38	105.83
11	16	307	CLA	C4A-NA-C1A	-4.72	104.58	106.71
11	13	301	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
12	14	308	KC1	C2C-C1C-NC	4.72	115.72	110.57
14	16	312	A86	C9-C10-C11	-4.72	112.74	126.61
14	13	313	A86	C41-C32-C31	-4.72	106.25	110.47
12	8	310	KC1	CMD-C2D-C1D	4.72	135.71	128.46
12	6	308	KC1	CHC-C1C-C2C	-4.72	117.61	124.98
12	13	308	KC1	CHD-C4C-C3C	-4.71	116.48	125.33
11	14	307	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
12	12	309	KC1	CHD-C4C-C3C	-4.71	116.48	125.33
11	15	302	CLA	C3D-C4D-ND	4.71	117.86	110.24
11	15	311	CLA	O2D-CGD-CBD	4.71	119.64	111.27
11	13	302	CLA	C4A-NA-C1A	-4.71	104.59	106.71
12	6	308	KC1	CHD-C4C-C3C	-4.71	116.49	125.33
12	11	304	KC1	CHD-C4C-C3C	-4.71	116.49	125.33
12	11	304	KC1	C1A-NA-C4A	-4.71	104.59	106.71
14	14	316	A86	C41-C32-C31	-4.70	106.27	110.47
11	10	311	CLA	O2D-CGD-CBD	4.70	119.62	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	6	303	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
14	16	312	A86	O4-C38-C39	4.70	119.73	111.09
14	14	318	A86	O4-C38-C39	4.70	119.73	111.09
11	15	311	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
11	15	310	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
11	15	304	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
12	7	312	KC1	CHD-C4C-C3C	-4.69	116.53	125.33
12	11	311	KC1	C2C-C1C-NC	4.68	115.68	110.57
13	10	314	DD6	C21-C20-C19	-4.68	109.02	114.28
11	16	303	CLA	C2C-C1C-NC	4.68	114.36	109.97
12	13	305	KC1	CHD-C4C-C3C	-4.68	116.55	125.33
12	11	306	KC1	CHD-C4C-C3C	-4.68	116.55	125.33
11	8	301	CLA	O2D-CGD-CBD	4.68	119.58	111.27
11	15	313	CLA	C3D-C2D-C1D	-4.67	99.45	105.83
12	13	305	KC1	CMD-C2D-C1D	4.67	135.64	128.46
11	8	308	CLA	C4A-NA-C1A	-4.67	104.61	106.71
12	16	311	KC1	CMA-C3A-C2A	-4.67	116.87	128.30
12	12	309	KC1	C1A-C2A-C3A	-4.67	103.41	107.11
11	8	301	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
12	16	311	KC1	CHD-C4C-C3C	-4.66	116.58	125.33
12	11	311	KC1	CHD-C4C-C3C	-4.66	116.58	125.33
11	10	304	CLA	C4A-NA-C1A	-4.66	104.61	106.71
11	10	308	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
13	10	314	DD6	C15-C14-C13	-4.66	116.15	125.99
12	8	312	KC1	CHD-C4C-C3C	-4.66	116.59	125.33
11	10	311	CLA	C3D-C2D-C1D	-4.66	99.48	105.83
11	11	308	CLA	C4A-NA-C1A	-4.65	104.61	106.71
11	15	308	CLA	C3C-C4C-NC	4.65	115.79	110.57
11	15	309	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
11	11	305	CLA	C2C-C1C-NC	4.64	114.32	109.97
12	10	310	KC1	O2D-CGD-CBD	4.64	119.52	111.27
14	10	316	A86	C4-C3-C2	-4.64	113.97	123.47
12	13	310	KC1	CMD-C2D-C1D	4.64	135.60	128.46
14	14	316	A86	O4-C38-C39	4.64	119.63	111.09
11	7	302	CLA	CMD-C2D-C1D	4.64	132.89	124.71
11	15	313	CLA	O2D-CGD-CBD	4.64	119.51	111.27
11	10	309	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
11	10	304	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
13	7	301	DD6	C7-C6-C8	-4.64	110.77	118.08
13	7	313	DD6	C35-C36-C31	-4.63	110.05	120.57
14	15	322	A86	C33-C32-C31	4.63	113.71	109.21
13	6	316	DD6	C21-C20-C15	-4.63	114.50	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	12	316	A86	O4-C38-C39	4.63	119.61	111.09
13	8	316	DD6	O1-C20-C21	-4.63	109.51	115.06
11	13	302	CLA	C3D-C2D-C1D	-4.63	99.52	105.83
14	12	314	A86	O4-C38-C39	4.63	119.60	111.09
14	14	315	A86	C17-C16-C15	4.62	113.88	109.16
11	16	302	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
11	16	308	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
11	6	301	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
11	16	303	CLA	C4A-NA-C1A	-4.62	104.63	106.71
13	7	301	DD6	C-C1-C24	-4.62	110.80	118.08
12	14	308	KC1	CHD-C4C-C3C	-4.62	116.66	125.33
11	14	312	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
12	8	310	KC1	CHC-C1C-C2C	-4.61	117.77	124.98
11	15	302	CLA	C2C-C1C-NC	4.61	114.29	109.97
14	10	301	A86	C12-C11-C13	4.61	123.77	116.02
11	12	303	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
11	12	304	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
13	7	301	DD6	C21-C20-C19	-4.61	109.09	114.28
12	8	306	KC1	CHD-C4C-C3C	-4.61	116.67	125.33
12	10	310	KC1	C2C-C1C-NC	4.61	115.61	110.57
12	6	308	KC1	C2A-C1A-NA	4.61	116.79	109.40
11	15	303	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
14	7	315	A86	O4-C38-C39	4.61	119.56	111.09
12	13	311	KC1	C2C-C1C-NC	4.60	115.60	110.57
12	13	305	KC1	CHC-C1C-C2C	-4.60	117.79	124.98
13	7	316	DD6	C15-C14-C13	4.60	135.72	125.99
11	6	301	CLA	O2D-CGD-CBD	4.60	119.44	111.27
11	14	307	CLA	C3D-C4D-ND	4.60	117.68	110.24
11	14	304	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
11	12	304	CLA	C4A-NA-C1A	-4.60	104.64	106.71
12	6	308	KC1	CMD-C2D-C1D	4.60	135.53	128.46
12	12	311	KC1	CHC-C1C-C2C	-4.60	117.80	124.98
11	7	311	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
14	14	301	A86	C40-C32-C31	-4.59	106.36	110.47
11	13	304	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
11	13	303	CLA	C4A-NA-C1A	-4.59	104.64	106.71
12	13	312	KC1	CHD-C4C-C3C	-4.59	116.71	125.33
11	16	310	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
11	15	314	CLA	O2D-CGD-CBD	4.59	119.42	111.27
11	11	307	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
11	13	303	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
12	14	306	KC1	CHC-C1C-C2C	-4.59	117.82	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	14	302	CLA	C2C-C1C-NC	4.58	114.27	109.97
14	8	318	A86	C4-C3-C2	-4.58	114.09	123.47
13	12	315	DD6	C7-C6-C8	-4.58	110.86	118.08
11	11	305	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
11	8	304	CLA	O2D-CGD-CBD	4.58	119.40	111.27
11	16	309	CLA	C3D-C2D-C1D	-4.58	99.59	105.83
11	6	313	CLA	C4A-NA-C1A	-4.58	104.65	106.71
11	14	309	CLA	C4A-NA-C1A	-4.58	104.65	106.71
11	11	309	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
12	10	306	KC1	CHD-C4C-C3C	-4.57	116.74	125.33
12	8	311	KC1	CHC-C1C-C2C	-4.57	117.84	124.98
12	10	310	KC1	CMD-C2D-C1D	4.57	135.48	128.46
12	12	305	KC1	C2C-C1C-NC	4.57	115.56	110.57
11	6	314	CLA	C3D-C2D-C1D	-4.56	99.60	105.83
11	14	313	CLA	C4A-NA-C1A	-4.56	104.65	106.71
11	16	303	CLA	C3D-C4D-ND	4.56	117.62	110.24
14	8	315	A86	C26-C25-C24	-4.56	108.98	123.22
11	12	321	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
11	14	310	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
12	13	311	KC1	C1A-NA-C4A	-4.56	104.66	106.71
12	6	305	KC1	O2D-CGD-CBD	4.56	119.36	111.27
11	8	308	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
13	8	316	DD6	C13-C11-C10	-4.55	111.95	118.94
11	7	308	CLA	O2D-CGD-CBD	4.55	119.36	111.27
11	11	303	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
11	11	308	CLA	C3D-C4D-ND	4.55	117.60	110.24
12	10	310	KC1	CHC-C1C-C2C	-4.55	117.87	124.98
11	13	303	CLA	C3D-C4D-ND	4.55	117.60	110.24
13	15	318	DD6	C35-C36-C31	-4.55	110.24	120.57
13	6	316	DD6	C13-C11-C10	-4.55	111.96	118.94
12	14	308	KC1	CHC-C1C-C2C	-4.55	117.87	124.98
12	12	305	KC1	CHC-C1C-C2C	-4.55	117.88	124.98
12	8	312	KC1	C2A-C1A-NA	4.55	116.69	109.40
12	12	313	KC1	CMA-C3A-C2A	-4.55	117.17	128.30
12	7	307	KC1	CHC-C1C-C2C	-4.55	117.88	124.98
13	7	316	DD6	C-C1-C24	-4.55	110.92	118.08
12	6	305	KC1	C1A-NA-C4A	-4.54	104.66	106.71
11	15	312	CLA	C4A-NA-C1A	-4.54	104.66	106.71
12	8	307	KC1	C1A-NA-C4A	-4.54	104.66	106.71
11	11	303	CLA	C2C-C1C-NC	4.54	114.23	109.97
12	14	306	KC1	C4B-C3B-C2B	-4.54	103.02	106.75
11	6	302	CLA	C3D-C2D-C1D	-4.54	99.64	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	16	303	CLA	O2D-CGD-CBD	4.54	119.33	111.27
11	8	301	CLA	C3C-C4C-NC	4.54	115.66	110.57
12	8	314	KC1	CHC-C1C-C2C	-4.53	117.89	124.98
11	14	305	CLA	C3D-C2D-C1D	-4.53	99.64	105.83
14	14	301	A86	C4-C5-C6	-4.53	120.84	127.31
12	7	307	KC1	CMD-C2D-C1D	4.53	135.43	128.46
11	7	309	CLA	C4A-NA-C1A	-4.53	104.67	106.71
12	8	314	KC1	CHD-C4C-C3C	-4.53	116.83	125.33
11	6	307	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
11	13	309	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
11	8	304	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
11	14	313	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
12	6	309	KC1	O2D-CGD-CBD	4.52	119.30	111.27
11	12	310	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
13	8	317	DD6	C-C1-C24	-4.52	110.96	118.08
14	8	315	A86	C3-C2-C1	-4.52	120.86	127.31
14	10	315	A86	C25-C26-C27	-4.52	120.86	127.31
11	7	305	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
11	15	303	CLA	O2D-CGD-CBD	4.52	119.30	111.27
11	7	310	CLA	C3D-C2D-C1D	-4.52	99.67	105.83
11	15	308	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
14	16	312	A86	C8-C6-C5	4.51	125.87	118.94
11	15	306	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
14	8	315	A86	C4-C5-C6	-4.51	120.87	127.31
11	16	305	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
13	10	313	DD6	C12-C11-C13	-4.51	110.98	118.08
11	12	312	CLA	O2D-CGD-CBD	4.51	119.28	111.27
12	8	311	KC1	CHD-C4C-C3C	-4.50	116.88	125.33
11	16	309	CLA	C4A-NA-C1A	-4.50	104.68	106.71
12	13	311	KC1	CHD-C4C-C3C	-4.50	116.89	125.33
11	14	305	CLA	O2D-CGD-CBD	4.50	119.26	111.27
11	7	302	CLA	C3D-C2D-C1D	-4.50	99.70	105.83
12	14	311	KC1	O2D-CGD-CBD	4.50	119.26	111.27
14	7	314	A86	C23-C16-C22	-4.49	100.74	107.37
11	14	313	CLA	C3D-C4D-ND	4.49	117.50	110.24
11	10	305	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
11	14	302	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
14	7	318	A86	C36-C31-C32	-4.49	115.25	119.70
14	15	321	A86	C3-C2-C1	-4.49	120.91	127.31
14	7	318	A86	C20-C19-C18	-4.48	103.88	112.75
13	7	313	DD6	C37-C36-C35	-4.48	106.05	114.36
12	14	306	KC1	C2A-C1A-NA	4.48	116.59	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	6	309	KC1	C1A-NA-C4A	-4.48	104.69	106.71
14	7	314	A86	C26-C25-C24	-4.48	109.25	123.22
11	7	309	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
11	6	306	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
12	12	311	KC1	CHD-C4C-C3C	-4.47	116.94	125.33
12	11	304	KC1	C2A-C1A-NA	4.47	116.57	109.40
13	12	317	DD6	C35-C36-C31	-4.47	110.42	120.57
14	7	315	A86	C20-C19-C18	-4.46	103.92	112.75
12	6	310	KC1	O2D-CGD-CBD	4.46	119.19	111.27
14	7	318	A86	C25-C24-C1	-4.46	113.89	126.42
11	8	302	CLA	CMB-C2B-C3B	4.46	133.02	124.68
12	10	306	KC1	CHC-C1C-C2C	-4.46	118.02	124.98
14	16	314	A86	C4-C5-C6	-4.46	120.95	127.31
11	15	305	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
11	13	307	CLA	C4A-NA-C1A	-4.46	104.70	106.71
12	10	310	KC1	CHD-C4C-C3C	-4.45	116.97	125.33
11	11	305	CLA	C3D-C4D-ND	4.45	117.44	110.24
14	12	316	A86	C40-C32-C31	-4.45	106.49	110.47
11	14	303	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
11	6	311	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
11	15	310	CLA	C4A-NA-C1A	-4.45	104.71	106.71
13	6	316	DD6	C21-C20-C19	-4.44	109.28	114.28
12	8	314	KC1	C2C-C1C-NC	4.44	115.42	110.57
11	7	302	CLA	C2C-C1C-NC	4.44	114.13	109.97
12	13	312	KC1	CHC-C1C-C2C	-4.44	118.04	124.98
11	14	304	CLA	C4A-NA-C1A	-4.44	104.71	106.71
11	11	303	CLA	C3D-C4D-ND	4.43	117.41	110.24
11	14	307	CLA	CHD-C4C-C3C	-4.43	118.33	124.84
11	13	307	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
12	12	309	KC1	CHC-C1C-C2C	-4.42	118.07	124.98
13	15	319	DD6	C35-C36-C31	-4.42	110.53	120.57
12	7	307	KC1	C2C-C1C-NC	4.42	115.40	110.57
11	10	308	CLA	C3D-C4D-ND	4.42	117.39	110.24
12	13	305	KC1	C2C-C1C-NC	4.41	115.39	110.57
11	13	304	CLA	C4A-NA-C1A	-4.41	104.72	106.71
11	12	310	CLA	C3C-C4C-NC	4.41	115.52	110.57
11	15	303	CLA	C3C-C4C-NC	4.41	115.52	110.57
12	8	306	KC1	CHC-C1C-C2C	-4.41	118.09	124.98
14	14	319	A86	C41-C32-C31	-4.41	106.53	110.47
11	7	304	CLA	C3D-C4D-ND	4.41	117.37	110.24
11	6	312	CLA	C3D-C2D-C1D	-4.41	99.82	105.83
13	7	317	DD6	C21-C20-C15	-4.40	114.88	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	7	307	KC1	C4B-C3B-C2B	-4.40	103.14	106.75
11	7	311	CLA	O2D-CGD-CBD	4.40	119.08	111.27
11	10	308	CLA	O2D-CGD-CBD	4.40	119.08	111.27
12	13	310	KC1	C2C-C1C-NC	4.40	115.37	110.57
11	6	304	CLA	C4A-NA-C1A	-4.40	104.73	106.71
12	10	312	KC1	C2A-C1A-NA	4.39	116.45	109.40
11	6	314	CLA	O2D-CGD-CBD	4.39	119.08	111.27
11	15	314	CLA	C3D-C4D-ND	4.39	117.34	110.24
14	10	316	A86	C10-C9-C8	-4.39	109.52	123.22
11	8	303	CLA	C4A-NA-C1A	-4.39	104.73	106.71
11	15	307	CLA	C3D-C2D-C1D	-4.38	99.85	105.83
11	13	309	CLA	O2D-CGD-CBD	4.38	119.05	111.27
14	12	316	A86	C10-C9-C8	-4.38	109.56	123.22
12	8	306	KC1	C2C-C1C-NC	4.38	115.35	110.57
11	10	305	CLA	C3D-C4D-ND	4.37	117.31	110.24
11	14	309	CLA	C3D-C2D-C1D	-4.37	99.86	105.83
12	16	304	KC1	C2C-C1C-NC	4.37	115.35	110.57
14	16	314	A86	C40-C32-C31	-4.37	106.56	110.47
14	7	318	A86	C9-C8-C6	-4.37	114.14	126.42
12	16	304	KC1	C2A-C1A-NA	4.37	116.41	109.40
14	15	320	A86	C41-C32-C31	-4.37	106.56	110.47
11	7	304	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
14	15	321	A86	C17-C16-C15	4.37	113.62	109.16
11	6	311	CLA	C3D-C4D-ND	4.37	117.30	110.24
12	8	307	KC1	C2A-C1A-NA	4.36	116.39	109.40
12	8	306	KC1	C4B-C3B-C2B	-4.35	103.18	106.75
12	14	306	KC1	CMD-C2D-C1D	4.35	135.16	128.46
11	16	301	CLA	O2D-CGD-CBD	4.35	119.00	111.27
12	10	310	KC1	C2A-C1A-NA	4.35	116.38	109.40
11	15	309	CLA	C3D-C4D-ND	4.35	117.27	110.24
12	8	307	KC1	O2D-CGD-CBD	4.35	118.99	111.27
11	8	303	CLA	C3D-C4D-ND	4.34	117.27	110.24
12	13	311	KC1	C2A-C1A-NA	4.34	116.36	109.40
13	8	316	DD6	C23-C16-C17	-4.34	101.45	108.98
11	8	305	CLA	C3C-C4C-NC	4.33	115.43	110.57
11	15	307	CLA	C4A-NA-C1A	-4.33	104.76	106.71
11	16	301	CLA	C3C-C4C-NC	4.33	115.43	110.57
11	15	304	CLA	C3C-C4C-NC	4.33	115.43	110.57
12	11	310	KC1	C2A-C1A-NA	4.33	116.34	109.40
13	11	312	DD6	C21-C20-C15	-4.32	115.02	122.26
11	12	304	CLA	C3D-C4D-ND	4.32	117.22	110.24
14	14	320	A86	C9-C8-C6	-4.32	114.28	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	13	311	KC1	CBA-CAA-C2A	-4.32	108.81	125.27
11	8	304	CLA	C1D-CHD-C4C	-4.31	116.75	126.06
11	16	307	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
12	12	313	KC1	CHB-C4A-C3A	-4.31	118.25	124.98
12	8	307	KC1	CHC-C1C-C2C	-4.31	118.25	124.98
11	13	301	CLA	C4A-NA-C1A	-4.30	104.77	106.71
14	6	317	A86	C40-C32-C31	-4.30	106.62	110.47
12	11	306	KC1	CHC-C1C-C2C	-4.30	118.26	124.98
12	13	308	KC1	CBA-CAA-C2A	-4.30	108.88	125.27
11	15	312	CLA	C3D-C2D-C1D	-4.30	99.97	105.83
12	10	306	KC1	C2A-C1A-NA	4.30	116.29	109.40
11	12	308	CLA	C3D-C2D-C1D	-4.29	99.97	105.83
13	8	316	DD6	C15-C14-C13	4.29	135.07	125.99
11	11	309	CLA	C4A-NA-C1A	-4.29	104.78	106.71
12	13	308	KC1	C2C-C1C-NC	4.29	115.25	110.57
11	6	313	CLA	C3D-C2D-C1D	-4.29	99.98	105.83
12	8	306	KC1	C2A-C1A-NA	4.29	116.28	109.40
12	6	308	KC1	C4B-C3B-C2B	-4.29	103.23	106.75
11	6	313	CLA	O2D-CGD-CBD	4.29	118.88	111.27
14	10	301	A86	C36-C31-C32	-4.28	115.44	119.70
11	10	309	CLA	C3D-C4D-ND	4.28	117.17	110.24
11	12	307	CLA	C3D-C2D-C1D	-4.28	99.98	105.83
11	12	302	CLA	C3C-C4C-NC	4.28	115.37	110.57
13	8	317	DD6	C7-C6-C8	-4.28	111.33	118.08
11	16	306	CLA	C3D-C4D-ND	4.28	117.17	110.24
14	11	301	A86	C7-C6-C5	-4.28	116.92	122.92
12	11	304	KC1	O2D-CGD-CBD	4.28	118.87	111.27
12	10	306	KC1	C2C-C1C-NC	4.28	115.24	110.57
11	7	302	CLA	C3C-C4C-NC	4.28	115.37	110.57
12	11	304	KC1	C2C-C1C-NC	4.28	115.24	110.57
11	15	314	CLA	C4A-NA-C1A	-4.27	104.78	106.71
11	12	307	CLA	CAC-C3C-C4C	4.27	130.35	124.81
15	6	319	LHG	O4-P-O5	4.27	133.34	112.24
12	16	304	KC1	CHD-C4C-C3C	-4.27	117.32	125.33
12	12	313	KC1	C2C-C1C-NC	4.27	115.23	110.57
11	10	307	CLA	O2D-CGD-CBD	4.26	118.84	111.27
12	7	312	KC1	O2D-CGD-CBD	4.26	118.84	111.27
11	7	302	CLA	C3D-C4D-ND	4.26	117.13	110.24
12	6	309	KC1	C2A-C1A-NA	4.26	116.23	109.40
12	13	308	KC1	CHC-C1C-C2C	-4.25	118.33	124.98
11	6	304	CLA	C3D-C2D-C1D	-4.25	100.03	105.83
12	16	311	KC1	CBA-CAA-C2A	-4.25	109.08	125.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	10	308	CLA	C4A-NA-C1A	-4.25	104.80	106.71
11	12	307	CLA	C3D-C4D-ND	4.25	117.11	110.24
11	14	302	CLA	C3D-C4D-ND	4.25	117.11	110.24
11	12	302	CLA	C1D-CHD-C4C	-4.25	116.90	126.06
11	15	304	CLA	C3D-C4D-ND	4.24	117.10	110.24
11	14	304	CLA	C3D-C4D-ND	4.24	117.10	110.24
11	12	306	CLA	C3D-C2D-C1D	-4.24	100.05	105.83
13	8	316	DD6	C-C1-C24	-4.24	111.40	118.08
14	10	317	A86	C25-C26-C27	-4.23	121.27	127.31
11	15	312	CLA	C1C-C2C-C3C	-4.23	102.51	106.96
12	13	308	KC1	C2A-C1A-NA	4.23	116.19	109.40
14	14	314	A86	C4-C3-C2	-4.23	114.81	123.47
12	11	310	KC1	CHC-C1C-C2C	-4.23	118.37	124.98
12	12	311	KC1	C1A-NA-C4A	-4.23	104.81	106.71
14	10	302	A86	C3-C2-C1	-4.23	121.28	127.31
11	6	314	CLA	C4A-NA-C1A	-4.23	104.81	106.71
11	12	310	CLA	C4A-NA-C1A	-4.22	104.81	106.71
11	12	312	CLA	C3D-C4D-ND	4.22	117.07	110.24
11	6	302	CLA	O2D-CGD-CBD	4.22	118.77	111.27
12	8	314	KC1	O2D-CGD-O1D	-4.22	115.58	123.84
12	11	304	KC1	CHC-C1C-C2C	-4.22	118.39	124.98
11	12	302	CLA	O2D-CGD-CBD	4.22	118.77	111.27
11	12	310	CLA	C3D-C4D-ND	4.22	117.06	110.24
14	14	320	A86	C25-C24-C1	-4.22	114.56	126.42
12	8	313	KC1	O2D-CGD-CBD	4.22	118.76	111.27
12	6	308	KC1	C1C-C2C-C3C	-4.22	102.52	106.96
11	8	309	CLA	C3D-C4D-ND	4.22	117.06	110.24
11	14	312	CLA	O2D-CGD-CBD	4.21	118.76	111.27
11	11	307	CLA	C3D-C4D-ND	4.21	117.05	110.24
12	13	312	KC1	C1A-NA-C4A	-4.21	104.81	106.71
14	7	314	A86	C25-C26-C27	-4.21	121.30	127.31
11	7	306	CLA	C3D-C4D-ND	4.21	117.05	110.24
12	13	312	KC1	C2C-C1C-NC	4.21	115.17	110.57
11	10	307	CLA	C4A-NA-C1A	-4.21	104.81	106.71
12	6	310	KC1	CHC-C1C-C2C	-4.21	118.40	124.98
14	12	314	A86	C4-C3-C2	-4.21	114.85	123.47
12	12	313	KC1	CHC-C1C-C2C	-4.21	118.40	124.98
12	8	311	KC1	C2C-C1C-NC	4.21	115.17	110.57
11	12	308	CLA	C3C-C4C-NC	4.21	115.29	110.57
11	8	309	CLA	C3D-C2D-C1D	-4.21	100.09	105.83
12	7	312	KC1	C2A-C1A-NA	4.20	116.14	109.40
13	13	314	DD6	C15-C14-C13	4.20	134.88	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	13	313	A86	C9-C10-C11	-4.20	114.26	126.61
11	16	309	CLA	C3D-C4D-ND	4.20	117.03	110.24
11	10	309	CLA	C4A-NA-C1A	-4.20	104.82	106.71
14	15	316	A86	C9-C8-C6	-4.20	114.63	126.42
12	12	311	KC1	C2A-C1A-NA	4.19	116.12	109.40
11	8	305	CLA	C1-C2-C3	-4.19	118.80	126.04
13	15	318	DD6	C23-C16-C15	4.19	121.34	110.05
11	14	310	CLA	C3D-C4D-ND	4.18	117.00	110.24
12	14	308	KC1	CBA-CAA-C2A	-4.18	109.33	125.27
11	8	301	CLA	C3D-C4D-ND	4.18	117.00	110.24
11	12	303	CLA	C3C-C4C-NC	4.18	115.26	110.57
11	15	307	CLA	C1C-C2C-C3C	-4.18	102.56	106.96
14	7	318	A86	C4-C5-C6	-4.18	121.34	127.31
11	10	304	CLA	C3C-C4C-NC	4.18	115.26	110.57
11	13	309	CLA	C3C-C4C-NC	4.18	115.26	110.57
11	15	306	CLA	C3C-C4C-NC	4.18	115.26	110.57
14	14	315	A86	C36-C31-C32	-4.18	115.55	119.70
11	6	303	CLA	C3D-C4D-ND	4.18	117.00	110.24
11	10	311	CLA	C3D-C4D-ND	4.18	117.00	110.24
11	12	308	CLA	C4A-NA-C1A	-4.18	104.83	106.71
12	14	311	KC1	C1A-NA-C4A	-4.18	104.83	106.71
14	10	301	A86	C22-C16-C17	-4.18	101.73	108.98
11	13	302	CLA	O2D-CGD-CBD	4.18	118.69	111.27
11	14	302	CLA	C4A-NA-C1A	-4.18	104.83	106.71
11	14	303	CLA	C4A-NA-C1A	-4.18	104.83	106.71
11	15	313	CLA	C3D-C4D-ND	4.17	116.99	110.24
11	16	307	CLA	C3D-C4D-ND	4.17	116.99	110.24
14	15	322	A86	C9-C8-C6	-4.17	114.69	126.42
11	7	308	CLA	C4A-NA-C1A	-4.17	104.83	106.71
11	15	309	CLA	C4A-NA-C1A	-4.17	104.83	106.71
12	7	312	KC1	C1A-NA-C4A	-4.17	104.83	106.71
13	7	317	DD6	C22-C16-C15	4.17	121.30	110.05
14	15	321	A86	C4-C5-C6	-4.17	121.36	127.31
12	13	311	KC1	C3B-C2B-C1B	-4.16	103.10	107.08
12	6	310	KC1	C2C-C1C-NC	4.16	115.12	110.57
11	7	305	CLA	C3C-C4C-NC	4.16	115.24	110.57
12	7	312	KC1	CHC-C1C-C2C	-4.16	118.48	124.98
14	14	317	A86	C12-C11-C13	4.16	123.01	116.02
11	15	304	CLA	C1D-CHD-C4C	-4.16	117.09	126.06
13	15	319	DD6	C15-C14-C13	4.16	134.78	125.99
13	13	314	DD6	C8-C6-C5	-4.16	112.56	118.94
11	6	307	CLA	C1C-C2C-C3C	-4.15	102.59	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	7	313	DD6	C21-C20-C19	-4.15	109.61	114.28
12	16	304	KC1	C1A-NA-C4A	-4.15	104.84	106.71
14	6	317	A86	C4-C3-C2	-4.15	114.98	123.47
11	7	308	CLA	C1D-CHD-C4C	-4.15	117.11	126.06
12	13	312	KC1	C2A-C1A-NA	4.15	116.05	109.40
14	14	319	A86	C36-C31-C32	-4.15	115.58	119.70
11	15	307	CLA	CAA-C2A-C3A	-4.15	101.43	112.78
14	15	322	A86	C25-C24-C1	-4.15	114.77	126.42
14	15	317	A86	C33-C32-C31	4.14	113.24	109.21
12	12	313	KC1	C1A-C2A-C3A	4.14	110.40	107.11
11	13	301	CLA	C3D-C4D-ND	4.14	116.94	110.24
11	14	312	CLA	C3D-C4D-ND	4.14	116.94	110.24
11	10	307	CLA	C3C-C4C-NC	4.14	115.22	110.57
11	14	307	CLA	C3C-C4C-NC	4.14	115.22	110.57
11	16	303	CLA	CAA-C2A-C3A	-4.14	101.44	112.78
12	12	311	KC1	C2C-C1C-NC	4.14	115.09	110.57
11	15	314	CLA	C3C-C4C-NC	4.14	115.21	110.57
12	8	306	KC1	C1C-C2C-C3C	-4.13	102.61	106.96
12	6	310	KC1	C2A-C1A-NA	4.13	116.03	109.40
11	13	309	CLA	C1C-C2C-C3C	-4.13	102.61	106.96
11	11	308	CLA	C3D-C2D-C1D	-4.13	100.19	105.83
11	15	306	CLA	C1D-CHD-C4C	-4.13	117.15	126.06
11	14	303	CLA	C3D-C4D-ND	4.13	116.91	110.24
14	6	317	A86	C36-C31-C32	-4.13	115.60	119.70
12	16	311	KC1	C2C-C1C-NC	4.13	115.08	110.57
14	15	315	A86	C41-C32-C31	-4.12	106.78	110.47
12	11	311	KC1	C2A-C1A-NA	4.12	116.01	109.40
11	13	304	CLA	C3D-C4D-ND	4.12	116.90	110.24
11	16	308	CLA	C3D-C4D-ND	4.12	116.90	110.24
14	15	320	A86	C9-C10-C11	-4.12	114.50	126.61
13	8	316	DD6	C35-C36-C31	-4.12	111.23	120.57
11	16	301	CLA	C3D-C4D-ND	4.11	116.89	110.24
13	15	318	DD6	C15-C14-C13	4.11	134.69	125.99
12	10	312	KC1	C4B-C3B-C2B	-4.11	103.38	106.75
12	6	310	KC1	C1A-NA-C4A	-4.11	104.86	106.71
12	8	314	KC1	CBA-CAA-C2A	-4.11	109.61	125.27
13	15	318	DD6	O1-C20-C21	-4.11	110.13	115.06
11	15	310	CLA	C3D-C4D-ND	4.11	116.88	110.24
11	15	303	CLA	C1D-CHD-C4C	-4.11	117.20	126.06
11	7	310	CLA	C4A-NA-C1A	-4.11	104.86	106.71
11	6	301	CLA	C3D-C4D-ND	4.10	116.87	110.24
11	15	311	CLA	C3D-C4D-ND	4.10	116.87	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	14	315	A86	C10-C9-C8	-4.10	110.43	123.22
11	6	304	CLA	C3D-C4D-ND	4.10	116.86	110.24
11	10	303	CLA	O2D-CGD-CBD	4.09	118.54	111.27
14	14	321	A86	C41-C32-C31	-4.09	106.81	110.47
11	11	307	CLA	C1D-CHD-C4C	-4.09	117.23	126.06
11	7	306	CLA	C2C-C1C-NC	4.09	113.81	109.97
11	7	309	CLA	C3D-C4D-ND	4.09	116.85	110.24
12	10	306	KC1	C1A-NA-C4A	-4.09	104.87	106.71
12	12	309	KC1	C2C-C1C-NC	4.09	115.03	110.57
11	15	312	CLA	C3D-C4D-ND	4.09	116.85	110.24
12	14	311	KC1	C2C-C1C-NC	4.09	115.03	110.57
11	6	312	CLA	C3D-C4D-ND	4.08	116.84	110.24
14	14	318	A86	C3-C2-C1	-4.08	121.48	127.31
14	14	317	A86	C36-C31-C32	-4.08	115.65	119.70
11	10	304	CLA	O2D-CGD-CBD	4.08	118.52	111.27
11	8	303	CLA	C3D-C2D-C1D	-4.08	100.26	105.83
14	10	302	A86	C12-C11-C13	4.08	122.87	116.02
12	7	307	KC1	O2D-CGD-CBD	4.08	118.51	111.27
12	7	307	KC1	C2A-C1A-NA	4.08	115.94	109.40
12	11	310	KC1	C2C-C1C-NC	4.08	115.02	110.57
14	14	321	A86	C25-C24-C1	-4.08	114.97	126.42
11	8	309	CLA	C1C-C2C-C3C	-4.08	102.67	106.96
12	11	306	KC1	C2C-C1C-NC	4.07	115.02	110.57
12	6	305	KC1	CMD-C2D-C1D	4.07	134.72	128.46
11	7	311	CLA	C3D-C4D-ND	4.07	116.83	110.24
11	14	310	CLA	C1D-CHD-C4C	-4.07	117.28	126.06
14	13	315	A86	C40-C32-C31	-4.07	106.83	110.47
12	14	311	KC1	CBA-CAA-C2A	-4.07	109.76	125.27
12	13	311	KC1	C1C-C2C-C3C	-4.07	102.68	106.96
11	14	305	CLA	C3D-C4D-ND	4.07	116.82	110.24
14	15	316	A86	C12-C11-C13	4.07	122.85	116.02
11	8	301	CLA	CMB-C2B-C3B	4.07	132.29	124.68
11	15	305	CLA	C4A-NA-C1A	-4.07	104.88	106.71
11	12	308	CLA	C3D-C4D-ND	4.07	116.81	110.24
14	14	301	A86	C12-C11-C13	4.06	122.85	116.02
11	16	306	CLA	C3C-C4C-NC	4.06	115.13	110.57
13	8	317	DD6	C37-C36-C35	-4.06	106.83	114.36
11	12	312	CLA	C4A-NA-C1A	-4.06	104.88	106.71
12	8	311	KC1	C2A-C1A-NA	4.06	115.91	109.40
13	8	316	DD6	C12-C11-C13	-4.06	111.68	118.08
14	10	316	A86	C12-C11-C13	4.06	122.84	116.02
11	8	305	CLA	C1D-CHD-C4C	-4.06	117.31	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	15	303	CLA	C3D-C4D-ND	4.06	116.80	110.24
14	11	314	A86	C4-C3-C2	-4.06	115.17	123.47
11	11	309	CLA	C3D-C4D-ND	4.05	116.80	110.24
11	15	305	CLA	C3D-C4D-ND	4.05	116.79	110.24
11	12	302	CLA	C3D-C4D-ND	4.05	116.79	110.24
11	16	302	CLA	C3C-C4C-NC	4.05	115.11	110.57
11	16	302	CLA	O2D-CGD-CBD	4.05	118.47	111.27
12	8	313	KC1	C2A-C1A-NA	4.05	115.90	109.40
12	6	310	KC1	CAA-CBA-CGA	-4.05	106.45	127.26
11	10	303	CLA	C1D-CHD-C4C	-4.05	117.33	126.06
11	11	305	CLA	O2D-CGD-CBD	4.05	118.46	111.27
14	15	321	A86	C12-C11-C13	4.04	122.81	116.02
13	7	316	DD6	C22-C16-C15	4.04	120.96	110.05
11	16	310	CLA	C3C-C4C-NC	4.04	115.10	110.57
12	8	310	KC1	C2A-C1A-NA	4.04	115.88	109.40
11	15	307	CLA	C3C-C4C-NC	4.04	115.10	110.57
11	15	306	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
11	7	309	CLA	O2D-CGD-CBD	4.03	118.44	111.27
11	10	311	CLA	C4A-NA-C1A	-4.03	104.89	106.71
11	16	310	CLA	C4A-NA-C1A	-4.03	104.89	106.71
12	8	312	KC1	C2C-C1C-NC	4.03	114.97	110.57
14	16	314	A86	C36-C31-C32	-4.03	115.70	119.70
12	11	306	KC1	C1A-NA-C4A	-4.03	104.90	106.71
12	11	311	KC1	CMA-C3A-C2A	-4.02	118.45	128.30
11	16	310	CLA	C3D-C4D-ND	4.02	116.75	110.24
11	6	312	CLA	C4A-NA-C1A	-4.02	104.90	106.71
11	15	308	CLA	C4A-NA-C1A	-4.02	104.90	106.71
11	16	305	CLA	C1D-CHD-C4C	-4.02	117.38	126.06
12	13	312	KC1	C4B-C3B-C2B	-4.02	103.45	106.75
14	10	315	A86	C40-C32-C31	-4.02	106.87	110.47
11	15	307	CLA	O2D-CGD-CBD	4.02	118.41	111.27
13	16	313	DD6	C37-C36-C35	-4.02	106.91	114.36
11	12	310	CLA	C1D-CHD-C4C	-4.02	117.39	126.06
14	7	314	A86	C20-C19-C18	-4.01	104.81	112.75
12	8	314	KC1	C2A-C1A-NA	4.01	115.84	109.40
14	8	315	A86	C3-C4-C5	-4.01	115.25	123.47
14	15	316	A86	C4-C5-C6	-4.01	121.58	127.31
11	16	301	CLA	C1D-CHD-C4C	-4.01	117.40	126.06
14	8	318	A86	C33-C32-C31	4.01	113.11	109.21
12	8	312	KC1	CBA-CAA-C2A	-4.01	109.98	125.27
13	10	314	DD6	C37-C36-C35	-4.01	106.92	114.36
12	16	311	KC1	CHC-C1C-C2C	-4.01	118.71	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	8	305	CLA	C4A-NA-C1A	-4.01	104.90	106.71
11	12	307	CLA	C1D-CHD-C4C	-4.01	117.41	126.06
11	14	309	CLA	C3D-C4D-ND	4.01	116.72	110.24
14	15	322	A86	C-C1-C2	-4.01	117.31	122.92
12	11	306	KC1	CBA-CAA-C2A	-4.01	110.00	125.27
11	15	314	CLA	C1D-CHD-C4C	-4.01	117.42	126.06
11	6	314	CLA	C3D-C4D-ND	4.00	116.71	110.24
12	13	310	KC1	C2A-C1A-NA	4.00	115.82	109.40
11	6	311	CLA	C1D-CHD-C4C	-4.00	117.43	126.06
13	15	318	DD6	C21-C20-C19	-4.00	109.78	114.28
12	6	305	KC1	C2A-C1A-NA	4.00	115.81	109.40
11	12	321	CLA	C3D-C4D-ND	4.00	116.71	110.24
12	14	308	KC1	C1A-NA-C4A	-4.00	104.91	106.71
11	15	307	CLA	C3D-C4D-ND	3.99	116.70	110.24
14	15	317	A86	C25-C26-C27	-3.99	121.61	127.31
12	13	306	KC1	C4B-C3B-C2B	-3.99	103.47	106.75
14	10	316	A86	C40-C32-C31	-3.99	106.90	110.47
11	13	301	CLA	C1D-CHD-C4C	-3.99	117.45	126.06
11	8	304	CLA	C3D-C4D-ND	3.99	116.69	110.24
11	12	304	CLA	O2A-CGA-CBA	3.99	124.42	111.91
11	7	308	CLA	C1C-C2C-C3C	-3.99	102.76	106.96
11	10	304	CLA	C3D-C4D-ND	3.99	116.69	110.24
11	10	308	CLA	C2C-C1C-NC	3.99	113.71	109.97
11	15	308	CLA	CAC-C3C-C4C	3.99	129.98	124.81
12	12	311	KC1	C4B-C3B-C2B	-3.99	103.48	106.75
12	14	308	KC1	CMD-C2D-C1D	3.98	134.59	128.46
12	16	304	KC1	CBA-CAA-C2A	-3.98	110.08	125.27
12	13	310	KC1	C1C-C2C-C3C	-3.98	102.77	106.96
14	11	315	A86	C25-C24-C1	-3.98	115.23	126.42
11	8	302	CLA	C3D-C4D-ND	3.98	116.68	110.24
11	15	306	CLA	C3D-C4D-ND	3.98	116.67	110.24
11	6	306	CLA	C3D-C4D-ND	3.98	116.67	110.24
11	7	305	CLA	C1D-CHD-C4C	-3.98	117.48	126.06
11	13	302	CLA	C3C-C4C-NC	3.98	115.03	110.57
12	14	306	KC1	CHD-C4C-C3C	-3.97	117.87	125.33
11	14	305	CLA	C3C-C4C-NC	3.97	115.03	110.57
12	8	306	KC1	O2D-CGD-CBD	3.97	118.32	111.27
11	6	302	CLA	C3D-C4D-ND	3.97	116.66	110.24
11	10	303	CLA	C3C-C4C-NC	3.97	115.02	110.57
12	10	312	KC1	CHC-C1C-C2C	-3.97	118.78	124.98
14	15	317	A86	C3-C2-C1	-3.96	121.65	127.31
11	8	302	CLA	O2D-CGD-CBD	3.96	118.31	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	14	315	A86	C12-C11-C13	3.96	122.68	116.02
11	7	303	CLA	C3D-C4D-ND	3.96	116.65	110.24
11	16	302	CLA	C3D-C4D-ND	3.96	116.64	110.24
11	12	321	CLA	C1D-CHD-C4C	-3.96	117.52	126.06
11	10	305	CLA	CBA-CAA-C2A	3.96	125.55	113.86
13	10	314	DD6	C25-C24-C1	-3.96	115.30	126.42
12	6	309	KC1	C4B-C3B-C2B	-3.96	103.50	106.75
12	12	313	KC1	C1C-C2C-C3C	-3.96	102.80	106.96
11	12	307	CLA	CAA-C2A-C3A	-3.96	101.94	112.78
11	11	305	CLA	CBA-CAA-C2A	3.96	125.55	113.86
12	8	312	KC1	O2D-CGD-CBD	3.96	118.30	111.27
11	7	311	CLA	C1D-CHD-C4C	-3.96	117.52	126.06
11	11	303	CLA	C1D-CHD-C4C	-3.95	117.53	126.06
11	10	303	CLA	C3D-C4D-ND	3.95	116.63	110.24
11	6	303	CLA	C3C-C4C-NC	3.95	115.00	110.57
11	8	302	CLA	C3C-C4C-NC	3.95	115.00	110.57
11	7	303	CLA	C1C-C2C-C3C	-3.95	102.81	106.96
13	6	316	DD6	C7-C6-C8	-3.95	111.86	118.08
11	13	302	CLA	C3D-C4D-ND	3.95	116.62	110.24
14	11	313	A86	C25-C26-C27	-3.94	121.68	127.31
14	15	315	A86	C-C1-C24	-3.94	111.86	118.08
11	12	306	CLA	C3C-C4C-NC	3.94	114.99	110.57
11	16	305	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
14	16	312	A86	C26-C25-C24	-3.94	110.93	123.22
12	14	308	KC1	C2A-C1A-NA	3.94	115.72	109.40
11	8	308	CLA	C3D-C4D-ND	3.93	116.60	110.24
14	7	315	A86	C4-C3-C2	-3.93	115.42	123.47
11	12	306	CLA	C1D-CHD-C4C	-3.93	117.58	126.06
14	14	321	A86	C3-C4-C5	-3.93	115.42	123.47
12	12	305	KC1	C1C-C2C-C3C	-3.93	102.83	106.96
11	16	305	CLA	C3C-C4C-NC	3.93	114.98	110.57
12	11	306	KC1	C2A-C1A-NA	3.93	115.70	109.40
11	15	311	CLA	C1D-CHD-C4C	-3.93	117.58	126.06
11	16	309	CLA	C1C-C2C-C3C	-3.92	102.83	106.96
12	11	304	KC1	C4B-C3B-C2B	-3.92	103.53	106.75
11	11	307	CLA	C4A-NA-C1A	-3.92	104.94	106.71
12	13	308	KC1	C1C-C2C-C3C	-3.92	102.83	106.96
11	16	306	CLA	CAA-C2A-C3A	-3.92	102.04	112.78
11	16	309	CLA	C1D-CHD-C4C	-3.92	117.60	126.06
11	16	306	CLA	C3D-C2D-C1D	-3.92	100.48	105.83
14	7	315	A86	C4-C5-C6	-3.92	121.72	127.31
11	6	307	CLA	O2D-CGD-CBD	3.92	118.22	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	13	312	KC1	C1C-C2C-C3C	-3.91	102.84	106.96
12	14	308	KC1	C4B-C3B-C2B	-3.91	103.54	106.75
11	10	311	CLA	C1D-CHD-C4C	-3.91	117.62	126.06
11	16	309	CLA	C3C-C4C-NC	3.91	114.96	110.57
11	12	303	CLA	CMB-C2B-C3B	3.91	132.00	124.68
11	8	309	CLA	C1D-CHD-C4C	-3.91	117.62	126.06
11	6	311	CLA	CBC-CAC-C3C	-3.91	101.65	112.43
11	14	304	CLA	C1D-CHD-C4C	-3.91	117.63	126.06
11	8	301	CLA	C1C-C2C-C3C	-3.91	102.85	106.96
11	7	308	CLA	C3D-C4D-ND	3.91	116.56	110.24
14	14	320	A86	C41-C32-C31	-3.91	106.98	110.47
12	11	310	KC1	C4B-C3B-C2B	-3.91	103.54	106.75
11	12	307	CLA	CMC-C2C-C1C	3.91	130.99	125.04
11	15	304	CLA	O2D-CGD-CBD	3.91	118.21	111.27
12	10	310	KC1	C1C-C2C-C3C	-3.90	102.85	106.96
12	11	310	KC1	CBA-CAA-C2A	-3.90	110.39	125.27
12	12	313	KC1	CAA-CBA-CGA	-3.90	107.21	127.26
13	6	315	DD6	C7-C6-C8	-3.90	111.93	118.08
12	14	306	KC1	C2C-C1C-NC	3.90	114.83	110.57
11	16	308	CLA	C1D-CHD-C4C	-3.90	117.65	126.06
11	12	308	CLA	O2D-CGD-CBD	3.90	118.19	111.27
11	16	306	CLA	C1D-CHD-C4C	-3.90	117.65	126.06
11	13	304	CLA	C3C-C4C-NC	3.89	114.94	110.57
12	8	307	KC1	CMB-C2B-C1B	3.89	131.58	124.71
11	6	313	CLA	C3D-C4D-ND	3.89	116.54	110.24
11	15	302	CLA	C1D-CHD-C4C	-3.89	117.66	126.06
11	7	305	CLA	C1C-C2C-C3C	-3.89	102.86	106.96
12	11	311	KC1	C1C-C2C-C3C	-3.89	102.86	106.96
12	13	306	KC1	CHC-C1C-C2C	-3.89	118.90	124.98
11	6	306	CLA	CMB-C2B-C3B	3.89	131.96	124.68
11	12	306	CLA	C1C-C2C-C3C	-3.89	102.86	106.96
11	6	313	CLA	C1C-C2C-C3C	-3.89	102.87	106.96
13	12	315	DD6	C37-C36-C35	-3.89	107.15	114.36
13	6	315	DD6	C21-C20-C19	-3.89	109.91	114.28
12	6	308	KC1	CBA-CAA-C2A	-3.89	110.44	125.27
11	12	306	CLA	C3D-C4D-ND	3.89	116.53	110.24
13	16	313	DD6	C21-C20-C15	-3.89	115.75	122.26
12	12	305	KC1	C4B-C3B-C2B	-3.89	103.56	106.75
11	8	301	CLA	C1D-CHD-C4C	-3.88	117.68	126.06
11	15	310	CLA	C3C-C4C-NC	3.88	114.92	110.57
11	16	302	CLA	C1D-CHD-C4C	-3.88	117.68	126.06
12	10	312	KC1	C2C-C1C-NC	3.88	114.81	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	14	305	CLA	CAA-C2A-C3A	-3.88	102.16	112.78
12	7	307	KC1	C1C-C2C-C3C	-3.88	102.88	106.96
11	12	303	CLA	C1C-C2C-C3C	-3.88	102.88	106.96
11	15	314	CLA	C1C-C2C-C3C	-3.88	102.88	106.96
11	15	311	CLA	C1C-C2C-C3C	-3.87	102.88	106.96
12	16	311	KC1	C1C-C2C-C3C	-3.87	102.88	106.96
11	7	310	CLA	C3D-C4D-ND	3.87	116.50	110.24
13	12	317	DD6	C21-C20-C15	-3.87	115.77	122.26
12	8	306	KC1	CBA-CAA-C2A	-3.87	110.51	125.27
12	8	310	KC1	CAC-C3C-C4C	3.87	129.83	124.81
11	12	302	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
11	13	304	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
12	12	305	KC1	C2A-C1A-NA	3.87	115.61	109.40
13	6	316	DD6	C35-C36-C31	-3.87	111.79	120.57
11	13	309	CLA	C4A-NA-C1A	-3.87	104.97	106.71
11	13	307	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
11	12	308	CLA	C1D-CHD-C4C	-3.86	117.72	126.06
14	11	301	A86	C36-C31-C32	-3.86	115.86	119.70
11	7	304	CLA	C3B-C4B-NB	3.86	114.20	109.21
11	14	309	CLA	C1D-CHD-C4C	-3.86	117.73	126.06
11	7	302	CLA	C4A-NA-C1A	-3.86	104.97	106.71
11	16	306	CLA	CAC-C3C-C4C	3.86	129.82	124.81
11	14	307	CLA	O2D-CGD-CBD	3.86	118.13	111.27
14	7	315	A86	C26-C25-C24	-3.86	111.17	123.22
11	16	303	CLA	C3C-C4C-NC	3.86	114.90	110.57
11	16	305	CLA	C3D-C4D-ND	3.86	116.48	110.24
11	7	306	CLA	C4A-NA-C1A	-3.86	104.97	106.71
11	12	303	CLA	C3D-C4D-ND	3.85	116.47	110.24
11	14	309	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
12	14	311	KC1	CHC-C1C-C2C	-3.85	118.96	124.98
14	7	314	A86	O4-C38-C39	3.85	118.17	111.09
12	7	307	KC1	C1A-NA-C4A	-3.85	104.98	106.71
11	6	301	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
11	14	310	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
11	7	306	CLA	C1D-CHD-C4C	-3.84	117.77	126.06
11	6	314	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
11	15	310	CLA	C3B-C4B-NB	3.84	114.18	109.21
13	7	301	DD6	C15-C14-C13	-3.84	117.87	125.99
11	16	307	CLA	C1D-CHD-C4C	-3.84	117.78	126.06
11	15	313	CLA	C1D-CHD-C4C	-3.83	117.78	126.06
11	6	307	CLA	C4A-NA-C1A	-3.83	104.98	106.71
11	6	314	CLA	C1D-CHD-C4C	-3.83	117.79	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	13	309	CLA	C1D-CHD-C4C	-3.83	117.79	126.06
11	6	312	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
11	15	303	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
11	14	305	CLA	C4A-NA-C1A	-3.83	104.98	106.71
12	10	310	KC1	CBA-CAA-C2A	-3.83	110.67	125.27
13	7	317	DD6	C15-C14-C13	3.83	134.09	125.99
11	13	307	CLA	C3C-C4C-NC	3.83	114.87	110.57
14	8	315	A86	C33-C32-C31	3.83	112.93	109.21
11	10	307	CLA	C1D-CHD-C4C	-3.83	117.80	126.06
14	13	313	A86	C36-C35-C34	3.83	116.28	111.75
11	13	301	CLA	C3C-C4C-NC	3.83	114.86	110.57
11	14	312	CLA	C3C-C4C-NC	3.83	114.86	110.57
11	15	305	CLA	C3C-C4C-NC	3.83	114.86	110.57
11	15	311	CLA	C3C-C4C-NC	3.83	114.86	110.57
11	8	303	CLA	C3B-C4B-NB	3.83	114.16	109.21
11	13	304	CLA	C1D-CHD-C4C	-3.83	117.81	126.06
12	13	310	KC1	CHC-C1C-C2C	-3.82	119.00	124.98
11	7	309	CLA	C3C-C4C-NC	3.82	114.86	110.57
12	11	311	KC1	C4B-C3B-C2B	-3.82	103.61	106.75
12	13	308	KC1	C4B-C3B-C2B	-3.82	103.61	106.75
11	15	312	CLA	C1D-CHD-C4C	-3.82	117.82	126.06
11	14	310	CLA	C3C-C4C-NC	3.82	114.85	110.57
11	6	312	CLA	C1D-CHD-C4C	-3.82	117.83	126.06
11	6	304	CLA	C3C-C4C-NC	3.82	114.85	110.57
11	8	308	CLA	C3C-C4C-NC	3.82	114.85	110.57
11	12	307	CLA	C2C-C1C-NC	3.82	113.55	109.97
11	6	301	CLA	C1D-CHD-C4C	-3.81	117.83	126.06
11	15	308	CLA	C3D-C4D-ND	3.81	116.41	110.24
11	7	310	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
13	11	312	DD6	C35-C36-C31	-3.81	111.92	120.57
11	14	304	CLA	C3C-C4C-NC	3.81	114.84	110.57
14	15	322	A86	C9-C10-C11	-3.81	115.41	126.61
11	10	311	CLA	C3C-C4C-NC	3.81	114.84	110.57
11	11	303	CLA	C3C-C4C-NC	3.81	114.84	110.57
11	15	309	CLA	C1D-CHD-C4C	-3.81	117.85	126.06
11	12	312	CLA	C1D-CHD-C4C	-3.80	117.85	126.06
12	14	311	KC1	C2A-C1A-NA	3.80	115.50	109.40
11	12	304	CLA	CBA-CAA-C2A	3.80	125.09	113.86
11	7	311	CLA	C4A-NA-C1A	-3.80	105.00	106.71
13	15	319	DD6	C21-C20-C15	-3.80	115.89	122.26
11	13	302	CLA	C1C-C2C-C3C	-3.80	102.96	106.96
11	8	303	CLA	C1C-C2C-C3C	-3.80	102.96	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	16	303	CLA	C1D-CHD-C4C	-3.80	117.86	126.06
12	8	307	KC1	C2C-C1C-NC	3.80	114.72	110.57
11	6	302	CLA	C1C-C2C-C3C	-3.80	102.96	106.96
12	10	306	KC1	C1C-C2C-C3C	-3.80	102.96	106.96
11	8	302	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
11	12	303	CLA	C1D-CHD-C4C	-3.79	117.87	126.06
14	14	320	A86	C-C1-C2	-3.79	117.61	122.92
11	10	305	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
11	16	308	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
11	16	310	CLA	O2D-CGD-O1D	-3.79	116.43	123.84
12	6	310	KC1	C1C-C2C-C3C	-3.79	102.97	106.96
11	13	309	CLA	C3D-C4D-ND	3.79	116.37	110.24
12	8	314	KC1	C1C-C2C-C3C	-3.79	102.97	106.96
12	8	313	KC1	CAA-CBA-CGA	-3.79	107.80	127.26
11	6	311	CLA	C1C-C2C-C3C	-3.79	102.98	106.96
11	12	307	CLA	C3C-C4C-NC	3.78	114.81	110.57
13	7	317	DD6	C35-C36-C31	-3.78	111.98	120.57
11	8	303	CLA	C3C-C4C-NC	3.78	114.81	110.57
11	6	302	CLA	C1D-CHD-C4C	-3.78	117.90	126.06
12	13	310	KC1	C1A-NA-C4A	-3.78	105.01	106.71
12	13	305	KC1	C1C-C2C-C3C	-3.78	102.99	106.96
12	8	313	KC1	CHC-C1C-C2C	-3.78	119.08	124.98
11	6	303	CLA	O2A-CGA-CBA	3.77	123.75	111.91
11	8	308	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
13	10	313	DD6	C3-C4-C5	-3.77	115.75	123.47
11	15	307	CLA	C1D-CHD-C4C	-3.77	117.93	126.06
11	11	309	CLA	C1D-CHD-C4C	-3.77	117.93	126.06
11	11	303	CLA	C4A-NA-C1A	-3.77	105.01	106.71
11	12	312	CLA	C1C-C2C-C3C	-3.77	103.00	106.96
11	6	307	CLA	C3D-C4D-ND	3.76	116.33	110.24
14	14	320	A86	C3-C4-C5	3.76	131.18	123.47
11	7	305	CLA	C3D-C4D-ND	3.76	116.32	110.24
11	7	311	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
11	7	308	CLA	C3C-C4C-NC	3.76	114.79	110.57
11	6	306	CLA	C3C-C4C-NC	3.76	114.79	110.57
14	7	318	A86	C9-C10-C11	-3.76	115.56	126.61
11	8	305	CLA	C3D-C4D-ND	3.76	116.31	110.24
11	13	307	CLA	C3D-C4D-ND	3.76	116.31	110.24
11	16	307	CLA	C3C-C4C-NC	3.76	114.78	110.57
13	7	301	DD6	C12-C11-C13	-3.76	112.16	118.08
11	6	306	CLA	C1D-CHD-C4C	-3.76	117.96	126.06
11	7	303	CLA	C3B-C4B-NB	3.75	114.06	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	8	312	KC1	CHC-C1C-C2C	-3.75	119.12	124.98
12	13	305	KC1	C4B-C3B-C2B	-3.75	103.67	106.75
11	12	312	CLA	C3C-C4C-NC	3.75	114.78	110.57
11	15	313	CLA	C3C-C4C-NC	3.75	114.78	110.57
14	14	314	A86	C41-C32-C31	-3.75	107.11	110.47
14	7	314	A86	C40-C32-C31	-3.75	107.12	110.47
11	14	313	CLA	C1D-CHD-C4C	-3.75	117.97	126.06
11	15	310	CLA	C1C-C2C-C3C	-3.75	103.02	106.96
13	10	313	DD6	C15-C14-C13	3.75	133.92	125.99
11	16	310	CLA	C1D-CHD-C4C	-3.75	117.97	126.06
12	10	310	KC1	CHC-C4B-NB	-3.75	121.01	124.45
14	15	321	A86	C36-C31-C32	-3.74	115.98	119.70
11	13	302	CLA	C1D-CHD-C4C	-3.74	117.99	126.06
12	8	310	KC1	CAA-CBA-CGA	-3.74	108.03	127.26
11	13	303	CLA	C1C-C2C-C3C	-3.74	103.02	106.96
11	11	308	CLA	CAC-C3C-C4C	3.74	129.66	124.81
14	12	314	A86	C40-C32-C31	-3.74	107.13	110.47
13	10	313	DD6	C14-C13-C11	3.74	131.33	125.53
12	11	304	KC1	C1C-C2C-C3C	-3.74	103.03	106.96
14	15	320	A86	C35-C34-C33	3.74	116.39	109.88
11	15	310	CLA	C1D-CHD-C4C	-3.74	118.00	126.06
11	15	311	CLA	C4A-NA-C1A	-3.73	105.03	106.71
11	10	309	CLA	C3C-C4C-NC	3.73	114.76	110.57
11	6	304	CLA	C1D-CHD-C4C	-3.73	118.01	126.06
11	14	313	CLA	C3C-C4C-NC	3.73	114.75	110.57
13	6	318	DD6	C21-C20-C15	-3.73	116.01	122.26
11	10	304	CLA	C1D-CHD-C4C	-3.73	118.02	126.06
11	13	303	CLA	C1D-CHD-C4C	-3.73	118.02	126.06
11	11	309	CLA	C1C-C2C-C3C	-3.73	103.04	106.96
11	16	310	CLA	C1C-C2C-C3C	-3.73	103.04	106.96
12	6	310	KC1	C4B-C3B-C2B	-3.72	103.69	106.75
12	14	306	KC1	C4C-C3C-C2C	-3.72	101.47	106.90
12	8	314	KC1	CMA-C3A-C2A	-3.72	119.19	128.30
11	6	313	CLA	C1D-CHD-C4C	-3.72	118.04	126.06
11	12	307	CLA	CMB-C2B-C3B	3.72	131.63	124.68
12	11	310	KC1	C1C-C2C-C3C	-3.72	103.05	106.96
11	16	308	CLA	C3C-C4C-NC	3.72	114.74	110.57
13	10	313	DD6	C37-C36-C35	-3.72	107.47	114.36
12	12	309	KC1	C1C-C2C-C3C	-3.71	103.05	106.96
11	10	309	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
11	7	310	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
12	7	307	KC1	CBA-CAA-C2A	-3.71	111.12	125.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	13	307	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
13	7	313	DD6	C7-C6-C8	-3.71	112.24	118.08
12	8	306	KC1	C1A-NA-C4A	-3.71	105.04	106.71
12	6	305	KC1	CHC-C1C-C2C	-3.70	119.19	124.98
11	12	302	CLA	C4A-NA-C1A	-3.70	105.04	106.71
12	8	312	KC1	C1A-NA-C4A	-3.70	105.04	106.71
11	7	309	CLA	C1C-C2C-C3C	-3.70	103.06	106.96
11	12	304	CLA	C1D-CHD-C4C	-3.70	118.07	126.06
13	16	313	DD6	C23-C16-C17	-3.70	102.55	108.98
14	11	315	A86	C3-C4-C5	-3.70	115.90	123.47
11	8	303	CLA	C1D-CHD-C4C	-3.70	118.08	126.06
11	8	301	CLA	C1-C2-C3	-3.70	119.65	126.04
12	16	304	KC1	C4B-C3B-C2B	-3.70	103.72	106.75
12	7	312	KC1	CAA-C2A-C1A	-3.69	107.77	124.75
14	11	314	A86	C3-C2-C1	-3.69	122.04	127.31
11	6	314	CLA	C3C-C4C-NC	3.69	114.71	110.57
11	8	301	CLA	C3B-C4B-NB	3.69	113.98	109.21
12	11	306	KC1	C1C-C2C-C3C	-3.69	103.08	106.96
11	6	307	CLA	C3C-C4C-NC	3.69	114.71	110.57
12	13	305	KC1	C1A-NA-C4A	-3.69	105.05	106.71
13	7	301	DD6	C35-C36-C31	-3.69	112.20	120.57
11	8	304	CLA	CAA-C2A-C1A	-3.69	99.90	111.97
14	14	320	A86	C8-C6-C5	-3.68	113.29	118.94
11	7	310	CLA	C3C-C4C-NC	3.68	114.70	110.57
11	8	305	CLA	CMB-C2B-C3B	3.68	131.57	124.68
11	6	313	CLA	CMB-C2B-C3B	3.68	131.57	124.68
11	15	306	CLA	O2D-CGD-O1D	-3.68	116.64	123.84
14	14	317	A86	C3-C2-C1	-3.68	122.06	127.31
11	8	304	CLA	C3C-C4C-NC	3.68	114.70	110.57
11	14	312	CLA	C1D-CHD-C4C	-3.68	118.12	126.06
13	15	318	DD6	C21-C20-C15	-3.68	116.10	122.26
12	6	305	KC1	C2C-C1C-NC	3.68	114.59	110.57
13	15	319	DD6	C37-C36-C35	-3.68	107.54	114.36
11	14	303	CLA	C1D-CHD-C4C	-3.68	118.13	126.06
11	16	307	CLA	C1C-C2C-C3C	-3.67	103.09	106.96
11	6	307	CLA	C1D-CHD-C4C	-3.67	118.13	126.06
11	14	305	CLA	C1C-C2C-C3C	-3.67	103.09	106.96
12	14	311	KC1	C1C-C2C-C3C	-3.67	103.09	106.96
12	8	310	KC1	C4C-C3C-C2C	-3.67	101.55	106.90
14	14	314	A86	C10-C9-C8	-3.67	111.76	123.22
11	12	302	CLA	O2A-CGA-CBA	3.67	123.43	111.91
11	11	309	CLA	C3C-C4C-NC	3.67	114.69	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	8	318	A86	C35-C34-C33	3.67	116.28	109.88
11	12	310	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
12	16	304	KC1	C1C-C2C-C3C	-3.67	103.10	106.96
11	7	304	CLA	C3C-C4C-NC	3.67	114.68	110.57
11	7	303	CLA	C3C-C4C-NC	3.67	114.68	110.57
11	6	306	CLA	O2A-CGA-CBA	3.67	123.41	111.91
11	7	303	CLA	C1D-CHD-C4C	-3.67	118.15	126.06
13	15	319	DD6	C23-C16-C15	3.67	119.94	110.05
11	8	309	CLA	C4A-NA-C1A	-3.67	105.06	106.71
11	10	303	CLA	C4A-NA-C1A	-3.67	105.06	106.71
11	15	310	CLA	CMB-C2B-C3B	3.66	131.53	124.68
11	10	305	CLA	C1D-CHD-C4C	-3.66	118.16	126.06
11	8	309	CLA	C3C-C4C-NC	3.66	114.68	110.57
11	7	309	CLA	C1D-CHD-C4C	-3.66	118.16	126.06
11	8	302	CLA	C1D-CHD-C4C	-3.66	118.16	126.06
14	11	314	A86	C36-C31-C32	-3.66	116.06	119.70
12	13	305	KC1	C2A-C1A-NA	3.66	115.27	109.40
12	6	309	KC1	C2C-C1C-NC	3.66	114.56	110.57
11	14	310	CLA	C4A-NA-C1A	-3.65	105.06	106.71
11	6	312	CLA	C3C-C4C-NC	3.65	114.67	110.57
11	15	313	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
11	12	303	CLA	C3B-C4B-NB	3.65	113.93	109.21
12	10	306	KC1	C4B-C3B-C2B	-3.65	103.75	106.75
12	8	314	KC1	C1A-NA-C4A	-3.65	105.06	106.71
11	14	302	CLA	C1D-CHD-C4C	-3.65	118.19	126.06
12	7	312	KC1	C2C-C1C-NC	3.65	114.56	110.57
11	7	302	CLA	C1D-CHD-C4C	-3.65	118.19	126.06
11	14	309	CLA	C3C-C4C-NC	3.65	114.66	110.57
11	15	309	CLA	C3C-C4C-NC	3.65	114.66	110.57
11	15	305	CLA	C1C-C2C-C3C	-3.64	103.12	106.96
12	13	312	KC1	CAA-CBA-CGA	-3.64	108.54	127.26
12	10	312	KC1	C1C-C2C-C3C	-3.64	103.13	106.96
11	8	308	CLA	C1D-CHD-C4C	-3.64	118.20	126.06
11	8	303	CLA	CAA-C2A-C3A	-3.64	102.81	112.78
11	12	303	CLA	O2D-CGD-CBD	3.64	117.73	111.27
12	8	314	KC1	C4B-C3B-C2B	-3.64	103.77	106.75
14	7	315	A86	C8-C6-C5	-3.64	113.36	118.94
11	15	309	CLA	O2D-CGD-CBD	3.63	117.72	111.27
11	15	305	CLA	C1D-CHD-C4C	-3.63	118.22	126.06
12	14	306	KC1	CBA-CAA-C2A	-3.63	111.42	125.27
12	8	307	KC1	C1C-C2C-C3C	-3.63	103.14	106.96
13	15	318	DD6	C37-C36-C35	-3.63	107.63	114.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	11	312	DD6	C13-C11-C10	-3.63	113.37	118.94
11	16	305	CLA	CAA-C2A-C3A	-3.63	102.85	112.78
11	11	308	CLA	O2A-CGA-CBA	3.63	123.29	111.91
11	10	304	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
13	8	316	DD6	C21-C20-C19	-3.62	110.20	114.28
11	7	304	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
12	8	310	KC1	C4B-C3B-C2B	-3.62	103.78	106.75
11	15	302	CLA	C3C-C4C-NC	3.62	114.63	110.57
11	12	308	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
14	15	321	A86	C41-C32-C31	-3.62	107.23	110.47
14	11	315	A86	C36-C31-C32	-3.61	116.11	119.70
11	7	306	CLA	C3C-C4C-NC	3.61	114.62	110.57
11	10	305	CLA	C3C-C4C-NC	3.61	114.62	110.57
11	16	310	CLA	CED-O2D-CGD	3.61	124.09	115.94
11	10	308	CLA	C1D-CHD-C4C	-3.61	118.28	126.06
12	8	311	KC1	C4B-C3B-C2B	-3.60	103.79	106.75
11	8	301	CLA	C4A-NA-C1A	-3.60	105.09	106.71
11	14	303	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
12	8	312	KC1	C1C-C2C-C3C	-3.60	103.17	106.96
13	6	315	DD6	C15-C14-C13	-3.60	118.38	125.99
14	11	313	A86	C4-C3-C2	-3.60	116.10	123.47
14	15	322	A86	C24-C1-C2	3.60	124.46	118.94
12	6	309	KC1	CHC-C1C-C2C	-3.59	119.37	124.98
11	10	307	CLA	C3D-C4D-ND	3.59	116.05	110.24
13	6	318	DD6	C21-C20-C19	-3.59	110.24	114.28
11	10	309	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
12	14	308	KC1	C4C-C3C-C2C	-3.58	101.67	106.90
11	10	303	CLA	C3B-C4B-NB	3.58	113.84	109.21
12	11	306	KC1	C4B-C3B-C2B	-3.58	103.81	106.75
11	6	303	CLA	C4A-NA-C1A	-3.58	105.10	106.71
13	7	313	DD6	C22-C16-C15	3.58	119.71	110.05
11	12	304	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
11	15	308	CLA	C4C-C3C-C2C	-3.58	101.68	106.90
11	6	303	CLA	C1D-CHD-C4C	-3.58	118.34	126.06
13	7	316	DD6	C37-C36-C35	-3.57	107.73	114.36
11	13	303	CLA	CAA-C2A-C3A	-3.57	102.99	112.78
11	14	303	CLA	CAA-C2A-C3A	-3.57	103.00	112.78
13	7	317	DD6	C21-C20-C19	-3.57	110.26	114.28
14	14	317	A86	C4-C3-C2	-3.57	116.16	123.47
11	14	304	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
11	6	302	CLA	C3C-C4C-NC	3.57	114.57	110.57
13	12	317	DD6	O1-C20-C21	-3.57	110.78	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	11	307	CLA	C1C-C2C-C3C	-3.57	103.21	106.96
13	12	315	DD6	C21-C20-C15	-3.56	116.29	122.26
11	7	311	CLA	C3C-C4C-NC	3.56	114.56	110.57
12	14	306	KC1	CAB-C3B-C4B	3.56	133.50	124.90
11	11	308	CLA	C3C-C4C-NC	3.56	114.56	110.57
15	6	319	LHG	O8-C23-C24	3.56	120.71	111.38
11	15	302	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
11	15	306	CLA	C3B-C4B-NB	3.56	113.81	109.21
11	11	308	CLA	C1D-CHD-C4C	-3.55	118.39	126.06
11	6	313	CLA	C3C-C4C-NC	3.55	114.56	110.57
14	14	320	A86	C9-C10-C11	-3.55	116.16	126.61
13	8	316	DD6	C7-C6-C8	-3.55	112.48	118.08
14	8	315	A86	C4-C3-C2	-3.55	116.20	123.47
14	10	301	A86	C10-C9-C8	-3.55	112.13	123.22
11	6	304	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
11	13	301	CLA	CAC-C3C-C4C	3.55	129.42	124.81
11	16	301	CLA	C4A-NA-C1A	-3.55	105.11	106.71
11	12	312	CLA	CAA-C2A-C3A	-3.55	103.06	112.78
13	12	315	DD6	C35-C36-C31	-3.54	112.53	120.57
12	6	309	KC1	C1C-C2C-C3C	-3.54	103.23	106.96
14	8	315	A86	C8-C6-C5	-3.54	113.51	118.94
11	10	303	CLA	C1C-C2C-C3C	-3.54	103.24	106.96
11	11	305	CLA	C1D-CHD-C4C	-3.54	118.43	126.06
11	11	305	CLA	C3C-C4C-NC	3.53	114.53	110.57
12	14	311	KC1	CMB-C2B-C1B	3.53	130.94	124.71
12	8	312	KC1	C4B-C3B-C2B	-3.53	103.85	106.75
14	10	301	A86	O-C13-C11	-3.53	113.35	121.15
11	10	303	CLA	CMB-C2B-C3B	3.53	131.28	124.68
11	15	304	CLA	C1C-C2C-C3C	-3.53	103.25	106.96
13	16	313	DD6	O1-C20-C21	-3.52	110.83	115.06
13	6	316	DD6	C23-C16-C22	-3.52	102.17	107.37
12	10	306	KC1	CAA-CBA-CGA	-3.52	109.16	127.26
11	7	303	CLA	CAA-C2A-C3A	-3.52	103.13	112.78
11	12	321	CLA	C1C-C2C-C3C	-3.52	103.25	106.96
14	14	319	A86	C34-O4-C38	-3.52	111.34	117.90
12	12	311	KC1	C1C-C2C-C3C	-3.52	103.26	106.96
11	6	302	CLA	CMB-C2B-C3B	3.52	131.26	124.68
14	13	313	A86	C7-C6-C5	-3.52	118.00	122.92
11	13	301	CLA	C1-C2-C3	-3.52	119.96	126.04
11	10	307	CLA	C1C-C2C-C3C	-3.52	103.26	106.96
14	14	314	A86	C7-C6-C5	-3.51	118.00	122.92
11	10	308	CLA	C3C-C4C-NC	3.51	114.51	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	7	310	CLA	CAC-C3C-C4C	3.51	129.36	124.81
13	13	314	DD6	C21-C20-C15	-3.50	116.39	122.26
13	10	313	DD6	C21-C20-C15	-3.50	116.39	122.26
11	14	313	CLA	C1C-C2C-C3C	-3.50	103.27	106.96
11	12	304	CLA	C3C-C4C-NC	3.50	114.50	110.57
11	14	305	CLA	C1D-CHD-C4C	-3.50	118.50	126.06
12	11	304	KC1	CBA-CAA-C2A	-3.50	111.92	125.27
12	11	304	KC1	CAA-CBA-CGA	-3.50	109.28	127.26
14	14	315	A86	C25-C26-C27	-3.50	122.32	127.31
14	14	321	A86	C9-C10-C11	-3.50	116.33	126.61
11	6	301	CLA	CBC-CAC-C3C	-3.49	102.80	112.43
11	16	306	CLA	CMB-C2B-C3B	3.49	131.22	124.68
13	6	315	DD6	C25-C24-C1	-3.49	116.61	126.42
11	15	308	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
11	7	311	CLA	C3B-C4B-NB	3.49	113.72	109.21
14	8	315	A86	C36-C31-C32	-3.48	116.24	119.70
11	6	311	CLA	C3B-C4B-NB	3.48	113.71	109.21
11	7	304	CLA	C1D-CHD-C4C	-3.48	118.56	126.06
12	12	309	KC1	C4B-C3B-C2B	-3.48	103.90	106.75
12	6	305	KC1	C4B-C3B-C2B	-3.47	103.90	106.75
11	14	303	CLA	C3C-C4C-NC	3.47	114.47	110.57
11	8	304	CLA	C4-C3-C5	3.47	121.11	115.27
11	16	301	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
11	8	304	CLA	C4A-NA-C1A	-3.47	105.15	106.71
11	15	305	CLA	CAC-C3C-C4C	3.47	129.31	124.81
11	7	309	CLA	C3B-C4B-NB	3.47	113.69	109.21
12	14	306	KC1	CHC-C4B-NB	-3.47	121.27	124.45
14	11	313	A86	C10-C9-C8	-3.46	112.41	123.22
11	13	309	CLA	C3B-C4B-NB	3.46	113.69	109.21
12	16	311	KC1	C4B-C3B-C2B	-3.46	103.91	106.75
11	8	309	CLA	O2D-CGD-O1D	-3.46	117.07	123.84
12	8	313	KC1	C4C-C3C-C2C	-3.46	101.86	106.90
14	7	318	A86	C3-C4-C5	-3.46	116.39	123.47
12	14	308	KC1	C1C-C2C-C3C	-3.45	103.33	106.96
12	6	310	KC1	CAA-C2A-C1A	-3.45	108.88	124.75
11	14	312	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
13	8	317	DD6	C21-C20-C19	-3.45	110.40	114.28
12	10	312	KC1	CAA-CBA-CGA	-3.45	109.53	127.26
12	10	312	KC1	CBA-CAA-C2A	-3.45	112.12	125.27
12	8	311	KC1	C1C-C2C-C3C	-3.45	103.33	106.96
13	11	312	DD6	C37-C36-C35	-3.45	107.97	114.36
13	6	318	DD6	C33-C32-C31	3.45	116.61	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	8	310	KC1	C1A-NA-C4A	-3.44	105.16	106.71
12	13	306	KC1	C2C-C1C-NC	3.44	114.33	110.57
11	12	302	CLA	CAA-C2A-C1A	-3.44	100.71	111.97
12	14	311	KC1	C4B-C3B-C2B	-3.44	103.93	106.75
11	15	309	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
11	11	307	CLA	C3C-C4C-NC	3.43	114.42	110.57
11	15	305	CLA	C3B-C4B-NB	3.43	113.65	109.21
12	8	310	KC1	C2C-C1C-NC	3.43	114.32	110.57
13	6	318	DD6	C15-C14-C13	-3.43	118.74	125.99
14	7	318	A86	C3-C2-C1	-3.43	122.42	127.31
11	14	307	CLA	C1D-CHD-C4C	-3.43	118.67	126.06
12	12	311	KC1	CAC-C3C-C4C	3.43	129.26	124.81
12	13	311	KC1	CAA-CBA-CGA	-3.42	109.67	127.26
11	16	303	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
11	7	305	CLA	C4A-NA-C1A	-3.42	105.17	106.71
11	11	308	CLA	CMB-C2B-C3B	3.42	131.07	124.68
11	16	302	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
11	12	321	CLA	C3B-C4B-NB	3.42	113.63	109.21
11	15	308	CLA	O2A-CGA-CBA	3.41	125.00	114.03
11	13	303	CLA	C3C-C4C-NC	3.41	114.39	110.57
11	8	309	CLA	C3B-C4B-NB	3.41	113.62	109.21
14	10	316	A86	C20-C19-C18	-3.41	106.01	112.75
11	12	321	CLA	C3C-C4C-NC	3.40	114.39	110.57
11	6	302	CLA	C3B-C4B-NB	3.40	113.61	109.21
14	14	314	A86	C40-C32-C31	-3.40	107.43	110.47
11	16	308	CLA	CAC-C3C-C4C	3.40	129.22	124.81
11	6	303	CLA	C1C-C2C-C3C	-3.40	103.38	106.96
14	13	315	A86	C41-C32-C31	-3.39	107.43	110.47
12	6	309	KC1	CAA-CBA-CGA	-3.39	109.82	127.26
12	6	305	KC1	CAA-CBA-CGA	-3.39	109.83	127.26
12	12	309	KC1	C1A-NA-C4A	-3.39	105.18	106.71
12	12	313	KC1	C4B-C3B-C2B	-3.39	103.97	106.75
11	14	302	CLA	C3C-C4C-NC	3.39	114.37	110.57
14	7	315	A86	C36-C31-C32	-3.38	116.34	119.70
11	14	307	CLA	C1C-C2C-C3C	-3.38	103.40	106.96
13	10	314	DD6	C35-C36-C31	-3.38	112.89	120.57
12	10	310	KC1	CAA-CBA-CGA	-3.38	109.87	127.26
11	6	301	CLA	C3C-C4C-NC	3.38	114.36	110.57
14	8	315	A86	C7-C6-C8	3.38	123.40	118.08
11	6	312	CLA	C3B-C4B-NB	3.38	113.58	109.21
11	7	310	CLA	C3B-C4B-NB	3.37	113.57	109.21
11	15	302	CLA	CMB-C2B-C3B	3.37	130.99	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	16	309	CLA	C3B-C4B-NB	3.37	113.57	109.21
14	10	317	A86	C40-C32-C31	-3.37	107.46	110.47
11	8	305	CLA	C4C-C3C-C2C	-3.37	101.99	106.90
11	12	321	CLA	O2D-CGD-CBD	3.37	117.25	111.27
11	15	311	CLA	C3B-C4B-NB	3.36	113.56	109.21
11	15	304	CLA	C4C-C3C-C2C	-3.36	102.00	106.90
11	6	311	CLA	C3C-C4C-NC	3.36	114.34	110.57
11	11	305	CLA	C1C-C2C-C3C	-3.35	103.43	106.96
13	10	314	DD6	C12-C11-C13	-3.35	112.80	118.08
13	7	317	DD6	O1-C20-C21	-3.35	111.04	115.06
11	12	304	CLA	C3B-C4B-NB	3.35	113.54	109.21
11	15	303	CLA	O2A-CGA-CBA	3.35	122.42	111.91
11	15	302	CLA	C1C-C2C-C3C	-3.35	103.44	106.96
11	10	311	CLA	C3B-C4B-NB	3.35	113.54	109.21
11	6	306	CLA	C1C-C2C-C3C	-3.35	103.44	106.96
11	8	304	CLA	C1C-C2C-C3C	-3.35	103.44	106.96
11	14	302	CLA	C1C-C2C-C3C	-3.34	103.44	106.96
13	13	314	DD6	O1-C20-C21	-3.34	111.05	115.06
11	12	302	CLA	C3B-C4B-NB	3.34	113.52	109.21
11	10	304	CLA	C3B-C4B-NB	3.34	113.52	109.21
11	16	310	CLA	CAA-C2A-C3A	-3.34	103.64	112.78
11	7	303	CLA	O2D-CGD-CBD	3.34	117.19	111.27
11	16	305	CLA	C3B-C4B-NB	3.34	113.52	109.21
12	12	305	KC1	CBA-CAA-C2A	-3.34	112.56	125.27
11	8	304	CLA	C3B-C4B-NB	3.33	113.52	109.21
12	6	310	KC1	CBA-CAA-C2A	-3.33	112.56	125.27
11	7	302	CLA	CMC-C2C-C1C	3.33	130.11	125.04
14	11	315	A86	C10-C9-C8	-3.33	112.83	123.22
11	10	303	CLA	C1-C2-C3	-3.33	120.29	126.04
11	13	301	CLA	C1C-C2C-C3C	-3.32	103.46	106.96
14	14	301	A86	C10-C9-C8	-3.32	112.86	123.22
16	8	321	LMG	O7-C10-O9	-3.32	115.68	123.70
11	14	310	CLA	C3B-C4B-NB	3.32	113.50	109.21
13	15	319	DD6	C33-C34-C35	3.32	114.84	110.30
11	6	307	CLA	C3B-C4B-NB	3.32	113.50	109.21
11	15	303	CLA	C4-C3-C5	3.32	120.85	115.27
11	16	306	CLA	C4C-C3C-C2C	-3.32	102.06	106.90
13	13	314	DD6	C23-C16-C17	-3.31	103.22	108.98
11	10	305	CLA	C3B-C4B-NB	3.31	113.49	109.21
14	11	313	A86	C36-C31-C32	-3.31	116.41	119.70
12	13	306	KC1	C4C-C3C-C2C	-3.30	102.08	106.90
13	7	301	DD6	C37-C36-C35	-3.30	108.23	114.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	6	313	CLA	CHC-C1C-C2C	-3.30	117.58	126.72
11	15	312	CLA	CBC-CAC-C3C	-3.30	103.32	112.43
11	14	307	CLA	C4C-C3C-C2C	-3.30	102.08	106.90
11	10	311	CLA	C1C-C2C-C3C	-3.30	103.48	106.96
11	14	309	CLA	CHC-C1C-C2C	-3.30	117.59	126.72
14	14	320	A86	C24-C1-C2	3.30	124.00	118.94
11	11	303	CLA	C1C-C2C-C3C	-3.30	103.49	106.96
12	13	310	KC1	C4B-C3B-C2B	-3.29	104.05	106.75
12	8	313	KC1	CAA-C2A-C1A	-3.29	109.61	124.75
11	15	309	CLA	C3B-C4B-NB	3.29	113.47	109.21
13	6	315	DD6	C19-C18-C17	3.29	117.13	110.77
11	10	309	CLA	C4-C3-C5	3.29	120.81	115.27
11	16	308	CLA	C3B-C4B-NB	3.29	113.46	109.21
12	7	312	KC1	C1C-C2C-C3C	-3.29	103.50	106.96
12	13	306	KC1	CAC-C3C-C4C	3.29	129.08	124.81
12	6	309	KC1	CHD-C4C-NC	3.29	129.19	124.20
12	14	311	KC1	CAA-CBA-CGA	-3.29	110.37	127.26
11	11	308	CLA	C1C-C2C-C3C	-3.29	103.50	106.96
11	13	307	CLA	CAC-C3C-C4C	3.28	129.07	124.81
12	8	313	KC1	CHD-C4C-NC	3.28	129.19	124.20
12	11	311	KC1	C1A-NA-C4A	-3.28	105.23	106.71
11	16	302	CLA	C3B-C4B-NB	3.28	113.45	109.21
11	13	309	CLA	CHC-C1C-C2C	-3.28	117.64	126.72
13	8	316	DD6	C37-C36-C35	-3.28	108.28	114.36
13	13	314	DD6	C35-C36-C31	-3.28	113.13	120.57
11	6	307	CLA	CHC-C1C-C2C	-3.28	117.66	126.72
11	6	311	CLA	CAA-C2A-C3A	-3.28	103.81	112.78
12	13	308	KC1	CAA-CBA-CGA	-3.28	110.43	127.26
11	14	309	CLA	C3B-C4B-NB	3.27	113.44	109.21
12	11	311	KC1	CBA-CAA-C2A	-3.27	112.79	125.27
13	6	315	DD6	C35-C36-C31	-3.27	113.14	120.57
12	10	310	KC1	CAB-C3B-C4B	3.27	132.79	124.90
11	7	306	CLA	CHD-C4C-NC	3.27	129.35	124.20
12	12	313	KC1	CHD-C4C-NC	3.27	129.16	124.20
12	7	307	KC1	CAA-CBA-CGA	-3.27	110.46	127.26
14	16	312	A86	C24-C1-C2	3.27	123.96	118.94
12	11	311	KC1	CAC-C3C-C4C	3.27	129.05	124.81
12	6	305	KC1	C4C-C3C-C2C	-3.27	102.14	106.90
12	8	306	KC1	CAB-C3B-C4B	3.27	132.79	124.90
13	10	314	DD6	C19-C18-C17	3.27	117.08	110.77
12	10	306	KC1	CAC-C3C-C4C	3.27	129.05	124.81
14	14	316	A86	C12-C11-C13	3.27	121.51	116.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	12	304	CLA	CMB-C2B-C3B	3.27	130.79	124.68
11	14	302	CLA	C4-C3-C5	3.26	120.76	115.27
14	14	315	A86	C41-C32-C31	-3.26	107.55	110.47
11	7	303	CLA	CHC-C1C-C2C	-3.26	117.70	126.72
11	14	303	CLA	C3B-C4B-NB	3.26	113.42	109.21
12	8	307	KC1	CBA-CAA-C2A	-3.26	112.84	125.27
11	14	313	CLA	CAA-C2A-C3A	-3.26	103.85	112.78
14	15	321	A86	C40-C32-C31	-3.26	107.56	110.47
11	6	304	CLA	CAA-C2A-C3A	-3.26	103.86	112.78
11	6	312	CLA	CHC-C1C-C2C	-3.26	117.71	126.72
11	16	305	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
12	10	306	KC1	O2D-CGD-O1D	-3.25	117.48	123.84
11	11	309	CLA	C3B-C4B-NB	3.25	113.42	109.21
11	14	302	CLA	CAC-C3C-C4C	3.25	129.03	124.81
14	7	314	A86	C41-C32-C31	-3.25	107.56	110.47
12	8	314	KC1	CAA-CBA-CGA	-3.25	110.55	127.26
11	10	308	CLA	O2A-CGA-CBA	3.25	122.11	111.91
11	16	308	CLA	CHC-C1C-C2C	-3.25	117.73	126.72
11	15	306	CLA	CHC-C1C-C2C	-3.25	117.74	126.72
11	15	312	CLA	C3B-C4B-NB	3.25	113.41	109.21
11	7	302	CLA	C1C-C2C-C3C	-3.25	103.54	106.96
11	7	304	CLA	CMB-C2B-C3B	3.25	130.75	124.68
11	7	308	CLA	C3B-C4B-NB	3.24	113.40	109.21
13	12	317	DD6	C37-C36-C35	-3.24	108.35	114.36
12	6	305	KC1	C1C-C2C-C3C	-3.24	103.55	106.96
12	11	306	KC1	CAA-CBA-CGA	-3.24	110.61	127.26
14	15	315	A86	C8-C6-C5	-3.24	113.97	118.94
14	16	312	A86	C10-C9-C8	3.24	133.32	123.22
11	7	311	CLA	CHC-C1C-C2C	-3.24	117.76	126.72
11	7	302	CLA	O2A-CGA-CBA	3.24	122.07	111.91
13	10	314	DD6	C14-C13-C11	3.23	130.55	125.53
11	6	314	CLA	C3B-C4B-NB	3.23	113.39	109.21
14	15	321	A86	C4-C3-C2	-3.23	116.86	123.47
12	16	311	KC1	CAA-CBA-CGA	-3.23	110.67	127.26
11	12	307	CLA	CHD-C4C-NC	3.23	129.29	124.20
14	16	312	A86	C4-C3-C2	-3.22	116.87	123.47
14	6	317	A86	C9-C8-C6	-3.22	117.36	126.42
14	14	301	A86	C25-C26-C27	-3.22	122.71	127.31
11	6	306	CLA	C3B-C4B-NB	3.22	113.38	109.21
11	12	306	CLA	C3B-C4B-NB	3.22	113.38	109.21
12	8	311	KC1	C4C-C3C-C2C	-3.22	102.20	106.90
14	15	321	A86	C34-O4-C38	-3.22	111.89	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	10	309	CLA	C3B-C4B-NB	3.21	113.36	109.21
12	8	310	KC1	CHD-C4C-NC	3.21	129.08	124.20
16	8	321	LMG	O6-C1-O1	-3.21	102.37	109.97
11	13	302	CLA	C3B-C4B-NB	3.21	113.36	109.21
11	12	306	CLA	CHC-C1C-C2C	-3.21	117.84	126.72
11	12	312	CLA	C3B-C4B-NB	3.21	113.36	109.21
11	16	310	CLA	C3B-C4B-NB	3.21	113.36	109.21
11	10	308	CLA	CHD-C4C-NC	3.21	129.26	124.20
11	8	309	CLA	CHC-C1C-C2C	-3.21	117.85	126.72
12	12	305	KC1	C1A-NA-C4A	-3.21	105.27	106.71
12	6	309	KC1	CAB-C3B-C4B	3.20	132.64	124.90
14	8	318	A86	C36-C31-C32	-3.20	116.52	119.70
11	16	301	CLA	CHD-C4C-NC	3.20	129.25	124.20
11	13	304	CLA	C3B-C4B-NB	3.20	113.35	109.21
11	16	306	CLA	C1C-C2C-C3C	-3.20	103.59	106.96
11	14	305	CLA	C3B-C4B-NB	3.20	113.34	109.21
11	14	313	CLA	C3B-C4B-NB	3.20	113.34	109.21
11	6	306	CLA	CAC-C3C-C4C	3.20	128.96	124.81
11	15	304	CLA	C1-O2A-CGA	3.20	124.83	116.44
12	13	310	KC1	CHB-C1B-NB	-3.19	121.52	124.45
11	15	302	CLA	CAA-C2A-C3A	-3.19	104.03	112.78
13	16	313	DD6	C22-C16-C15	3.19	118.67	110.05
13	10	313	DD6	O1-C20-C21	-3.19	111.23	115.06
11	7	306	CLA	CMC-C2C-C1C	3.19	129.90	125.04
12	8	307	KC1	C4B-C3B-C2B	-3.19	104.13	106.75
11	8	305	CLA	C3B-C4B-NB	3.19	113.33	109.21
11	16	309	CLA	CAA-C2A-C3A	-3.19	104.05	112.78
14	8	318	A86	C12-C11-C13	3.19	121.38	116.02
11	15	304	CLA	C3B-C4B-NB	3.18	113.33	109.21
11	6	313	CLA	C3B-C4B-NB	3.18	113.33	109.21
11	15	307	CLA	C3B-C4B-NB	3.18	113.33	109.21
11	14	304	CLA	CAC-C3C-C4C	3.18	128.94	124.81
11	8	302	CLA	CAA-C2A-C3A	-3.18	104.07	112.78
12	8	313	KC1	CBA-CAA-C2A	-3.18	113.15	125.27
13	10	313	DD6	C35-C36-C31	-3.18	113.35	120.57
14	7	314	A86	C4-C3-C2	-3.18	116.97	123.47
11	8	301	CLA	C4C-C3C-C2C	-3.18	102.27	106.90
11	14	304	CLA	C3B-C4B-NB	3.17	113.31	109.21
14	10	316	A86	C-C1-C24	3.17	123.08	118.08
11	11	303	CLA	CHD-C4C-NC	3.17	129.20	124.20
11	11	305	CLA	CAC-C3C-C4C	3.17	128.93	124.81
11	7	305	CLA	C1-C2-C3	-3.17	120.56	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	12	314	A86	C36-C31-C32	-3.17	116.55	119.70
11	15	303	CLA	C3B-C4B-NB	3.17	113.30	109.21
11	7	310	CLA	CHC-C1C-C2C	-3.16	117.97	126.72
14	15	315	A86	C25-C24-C1	3.16	135.30	126.42
11	11	307	CLA	CAA-C2A-C3A	-3.16	104.12	112.78
11	8	303	CLA	CAC-C3C-C4C	3.16	128.91	124.81
11	8	302	CLA	C3B-C4B-NB	3.16	113.30	109.21
12	13	306	KC1	CHD-C4C-NC	3.16	129.00	124.20
11	8	308	CLA	O2A-CGA-CBA	3.16	121.83	111.91
14	15	321	A86	C10-C9-C8	-3.16	113.35	123.22
11	7	308	CLA	CHC-C1C-C2C	-3.16	117.98	126.72
11	7	302	CLA	CAC-C3C-C4C	3.16	128.91	124.81
11	16	310	CLA	CGD-CBD-CAD	-3.16	100.51	110.73
13	7	301	DD6	C14-C13-C11	3.16	130.43	125.53
13	7	317	DD6	C37-C36-C35	-3.15	108.51	114.36
11	15	312	CLA	C3C-C4C-NC	3.15	114.11	110.57
11	13	307	CLA	C3B-C4B-NB	3.15	113.29	109.21
11	15	302	CLA	O2A-CGA-CBA	3.15	121.80	111.91
11	8	303	CLA	CHC-C1C-C2C	-3.15	118.00	126.72
14	7	318	A86	C-C1-C2	-3.15	118.51	122.92
11	10	303	CLA	CAC-C3C-C4C	3.15	128.90	124.81
14	6	317	A86	C35-C34-C33	3.15	115.38	109.88
11	7	305	CLA	C3B-C4B-NB	3.15	113.28	109.21
11	10	311	CLA	CAA-C2A-C3A	-3.15	104.15	112.78
11	16	307	CLA	CAA-C2A-C3A	-3.15	104.15	112.78
13	8	317	DD6	C12-C11-C13	-3.15	113.12	118.08
11	13	307	CLA	CHC-C1C-C2C	-3.15	118.01	126.72
12	8	307	KC1	CHD-C4C-NC	3.15	128.98	124.20
11	15	307	CLA	CHC-C1C-C2C	-3.15	118.02	126.72
11	15	312	CLA	CHC-C1C-C2C	-3.15	118.02	126.72
11	12	310	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
12	7	312	KC1	CAA-CBA-CGA	-3.14	111.12	127.26
14	11	313	A86	C35-C34-C33	3.14	115.36	109.88
11	15	313	CLA	C3B-C4B-NB	3.14	113.27	109.21
11	14	307	CLA	CMB-C2B-C3B	3.14	130.55	124.68
11	16	306	CLA	C3B-C4B-NB	3.14	113.27	109.21
11	7	304	CLA	O2D-CGD-O1D	-3.14	117.71	123.84
11	10	303	CLA	CHC-C1C-C2C	-3.13	118.05	126.72
11	14	310	CLA	C1-C2-C3	-3.13	121.68	126.75
11	8	304	CLA	C1-O2A-CGA	3.13	124.67	116.44
11	16	303	CLA	C3B-C4B-NB	3.13	113.26	109.21
11	15	312	CLA	CMB-C2B-C3B	3.13	130.54	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	10	317	A86	C23-C16-C17	-3.13	103.54	108.98
11	7	302	CLA	C4C-C3C-C2C	-3.13	102.34	106.90
11	12	308	CLA	C4C-C3C-C2C	-3.13	102.34	106.90
11	14	313	CLA	CHD-C4C-NC	3.13	129.13	124.20
11	10	311	CLA	C4C-C3C-C2C	-3.13	102.34	106.90
11	7	305	CLA	CHC-C1C-C2C	-3.12	118.08	126.72
13	6	318	DD6	C33-C34-C35	3.12	114.58	110.30
11	13	301	CLA	CHD-C4C-NC	3.12	129.12	124.20
14	15	322	A86	C3-C4-C5	3.12	129.86	123.47
11	15	311	CLA	CHC-C1C-C2C	-3.12	118.09	126.72
12	14	311	KC1	CMC-C2C-C1C	3.12	129.78	125.04
11	12	310	CLA	C3B-C4B-NB	3.11	113.23	109.21
11	12	321	CLA	CHC-C1C-C2C	-3.11	118.12	126.72
13	15	319	DD6	O1-C20-C21	-3.11	111.33	115.06
11	15	314	CLA	C3B-C4B-NB	3.11	113.23	109.21
11	16	307	CLA	C3B-C4B-NB	3.11	113.23	109.21
11	15	306	CLA	CAA-C2A-C3A	-3.11	104.26	112.78
11	15	314	CLA	CAC-C3C-C4C	3.11	128.84	124.81
11	6	306	CLA	CAA-C2A-C3A	-3.11	104.27	112.78
11	10	304	CLA	CMB-C2B-C3B	3.11	130.49	124.68
13	7	301	DD6	C19-C18-C17	3.11	116.77	110.77
11	16	305	CLA	CHC-C1C-C2C	-3.11	118.13	126.72
11	10	311	CLA	CHC-C1C-C2C	-3.10	118.13	126.72
12	14	306	KC1	CAA-CBA-CGA	-3.10	111.32	127.26
12	8	310	KC1	CBA-CAA-C2A	-3.10	113.45	125.27
12	12	309	KC1	C2A-C1A-NA	3.10	114.38	109.40
12	6	309	KC1	CBA-CAA-C2A	-3.10	113.45	125.27
11	15	304	CLA	CHC-C1C-C2C	-3.10	118.15	126.72
11	8	305	CLA	C1C-C2C-C3C	-3.10	103.70	106.96
12	8	306	KC1	CMB-C2B-C1B	3.10	130.18	124.71
11	8	308	CLA	C3B-C4B-NB	3.10	113.22	109.21
12	8	313	KC1	C2C-C1C-NC	3.10	113.95	110.57
14	14	315	A86	C24-C1-C2	-3.09	114.19	118.94
11	12	312	CLA	CHC-C1C-C2C	-3.09	118.16	126.72
13	15	319	DD6	C25-C24-C1	-3.09	117.73	126.42
11	12	306	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
12	8	312	KC1	CAA-CBA-CGA	-3.09	111.37	127.26
13	6	316	DD6	C25-C24-C1	-3.09	117.73	126.42
11	6	304	CLA	C3B-C4B-NB	3.09	113.21	109.21
11	7	305	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
11	11	308	CLA	C3B-C4B-NB	3.09	113.21	109.21
14	11	301	A86	C25-C24-C1	-3.09	117.73	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	6	318	DD6	C32-C31-C36	-3.09	118.27	122.63
13	7	316	DD6	C19-C18-C17	3.09	116.74	110.77
11	14	305	CLA	CHB-C4A-NA	3.09	128.78	124.51
14	15	315	A86	C7-C6-C8	3.09	122.94	118.08
11	13	304	CLA	CAA-C2A-C3A	-3.09	104.32	112.78
14	16	312	A86	C40-C32-C31	-3.09	107.71	110.47
14	11	315	A86	C12-C11-C13	3.09	121.21	116.02
11	16	302	CLA	C4C-C3C-C2C	-3.09	102.40	106.90
11	6	304	CLA	C4-C3-C5	3.09	120.46	115.27
12	12	313	KC1	O2D-CGD-O1D	-3.09	117.81	123.84
11	16	302	CLA	CAA-C2A-C3A	-3.09	104.33	112.78
11	14	312	CLA	C3B-C4B-NB	3.08	113.20	109.21
11	12	306	CLA	CAA-C2A-C3A	-3.08	104.34	112.78
11	15	303	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
11	8	302	CLA	CHD-C4C-NC	3.08	129.06	124.20
12	12	311	KC1	C4C-C3C-C2C	-3.08	102.41	106.90
11	14	304	CLA	CHC-C1C-C2C	-3.08	118.20	126.72
12	10	306	KC1	CBA-CAA-C2A	-3.08	113.53	125.27
11	8	303	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
14	7	318	A86	C40-C32-C31	-3.08	107.72	110.47
13	12	315	DD6	C25-C24-C1	-3.08	117.77	126.42
11	11	309	CLA	CHC-C1C-C2C	-3.08	118.21	126.72
11	14	305	CLA	CHC-C1C-C2C	-3.08	118.21	126.72
14	11	313	A86	C12-C11-C13	3.08	121.19	116.02
11	15	313	CLA	CHC-C1C-C2C	-3.07	118.22	126.72
12	8	312	KC1	C4C-C3C-C2C	-3.07	102.42	106.90
12	11	311	KC1	CMB-C2B-C1B	3.07	130.12	124.71
12	14	311	KC1	CHD-C4C-NC	3.07	128.86	124.20
12	16	304	KC1	CAA-CBA-CGA	-3.07	111.48	127.26
11	13	303	CLA	C3B-C4B-NB	3.07	113.18	109.21
12	16	304	KC1	C4C-C3C-C2C	-3.07	102.42	106.90
11	12	302	CLA	CHD-C4C-NC	3.07	129.04	124.20
13	6	318	DD6	C12-C11-C13	-3.07	113.24	118.08
14	14	319	A86	C3-C4-C5	-3.07	117.19	123.47
13	11	312	DD6	O1-C20-C21	-3.07	111.38	115.06
11	16	307	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
14	13	315	A86	C25-C24-C1	-3.06	117.81	126.42
11	14	307	CLA	C3B-C4B-NB	3.06	113.17	109.21
12	12	309	KC1	CHD-C4C-NC	3.06	128.85	124.20
11	8	304	CLA	CHC-C1C-C2C	-3.06	118.25	126.72
11	7	304	CLA	CHC-C1C-C2C	-3.06	118.25	126.72
11	15	309	CLA	CHC-C1C-C2C	-3.06	118.25	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	12	313	KC1	CMC-C2C-C1C	3.06	129.70	125.04
11	15	310	CLA	CHC-C1C-C2C	-3.06	118.26	126.72
11	6	303	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
11	16	309	CLA	CHC-C1C-C2C	-3.06	118.26	126.72
11	6	314	CLA	CHC-C1C-C2C	-3.06	118.27	126.72
12	6	305	KC1	CHD-C4C-NC	3.06	128.84	124.20
12	12	313	KC1	CHB-C1B-NB	-3.06	121.64	124.45
12	16	311	KC1	CHB-C1B-NB	-3.06	121.64	124.45
12	8	310	KC1	CMB-C2B-C1B	3.06	130.10	124.71
12	8	313	KC1	C4B-C3B-C2B	-3.06	104.24	106.75
11	6	311	CLA	CHD-C4C-NC	3.06	129.02	124.20
12	12	305	KC1	CHB-C1B-NB	-3.05	121.65	124.45
11	16	303	CLA	CHD-C4C-NC	3.05	129.01	124.20
11	10	307	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
14	15	315	A86	C-C1-C2	-3.05	118.65	122.92
14	7	315	A86	C7-C6-C8	3.05	122.89	118.08
12	7	307	KC1	C4C-C3C-C2C	-3.05	102.45	106.90
11	14	303	CLA	CHC-C1C-C2C	-3.05	118.28	126.72
11	6	312	CLA	CAC-C3C-C4C	3.05	128.77	124.81
12	16	311	KC1	C2A-C1A-NA	3.05	114.29	109.40
12	10	306	KC1	CMB-C2B-C1B	3.05	130.09	124.71
12	11	304	KC1	CAC-C3C-C4C	3.05	128.76	124.81
12	10	312	KC1	CHD-C4C-NC	3.05	128.83	124.20
12	8	311	KC1	CBA-CAA-C2A	-3.05	113.66	125.27
11	10	304	CLA	C4C-C3C-C2C	-3.05	102.46	106.90
11	13	304	CLA	CHC-C1C-C2C	-3.04	118.30	126.72
14	12	316	A86	C25-C26-C27	-3.04	122.97	127.31
12	10	310	KC1	C4C-C3C-C2C	-3.04	102.46	106.90
11	14	303	CLA	CAC-C3C-C4C	3.04	128.76	124.81
13	10	313	DD6	C7-C6-C8	-3.04	113.29	118.08
12	7	312	KC1	CHD-C4C-NC	3.04	128.81	124.20
11	10	308	CLA	CMC-C2C-C1C	3.04	129.67	125.04
11	15	302	CLA	CAC-C3C-C4C	3.04	128.75	124.81
11	16	305	CLA	C1-C2-C3	-3.04	121.84	126.75
11	13	301	CLA	CMC-C2C-C1C	3.03	129.66	125.04
11	11	303	CLA	C1-C2-C3	-3.03	120.80	126.04
11	6	314	CLA	CAA-C2A-C3A	-3.03	104.48	112.78
11	8	304	CLA	CHD-C4C-NC	3.03	128.98	124.20
11	13	309	CLA	CAC-C3C-C4C	3.03	128.74	124.81
12	6	309	KC1	CHC-C4B-NB	-3.03	121.67	124.45
12	8	311	KC1	CAC-C3C-C4C	3.03	128.74	124.81
11	16	307	CLA	CHC-C1C-C2C	-3.03	118.35	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	16	303	CLA	C1-C2-C3	-3.03	120.81	126.04
14	16	314	A86	C35-C34-C33	3.02	115.15	109.88
11	12	304	CLA	CHC-C1C-C2C	-3.02	118.36	126.72
14	8	315	A86	C-C1-C24	3.02	122.84	118.08
11	7	304	CLA	CAA-C2A-C3A	-3.02	104.50	112.78
11	12	306	CLA	CHB-C4A-NA	3.02	128.69	124.51
11	16	302	CLA	C1-C2-C3	-3.02	120.82	126.04
11	6	303	CLA	C3B-C4B-NB	3.02	113.12	109.21
14	14	316	A86	C10-C9-C8	-3.02	113.79	123.22
12	6	308	KC1	CAA-CBA-CGA	-3.02	111.74	127.26
11	14	312	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
11	16	301	CLA	C3B-C4B-NB	3.02	113.11	109.21
11	16	301	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
11	7	308	CLA	CAC-C3C-C4C	3.02	128.72	124.81
13	7	316	DD6	C35-C36-C31	-3.01	113.73	120.57
11	7	304	CLA	CAC-C3C-C4C	3.01	128.72	124.81
14	15	315	A86	C36-C31-C32	-3.01	116.71	119.70
11	13	302	CLA	CHC-C1C-C2C	-3.01	118.39	126.72
11	12	302	CLA	C4-C3-C5	3.01	120.34	115.27
14	11	301	A86	C40-C32-C31	-3.01	107.78	110.47
14	11	313	A86	C26-C25-C24	-3.01	113.82	123.22
12	16	311	KC1	C4C-C3C-C2C	-3.01	102.51	106.90
11	12	308	CLA	C3B-C4B-NB	3.01	113.10	109.21
11	16	303	CLA	CBA-CAA-C2A	3.01	122.74	113.86
14	14	319	A86	C12-C11-C10	-3.01	116.15	123.42
14	14	318	A86	C25-C24-C1	-3.01	117.97	126.42
11	12	306	CLA	C4A-NA-C1A	-3.01	105.36	106.71
12	7	312	KC1	CMB-C2B-C1B	3.00	130.01	124.71
11	16	301	CLA	CMC-C2C-C1C	3.00	129.61	125.04
11	10	303	CLA	C4C-C3C-C2C	-3.00	102.52	106.90
12	8	314	KC1	C4C-C3C-C2C	-3.00	102.52	106.90
11	12	307	CLA	C4C-C3C-C2C	-3.00	102.52	106.90
14	7	318	A86	C7-C6-C5	-3.00	118.72	122.92
11	14	312	CLA	CHC-C1C-C2C	-3.00	118.42	126.72
11	12	303	CLA	C4C-C3C-C2C	-3.00	102.52	106.90
12	13	310	KC1	CMB-C2B-C1B	3.00	130.00	124.71
11	12	303	CLA	CHC-C1C-C2C	-3.00	118.42	126.72
13	8	316	DD6	C25-C24-C1	-3.00	117.99	126.42
12	13	305	KC1	C4C-C3C-C2C	-3.00	102.53	106.90
11	6	306	CLA	CHC-C1C-C2C	-3.00	118.43	126.72
16	7	319	LMG	C1-C2-C3	-3.00	103.75	110.00
13	7	317	DD6	C19-C18-C17	3.00	116.56	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	10	302	A86	C23-C16-C17	-3.00	103.78	108.98
11	12	302	CLA	C4C-C3C-C2C	-2.99	102.53	106.90
11	16	310	CLA	C4C-C3C-C2C	-2.99	102.53	106.90
12	7	312	KC1	C4C-C3C-C2C	-2.99	102.53	106.90
14	6	317	A86	C25-C24-C1	-2.99	118.01	126.42
13	8	317	DD6	C10-C9-C8	-2.99	113.88	123.22
11	6	301	CLA	C3B-C4B-NB	2.99	113.08	109.21
14	12	314	A86	C10-C9-C8	-2.99	113.88	123.22
11	16	302	CLA	CAC-C3C-C4C	2.99	128.69	124.81
11	10	303	CLA	CHD-C4C-NC	2.99	128.91	124.20
12	6	309	KC1	C4C-C3C-C2C	-2.99	102.54	106.90
14	15	320	A86	C36-C31-C32	-2.99	116.73	119.70
11	16	303	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
11	11	307	CLA	CHC-C1C-C2C	-2.99	118.46	126.72
11	11	307	CLA	CHD-C4C-NC	2.99	128.91	124.20
14	10	317	A86	C36-C31-C32	-2.99	116.73	119.70
11	6	313	CLA	C1-C2-C3	-2.99	120.88	126.04
12	8	306	KC1	CAA-CBA-CGA	-2.98	111.92	127.26
11	15	302	CLA	CHD-C4C-NC	2.98	128.91	124.20
11	15	310	CLA	CAC-C3C-C4C	2.98	128.68	124.81
11	12	306	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
12	13	310	KC1	CHD-C4C-NC	2.98	128.72	124.20
12	7	312	KC1	C4B-C3B-C2B	-2.98	104.31	106.75
13	16	313	DD6	C35-C36-C31	-2.98	113.81	120.57
11	15	305	CLA	CAA-C2A-C3A	-2.98	104.62	112.78
13	6	318	DD6	C40-C32-C31	-2.98	105.74	110.47
11	16	307	CLA	CAC-C3C-C4C	2.98	128.67	124.81
11	15	306	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
12	12	305	KC1	C4C-C3C-C2C	-2.98	102.56	106.90
11	15	312	CLA	CHD-C4C-NC	2.98	128.89	124.20
12	8	311	KC1	C1A-NA-C4A	-2.98	105.37	106.71
14	7	315	A86	C3-C4-C5	-2.98	117.38	123.47
11	13	309	CLA	CAA-C2A-C3A	-2.98	104.63	112.78
14	14	320	A86	C4-C5-C6	2.98	131.56	127.31
11	6	302	CLA	CHC-C1C-C2C	-2.97	118.49	126.72
11	6	302	CLA	CAC-C3C-C4C	2.97	128.67	124.81
14	7	315	A86	C25-C26-C27	-2.97	123.07	127.31
12	13	306	KC1	CBA-CAA-C2A	-2.97	113.94	125.27
14	14	301	A86	C35-C34-C33	2.97	115.06	109.88
11	12	321	CLA	CAC-C3C-C4C	2.97	128.66	124.81
14	6	317	A86	C3-C2-C1	-2.97	123.07	127.31
11	7	306	CLA	CAC-C3C-C4C	2.97	128.66	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	6	306	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
11	14	304	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
11	14	310	CLA	CHC-C1C-C2C	-2.97	118.51	126.72
11	16	310	CLA	CHC-C1C-C2C	-2.97	118.51	126.72
11	7	306	CLA	C1C-C2C-C3C	-2.97	103.84	106.96
11	10	307	CLA	C4-C3-C5	2.97	120.26	115.27
11	15	307	CLA	C1-C2-C3	-2.97	121.95	126.75
12	8	306	KC1	CBC-CAC-C3C	-2.97	104.25	112.43
11	15	305	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
12	14	311	KC1	C4C-C3C-C2C	-2.96	102.58	106.90
11	10	308	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
11	14	305	CLA	C1-C2-C3	-2.96	121.96	126.75
11	10	304	CLA	CHC-C1C-C2C	-2.96	118.53	126.72
11	15	305	CLA	CHC-C1C-C2C	-2.96	118.53	126.72
11	13	307	CLA	CMB-C2B-C3B	2.96	130.22	124.68
11	13	307	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
11	8	304	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
11	12	302	CLA	CAA-C2A-C3A	-2.96	104.68	112.78
14	13	315	A86	C12-C11-C10	-2.96	116.27	123.42
11	14	302	CLA	CHD-C4C-NC	2.96	128.86	124.20
12	11	304	KC1	C4C-C3C-C2C	-2.95	102.59	106.90
11	10	303	CLA	CBC-CAC-C3C	-2.95	104.29	112.43
11	16	309	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
11	14	309	CLA	CAC-C3C-C4C	2.95	128.64	124.81
11	8	305	CLA	CMC-C2C-C1C	2.95	129.53	125.04
11	7	306	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
11	15	309	CLA	CAC-C3C-C4C	2.95	128.64	124.81
11	15	309	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
11	13	303	CLA	CHC-C1C-C2C	-2.95	118.57	126.72
12	13	308	KC1	CHD-C4C-NC	2.95	128.67	124.20
11	10	305	CLA	CHC-C1C-C2C	-2.95	118.57	126.72
11	8	309	CLA	CAC-C3C-C4C	2.94	128.63	124.81
11	14	305	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
11	10	309	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
14	10	315	A86	C4-C3-C2	-2.94	117.45	123.47
12	12	313	KC1	CMB-C2B-C1B	2.94	129.89	124.71
11	10	309	CLA	CHC-C1C-C2C	-2.94	118.60	126.72
14	11	301	A86	C12-C11-C10	-2.94	116.32	123.42
12	14	311	KC1	CAC-C3C-C4C	2.94	128.62	124.81
11	6	311	CLA	CAC-C3C-C4C	2.93	128.62	124.81
11	8	308	CLA	C1-C2-C3	-2.93	120.97	126.04
11	10	308	CLA	CAA-C2A-C3A	-2.93	104.75	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	10	308	CLA	CAC-C3C-C4C	2.93	128.62	124.81
11	6	302	CLA	O2A-CGA-CBA	2.93	121.11	111.91
12	13	305	KC1	CAC-C3C-C4C	2.93	128.61	124.81
11	7	309	CLA	CHC-C1C-C2C	-2.93	118.61	126.72
14	8	318	A86	C3-C4-C5	2.93	129.48	123.47
11	10	308	CLA	C1C-C2C-C3C	-2.93	103.88	106.96
11	14	302	CLA	C3B-C4B-NB	2.93	113.00	109.21
12	11	304	KC1	CAA-C2A-C1A	-2.93	111.28	124.75
11	10	307	CLA	CMB-C2B-C3B	2.93	130.16	124.68
11	8	303	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
12	13	310	KC1	CBA-CAA-C2A	-2.93	114.11	125.27
11	11	303	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
11	12	306	CLA	C1-C2-C3	-2.93	120.98	126.04
14	16	312	A86	C7-C6-C5	-2.93	118.82	122.92
11	13	303	CLA	CAC-C3C-C4C	2.93	128.61	124.81
13	8	317	DD6	C25-C24-C1	-2.93	118.20	126.42
11	15	308	CLA	C1C-C2C-C3C	-2.93	103.88	106.96
12	11	310	KC1	C4C-C3C-C2C	-2.93	102.63	106.90
13	6	315	DD6	C9-C8-C6	-2.93	118.20	126.42
12	16	311	KC1	C1A-NA-C4A	-2.92	105.39	106.71
11	6	304	CLA	CHC-C1C-C2C	-2.92	118.63	126.72
12	8	314	KC1	CAC-C3C-C4C	2.92	128.60	124.81
13	13	314	DD6	C37-C36-C35	-2.92	108.94	114.36
16	8	320	LMG	O6-C1-O1	-2.92	103.06	109.97
12	13	306	KC1	CAA-CBA-CGA	-2.92	112.25	127.26
11	15	308	CLA	CHC-C1C-C2C	-2.92	118.64	126.72
11	6	304	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
11	12	304	CLA	CAC-C3C-C4C	2.92	128.60	124.81
11	14	312	CLA	CAA-C2A-C3A	-2.92	104.78	112.78
11	14	312	CLA	CAC-C3C-C4C	2.92	128.60	124.81
11	13	301	CLA	CHC-C1C-C2C	-2.92	118.65	126.72
12	13	310	KC1	C4C-C3C-C2C	-2.92	102.65	106.90
13	6	316	DD6	C34-C35-C36	-2.92	106.05	111.85
12	11	306	KC1	C4C-C3C-C2C	-2.91	102.65	106.90
11	16	302	CLA	CHC-C1C-C2C	-2.91	118.66	126.72
11	11	308	CLA	CHC-C1C-C2C	-2.91	118.66	126.72
11	15	310	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
11	6	301	CLA	CHD-C4C-NC	2.91	128.79	124.20
11	8	308	CLA	CHD-C4C-NC	2.91	128.79	124.20
11	8	302	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
11	7	311	CLA	CAC-C3C-C4C	2.91	128.59	124.81
11	7	306	CLA	C3B-C4B-NB	2.91	112.97	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	14	313	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
11	7	304	CLA	O1D-CGD-CBD	-2.91	118.53	124.48
11	15	314	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
13	11	312	DD6	C19-C18-C17	2.91	116.39	110.77
11	13	301	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
11	6	313	CLA	CAC-C3C-C4C	2.91	128.58	124.81
11	7	305	CLA	CAC-C3C-C4C	2.91	128.58	124.81
12	11	311	KC1	C4C-C3C-C2C	-2.91	102.66	106.90
12	14	308	KC1	CMB-C2B-C1B	2.91	129.83	124.71
11	13	307	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
14	11	314	A86	C40-C32-C31	-2.90	107.87	110.47
12	6	308	KC1	C4C-C3C-C2C	-2.90	102.67	106.90
12	8	311	KC1	CAA-CBA-CGA	-2.90	112.34	127.26
11	12	308	CLA	CHC-C1C-C2C	-2.90	118.69	126.72
11	7	304	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
11	15	313	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
11	6	311	CLA	C4-C3-C5	2.90	120.15	115.27
11	8	305	CLA	CAA-C2A-C3A	-2.90	104.83	112.78
11	11	303	CLA	C4-C3-C5	2.90	120.15	115.27
11	16	305	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
11	12	310	CLA	O2A-CGA-CBA	2.90	121.00	111.91
11	6	311	CLA	CHC-C1C-C2C	-2.90	118.71	126.72
11	15	313	CLA	CHD-C4C-NC	2.89	128.76	124.20
12	11	310	KC1	CHD-C4C-NC	2.89	128.59	124.20
12	8	312	KC1	CAC-C3C-C4C	2.89	128.56	124.81
12	11	310	KC1	CAA-CBA-CGA	-2.89	112.39	127.26
11	12	321	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
11	14	313	CLA	CHC-C1C-C2C	-2.89	118.72	126.72
11	15	309	CLA	CMB-C2B-C3B	2.89	130.09	124.68
12	6	310	KC1	CHD-C4C-NC	2.89	128.59	124.20
13	10	314	DD6	C23-C16-C22	-2.89	103.10	107.37
11	7	303	CLA	C4-C3-C5	2.89	120.14	115.27
11	13	302	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
11	15	307	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
11	16	308	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
11	6	301	CLA	O2A-CGA-CBA	2.89	120.98	111.91
14	16	312	A86	C35-C34-C33	2.89	114.92	109.88
11	16	307	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
12	13	312	KC1	CHD-C4C-NC	2.89	128.59	124.20
11	8	305	CLA	CAC-C3C-C4C	2.89	128.56	124.81
11	11	308	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
11	6	307	CLA	CMB-C2B-C3B	2.89	130.08	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	7	311	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
11	6	303	CLA	C1-O2A-CGA	2.89	124.02	116.44
11	6	301	CLA	CHC-C1C-C2C	-2.89	118.73	126.72
11	16	302	CLA	CHD-C4C-NC	2.89	128.75	124.20
11	6	306	CLA	CHD-C4C-NC	2.89	128.75	124.20
11	7	309	CLA	C4C-C3C-C2C	-2.88	102.69	106.90
11	7	302	CLA	CMB-C2B-C3B	2.88	130.07	124.68
13	11	312	DD6	C9-C8-C6	-2.88	118.32	126.42
11	15	314	CLA	CMC-C2C-C1C	2.88	129.43	125.04
11	16	305	CLA	CHB-C4A-NA	2.88	128.49	124.51
11	13	309	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
14	12	314	A86	C41-C32-C31	-2.88	107.90	110.47
11	11	307	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
12	7	307	KC1	CHD-C4C-NC	2.88	128.57	124.20
11	16	309	CLA	C4C-C3C-C2C	-2.88	102.71	106.90
11	12	312	CLA	CAC-C3C-C4C	2.88	128.54	124.81
13	15	319	DD6	C21-C20-C19	-2.87	111.05	114.28
11	11	305	CLA	C3B-C4B-NB	2.87	112.93	109.21
11	15	312	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
12	13	310	KC1	CMC-C2C-C1C	2.87	129.41	125.04
11	7	304	CLA	CHB-C4A-NA	2.87	128.48	124.51
11	15	303	CLA	CHC-C1C-C2C	-2.87	118.78	126.72
11	14	303	CLA	CHD-C4C-NC	2.87	128.73	124.20
12	13	306	KC1	C1C-C2C-C3C	-2.87	103.94	106.96
11	8	301	CLA	CMC-C2C-C1C	2.87	129.41	125.04
12	6	310	KC1	C4C-C3C-C2C	-2.87	102.72	106.90
11	6	303	CLA	CHC-C1C-C2C	-2.87	118.79	126.72
11	8	305	CLA	CHD-C4C-NC	2.87	128.72	124.20
11	10	308	CLA	C3B-C4B-NB	2.87	112.92	109.21
11	12	312	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
11	15	303	CLA	CAA-C2A-C3A	-2.87	104.93	112.78
11	11	303	CLA	CMC-C2C-C1C	2.86	129.40	125.04
13	7	301	DD6	C25-C24-C1	-2.86	118.37	126.42
12	12	313	KC1	CBD-CHA-C1A	2.86	134.22	128.88
11	14	310	CLA	CHB-C4A-NA	2.86	128.47	124.51
13	12	317	DD6	C15-C14-C13	2.86	132.05	125.99
14	7	315	A86	C41-C32-C31	-2.86	107.91	110.47
14	11	315	A86	C40-C32-C31	-2.86	107.91	110.47
11	12	312	CLA	CHD-C4C-NC	2.86	128.71	124.20
11	16	306	CLA	C1-C2-C3	-2.86	121.09	126.04
14	10	316	A86	C26-C25-C24	-2.86	114.29	123.22
12	10	312	KC1	CAA-C2A-C1A	-2.86	111.61	124.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	16	306	CLA	CHC-C1C-C2C	-2.86	118.82	126.72
12	13	305	KC1	O2D-CGD-O1D	-2.86	118.25	123.84
11	10	309	CLA	CAA-C2A-C3A	-2.86	104.95	112.78
12	8	311	KC1	CMB-C2B-C1B	2.86	129.75	124.71
14	14	314	A86	C12-C11-C10	-2.86	116.51	123.42
12	8	306	KC1	CHC-C4B-NB	-2.86	121.83	124.45
11	12	304	CLA	C4C-C3C-C2C	-2.86	102.74	106.90
13	15	318	DD6	C19-C18-C17	2.85	116.29	110.77
11	11	305	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
11	12	302	CLA	CHB-C4A-NA	2.85	128.46	124.51
12	6	310	KC1	CAC-C3C-C4C	2.85	128.51	124.81
12	16	304	KC1	CAC-C3C-C4C	2.85	128.51	124.81
11	14	313	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
13	15	318	DD6	C14-C13-C11	-2.85	121.11	125.53
11	7	303	CLA	CBC-CAC-C3C	-2.85	104.57	112.43
14	14	315	A86	C26-C25-C24	-2.85	114.32	123.22
11	10	304	CLA	CAA-C2A-C3A	-2.85	104.97	112.78
11	14	302	CLA	CHC-C1C-C2C	-2.85	118.84	126.72
11	12	302	CLA	CMC-C2C-C1C	2.85	129.38	125.04
11	14	310	CLA	CAC-C3C-C4C	2.85	128.51	124.81
11	11	305	CLA	C1-C2-C3	-2.85	121.12	126.04
11	6	301	CLA	C1-C2-C3	-2.85	121.12	126.04
12	12	313	KC1	C4C-C3C-C2C	-2.85	102.75	106.90
14	14	319	A86	C25-C24-C1	-2.85	118.42	126.42
12	8	314	KC1	CMB-C2B-C1B	2.85	129.73	124.71
11	15	302	CLA	CMC-C2C-C1C	2.84	129.37	125.04
11	15	302	CLA	C4C-C3C-C2C	-2.84	102.75	106.90
14	7	318	A86	C24-C1-C2	2.84	123.30	118.94
11	6	314	CLA	CAC-C3C-C4C	2.84	128.50	124.81
11	15	313	CLA	C4-C3-C5	2.84	120.05	115.27
11	15	311	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
11	13	304	CLA	CAC-C3C-C4C	2.84	128.50	124.81
11	13	304	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
12	12	305	KC1	CHD-C4C-NC	2.84	128.51	124.20
17	15	301	LMT	C1B-O5B-C5B	2.84	119.26	113.69
11	10	311	CLA	CAC-C3C-C4C	2.84	128.49	124.81
12	13	311	KC1	CAC-C3C-C4C	2.84	128.49	124.81
11	15	314	CLA	CHC-C1C-C2C	-2.84	118.87	126.72
12	11	304	KC1	CHD-C4C-NC	2.84	128.51	124.20
12	11	306	KC1	CHD-C4C-NC	2.84	128.51	124.20
12	8	312	KC1	CMB-C2B-C1B	2.84	129.71	124.71
11	10	311	CLA	CHD-C4C-NC	2.84	128.67	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	11	305	CLA	CHC-C1C-C2C	-2.83	118.88	126.72
11	7	302	CLA	CAA-C2A-C3A	-2.83	105.02	112.78
11	16	303	CLA	O2A-CGA-CBA	2.83	120.80	111.91
11	12	306	CLA	CAC-C3C-C4C	2.83	128.48	124.81
11	6	314	CLA	CHD-C4C-NC	2.83	128.66	124.20
11	6	312	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
13	15	318	DD6	C33-C32-C31	2.83	115.36	109.62
14	10	316	A86	C24-C1-C2	-2.83	114.60	118.94
11	6	303	CLA	CAC-C3C-C4C	2.83	128.48	124.81
11	8	302	CLA	C4-C3-C5	2.83	120.03	115.27
11	14	310	CLA	C4C-C3C-C2C	-2.83	102.78	106.90
12	13	308	KC1	C4C-C3C-C2C	-2.83	102.78	106.90
11	11	309	CLA	C4C-C3C-C2C	-2.83	102.78	106.90
11	14	309	CLA	C4C-C3C-C2C	-2.83	102.78	106.90
12	12	309	KC1	CAA-CBA-CGA	-2.83	112.74	127.26
11	12	303	CLA	CAA-C2A-C3A	-2.82	105.04	112.78
11	10	307	CLA	CHB-C4A-NA	2.82	128.42	124.51
14	15	316	A86	C25-C24-C1	-2.82	118.48	126.42
12	10	306	KC1	C4C-C3C-C2C	-2.82	102.78	106.90
13	15	318	DD6	C25-C24-C1	-2.82	118.48	126.42
11	16	301	CLA	CAC-C3C-C4C	2.82	128.47	124.81
12	13	311	KC1	CHD-C4C-NC	2.82	128.48	124.20
11	8	305	CLA	OBD-CAD-C3D	-2.82	121.73	128.52
12	11	310	KC1	CAC-C3C-C4C	2.82	128.47	124.81
11	14	302	CLA	O2A-CGA-CBA	2.82	120.75	111.91
11	15	311	CLA	CHD-C4C-NC	2.82	128.64	124.20
11	8	301	CLA	CAC-C3C-C4C	2.82	128.47	124.81
13	11	312	DD6	C15-C14-C13	-2.82	120.04	125.99
11	13	301	CLA	C3B-C4B-NB	2.82	112.85	109.21
14	16	312	A86	C-C1-C2	-2.82	118.98	122.92
17	15	301	LMT	O1B-C4'-C3'	2.82	114.77	107.28
12	13	305	KC1	CMB-C2B-C1B	2.82	129.68	124.71
12	12	311	KC1	CHB-C4A-NA	2.81	128.64	124.20
12	12	305	KC1	CAA-CBA-CGA	-2.81	112.79	127.26
14	15	315	A86	C4-C5-C6	2.81	131.33	127.31
11	6	313	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
12	10	312	KC1	C4C-C3C-C2C	-2.81	102.80	106.90
11	12	302	CLA	CBC-CAC-C3C	-2.81	104.67	112.43
11	12	308	CLA	CAA-C2A-C3A	-2.81	105.07	112.78
14	11	314	A86	C9-C10-C11	-2.81	118.34	126.61
12	12	309	KC1	C4C-C3C-C2C	-2.81	102.80	106.90
14	14	319	A86	C10-C9-C8	-2.81	114.44	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	12	308	CLA	CAC-C3C-C4C	2.81	128.46	124.81
14	11	301	A86	C3-C4-C5	-2.81	117.72	123.47
11	16	301	CLA	CHC-C1C-C2C	-2.81	118.94	126.72
11	6	303	CLA	CHD-C4C-NC	2.81	128.63	124.20
11	7	309	CLA	CHD-C4C-NC	2.81	128.63	124.20
11	13	303	CLA	CHD-C4C-NC	2.81	128.63	124.20
12	6	309	KC1	CMC-C2C-C1C	2.81	129.31	125.04
12	14	308	KC1	CAA-CBA-CGA	-2.81	112.84	127.26
12	7	312	KC1	CBA-CAA-C2A	-2.81	114.58	125.27
11	10	305	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
11	12	302	CLA	CMB-C2B-C3B	2.80	129.93	124.68
11	8	304	CLA	CAA-CBA-CGA	-2.80	105.06	113.25
12	10	306	KC1	CHD-C4C-NC	2.80	128.46	124.20
12	10	312	KC1	CAC-C3C-C4C	2.80	128.45	124.81
11	8	304	CLA	O2A-CGA-CBA	2.80	120.71	111.91
12	12	309	KC1	CAC-C3C-C4C	2.80	128.45	124.81
14	16	314	A86	C3-C4-C5	-2.80	117.74	123.47
11	12	321	CLA	CHD-C4C-NC	2.80	128.62	124.20
11	7	308	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
12	8	307	KC1	C4C-C3C-C2C	-2.80	102.82	106.90
11	10	307	CLA	CHC-C1C-C2C	-2.80	118.98	126.72
11	8	309	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
11	8	308	CLA	CHC-C1C-C2C	-2.80	118.98	126.72
12	14	306	KC1	O2D-CGD-O1D	-2.80	118.37	123.84
11	6	312	CLA	O2D-CGD-O1D	-2.79	118.37	123.84
11	6	302	CLA	CHD-C4C-NC	2.79	128.61	124.20
11	11	305	CLA	CHD-C4C-NC	2.79	128.61	124.20
13	6	316	DD6	C37-C36-C35	-2.79	109.18	114.36
13	15	319	DD6	C14-C13-C11	-2.79	121.20	125.53
14	7	314	A86	C4-C5-C6	-2.79	123.33	127.31
11	10	309	CLA	CHD-C4C-NC	2.79	128.60	124.20
11	10	304	CLA	CAC-C3C-C4C	2.79	128.43	124.81
11	7	310	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
14	10	301	A86	C33-C32-C31	2.79	111.92	109.21
11	7	302	CLA	CHD-C4C-NC	2.79	128.60	124.20
11	15	304	CLA	C4-C3-C5	2.79	119.96	115.27
11	12	310	CLA	CHC-C1C-C2C	-2.79	119.01	126.72
11	11	307	CLA	CHB-C4A-NA	2.79	128.37	124.51
11	6	313	CLA	CHB-C4A-NA	2.78	128.36	124.51
14	13	315	A86	C7-C6-C5	-2.78	119.02	122.92
14	10	316	A86	O-C13-C11	-2.78	115.00	121.15
12	8	307	KC1	CHB-C1B-NB	-2.78	121.89	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	6	310	KC1	CMB-C2B-C1B	2.78	129.62	124.71
11	8	308	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
13	6	316	DD6	C33-C32-C31	2.78	115.26	109.62
14	15	320	A86	C25-C24-C1	-2.78	118.61	126.42
11	8	308	CLA	CMC-C2C-C1C	2.78	129.27	125.04
11	6	304	CLA	CAC-C3C-C4C	2.78	128.41	124.81
11	11	303	CLA	C3B-C4B-NB	2.78	112.80	109.21
11	12	312	CLA	O2A-CGA-CBA	2.78	120.62	111.91
12	10	312	KC1	CMC-C2C-C1C	2.77	129.26	125.04
11	16	310	CLA	CHD-C4C-NC	2.77	128.57	124.20
11	10	308	CLA	CMB-C2B-C3B	2.77	129.87	124.68
11	16	305	CLA	C4A-NA-C1A	-2.77	105.46	106.71
13	12	317	DD6	C23-C16-C17	-2.77	104.17	108.98
11	15	309	CLA	CHD-C4C-NC	2.77	128.57	124.20
11	15	313	CLA	CAC-C3C-C4C	2.77	128.40	124.81
14	14	318	A86	C12-C11-C13	2.77	120.67	116.02
11	7	303	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
11	6	313	CLA	CAA-C2A-C3A	-2.77	105.20	112.78
11	6	301	CLA	CBA-CAA-C2A	2.77	122.03	113.86
11	14	302	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
13	6	318	DD6	C37-C36-C35	-2.76	109.23	114.36
11	10	307	CLA	CAC-C3C-C4C	2.76	128.40	124.81
11	6	314	CLA	C4C-C3C-C2C	-2.76	102.87	106.90
13	6	316	DD6	C19-C18-C17	2.76	116.11	110.77
11	7	311	CLA	CHD-C4C-NC	2.76	128.56	124.20
11	13	307	CLA	O2A-CGA-CBA	2.76	120.57	111.91
11	16	305	CLA	CAC-C3C-C4C	2.76	128.39	124.81
11	10	309	CLA	CED-O2D-CGD	2.76	122.18	115.94
11	15	308	CLA	O2A-CGA-O1A	-2.76	116.43	123.30
14	13	313	A86	C25-C26-C27	2.76	131.24	127.31
12	8	306	KC1	C4C-C3C-C2C	-2.75	102.88	106.90
11	6	304	CLA	CHD-C4C-NC	2.75	128.54	124.20
12	7	312	KC1	CAC-C3C-C4C	2.75	128.38	124.81
11	8	304	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
11	10	304	CLA	CHD-C4C-NC	2.75	128.54	124.20
11	15	313	CLA	O2A-CGA-CBA	2.75	120.54	111.91
12	11	306	KC1	CAC-C3C-C4C	2.75	128.38	124.81
11	13	302	CLA	CHD-C4C-NC	2.75	128.53	124.20
12	12	305	KC1	CMB-C2B-C1B	2.75	129.55	124.71
11	12	321	CLA	CAA-C2A-C3A	-2.75	105.26	112.78
14	13	315	A86	C36-C31-C32	-2.75	116.97	119.70
11	14	302	CLA	C4C-C3C-C2C	-2.74	102.90	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	14	314	A86	C3-C4-C5	2.74	129.09	123.47
11	13	302	CLA	CAC-C3C-C4C	2.74	128.37	124.81
11	12	308	CLA	C1-C2-C3	-2.74	121.30	126.04
11	12	303	CLA	CHD-C4C-NC	2.74	128.52	124.20
11	6	303	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
11	14	302	CLA	CMC-C2C-C1C	2.74	129.21	125.04
11	13	307	CLA	CAA-C2A-C3A	-2.74	105.29	112.78
11	7	302	CLA	C3B-C4B-NB	2.74	112.75	109.21
11	15	302	CLA	C3B-C4B-NB	2.74	112.75	109.21
11	6	306	CLA	O2A-CGA-O1A	-2.73	116.69	123.59
11	7	303	CLA	CHD-C4C-NC	2.73	128.51	124.20
14	6	317	A86	C28-C27-C26	-2.73	119.10	122.92
13	7	316	DD6	O1-C20-C21	-2.73	111.78	115.06
13	8	316	DD6	C20-C19-C18	-2.73	107.34	112.75
11	6	304	CLA	O2A-CGA-CBA	2.73	120.48	111.91
11	15	307	CLA	CBC-CAC-C3C	-2.73	104.90	112.43
11	16	309	CLA	CAC-C3C-C4C	2.73	128.35	124.81
11	7	302	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
11	7	309	CLA	C4-C3-C5	2.73	119.86	115.27
11	8	302	CLA	CHC-C1C-C2C	-2.73	119.18	126.72
11	11	309	CLA	CHD-C4C-NC	2.73	128.50	124.20
12	8	306	KC1	CAC-C3C-C4C	2.73	128.35	124.81
12	8	306	KC1	CHD-C4C-NC	2.72	128.34	124.20
11	7	308	CLA	CHD-C4C-NC	2.72	128.49	124.20
11	14	303	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
13	7	316	DD6	C21-C20-C19	-2.72	111.22	114.28
11	12	310	CLA	CAC-C3C-C4C	2.72	128.34	124.81
11	14	307	CLA	CHC-C1C-C2C	-2.72	119.20	126.72
12	13	305	KC1	CAA-CBA-CGA	-2.72	113.30	127.26
12	11	311	KC1	CHD-C4C-NC	2.72	128.32	124.20
11	12	302	CLA	C1-C2-C3	-2.72	121.35	126.04
13	12	317	DD6	C22-C16-C15	2.71	117.38	110.05
11	13	307	CLA	C4-C3-C5	2.71	119.84	115.27
12	13	310	KC1	CAA-CBA-CGA	-2.71	113.31	127.26
11	12	308	CLA	CHD-C4C-NC	2.71	128.48	124.20
11	13	303	CLA	C4C-C3C-C2C	-2.71	102.94	106.90
11	13	301	CLA	CHB-C4A-NA	2.71	128.26	124.51
11	6	301	CLA	CAC-C3C-C4C	2.71	128.33	124.81
11	11	309	CLA	CMB-C2B-C3B	2.71	129.75	124.68
14	10	301	A86	O1-C15-C14	-2.71	107.77	113.21
11	12	321	CLA	O2A-CGA-CBA	2.71	120.41	111.91
11	16	310	CLA	CAC-C3C-C4C	2.71	128.32	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	15	315	A86	C10-C9-C8	2.71	131.67	123.22
11	6	313	CLA	O2A-CGA-CBA	2.71	120.41	111.91
11	12	304	CLA	O2A-CGA-O1A	-2.71	116.76	123.59
11	14	305	CLA	CMB-C2B-C3B	2.71	129.74	124.68
11	6	302	CLA	C4C-C3C-C2C	-2.71	102.95	106.90
11	11	308	CLA	CMC-C2C-C1C	2.71	129.16	125.04
11	8	301	CLA	CHB-C4A-NA	2.71	128.25	124.51
12	13	312	KC1	C4C-C3C-C2C	-2.71	102.95	106.90
11	7	305	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
11	12	306	CLA	CBC-CAC-C3C	-2.70	104.98	112.43
11	15	308	CLA	CHB-C4A-NA	2.70	128.25	124.51
11	11	303	CLA	CHC-C1C-C2C	-2.70	119.25	126.72
11	10	305	CLA	CHD-C4C-NC	2.70	128.46	124.20
11	16	305	CLA	CHD-C4C-NC	2.70	128.46	124.20
11	6	307	CLA	C4C-C3C-C2C	-2.70	102.96	106.90
11	7	306	CLA	CMB-C2B-C3B	2.70	129.73	124.68
11	11	307	CLA	CMB-C2B-C3B	2.70	129.73	124.68
11	10	307	CLA	CHD-C4C-NC	2.70	128.45	124.20
11	15	305	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
14	15	316	A86	C3-C4-C5	-2.70	117.95	123.47
14	7	314	A86	C9-C10-C11	-2.70	118.68	126.61
14	15	322	A86	C4-C5-C6	-2.69	123.47	127.31
14	14	321	A86	C4-C3-C2	2.69	128.99	123.47
11	16	305	CLA	CBC-CAC-C3C	-2.69	105.02	112.43
11	16	303	CLA	CHC-C1C-C2C	-2.69	119.28	126.72
11	10	305	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
14	7	315	A86	C9-C8-C6	-2.69	118.86	126.42
11	16	306	CLA	CMA-C3A-C2A	-2.69	102.98	113.83
11	15	308	CLA	C3B-C4B-NB	2.69	112.69	109.21
11	10	309	CLA	CAC-C3C-C4C	2.69	128.29	124.81
11	14	303	CLA	CHB-C4A-NA	2.68	128.22	124.51
11	12	308	CLA	O2A-CGA-CBA	2.68	120.33	111.91
11	10	305	CLA	CAC-C3C-C4C	2.68	128.29	124.81
11	15	311	CLA	CAC-C3C-C4C	2.68	128.29	124.81
11	15	313	CLA	CAA-C2A-C3A	-2.68	105.44	112.78
12	14	308	KC1	O2D-CGD-O1D	-2.68	118.60	123.84
14	12	316	A86	C36-C31-C32	-2.68	117.04	119.70
11	12	304	CLA	CHD-C4C-NC	2.68	128.42	124.20
11	7	309	CLA	CHB-C4A-NA	2.68	128.22	124.51
14	15	315	A86	C22-C16-C17	-2.68	104.33	108.98
12	8	313	KC1	CMB-C2B-C1B	2.68	129.43	124.71
14	14	315	A86	C4-C3-C2	-2.68	117.99	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	8	317	DD6	C21-C20-C15	-2.67	117.78	122.26
14	12	314	A86	C9-C10-C11	-2.67	118.75	126.61
13	8	317	DD6	C4-C3-C2	-2.67	118.00	123.47
12	10	310	KC1	CAC-C3C-C4C	2.67	128.28	124.81
11	16	302	CLA	C4-C3-C5	2.67	119.77	115.27
12	6	308	KC1	CHD-C4C-NC	2.67	128.26	124.20
14	12	316	A86	C3-C4-C5	-2.67	118.00	123.47
12	8	312	KC1	CHD-C4C-NC	2.67	128.25	124.20
11	11	307	CLA	C3B-C4B-NB	2.67	112.66	109.21
13	7	316	DD6	C23-C16-C17	-2.67	104.34	108.98
11	12	310	CLA	CHD-C4C-NC	2.67	128.41	124.20
12	13	312	KC1	CAC-C3C-C4C	2.67	128.27	124.81
13	7	316	DD6	C14-C13-C11	-2.67	121.39	125.53
12	13	305	KC1	CHD-C4C-NC	2.67	128.25	124.20
11	12	308	CLA	CMB-C2B-C3B	2.67	129.67	124.68
11	14	305	CLA	CAC-C3C-C4C	2.67	128.27	124.81
14	12	314	A86	C12-C11-C13	2.67	120.50	116.02
11	6	304	CLA	C1-C2-C3	-2.67	121.43	126.04
11	15	304	CLA	O2A-C1-C2	2.67	115.64	108.64
13	6	315	DD6	C37-C36-C35	-2.67	109.42	114.36
11	13	304	CLA	CHD-C4C-NC	2.66	128.40	124.20
11	6	302	CLA	CBC-CAC-C3C	-2.66	105.09	112.43
11	6	306	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
11	6	302	CLA	CAA-C2A-C3A	-2.66	105.49	112.78
11	11	309	CLA	CAC-C3C-C4C	2.66	128.26	124.81
14	14	301	A86	C20-C19-C18	-2.66	107.49	112.75
11	15	303	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
12	12	305	KC1	CAC-C3C-C4C	2.66	128.26	124.81
11	8	302	CLA	O2A-CGA-CBA	2.66	120.25	111.91
11	16	307	CLA	CHD-C4C-NC	2.66	128.39	124.20
11	14	312	CLA	CHD-C4C-NC	2.66	128.39	124.20
11	7	310	CLA	C1-C2-C3	-2.66	121.45	126.04
11	13	302	CLA	CAA-C2A-C3A	-2.66	105.51	112.78
11	7	306	CLA	O2A-CGA-CBA	2.66	120.24	111.91
11	7	303	CLA	CAC-C3C-C4C	2.66	128.25	124.81
11	16	309	CLA	CHD-C4C-NC	2.65	128.39	124.20
13	16	313	DD6	C23-C16-C15	-2.65	102.88	110.05
11	14	304	CLA	CHD-C4C-NC	2.65	128.39	124.20
11	12	302	CLA	O2A-CGA-O1A	-2.65	116.89	123.59
11	13	303	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
11	10	308	CLA	C1-C2-C3	-2.65	121.46	126.04
12	13	311	KC1	C4C-C3C-C2C	-2.65	103.03	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	12	316	A86	C9-C10-C11	-2.65	118.82	126.61
14	14	318	A86	C4-C3-C2	-2.65	118.05	123.47
11	15	309	CLA	O2A-CGA-CBA	2.65	120.22	111.91
14	16	312	A86	C9-C8-C6	2.65	133.85	126.42
14	14	317	A86	C35-C34-C33	2.65	114.49	109.88
11	11	303	CLA	CAC-C3C-C4C	2.65	128.24	124.81
11	14	313	CLA	CAC-C3C-C4C	2.65	128.24	124.81
12	12	311	KC1	CHD-C4C-NC	2.65	128.22	124.20
14	14	320	A86	C40-C32-C31	-2.64	108.11	110.47
11	14	312	CLA	CMB-C2B-C3B	2.64	129.62	124.68
11	14	303	CLA	C1-C2-C3	-2.64	121.47	126.04
14	10	302	A86	C40-C32-C31	-2.64	108.11	110.47
11	11	309	CLA	C1-C2-C3	-2.64	121.47	126.04
11	6	311	CLA	C1-C2-C3	-2.64	121.48	126.04
11	11	307	CLA	C1-O2A-CGA	2.64	123.36	116.44
13	15	318	DD6	C32-C33-C34	2.64	119.60	113.64
11	6	314	CLA	CMB-C2B-C3B	2.64	129.61	124.68
11	15	302	CLA	CHC-C1C-C2C	-2.64	119.43	126.72
11	6	302	CLA	C1-C2-C3	-2.64	121.48	126.04
11	12	312	CLA	CBC-CAC-C3C	-2.64	105.17	112.43
14	14	317	A86	C9-C10-C11	-2.63	118.86	126.61
11	15	304	CLA	CHB-C4A-NA	2.63	128.15	124.51
11	15	312	CLA	C2A-C3A-C4A	-2.63	97.62	101.87
11	8	301	CLA	CHC-C1C-C2C	-2.63	119.44	126.72
12	12	309	KC1	O2D-CGD-O1D	-2.63	118.69	123.84
14	7	318	A86	C23-C16-C17	-2.63	104.41	108.98
14	8	315	A86	C20-C19-C18	-2.63	107.54	112.75
11	15	309	CLA	C4-C3-C5	2.63	119.70	115.27
11	7	304	CLA	CHD-C4C-NC	2.63	128.35	124.20
11	6	307	CLA	CHD-C4C-NC	2.63	128.35	124.20
11	10	307	CLA	C3B-C4B-NB	2.63	112.61	109.21
11	15	307	CLA	CAC-C3C-C4C	2.63	128.22	124.81
11	7	305	CLA	CAA-C2A-C3A	-2.63	105.58	112.78
11	7	310	CLA	O2A-CGA-CBA	2.63	120.16	111.91
11	15	308	CLA	CAA-C2A-C3A	-2.63	105.58	112.78
11	7	304	CLA	CBC-CAC-C3C	-2.63	105.19	112.43
11	11	309	CLA	O2A-CGA-CBA	2.63	120.15	111.91
11	6	303	CLA	CMB-C2B-C3B	2.63	129.59	124.68
11	14	307	CLA	C1-C2-C3	-2.63	121.50	126.04
11	8	303	CLA	CMB-C2B-C3B	2.63	129.59	124.68
12	16	304	KC1	O2D-CGD-O1D	-2.62	118.71	123.84
11	7	306	CLA	C4-C3-C5	2.62	119.69	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	13	301	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
11	15	308	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
14	13	313	A86	C4-C3-C2	-2.62	118.10	123.47
11	16	301	CLA	C4-C3-C5	2.62	119.68	115.27
12	8	313	KC1	C1C-C2C-C3C	-2.62	104.20	106.96
11	6	311	CLA	CMC-C2C-C1C	2.62	129.03	125.04
12	12	311	KC1	O2D-CGD-O1D	-2.62	118.71	123.84
13	7	301	DD6	O1-C20-C21	-2.62	111.92	115.06
11	8	301	CLA	O2A-CGA-CBA	2.62	120.13	111.91
11	14	310	CLA	CMB-C2B-C3B	2.62	129.58	124.68
12	16	311	KC1	O2D-CGD-O1D	-2.62	118.72	123.84
11	15	303	CLA	CAC-C3C-C4C	2.62	128.21	124.81
11	13	304	CLA	CMB-C2B-C3B	2.62	129.58	124.68
11	6	314	CLA	CHB-C4A-NA	2.62	128.13	124.51
12	16	311	KC1	CHD-C4C-NC	2.62	128.17	124.20
11	13	303	CLA	C4-C3-C5	2.62	119.67	115.27
14	14	315	A86	O1-C15-C14	2.62	118.46	113.21
14	12	314	A86	C26-C25-C24	-2.62	115.05	123.22
11	16	301	CLA	CHB-C4A-NA	2.62	128.13	124.51
11	7	311	CLA	CMB-C2B-C3B	2.61	129.57	124.68
12	7	312	KC1	CHB-C4A-NA	2.61	128.32	124.20
12	6	305	KC1	O2D-CGD-O1D	-2.61	118.73	123.84
12	8	313	KC1	CAC-C3C-C4C	2.61	128.20	124.81
11	7	310	CLA	CMB-C2B-C3B	2.61	129.56	124.68
11	14	304	CLA	CAA-C2A-C3A	-2.61	105.63	112.78
14	15	316	A86	C34-O4-C38	-2.61	113.03	117.90
11	6	301	CLA	CHB-C4A-NA	2.61	128.12	124.51
11	14	305	CLA	CHD-C4C-NC	2.61	128.31	124.20
11	14	310	CLA	CHD-C4C-NC	2.61	128.31	124.20
11	10	304	CLA	C1-C2-C3	-2.61	121.53	126.04
11	12	307	CLA	CMA-C3A-C2A	-2.61	103.31	113.83
12	8	314	KC1	CHD-C4C-NC	2.61	128.16	124.20
11	8	309	CLA	CHD-C4C-NC	2.61	128.31	124.20
11	7	306	CLA	CHC-C1C-C2C	-2.61	119.51	126.72
12	8	311	KC1	O1D-CGD-CBD	-2.61	119.15	124.48
11	14	302	CLA	CMB-C2B-C3B	2.60	129.55	124.68
11	11	303	CLA	CMB-C2B-C3B	2.60	129.55	124.68
12	13	311	KC1	CMB-C2B-C1B	2.60	129.30	124.71
11	8	308	CLA	CHB-C4A-NA	2.60	128.11	124.51
11	12	310	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
11	7	310	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
12	13	312	KC1	CBA-CAA-C2A	-2.60	115.36	125.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	6	312	CLA	CHD-C4C-NC	2.60	128.30	124.20
12	8	306	KC1	CMC-C2C-C1C	2.60	129.00	125.04
11	15	308	CLA	CAA-CBA-CGA	2.60	119.40	112.51
11	11	308	CLA	CHD-C4C-NC	2.60	128.29	124.20
11	13	309	CLA	CHB-C4A-NA	2.60	128.10	124.51
11	15	309	CLA	CHB-C4A-NA	2.60	128.10	124.51
11	11	308	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
11	6	306	CLA	O2A-C1-C2	2.60	115.46	108.64
14	12	316	A86	O-C13-C11	-2.59	115.42	121.15
14	15	317	A86	C3-C4-C5	-2.59	118.16	123.47
11	14	303	CLA	CBC-CAC-C3C	-2.59	105.28	112.43
12	13	306	KC1	CMC-C2C-C1C	2.59	128.99	125.04
14	11	314	A86	C26-C25-C24	-2.59	115.13	123.22
11	12	307	CLA	C3B-C4B-NB	2.59	112.56	109.21
11	12	303	CLA	C4-C3-C5	2.59	119.63	115.27
11	12	307	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
11	13	302	CLA	C4-C3-C5	2.59	119.62	115.27
11	15	310	CLA	CHD-C4C-NC	2.59	128.28	124.20
11	6	301	CLA	C4C-C3C-C2C	-2.59	103.13	106.90
14	7	315	A86	C12-C11-C13	2.59	120.37	116.02
14	15	321	A86	C7-C6-C8	2.59	122.15	118.08
11	12	302	CLA	CHC-C1C-C2C	-2.58	119.57	126.72
11	14	313	CLA	CBC-CAC-C3C	-2.58	105.31	112.43
12	11	306	KC1	O2D-CGD-O1D	-2.58	118.79	123.84
13	7	313	DD6	C10-C9-C8	-2.58	115.16	123.22
12	8	314	KC1	CHB-C4A-NA	2.58	128.27	124.20
12	11	306	KC1	CMB-C2B-C1B	2.58	129.26	124.71
11	11	308	CLA	C1-C2-C3	-2.58	121.58	126.04
13	6	316	DD6	C9-C8-C6	-2.58	119.17	126.42
13	13	314	DD6	C19-C18-C17	2.58	115.75	110.77
11	16	307	CLA	CMB-C2B-C3B	2.58	129.50	124.68
14	10	315	A86	C22-C16-C17	-2.58	104.51	108.98
13	15	319	DD6	C19-C18-C17	2.57	115.75	110.77
11	15	306	CLA	CAC-C3C-C4C	2.57	128.15	124.81
11	6	311	CLA	C4C-C3C-C2C	-2.57	103.15	106.90
11	15	313	CLA	CMB-C2B-C3B	2.57	129.49	124.68
16	8	323	LMG	O2-C2-C1	-2.57	103.80	110.05
13	8	316	DD6	C4-C3-C2	-2.57	118.20	123.47
11	7	304	CLA	C1-C2-C3	-2.57	121.59	126.04
11	10	308	CLA	CHC-C1C-C2C	-2.57	119.61	126.72
11	7	308	CLA	CMC-C2C-C1C	2.57	128.96	125.04
11	8	305	CLA	CHC-C1C-C2C	-2.57	119.61	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	8	308	CLA	CAC-C3C-C4C	2.57	128.14	124.81
14	8	318	A86	C7-C6-C5	2.57	126.52	122.92
11	7	305	CLA	CHB-C4A-NA	2.57	128.06	124.51
11	12	304	CLA	C1-C2-C3	-2.57	121.60	126.04
11	16	305	CLA	O2A-CGA-CBA	2.57	119.96	111.91
14	15	315	A86	C20-C19-C18	-2.57	107.67	112.75
11	10	305	CLA	C4-C3-C5	2.56	119.58	115.27
11	10	309	CLA	O2D-CGD-CBD	2.56	115.82	111.27
11	8	309	CLA	CHB-C4A-NA	2.56	128.05	124.51
14	7	315	A86	C40-C32-C31	-2.56	108.18	110.47
11	13	301	CLA	O2A-CGA-CBA	2.56	119.94	111.91
11	15	314	CLA	CAA-C2A-C3A	-2.56	105.77	112.78
12	12	309	KC1	CBC-CAC-C3C	-2.56	105.38	112.43
11	6	301	CLA	CMC-C2C-C1C	2.56	128.93	125.04
11	12	310	CLA	CMC-C2C-C1C	2.56	128.93	125.04
11	8	303	CLA	O2A-CGA-CBA	2.56	119.93	111.91
15	6	319	LHG	C11-C10-C9	-2.56	101.45	114.42
14	12	314	A86	C24-C1-C2	-2.56	115.02	118.94
11	15	312	CLA	CMD-C2D-C3D	-2.56	121.74	127.61
11	14	307	CLA	CMC-C2C-C1C	2.56	128.93	125.04
11	16	308	CLA	CHD-C4C-NC	2.55	128.23	124.20
11	7	302	CLA	C6-C7-C8	-2.55	107.66	115.92
11	13	307	CLA	CHB-C4A-NA	2.55	128.04	124.51
12	8	307	KC1	CBC-CAC-C3C	-2.55	105.39	112.43
12	13	310	KC1	O2D-CGD-O1D	-2.55	118.85	123.84
12	10	310	KC1	CHD-C4C-NC	2.55	128.07	124.20
11	6	302	CLA	CMC-C2C-C1C	2.55	128.93	125.04
13	10	313	DD6	C25-C24-C1	-2.55	119.25	126.42
11	6	304	CLA	CMB-C2B-C3B	2.55	129.45	124.68
14	15	322	A86	C23-C16-C17	-2.55	104.55	108.98
11	12	304	CLA	CBC-CAC-C3C	-2.55	105.40	112.43
11	14	307	CLA	C1-O2A-CGA	2.55	123.13	116.44
11	15	307	CLA	CHD-C4C-NC	2.55	128.21	124.20
11	6	307	CLA	C4-C3-C5	2.54	119.55	115.27
12	16	304	KC1	CMB-C2B-C1B	2.54	129.19	124.71
11	15	314	CLA	CHD-C4C-NC	2.54	128.21	124.20
13	10	313	DD6	C22-C16-C17	-2.54	104.57	108.98
12	6	305	KC1	CMC-C2C-C1C	2.54	128.91	125.04
11	10	303	CLA	CBA-CAA-C2A	2.54	121.36	113.86
11	8	308	CLA	CMB-C2B-C3B	2.54	129.43	124.68
13	8	317	DD6	C15-C14-C13	-2.54	120.62	125.99
12	12	309	KC1	CHB-C4A-NA	2.54	128.21	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	7	319	LMG	O1-C7-C8	-2.54	104.77	110.90
11	15	303	CLA	CHD-C4C-NC	2.54	128.20	124.20
13	12	317	DD6	C3-C4-C5	-2.54	118.28	123.47
11	14	303	CLA	CMC-C2C-C1C	2.54	128.90	125.04
11	14	303	CLA	CBA-CAA-C2A	2.54	121.35	113.86
11	14	302	CLA	CHB-C4A-NA	2.54	128.02	124.51
12	13	312	KC1	CMB-C2B-C1B	2.54	129.19	124.71
11	15	309	CLA	CAA-C2A-C3A	-2.54	105.83	112.78
11	8	303	CLA	CHD-C4C-NC	2.53	128.20	124.20
12	10	306	KC1	CHB-C4A-NA	2.53	128.20	124.20
17	12	322	LMT	O1B-C4'-C3'	2.53	114.02	107.28
14	14	321	A86	C3-C2-C1	2.53	130.92	127.31
13	10	314	DD6	C23-C16-C15	2.53	116.88	110.05
11	6	314	CLA	O2A-CGA-CBA	2.53	119.85	111.91
14	11	314	A86	C23-C16-C22	-2.53	103.64	107.37
14	14	319	A86	C7-C6-C5	-2.53	119.38	122.92
11	11	309	CLA	CAA-C2A-C3A	-2.53	105.86	112.78
11	11	309	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
14	10	301	A86	C7-C6-C8	2.53	122.06	118.08
11	8	309	CLA	O2A-CGA-CBA	2.53	119.83	111.91
12	12	313	KC1	CAC-C3C-C4C	2.52	128.09	124.81
13	12	317	DD6	C20-C19-C18	2.52	117.74	112.75
11	13	303	CLA	CMB-C2B-C3B	2.52	129.40	124.68
12	13	308	KC1	CAC-C3C-C4C	2.52	128.08	124.81
11	7	305	CLA	CMB-C2B-C3B	2.52	129.40	124.68
14	14	314	A86	C34-O4-C38	-2.52	113.19	117.90
11	15	304	CLA	CMB-C2B-C3B	2.52	129.40	124.68
11	11	307	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
11	15	313	CLA	CBC-CAC-C3C	-2.52	105.48	112.43
12	13	311	KC1	CBC-CAC-C3C	-2.52	105.48	112.43
11	12	310	CLA	C4-C3-C5	2.52	119.51	115.27
12	8	311	KC1	CHD-C4C-NC	2.52	128.03	124.20
12	8	314	KC1	O1D-CGD-CBD	-2.52	119.33	124.48
12	6	305	KC1	CAC-C3C-C4C	2.52	128.08	124.81
11	11	305	CLA	CMC-C2C-C1C	2.52	128.88	125.04
11	7	305	CLA	O2A-CGA-CBA	2.52	119.81	111.91
11	13	303	CLA	C1-C2-C3	-2.52	121.69	126.04
14	14	314	A86	C23-C16-C17	-2.52	104.61	108.98
11	6	313	CLA	CHD-C4C-NC	2.52	128.17	124.20
12	8	311	KC1	CHB-C4A-NA	2.52	128.17	124.20
11	8	301	CLA	CBA-CAA-C2A	2.51	121.28	113.86
11	12	303	CLA	CAC-C3C-C4C	2.51	128.07	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	13	305	KC1	CHB-C4A-NA	2.51	128.16	124.20
12	6	310	KC1	CMC-C2C-C1C	2.51	128.86	125.04
11	12	303	CLA	O2A-CGA-CBA	2.51	119.78	111.91
12	12	311	KC1	CAA-CBA-CGA	-2.51	114.36	127.26
11	7	310	CLA	CHD-C4C-NC	2.51	128.16	124.20
12	8	312	KC1	CMC-C2C-C1C	2.51	128.86	125.04
14	11	313	A86	C7-C6-C5	-2.51	119.41	122.92
12	13	308	KC1	O2D-CGD-O1D	-2.51	118.94	123.84
11	12	306	CLA	CHD-C4C-NC	2.51	128.15	124.20
11	16	302	CLA	CMC-C2C-C1C	2.50	128.85	125.04
14	10	315	A86	C12-C11-C13	2.50	120.23	116.02
11	10	304	CLA	CMC-C2C-C1C	2.50	128.85	125.04
12	7	312	KC1	CBC-CAC-C3C	-2.50	105.53	112.43
14	14	314	A86	C25-C24-C1	-2.50	119.39	126.42
12	8	307	KC1	CAC-C3C-C4C	2.50	128.06	124.81
11	8	309	CLA	CBC-CAC-C3C	-2.50	105.54	112.43
12	11	311	KC1	CHB-C4A-NA	2.50	128.14	124.20
11	10	309	CLA	O2A-CGA-CBA	2.50	119.75	111.91
12	11	311	KC1	CAA-CBA-CGA	-2.50	114.42	127.26
11	12	308	CLA	C4-C3-C5	2.50	119.47	115.27
14	15	317	A86	C12-C11-C13	2.50	120.22	116.02
11	16	310	CLA	CBC-CAC-C3C	-2.50	105.54	112.43
11	14	310	CLA	CMC-C2C-C1C	2.50	128.84	125.04
11	12	321	CLA	C4-C3-C5	2.50	119.47	115.27
14	15	315	A86	C9-C8-C6	2.50	133.43	126.42
11	13	304	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
11	12	310	CLA	CAA-C2A-C3A	-2.49	105.95	112.78
13	10	313	DD6	C19-C18-C17	2.49	115.58	110.77
11	15	313	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
11	10	307	CLA	CMC-C2C-C1C	2.49	128.83	125.04
11	7	305	CLA	C4-C3-C5	2.49	119.46	115.27
13	7	301	DD6	C23-C16-C22	-2.49	103.70	107.37
11	7	306	CLA	CHB-C4A-NA	2.49	127.95	124.51
11	14	302	CLA	CBC-CAC-C3C	-2.49	105.58	112.43
12	11	311	KC1	CHB-C1B-NB	-2.49	122.17	124.45
14	13	315	A86	C9-C8-C6	-2.49	119.43	126.42
12	14	306	KC1	O1D-CGD-CBD	-2.49	119.40	124.48
12	13	308	KC1	CMB-C2B-C1B	2.49	129.09	124.71
12	6	308	KC1	CHC-C4B-NB	-2.48	122.17	124.45
11	8	304	CLA	CAC-C3C-C4C	2.48	128.03	124.81
11	14	310	CLA	CBC-CAC-C3C	-2.48	105.58	112.43
11	14	307	CLA	O2A-CGA-CBA	2.48	119.70	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	6	312	CLA	CAA-C2A-C3A	-2.48	105.98	112.78
11	8	301	CLA	CHD-C4C-NC	2.48	128.12	124.20
11	7	310	CLA	CBC-CAC-C3C	-2.48	105.59	112.43
11	12	307	CLA	CHC-C1C-C2C	-2.48	119.86	126.72
12	7	307	KC1	CAA-C2A-C1A	-2.48	113.35	124.75
16	8	323	LMG	O3-C3-C2	-2.48	104.62	110.35
11	6	311	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
11	7	309	CLA	O2A-CGA-CBA	2.48	119.68	111.91
11	16	308	CLA	CAA-C2A-C3A	-2.48	106.00	112.78
14	10	317	A86	C12-C11-C10	-2.48	117.43	123.42
11	14	309	CLA	CHD-C4C-NC	2.48	128.10	124.20
11	6	311	CLA	O2A-CGA-CBA	2.47	119.67	111.91
14	16	314	A86	C12-C11-C13	2.47	120.18	116.02
11	6	307	CLA	CAC-C3C-C4C	2.47	128.02	124.81
11	7	302	CLA	CHC-C1C-C2C	-2.47	119.89	126.72
11	12	312	CLA	CMB-C2B-C3B	2.47	129.30	124.68
11	13	303	CLA	CBC-CAC-C3C	-2.47	105.62	112.43
11	7	302	CLA	CHB-C4A-NA	2.47	127.93	124.51
11	13	302	CLA	CMC-C2C-C1C	2.47	128.80	125.04
11	8	304	CLA	CHB-C4A-NA	2.47	127.92	124.51
12	11	304	KC1	CHB-C1B-NB	-2.46	122.19	124.45
12	16	304	KC1	CHD-C4C-NC	2.46	127.94	124.20
14	11	315	A86	C-C1-C24	2.46	121.96	118.08
12	8	307	KC1	CAA-CBA-CGA	-2.46	114.60	127.26
11	15	305	CLA	CHD-C4C-NC	2.46	128.08	124.20
11	11	305	CLA	O2A-CGA-CBA	2.46	119.64	111.91
11	8	309	CLA	CMB-C2B-C3B	2.46	129.28	124.68
11	15	306	CLA	CMB-C2B-C3B	2.46	129.28	124.68
11	16	310	CLA	O1D-CGD-CBD	2.46	129.52	124.48
11	14	310	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
12	11	304	KC1	CMB-C2B-C1B	2.46	129.05	124.71
16	8	321	LMG	O3-C3-C2	-2.46	104.67	110.35
12	8	310	KC1	CHB-C1B-NB	-2.46	122.20	124.45
14	10	302	A86	C3-C4-C5	-2.46	118.44	123.47
11	12	304	CLA	CHB-C4A-NA	2.45	127.91	124.51
11	6	304	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
11	15	308	CLA	CAA-C2A-C1A	2.45	120.01	111.97
14	10	315	A86	C36-C31-C32	-2.45	117.26	119.70
14	15	317	A86	C10-C9-C8	-2.45	115.57	123.22
11	13	301	CLA	CMB-C2B-C3B	2.45	129.26	124.68
12	6	308	KC1	O2D-CGD-O1D	-2.45	119.05	123.84
14	14	321	A86	C7-C6-C5	-2.45	119.49	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	7	307	KC1	CMB-C2B-C1B	2.45	129.03	124.71
14	14	316	A86	C4-C3-C2	-2.45	118.46	123.47
11	15	305	CLA	CMB-C2B-C3B	2.45	129.26	124.68
11	10	309	CLA	CMB-C2B-C3B	2.45	129.26	124.68
11	7	310	CLA	CAA-C2A-C3A	-2.45	106.07	112.78
11	6	312	CLA	CMB-C2B-C3B	2.45	129.26	124.68
12	12	311	KC1	CBA-CAA-C2A	-2.45	115.94	125.27
11	11	303	CLA	O2A-CGA-CBA	2.45	119.58	111.91
11	16	309	CLA	CMB-C2B-C3B	2.44	129.25	124.68
11	15	306	CLA	CHD-C4C-NC	2.44	128.05	124.20
11	10	308	CLA	CHB-C4A-NA	2.44	127.89	124.51
14	12	316	A86	C35-C34-C33	2.44	114.14	109.88
11	14	303	CLA	CMB-C2B-C3B	2.44	129.25	124.68
11	7	310	CLA	CMC-C2C-C1C	2.44	128.76	125.04
12	14	306	KC1	C1C-C2C-C3C	-2.44	104.39	106.96
12	6	309	KC1	CMB-C2B-C1B	2.44	129.01	124.71
14	7	315	A86	C19-C18-C17	-2.44	106.06	110.77
17	8	319	LMT	C1'-O5'-C5'	2.44	118.47	113.69
13	13	314	DD6	C12-C11-C13	-2.43	114.24	118.08
11	10	307	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
14	10	302	A86	C28-C27-C26	-2.43	119.51	122.92
12	12	313	KC1	CBA-CAA-C2A	-2.43	115.99	125.27
12	10	310	KC1	CAA-C2A-C1A	-2.43	113.56	124.75
11	11	308	CLA	O1D-CGD-CBD	-2.43	119.51	124.48
11	13	307	CLA	CHD-C4C-NC	2.43	128.04	124.20
11	15	310	CLA	CAA-C2A-C3A	-2.43	106.12	112.78
14	14	318	A86	C7-C6-C5	-2.43	119.52	122.92
11	6	303	CLA	CHB-C4A-NA	2.43	127.87	124.51
11	6	306	CLA	C4-C3-C5	2.43	119.36	115.27
11	7	306	CLA	C1-C2-C3	-2.43	121.84	126.04
12	16	304	KC1	CHB-C4A-NA	2.43	128.03	124.20
13	6	318	DD6	C23-C16-C17	-2.43	104.77	108.98
11	16	310	CLA	CMC-C2C-C1C	2.43	128.74	125.04
11	16	308	CLA	CMB-C2B-C3B	2.43	129.22	124.68
11	7	304	CLA	CMD-C2D-C3D	-2.43	122.03	127.61
11	15	304	CLA	CAA-C2A-C3A	-2.42	106.14	112.78
14	10	316	A86	C34-O4-C38	-2.42	113.38	117.90
12	11	310	KC1	CMC-C2C-C1C	2.42	128.73	125.04
14	14	317	A86	C34-O4-C38	-2.42	113.38	117.90
11	15	304	CLA	CED-O2D-CGD	2.42	121.41	115.94
12	10	312	KC1	O2D-CGD-O1D	-2.42	119.11	123.84
11	12	312	CLA	CMC-C2C-C1C	2.42	128.72	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	15	314	CLA	CHB-C4A-NA	2.42	127.85	124.51
11	8	304	CLA	CBC-CAC-C3C	-2.42	105.77	112.43
12	13	305	KC1	CBC-CAC-C3C	-2.42	105.77	112.43
11	10	307	CLA	CAA-C2A-C3A	-2.42	106.16	112.78
11	12	310	CLA	C1-C2-C3	-2.41	121.87	126.04
11	15	303	CLA	CMC-C2C-C1C	2.41	128.72	125.04
12	10	306	KC1	CMC-C2C-C1C	2.41	128.72	125.04
13	12	315	DD6	C4-C3-C2	-2.41	118.53	123.47
14	10	301	A86	C25-C24-C1	2.41	133.19	126.42
11	11	309	CLA	CHB-C4A-NA	2.41	127.85	124.51
12	8	311	KC1	CAA-C2A-C1A	-2.41	113.66	124.75
14	8	315	A86	C24-C1-C2	-2.41	115.24	118.94
11	16	303	CLA	CHB-C4A-NA	2.41	127.84	124.51
11	8	304	CLA	C1-C2-C3	-2.41	121.88	126.04
12	8	310	KC1	O2D-CGD-O1D	-2.41	119.13	123.84
11	8	305	CLA	O2D-CGD-O1D	-2.41	119.14	123.84
11	6	312	CLA	CHB-C4A-NA	2.41	127.84	124.51
11	15	302	CLA	C4-C3-C5	2.40	119.31	115.27
14	15	321	A86	C-C1-C24	2.40	121.86	118.08
11	14	310	CLA	O2A-CGA-CBA	2.40	119.45	111.91
12	11	310	KC1	O2D-CGD-O1D	-2.40	119.14	123.84
13	7	313	DD6	C3-C4-C5	-2.40	118.55	123.47
12	6	308	KC1	CMB-C2B-C1B	2.40	128.94	124.71
12	13	306	KC1	CMB-C2B-C1B	2.40	128.94	124.71
11	15	304	CLA	O2A-CGA-CBA	2.40	119.44	111.91
17	11	316	LMT	C1-O1'-C1'	-2.40	109.86	113.84
12	8	312	KC1	CED-O2D-CGD	2.40	121.36	115.94
13	7	317	DD6	C4-C3-C2	-2.40	118.56	123.47
12	13	306	KC1	O2D-CGD-O1D	-2.40	119.15	123.84
11	15	314	CLA	CBC-CAC-C3C	-2.40	105.82	112.43
11	15	310	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
11	7	302	CLA	O2A-C1-C2	2.40	114.94	108.64
14	11	315	A86	C41-C32-C31	-2.40	108.33	110.47
14	7	314	A86	C36-C31-C32	-2.40	117.32	119.70
12	10	306	KC1	CHB-C1B-NB	-2.40	122.25	124.45
11	15	302	CLA	CGD-CBD-CAD	-2.40	102.97	110.73
11	15	305	CLA	CMC-C2C-C1C	2.39	128.69	125.04
11	15	306	CLA	O1D-CGD-CBD	-2.39	119.59	124.48
11	7	303	CLA	C1-C2-C3	-2.39	121.90	126.04
13	13	314	DD6	C20-C19-C18	2.39	117.48	112.75
11	13	307	CLA	C1-O2A-CGA	2.39	122.72	116.44
11	11	305	CLA	CMB-C2B-C3B	2.39	129.15	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	8	305	CLA	O2A-CGA-CBA	2.39	119.42	111.91
11	6	314	CLA	CMC-C2C-C1C	2.39	128.68	125.04
12	12	311	KC1	CMB-C2B-C1B	2.39	128.93	124.71
11	8	308	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
11	14	309	CLA	CMB-C2B-C3B	2.39	129.15	124.68
13	16	313	DD6	C25-C24-C1	-2.39	119.71	126.42
11	12	307	CLA	CMA-C3A-C4A	-2.39	105.36	111.77
11	10	303	CLA	CHB-C4A-NA	2.39	127.81	124.51
13	8	317	DD6	C35-C36-C31	-2.39	115.16	120.57
11	7	309	CLA	CMB-C2B-C3B	2.38	129.14	124.68
11	10	311	CLA	CMB-C2B-C3B	2.38	129.14	124.68
11	14	305	CLA	CBC-CAC-C3C	-2.38	105.86	112.43
11	6	314	CLA	C4-C3-C5	2.38	119.28	115.27
14	10	316	A86	C7-C6-C8	2.38	121.83	118.08
14	14	319	A86	C40-C32-C31	-2.38	108.34	110.47
11	13	309	CLA	CMB-C2B-C3B	2.38	129.13	124.68
11	16	301	CLA	CMB-C2B-C3B	2.38	129.13	124.68
14	15	322	A86	O-C13-C14	-2.38	116.82	121.66
11	11	305	CLA	CHB-C4A-NA	2.38	127.80	124.51
13	16	313	DD6	C10-C9-C8	-2.38	115.80	123.22
11	7	311	CLA	CBC-CAC-C3C	-2.38	105.88	112.43
12	10	306	KC1	O1D-CGD-CBD	-2.38	119.62	124.48
11	16	303	CLA	CAC-C3C-C4C	2.37	127.89	124.81
11	10	305	CLA	CBC-CAC-C3C	-2.37	105.89	112.43
11	7	306	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
11	14	309	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
11	6	303	CLA	O2A-C1-C2	2.37	114.87	108.64
12	7	307	KC1	CAC-C3C-C4C	2.37	127.89	124.81
13	7	313	DD6	C21-C20-C15	-2.37	118.29	122.26
11	15	307	CLA	CHB-C4A-NA	2.37	127.79	124.51
13	13	314	DD6	C25-C24-C1	-2.37	119.76	126.42
11	10	304	CLA	O2A-CGA-CBA	2.37	119.34	111.91
11	16	306	CLA	CMC-C2C-C1C	2.37	128.64	125.04
11	14	303	CLA	C4-C3-C5	2.37	119.25	115.27
11	6	302	CLA	CHB-C4A-NA	2.37	127.78	124.51
12	12	305	KC1	O2D-CGD-O1D	-2.37	119.21	123.84
11	6	306	CLA	C1-C2-C3	-2.37	121.95	126.04
12	11	304	KC1	CMC-C2C-C1C	2.37	128.64	125.04
14	16	314	A86	C7-C6-C8	2.36	121.80	118.08
11	14	312	CLA	CHB-C4A-NA	2.36	127.78	124.51
11	8	302	CLA	CMC-C2C-C1C	2.36	128.64	125.04
14	15	320	A86	C23-C16-C17	-2.36	104.88	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	7	305	CLA	CHD-C4C-NC	2.36	127.93	124.20
11	6	314	CLA	CBC-CAC-C3C	-2.36	105.92	112.43
12	12	311	KC1	CHB-C1B-NB	-2.36	122.28	124.45
12	14	311	KC1	CHB-C1B-NB	-2.36	122.28	124.45
14	14	320	A86	C28-C27-C26	-2.36	119.62	122.92
14	10	301	A86	C23-C16-C22	-2.36	103.89	107.37
11	13	309	CLA	CHD-C4C-NC	2.36	127.92	124.20
11	12	312	CLA	CHB-C4A-NA	2.36	127.78	124.51
16	8	320	LMG	C38-C37-C36	-2.36	102.45	114.42
16	14	322	LMG	O6-C1-O1	-2.36	104.39	109.97
11	11	308	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
11	12	321	CLA	CMB-C2B-C3B	2.36	129.09	124.68
14	7	318	A86	C41-C32-C31	-2.36	108.36	110.47
11	15	314	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
13	6	318	DD6	C4-C3-C2	-2.36	118.65	123.47
11	15	312	CLA	CMC-C2C-C1C	2.36	128.63	125.04
11	16	303	CLA	CMC-C2C-C1C	2.35	128.62	125.04
12	8	310	KC1	CHC-C1C-NC	2.35	127.91	124.20
14	8	318	A86	O1-C15-C14	2.35	117.93	113.21
12	10	312	KC1	CBC-CAC-C3C	-2.35	105.94	112.43
11	16	305	CLA	CMC-C2C-C1C	2.35	128.62	125.04
11	6	311	CLA	CMB-C2B-C3B	2.35	129.08	124.68
14	7	318	A86	C8-C6-C5	2.35	122.55	118.94
13	6	316	DD6	O1-C20-C21	-2.35	112.24	115.06
11	15	309	CLA	C1-C2-C3	-2.35	121.98	126.04
12	6	305	KC1	CMB-C2B-C1B	2.35	128.86	124.71
12	13	306	KC1	OBD-CAD-C3D	-2.35	124.08	127.98
12	14	306	KC1	CAA-C2A-C1A	-2.35	113.95	124.75
11	15	302	CLA	C11-C12-C13	-2.35	108.33	115.92
12	11	306	KC1	CHB-C1B-NB	-2.35	122.30	124.45
13	13	314	DD6	C9-C8-C6	-2.35	119.82	126.42
16	8	323	LMG	O6-C1-O1	-2.35	104.42	109.97
11	12	312	CLA	C4-C3-C5	2.35	119.22	115.27
11	11	307	CLA	CBC-CAC-C3C	-2.35	105.97	112.43
14	15	320	A86	C7-C6-C5	-2.34	119.64	122.92
12	6	309	KC1	O2D-CGD-O1D	-2.34	119.26	123.84
11	8	302	CLA	C1-C2-C3	-2.34	121.99	126.04
11	10	311	CLA	CHB-C4A-NA	2.34	127.75	124.51
14	14	318	A86	C9-C10-C11	-2.34	119.72	126.61
11	10	305	CLA	C1-C2-C3	-2.34	121.99	126.04
11	7	308	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
13	13	314	DD6	C22-C16-C15	2.34	116.36	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	6	310	KC1	CHB-C1B-NB	-2.34	122.30	124.45
11	15	306	CLA	CHB-C4A-NA	2.34	127.75	124.51
11	16	310	CLA	CHB-C4A-NA	2.34	127.75	124.51
11	13	309	CLA	CED-O2D-CGD	2.34	121.22	115.94
11	12	306	CLA	CMB-C2B-C3B	2.34	129.05	124.68
13	10	314	DD6	C4-C3-C2	-2.34	118.69	123.47
11	7	303	CLA	O2A-CGA-CBA	2.34	119.24	111.91
11	10	308	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
12	11	310	KC1	CHB-C1B-NB	-2.33	122.31	124.45
14	10	315	A86	C23-C16-C22	-2.33	103.93	107.37
14	14	314	A86	C35-C34-C33	2.33	113.95	109.88
11	6	304	CLA	CHB-C4A-NA	2.33	127.74	124.51
12	6	308	KC1	CAC-C3C-C4C	2.33	127.83	124.81
12	8	307	KC1	CAA-C2A-C1A	-2.33	114.03	124.75
14	8	318	A86	C12-C11-C10	-2.33	117.78	123.42
16	8	320	LMG	O3-C3-C2	-2.33	104.96	110.35
11	12	308	CLA	CMC-C2C-C1C	2.33	128.59	125.04
14	10	317	A86	C-C1-C2	-2.33	119.66	122.92
11	15	310	CLA	CHB-C4A-NA	2.33	127.73	124.51
12	8	310	KC1	CHB-C4A-NA	2.33	127.87	124.20
11	8	308	CLA	CAA-C2A-C3A	-2.32	106.41	112.78
11	13	303	CLA	CHB-C4A-NA	2.32	127.73	124.51
14	15	321	A86	O1-C15-C14	2.32	117.87	113.21
11	16	302	CLA	CBC-CAC-C3C	-2.32	106.03	112.43
16	14	322	LMG	O3-C3-C2	-2.32	104.98	110.35
17	15	301	LMT	O5B-C5B-C4B	2.32	113.91	109.69
14	15	322	A86	O1-C15-C14	2.32	117.87	113.21
11	16	307	CLA	CMC-C2C-C1C	2.32	128.58	125.04
11	14	313	CLA	CMC-C2C-C1C	2.32	128.57	125.04
12	13	305	KC1	CAA-C2A-C1A	-2.32	114.08	124.75
11	14	302	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
11	12	304	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
12	12	309	KC1	CMB-C2B-C1B	2.32	128.80	124.71
11	15	304	CLA	CAC-C3C-C4C	2.32	127.82	124.81
11	13	303	CLA	CMC-C2C-C1C	2.32	128.57	125.04
16	7	319	LMG	O3-C3-C2	-2.32	105.00	110.35
11	10	309	CLA	CHB-C4A-NA	2.32	127.71	124.51
11	15	311	CLA	CBC-CAC-C3C	-2.31	106.05	112.43
14	12	316	A86	C20-C19-C18	-2.31	108.17	112.75
14	11	314	A86	C22-C16-C17	-2.31	104.96	108.98
14	13	315	A86	C3-C4-C5	-2.31	118.73	123.47
14	14	321	A86	C36-C31-C32	-2.31	117.40	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	8	306	KC1	CHB-C4A-NA	2.31	127.85	124.20
12	12	313	KC1	CGD-CBD-CAD	-2.31	103.25	110.73
11	11	305	CLA	C1-O2A-CGA	2.31	122.51	116.44
12	12	311	KC1	CAA-C2A-C1A	-2.31	114.13	124.75
13	8	317	DD6	C33-C32-C31	2.31	114.30	109.62
12	13	312	KC1	O2D-CGD-O1D	-2.31	119.32	123.84
13	16	313	DD6	C3-C4-C5	-2.31	118.74	123.47
11	14	304	CLA	CMC-C2C-C1C	2.31	128.56	125.04
11	6	307	CLA	CHB-C4A-NA	2.31	127.70	124.51
14	15	320	A86	C3-C2-C1	-2.31	124.02	127.31
12	16	304	KC1	CHB-C1B-NB	-2.31	122.33	124.45
11	6	301	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
11	16	302	CLA	CED-O2D-CGD	2.31	121.16	115.94
14	13	315	A86	C-C1-C2	-2.31	119.69	122.92
11	16	309	CLA	CHB-C4A-NA	2.30	127.70	124.51
11	11	307	CLA	CAC-C3C-C4C	2.30	127.80	124.81
11	11	303	CLA	CHB-C4A-NA	2.30	127.70	124.51
11	6	306	CLA	CMC-C2C-C1C	2.30	128.54	125.04
11	14	313	CLA	CMB-C2B-C3B	2.30	128.99	124.68
14	6	317	A86	C9-C10-C11	-2.30	119.84	126.61
11	10	305	CLA	O2A-CGA-CBA	2.30	119.13	111.91
14	12	314	A86	C-C1-C24	2.30	121.70	118.08
11	11	308	CLA	CHB-C4A-NA	2.30	127.69	124.51
14	14	315	A86	C8-C6-C5	2.30	122.47	118.94
11	10	308	CLA	CBC-CAC-C3C	-2.30	106.09	112.43
11	14	309	CLA	CHB-C4A-NA	2.30	127.69	124.51
11	7	311	CLA	CHB-C4A-NA	2.30	127.69	124.51
11	15	304	CLA	CHD-C4C-NC	2.30	127.82	124.20
12	13	312	KC1	CMC-C2C-C1C	2.30	128.53	125.04
11	12	312	CLA	C1-C2-C3	-2.30	122.07	126.04
11	11	308	CLA	CAA-C2A-C3A	-2.29	106.50	112.78
11	16	302	CLA	CMB-C2B-C3B	2.29	128.97	124.68
12	13	311	KC1	CAB-C3B-C4B	2.29	130.44	124.90
11	12	303	CLA	C1-C2-C3	-2.29	122.08	126.04
11	7	311	CLA	CAA-C2A-C3A	-2.29	106.50	112.78
13	12	317	DD6	C19-C18-C17	2.29	115.20	110.77
13	11	312	DD6	C20-C19-C18	2.29	117.29	112.75
11	10	308	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
12	7	312	KC1	CHB-C1B-NB	-2.29	122.35	124.45
11	15	313	CLA	CHB-C4A-NA	2.29	127.68	124.51
11	10	307	CLA	O2A-CGA-CBA	2.29	119.10	111.91
11	14	309	CLA	CBC-CAC-C3C	-2.29	106.12	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	13	304	CLA	CMC-C2C-C1C	2.29	128.53	125.04
12	8	314	KC1	CGD-CBD-CAD	-2.29	103.32	110.73
11	14	305	CLA	O2A-CGA-CBA	2.29	119.09	111.91
13	6	318	DD6	O1-C20-C21	-2.29	112.31	115.06
12	14	308	KC1	CAC-C3C-C4C	2.29	127.78	124.81
12	8	306	KC1	CAA-C2A-C1A	-2.29	114.22	124.75
11	7	311	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
12	6	305	KC1	CHB-C4A-NA	2.29	127.81	124.20
11	15	311	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
11	7	310	CLA	CHB-C4A-NA	2.29	127.67	124.51
11	6	302	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
11	8	301	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
11	10	303	CLA	CMC-C2C-C1C	2.29	128.52	125.04
14	16	314	A86	C10-C9-C8	-2.28	116.09	123.22
11	8	305	CLA	CHB-C4A-NA	2.28	127.67	124.51
11	15	311	CLA	CHB-C4A-NA	2.28	127.67	124.51
11	14	305	CLA	O2D-CGD-O1D	-2.28	119.37	123.84
11	13	303	CLA	O2A-CGA-CBA	2.28	119.07	111.91
14	11	314	A86	C19-C18-C17	2.28	115.18	110.77
12	12	309	KC1	CMC-C2C-C1C	2.28	128.51	125.04
11	15	307	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
14	15	317	A86	C7-C6-C5	-2.28	119.73	122.92
14	14	316	A86	C3-C4-C5	-2.28	118.80	123.47
14	10	316	A86	C7-C6-C5	-2.28	119.73	122.92
11	15	312	CLA	C4C-C3C-C2C	-2.28	103.58	106.90
11	14	303	CLA	O1D-CGD-CBD	-2.28	119.83	124.48
11	13	307	CLA	CMC-C2C-C1C	2.28	128.51	125.04
11	12	307	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
11	13	303	CLA	CBA-CAA-C2A	2.27	120.58	113.86
12	11	311	KC1	CMC-C2C-C1C	2.27	128.50	125.04
11	14	302	CLA	C4-C3-C2	-2.27	117.84	123.68
11	7	303	CLA	CMB-C2B-C3B	2.27	128.93	124.68
12	13	312	KC1	CBC-CAC-C3C	-2.27	106.17	112.43
11	16	308	CLA	CHB-C4A-NA	2.27	127.65	124.51
11	6	307	CLA	O2A-CGA-CBA	2.27	119.03	111.91
12	8	311	KC1	CHB-C1B-NB	-2.27	122.37	124.45
11	12	302	CLA	CAC-C3C-C4C	2.27	127.75	124.81
14	12	314	A86	C22-C16-C17	-2.27	105.04	108.98
12	13	310	KC1	CBC-CAC-C3C	-2.27	106.18	112.43
14	14	317	A86	C7-C6-C5	-2.27	119.75	122.92
12	13	312	KC1	CHB-C4A-NA	2.27	127.78	124.20
11	10	311	CLA	O2D-CGD-O1D	-2.27	119.41	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	6	311	CLA	CHB-C4A-NA	2.26	127.64	124.51
11	6	304	CLA	CMC-C2C-C1C	2.26	128.48	125.04
11	16	301	CLA	CBC-CAC-C3C	-2.26	106.20	112.43
11	6	303	CLA	CMC-C2C-C1C	2.26	128.48	125.04
11	15	311	CLA	CAA-C2A-C3A	-2.26	106.59	112.78
11	7	308	CLA	CHB-C4A-NA	2.26	127.64	124.51
11	16	305	CLA	C5-C3-C4	2.26	119.59	114.60
11	7	309	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
14	14	315	A86	C7-C6-C5	-2.26	119.76	122.92
12	11	311	KC1	O2D-CGD-O1D	-2.26	119.42	123.84
11	6	306	CLA	CBC-CAC-C3C	-2.26	106.21	112.43
13	8	316	DD6	C33-C32-C31	2.26	114.19	109.62
14	6	317	A86	C12-C11-C13	2.26	119.81	116.02
14	14	317	A86	O1-C15-C14	2.26	117.74	113.21
14	7	315	A86	C-C1-C24	2.26	121.63	118.08
12	13	310	KC1	CAC-C3C-C4C	2.25	127.73	124.81
12	14	308	KC1	CHB-C1B-NB	-2.25	122.38	124.45
11	12	307	CLA	CHB-C4A-NA	2.25	127.63	124.51
11	11	307	CLA	O2A-CGA-CBA	2.25	118.98	111.91
11	15	311	CLA	CMB-C2B-C3B	2.25	128.89	124.68
11	15	302	CLA	C1-C2-C3	-2.25	122.15	126.04
12	11	306	KC1	CHB-C4A-NA	2.25	127.75	124.20
11	16	302	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
12	8	310	KC1	C1C-C2C-C3C	-2.25	104.59	106.96
12	6	310	KC1	O2D-CGD-O1D	-2.25	119.44	123.84
12	8	314	KC1	CHB-C1B-NB	-2.25	122.39	124.45
11	11	307	CLA	C4-C3-C5	2.25	119.05	115.27
11	12	303	CLA	CED-O2D-CGD	2.25	121.02	115.94
11	11	309	CLA	C4-C3-C5	2.25	119.05	115.27
14	15	317	A86	C-C1-C24	2.25	121.61	118.08
11	6	301	CLA	CAA-C2A-C3A	-2.24	106.63	112.78
14	10	317	A86	C25-C24-C1	-2.24	120.11	126.42
11	12	321	CLA	C1-C2-C3	-2.24	122.16	126.04
14	14	316	A86	C25-C24-C1	-2.24	120.12	126.42
11	10	309	CLA	CMC-C2C-C1C	2.24	128.45	125.04
11	7	306	CLA	CBC-CAC-C3C	-2.24	106.25	112.43
13	7	316	DD6	C3-C4-C5	-2.24	118.89	123.47
13	8	316	DD6	C34-C35-C36	-2.24	107.40	111.85
11	16	308	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
17	11	316	LMT	C1B-O1B-C4'	-2.24	112.43	117.96
11	8	303	CLA	C4-C3-C5	2.24	119.03	115.27
13	15	319	DD6	C33-C32-C31	2.24	114.15	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	8	315	A86	C25-C26-C27	-2.24	124.12	127.31
11	10	304	CLA	O2D-CGD-O1D	-2.24	119.47	123.84
11	15	313	CLA	C1-C2-C3	-2.24	122.18	126.04
14	15	322	A86	C12-C11-C13	2.24	119.78	116.02
13	12	315	DD6	C3-C4-C5	-2.23	118.90	123.47
14	14	301	A86	C4-C3-C2	-2.23	118.90	123.47
11	16	301	CLA	CBA-CAA-C2A	2.23	120.45	113.86
11	14	304	CLA	CMB-C2B-C3B	2.23	128.85	124.68
14	11	313	A86	C34-O4-C38	-2.23	113.74	117.90
11	14	312	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
11	12	303	CLA	CMC-C2C-C1C	2.23	128.44	125.04
11	6	307	CLA	C1-O2A-CGA	2.23	122.30	116.44
12	16	311	KC1	CHB-C4A-NA	2.23	127.72	124.20
12	8	307	KC1	CMC-C2C-C1C	2.23	128.44	125.04
11	12	306	CLA	O2A-CGA-CBA	2.23	118.90	111.91
11	8	304	CLA	O2A-C1-C2	2.23	114.49	108.64
12	10	310	KC1	CHB-C1B-C2B	-2.23	120.81	125.48
14	13	315	A86	C28-C27-C26	-2.23	119.80	122.92
11	8	303	CLA	C1-C2-C3	-2.23	122.19	126.04
14	16	314	A86	C34-O4-C38	-2.23	113.75	117.90
11	12	321	CLA	CBC-CAC-C3C	-2.23	106.29	112.43
14	16	312	A86	C22-C16-C17	-2.23	105.11	108.98
11	14	303	CLA	CMA-C3A-C4A	-2.23	105.79	111.77
11	11	303	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
11	15	307	CLA	CMB-C2B-C3B	2.23	128.84	124.68
11	12	302	CLA	O2D-CGD-O1D	-2.23	119.49	123.84
11	12	310	CLA	CHB-C4A-NA	2.23	127.59	124.51
11	10	304	CLA	C4-C3-C5	2.23	119.02	115.27
13	8	316	DD6	C22-C16-C15	2.22	116.05	110.05
11	10	305	CLA	CHB-C4A-NA	2.22	127.59	124.51
11	12	321	CLA	CHB-C4A-NA	2.22	127.59	124.51
12	16	311	KC1	CMB-C2B-C1B	2.22	128.63	124.71
14	15	316	A86	O-C13-C11	-2.22	116.24	121.15
12	14	306	KC1	CHB-C1B-C2B	-2.22	120.82	125.48
11	16	303	CLA	C4-C3-C5	2.22	119.01	115.27
11	11	308	CLA	CMA-C3A-C2A	-2.22	104.87	113.83
11	16	306	CLA	CHD-C4C-NC	2.22	127.70	124.20
14	14	315	A86	C40-C32-C31	-2.22	108.48	110.47
12	14	308	KC1	CHB-C4A-NA	2.22	127.70	124.20
11	7	309	CLA	CAC-C3C-C4C	2.22	127.69	124.81
13	15	318	DD6	C3-C4-C5	-2.22	118.93	123.47
12	14	306	KC1	CMC-C2C-C1C	2.22	128.42	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	10	316	A86	C28-C27-C26	-2.22	119.81	122.92
11	15	312	CLA	CAC-C3C-C4C	2.22	127.69	124.81
11	12	312	CLA	O2D-CGD-O1D	-2.22	119.51	123.84
13	15	319	DD6	C9-C8-C6	-2.22	120.19	126.42
17	11	302	LMT	O5B-C5B-C6B	2.21	111.94	106.44
11	14	313	CLA	CMA-C3A-C2A	-2.21	104.90	113.83
14	11	314	A86	C12-C11-C13	2.21	119.74	116.02
11	16	308	CLA	CMC-C2C-C1C	2.21	128.41	125.04
13	12	315	DD6	O1-C20-C21	-2.21	112.41	115.06
11	15	312	CLA	CHB-C4A-NA	2.21	127.57	124.51
11	16	301	CLA	C4-C3-C2	-2.21	118.00	123.68
13	6	315	DD6	O1-C20-C21	-2.21	112.41	115.06
12	6	310	KC1	CBC-CAC-C3C	-2.21	106.34	112.43
11	13	307	CLA	CBC-CAC-C3C	-2.21	106.34	112.43
11	10	303	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
12	13	312	KC1	CHB-C1B-NB	-2.21	122.42	124.45
11	13	304	CLA	CBC-CAC-C3C	-2.21	106.34	112.43
11	14	302	CLA	O1D-CGD-CBD	-2.20	119.98	124.48
12	14	311	KC1	CHB-C4A-NA	2.20	127.67	124.20
14	14	320	A86	C7-C6-C8	2.20	121.55	118.08
12	12	311	KC1	CHC-C4B-NB	-2.20	122.43	124.45
11	15	308	CLA	O1D-CGD-CBD	-2.20	119.98	124.48
11	7	303	CLA	CED-O2D-CGD	2.20	120.91	115.94
11	15	305	CLA	CHB-C4A-NA	2.20	127.55	124.51
11	8	303	CLA	CMC-C2C-C1C	2.20	128.39	125.04
12	12	305	KC1	CHB-C4A-NA	2.20	127.67	124.20
11	15	313	CLA	CMC-C2C-C1C	2.20	128.38	125.04
11	15	307	CLA	C5-C3-C4	2.20	119.45	114.60
14	15	321	A86	C8-C6-C5	-2.19	115.57	118.94
12	7	307	KC1	CHB-C1B-NB	-2.19	122.44	124.45
11	15	302	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
12	11	306	KC1	CMC-C2C-C1C	2.19	128.38	125.04
11	16	307	CLA	CHB-C4A-NA	2.19	127.55	124.51
14	7	318	A86	O-C13-C11	-2.19	116.30	121.15
14	11	314	A86	C9-C8-C6	-2.19	120.26	126.42
11	13	304	CLA	CHB-C4A-NA	2.19	127.54	124.51
13	6	318	DD6	C25-C24-C1	-2.19	120.26	126.42
11	13	302	CLA	CMB-C2B-C3B	2.19	128.78	124.68
11	16	309	CLA	CMC-C2C-C1C	2.19	128.38	125.04
12	8	306	KC1	CED-O2D-CGD	2.19	120.89	115.94
14	8	318	A86	O-C13-C11	-2.19	116.31	121.15
11	12	304	CLA	O1D-CGD-CBD	-2.19	120.01	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	14	302	CLA	CAA-C2A-C3A	-2.19	106.79	112.78
11	16	307	CLA	CBC-CAC-C3C	-2.19	106.40	112.43
17	11	302	LMT	C1B-O1B-C4'	-2.19	112.56	117.96
11	16	303	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
11	15	308	CLA	CHA-C1A-NA	-2.19	121.39	126.40
11	15	308	CLA	CMC-C2C-C1C	2.18	128.37	125.04
14	14	316	A86	C20-C19-C18	-2.18	108.43	112.75
12	8	313	KC1	CHB-C4A-NA	2.18	127.64	124.20
11	8	303	CLA	CHB-C4A-NA	2.18	127.53	124.51
16	14	322	LMG	O2-C2-C1	-2.18	104.75	110.05
12	6	309	KC1	CAC-C3C-C4C	2.18	127.64	124.81
11	8	302	CLA	CHB-C4A-NA	2.18	127.53	124.51
11	10	307	CLA	CHA-C1A-NA	-2.18	121.41	126.40
14	14	317	A86	C10-C9-C8	-2.18	116.42	123.22
14	10	316	A86	C19-C18-C17	-2.18	106.56	110.77
11	15	303	CLA	CBC-CAC-C3C	-2.18	106.42	112.43
12	13	308	KC1	CMC-C2C-C1C	2.18	128.36	125.04
11	14	304	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
12	10	306	KC1	CBC-CAC-C3C	-2.18	106.43	112.43
11	13	309	CLA	CBC-CAC-C3C	-2.18	106.43	112.43
14	15	322	A86	C28-C27-C26	-2.18	119.87	122.92
12	14	311	KC1	CBC-CAC-C3C	-2.18	106.43	112.43
14	15	320	A86	C10-C9-C8	2.17	130.00	123.22
14	7	315	A86	C23-C16-C22	-2.17	104.17	107.37
11	12	303	CLA	CHB-C4A-NA	2.17	127.51	124.51
11	7	309	CLA	CBA-CAA-C2A	2.17	120.27	113.86
12	13	311	KC1	O2D-CGD-O1D	-2.17	119.60	123.84
11	10	304	CLA	CHB-C4A-NA	2.17	127.51	124.51
12	11	311	KC1	CBC-CAC-C3C	-2.17	106.45	112.43
11	6	303	CLA	C4-C3-C5	2.17	118.92	115.27
11	14	309	CLA	CAA-C2A-C3A	-2.17	106.85	112.78
12	6	309	KC1	CHB-C4A-NA	2.17	127.62	124.20
11	16	310	CLA	CMB-C2B-C3B	2.17	128.73	124.68
11	8	301	CLA	O2A-C1-C2	2.16	114.32	108.64
12	8	307	KC1	CHB-C4A-NA	2.16	127.61	124.20
12	11	304	KC1	CBC-CAC-C3C	-2.16	106.47	112.43
12	13	308	KC1	CHB-C4A-NA	2.16	127.61	124.20
11	14	309	CLA	CHA-C1A-NA	-2.16	121.45	126.40
11	6	307	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
14	15	320	A86	C4-C3-C2	2.16	127.90	123.47
14	11	315	A86	O4-C38-O5	-2.16	118.67	122.96
14	10	301	A86	C26-C25-C24	2.16	129.95	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	11	314	A86	C23-C16-C17	2.16	112.73	108.98
11	15	305	CLA	O1D-CGD-CBD	-2.16	120.07	124.48
12	7	307	KC1	CHB-C4A-NA	2.16	127.61	124.20
11	7	305	CLA	CMC-C2C-C1C	2.16	128.32	125.04
11	16	301	CLA	O2D-CGD-O1D	-2.15	119.62	123.84
11	6	314	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
11	10	307	CLA	CBA-CAA-C2A	2.15	120.22	113.86
11	6	301	CLA	CMB-C2B-C3B	2.15	128.71	124.68
16	8	323	LMG	O1-C7-C8	-2.15	105.70	110.90
12	6	309	KC1	CAA-C2A-C1A	-2.15	114.85	124.75
11	16	309	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
12	13	310	KC1	CHB-C4A-NA	2.15	127.59	124.20
11	13	302	CLA	CHB-C4A-NA	2.15	127.48	124.51
11	14	303	CLA	O2A-CGA-CBA	2.15	118.65	111.91
12	6	308	KC1	CHB-C1B-NB	-2.15	122.48	124.45
14	14	321	A86	C24-C1-C2	-2.15	115.64	118.94
11	15	311	CLA	CMC-C2C-C1C	2.15	128.31	125.04
12	14	308	KC1	O1D-CGD-CBD	-2.15	120.09	124.48
11	11	308	CLA	C4-C3-C5	2.15	118.88	115.27
12	8	313	KC1	CED-O2D-CGD	2.15	120.79	115.94
14	14	318	A86	O1-C15-C14	2.15	117.52	113.21
12	14	308	KC1	CHD-C4C-NC	2.15	127.46	124.20
12	13	305	KC1	CMC-C2C-C1C	2.15	128.31	125.04
17	12	318	LMT	C2'-C3'-C4'	2.15	114.58	109.68
11	16	306	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
12	8	307	KC1	O2D-CGD-O1D	-2.14	119.65	123.84
14	10	315	A86	C-C1-C2	-2.14	119.92	122.92
14	16	314	A86	C26-C25-C24	-2.14	116.53	123.22
11	14	310	CLA	C5-C3-C4	2.14	119.33	114.60
11	6	307	CLA	CBC-CAC-C3C	-2.14	106.53	112.43
13	7	313	DD6	C26-C25-C24	-2.14	116.54	123.22
12	12	309	KC1	CHB-C1B-C2B	-2.14	120.99	125.48
12	14	308	KC1	CBD-CHA-C1A	2.14	132.87	128.88
12	8	312	KC1	CHB-C4A-NA	2.14	127.58	124.20
14	11	315	A86	C9-C10-C11	-2.14	120.32	126.61
13	10	314	DD6	C10-C9-C8	-2.14	116.54	123.22
11	8	304	CLA	C2A-C3A-C4A	-2.14	98.41	101.87
12	6	310	KC1	CHB-C4A-NA	2.14	127.58	124.20
12	13	311	KC1	CMC-C2C-C1C	2.14	128.30	125.04
11	13	309	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
11	13	302	CLA	CED-O2D-CGD	2.14	120.77	115.94
13	13	314	DD6	C4-C3-C2	-2.14	119.10	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	10	303	CLA	O2A-CGA-CBA	2.14	118.61	111.91
14	14	316	A86	C7-C6-C8	2.14	121.44	118.08
11	15	310	CLA	CMC-C2C-C1C	2.14	128.29	125.04
11	10	308	CLA	C4-C3-C5	2.14	118.86	115.27
13	6	316	DD6	C3-C4-C5	-2.14	119.10	123.47
11	7	309	CLA	CMC-C2C-C1C	2.13	128.29	125.04
14	14	315	A86	C22-C16-C17	-2.13	105.28	108.98
11	14	302	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
11	13	302	CLA	O2A-CGA-CBA	2.13	118.59	111.91
13	13	314	DD6	C33-C32-C31	2.13	113.94	109.62
11	12	304	CLA	CMC-C2C-C1C	2.13	128.28	125.04
12	6	308	KC1	CHB-C4A-NA	2.13	127.56	124.20
14	10	301	A86	O3-C36-C37	-2.13	105.61	109.39
14	14	315	A86	C3-C4-C5	-2.13	119.12	123.47
14	11	314	A86	C-C1-C24	2.13	121.43	118.08
12	10	312	KC1	CHB-C1B-NB	-2.13	122.50	124.45
12	7	312	KC1	O2D-CGD-O1D	-2.13	119.68	123.84
11	7	309	CLA	C1-C2-C3	-2.13	122.37	126.04
12	12	309	KC1	CHB-C1B-NB	-2.13	122.50	124.45
11	16	306	CLA	CHB-C4A-NA	2.12	127.45	124.51
14	14	318	A86	C10-C9-C8	-2.12	116.59	123.22
13	7	317	DD6	C25-C24-C1	-2.12	120.45	126.42
11	7	304	CLA	OBD-CAD-C3D	-2.12	123.41	128.52
14	15	315	A86	O-C13-C14	-2.12	117.34	121.66
11	6	306	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
11	14	312	CLA	CED-O2D-CGD	2.12	120.74	115.94
11	14	313	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
11	8	305	CLA	CBC-CAC-C3C	-2.12	106.58	112.43
12	13	308	KC1	CHB-C1B-NB	-2.12	122.50	124.45
11	16	308	CLA	CHA-C1A-NA	-2.12	121.54	126.40
12	14	311	KC1	CBD-CHA-C1A	2.12	132.83	128.88
16	8	323	LMG	C1-O6-C5	-2.12	109.53	113.69
11	13	301	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
11	13	304	CLA	O1D-CGD-CBD	-2.12	120.15	124.48
11	16	305	CLA	CMB-C2B-C3B	2.11	128.63	124.68
11	13	302	CLA	O2D-CGD-O1D	-2.11	119.70	123.84
12	13	305	KC1	CBD-CHA-C1A	2.11	132.82	128.88
14	11	313	A86	C8-C6-C5	2.11	122.19	118.94
11	6	312	CLA	CBC-CAC-C3C	-2.11	106.60	112.43
11	14	307	CLA	CHA-C1A-NA	-2.11	121.56	126.40
11	13	309	CLA	CMC-C2C-C1C	2.11	128.25	125.04
13	7	313	DD6	C23-C16-C17	-2.11	105.32	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	8	318	A86	C22-C16-C17	-2.11	105.32	108.98
11	15	309	CLA	CBC-CAC-C3C	-2.11	106.61	112.43
12	13	308	KC1	O1D-CGD-CBD	-2.11	120.17	124.48
11	15	302	CLA	CBC-CAC-C3C	-2.11	106.61	112.43
11	15	303	CLA	CHB-C4A-NA	2.11	127.43	124.51
12	10	312	KC1	CHB-C4A-NA	2.11	127.53	124.20
14	7	318	A86	C28-C27-C26	-2.11	119.97	122.92
12	6	305	KC1	CHB-C1B-NB	-2.11	122.52	124.45
11	14	304	CLA	CHB-C4A-NA	2.11	127.43	124.51
11	8	309	CLA	CMC-C2C-C1C	2.11	128.25	125.04
12	13	306	KC1	CED-O2D-CGD	2.11	120.70	115.94
11	6	313	CLA	CHA-C1A-NA	-2.11	121.57	126.40
11	10	309	CLA	C1-C2-C3	-2.11	122.40	126.04
12	12	313	KC1	CBC-CAC-C3C	-2.11	106.63	112.43
11	7	302	CLA	C1-O2A-CGA	2.10	121.96	116.44
14	8	315	A86	O4-C38-O5	-2.10	118.78	122.96
11	15	312	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
11	8	302	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
14	15	315	A86	C12-C11-C10	-2.10	118.34	123.42
14	14	319	A86	C8-C6-C5	2.10	122.16	118.94
14	15	320	A86	C9-C8-C6	2.10	132.31	126.42
12	12	311	KC1	CBC-CAC-C3C	-2.10	106.64	112.43
14	11	301	A86	C4-C3-C2	-2.10	119.17	123.47
12	10	306	KC1	CAA-C2A-C1A	-2.10	115.10	124.75
11	14	305	CLA	CMC-C2C-C1C	2.10	128.23	125.04
11	12	306	CLA	CMC-C2C-C1C	2.10	128.23	125.04
11	13	301	CLA	O2A-C1-C2	2.10	114.15	108.64
14	11	301	A86	C22-C16-C17	-2.10	105.34	108.98
11	12	321	CLA	CHA-C1A-NA	-2.10	121.60	126.40
12	10	310	KC1	CHB-C4A-NA	2.10	127.51	124.20
16	7	319	LMG	C9-C8-C7	-2.09	106.83	111.79
11	13	301	CLA	CBC-CAC-C3C	-2.09	106.66	112.43
11	16	301	CLA	C6-C7-C8	-2.09	109.15	115.92
11	6	306	CLA	CHB-C4A-NA	2.09	127.41	124.51
11	12	308	CLA	CHB-C4A-NA	2.09	127.41	124.51
11	13	301	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
14	14	301	A86	C36-C31-C32	-2.09	117.62	119.70
11	14	307	CLA	CED-O2D-CGD	2.09	120.67	115.94
12	11	304	KC1	O2D-CGD-O1D	-2.09	119.75	123.84
13	11	312	DD6	C22-C16-C15	2.09	115.69	110.05
16	8	321	LMG	O2-C2-C1	-2.09	104.97	110.05
11	6	303	CLA	CAA-C2A-C3A	-2.09	107.06	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	13	313	A86	C25-C24-C1	-2.09	120.55	126.42
11	11	305	CLA	CBC-CAC-C3C	-2.09	106.67	112.43
11	10	309	CLA	CBC-CAC-C3C	-2.09	106.67	112.43
12	8	306	KC1	CHB-C1B-NB	-2.09	122.53	124.45
11	15	303	CLA	CMB-C2B-C3B	2.09	128.58	124.68
11	16	306	CLA	C4-C3-C5	2.09	118.78	115.27
14	11	301	A86	C8-C6-C5	-2.09	115.74	118.94
17	11	316	LMT	C2'-C3'-C4'	2.08	114.44	109.68
11	13	309	CLA	CHA-C1A-NA	-2.08	121.63	126.40
12	11	310	KC1	CHB-C4A-NA	2.08	127.48	124.20
11	8	308	CLA	C4-C3-C5	2.08	118.77	115.27
11	15	303	CLA	CHA-C1A-NA	-2.08	121.63	126.40
11	13	303	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
14	7	315	A86	C35-C34-C33	2.08	113.51	109.88
14	8	318	A86	C25-C24-C1	-2.08	120.57	126.42
11	7	304	CLA	O2A-CGA-CBA	2.08	118.44	111.91
14	15	316	A86	C19-C18-C17	2.08	114.79	110.77
17	11	316	LMT	O5'-C5'-C6'	2.08	111.60	106.44
14	12	314	A86	C25-C26-C27	-2.08	124.35	127.31
11	13	302	CLA	C1-C2-C3	-2.08	122.45	126.04
11	7	308	CLA	CAA-C2A-C3A	-2.08	107.09	112.78
14	15	316	A86	C35-C34-C33	2.08	113.50	109.88
11	8	303	CLA	CBC-CAC-C3C	-2.08	106.71	112.43
13	6	316	DD6	C33-C34-C35	-2.07	107.47	110.30
12	8	313	KC1	CHB-C1B-NB	-2.07	122.55	124.45
13	8	316	DD6	C40-C32-C31	-2.07	107.18	110.47
12	14	311	KC1	O2D-CGD-O1D	-2.07	119.79	123.84
16	8	320	LMG	O2-C2-C1	-2.07	105.02	110.05
11	6	306	CLA	CBA-CAA-C2A	2.07	119.97	113.86
11	13	307	CLA	CED-O2D-CGD	2.07	120.61	115.94
14	10	315	A86	C7-C6-C8	2.07	121.33	118.08
11	7	305	CLA	CHA-C1A-NA	-2.07	121.67	126.40
11	15	312	CLA	CAA-C2A-C3A	-2.07	107.12	112.78
11	6	304	CLA	CBA-CAA-C2A	-2.06	107.77	113.86
13	7	317	DD6	C23-C16-C17	-2.06	105.40	108.98
13	7	301	DD6	C22-C16-C15	2.06	115.62	110.05
11	10	307	CLA	C1-O2A-CGA	2.06	121.86	116.44
11	7	308	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
11	16	306	CLA	O1D-CGD-CBD	-2.06	120.26	124.48
11	6	306	CLA	C2A-C3A-C4A	-2.06	98.54	101.87
11	10	305	CLA	CMC-C2C-C1C	2.06	128.18	125.04
14	10	317	A86	C9-C8-C6	-2.06	120.62	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	16	306	CLA	CAA-C2A-C1A	2.06	118.73	111.97
13	11	312	DD6	C23-C16-C17	-2.06	105.40	108.98
11	8	304	CLA	CHC-C1C-NC	2.06	127.33	124.20
11	7	303	CLA	CHB-C4A-NA	2.06	127.36	124.51
11	6	307	CLA	C1-C2-C3	-2.06	122.48	126.04
11	13	301	CLA	C4-C3-C5	2.06	118.73	115.27
13	7	313	DD6	C23-C16-C15	-2.06	104.49	110.05
12	11	310	KC1	CBC-CAC-C3C	-2.06	106.76	112.43
14	16	314	A86	C9-C10-C11	-2.06	120.56	126.61
17	7	320	LMT	C1B-O1B-C4'	-2.06	112.87	117.96
13	8	317	DD6	C3-C4-C5	-2.06	119.26	123.47
11	8	301	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
13	8	317	DD6	C23-C16-C15	2.06	115.60	110.05
14	10	301	A86	C34-O4-C38	-2.06	114.06	117.90
14	16	312	A86	C41-C32-C31	-2.05	108.63	110.47
14	10	315	A86	C10-C9-C8	-2.05	116.81	123.22
12	7	307	KC1	O2D-CGD-O1D	-2.05	119.82	123.84
13	11	312	DD6	C25-C24-C1	-2.05	120.65	126.42
12	8	306	KC1	O2D-CGD-O1D	-2.05	119.83	123.84
12	11	304	KC1	CHB-C4A-NA	2.05	127.44	124.20
14	15	315	A86	C28-C27-C26	-2.05	120.05	122.92
12	11	306	KC1	CBC-CAC-C3C	-2.05	106.78	112.43
14	16	314	A86	C28-C27-C26	-2.05	120.05	122.92
11	16	303	CLA	CMB-C2B-C3B	2.05	128.51	124.68
11	15	305	CLA	O2A-CGA-CBA	2.05	120.61	114.03
11	7	304	CLA	C4-C3-C5	2.05	118.72	115.27
11	11	309	CLA	CBC-CAC-C3C	-2.05	106.79	112.43
11	6	302	CLA	CMA-C3A-C4A	-2.04	106.28	111.77
12	14	306	KC1	CMB-C2B-C1B	2.04	128.31	124.71
14	14	314	A86	C26-C25-C24	-2.04	116.84	123.22
11	15	307	CLA	CMC-C2C-C1C	2.04	128.15	125.04
12	8	313	KC1	OBD-CAD-C3D	-2.04	124.59	127.98
11	6	301	CLA	C2A-C3A-C4A	-2.04	98.57	101.87
11	15	313	CLA	CGD-CBD-CAD	-2.04	104.12	110.73
13	6	315	DD6	C23-C16-C17	2.04	112.53	108.98
14	14	314	A86	C7-C6-C8	-2.04	114.86	118.08
11	12	321	CLA	CED-O2D-CGD	2.04	120.56	115.94
11	7	302	CLA	C6-C5-C3	-2.04	108.10	113.45
12	10	306	KC1	CBD-CHA-C1A	2.04	132.69	128.88
11	6	313	CLA	CED-O2D-CGD	2.04	120.55	115.94
11	7	302	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
14	14	318	A86	C-C1-C24	2.04	121.29	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	6	317	A86	C23-C16-C17	-2.04	105.44	108.98
14	14	301	A86	C3-C4-C5	-2.04	119.30	123.47
14	16	314	A86	C4-C3-C2	-2.04	119.30	123.47
11	6	302	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
12	13	306	KC1	CHB-C4A-NA	2.04	127.41	124.20
11	10	308	CLA	C6-C7-C8	-2.04	109.34	115.92
14	10	315	A86	C4-C5-C6	-2.04	124.41	127.31
13	7	316	DD6	C9-C8-C6	-2.04	120.70	126.42
12	8	312	KC1	O2A-CGA-O1A	-2.04	118.44	122.67
11	7	308	CLA	C1-C2-C3	-2.04	122.52	126.04
13	12	315	DD6	C33-C32-C31	2.03	113.74	109.62
14	14	301	A86	C7-C6-C8	2.03	121.28	118.08
17	11	316	LMT	O1B-C4'-C3'	2.03	112.69	107.28
11	12	302	CLA	C16-C15-C13	-2.03	109.35	115.92
12	13	306	KC1	O1D-CGD-CBD	-2.03	120.33	124.48
11	14	313	CLA	CGD-CBD-CAD	-2.03	104.15	110.73
11	12	303	CLA	CHA-C1A-NA	-2.03	121.75	126.40
12	12	309	KC1	O1D-CGD-CBD	-2.03	120.33	124.48
11	14	302	CLA	C1-O2A-CGA	2.03	121.77	116.44
14	10	316	A86	C41-C32-C31	-2.03	108.66	110.47
14	7	314	A86	C12-C11-C13	2.03	119.43	116.02
11	15	305	CLA	CHA-C1A-NA	-2.03	121.76	126.40
11	15	310	CLA	O1D-CGD-CBD	-2.03	120.34	124.48
11	11	307	CLA	C1-C2-C3	-2.02	122.54	126.04
14	8	318	A86	C40-C32-C31	-2.02	108.66	110.47
11	14	312	CLA	CMC-C2C-C1C	2.02	128.12	125.04
12	12	311	KC1	O2A-CGA-O1A	-2.02	118.47	122.67
11	6	307	CLA	CED-O2D-CGD	2.02	120.51	115.94
11	12	307	CLA	CAA-CBA-CGA	-2.02	107.34	113.25
14	10	302	A86	C-C1-C24	2.02	121.26	118.08
14	10	302	A86	O-C13-C11	-2.02	116.68	121.15
11	6	314	CLA	C1-C2-C3	-2.02	122.55	126.04
11	13	302	CLA	CBC-CAC-C3C	-2.02	106.86	112.43
11	10	303	CLA	CHA-C1A-NA	-2.02	121.77	126.40
11	14	305	CLA	C5-C3-C4	2.02	119.06	114.60
11	13	301	CLA	CHA-C1A-NA	-2.02	121.78	126.40
14	15	315	A86	C9-C10-C11	-2.02	120.67	126.61
14	11	314	A86	C35-C34-C33	2.02	113.40	109.88
11	15	306	CLA	O2A-CGA-CBA	2.02	120.51	114.03
14	10	302	A86	C-C1-C2	-2.02	120.10	122.92
11	7	303	CLA	C6-C7-C8	-2.01	109.41	115.92
12	8	311	KC1	CED-O2D-CGD	2.01	120.49	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	7	318	A86	C4-C3-C2	-2.01	119.35	123.47
11	16	303	CLA	CBC-CAC-C3C	-2.01	106.88	112.43
12	10	310	KC1	O2D-CGD-O1D	-2.01	119.90	123.84
11	7	311	CLA	O2A-CGA-CBA	2.01	120.19	112.23
14	15	322	A86	C34-O4-C38	-2.01	114.14	117.90
11	16	301	CLA	C11-C10-C8	-2.01	109.42	115.92
12	8	313	KC1	O1D-CGD-CBD	-2.01	120.37	124.48
11	16	302	CLA	C1-O2A-CGA	2.01	121.71	116.44
12	11	310	KC1	CMB-C2B-C1B	2.01	128.25	124.71
11	7	303	CLA	O2D-CGD-O1D	-2.01	119.92	123.84
11	6	311	CLA	C1B-CHB-C4A	-2.01	126.14	130.12
11	10	307	CLA	CBC-CAC-C3C	-2.01	106.90	112.43
11	6	307	CLA	O2D-CGD-O1D	-2.00	119.92	123.84
11	7	302	CLA	C4-C3-C2	-2.00	118.54	123.68
11	15	303	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
11	15	304	CLA	C2A-C3A-C4A	-2.00	98.64	101.87
14	14	314	A86	C9-C8-C6	2.00	132.04	126.42
12	10	310	KC1	CMB-C2B-C1B	2.00	128.24	124.71
14	10	317	A86	C3-C4-C5	-2.00	119.38	123.47

All (63) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	6	301	CLA	ND
11	6	302	CLA	ND
11	6	303	CLA	ND
11	6	304	CLA	ND
11	6	306	CLA	ND
11	6	307	CLA	ND
11	6	312	CLA	ND
11	6	313	CLA	ND
11	6	314	CLA	ND
11	7	302	CLA	ND
11	7	303	CLA	ND
11	7	304	CLA	ND
11	7	305	CLA	ND
11	7	308	CLA	ND
11	7	309	CLA	ND
11	7	310	CLA	ND
11	8	301	CLA	ND
11	8	302	CLA	ND
11	8	303	CLA	ND

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Mol	Chain	Res	Type	Atom
11	8	304	CLA	ND
11	8	308	CLA	ND
11	10	304	CLA	ND
11	10	305	CLA	ND
11	10	307	CLA	ND
11	10	308	CLA	ND
11	10	309	CLA	ND
11	11	305	CLA	ND
11	11	307	CLA	ND
11	11	309	CLA	ND
11	12	303	CLA	ND
11	12	304	CLA	ND
11	12	306	CLA	ND
11	12	307	CLA	ND
11	12	308	CLA	ND
11	12	312	CLA	ND
11	12	321	CLA	ND
11	13	302	CLA	ND
11	13	307	CLA	ND
11	13	309	CLA	ND
11	14	302	CLA	ND
11	14	303	CLA	ND
11	14	304	CLA	ND
11	14	305	CLA	ND
11	14	309	CLA	ND
11	14	310	CLA	ND
11	14	313	CLA	ND
11	15	303	CLA	ND
11	15	304	CLA	ND
11	15	305	CLA	ND
11	15	306	CLA	ND
11	15	307	CLA	ND
11	15	308	CLA	ND
11	15	309	CLA	ND
11	15	310	CLA	ND
11	15	311	CLA	ND
11	15	312	CLA	ND
11	16	302	CLA	ND
11	16	303	CLA	ND
11	16	305	CLA	ND
11	16	306	CLA	ND
11	16	307	CLA	ND

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Mol	Chain	Res	Type	Atom
11	16	308	CLA	ND
11	16	310	CLA	ND

All (1794) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	6	301	CLA	C1A-C2A-CAA-CBA
11	6	301	CLA	C3A-C2A-CAA-CBA
11	6	304	CLA	C2-C3-C5-C6
11	6	304	CLA	C4-C3-C5-C6
11	6	306	CLA	C1A-C2A-CAA-CBA
11	6	311	CLA	C4-C3-C5-C6
11	7	303	CLA	C2-C3-C5-C6
11	7	303	CLA	C4-C3-C5-C6
11	7	306	CLA	C1A-C2A-CAA-CBA
11	7	306	CLA	C3A-C2A-CAA-CBA
11	7	306	CLA	CBD-CGD-O2D-CED
11	7	306	CLA	C2-C3-C5-C6
11	7	306	CLA	C4-C3-C5-C6
11	7	309	CLA	C1A-C2A-CAA-CBA
11	7	309	CLA	C3A-C2A-CAA-CBA
11	7	309	CLA	CBD-CGD-O2D-CED
11	7	311	CLA	C2A-CAA-CBA-CGA
11	8	301	CLA	C3A-C2A-CAA-CBA
11	8	302	CLA	C2-C3-C5-C6
11	8	302	CLA	C4-C3-C5-C6
11	8	305	CLA	C1A-C2A-CAA-CBA
11	8	305	CLA	C2-C3-C5-C6
11	10	303	CLA	C3A-C2A-CAA-CBA
11	10	305	CLA	C1A-C2A-CAA-CBA
11	10	307	CLA	C1A-C2A-CAA-CBA
11	10	307	CLA	C3A-C2A-CAA-CBA
11	10	309	CLA	C4-C3-C5-C6
11	11	303	CLA	O1A-CGA-O2A-C1
11	11	305	CLA	C1A-C2A-CAA-CBA
11	11	307	CLA	C2-C1-O2A-CGA
11	12	302	CLA	C4-C3-C5-C6
11	12	312	CLA	C1A-C2A-CAA-CBA
11	13	301	CLA	C1A-C2A-CAA-CBA
11	13	301	CLA	C3A-C2A-CAA-CBA
11	13	303	CLA	C1A-C2A-CAA-CBA
11	13	307	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
11	13	307	CLA	C4-C3-C5-C6
11	13	309	CLA	C1A-C2A-CAA-CBA
11	14	303	CLA	C1A-C2A-CAA-CBA
11	14	312	CLA	CHA-CBD-CGD-O1D
11	14	312	CLA	CHA-CBD-CGD-O2D
11	14	313	CLA	C1A-C2A-CAA-CBA
11	14	313	CLA	CHA-CBD-CGD-O1D
11	14	313	CLA	CHA-CBD-CGD-O2D
11	15	302	CLA	C2-C3-C5-C6
11	15	302	CLA	C4-C3-C5-C6
11	15	303	CLA	C3A-C2A-CAA-CBA
11	15	303	CLA	C2-C3-C5-C6
11	15	303	CLA	C4-C3-C5-C6
11	15	305	CLA	CHA-CBD-CGD-O2D
11	15	306	CLA	CHA-CBD-CGD-O1D
11	15	306	CLA	CHA-CBD-CGD-O2D
11	15	308	CLA	C1A-C2A-CAA-CBA
11	15	309	CLA	CBD-CGD-O2D-CED
11	15	310	CLA	CHA-CBD-CGD-O2D
11	15	311	CLA	C1A-C2A-CAA-CBA
11	15	313	CLA	CAD-CBD-CGD-O1D
11	15	313	CLA	C2-C3-C5-C6
11	15	313	CLA	C4-C3-C5-C6
11	16	301	CLA	C3A-C2A-CAA-CBA
11	16	303	CLA	C1A-C2A-CAA-CBA
11	16	303	CLA	C3A-C2A-CAA-CBA
11	16	303	CLA	C2-C3-C5-C6
11	16	303	CLA	C4-C3-C5-C6
11	16	306	CLA	C1A-C2A-CAA-CBA
11	16	307	CLA	C1A-C2A-CAA-CBA
11	16	307	CLA	CHA-CBD-CGD-O1D
11	16	307	CLA	CHA-CBD-CGD-O2D
11	16	308	CLA	C1A-C2A-CAA-CBA
11	16	309	CLA	CHA-CBD-CGD-O1D
11	16	309	CLA	CHA-CBD-CGD-O2D
11	16	310	CLA	CBD-CGD-O2D-CED
12	6	305	KC1	C1A-C2A-CAA-CBA
12	6	305	KC1	C2A-CAA-CBA-CGA
12	6	308	KC1	C3A-C2A-CAA-CBA
12	6	308	KC1	C2A-CAA-CBA-CGA
12	6	309	KC1	C3A-C2A-CAA-CBA
12	6	310	KC1	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	7	307	KC1	C2A-CAA-CBA-CGA
12	7	312	KC1	C2B-C3B-CAB-CBB
12	7	312	KC1	C4B-C3B-CAB-CBB
12	8	306	KC1	C3A-C2A-CAA-CBA
12	8	306	KC1	C2A-CAA-CBA-CGA
12	8	306	KC1	CAA-CBA-CGA-O1A
12	8	306	KC1	CAA-CBA-CGA-O2A
12	8	307	KC1	C3A-C2A-CAA-CBA
12	8	307	KC1	C2B-C3B-CAB-CBB
12	8	307	KC1	C4B-C3B-CAB-CBB
12	8	307	KC1	C2A-CAA-CBA-CGA
12	8	310	KC1	C3A-C2A-CAA-CBA
12	8	310	KC1	C2B-C3B-CAB-CBB
12	8	311	KC1	C3A-C2A-CAA-CBA
12	8	311	KC1	C2B-C3B-CAB-CBB
12	8	311	KC1	C2A-CAA-CBA-CGA
12	8	312	KC1	C3A-C2A-CAA-CBA
12	8	312	KC1	C2A-CAA-CBA-CGA
12	8	313	KC1	C3A-C2A-CAA-CBA
12	8	313	KC1	C2B-C3B-CAB-CBB
12	8	313	KC1	C4B-C3B-CAB-CBB
12	8	314	KC1	C1A-C2A-CAA-CBA
12	8	314	KC1	C3A-C2A-CAA-CBA
12	10	306	KC1	C2A-CAA-CBA-CGA
12	10	306	KC1	CHA-CBD-CGD-O2D
12	10	310	KC1	C3A-C2A-CAA-CBA
12	10	310	KC1	C2A-CAA-CBA-CGA
12	10	312	KC1	C2A-CAA-CBA-CGA
12	11	304	KC1	C3A-C2A-CAA-CBA
12	11	304	KC1	C2A-CAA-CBA-CGA
12	11	306	KC1	C3A-C2A-CAA-CBA
12	11	306	KC1	C2A-CAA-CBA-CGA
12	11	306	KC1	CHA-CBD-CGD-O2D
12	11	310	KC1	C3A-C2A-CAA-CBA
12	11	310	KC1	C2A-CAA-CBA-CGA
12	11	311	KC1	C1A-C2A-CAA-CBA
12	11	311	KC1	C2B-C3B-CAB-CBB
12	11	311	KC1	C2A-CAA-CBA-CGA
12	12	305	KC1	C1A-C2A-CAA-CBA
12	12	305	KC1	C2A-CAA-CBA-CGA
12	12	309	KC1	C3A-C2A-CAA-CBA
12	12	311	KC1	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
12	12	313	KC1	C1A-C2A-CAA-CBA
12	12	313	KC1	C3A-C2A-CAA-CBA
12	13	305	KC1	C1A-C2A-CAA-CBA
12	13	305	KC1	C2A-CAA-CBA-CGA
12	13	305	KC1	CHA-CBD-CGD-O2D
12	13	306	KC1	C1A-C2A-CAA-CBA
12	13	306	KC1	C2A-CAA-CBA-CGA
12	13	306	KC1	CHA-CBD-CGD-O1D
12	13	306	KC1	CHA-CBD-CGD-O2D
12	13	308	KC1	C3A-C2A-CAA-CBA
12	13	308	KC1	C2A-CAA-CBA-CGA
12	13	308	KC1	CHA-CBD-CGD-O1D
12	13	308	KC1	CHA-CBD-CGD-O2D
12	13	310	KC1	C1A-C2A-CAA-CBA
12	13	310	KC1	C2B-C3B-CAB-CBB
12	13	310	KC1	C4B-C3B-CAB-CBB
12	13	310	KC1	C2A-CAA-CBA-CGA
12	13	311	KC1	C3A-C2A-CAA-CBA
12	13	311	KC1	CAA-CBA-CGA-O1A
12	13	311	KC1	CAA-CBA-CGA-O2A
12	13	312	KC1	C1A-C2A-CAA-CBA
12	14	306	KC1	C2A-CAA-CBA-CGA
12	14	308	KC1	C3A-C2A-CAA-CBA
12	14	308	KC1	C2A-CAA-CBA-CGA
12	14	308	KC1	CHA-CBD-CGD-O1D
12	14	308	KC1	CHA-CBD-CGD-O2D
12	14	311	KC1	C3A-C2A-CAA-CBA
12	16	304	KC1	C1A-C2A-CAA-CBA
12	16	304	KC1	C3A-C2A-CAA-CBA
12	16	304	KC1	C2A-CAA-CBA-CGA
12	16	304	KC1	CAA-CBA-CGA-O1A
12	16	304	KC1	CAA-CBA-CGA-O2A
12	16	311	KC1	C3A-C2A-CAA-CBA
12	16	311	KC1	C2B-C3B-CAB-CBB
12	16	311	KC1	C4B-C3B-CAB-CBB
12	16	311	KC1	C2A-CAA-CBA-CGA
13	6	315	DD6	C-C1-C2-C3
13	6	315	DD6	C-C1-C24-C25
13	6	315	DD6	C9-C10-C11-C12
13	6	315	DD6	C11-C10-C9-C8
13	6	315	DD6	C4-C5-C6-C7
13	6	316	DD6	C-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
13	6	316	DD6	C-C1-C24-C25
13	6	316	DD6	C4-C5-C6-C8
13	6	316	DD6	C7-C6-C8-C9
13	6	318	DD6	C-C1-C2-C3
13	6	318	DD6	C2-C1-C24-C25
13	6	318	DD6	C9-C10-C11-C12
13	6	318	DD6	C4-C5-C6-C7
13	7	301	DD6	C-C1-C2-C3
13	7	301	DD6	C-C1-C24-C25
13	7	301	DD6	C2-C1-C24-C25
13	7	301	DD6	C9-C10-C11-C12
13	7	301	DD6	C10-C11-C13-C14
13	7	301	DD6	C4-C5-C6-C7
13	7	301	DD6	C5-C6-C8-C9
13	7	313	DD6	C-C1-C2-C3
13	7	313	DD6	C-C1-C24-C25
13	7	313	DD6	C9-C10-C11-C12
13	7	313	DD6	C10-C11-C13-C14
13	7	313	DD6	C12-C11-C13-C14
13	7	313	DD6	C4-C5-C6-C7
13	7	313	DD6	C7-C6-C8-C9
13	7	316	DD6	C-C1-C2-C3
13	7	316	DD6	C2-C1-C24-C25
13	7	316	DD6	C9-C10-C11-C12
13	7	316	DD6	C10-C11-C13-C14
13	7	316	DD6	C12-C11-C13-C14
13	7	316	DD6	C13-C14-C15-C16
13	7	316	DD6	C4-C5-C6-C8
13	7	317	DD6	C-C1-C2-C3
13	7	317	DD6	C9-C10-C11-C13
13	7	317	DD6	C24-C25-C26-C27
13	7	317	DD6	C3-C4-C5-C6
13	7	317	DD6	C4-C5-C6-C8
13	8	316	DD6	C-C1-C2-C3
13	8	316	DD6	C9-C10-C11-C12
13	8	316	DD6	C12-C11-C13-C14
13	8	316	DD6	C4-C5-C6-C7
13	8	317	DD6	C-C1-C2-C3
13	8	317	DD6	C-C1-C24-C25
13	8	317	DD6	C9-C10-C11-C13
13	8	317	DD6	C10-C11-C13-C14
13	8	317	DD6	C12-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
13	8	317	DD6	C13-C14-C15-O1
13	8	317	DD6	C4-C5-C6-C7
13	8	317	DD6	C5-C6-C8-C9
13	10	313	DD6	C-C1-C2-C3
13	10	313	DD6	C-C1-C24-C25
13	10	313	DD6	C9-C10-C11-C13
13	10	313	DD6	C13-C14-C15-O1
13	10	313	DD6	C4-C5-C6-C7
13	10	314	DD6	C-C1-C2-C3
13	10	314	DD6	C9-C10-C11-C12
13	10	314	DD6	C4-C5-C6-C7
13	10	314	DD6	C7-C6-C8-C9
13	11	312	DD6	C-C1-C2-C3
13	11	312	DD6	C-C1-C24-C25
13	11	312	DD6	C9-C10-C11-C13
13	11	312	DD6	C4-C5-C6-C7
13	11	312	DD6	C7-C6-C8-C9
13	12	315	DD6	C-C1-C2-C3
13	12	315	DD6	C9-C10-C11-C12
13	12	315	DD6	C10-C11-C13-C14
13	12	315	DD6	C12-C11-C13-C14
13	12	315	DD6	C4-C5-C6-C7
13	12	317	DD6	C-C1-C2-C3
13	12	317	DD6	C2-C1-C24-C25
13	12	317	DD6	C9-C10-C11-C13
13	12	317	DD6	C10-C11-C13-C14
13	12	317	DD6	C12-C11-C13-C14
13	12	317	DD6	C4-C5-C6-C7
13	12	317	DD6	C5-C6-C8-C9
13	12	317	DD6	C7-C6-C8-C9
13	13	314	DD6	C-C1-C2-C3
13	13	314	DD6	C9-C10-C11-C12
13	13	314	DD6	C13-C14-C15-O1
13	13	314	DD6	C4-C5-C6-C7
13	13	314	DD6	C5-C6-C8-C9
13	13	314	DD6	C7-C6-C8-C9
13	15	318	DD6	C24-C1-C2-C3
13	15	318	DD6	C-C1-C24-C25
13	15	318	DD6	C9-C10-C11-C13
13	15	318	DD6	C13-C14-C15-C16
13	15	318	DD6	C1-C2-C3-C4
13	15	318	DD6	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
13	15	318	DD6	C7-C6-C8-C9
13	15	319	DD6	C-C1-C2-C3
13	15	319	DD6	C2-C1-C24-C25
13	15	319	DD6	C9-C10-C11-C12
13	15	319	DD6	C13-C14-C15-C16
13	15	319	DD6	C1-C2-C3-C4
13	15	319	DD6	C4-C5-C6-C7
13	15	319	DD6	C5-C6-C8-C9
13	16	313	DD6	C-C1-C2-C3
13	16	313	DD6	C9-C10-C11-C13
13	16	313	DD6	C13-C14-C15-C20
13	16	313	DD6	C13-C14-C15-O1
13	16	313	DD6	C4-C5-C6-C7
13	16	313	DD6	C5-C6-C8-C9
13	16	313	DD6	C7-C6-C8-C9
14	6	317	A86	C5-C6-C8-C9
14	6	317	A86	C7-C6-C8-C9
14	7	314	A86	C13-C14-C15-O1
14	7	314	A86	C1-C2-C3-C4
14	7	314	A86	C26-C27-C29-C30
14	7	314	A86	C39-C38-O4-C34
14	7	314	A86	O5-C38-O4-C34
14	7	314	A86	C3-C4-C5-C6
14	7	314	A86	C5-C6-C8-C9
14	7	314	A86	C7-C6-C8-C9
14	7	315	A86	C11-C10-C9-C8
14	7	315	A86	C10-C11-C13-O
14	7	315	A86	C10-C11-C13-C14
14	7	315	A86	C12-C11-C13-O
14	7	315	A86	C5-C6-C8-C9
14	7	315	A86	C7-C6-C8-C9
14	7	318	A86	C13-C14-C15-O1
14	7	318	A86	C39-C38-O4-C34
14	8	315	A86	C-C1-C24-C25
14	8	315	A86	C2-C1-C24-C25
14	8	315	A86	O5-C38-O4-C34
14	8	318	A86	C-C1-C24-C25
14	8	318	A86	C11-C13-C14-C15
14	8	318	A86	C5-C6-C8-C9
14	10	301	A86	C39-C38-O4-C34
14	10	302	A86	C10-C11-C13-O
14	10	302	A86	C12-C11-C13-O

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Mol	Chain	Res	Type	Atoms
14	10	315	A86	O-C13-C14-C15
14	10	315	A86	C11-C13-C14-C15
14	10	315	A86	C35-C34-O4-C38
14	10	315	A86	C3-C4-C5-C6
14	10	316	A86	C-C1-C24-C25
14	10	316	A86	C2-C1-C24-C25
14	10	316	A86	C13-C14-C15-C16
14	10	316	A86	C24-C25-C26-C27
14	10	316	A86	C39-C38-O4-C34
14	10	316	A86	O5-C38-O4-C34
14	10	316	A86	C5-C6-C8-C9
14	10	316	A86	C7-C6-C8-C9
14	10	317	A86	C11-C13-C14-C15
14	11	301	A86	C39-C38-O4-C34
14	11	301	A86	O5-C38-O4-C34
14	11	313	A86	C11-C10-C9-C8
14	11	313	A86	O-C13-C14-C15
14	11	313	A86	C11-C13-C14-C15
14	11	313	A86	C13-C14-C15-C16
14	11	313	A86	C13-C14-C15-O1
14	11	313	A86	C39-C38-O4-C34
14	11	314	A86	C-C1-C24-C25
14	11	314	A86	C2-C1-C24-C25
14	11	314	A86	C26-C27-C29-C30
14	11	314	A86	C28-C27-C29-C30
14	11	314	A86	C33-C34-O4-C38
14	11	314	A86	C39-C38-O4-C34
14	11	314	A86	O5-C38-O4-C34
14	11	314	A86	C7-C6-C8-C9
14	11	315	A86	C13-C14-C15-C16
14	11	315	A86	C1-C2-C3-C4
14	11	315	A86	C24-C25-C26-C27
14	12	314	A86	C-C1-C24-C25
14	12	314	A86	C2-C1-C24-C25
14	12	314	A86	C13-C14-C15-C16
14	12	314	A86	C5-C6-C8-C9
14	12	314	A86	C7-C6-C8-C9
14	12	316	A86	C12-C11-C13-O
14	12	316	A86	C13-C14-C15-C16
14	12	316	A86	C24-C25-C26-C27
14	12	316	A86	C5-C6-C8-C9
14	13	313	A86	C-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
14	13	313	A86	C2-C1-C24-C25
14	13	313	A86	C10-C11-C13-O
14	13	313	A86	C12-C11-C13-O
14	13	315	A86	C-C1-C24-C25
14	13	315	A86	C11-C10-C9-C8
14	13	315	A86	C12-C11-C13-C14
14	13	315	A86	C13-C14-C15-C16
14	13	315	A86	C26-C27-C29-C30
14	13	315	A86	C28-C27-C29-C30
14	14	301	A86	C39-C38-O4-C34
14	14	314	A86	C-C1-C24-C25
14	14	314	A86	C2-C1-C24-C25
14	14	314	A86	C10-C11-C13-O
14	14	314	A86	C10-C11-C13-C14
14	14	314	A86	C12-C11-C13-O
14	14	315	A86	C-C1-C24-C25
14	14	315	A86	C2-C1-C24-C25
14	14	315	A86	C11-C10-C9-C8
14	14	315	A86	O-C13-C14-C15
14	14	315	A86	C11-C13-C14-C15
14	14	315	A86	C24-C25-C26-C27
14	14	316	A86	C-C1-C24-C25
14	14	316	A86	C13-C14-C15-C16
14	14	317	A86	C-C1-C24-C25
14	14	317	A86	C2-C1-C24-C25
14	14	317	A86	C11-C13-C14-C15
14	14	317	A86	C13-C14-C15-C16
14	14	317	A86	C26-C27-C29-C30
14	14	317	A86	C3-C4-C5-C6
14	14	318	A86	C-C1-C24-C25
14	14	318	A86	C2-C1-C24-C25
14	14	318	A86	O-C13-C14-C15
14	14	318	A86	C11-C13-C14-C15
14	14	318	A86	C13-C14-C15-C16
14	14	318	A86	C24-C25-C26-C27
14	14	319	A86	C10-C11-C13-O
14	14	319	A86	C10-C11-C13-C14
14	14	319	A86	C12-C11-C13-O
14	14	319	A86	C1-C2-C3-C4
14	14	319	A86	C24-C25-C26-C27
14	14	320	A86	C13-C14-C15-O1
14	14	320	A86	O5-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
14	14	320	A86	C3-C4-C5-C6
14	14	321	A86	C-C1-C24-C25
14	14	321	A86	C2-C1-C24-C25
14	14	321	A86	C13-C14-C15-O1
14	14	321	A86	C24-C25-C26-C27
14	14	321	A86	C39-C38-O4-C34
14	14	321	A86	O5-C38-O4-C34
14	15	316	A86	C11-C10-C9-C8
14	15	316	A86	C10-C11-C13-O
14	15	316	A86	C10-C11-C13-C14
14	15	316	A86	C12-C11-C13-O
14	15	316	A86	C13-C14-C15-O1
14	15	316	A86	C24-C25-C26-C27
14	15	316	A86	C39-C38-O4-C34
14	15	317	A86	C11-C13-C14-C15
14	15	317	A86	C13-C14-C15-O1
14	15	320	A86	C-C1-C24-C25
14	15	320	A86	C2-C1-C24-C25
14	15	320	A86	C10-C11-C13-O
14	15	320	A86	C12-C11-C13-O
14	15	320	A86	C13-C14-C15-O1
14	15	320	A86	C24-C25-C26-C27
14	15	320	A86	C39-C38-O4-C34
14	15	320	A86	C5-C6-C8-C9
14	15	320	A86	C7-C6-C8-C9
14	15	321	A86	C-C1-C24-C25
14	15	321	A86	C2-C1-C24-C25
14	15	321	A86	C13-C14-C15-C16
14	15	321	A86	C24-C25-C26-C27
14	15	322	A86	O-C13-C14-C15
14	15	322	A86	C11-C13-C14-C15
14	15	322	A86	C13-C14-C15-O1
14	15	322	A86	C26-C27-C29-C30
14	15	322	A86	C28-C27-C29-C30
14	15	322	A86	C3-C4-C5-C6
14	15	322	A86	C5-C6-C8-C9
14	15	322	A86	C7-C6-C8-C9
14	16	312	A86	C13-C14-C15-O1
14	16	312	A86	C28-C27-C29-C30
14	16	314	A86	C-C1-C24-C25
14	16	314	A86	C2-C1-C24-C25
14	16	314	A86	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
14	16	314	A86	C5-C6-C8-C9
14	16	314	A86	C7-C6-C8-C9
16	8	320	LMG	O10-C28-O8-C9
16	8	321	LMG	O1-C7-C8-O7
16	8	321	LMG	C11-C10-O7-C8
17	8	319	LMT	C2'-C1'-O1'-C1
17	8	319	LMT	O5'-C1'-O1'-C1
17	8	319	LMT	C2-C1-O1'-C1'
17	12	301	LMT	O5'-C1'-O1'-C1
14	7	318	A86	O5-C38-O4-C34
14	10	315	A86	C39-C38-O4-C34
14	10	317	A86	C39-C38-O4-C34
14	11	313	A86	O5-C38-O4-C34
14	13	315	A86	C39-C38-O4-C34
14	14	301	A86	O5-C38-O4-C34
14	14	320	A86	C39-C38-O4-C34
14	15	315	A86	C39-C38-O4-C34
14	15	317	A86	C39-C38-O4-C34
14	15	321	A86	C39-C38-O4-C34
14	15	322	A86	C39-C38-O4-C34
14	16	314	A86	C39-C38-O4-C34
14	8	315	A86	C39-C38-O4-C34
14	10	301	A86	O5-C38-O4-C34
14	13	315	A86	O5-C38-O4-C34
14	14	316	A86	C39-C38-O4-C34
14	14	317	A86	C39-C38-O4-C34
14	15	320	A86	O5-C38-O4-C34
14	15	321	A86	O5-C38-O4-C34
14	15	322	A86	O5-C38-O4-C34
11	15	304	CLA	O1D-CGD-O2D-CED
11	15	314	CLA	O1D-CGD-O2D-CED
11	16	310	CLA	O1D-CGD-O2D-CED
11	12	308	CLA	CBD-CGD-O2D-CED
11	14	310	CLA	CBD-CGD-O2D-CED
11	15	304	CLA	CBD-CGD-O2D-CED
11	15	314	CLA	CBD-CGD-O2D-CED
12	7	307	KC1	CBD-CGD-O2D-CED
12	8	311	KC1	CBD-CGD-O2D-CED
11	7	306	CLA	O1A-CGA-O2A-C1
14	15	315	A86	O5-C38-O4-C34
11	7	306	CLA	O1D-CGD-O2D-CED
17	15	301	LMT	O5B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
11	8	301	CLA	CBD-CGD-O2D-CED
12	10	306	KC1	CBD-CGD-O2D-CED
12	11	306	KC1	CBD-CGD-O2D-CED
12	13	305	KC1	CBD-CGD-O2D-CED
12	13	306	KC1	CBD-CGD-O2D-CED
14	10	317	A86	O5-C38-O4-C34
11	12	306	CLA	O1A-CGA-O2A-C1
14	10	315	A86	O5-C38-O4-C34
14	15	317	A86	O5-C38-O4-C34
11	15	309	CLA	O1D-CGD-O2D-CED
16	8	323	LMG	O9-C10-O7-C8
14	12	316	A86	C39-C38-O4-C34
11	6	302	CLA	C3-C5-C6-C7
11	6	304	CLA	C3-C5-C6-C7
11	6	306	CLA	C3-C5-C6-C7
11	6	311	CLA	C3-C5-C6-C7
11	6	313	CLA	C3-C5-C6-C7
11	7	309	CLA	C3-C5-C6-C7
11	7	310	CLA	C3-C5-C6-C7
11	8	305	CLA	C3-C5-C6-C7
11	10	304	CLA	C3-C5-C6-C7
11	10	308	CLA	C3-C5-C6-C7
11	11	308	CLA	C3-C5-C6-C7
11	14	303	CLA	C3-C5-C6-C7
11	16	302	CLA	C3-C5-C6-C7
11	7	306	CLA	CBA-CGA-O2A-C1
11	11	303	CLA	CBA-CGA-O2A-C1
11	12	306	CLA	CBA-CGA-O2A-C1
14	14	318	A86	C39-C38-O4-C34
11	7	309	CLA	O1D-CGD-O2D-CED
11	15	306	CLA	CBD-CGD-O2D-CED
14	10	302	A86	C39-C38-O4-C34
14	10	302	A86	O5-C38-O4-C34
11	14	310	CLA	O1A-CGA-O2A-C1
14	15	316	A86	O5-C38-O4-C34
14	16	314	A86	O5-C38-O4-C34
11	7	305	CLA	C4-C3-C5-C6
11	13	303	CLA	C4-C3-C5-C6
11	6	311	CLA	C2-C3-C5-C6
11	10	309	CLA	C2-C3-C5-C6
11	13	303	CLA	C2-C3-C5-C6
11	11	308	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
11	6	314	CLA	C2A-CAA-CBA-CGA
11	16	310	CLA	C2A-CAA-CBA-CGA
11	12	312	CLA	O1A-CGA-O2A-C1
11	6	307	CLA	C3-C5-C6-C7
11	7	302	CLA	C3-C5-C6-C7
11	7	305	CLA	C3-C5-C6-C7
11	12	312	CLA	C3-C5-C6-C7
11	14	302	CLA	C3-C5-C6-C7
11	7	305	CLA	CBA-CGA-O2A-C1
11	12	312	CLA	CBA-CGA-O2A-C1
11	14	302	CLA	CBA-CGA-O2A-C1
16	8	320	LMG	C29-C28-O8-C9
14	14	317	A86	O5-C38-O4-C34
11	10	309	CLA	CBD-CGD-O2D-CED
11	12	307	CLA	CBD-CGD-O2D-CED
11	12	308	CLA	O1D-CGD-O2D-CED
11	7	305	CLA	O1A-CGA-O2A-C1
11	14	302	CLA	O1A-CGA-O2A-C1
11	15	307	CLA	O1A-CGA-O2A-C1
11	16	306	CLA	O1A-CGA-O2A-C1
14	14	316	A86	O5-C38-O4-C34
11	14	310	CLA	O1D-CGD-O2D-CED
13	6	318	DD6	C11-C10-C9-C8
13	7	301	DD6	C24-C25-C26-C27
13	12	317	DD6	C11-C10-C9-C8
13	13	314	DD6	C11-C10-C9-C8
13	15	318	DD6	C24-C25-C26-C27
13	15	319	DD6	C11-C10-C9-C8
14	8	315	A86	C24-C25-C26-C27
14	8	318	A86	C24-C25-C26-C27
14	8	318	A86	C3-C4-C5-C6
14	11	315	A86	C11-C10-C9-C8
14	14	315	A86	C3-C4-C5-C6
14	14	317	A86	C24-C25-C26-C27
14	14	321	A86	C1-C2-C3-C4
14	15	322	A86	C11-C10-C9-C8
14	16	314	A86	C11-C10-C9-C8
16	8	321	LMG	O6-C5-C6-O5
14	11	315	A86	C39-C38-O4-C34
11	10	311	CLA	CBD-CGD-O2D-CED
11	12	302	CLA	CBD-CGD-O2D-CED
11	12	321	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
11	15	303	CLA	CBD-CGD-O2D-CED
12	11	311	KC1	CBD-CGD-O2D-CED
12	8	311	KC1	O1D-CGD-O2D-CED
11	10	303	CLA	C3-C5-C6-C7
11	13	302	CLA	C3-C5-C6-C7
11	16	303	CLA	C3-C5-C6-C7
11	7	302	CLA	CBA-CGA-O2A-C1
11	14	310	CLA	CBA-CGA-O2A-C1
14	11	315	A86	O5-C38-O4-C34
16	8	321	LMG	C4-C5-C6-O5
11	8	305	CLA	CBD-CGD-O2D-CED
11	10	308	CLA	CBD-CGD-O2D-CED
12	10	310	KC1	CBD-CGD-O2D-CED
11	15	307	CLA	CBA-CGA-O2A-C1
11	16	306	CLA	CBA-CGA-O2A-C1
16	8	320	LMG	O6-C5-C6-O5
12	6	308	KC1	CAA-CBA-CGA-O2A
12	8	313	KC1	CAA-CBA-CGA-O2A
12	13	305	KC1	CAA-CBA-CGA-O1A
12	13	308	KC1	CAA-CBA-CGA-O2A
12	13	312	KC1	CAA-CBA-CGA-O1A
12	14	306	KC1	CAA-CBA-CGA-O2A
11	6	306	CLA	C4-C3-C5-C6
11	8	304	CLA	C4-C3-C5-C6
11	11	303	CLA	C4-C3-C5-C6
11	14	302	CLA	C4-C3-C5-C6
11	8	304	CLA	C2-C3-C5-C6
11	11	303	CLA	C2-C3-C5-C6
11	12	302	CLA	C2-C3-C5-C6
11	14	302	CLA	C2-C3-C5-C6
11	7	304	CLA	C2A-CAA-CBA-CGA
11	14	312	CLA	C2A-CAA-CBA-CGA
11	16	307	CLA	C2A-CAA-CBA-CGA
11	7	302	CLA	O1A-CGA-O2A-C1
11	12	310	CLA	CBA-CGA-O2A-C1
14	14	314	A86	C39-C38-O4-C34
12	6	305	KC1	CAA-CBA-CGA-O1A
12	6	308	KC1	CAA-CBA-CGA-O1A
12	7	307	KC1	CAA-CBA-CGA-O1A
12	10	310	KC1	CAA-CBA-CGA-O1A
12	10	312	KC1	CAA-CBA-CGA-O1A
12	11	304	KC1	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
12	11	304	KC1	CAA-CBA-CGA-O2A
12	11	310	KC1	CAA-CBA-CGA-O1A
12	12	313	KC1	CAA-CBA-CGA-O1A
12	13	308	KC1	CAA-CBA-CGA-O1A
12	13	312	KC1	CAA-CBA-CGA-O2A
12	14	306	KC1	CAA-CBA-CGA-O1A
12	14	308	KC1	CAA-CBA-CGA-O1A
12	14	308	KC1	CAA-CBA-CGA-O2A
16	8	323	LMG	C11-C10-O7-C8
12	7	307	KC1	O1D-CGD-O2D-CED
11	13	307	CLA	O1A-CGA-O2A-C1
11	6	314	CLA	C3-C5-C6-C7
11	6	314	CLA	CBA-CGA-O2A-C1
11	7	303	CLA	CBA-CGA-O2A-C1
11	7	310	CLA	CBA-CGA-O2A-C1
11	8	303	CLA	CBA-CGA-O2A-C1
11	8	308	CLA	CBA-CGA-O2A-C1
11	10	309	CLA	CBA-CGA-O2A-C1
11	11	307	CLA	CBA-CGA-O2A-C1
11	11	309	CLA	CBA-CGA-O2A-C1
11	12	308	CLA	CBA-CGA-O2A-C1
11	13	307	CLA	CBA-CGA-O2A-C1
11	15	302	CLA	CBA-CGA-O2A-C1
11	15	304	CLA	CBA-CGA-O2A-C1
11	16	303	CLA	CBA-CGA-O2A-C1
13	6	316	DD6	C11-C10-C9-C8
14	10	315	A86	C11-C10-C9-C8
14	12	314	A86	C11-C10-C9-C8
14	14	317	A86	C11-C10-C9-C8
14	14	318	A86	C3-C4-C5-C6
14	15	316	A86	C3-C4-C5-C6
14	15	317	A86	C24-C25-C26-C27
11	14	302	CLA	C13-C15-C16-C17
12	6	305	KC1	CAA-CBA-CGA-O2A
12	7	312	KC1	CAA-CBA-CGA-O2A
12	8	313	KC1	CAA-CBA-CGA-O1A
12	8	314	KC1	CAA-CBA-CGA-O2A
12	10	310	KC1	CAA-CBA-CGA-O2A
12	10	312	KC1	CAA-CBA-CGA-O2A
12	11	311	KC1	CAA-CBA-CGA-O2A
12	12	313	KC1	CAA-CBA-CGA-O2A
12	13	305	KC1	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
12	13	306	KC1	CAA-CBA-CGA-O1A
12	13	306	KC1	CAA-CBA-CGA-O2A
11	6	306	CLA	C10-C11-C12-C13
11	7	309	CLA	C8-C10-C11-C12
11	11	307	CLA	C8-C10-C11-C12
11	11	309	CLA	C15-C16-C17-C18
11	13	302	CLA	C5-C6-C7-C8
11	12	310	CLA	C3-C5-C6-C7
16	7	319	LMG	C2-C1-O1-C7
16	8	320	LMG	O7-C8-C9-O8
11	10	309	CLA	O1A-CGA-O2A-C1
11	15	302	CLA	O1A-CGA-O2A-C1
11	6	306	CLA	C2-C3-C5-C6
11	6	304	CLA	C11-C12-C13-C14
11	11	308	CLA	C11-C10-C8-C9
11	16	303	CLA	C11-C12-C13-C14
12	11	306	KC1	O1D-CGD-O2D-CED
11	15	311	CLA	CBD-CGD-O2D-CED
11	7	303	CLA	C10-C11-C12-C13
13	6	315	DD6	C7-C6-C8-C9
13	6	318	DD6	C7-C6-C8-C9
13	7	316	DD6	C7-C6-C8-C9
13	7	317	DD6	C12-C11-C13-C14
13	8	316	DD6	C-C1-C24-C25
13	8	316	DD6	C7-C6-C8-C9
13	10	313	DD6	C12-C11-C13-C14
13	10	313	DD6	C7-C6-C8-C9
13	10	314	DD6	C-C1-C24-C25
13	10	314	DD6	C12-C11-C13-C14
13	11	312	DD6	C12-C11-C13-C14
13	12	315	DD6	C-C1-C24-C25
13	12	315	DD6	C7-C6-C8-C9
13	13	314	DD6	C-C1-C24-C25
13	13	314	DD6	C12-C11-C13-C14
13	15	318	DD6	C12-C11-C13-C14
13	15	319	DD6	C-C1-C24-C25
13	15	319	DD6	C12-C11-C13-C14
13	15	319	DD6	C7-C6-C8-C9
13	16	313	DD6	C-C1-C24-C25
13	16	313	DD6	C12-C11-C13-C14
14	6	317	A86	C-C1-C24-C25
14	7	314	A86	C-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
14	8	318	A86	C7-C6-C8-C9
14	10	302	A86	C-C1-C24-C25
14	10	315	A86	C-C1-C24-C25
14	11	315	A86	C7-C6-C8-C9
14	12	316	A86	C7-C6-C8-C9
14	13	313	A86	C7-C6-C8-C9
14	14	314	A86	C7-C6-C8-C9
14	14	315	A86	C7-C6-C8-C9
14	14	317	A86	C7-C6-C8-C9
14	14	318	A86	C7-C6-C8-C9
14	14	320	A86	C7-C6-C8-C9
14	14	321	A86	C7-C6-C8-C9
14	15	315	A86	C-C1-C24-C25
14	15	321	A86	C7-C6-C8-C9
14	16	312	A86	C7-C6-C8-C9
13	6	315	DD6	C10-C11-C13-C14
13	6	316	DD6	C10-C11-C13-C14
13	6	316	DD6	C5-C6-C8-C9
13	6	318	DD6	C10-C11-C13-C14
13	7	317	DD6	C5-C6-C8-C9
13	8	316	DD6	C10-C11-C13-C14
13	16	313	DD6	C10-C11-C13-C14
14	6	317	A86	C2-C1-C24-C25
14	7	314	A86	C2-C1-C24-C25
14	8	318	A86	C2-C1-C24-C25
14	10	302	A86	C2-C1-C24-C25
14	11	314	A86	C5-C6-C8-C9
14	11	315	A86	C5-C6-C8-C9
14	13	313	A86	C5-C6-C8-C9
14	13	315	A86	C2-C1-C24-C25
14	14	314	A86	C5-C6-C8-C9
14	14	315	A86	C5-C6-C8-C9
14	14	316	A86	C2-C1-C24-C25
14	14	317	A86	C5-C6-C8-C9
14	14	318	A86	C5-C6-C8-C9
14	14	320	A86	C5-C6-C8-C9
14	14	321	A86	C5-C6-C8-C9
14	15	315	A86	C2-C1-C24-C25
14	16	312	A86	C5-C6-C8-C9
11	11	307	CLA	O1A-CGA-O2A-C1
11	6	306	CLA	C15-C16-C17-C18
11	13	302	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
12	13	306	KC1	O1D-CGD-O2D-CED
12	7	307	KC1	CAA-CBA-CGA-O2A
12	7	312	KC1	CAA-CBA-CGA-O1A
12	11	311	KC1	CAA-CBA-CGA-O1A
11	12	308	CLA	C10-C11-C12-C13
11	14	302	CLA	C10-C11-C12-C13
11	15	304	CLA	C8-C10-C11-C12
11	16	302	CLA	C8-C10-C11-C12
16	8	320	LMG	C4-C5-C6-O5
11	11	309	CLA	O1A-CGA-O2A-C1
11	16	303	CLA	O1A-CGA-O2A-C1
11	6	303	CLA	C8-C10-C11-C12
11	7	302	CLA	C10-C11-C12-C13
11	7	306	CLA	C13-C15-C16-C17
11	7	306	CLA	C15-C16-C17-C18
11	7	308	CLA	C13-C15-C16-C17
11	8	301	CLA	C8-C10-C11-C12
11	8	301	CLA	C10-C11-C12-C13
11	10	309	CLA	C10-C11-C12-C13
11	11	308	CLA	C8-C10-C11-C12
11	8	301	CLA	O1D-CGD-O2D-CED
11	6	314	CLA	O1A-CGA-O2A-C1
11	8	303	CLA	O1A-CGA-O2A-C1
11	6	311	CLA	CBD-CGD-O2D-CED
11	8	302	CLA	C15-C16-C17-C18
11	10	305	CLA	C8-C10-C11-C12
11	12	312	CLA	C10-C11-C12-C13
11	8	301	CLA	C3-C5-C6-C7
14	11	314	A86	C35-C34-O4-C38
12	10	306	KC1	O1D-CGD-O2D-CED
12	8	314	KC1	CAA-CBA-CGA-O1A
12	11	306	KC1	CAA-CBA-CGA-O2A
12	11	310	KC1	CAA-CBA-CGA-O2A
11	6	302	CLA	C13-C15-C16-C17
11	7	302	CLA	C8-C10-C11-C12
11	7	305	CLA	C5-C6-C7-C8
11	12	306	CLA	C10-C11-C12-C13
11	13	307	CLA	C10-C11-C12-C13
11	15	302	CLA	C5-C6-C7-C8
11	16	301	CLA	C13-C15-C16-C17
11	11	303	CLA	CBD-CGD-O2D-CED
11	11	307	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
11	14	303	CLA	C8-C10-C11-C12
11	14	302	CLA	C15-C16-C17-C18
11	15	313	CLA	C5-C6-C7-C8
11	6	304	CLA	C11-C12-C13-C15
11	13	303	CLA	C11-C12-C13-C15
11	15	304	CLA	C11-C12-C13-C15
11	16	301	CLA	C3-C5-C6-C7
11	7	303	CLA	O1A-CGA-O2A-C1
11	7	310	CLA	O1A-CGA-O2A-C1
13	7	301	DD6	C3-C4-C5-C6
13	11	312	DD6	C11-C10-C9-C8
14	7	314	A86	C24-C25-C26-C27
14	7	315	A86	C24-C25-C26-C27
14	10	302	A86	C1-C2-C3-C4
14	10	315	A86	C1-C2-C3-C4
14	10	317	A86	C3-C4-C5-C6
14	11	313	A86	C24-C25-C26-C27
14	11	313	A86	C3-C4-C5-C6
14	11	314	A86	C11-C10-C9-C8
14	14	316	A86	C24-C25-C26-C27
14	14	319	A86	C3-C4-C5-C6
14	15	317	A86	C11-C10-C9-C8
11	8	308	CLA	C2A-CAA-CBA-CGA
11	13	301	CLA	C2A-CAA-CBA-CGA
11	13	309	CLA	C2A-CAA-CBA-CGA
11	15	307	CLA	C2A-CAA-CBA-CGA
11	15	314	CLA	C2A-CAA-CBA-CGA
12	13	305	KC1	O1D-CGD-O2D-CED
11	13	302	CLA	C8-C10-C11-C12
14	12	316	A86	O5-C38-O4-C34
11	12	310	CLA	O1A-CGA-O2A-C1
11	15	304	CLA	O1A-CGA-O2A-C1
11	13	301	CLA	CBD-CGD-O2D-CED
16	7	319	LMG	O6-C1-O1-C7
17	15	301	LMT	O5'-C1'-O1'-C1
14	14	301	A86	C33-C34-O4-C38
11	11	303	CLA	C3-C5-C6-C7
11	14	307	CLA	C3-C5-C6-C7
11	8	302	CLA	C5-C6-C7-C8
11	8	308	CLA	O1A-CGA-O2A-C1
11	12	308	CLA	O1A-CGA-O2A-C1
14	14	318	A86	O5-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
12	11	306	KC1	CAA-CBA-CGA-O1A
11	6	304	CLA	C5-C6-C7-C8
11	7	310	CLA	C15-C16-C17-C18
11	8	303	CLA	C10-C11-C12-C13
11	12	304	CLA	C10-C11-C12-C13
11	12	312	CLA	C8-C10-C11-C12
11	12	304	CLA	C3-C5-C6-C7
11	16	303	CLA	C15-C16-C17-C18
11	7	304	CLA	C4-C3-C5-C6
11	7	309	CLA	C4-C3-C5-C6
11	7	305	CLA	C2-C3-C5-C6
11	7	309	CLA	C2A-CAA-CBA-CGA
11	16	302	CLA	C16-C17-C18-C20
12	8	307	KC1	CAA-CBA-CGA-O2A
12	8	311	KC1	CAA-CBA-CGA-O2A
12	8	312	KC1	CAA-CBA-CGA-O2A
11	12	302	CLA	CBA-CGA-O2A-C1
11	16	305	CLA	CBA-CGA-O2A-C1
16	7	319	LMG	C29-C28-O8-C9
17	16	315	LMT	C5'-C4'-O1B-C1B
13	7	317	DD6	C11-C10-C9-C8
13	10	314	DD6	C24-C25-C26-C27
13	13	314	DD6	C3-C4-C5-C6
14	10	317	A86	C1-C2-C3-C4
14	11	314	A86	C24-C25-C26-C27
14	12	316	A86	C11-C10-C9-C8
14	13	315	A86	C3-C4-C5-C6
14	14	318	A86	C11-C10-C9-C8
14	14	321	A86	C3-C4-C5-C6
14	15	317	A86	C3-C4-C5-C6
14	15	320	A86	C1-C2-C3-C4
14	15	320	A86	C3-C4-C5-C6
17	15	301	LMT	C3-C4-C5-C6
13	6	316	DD6	C9-C10-C11-C12
13	7	317	DD6	C9-C10-C11-C12
13	7	317	DD6	C4-C5-C6-C7
13	8	317	DD6	C9-C10-C11-C12
13	12	317	DD6	C9-C10-C11-C12
13	15	318	DD6	C-C1-C2-C3
11	12	303	CLA	C3-C5-C6-C7
12	12	309	KC1	C2A-CAA-CBA-CGA
12	12	313	KC1	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
12	13	311	KC1	C2A-CAA-CBA-CGA
12	13	312	KC1	C2A-CAA-CBA-CGA
12	14	311	KC1	C2A-CAA-CBA-CGA
16	8	321	LMG	C15-C16-C17-C18
12	8	307	KC1	CAA-CBA-CGA-O1A
11	7	306	CLA	C10-C11-C12-C13
12	13	308	KC1	CBD-CGD-O2D-CED
11	15	306	CLA	O1D-CGD-O2D-CED
11	12	302	CLA	C3-C5-C6-C7
11	10	309	CLA	O1D-CGD-O2D-CED
13	6	316	DD6	C9-C10-C11-C13
13	7	301	DD6	C9-C10-C11-C13
13	7	316	DD6	C9-C10-C11-C13
13	8	317	DD6	C24-C1-C2-C3
13	12	315	DD6	C24-C1-C2-C3
13	12	317	DD6	C24-C1-C2-C3
13	13	314	DD6	C4-C5-C6-C8
13	15	318	DD6	C4-C5-C6-C8
13	16	313	DD6	C4-C5-C6-C8
16	14	322	LMG	C4-C5-C6-O5
16	7	319	LMG	C30-C31-C32-C33
11	13	302	CLA	C10-C11-C12-C13
11	13	301	CLA	C16-C17-C18-C19
16	8	321	LMG	C16-C17-C18-C19
11	7	304	CLA	C2-C3-C5-C6
11	6	307	CLA	C6-C7-C8-C9
11	7	306	CLA	C11-C12-C13-C14
11	7	308	CLA	C6-C7-C8-C9
11	13	303	CLA	C14-C13-C15-C16
16	8	320	LMG	C28-C29-C30-C31
12	8	311	KC1	CAA-CBA-CGA-O1A
11	12	302	CLA	C2A-CAA-CBA-CGA
16	8	321	LMG	O10-C28-O8-C9
13	7	317	DD6	C-C1-C24-C25
14	14	301	A86	C7-C6-C8-C9
14	15	316	A86	C7-C6-C8-C9
15	6	319	LHG	O1-C1-C2-C3
13	11	312	DD6	C5-C6-C8-C9
13	15	318	DD6	C2-C1-C24-C25
14	10	315	A86	C2-C1-C24-C25
14	15	316	A86	C5-C6-C8-C9
11	8	304	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
11	15	309	CLA	C10-C11-C12-C13
16	8	320	LMG	C11-C10-O7-C8
11	15	307	CLA	CBD-CGD-O2D-CED
11	10	308	CLA	C16-C17-C18-C19
11	10	308	CLA	C16-C17-C18-C20
11	16	302	CLA	C16-C17-C18-C19
11	11	309	CLA	C10-C11-C12-C13
11	12	307	CLA	O1D-CGD-O2D-CED
12	8	307	KC1	CBD-CGD-O2D-CED
11	16	303	CLA	C8-C10-C11-C12
12	6	310	KC1	CAA-CBA-CGA-O1A
12	6	310	KC1	CAA-CBA-CGA-O2A
12	8	312	KC1	CAA-CBA-CGA-O1A
16	14	322	LMG	O10-C28-O8-C9
11	11	308	CLA	O1D-CGD-O2D-CED
11	12	321	CLA	O1D-CGD-O2D-CED
11	8	304	CLA	C3A-C2A-CAA-CBA
11	10	305	CLA	C3A-C2A-CAA-CBA
11	10	311	CLA	C3A-C2A-CAA-CBA
11	11	305	CLA	C3A-C2A-CAA-CBA
11	13	303	CLA	C3A-C2A-CAA-CBA
11	13	304	CLA	C3A-C2A-CAA-CBA
11	13	309	CLA	C3A-C2A-CAA-CBA
11	14	303	CLA	C3A-C2A-CAA-CBA
11	14	313	CLA	C3A-C2A-CAA-CBA
11	15	305	CLA	C3A-C2A-CAA-CBA
11	15	308	CLA	C3A-C2A-CAA-CBA
11	15	311	CLA	C3A-C2A-CAA-CBA
11	15	312	CLA	C3A-C2A-CAA-CBA
11	16	306	CLA	C3A-C2A-CAA-CBA
11	16	307	CLA	C3A-C2A-CAA-CBA
11	16	308	CLA	C3A-C2A-CAA-CBA
11	16	309	CLA	C3A-C2A-CAA-CBA
17	8	319	LMT	C11-C10-C9-C8
11	16	301	CLA	C16-C17-C18-C20
12	11	311	KC1	O1D-CGD-O2D-CED
16	8	321	LMG	C11-C12-C13-C14
11	6	306	CLA	CBA-CGA-O2A-C1
11	10	308	CLA	CBA-CGA-O2A-C1
17	8	319	LMT	O1'-C1-C2-C3
17	16	315	LMT	C3'-C4'-O1B-C1B
15	6	319	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
16	7	319	LMG	C11-C12-C13-C14
16	8	321	LMG	C12-C13-C14-C15
11	13	301	CLA	C16-C17-C18-C20
11	16	305	CLA	O1A-CGA-O2A-C1
12	12	309	KC1	CAA-CBA-CGA-O1A
11	13	301	CLA	C3-C5-C6-C7
11	15	313	CLA	CBA-CGA-O2A-C1
11	6	304	CLA	C13-C15-C16-C17
11	7	309	CLA	C15-C16-C17-C18
11	8	305	CLA	C4-C3-C5-C6
11	6	301	CLA	C12-C13-C15-C16
11	6	304	CLA	C11-C10-C8-C7
11	7	306	CLA	C12-C13-C15-C16
11	7	308	CLA	C6-C7-C8-C10
11	12	303	CLA	C6-C7-C8-C10
11	13	303	CLA	C12-C13-C15-C16
11	16	302	CLA	C2-C3-C5-C6
11	16	303	CLA	C11-C12-C13-C15
11	15	313	CLA	O1A-CGA-O2A-C1
16	8	320	LMG	C36-C37-C38-C39
13	6	318	DD6	C1-C2-C3-C4
13	8	317	DD6	C3-C4-C5-C6
14	10	316	A86	C11-C10-C9-C8
14	15	322	A86	C24-C25-C26-C27
17	16	315	LMT	O5'-C5'-C6'-O6'
11	6	307	CLA	CBA-CGA-O2A-C1
11	8	304	CLA	CBA-CGA-O2A-C1
11	10	311	CLA	O1D-CGD-O2D-CED
11	6	307	CLA	C10-C11-C12-C13
11	10	305	CLA	C15-C16-C17-C18
17	16	315	LMT	C7-C8-C9-C10
16	8	320	LMG	C10-C11-C12-C13
16	8	321	LMG	C32-C33-C34-C35
12	6	305	KC1	C2B-C3B-CAB-CBB
12	6	308	KC1	C2B-C3B-CAB-CBB
12	6	310	KC1	C2B-C3B-CAB-CBB
12	8	312	KC1	C2B-C3B-CAB-CBB
12	8	314	KC1	C2B-C3B-CAB-CBB
12	10	306	KC1	C2B-C3B-CAB-CBB
12	11	304	KC1	C2B-C3B-CAB-CBB
12	11	306	KC1	C2B-C3B-CAB-CBB
12	12	305	KC1	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
12	12	313	KC1	C2B-C3B-CAB-CBB
12	13	305	KC1	C2B-C3B-CAB-CBB
12	13	306	KC1	C2B-C3B-CAB-CBB
12	13	308	KC1	C2B-C3B-CAB-CBB
12	13	312	KC1	C2B-C3B-CAB-CBB
12	14	311	KC1	C2B-C3B-CAB-CBB
12	16	304	KC1	C2B-C3B-CAB-CBB
11	10	305	CLA	C3-C5-C6-C7
11	10	309	CLA	C3-C5-C6-C7
11	15	309	CLA	CBA-CGA-O2A-C1
15	6	319	LHG	C8-C7-O7-C5
16	7	319	LMG	C11-C10-O7-C8
14	14	314	A86	O5-C38-O4-C34
12	6	305	KC1	C4B-C3B-CAB-CBB
12	6	308	KC1	C4B-C3B-CAB-CBB
12	6	310	KC1	C4B-C3B-CAB-CBB
12	8	310	KC1	C4B-C3B-CAB-CBB
12	8	311	KC1	C4B-C3B-CAB-CBB
12	8	312	KC1	C4B-C3B-CAB-CBB
12	8	314	KC1	C4B-C3B-CAB-CBB
12	10	306	KC1	C4B-C3B-CAB-CBB
12	11	306	KC1	C4B-C3B-CAB-CBB
12	11	311	KC1	C4B-C3B-CAB-CBB
12	12	305	KC1	C4B-C3B-CAB-CBB
12	12	313	KC1	C4B-C3B-CAB-CBB
12	13	305	KC1	C4B-C3B-CAB-CBB
12	13	306	KC1	C4B-C3B-CAB-CBB
12	13	308	KC1	C4B-C3B-CAB-CBB
12	13	312	KC1	C4B-C3B-CAB-CBB
12	14	311	KC1	C4B-C3B-CAB-CBB
12	16	304	KC1	C4B-C3B-CAB-CBB
11	6	307	CLA	C13-C15-C16-C17
11	7	308	CLA	C5-C6-C7-C8
11	15	302	CLA	C10-C11-C12-C13
16	8	320	LMG	O9-C10-O7-C8
14	7	315	A86	C39-C38-O4-C34
12	12	309	KC1	CAA-CBA-CGA-O2A
11	16	302	CLA	C4-C3-C5-C6
11	7	309	CLA	C2-C3-C5-C6
16	8	321	LMG	C30-C31-C32-C33
11	7	302	CLA	C11-C10-C8-C9
11	12	303	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
11	13	303	CLA	C11-C12-C13-C14
11	16	303	CLA	C11-C10-C8-C9
11	7	302	CLA	C2A-CAA-CBA-CGA
11	16	301	CLA	C2A-CAA-CBA-CGA
17	8	319	LMT	C5-C6-C7-C8
17	7	320	LMT	O5B-C5B-C6B-O6B
14	10	315	A86	C7-C6-C8-C9
14	14	319	A86	C7-C6-C8-C9
14	10	315	A86	C5-C6-C8-C9
14	14	319	A86	C5-C6-C8-C9
11	8	304	CLA	O1A-CGA-O2A-C1
11	6	311	CLA	C1A-C2A-CAA-CBA
11	6	314	CLA	C1A-C2A-CAA-CBA
11	7	304	CLA	C1A-C2A-CAA-CBA
11	7	310	CLA	C1A-C2A-CAA-CBA
11	8	301	CLA	C1A-C2A-CAA-CBA
11	8	303	CLA	C1A-C2A-CAA-CBA
11	10	303	CLA	C1A-C2A-CAA-CBA
11	10	308	CLA	C1A-C2A-CAA-CBA
11	10	309	CLA	C1A-C2A-CAA-CBA
11	10	311	CLA	C1A-C2A-CAA-CBA
11	11	303	CLA	C1A-C2A-CAA-CBA
11	11	308	CLA	C1A-C2A-CAA-CBA
11	11	309	CLA	C1A-C2A-CAA-CBA
11	12	308	CLA	C1A-C2A-CAA-CBA
11	12	310	CLA	C1A-C2A-CAA-CBA
11	13	304	CLA	C1A-C2A-CAA-CBA
11	13	307	CLA	C1A-C2A-CAA-CBA
11	14	305	CLA	C1A-C2A-CAA-CBA
11	14	312	CLA	C1A-C2A-CAA-CBA
11	15	302	CLA	C1A-C2A-CAA-CBA
11	15	303	CLA	C1A-C2A-CAA-CBA
11	15	305	CLA	C1A-C2A-CAA-CBA
11	15	307	CLA	C1A-C2A-CAA-CBA
11	15	309	CLA	C1A-C2A-CAA-CBA
11	15	312	CLA	C1A-C2A-CAA-CBA
11	15	314	CLA	C1A-C2A-CAA-CBA
11	16	301	CLA	C1A-C2A-CAA-CBA
11	16	309	CLA	C1A-C2A-CAA-CBA
11	16	310	CLA	C1A-C2A-CAA-CBA
16	8	321	LMG	O9-C10-O7-C8
14	10	301	A86	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
14	11	315	A86	C3-C4-C5-C6
14	14	315	A86	C1-C2-C3-C4
11	7	309	CLA	C13-C15-C16-C17
11	8	302	CLA	C13-C15-C16-C17
11	11	303	CLA	C13-C15-C16-C17
15	6	319	LHG	C4-O6-P-O3
11	13	303	CLA	C3-C5-C6-C7
11	12	302	CLA	O1D-CGD-O2D-CED
11	12	302	CLA	O1A-CGA-O2A-C1
11	15	303	CLA	O1D-CGD-O2D-CED
11	16	301	CLA	C16-C17-C18-C19
16	8	320	LMG	C33-C34-C35-C36
11	16	306	CLA	C4-C3-C5-C6
16	8	320	LMG	C7-C8-C9-O8
16	8	321	LMG	O1-C7-C8-C9
17	8	322	LMT	O5B-C5B-C6B-O6B
11	10	305	CLA	C13-C15-C16-C17
11	6	307	CLA	O1A-CGA-O2A-C1
11	10	308	CLA	O1A-CGA-O2A-C1
17	8	319	LMT	O5B-C5B-C6B-O6B
11	15	305	CLA	CBD-CGD-O2D-CED
17	7	320	LMT	C6-C7-C8-C9
16	7	319	LMG	C28-C29-C30-C31
11	12	307	CLA	CBA-CGA-O2A-C1
11	15	303	CLA	C10-C11-C12-C13
12	14	308	KC1	C2C-C3C-CAC-CBC
11	6	302	CLA	C4-C3-C5-C6
16	8	321	LMG	C29-C30-C31-C32
12	10	310	KC1	O1D-CGD-O2D-CED
11	8	305	CLA	CBA-CGA-O2A-C1
16	14	322	LMG	C29-C28-O8-C9
11	16	302	CLA	C10-C11-C12-C13
11	7	304	CLA	C3-C5-C6-C7
11	12	304	CLA	CBA-CGA-O2A-C1
11	8	305	CLA	O1A-CGA-O2A-C1
11	15	309	CLA	O1A-CGA-O2A-C1
13	7	301	DD6	C24-C1-C2-C3
16	8	323	LMG	O7-C8-C9-O8
16	8	321	LMG	C29-C28-O8-C9
11	6	306	CLA	O1A-CGA-O2A-C1
11	6	302	CLA	C2-C3-C5-C6
11	6	307	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
11	6	307	CLA	C12-C13-C15-C16
11	6	311	CLA	C11-C12-C13-C15
11	7	302	CLA	C11-C10-C8-C7
11	7	306	CLA	C11-C10-C8-C7
11	7	309	CLA	C12-C13-C15-C16
11	8	301	CLA	C11-C12-C13-C15
11	8	303	CLA	C11-C12-C13-C15
11	11	307	CLA	C11-C12-C13-C15
11	11	307	CLA	C12-C13-C15-C16
11	11	308	CLA	C12-C13-C15-C16
11	12	302	CLA	C11-C12-C13-C15
11	13	302	CLA	C11-C12-C13-C15
11	15	304	CLA	C6-C7-C8-C10
11	15	304	CLA	C12-C13-C15-C16
11	16	303	CLA	C6-C7-C8-C10
11	16	303	CLA	C11-C10-C8-C7
11	16	306	CLA	C2-C3-C5-C6
11	12	304	CLA	CAA-CBA-CGA-O2A
11	6	301	CLA	C14-C13-C15-C16
11	6	311	CLA	C11-C12-C13-C14
11	7	306	CLA	C11-C10-C8-C9
11	7	306	CLA	C14-C13-C15-C16
11	7	309	CLA	C14-C13-C15-C16
11	7	310	CLA	C6-C7-C8-C9
11	8	303	CLA	C11-C12-C13-C14
11	11	307	CLA	C11-C12-C13-C14
11	11	308	CLA	C14-C13-C15-C16
11	11	309	CLA	C6-C7-C8-C9
11	11	309	CLA	C14-C13-C15-C16
11	12	304	CLA	C11-C10-C8-C9
11	13	302	CLA	C6-C7-C8-C9
11	14	303	CLA	C11-C10-C8-C9
11	15	304	CLA	C6-C7-C8-C9
11	16	303	CLA	C6-C7-C8-C9
16	14	322	LMG	C29-C30-C31-C32
11	11	308	CLA	CBA-CGA-O2A-C1
11	13	303	CLA	CBA-CGA-O2A-C1
11	10	307	CLA	C2A-CAA-CBA-CGA
11	8	305	CLA	O1D-CGD-O2D-CED
11	10	308	CLA	O1D-CGD-O2D-CED
11	15	311	CLA	O1D-CGD-O2D-CED
14	11	315	A86	C-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
14	14	319	A86	C-C1-C24-C25
14	16	312	A86	C-C1-C24-C25
17	8	324	LMT	C7-C8-C9-C10
13	11	312	DD6	C10-C11-C13-C14
14	11	313	A86	C5-C6-C8-C9
14	11	315	A86	C2-C1-C24-C25
14	14	319	A86	C2-C1-C24-C25
14	15	317	A86	C5-C6-C8-C9
14	16	312	A86	C2-C1-C24-C25
11	13	301	CLA	O1D-CGD-O2D-CED
11	6	301	CLA	CBA-CGA-O2A-C1
11	8	301	CLA	CBA-CGA-O2A-C1
12	8	310	KC1	CAA-CBA-CGA-O2A
11	16	306	CLA	CBD-CGD-O2D-CED
11	7	304	CLA	C16-C17-C18-C19
11	15	304	CLA	C10-C11-C12-C13
11	13	302	CLA	C4-C3-C5-C6
12	8	310	KC1	CAA-CBA-CGA-O1A
17	8	324	LMT	C4-C5-C6-C7
11	15	302	CLA	C16-C17-C18-C19
15	6	319	LHG	C11-C10-C9-C8
11	6	304	CLA	CBA-CGA-O2A-C1
11	13	301	CLA	CBA-CGA-O2A-C1
16	14	322	LMG	O6-C5-C6-O5
11	6	303	CLA	C3A-C2A-CAA-CBA
11	11	303	CLA	C3A-C2A-CAA-CBA
11	11	307	CLA	C13-C15-C16-C17
13	6	315	DD6	C3-C4-C5-C6
13	16	313	DD6	C24-C25-C26-C27
14	8	315	A86	O-C13-C14-C15
14	12	316	A86	O-C13-C14-C15
14	14	316	A86	O-C13-C14-C15
14	15	320	A86	O-C13-C14-C15
14	16	314	A86	O-C13-C14-C15
15	6	319	LHG	C10-C11-C12-C13
16	8	323	LMG	C7-C8-C9-O8
16	14	322	LMG	C7-C8-C9-O8
11	6	311	CLA	O1D-CGD-O2D-CED
11	8	302	CLA	C3-C5-C6-C7
11	8	303	CLA	C4-C3-C5-C6
11	12	321	CLA	C3-C5-C6-C7
11	16	301	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
15	6	319	LHG	O6-C4-C5-O7
17	15	301	LMT	C7-C8-C9-C10
12	10	306	KC1	C3A-C2A-CAA-CBA
12	11	311	KC1	C3A-C2A-CAA-CBA
12	12	305	KC1	C3A-C2A-CAA-CBA
12	13	306	KC1	C3A-C2A-CAA-CBA
12	13	310	KC1	C3A-C2A-CAA-CBA
11	12	304	CLA	O1A-CGA-O2A-C1
11	15	313	CLA	C10-C11-C12-C13
16	14	322	LMG	C16-C17-C18-C19
14	16	314	A86	C33-C34-O4-C38
16	8	321	LMG	O6-C1-O1-C7
12	13	308	KC1	O1D-CGD-O2D-CED
14	8	318	A86	C10-C11-C13-C14
14	10	302	A86	C10-C11-C13-C14
14	11	314	A86	C10-C11-C13-C14
14	11	315	A86	C10-C11-C13-C14
14	13	313	A86	C10-C11-C13-C14
14	14	318	A86	C10-C11-C13-C14
14	15	320	A86	C10-C11-C13-C14
14	16	312	A86	C10-C11-C13-C14
11	7	304	CLA	C2-C1-O2A-CGA
11	7	310	CLA	C2-C1-O2A-CGA
11	12	304	CLA	C2-C1-O2A-CGA
11	13	307	CLA	C2-C1-O2A-CGA
11	16	301	CLA	C2-C1-O2A-CGA
11	6	301	CLA	C11-C12-C13-C14
11	8	301	CLA	C11-C12-C13-C14
11	10	309	CLA	C11-C10-C8-C9
11	12	310	CLA	C11-C12-C13-C14
11	14	307	CLA	C11-C10-C8-C9
11	15	302	CLA	C14-C13-C15-C16
11	15	304	CLA	C14-C13-C15-C16
11	11	305	CLA	CBA-CGA-O2A-C1
11	13	303	CLA	O1A-CGA-O2A-C1
14	15	317	A86	C7-C6-C8-C9
13	11	312	DD6	C2-C1-C24-C25
14	15	321	A86	C5-C6-C8-C9
11	10	304	CLA	C8-C10-C11-C12
11	11	308	CLA	C10-C11-C12-C13
17	15	301	LMT	C4'-C5'-C6'-O6'
15	6	319	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
11	6	301	CLA	C11-C12-C13-C15
11	7	310	CLA	C6-C7-C8-C10
11	11	309	CLA	C6-C7-C8-C10
11	11	309	CLA	C12-C13-C15-C16
11	12	304	CLA	C11-C10-C8-C7
11	13	302	CLA	C2-C3-C5-C6
11	13	302	CLA	C6-C7-C8-C10
11	14	303	CLA	C11-C10-C8-C7
11	14	307	CLA	C11-C10-C8-C7
11	15	302	CLA	C12-C13-C15-C16
17	12	301	LMT	C1-C2-C3-C4
17	8	319	LMT	C6-C7-C8-C9
13	8	316	DD6	C3-C4-C5-C6
14	10	302	A86	C3-C4-C5-C6
14	12	314	A86	C24-C25-C26-C27
14	13	313	A86	C24-C25-C26-C27
14	13	313	A86	C3-C4-C5-C6
14	15	321	A86	C11-C10-C9-C8
11	7	304	CLA	C16-C17-C18-C20
17	7	320	LMT	C1-C2-C3-C4
12	14	308	KC1	C4C-C3C-CAC-CBC
11	6	306	CLA	CAD-CBD-CGD-O2D
11	7	308	CLA	CAD-CBD-CGD-O2D
11	8	304	CLA	CAD-CBD-CGD-O2D
11	11	308	CLA	CAD-CBD-CGD-O2D
11	12	306	CLA	CAD-CBD-CGD-O2D
11	12	307	CLA	CAD-CBD-CGD-O2D
11	13	304	CLA	CAD-CBD-CGD-O2D
11	14	302	CLA	CAD-CBD-CGD-O2D
11	14	310	CLA	CAD-CBD-CGD-O2D
11	15	311	CLA	CAD-CBD-CGD-O2D
11	16	302	CLA	CAD-CBD-CGD-O2D
11	16	308	CLA	CAD-CBD-CGD-O2D
12	6	310	KC1	CAD-CBD-CGD-O2D
12	7	307	KC1	C2B-C3B-CAB-CBB
12	10	310	KC1	CAD-CBD-CGD-O2D
12	11	304	KC1	CAD-CBD-CGD-O2D
12	12	309	KC1	C2B-C3B-CAB-CBB
12	13	311	KC1	CAD-CBD-CGD-O2D
12	14	308	KC1	C2B-C3B-CAB-CBB
12	14	311	KC1	CAD-CBD-CGD-O2D
12	16	304	KC1	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
14	6	317	A86	C28-C27-C29-C30
14	7	314	A86	C28-C27-C29-C30
14	15	317	A86	C28-C27-C29-C30
14	7	315	A86	O5-C38-O4-C34
16	7	319	LMG	O10-C28-O8-C9
11	15	309	CLA	C4-C3-C5-C6
11	6	301	CLA	C10-C11-C12-C13
16	8	320	LMG	C37-C38-C39-C40
14	10	301	A86	C12-C11-C13-O
14	11	301	A86	C12-C11-C13-O
14	11	314	A86	C12-C11-C13-O
14	13	315	A86	C12-C11-C13-O
14	14	316	A86	C12-C11-C13-O
14	15	317	A86	C12-C11-C13-O
14	16	312	A86	C12-C11-C13-O
12	6	309	KC1	C4B-C3B-CAB-CBB
12	10	310	KC1	C4B-C3B-CAB-CBB
12	14	306	KC1	C4B-C3B-CAB-CBB
11	10	308	CLA	C2A-CAA-CBA-CGA
11	15	302	CLA	C16-C17-C18-C20
11	6	312	CLA	CHA-CBD-CGD-O1D
11	6	312	CLA	CHA-CBD-CGD-O2D
11	7	311	CLA	CHA-CBD-CGD-O1D
11	7	311	CLA	CHA-CBD-CGD-O2D
11	8	308	CLA	CHA-CBD-CGD-O1D
11	8	308	CLA	CHA-CBD-CGD-O2D
11	13	307	CLA	CHA-CBD-CGD-O1D
11	13	307	CLA	CHA-CBD-CGD-O2D
11	14	304	CLA	CHA-CBD-CGD-O1D
11	14	304	CLA	CHA-CBD-CGD-O2D
11	15	305	CLA	CHA-CBD-CGD-O1D
11	15	310	CLA	CHA-CBD-CGD-O1D
11	15	313	CLA	CHA-CBD-CGD-O1D
11	15	313	CLA	CHA-CBD-CGD-O2D
11	16	306	CLA	CHA-CBD-CGD-O1D
11	16	306	CLA	CHA-CBD-CGD-O2D
11	16	308	CLA	CHA-CBD-CGD-O1D
12	6	308	KC1	CHA-CBD-CGD-O1D
12	6	308	KC1	CHA-CBD-CGD-O2D
12	6	309	KC1	CHA-CBD-CGD-O1D
12	6	309	KC1	CHA-CBD-CGD-O2D
12	8	310	KC1	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
12	10	306	KC1	CHA-CBD-CGD-O1D
12	11	306	KC1	CHA-CBD-CGD-O1D
12	11	310	KC1	CHA-CBD-CGD-O1D
12	11	310	KC1	CHA-CBD-CGD-O2D
12	12	311	KC1	CHA-CBD-CGD-O1D
12	12	311	KC1	CHA-CBD-CGD-O2D
12	13	305	KC1	CHA-CBD-CGD-O1D
11	11	305	CLA	O1A-CGA-O2A-C1
11	13	301	CLA	O1A-CGA-O2A-C1
13	10	314	DD6	C24-C1-C2-C3
11	7	306	CLA	C8-C10-C11-C12
11	6	304	CLA	O1A-CGA-O2A-C1
11	10	305	CLA	O1A-CGA-O2A-C1
14	7	314	A86	C10-C11-C13-O
14	8	315	A86	C13-C14-C15-O1
14	10	301	A86	C13-C14-C15-O1
14	10	302	A86	C13-C14-C15-O1
14	10	316	A86	C13-C14-C15-O1
14	11	301	A86	C10-C11-C13-O
14	11	301	A86	C13-C14-C15-O1
14	11	314	A86	C10-C11-C13-O
14	11	315	A86	C13-C14-C15-O1
14	12	314	A86	C13-C14-C15-O1
14	12	316	A86	C13-C14-C15-O1
14	13	315	A86	C10-C11-C13-O
14	13	315	A86	C13-C14-C15-O1
14	14	316	A86	C13-C14-C15-O1
14	14	317	A86	C13-C14-C15-O1
14	14	318	A86	C10-C11-C13-O
14	14	318	A86	C13-C14-C15-O1
14	15	321	A86	C13-C14-C15-O1
14	16	312	A86	C10-C11-C13-O
16	8	320	LMG	C35-C36-C37-C38
16	8	323	LMG	C28-C29-C30-C31
11	6	301	CLA	O1A-CGA-O2A-C1
11	8	301	CLA	O1A-CGA-O2A-C1
12	8	307	KC1	O1D-CGD-O2D-CED
11	11	308	CLA	O1A-CGA-O2A-C1
13	6	315	DD6	C12-C11-C13-C14
13	6	316	DD6	C12-C11-C13-C14
13	6	318	DD6	C-C1-C24-C25
13	7	317	DD6	C7-C6-C8-C9

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Mol	Chain	Res	Type	Atoms
14	10	317	A86	C-C1-C24-C25
14	11	313	A86	C7-C6-C8-C9
14	15	316	A86	C-C1-C24-C25
11	7	310	CLA	C13-C15-C16-C17
13	7	317	DD6	C10-C11-C13-C14
13	15	318	DD6	C10-C11-C13-C14
13	15	319	DD6	C10-C11-C13-C14
14	15	316	A86	C2-C1-C24-C25
16	7	319	LMG	C13-C14-C15-C16
11	15	305	CLA	O1D-CGD-O2D-CED
11	6	312	CLA	C1A-C2A-CAA-CBA
11	7	302	CLA	C15-C16-C17-C18
11	15	313	CLA	C13-C15-C16-C17
11	6	303	CLA	C2-C1-O2A-CGA
11	15	304	CLA	C2-C1-O2A-CGA
11	6	311	CLA	CBA-CGA-O2A-C1
11	15	307	CLA	O1D-CGD-O2D-CED
11	6	306	CLA	CBD-CGD-O2D-CED
17	12	320	LMT	C5-C6-C7-C8
11	6	303	CLA	C3-C5-C6-C7
11	15	302	CLA	C3-C5-C6-C7
11	11	303	CLA	O1D-CGD-O2D-CED
15	6	319	LHG	C4-O6-P-O4
17	8	319	LMT	C2-C3-C4-C5
11	10	303	CLA	CBA-CGA-O2A-C1
11	11	307	CLA	O1D-CGD-O2D-CED
11	12	312	CLA	C2A-CAA-CBA-CGA
11	15	304	CLA	C3-C5-C6-C7
16	14	322	LMG	C17-C18-C19-C20
16	14	322	LMG	C11-C10-O7-C8
11	15	309	CLA	C16-C17-C18-C20
11	6	312	CLA	CAD-CBD-CGD-O1D
11	7	311	CLA	CAD-CBD-CGD-O1D
11	8	308	CLA	CAD-CBD-CGD-O1D
11	13	303	CLA	CAD-CBD-CGD-O1D
11	14	312	CLA	CAD-CBD-CGD-O1D
12	6	309	KC1	CAD-CBD-CGD-O1D
12	12	311	KC1	CAD-CBD-CGD-O1D
14	6	317	A86	C26-C27-C29-C30
14	15	317	A86	C26-C27-C29-C30
14	16	312	A86	C26-C27-C29-C30
11	10	307	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
11	12	302	CLA	C15-C16-C17-C18
11	13	301	CLA	C13-C15-C16-C17
17	8	324	LMT	O1'-C1-C2-C3
11	12	308	CLA	C4-C3-C5-C6
11	8	305	CLA	C12-C13-C15-C16
11	11	308	CLA	C11-C10-C8-C7
11	12	312	CLA	C11-C10-C8-C7
11	14	302	CLA	C3A-C2A-CAA-CBA
13	8	316	DD6	C11-C10-C9-C8
13	12	315	DD6	C24-C25-C26-C27
16	14	322	LMG	C30-C31-C32-C33
11	11	309	CLA	CBD-CGD-O2D-CED
11	11	308	CLA	C2A-CAA-CBA-CGA
16	8	320	LMG	O1-C7-C8-C9
16	14	322	LMG	C12-C13-C14-C15
16	8	320	LMG	O1-C7-C8-O7
16	14	322	LMG	O7-C8-C9-O8
11	6	311	CLA	O1A-CGA-O2A-C1
11	12	303	CLA	C15-C16-C17-C18
11	13	303	CLA	C13-C15-C16-C17
11	12	306	CLA	C4-C3-C5-C6
14	7	314	A86	C13-C14-C15-C20
14	7	318	A86	C13-C14-C15-C20
14	8	318	A86	C13-C14-C15-C20
14	14	314	A86	C13-C14-C15-C20
14	14	320	A86	C13-C14-C15-C20
14	14	321	A86	C13-C14-C15-C20
14	15	315	A86	C13-C14-C15-C20
14	15	316	A86	C13-C14-C15-C20
14	15	317	A86	C13-C14-C15-C20
11	6	304	CLA	C11-C10-C8-C9
11	7	302	CLA	C11-C12-C13-C14
11	15	304	CLA	C11-C12-C13-C14
13	10	313	DD6	C6-C8-C9-C10
14	10	301	A86	C1-C24-C25-C26
14	10	302	A86	C1-C24-C25-C26
14	10	302	A86	C6-C8-C9-C10
14	11	301	A86	C6-C8-C9-C10
14	13	313	A86	C6-C8-C9-C10
14	14	321	A86	C6-C8-C9-C10
14	15	315	A86	C1-C24-C25-C26
14	15	315	A86	C6-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
14	15	320	A86	C6-C8-C9-C10
14	16	312	A86	C6-C8-C9-C10
12	12	311	KC1	CAA-CBA-CGA-O1A
16	8	321	LMG	C17-C18-C19-C20
11	7	306	CLA	C16-C17-C18-C19
16	8	320	LMG	C32-C33-C34-C35
11	10	303	CLA	C15-C16-C17-C18
11	12	302	CLA	CAA-CBA-CGA-O2A
11	8	301	CLA	C2A-CAA-CBA-CGA
11	15	302	CLA	C2A-CAA-CBA-CGA
11	6	311	CLA	C2-C1-O2A-CGA
11	7	302	CLA	C2-C1-O2A-CGA
11	11	308	CLA	C2-C1-O2A-CGA
11	12	310	CLA	C2-C1-O2A-CGA
11	12	307	CLA	O1A-CGA-O2A-C1
11	15	313	CLA	C3-C5-C6-C7
17	8	319	LMT	C7-C8-C9-C10
17	12	301	LMT	O1'-C1-C2-C3
11	7	302	CLA	C13-C15-C16-C17
14	10	301	A86	C12-C11-C13-C14
14	10	302	A86	C12-C11-C13-C14
14	11	301	A86	C12-C11-C13-C14
14	11	314	A86	C12-C11-C13-C14
14	12	314	A86	C12-C11-C13-C14
14	14	316	A86	C12-C11-C13-C14
14	14	318	A86	C12-C11-C13-C14
14	16	312	A86	C12-C11-C13-C14
16	14	322	LMG	C14-C15-C16-C17
11	10	305	CLA	CBA-CGA-O2A-C1
17	12	318	LMT	C2-C3-C4-C5
17	16	315	LMT	C6-C7-C8-C9
11	6	304	CLA	CAA-CBA-CGA-O2A
11	6	301	CLA	C13-C15-C16-C17
11	7	310	CLA	C4-C3-C5-C6
11	16	306	CLA	O1D-CGD-O2D-CED
15	6	319	LHG	C3-O3-P-O6
17	8	324	LMT	C4'-C5'-C6'-O6'
11	7	308	CLA	C12-C13-C15-C16
11	12	310	CLA	C11-C12-C13-C15
11	13	301	CLA	C6-C7-C8-C10
11	16	303	CLA	C12-C13-C15-C16
11	6	303	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
11	6	307	CLA	C14-C13-C15-C16
11	8	305	CLA	C14-C13-C15-C16
11	12	302	CLA	C11-C12-C13-C14
11	13	302	CLA	C11-C12-C13-C14
13	6	316	DD6	C24-C25-C26-C27
13	7	317	DD6	C1-C2-C3-C4
13	8	316	DD6	C24-C25-C26-C27
14	10	317	A86	C24-C25-C26-C27
11	7	306	CLA	C16-C17-C18-C20
16	7	319	LMG	C32-C33-C34-C35
11	15	304	CLA	C13-C15-C16-C17
14	14	301	A86	C5-C6-C8-C9
11	15	312	CLA	CBD-CGD-O2D-CED
12	12	311	KC1	CAA-CBA-CGA-O2A
11	12	303	CLA	CBD-CGD-O2D-CED
16	8	321	LMG	C18-C19-C20-C21
11	15	309	CLA	C16-C17-C18-C19
13	7	313	DD6	C11-C10-C9-C8
13	7	316	DD6	C1-C2-C3-C4
14	7	314	A86	C11-C10-C9-C8
14	15	315	A86	C11-C10-C9-C8
11	10	303	CLA	O1A-CGA-O2A-C1
12	11	304	KC1	C4B-C3B-CAB-CBB
12	14	306	KC1	C2C-C3C-CAC-CBC
11	6	304	CLA	C15-C16-C17-C18
11	7	309	CLA	C10-C11-C12-C13
11	12	302	CLA	C5-C6-C7-C8
16	8	321	LMG	C31-C32-C33-C34
11	6	301	CLA	C2-C1-O2A-CGA
11	8	304	CLA	C2-C1-O2A-CGA
11	6	311	CLA	C2A-CAA-CBA-CGA
11	8	308	CLA	C3A-C2A-CAA-CBA
11	8	309	CLA	C3A-C2A-CAA-CBA
11	12	304	CLA	C3A-C2A-CAA-CBA
11	15	304	CLA	C3A-C2A-CAA-CBA
11	15	303	CLA	CAA-CBA-CGA-O2A
13	10	314	DD6	C3-C4-C5-C6
14	8	318	A86	O-C13-C14-C15
14	10	316	A86	O-C13-C14-C15
14	13	315	A86	O-C13-C14-C15
14	14	314	A86	O-C13-C14-C15
14	14	317	A86	O-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
14	15	317	A86	O-C13-C14-C15
11	15	306	CLA	CAA-CBA-CGA-O2A
13	7	317	DD6	C27-C29-C30-C31
16	8	321	LMG	C33-C34-C35-C36
11	15	302	CLA	C6-C7-C8-C9
11	13	304	CLA	CAA-CBA-CGA-O2A
13	10	313	DD6	C9-C10-C11-C12
14	7	318	A86	C-C1-C2-C3
14	7	318	A86	C4-C5-C6-C7
14	8	318	A86	C-C1-C2-C3
14	10	301	A86	C25-C26-C27-C28
14	11	301	A86	C-C1-C2-C3
14	11	301	A86	C4-C5-C6-C7
14	14	320	A86	C-C1-C2-C3
14	15	322	A86	C-C1-C2-C3
11	15	305	CLA	CAA-CBA-CGA-O1A
14	14	301	A86	C-C1-C24-C25
17	15	301	LMT	C2-C3-C4-C5
11	7	310	CLA	C5-C6-C7-C8
11	15	306	CLA	CAA-CBA-CGA-O1A
11	15	310	CLA	C1A-C2A-CAA-CBA
11	10	303	CLA	C11-C10-C8-C7
11	12	306	CLA	C2-C3-C5-C6
11	13	304	CLA	CAA-CBA-CGA-O1A
12	7	307	KC1	C3A-C2A-CAA-CBA
12	10	312	KC1	C3A-C2A-CAA-CBA
12	14	306	KC1	C3A-C2A-CAA-CBA
11	11	309	CLA	C4-C3-C5-C6
11	12	312	CLA	C4-C3-C5-C6
11	15	312	CLA	O1D-CGD-O2D-CED
14	7	318	A86	C24-C1-C2-C3
14	7	318	A86	C4-C5-C6-C8
14	10	301	A86	C25-C26-C27-C29
14	11	301	A86	C24-C1-C2-C3
14	11	301	A86	C4-C5-C6-C8
14	14	320	A86	C24-C1-C2-C3
14	15	322	A86	C24-C1-C2-C3
14	16	314	A86	C13-C14-C15-C16
11	13	309	CLA	CAA-CBA-CGA-O1A
13	15	319	DD6	C24-C25-C26-C27
14	11	313	A86	C1-C2-C3-C4
14	11	314	A86	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
14	14	314	A86	C3-C4-C5-C6
14	14	316	A86	C11-C10-C9-C8
14	15	317	A86	C1-C2-C3-C4
11	12	303	CLA	O1D-CGD-O2D-CED
16	7	319	LMG	C34-C35-C36-C37
14	10	315	A86	C10-C11-C13-C14
14	11	301	A86	C10-C11-C13-C14
14	11	313	A86	C10-C11-C13-C14
14	12	314	A86	C10-C11-C13-C14
14	13	315	A86	C10-C11-C13-C14
14	15	321	A86	C10-C11-C13-C14
11	8	308	CLA	C4-C3-C5-C6
11	10	307	CLA	C4-C3-C5-C6
11	12	303	CLA	C4-C3-C5-C6
11	12	304	CLA	C4-C3-C5-C6
11	12	310	CLA	C4-C3-C5-C6
11	7	310	CLA	C2-C3-C5-C6
17	8	324	LMT	C6-C7-C8-C9
11	13	309	CLA	CAA-CBA-CGA-O2A
12	8	312	KC1	C1A-C2A-CAA-CBA
12	13	311	KC1	C1A-C2A-CAA-CBA
15	6	319	LHG	O10-C23-O8-C6
11	16	302	CLA	C15-C16-C17-C18
11	6	301	CLA	C2A-CAA-CBA-CGA
11	6	313	CLA	C2A-CAA-CBA-CGA
11	12	304	CLA	CAA-CBA-CGA-O1A
11	14	309	CLA	CAA-CBA-CGA-O2A
11	6	304	CLA	C10-C11-C12-C13
13	11	312	DD6	C3-C4-C5-C6
14	10	315	A86	C24-C25-C26-C27
14	14	301	A86	C3-C4-C5-C6
11	14	307	CLA	C4-C3-C5-C6
14	14	301	A86	C2-C1-C24-C25
11	15	309	CLA	C2-C3-C5-C6
11	14	312	CLA	CAA-CBA-CGA-O2A
11	15	310	CLA	CAA-CBA-CGA-O2A
11	10	307	CLA	O1A-CGA-O2A-C1
11	7	302	CLA	C5-C6-C7-C8
11	6	304	CLA	C8-C10-C11-C12
16	7	319	LMG	C33-C34-C35-C36
11	10	307	CLA	CBA-CGA-O2A-C1
11	6	313	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
11	15	310	CLA	CAA-CBA-CGA-O1A
17	12	322	LMT	O5B-C1B-O1B-C4'
11	15	304	CLA	C11-C10-C8-C7
11	16	308	CLA	CAA-CBA-CGA-O2A
11	14	307	CLA	C8-C10-C11-C12
14	13	315	A86	C24-C25-C26-C27
11	8	305	CLA	C5-C6-C7-C8
11	8	309	CLA	C2A-CAA-CBA-CGA
11	6	303	CLA	C5-C6-C7-C8
11	8	303	CLA	C2-C3-C5-C6
11	8	308	CLA	C2-C3-C5-C6
11	12	308	CLA	C2-C3-C5-C6
11	12	312	CLA	C2-C3-C5-C6
11	6	314	CLA	C6-C7-C8-C9
11	7	308	CLA	C14-C13-C15-C16
11	12	304	CLA	C11-C12-C13-C14
11	12	312	CLA	C11-C10-C8-C9
11	13	301	CLA	C6-C7-C8-C9
11	13	307	CLA	C11-C12-C13-C14
11	16	303	CLA	C14-C13-C15-C16
11	6	304	CLA	C3A-C2A-CAA-CBA
11	6	306	CLA	C3A-C2A-CAA-CBA
11	15	310	CLA	C3A-C2A-CAA-CBA
17	11	316	LMT	C3'-C4'-O1B-C1B
11	15	305	CLA	CAA-CBA-CGA-O2A
11	7	303	CLA	CAD-CBD-CGD-O2D
11	8	305	CLA	CAD-CBD-CGD-O2D
11	10	307	CLA	CAD-CBD-CGD-O2D
11	10	311	CLA	CAD-CBD-CGD-O2D
11	12	321	CLA	CAD-CBD-CGD-O2D
11	13	309	CLA	CAD-CBD-CGD-O2D
11	15	303	CLA	CAD-CBD-CGD-O2D
11	15	307	CLA	CAD-CBD-CGD-O2D
11	16	303	CLA	CAD-CBD-CGD-O2D
11	16	305	CLA	CAD-CBD-CGD-O2D
11	16	310	CLA	CAD-CBD-CGD-O2D
14	12	316	A86	C28-C27-C29-C30
14	14	317	A86	C28-C27-C29-C30
14	14	321	A86	C28-C27-C29-C30
14	12	316	A86	C3-C4-C5-C6
11	6	306	CLA	C2-C1-O2A-CGA
11	16	306	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
11	15	311	CLA	CAA-CBA-CGA-O2A
11	16	310	CLA	CAA-CBA-CGA-O2A
11	14	312	CLA	CAA-CBA-CGA-O1A
11	8	303	CLA	C13-C15-C16-C17
11	11	309	CLA	C2-C3-C5-C6
11	12	310	CLA	C2-C3-C5-C6
11	6	313	CLA	CAA-CBA-CGA-O2A
11	7	311	CLA	CAA-CBA-CGA-O2A
11	13	301	CLA	CAA-CBA-CGA-O2A
14	10	317	A86	C2-C1-C24-C25
13	7	313	DD6	C13-C14-C15-O1
13	8	316	DD6	C13-C14-C15-O1
14	6	317	A86	C12-C11-C13-O
14	7	314	A86	C12-C11-C13-O
14	14	318	A86	C12-C11-C13-O
14	15	322	A86	C12-C11-C13-O
11	14	309	CLA	CAA-CBA-CGA-O1A
11	10	307	CLA	CAA-CBA-CGA-O2A
11	16	310	CLA	CAA-CBA-CGA-O1A
16	8	321	LMG	C34-C35-C36-C37
11	15	304	CLA	O2A-C1-C2-C3
12	12	309	KC1	C4B-C3B-CAB-CBB
11	14	304	CLA	CAA-CBA-CGA-O2A
12	8	306	KC1	CBD-CGD-O2D-CED
11	6	304	CLA	CHA-CBD-CGD-O2D
11	6	311	CLA	CHA-CBD-CGD-O1D
11	6	311	CLA	CHA-CBD-CGD-O2D
11	13	303	CLA	CHA-CBD-CGD-O1D
11	14	303	CLA	CHA-CBD-CGD-O1D
11	14	307	CLA	CHA-CBD-CGD-O1D
11	14	307	CLA	CHA-CBD-CGD-O2D
11	15	308	CLA	CHA-CBD-CGD-O1D
11	15	312	CLA	CHA-CBD-CGD-O2D
12	8	310	KC1	CHA-CBD-CGD-O2D
12	8	313	KC1	CHA-CBD-CGD-O1D
12	8	313	KC1	CHA-CBD-CGD-O2D
12	12	309	KC1	CHA-CBD-CGD-O2D
12	14	306	KC1	CHA-CBD-CGD-O1D
13	13	314	DD6	C24-C25-C26-C27
14	7	318	A86	C24-C25-C26-C27
11	14	304	CLA	CAA-CBA-CGA-O1A
11	6	307	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
11	16	306	CLA	CAA-CBA-CGA-O2A
11	14	307	CLA	C2-C3-C5-C6
11	10	303	CLA	CBD-CGD-O2D-CED
11	15	311	CLA	CAA-CBA-CGA-O1A
11	11	305	CLA	CAA-CBA-CGA-O2A
11	11	309	CLA	CAA-CBA-CGA-O2A
11	16	301	CLA	CAA-CBA-CGA-O2A
12	16	311	KC1	C4C-C3C-CAC-CBC
11	11	305	CLA	C6-C7-C8-C9
11	15	308	CLA	CAA-CBA-CGA-O2A
14	6	317	A86	C10-C11-C13-O
14	8	318	A86	C10-C11-C13-O
14	8	318	A86	C13-C14-C15-O1
14	10	315	A86	C10-C11-C13-O
14	10	317	A86	C13-C14-C15-O1
14	11	314	A86	C13-C14-C15-O1
14	11	315	A86	C10-C11-C13-O
14	12	314	A86	C10-C11-C13-O
14	12	316	A86	C10-C11-C13-O
14	13	313	A86	C13-C14-C15-O1
14	14	314	A86	C13-C14-C15-O1
14	14	315	A86	C13-C14-C15-O1
14	14	316	A86	C10-C11-C13-O
14	14	319	A86	C13-C14-C15-O1
14	14	321	A86	C10-C11-C13-O
14	15	315	A86	C13-C14-C15-O1
14	15	317	A86	C10-C11-C13-O
14	15	321	A86	C10-C11-C13-O
11	16	301	CLA	CBA-CGA-O2A-C1
11	12	307	CLA	CAA-CBA-CGA-O2A
11	8	301	CLA	C12-C13-C15-C16
11	12	304	CLA	C12-C13-C15-C16
11	8	304	CLA	CAA-CBA-CGA-O2A
11	8	301	CLA	C14-C13-C15-C16
15	6	319	LHG	C24-C23-O8-C6
11	16	308	CLA	CAA-CBA-CGA-O1A
11	14	305	CLA	C2A-CAA-CBA-CGA
11	6	313	CLA	CAA-CBA-CGA-O1A
11	12	302	CLA	C10-C11-C12-C13
11	13	301	CLA	C8-C10-C11-C12
14	8	318	A86	C39-C38-O4-C34
11	15	308	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
11	7	311	CLA	CAA-CBA-CGA-O1A
11	10	307	CLA	CAA-CBA-CGA-O1A
17	15	301	LMT	O5'-C5'-C6'-O6'
11	6	303	CLA	C1A-C2A-CAA-CBA
11	6	304	CLA	C1A-C2A-CAA-CBA
11	8	304	CLA	C1A-C2A-CAA-CBA
11	8	308	CLA	C1A-C2A-CAA-CBA
11	8	309	CLA	C1A-C2A-CAA-CBA
11	14	302	CLA	C1A-C2A-CAA-CBA
11	14	309	CLA	C1A-C2A-CAA-CBA
11	15	304	CLA	C1A-C2A-CAA-CBA
11	10	307	CLA	C2-C1-O2A-CGA
11	13	301	CLA	CAA-CBA-CGA-O1A
11	10	303	CLA	C2A-CAA-CBA-CGA
11	13	304	CLA	C2A-CAA-CBA-CGA
11	7	306	CLA	CAA-CBA-CGA-O2A
16	8	321	LMG	C2-C1-O1-C7
15	6	319	LHG	C4-O6-P-O5
11	8	301	CLA	CAA-CBA-CGA-O2A
13	7	313	DD6	C11-C13-C14-C15
13	10	313	DD6	C11-C13-C14-C15
13	12	317	DD6	C11-C13-C14-C15
13	13	314	DD6	C11-C13-C14-C15
13	16	313	DD6	C11-C13-C14-C15
11	11	309	CLA	CAA-CBA-CGA-O1A
11	16	301	CLA	CAA-CBA-CGA-O1A
11	16	306	CLA	CAA-CBA-CGA-O1A
11	15	311	CLA	C2A-CAA-CBA-CGA
11	15	304	CLA	C4C-C3C-CAC-CBC
12	12	305	KC1	CAA-CBA-CGA-O1A
11	15	308	CLA	CAA-CBA-CGA-O1A
11	16	303	CLA	C5-C6-C7-C8
17	7	320	LMT	O1'-C1-C2-C3
11	10	311	CLA	CAA-CBA-CGA-O2A
11	10	308	CLA	CAD-CBD-CGD-O1D
11	10	311	CLA	CAD-CBD-CGD-O1D
11	11	305	CLA	CAD-CBD-CGD-O1D
11	12	304	CLA	CAD-CBD-CGD-O1D
11	14	307	CLA	CAD-CBD-CGD-O1D
12	8	313	KC1	CAD-CBD-CGD-O1D
12	10	312	KC1	CAD-CBD-CGD-O1D
12	13	312	KC1	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
14	12	316	A86	C26-C27-C29-C30
14	14	321	A86	C26-C27-C29-C30
11	16	301	CLA	O1A-CGA-O2A-C1
11	8	304	CLA	CAA-CBA-CGA-O1A
11	12	307	CLA	CAA-CBA-CGA-O1A
16	14	322	LMG	C15-C16-C17-C18
11	10	303	CLA	C11-C10-C8-C9
11	10	309	CLA	C5-C6-C7-C8
11	10	309	CLA	CAA-CBA-CGA-O2A
11	12	308	CLA	CAA-CBA-CGA-O2A
11	15	304	CLA	C2C-C3C-CAC-CBC
12	12	305	KC1	CAA-CBA-CGA-O2A
11	8	305	CLA	CAA-CBA-CGA-O2A
11	14	302	CLA	CAA-CBA-CGA-O2A
11	7	308	CLA	C10-C11-C12-C13
11	12	312	CLA	C3A-C2A-CAA-CBA
11	15	302	CLA	C6-C7-C8-C10
11	11	305	CLA	CAA-CBA-CGA-O1A
11	10	303	CLA	CAA-CBA-CGA-O2A
11	13	303	CLA	CAA-CBA-CGA-O2A
11	16	307	CLA	CAA-CBA-CGA-O2A
13	6	315	DD6	C2-C1-C24-C25
13	7	313	DD6	C5-C6-C8-C9
11	16	307	CLA	CAA-CBA-CGA-O1A
12	16	311	KC1	C2C-C3C-CAC-CBC
14	10	317	A86	O-C13-C14-C15
14	11	315	A86	O-C13-C14-C15
14	12	314	A86	O-C13-C14-C15
14	15	321	A86	O-C13-C14-C15
11	7	306	CLA	CAA-CBA-CGA-O1A
11	13	303	CLA	C8-C10-C11-C12
11	14	302	CLA	C8-C10-C11-C12
11	14	302	CLA	CAA-CBA-CGA-O1A
11	8	303	CLA	C2A-CAA-CBA-CGA
11	11	309	CLA	C13-C15-C16-C17
11	10	303	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

88 monomers are involved in 141 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	14	322	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	12	301	LMT	1	0
11	11	307	CLA	1	0
17	12	322	LMT	1	0
13	6	315	DD6	2	0
17	8	324	LMT	1	0
11	6	302	CLA	1	0
11	11	308	CLA	1	0
11	12	308	CLA	3	0
17	12	320	LMT	2	0
11	8	309	CLA	1	0
11	15	303	CLA	3	0
11	13	307	CLA	4	0
11	7	309	CLA	1	0
13	10	313	DD6	1	0
11	6	304	CLA	2	0
11	12	306	CLA	2	0
11	16	303	CLA	3	0
11	7	310	CLA	2	0
13	6	318	DD6	1	0
14	11	314	A86	1	0
11	8	308	CLA	2	0
11	15	313	CLA	4	0
16	8	321	LMG	1	0
14	14	320	A86	1	0
12	8	313	KC1	1	0
11	14	303	CLA	3	0
11	14	305	CLA	1	0
13	11	312	DD6	1	0
11	6	303	CLA	1	0
11	16	310	CLA	2	0
11	13	302	CLA	2	0
11	7	308	CLA	4	0
11	13	303	CLA	1	0
11	14	302	CLA	2	0
11	10	305	CLA	2	0
11	10	309	CLA	1	0
11	15	309	CLA	2	0
11	8	301	CLA	1	0
11	16	301	CLA	7	0
11	7	305	CLA	2	0
13	6	316	DD6	1	0
11	12	303	CLA	3	0

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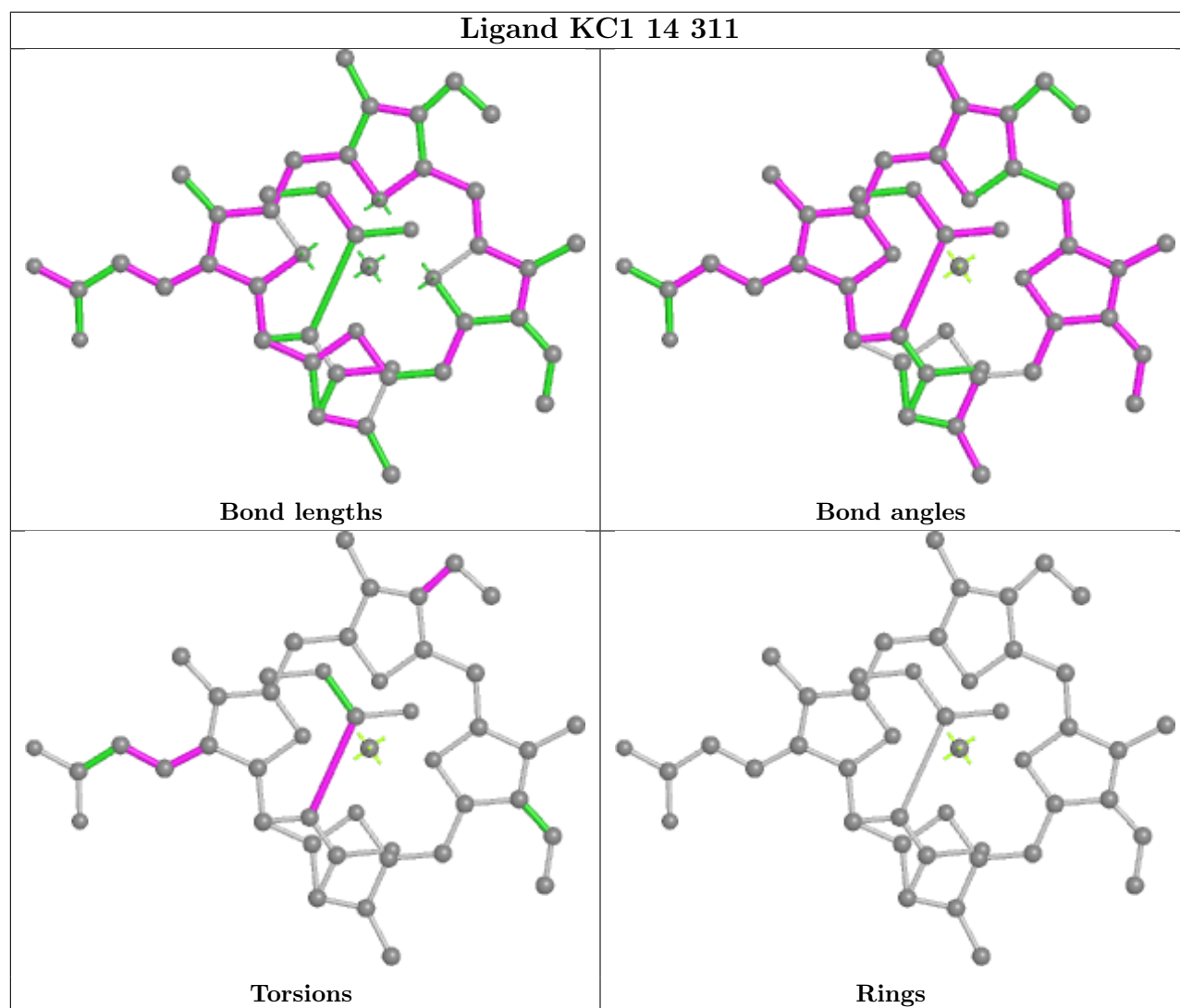
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	14	317	A86	1	0
14	8	315	A86	1	0
11	15	312	CLA	1	0
11	12	302	CLA	1	0
11	8	303	CLA	5	0
11	6	311	CLA	3	0
11	8	302	CLA	2	0
11	7	302	CLA	1	0
11	12	321	CLA	1	0
11	10	304	CLA	3	0
16	7	319	LMG	1	0
17	11	316	LMT	2	0
11	14	312	CLA	1	0
11	13	301	CLA	2	0
11	7	303	CLA	1	0
11	15	308	CLA	1	0
11	16	302	CLA	1	0
11	16	307	CLA	2	0
11	15	304	CLA	1	0
11	10	303	CLA	3	0
13	13	314	DD6	1	0
17	12	319	LMT	3	0
11	13	304	CLA	2	0
16	8	323	LMG	1	0
11	8	305	CLA	2	0
11	10	307	CLA	2	0
11	6	306	CLA	3	0
11	12	310	CLA	2	0
11	14	307	CLA	2	0
11	6	301	CLA	2	0
11	11	303	CLA	4	0
11	15	307	CLA	2	0
11	12	304	CLA	2	0
11	6	313	CLA	2	0
12	13	310	KC1	1	0
12	16	304	KC1	1	0
13	7	313	DD6	1	0
11	7	306	CLA	3	0
11	8	304	CLA	1	0
11	15	302	CLA	5	0
14	7	314	A86	1	0
16	8	320	LMG	1	0

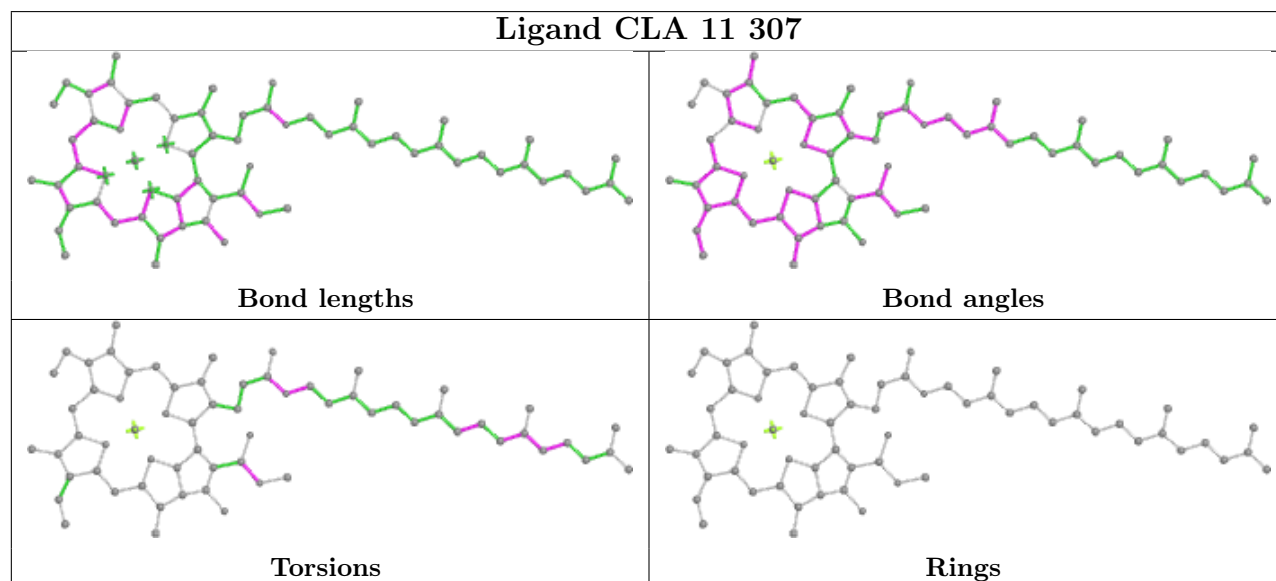
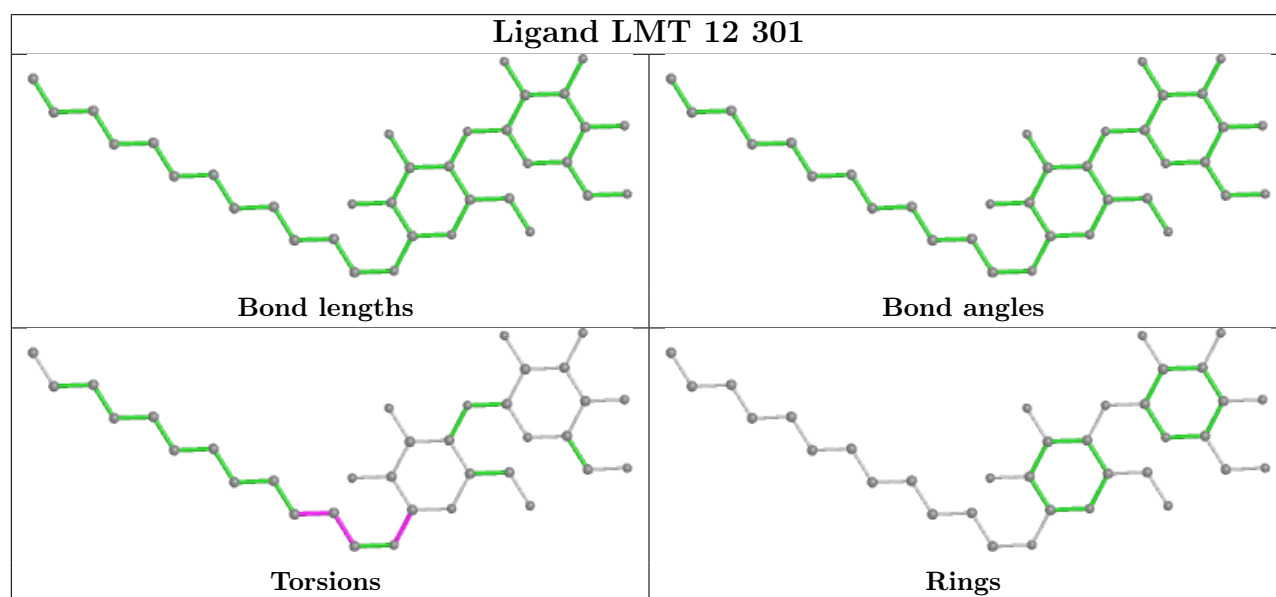
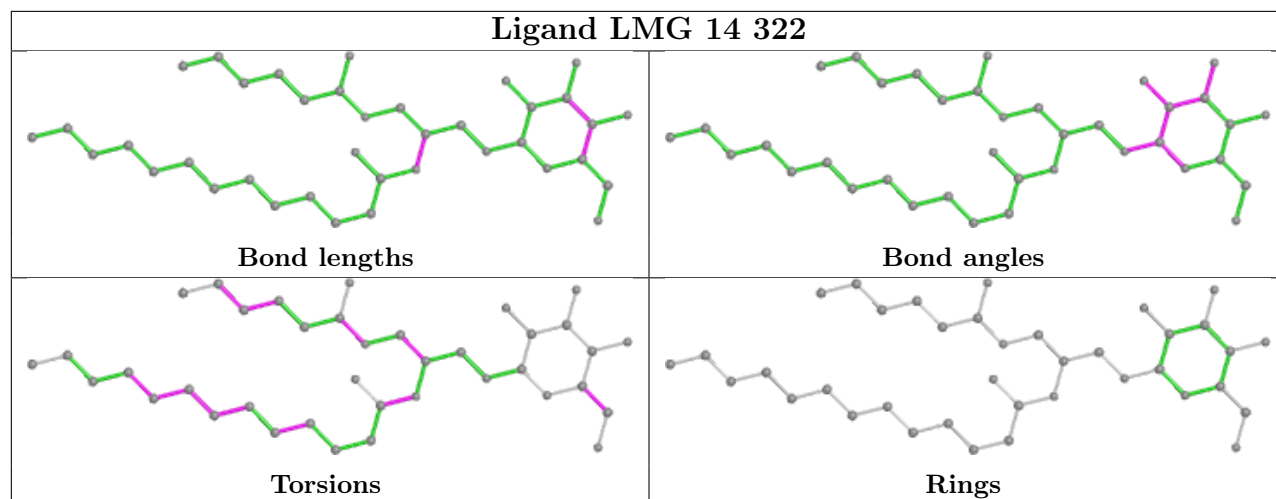
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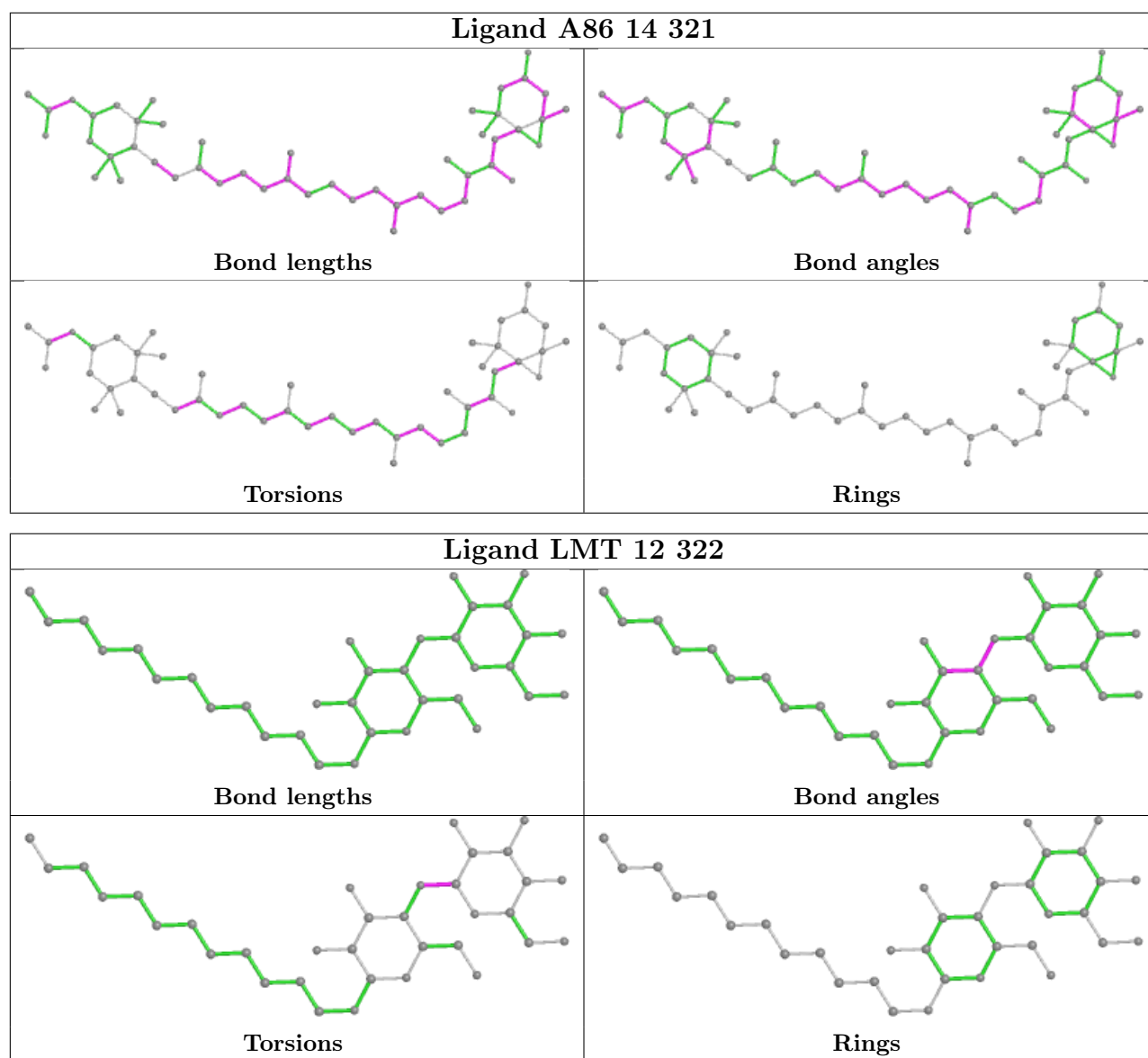
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	16	306	CLA	1	0
11	10	308	CLA	3	0
11	12	312	CLA	1	0

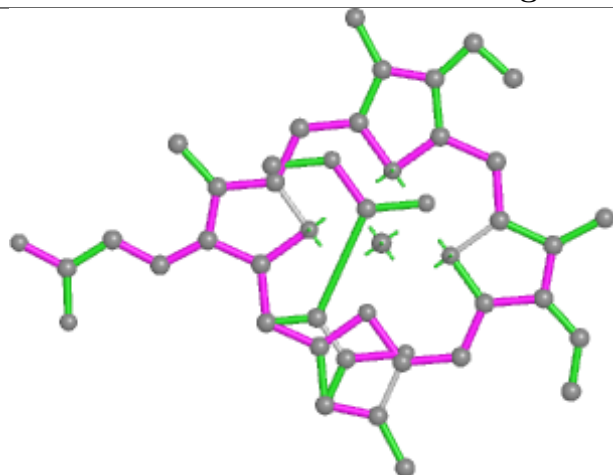
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



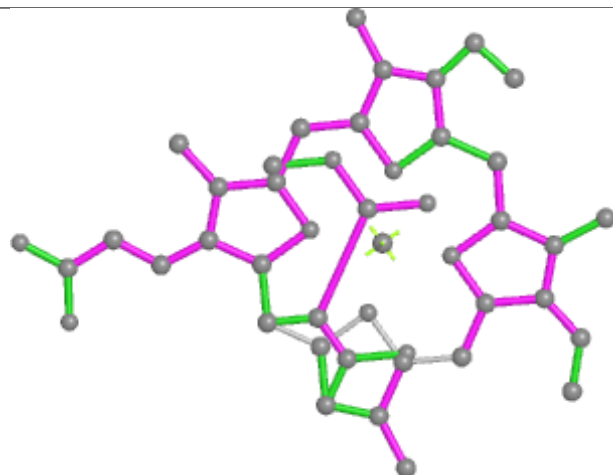




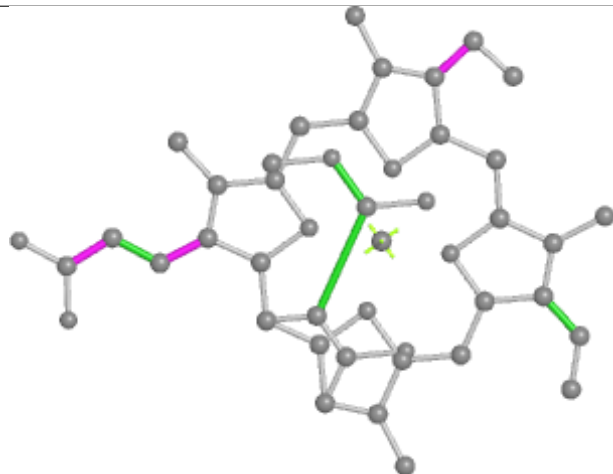
Ligand KC1 8 314



Bond lengths



Bond angles

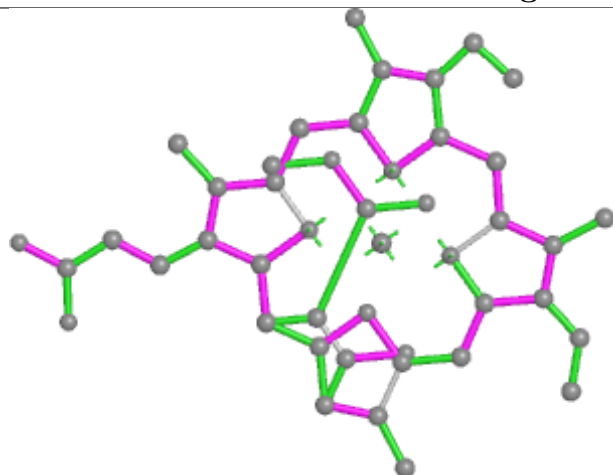


Torsions

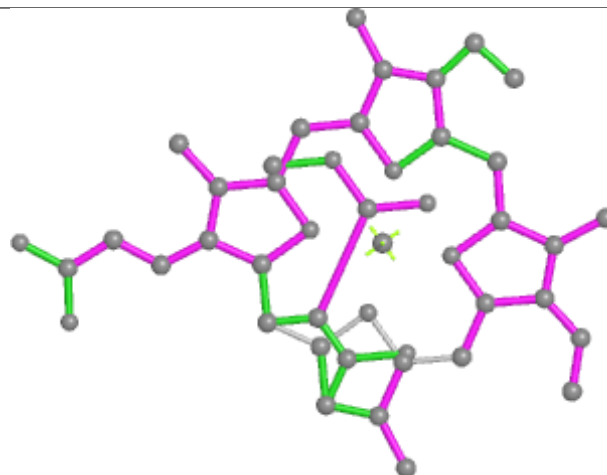


Rings

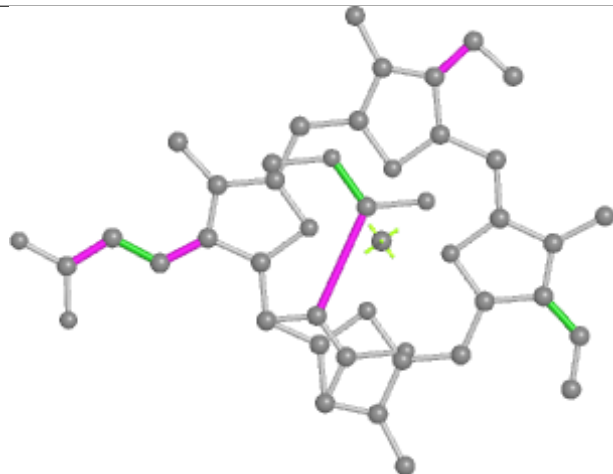
Ligand KC1 6 310



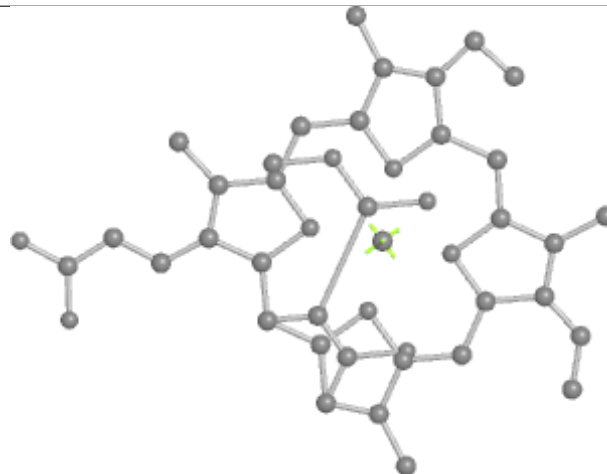
Bond lengths



Bond angles

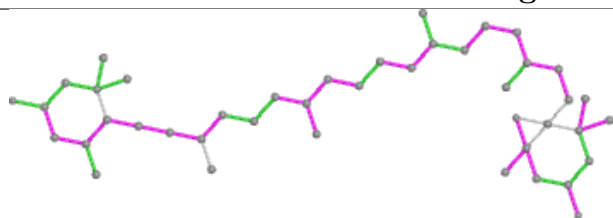


Torsions

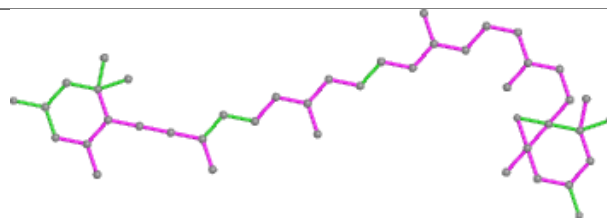


Rings

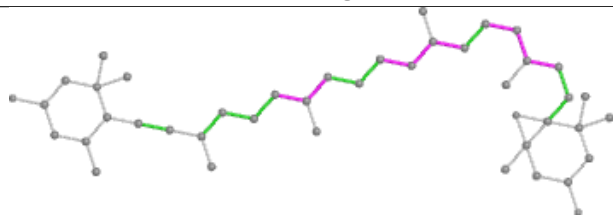
Ligand DD6 6 315



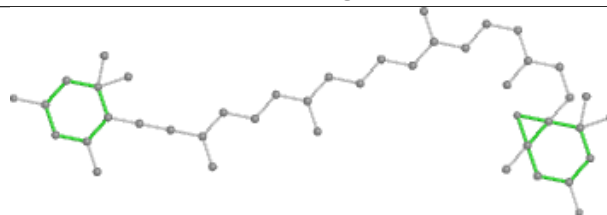
Bond lengths



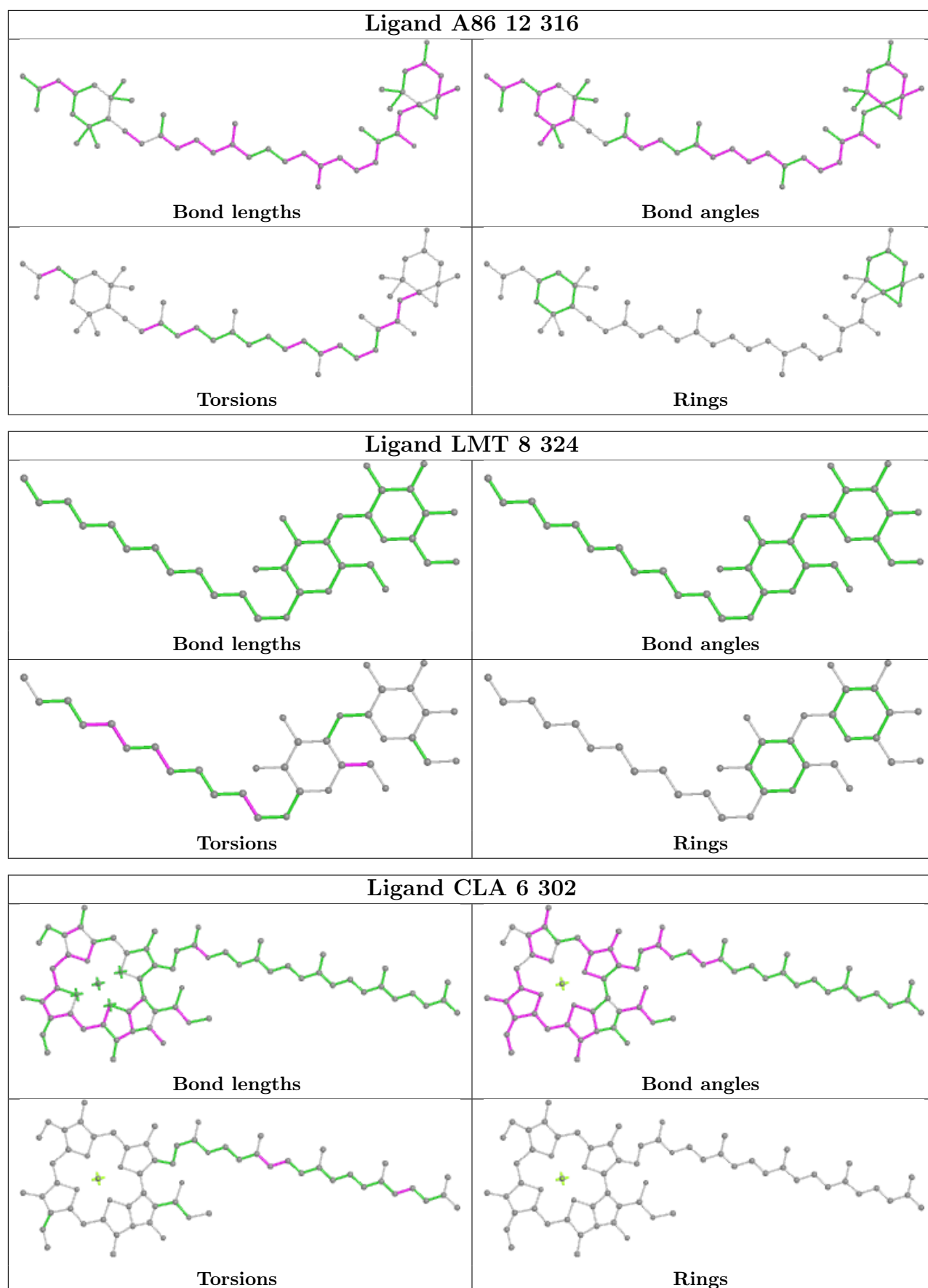
Bond angles

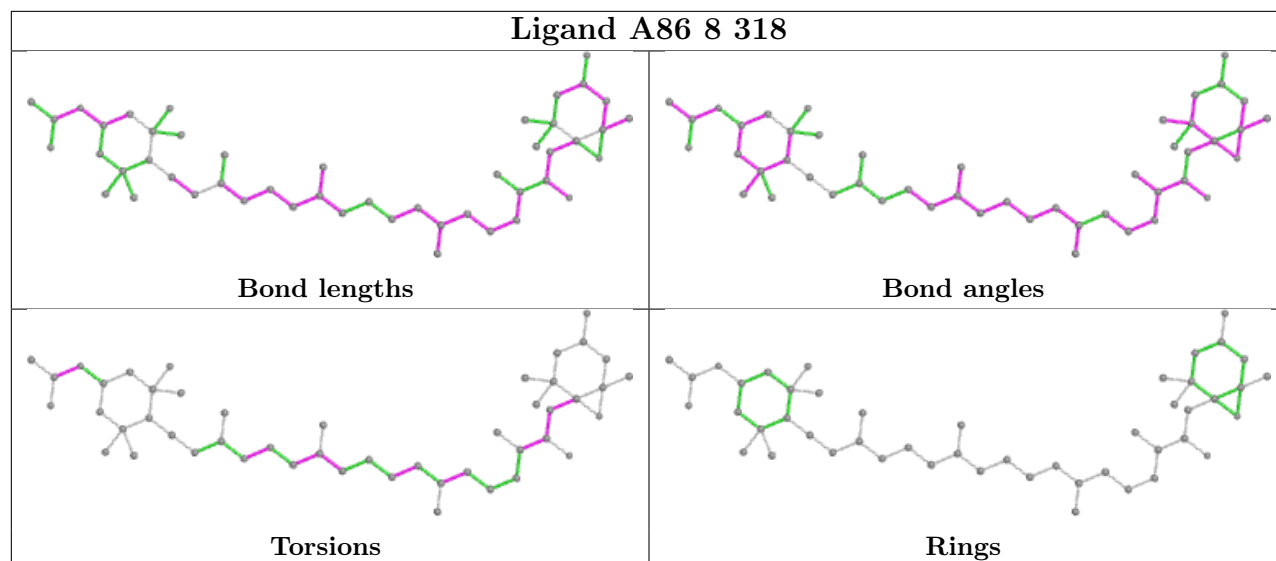
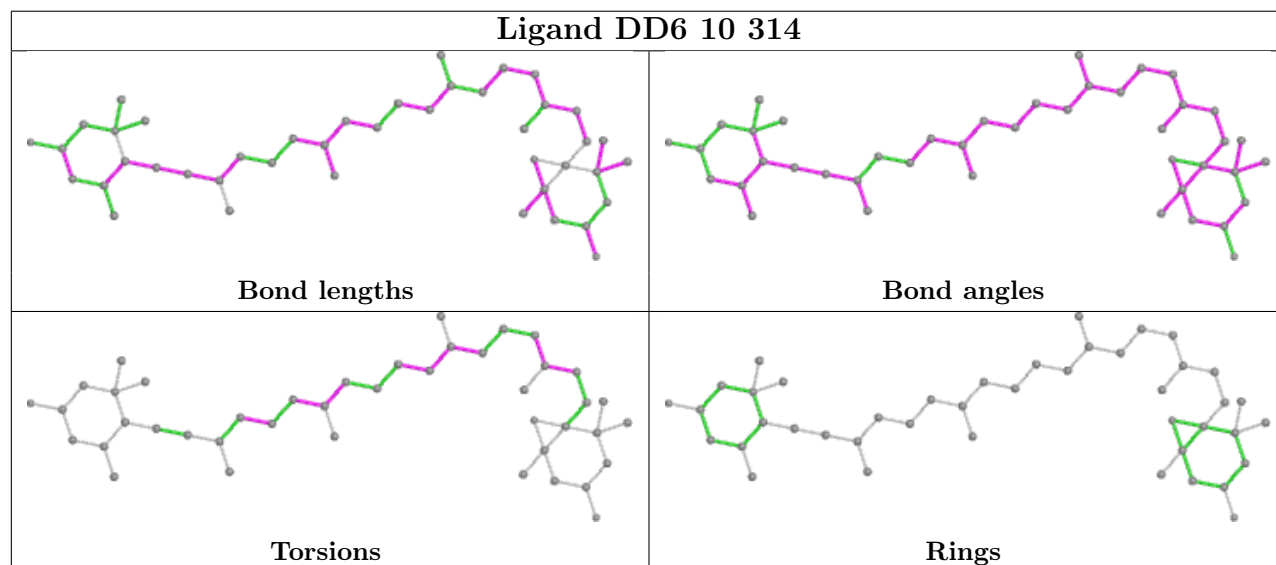
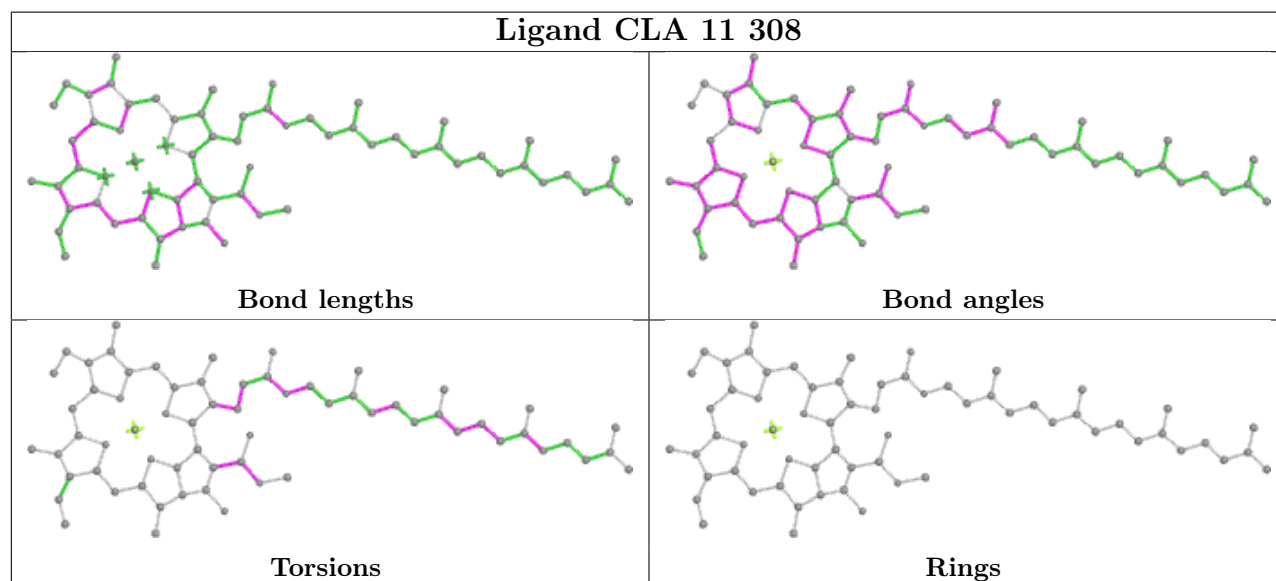


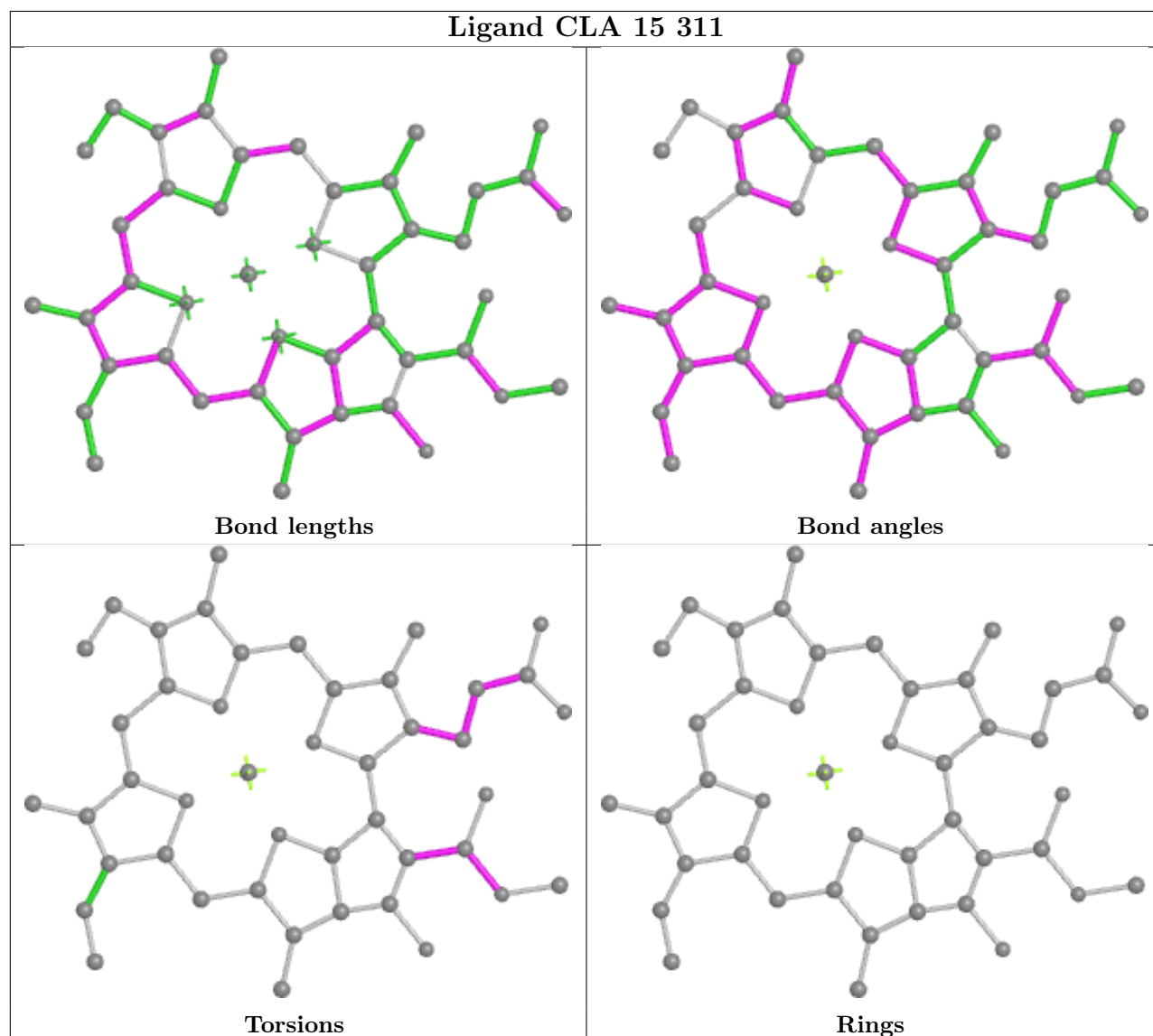
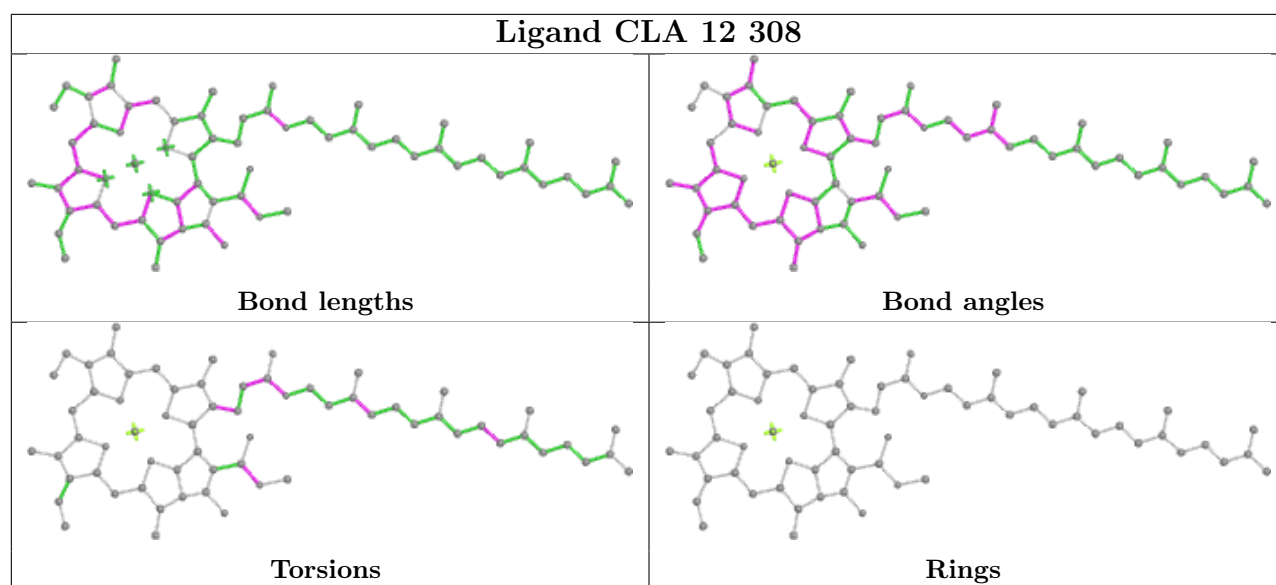
Torsions

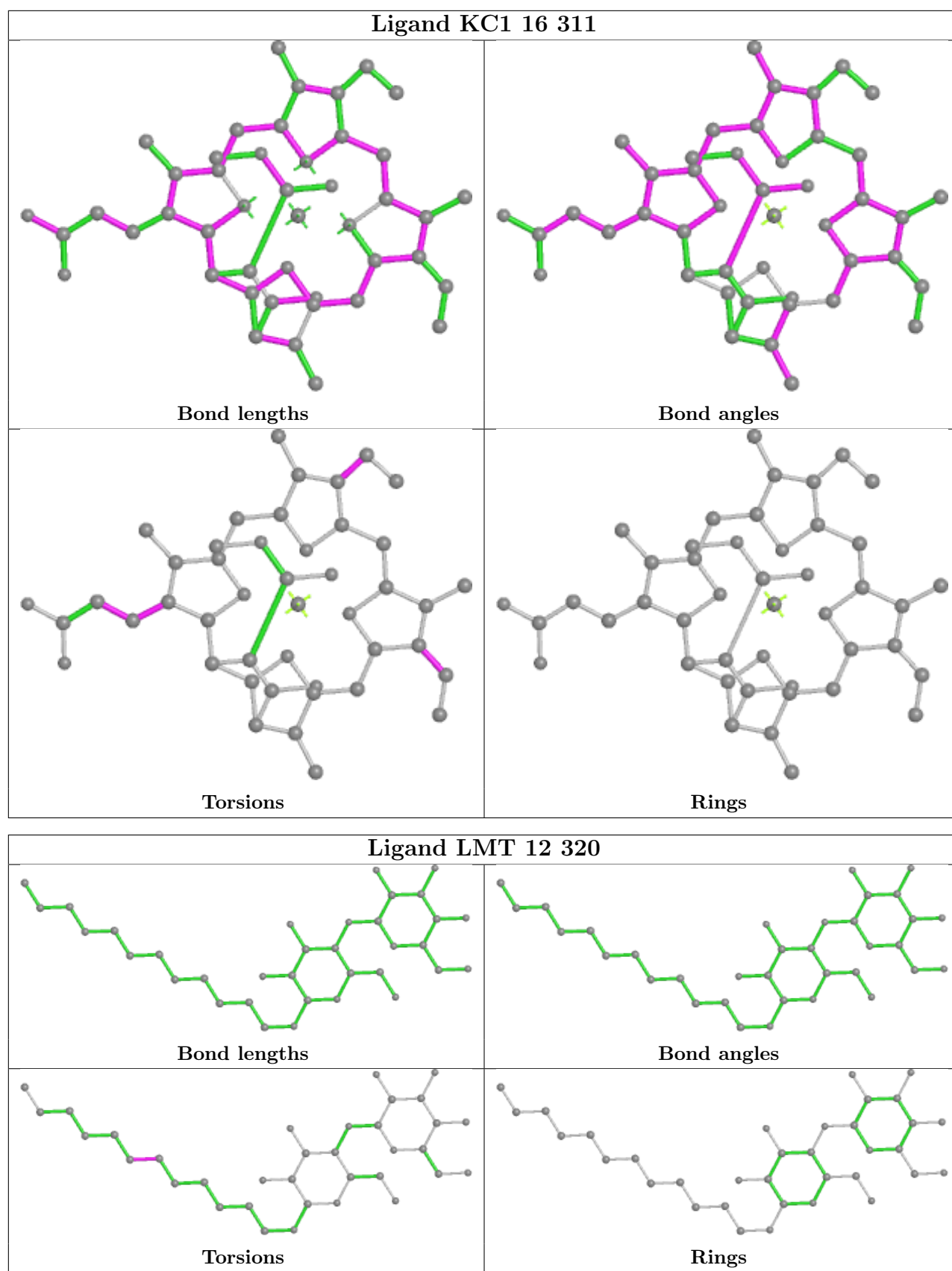


Rings

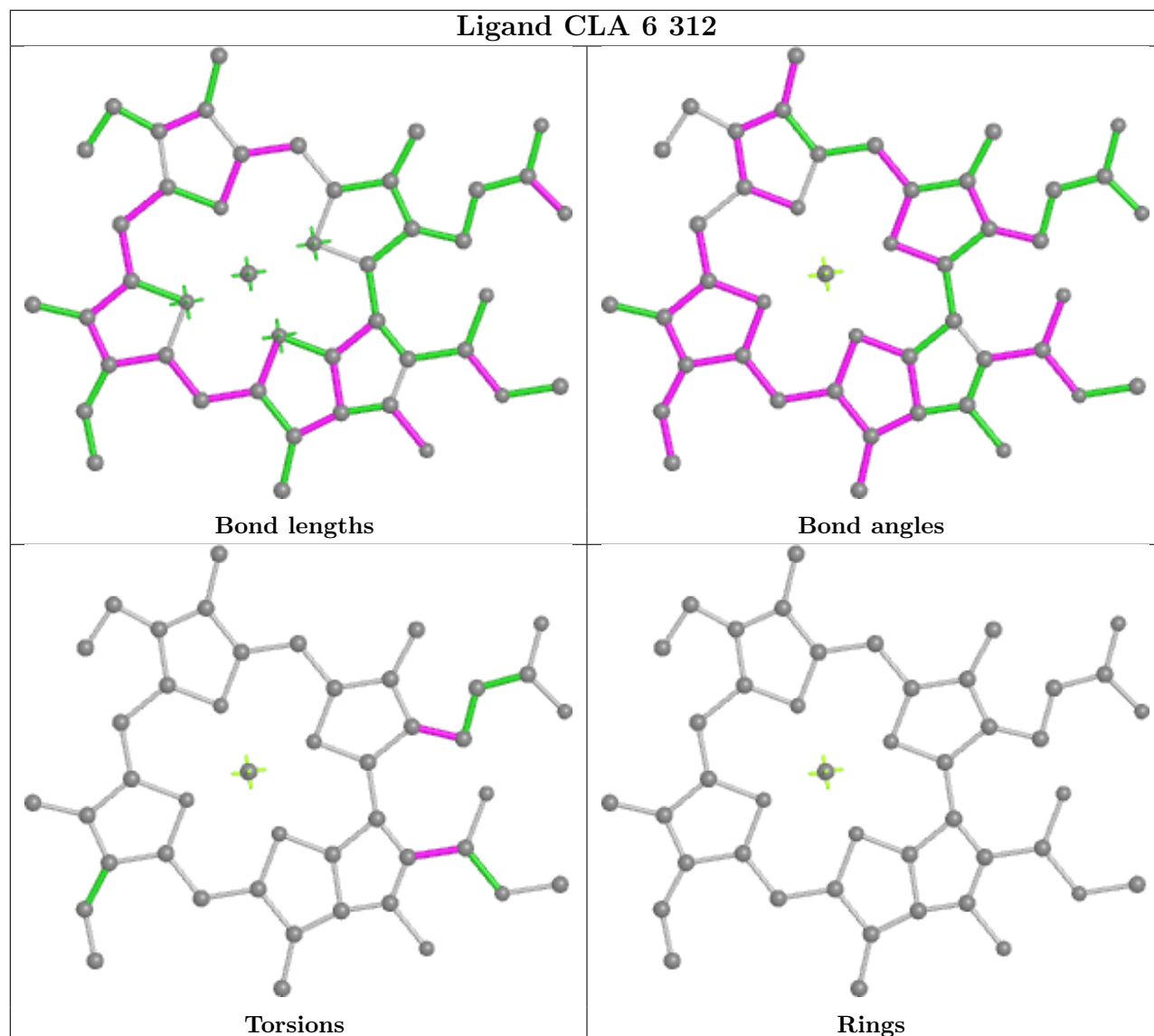


Ligand A86 8 318**Ligand DD6 10 314****Ligand CLA 11 308**

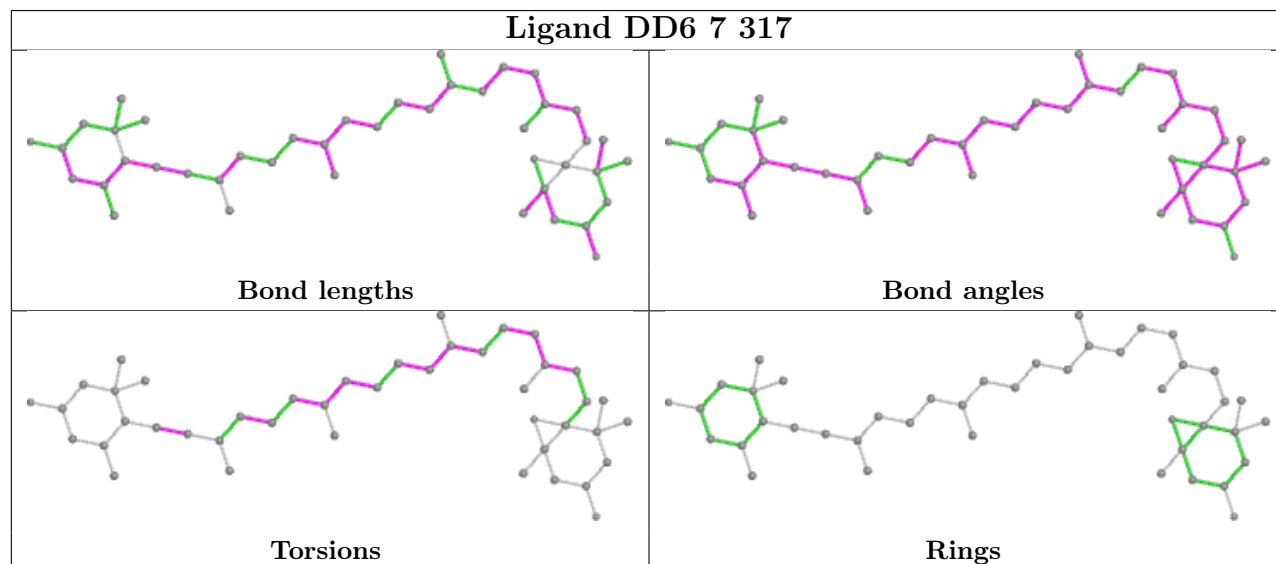




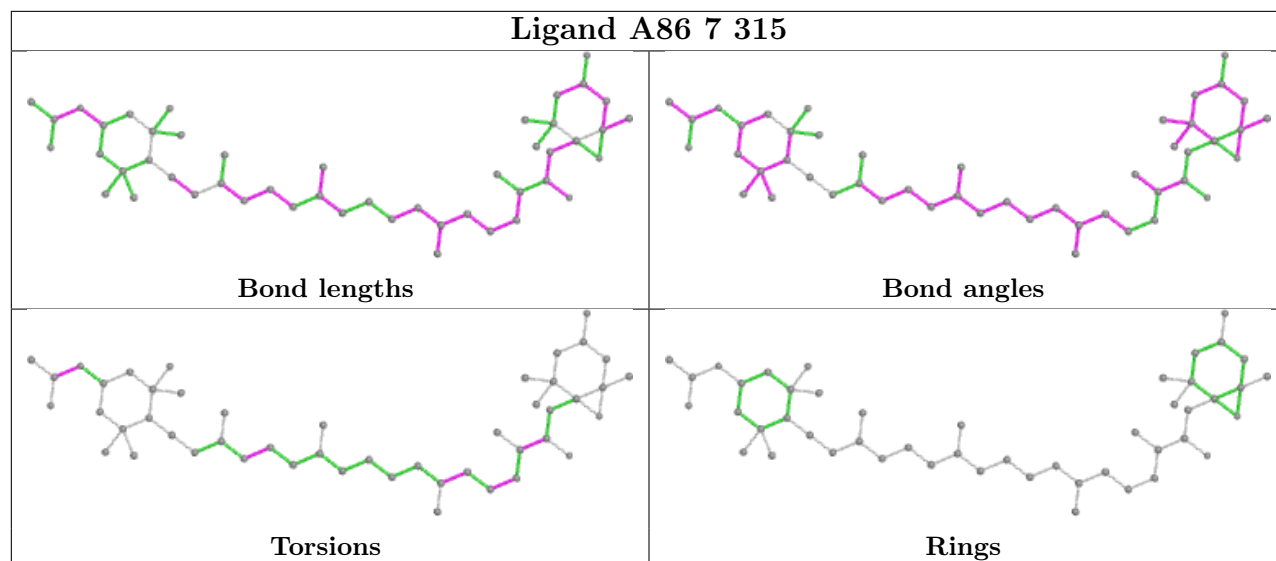
Ligand CLA 6 312



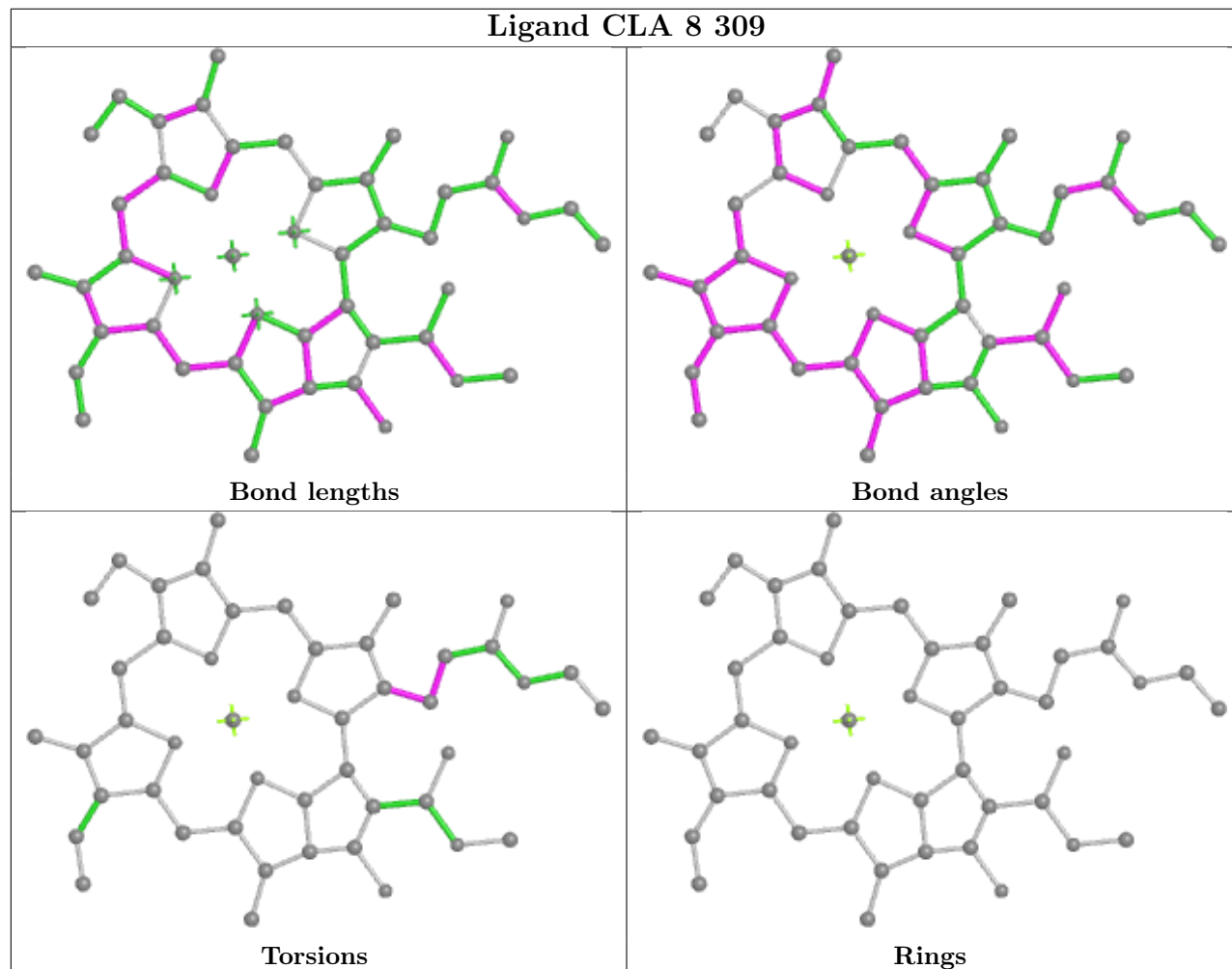
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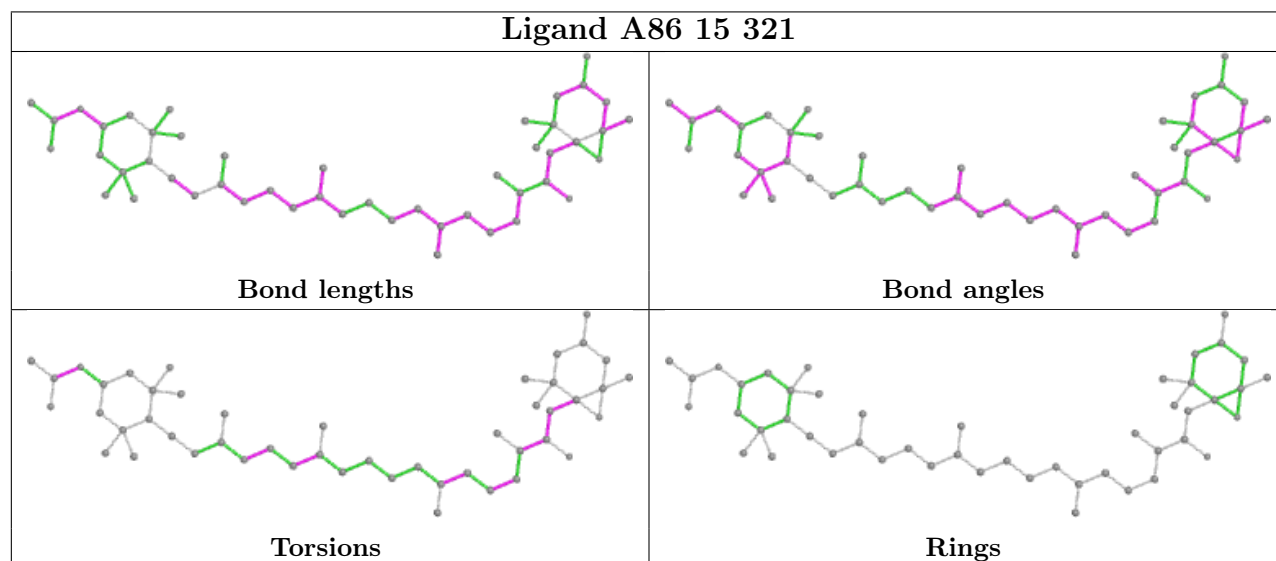
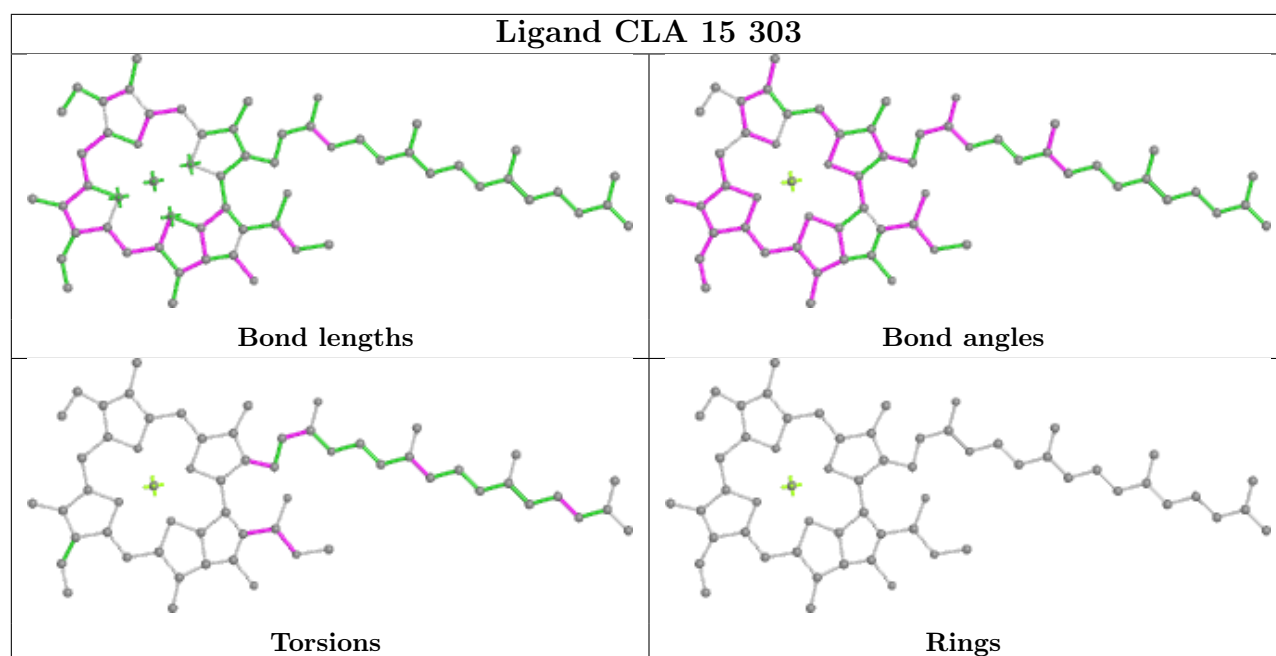


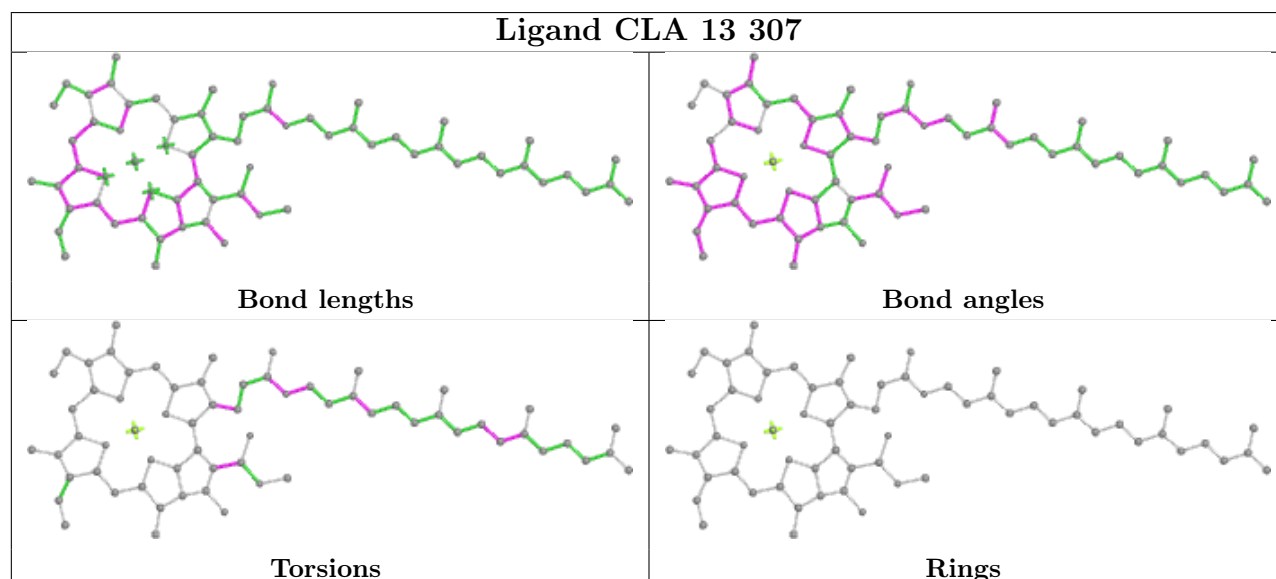
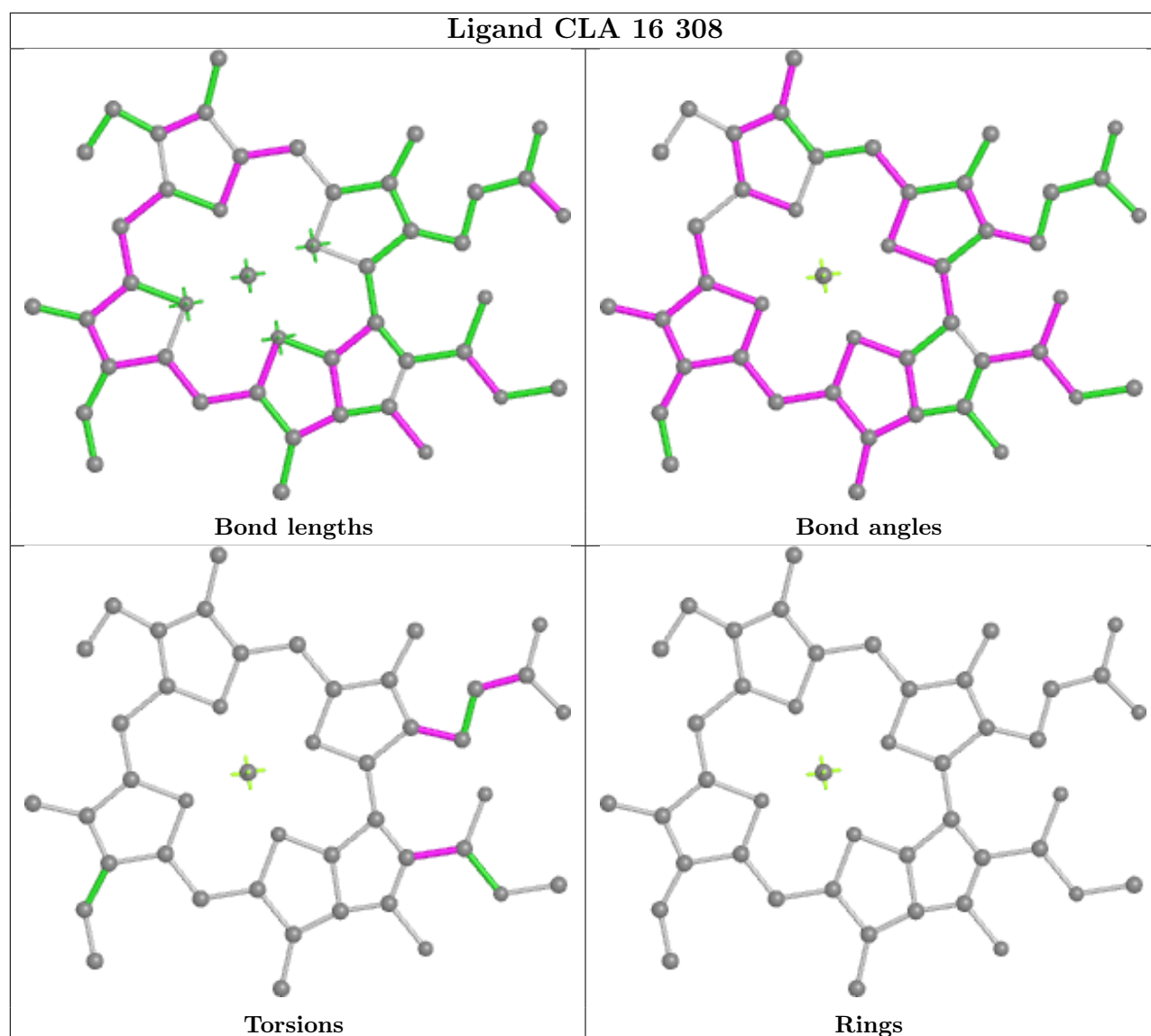
Ligand A86 7 315



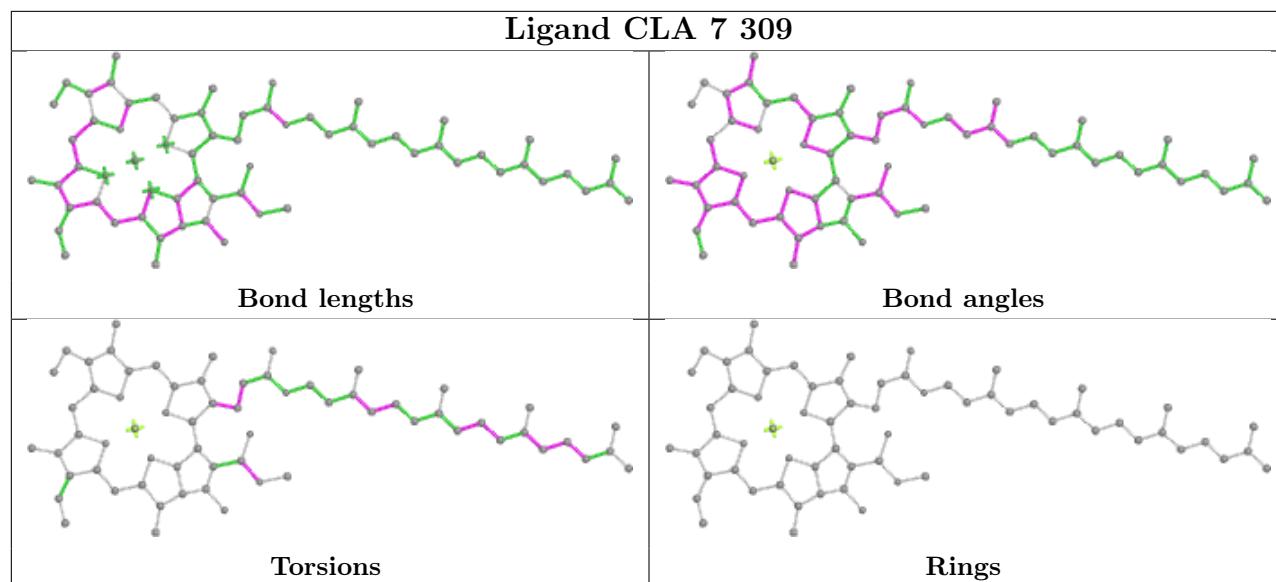
Ligand CLA 8 309



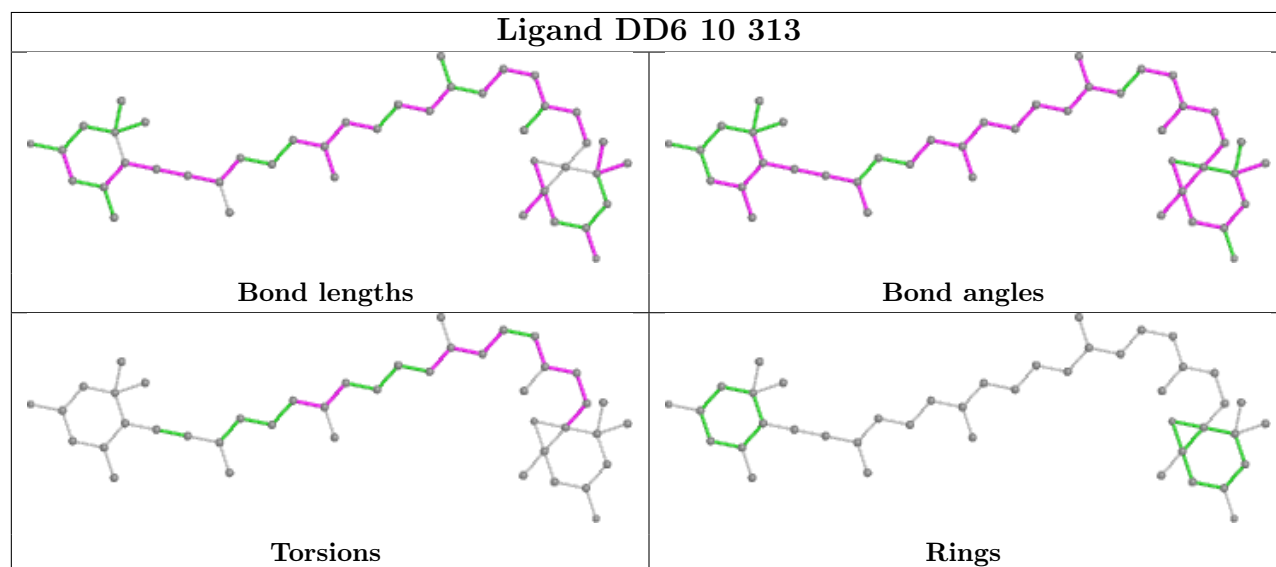




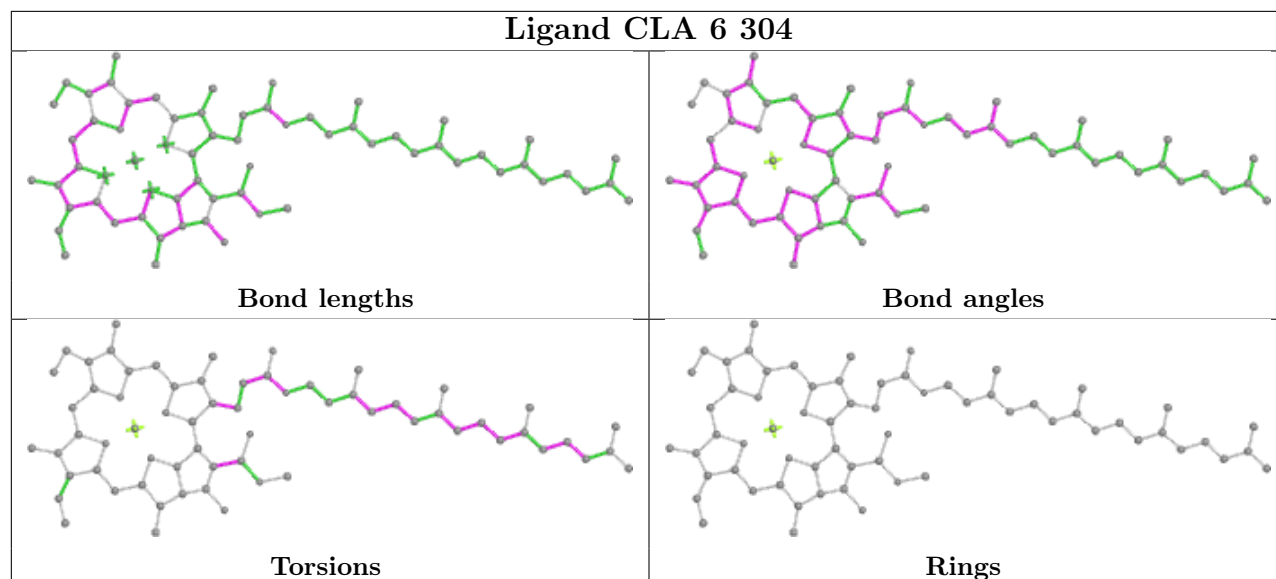
Ligand CLA 7 309

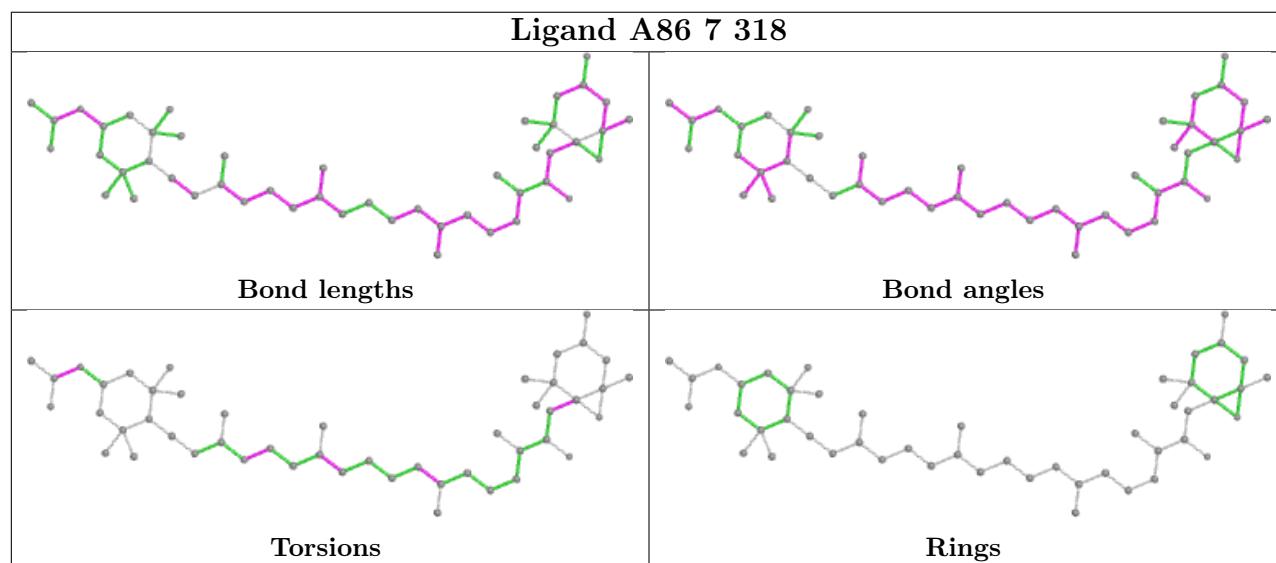
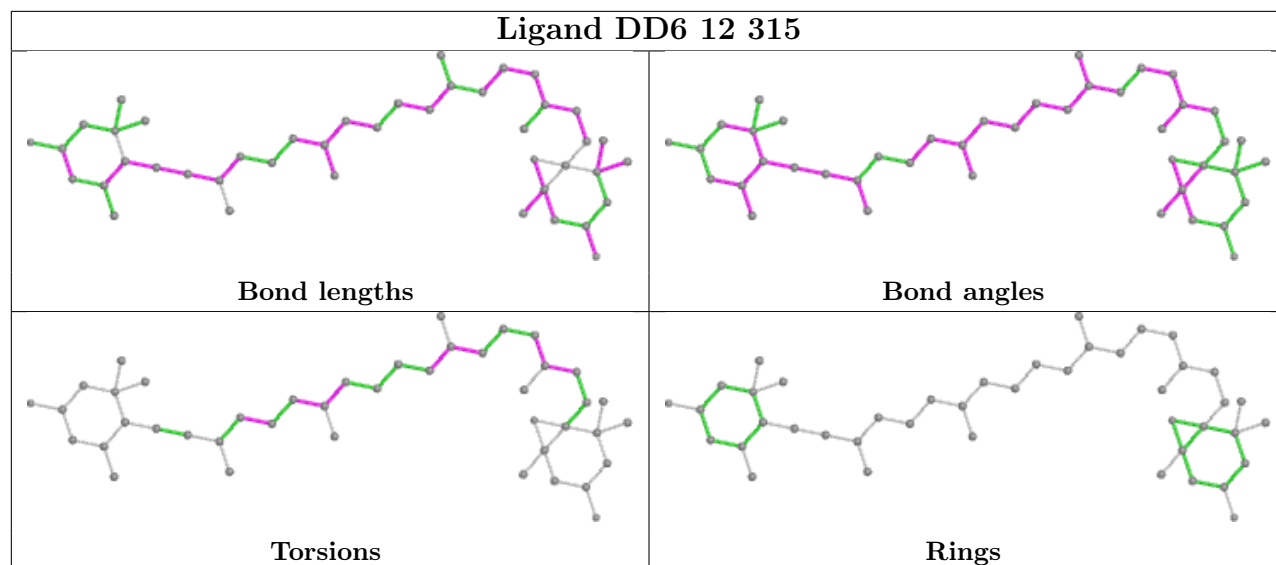


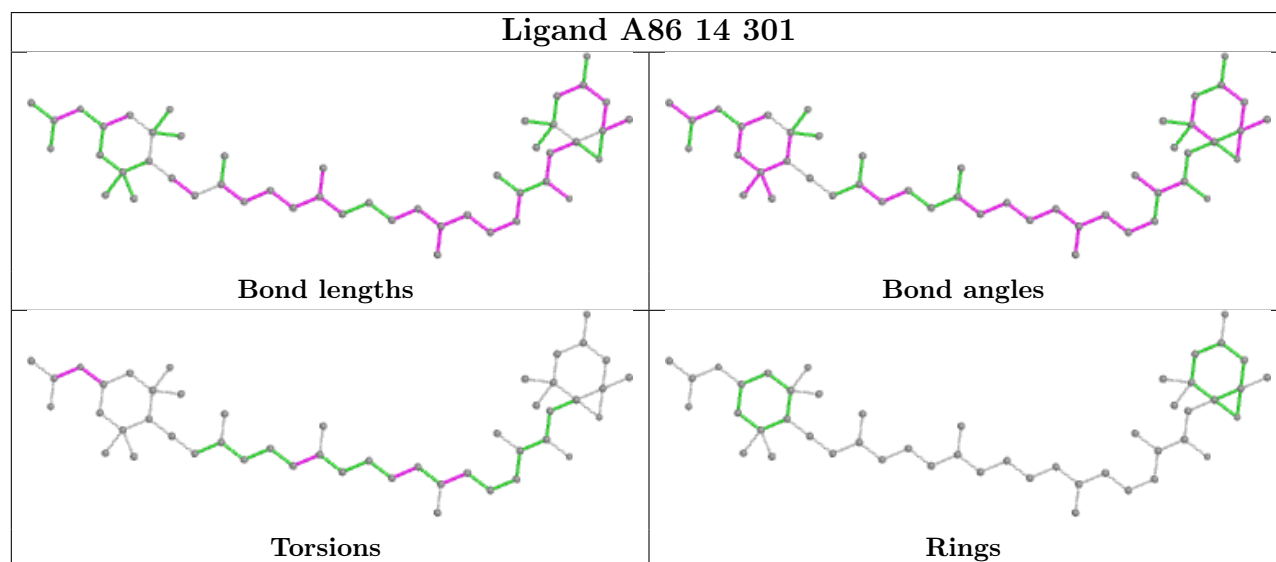
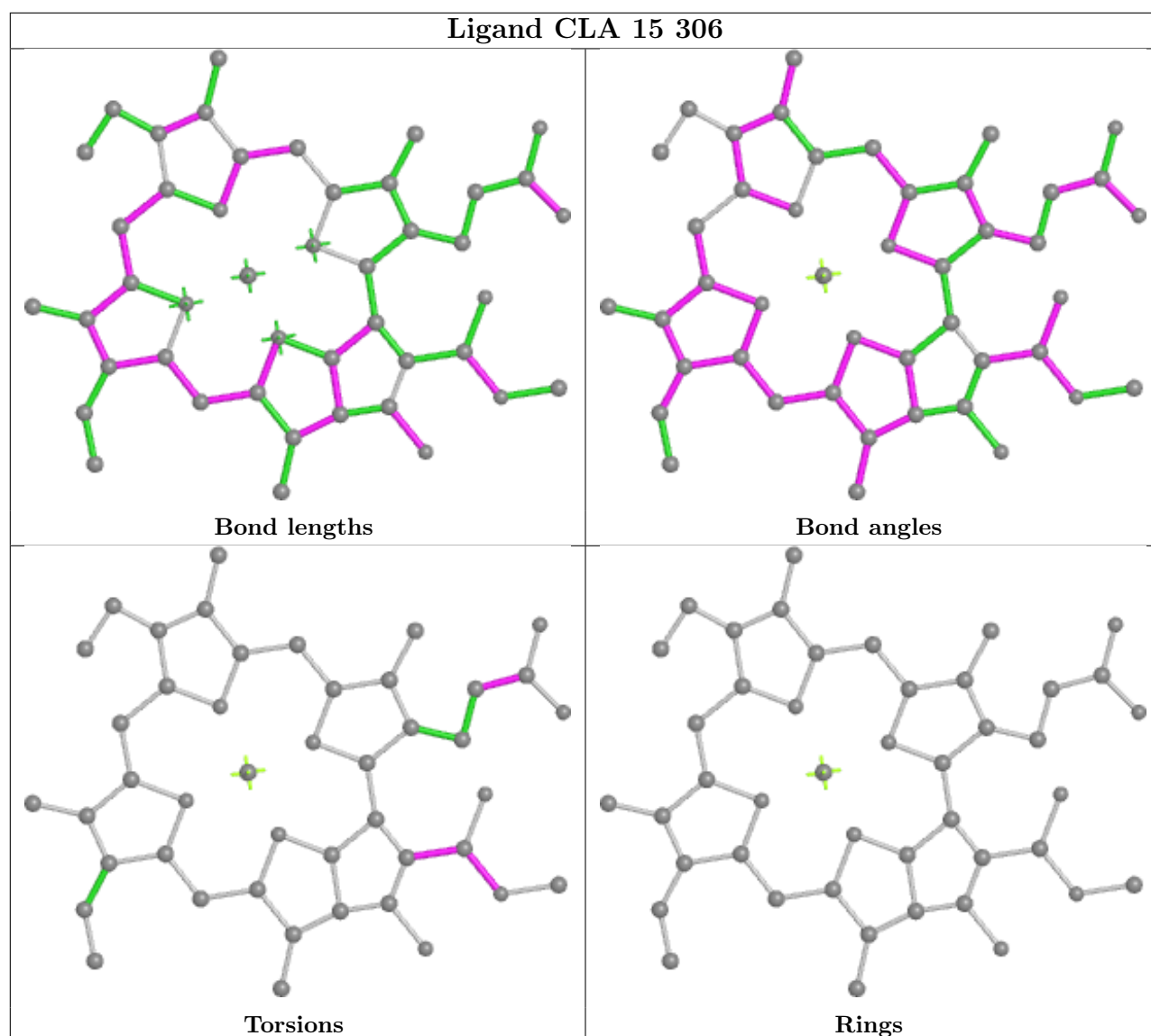
Ligand DD6 10 313

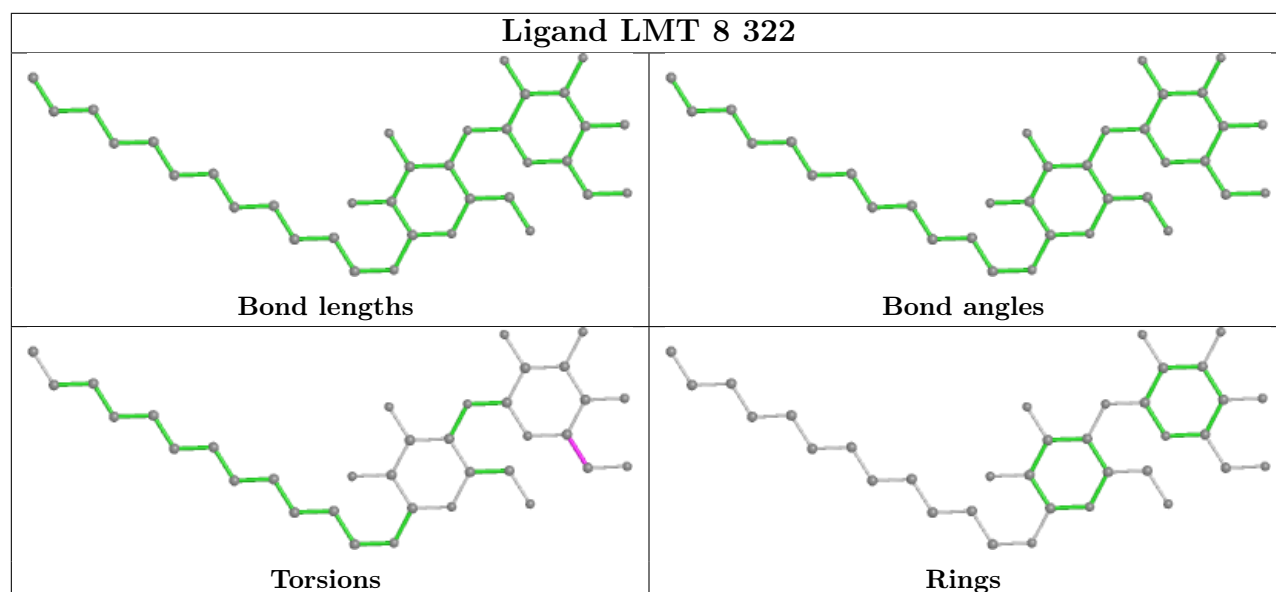
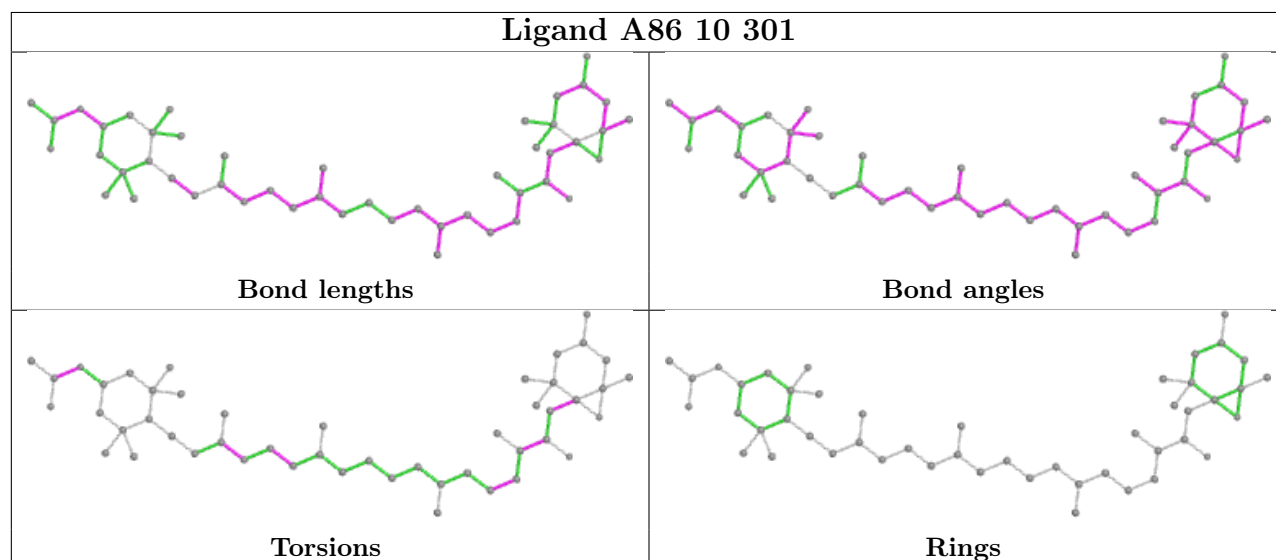
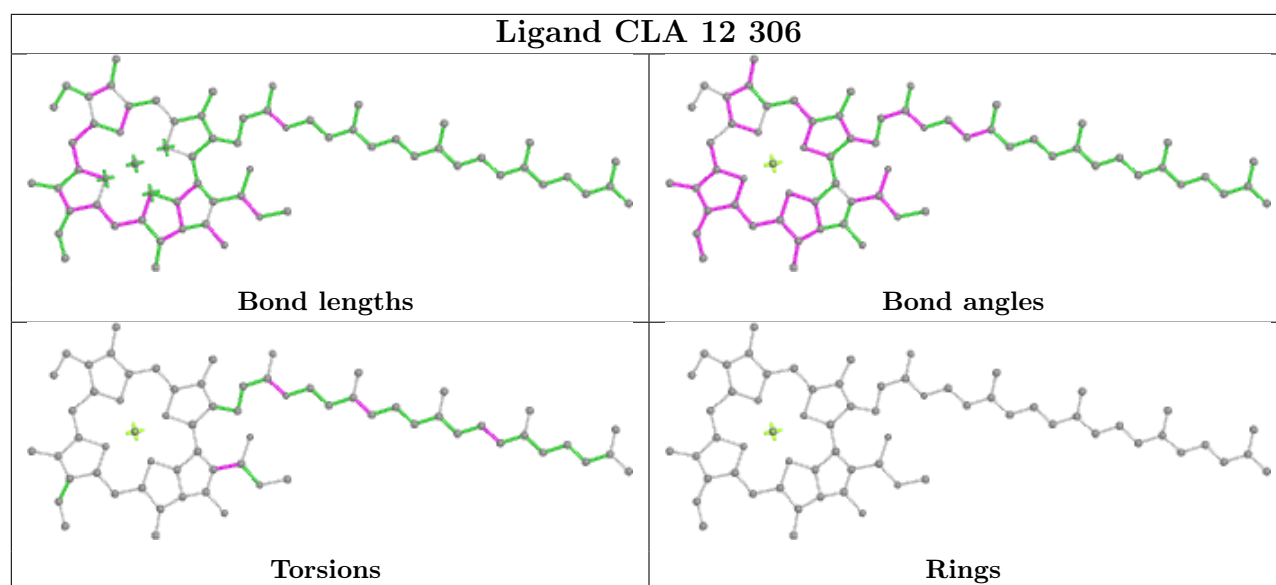


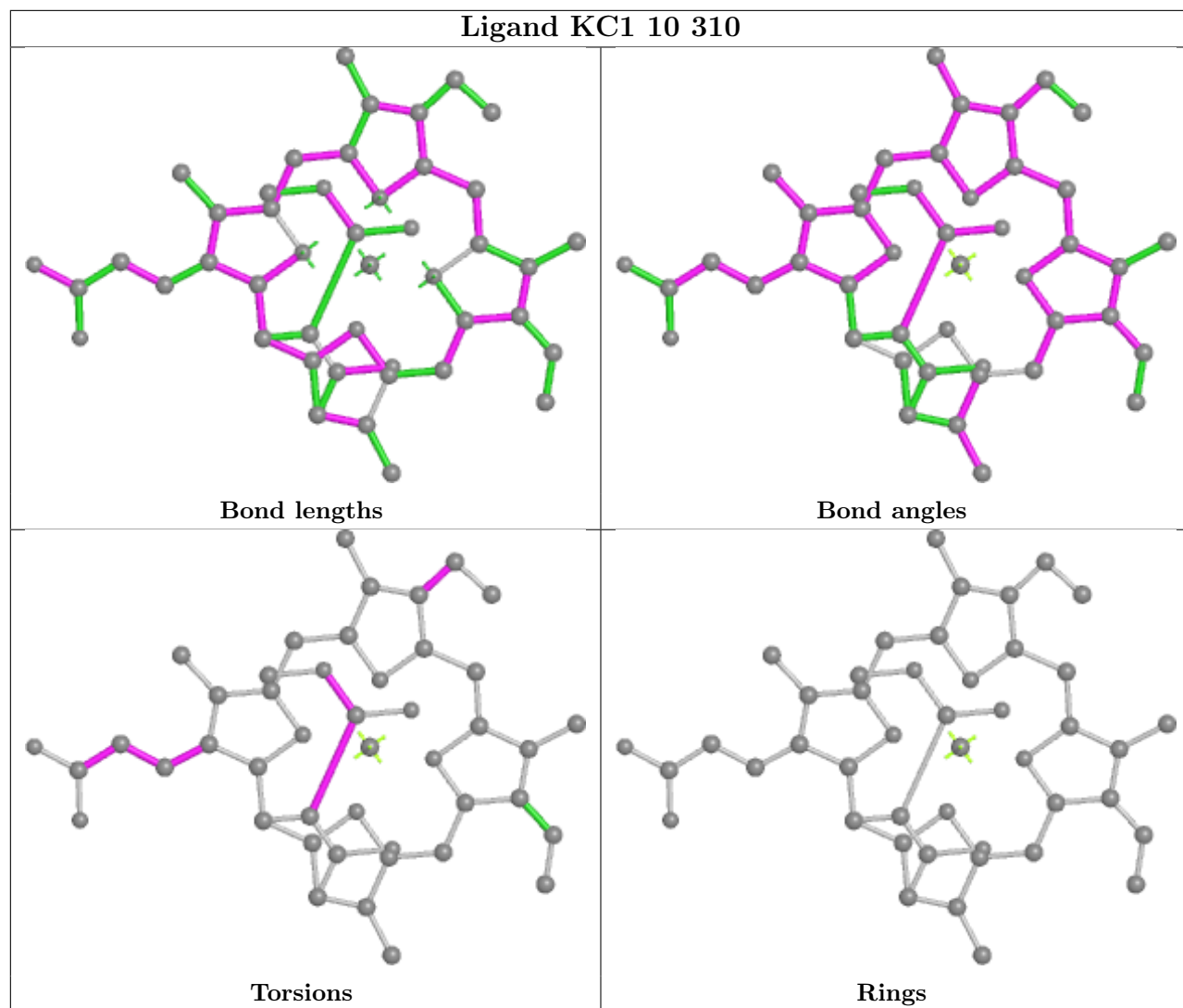
Ligand CLA 6 304

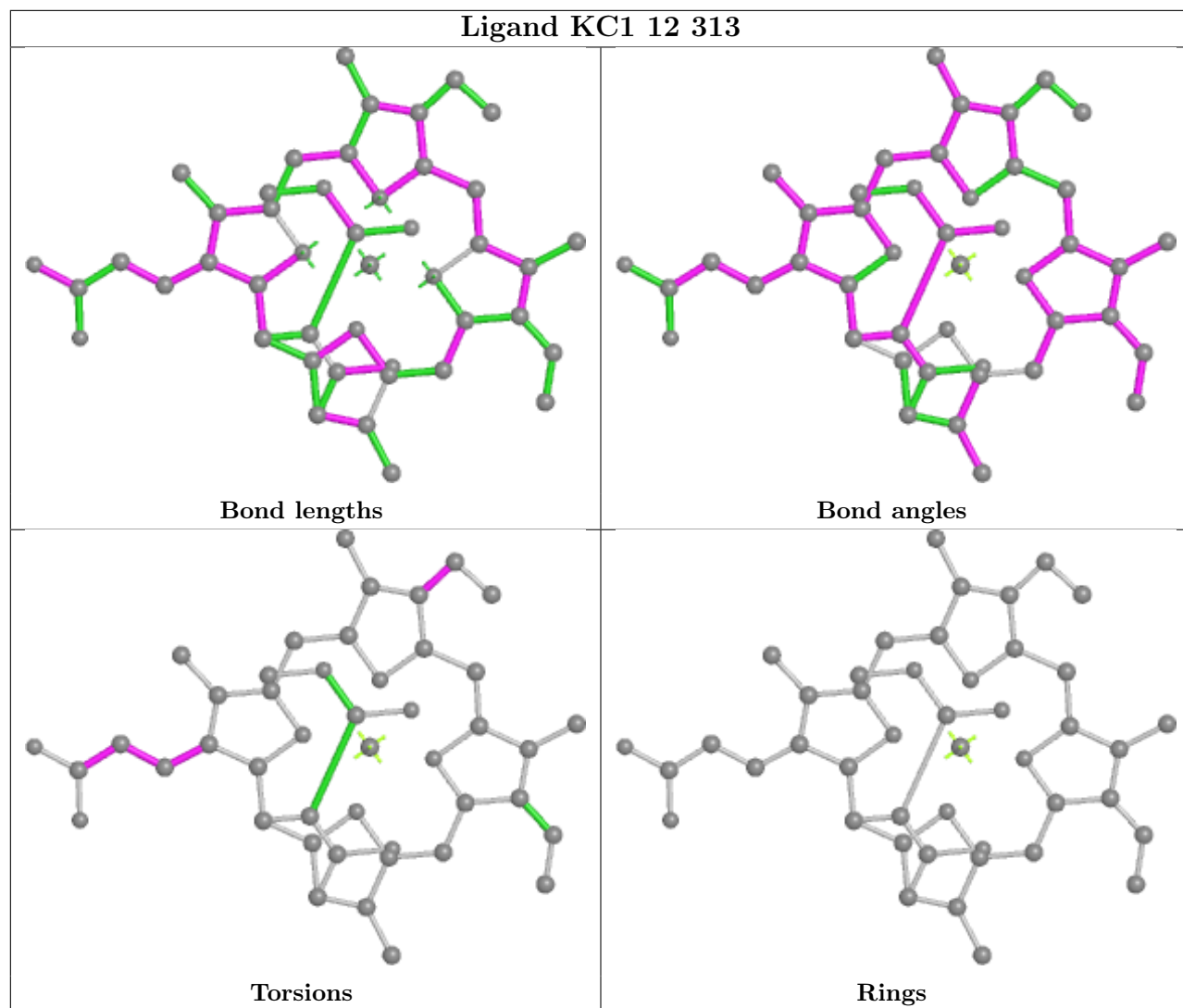




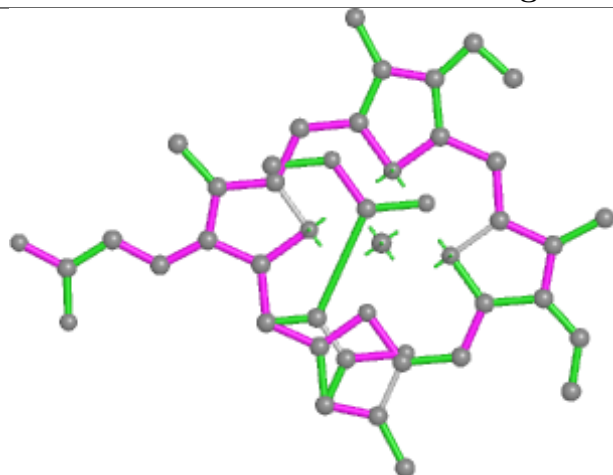




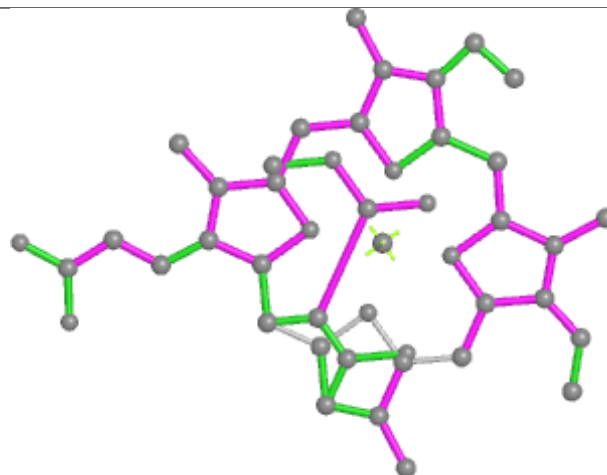




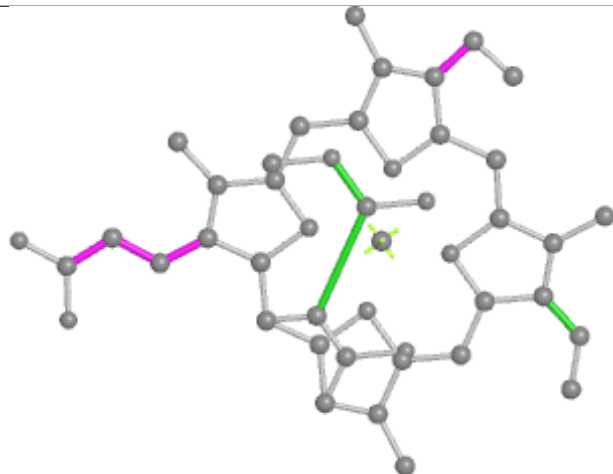
Ligand KC1 6 305



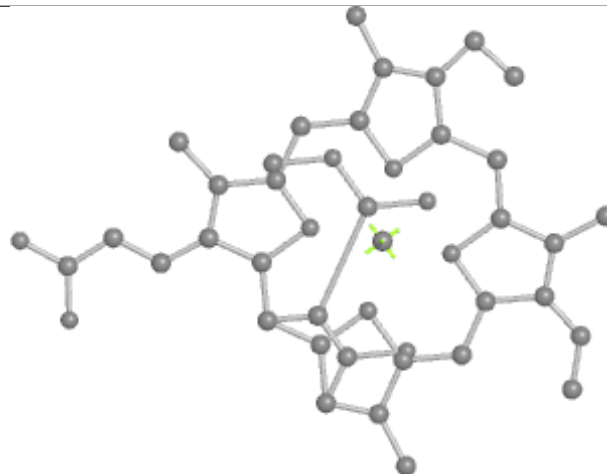
Bond lengths



Bond angles

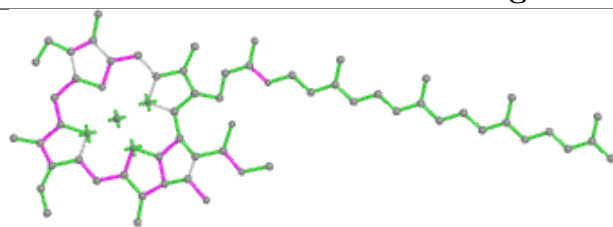


Torsions

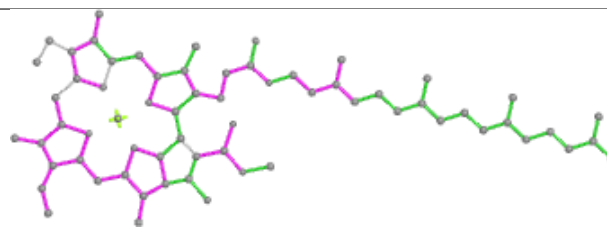


Rings

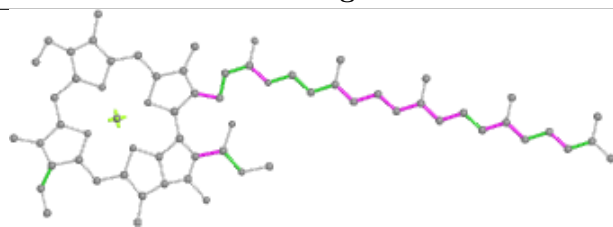
Ligand CLA 16 303



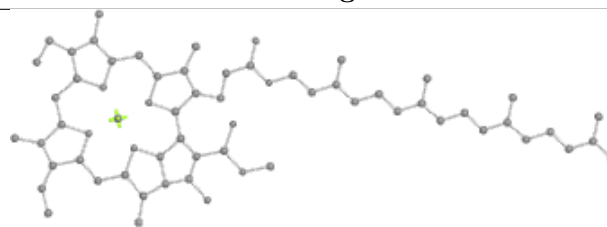
Bond lengths



Bond angles

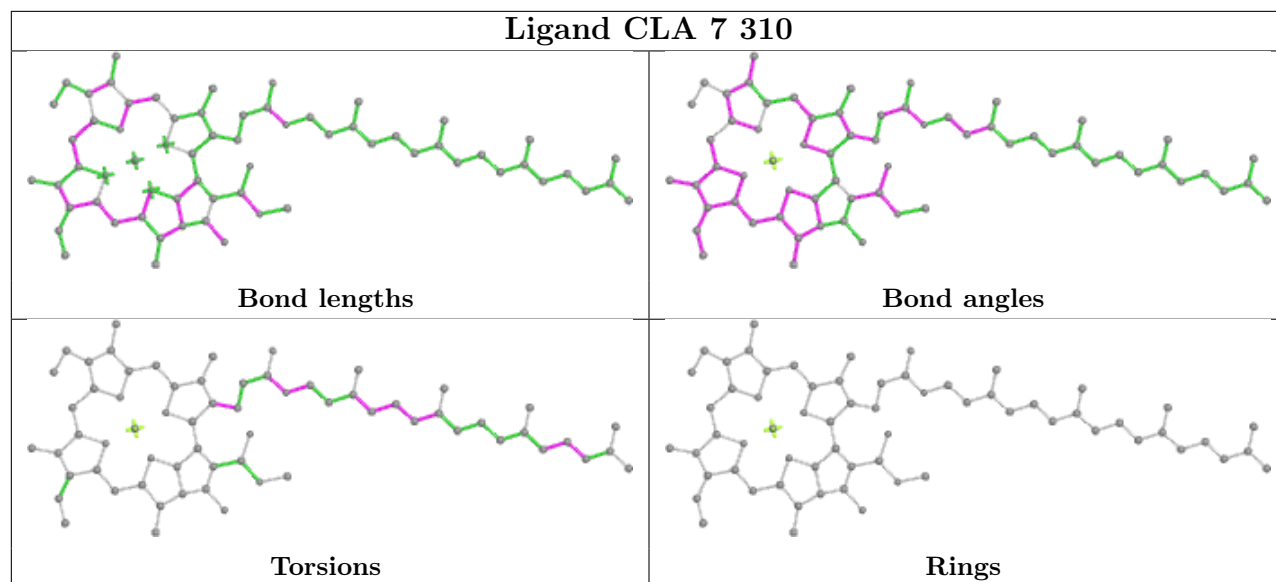


Torsions

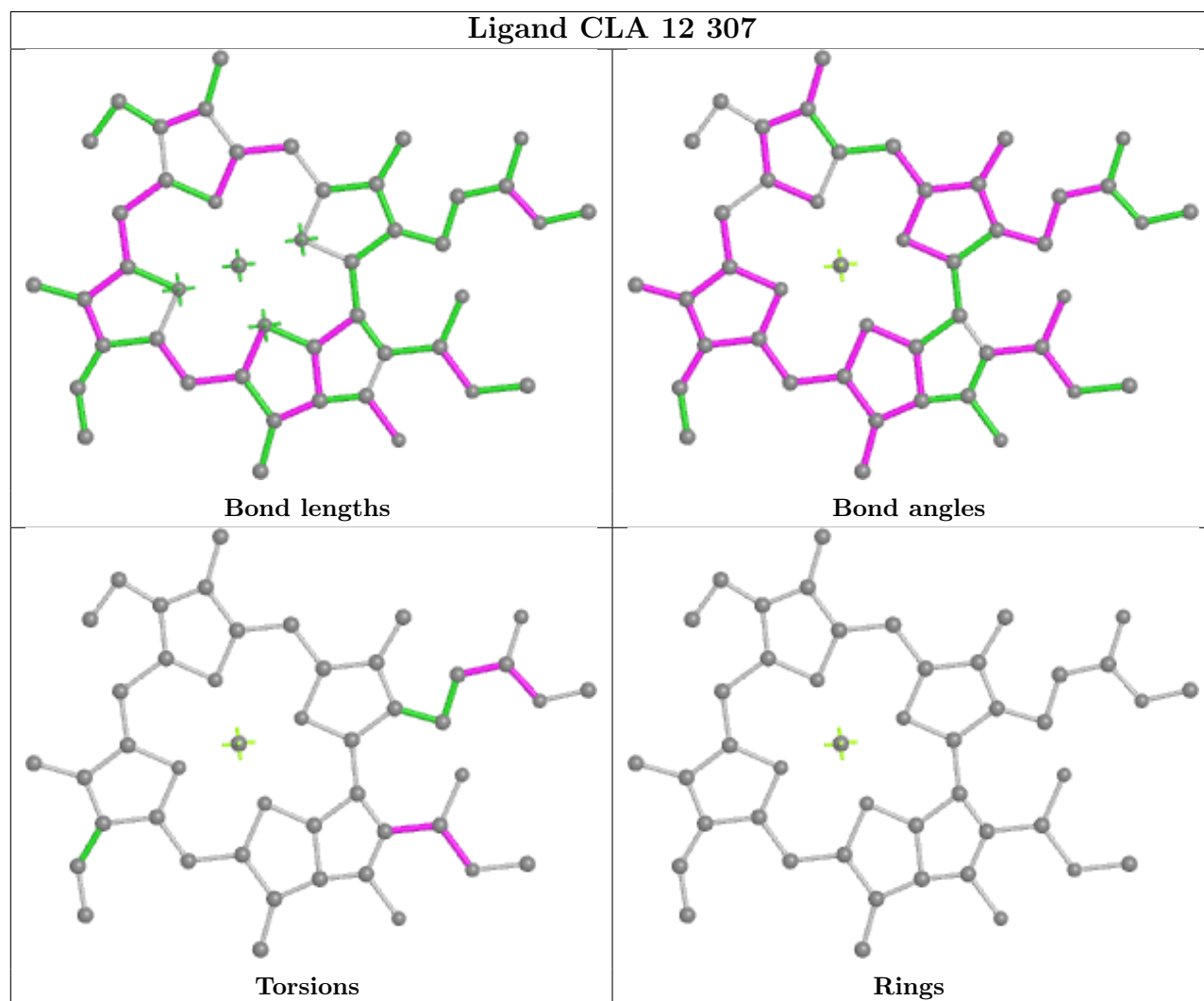


Rings

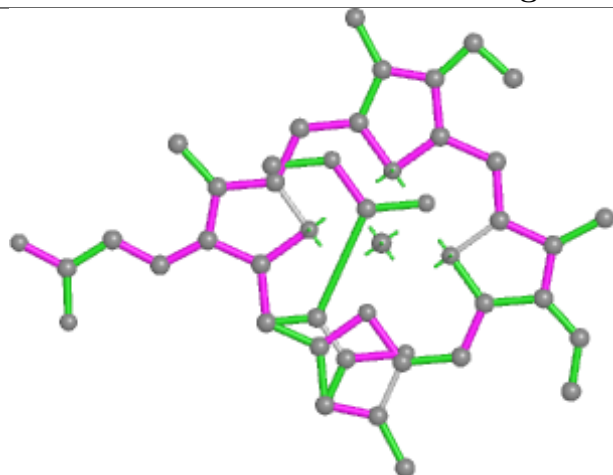
Ligand CLA 7 310



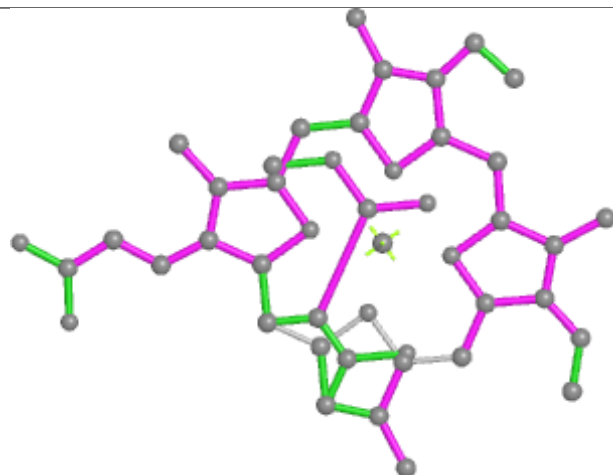
Ligand CLA 12 307



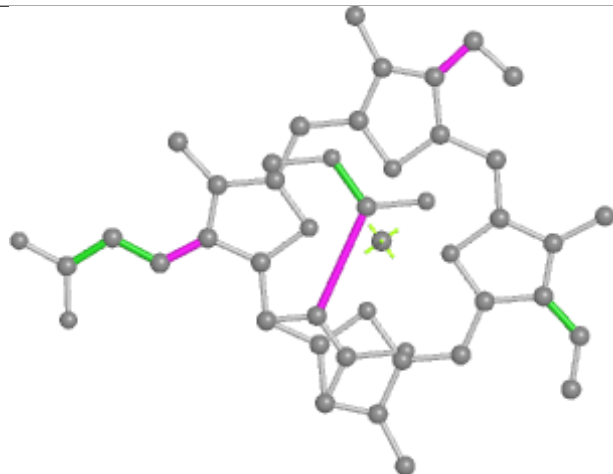
Ligand KC1 6 309



Bond lengths



Bond angles

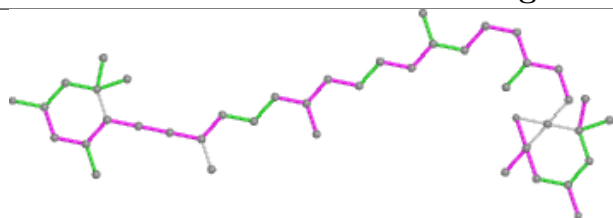


Torsions

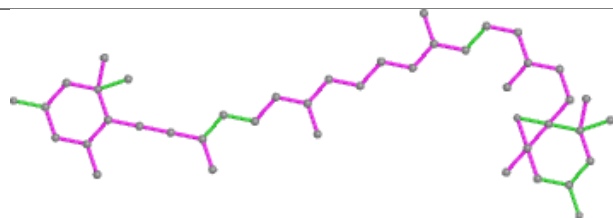


Rings

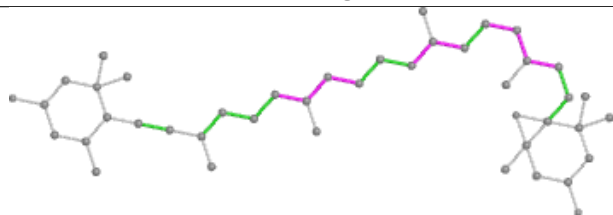
Ligand DD6 6 318



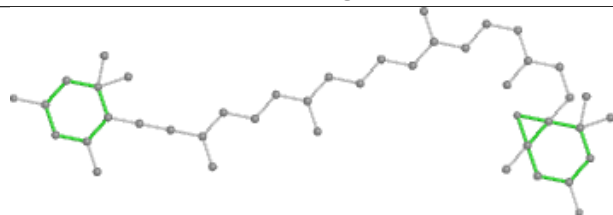
Bond lengths



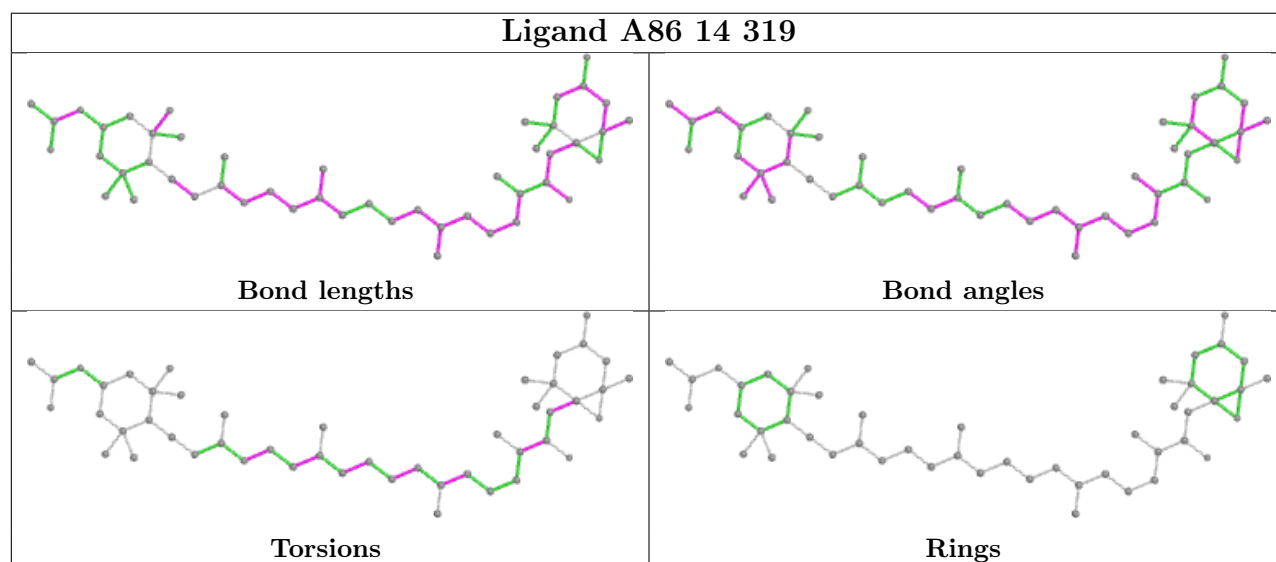
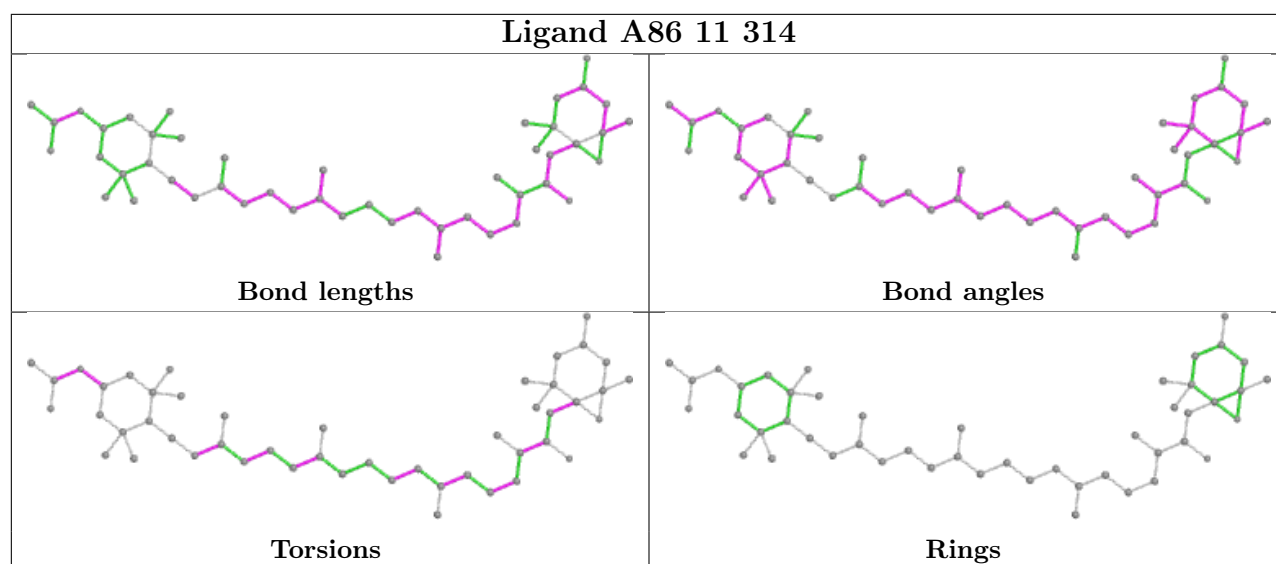
Bond angles



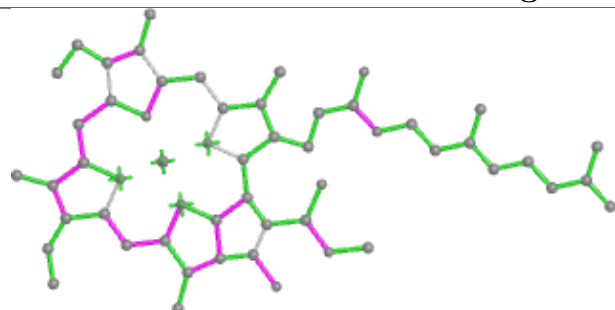
Torsions



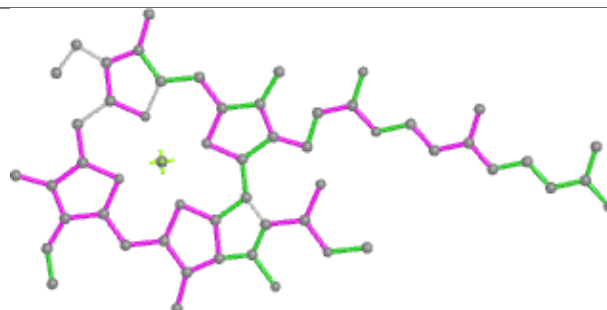
Rings



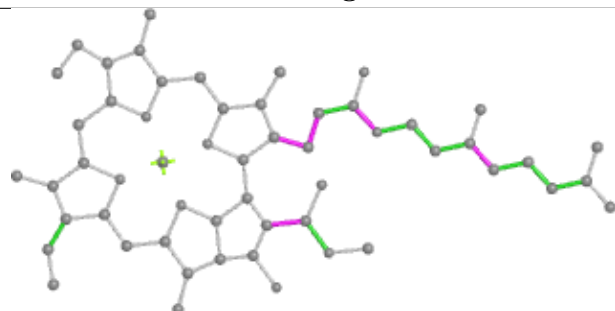
Ligand CLA 8 308



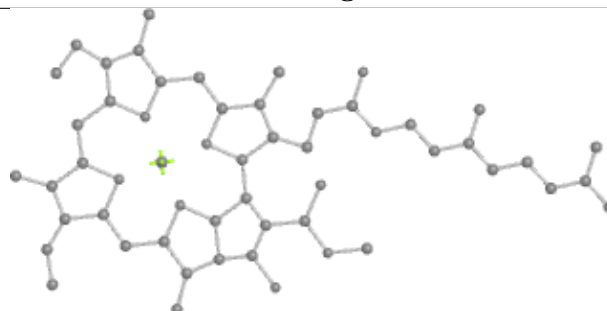
Bond lengths



Bond angles

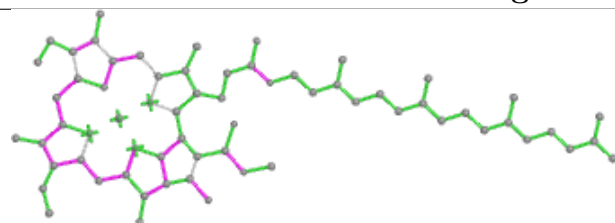


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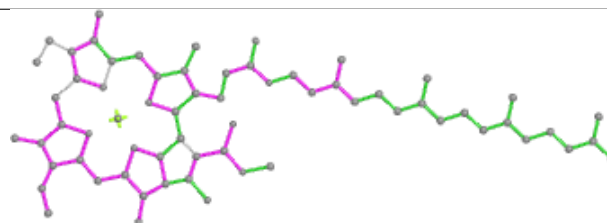


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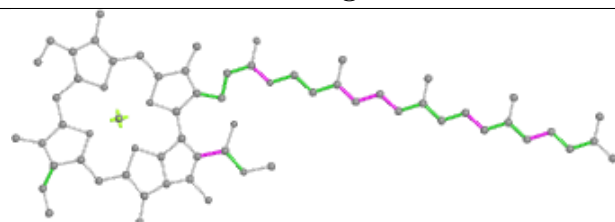
Ligand CLA 15 313



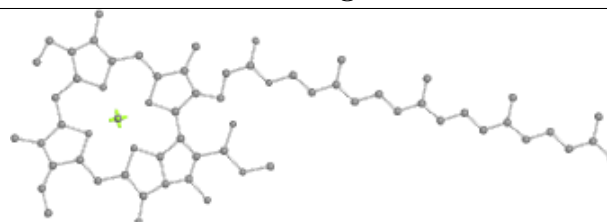
Bond lengths



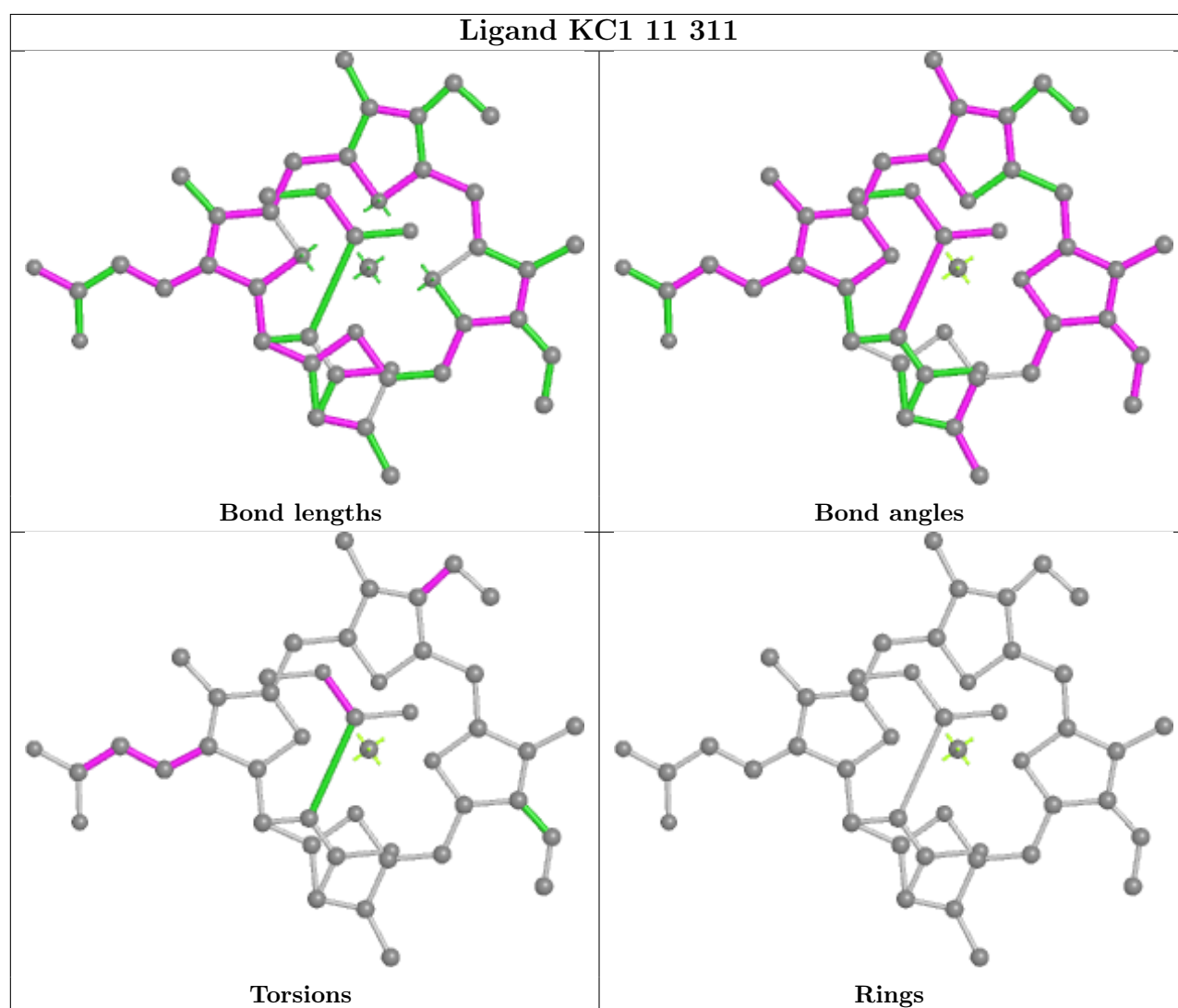
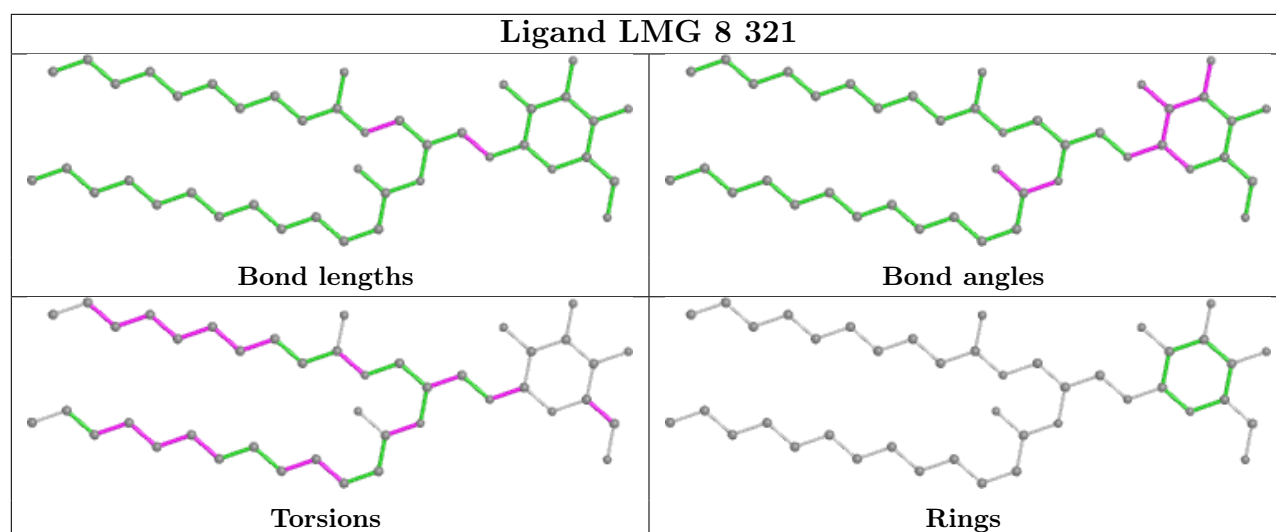
Bond angles



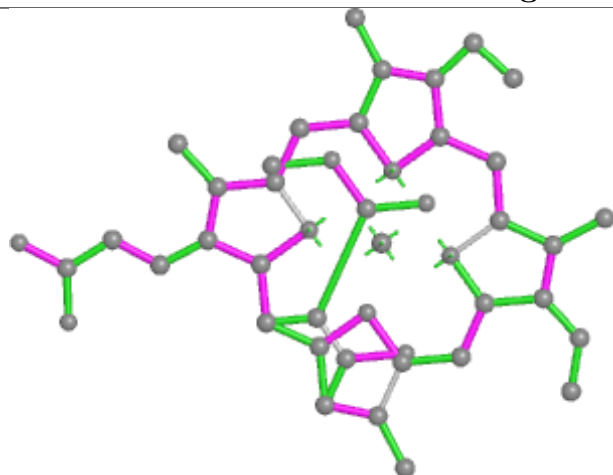
Torsions



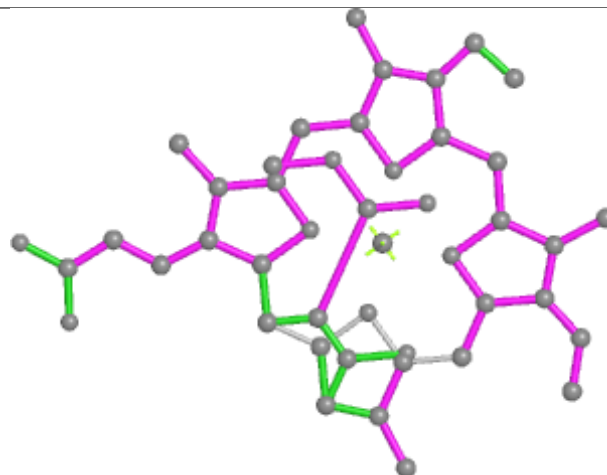
Rings



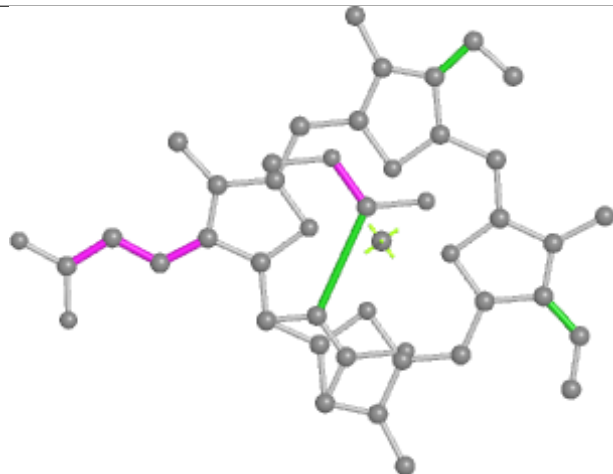
Ligand KC1 8 306



Bond lengths



Bond angles

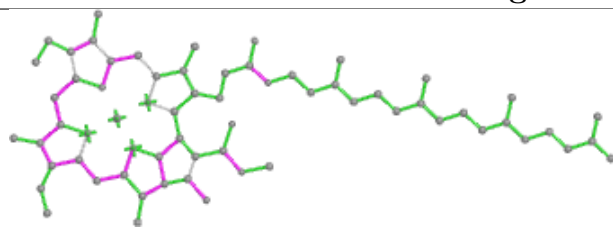


Torsions

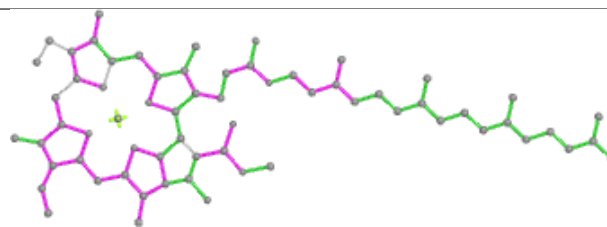


Rings

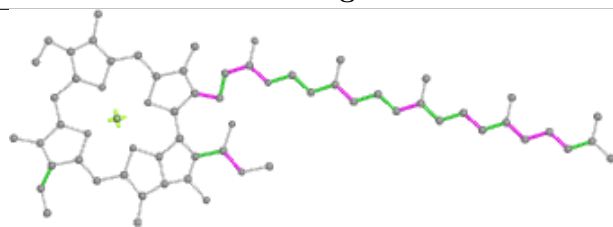
Ligand CLA 11 309



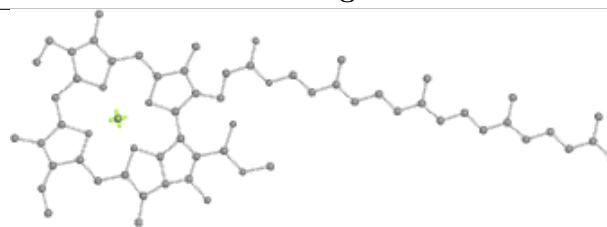
Bond lengths



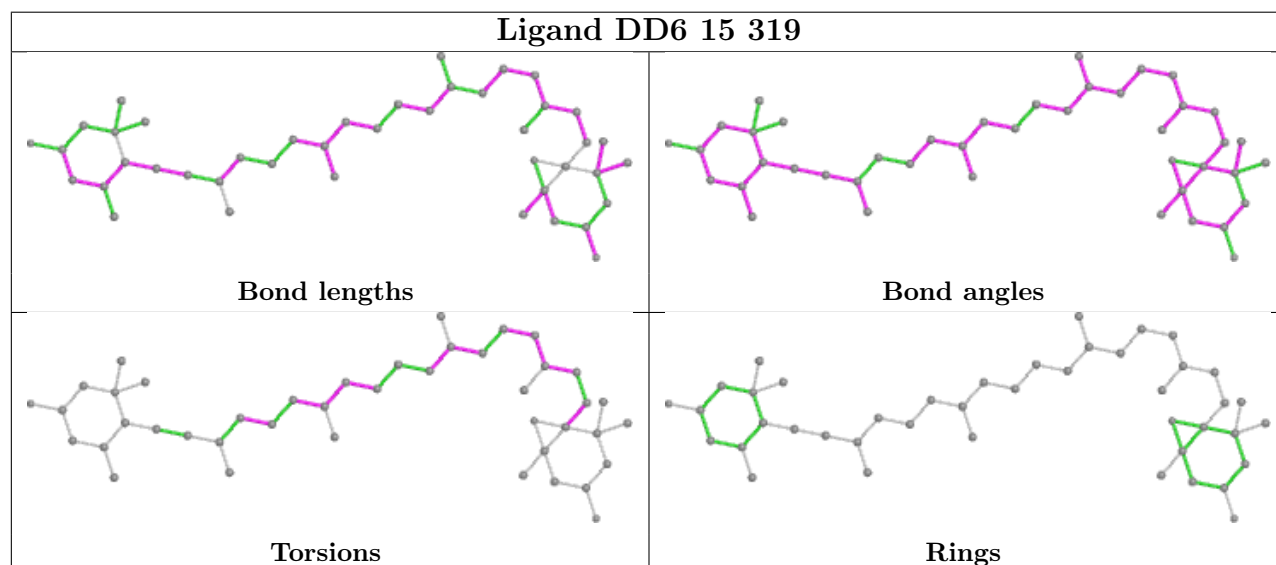
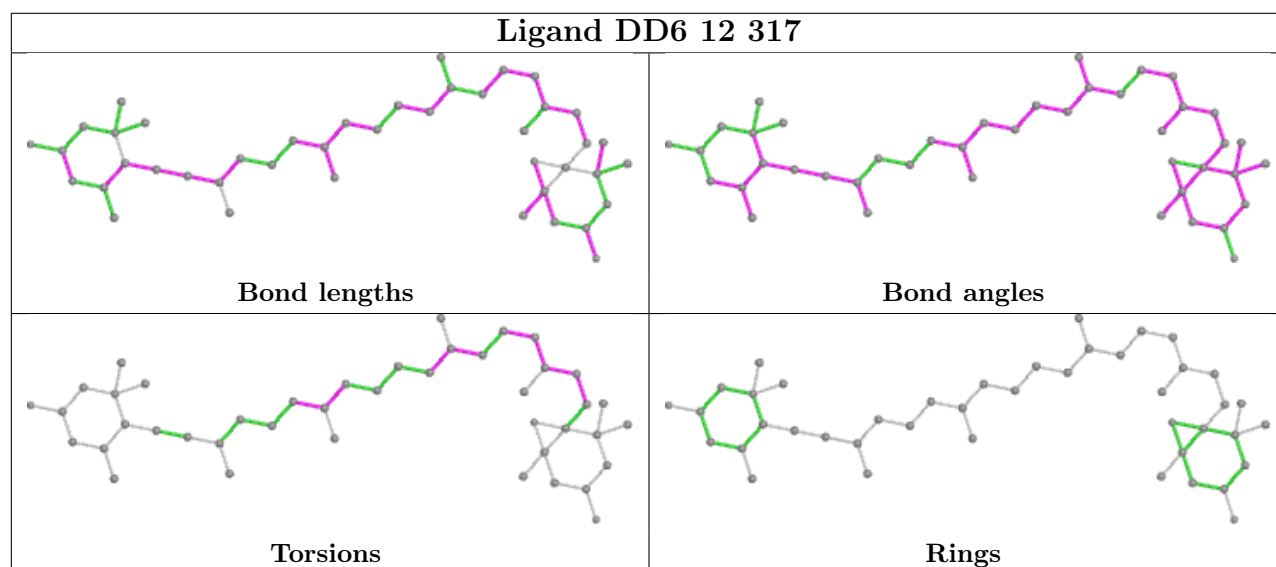
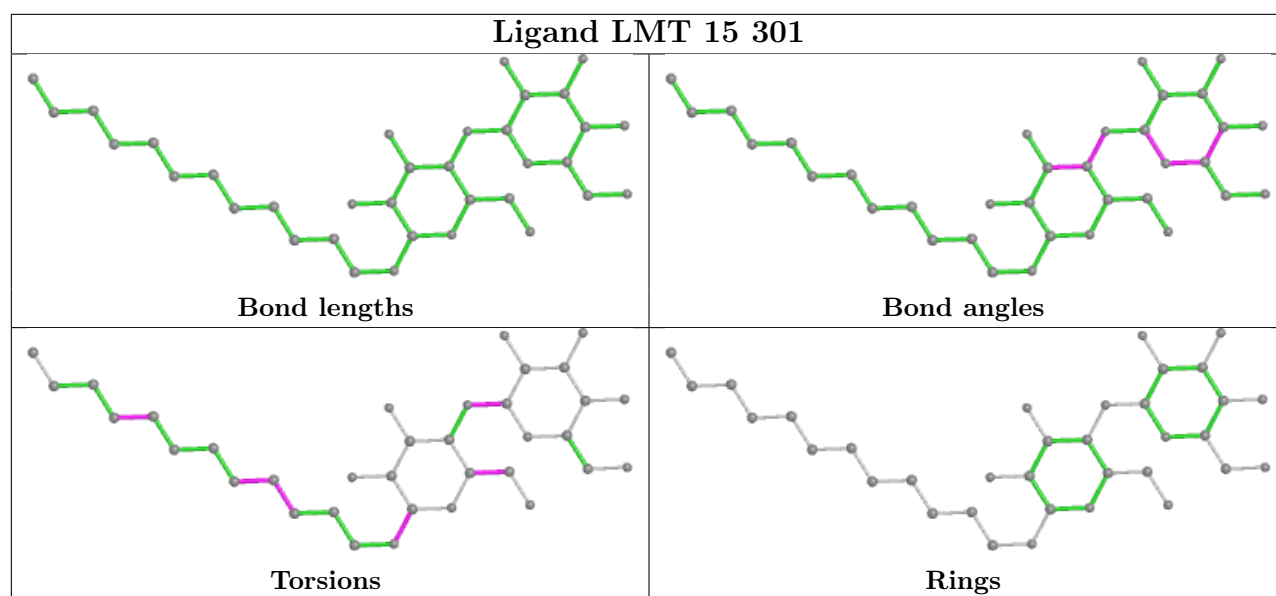
Bond angles



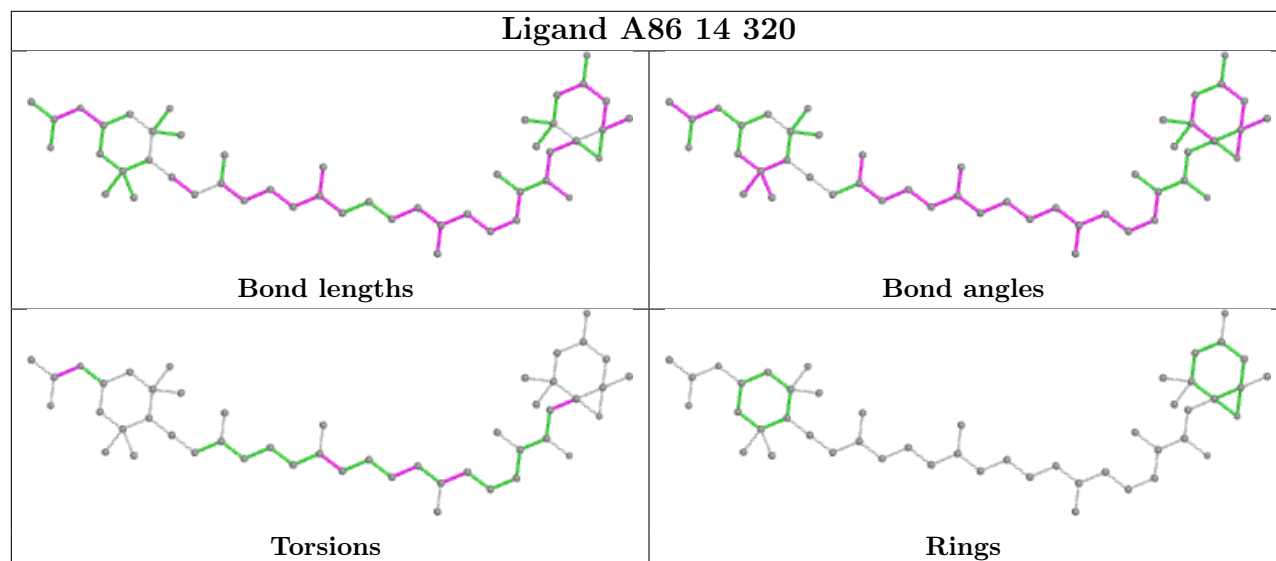
Torsions



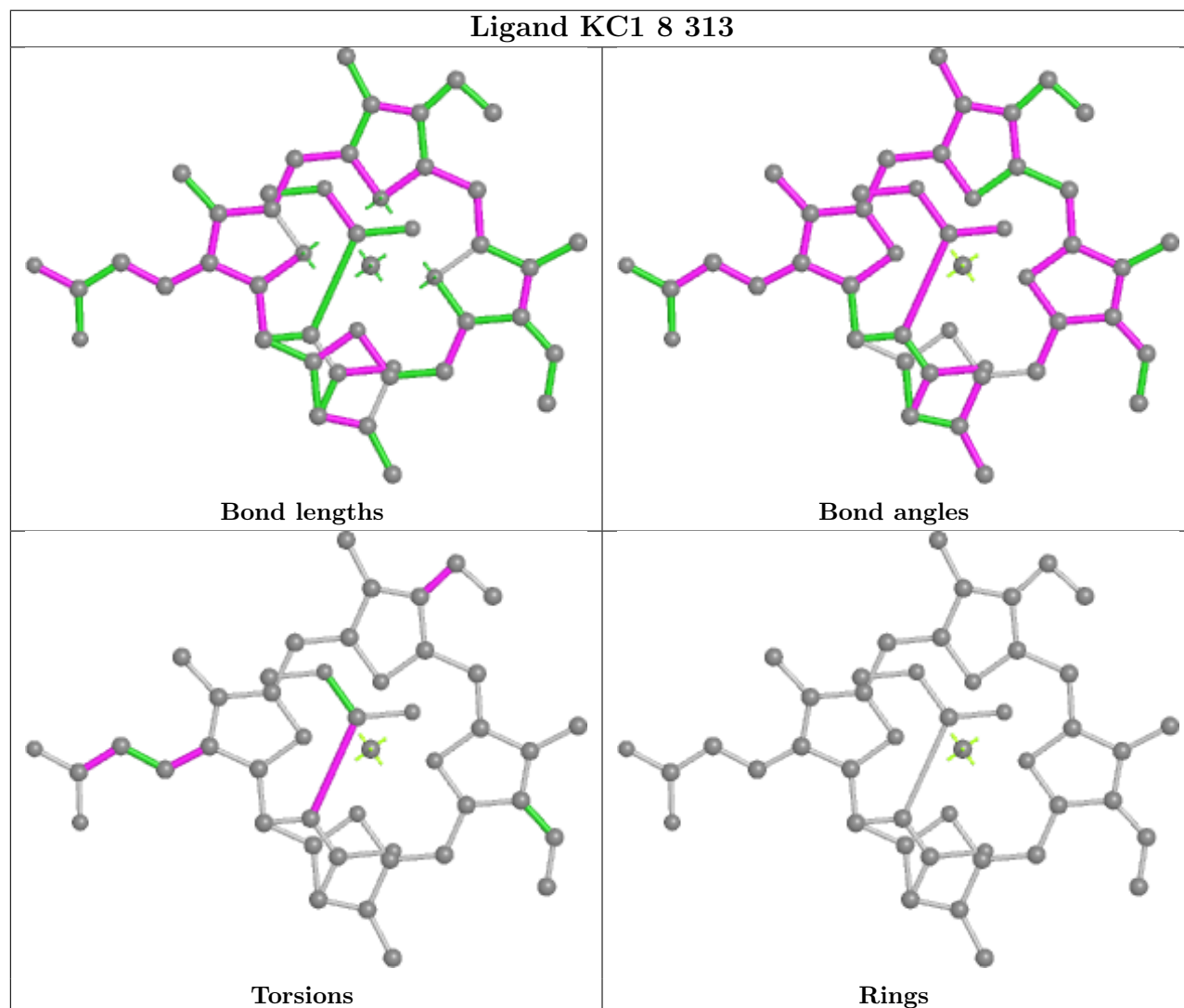
Rings

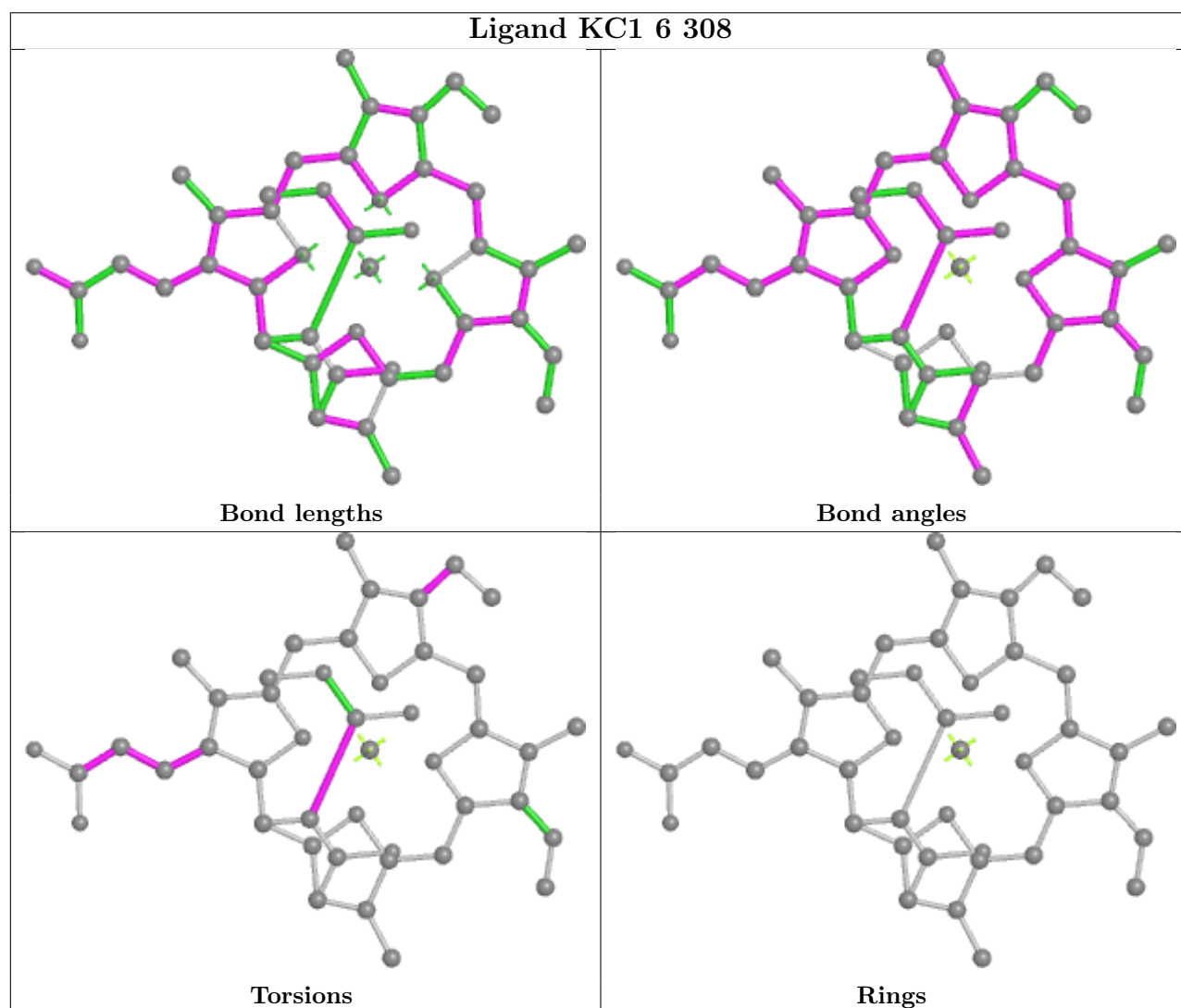
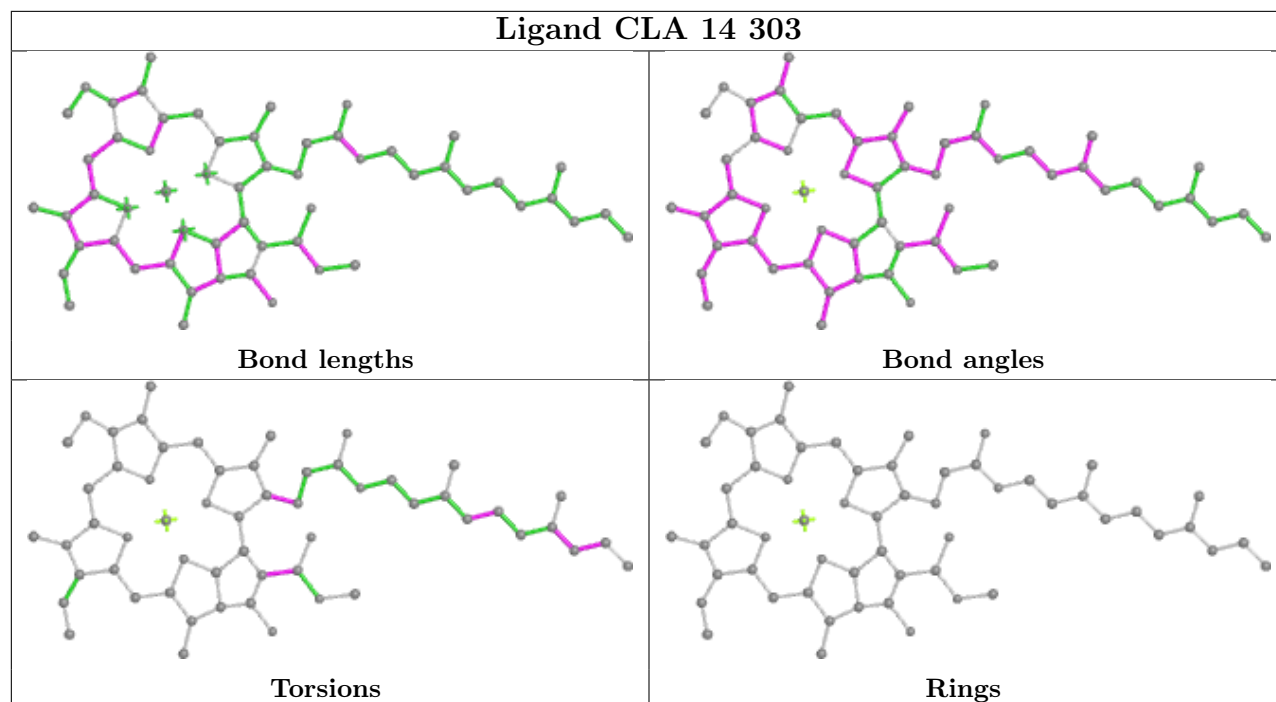


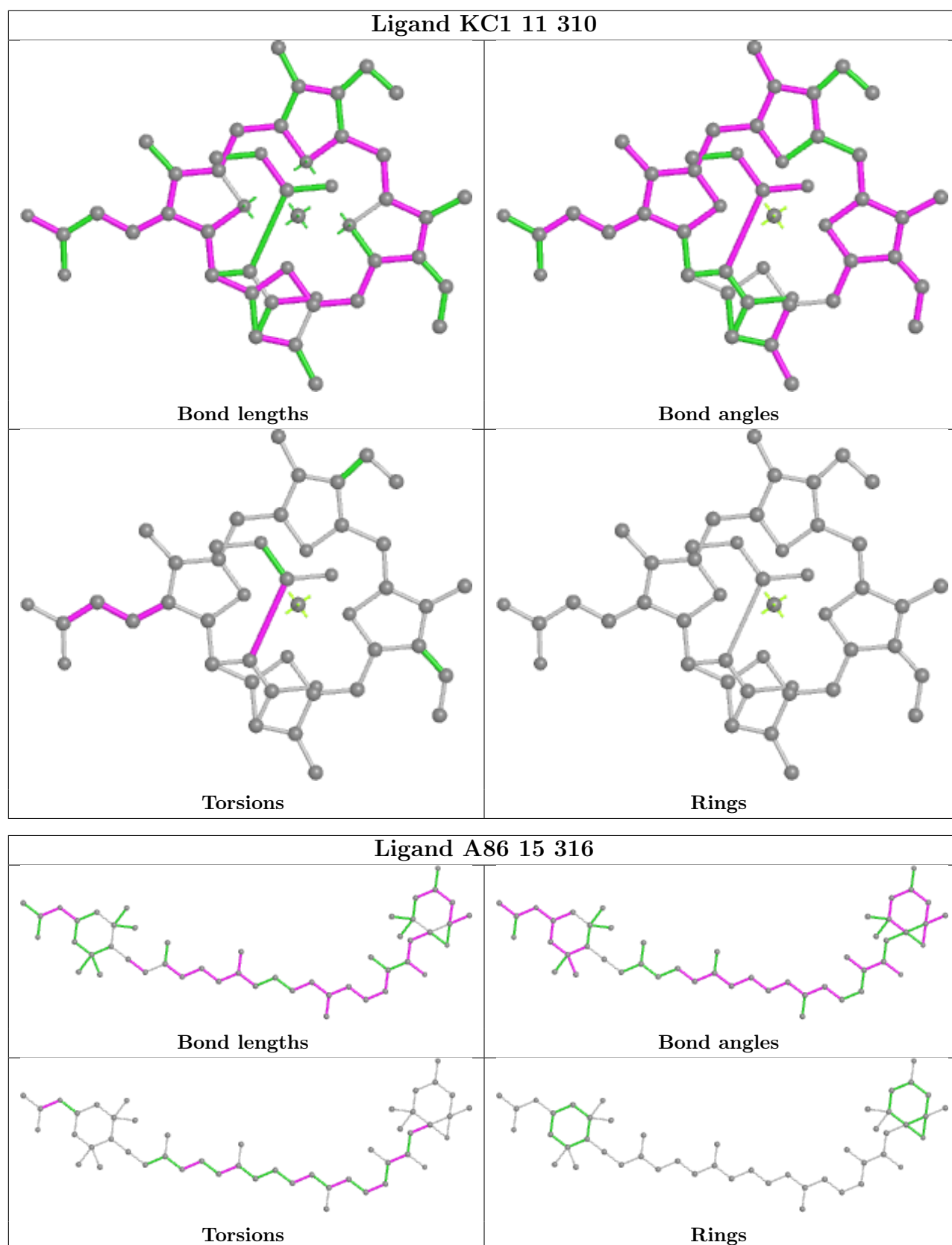
Ligand A86 14 320



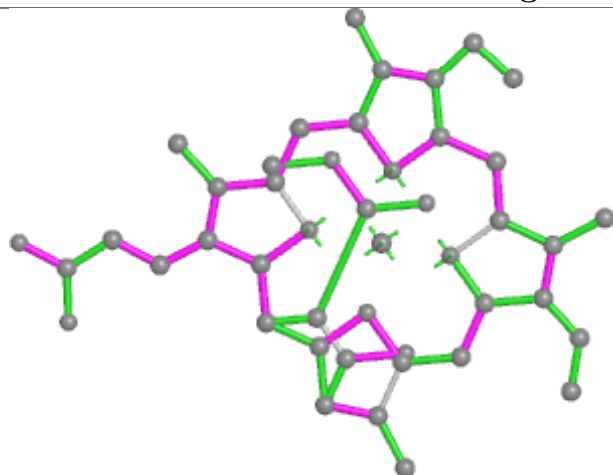
Ligand KC1 8 313



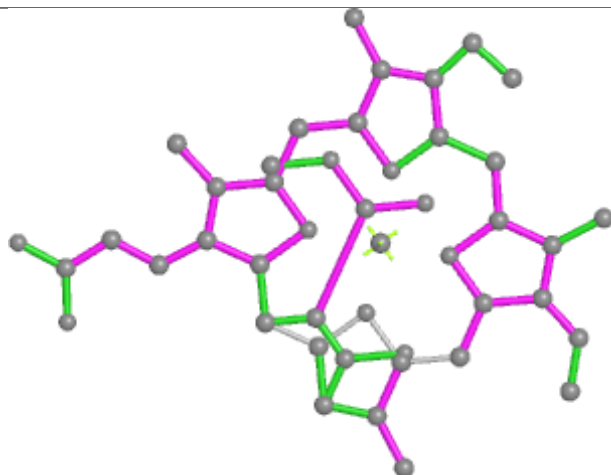




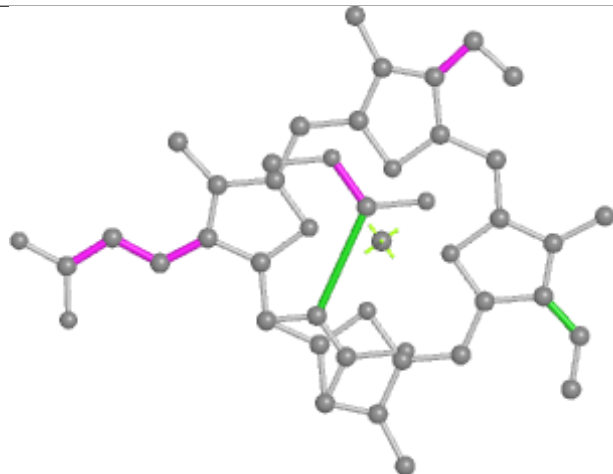
Ligand KC1 7 307



Bond lengths



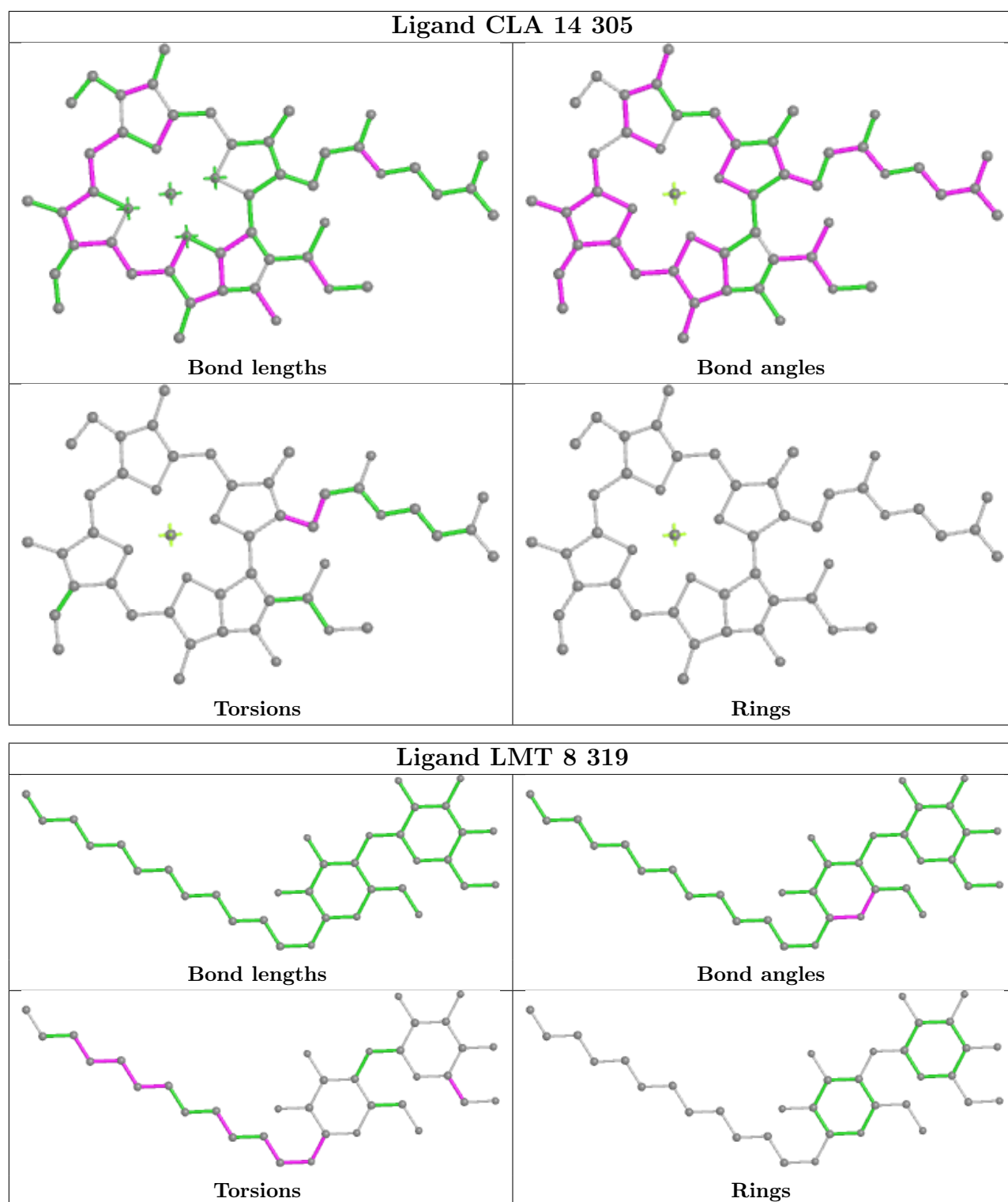
Bond angles

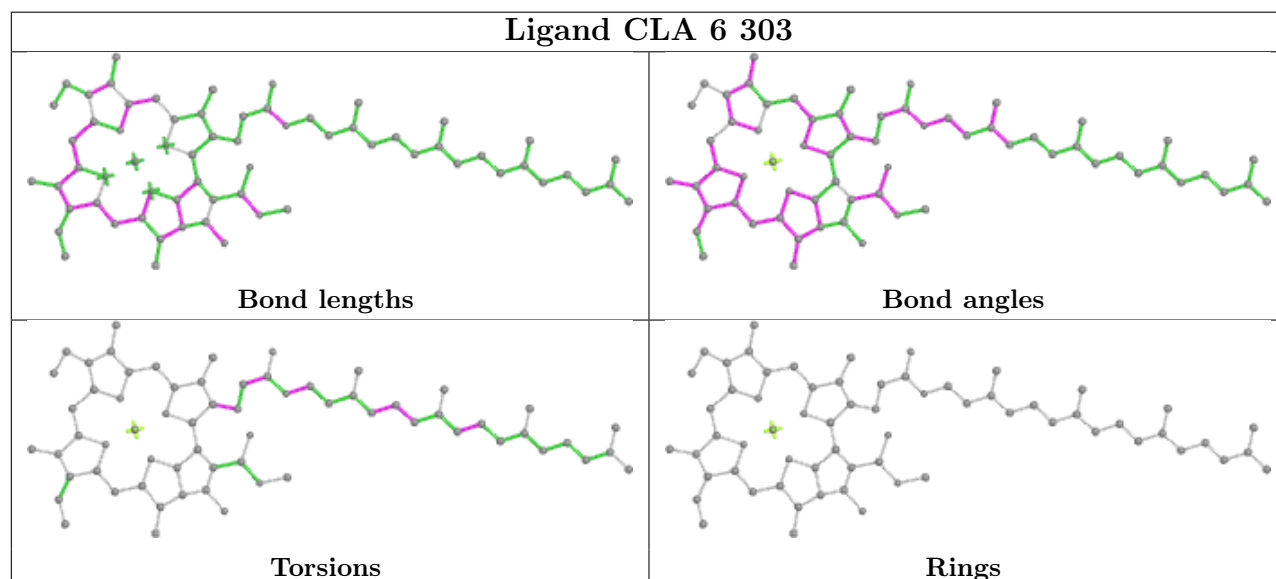
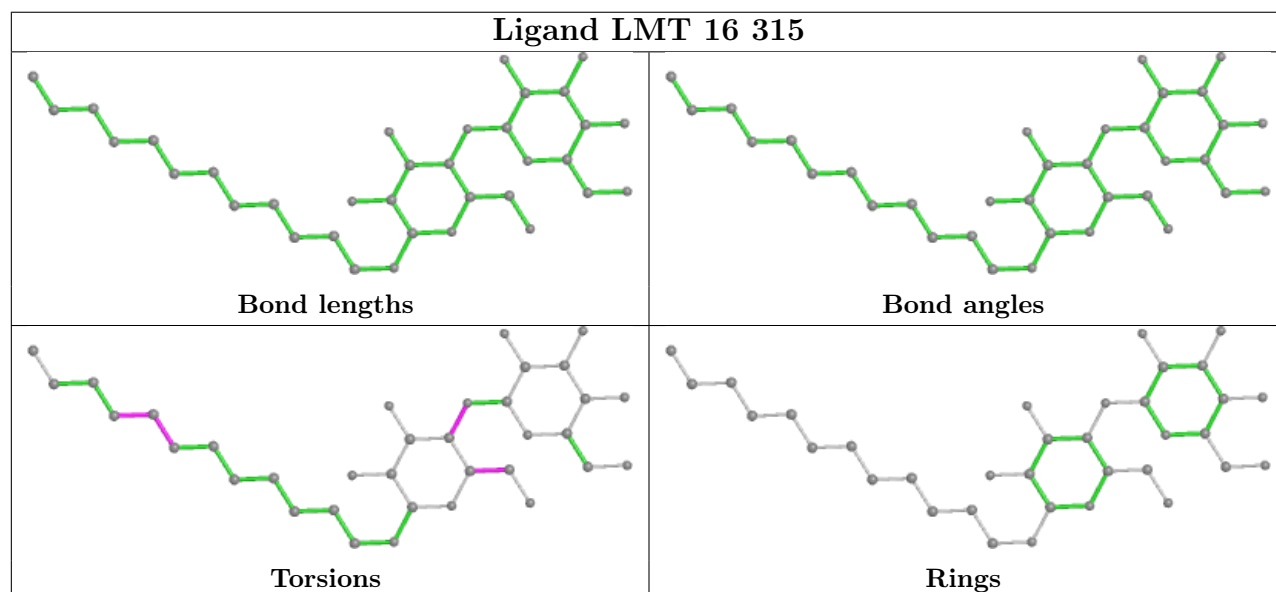
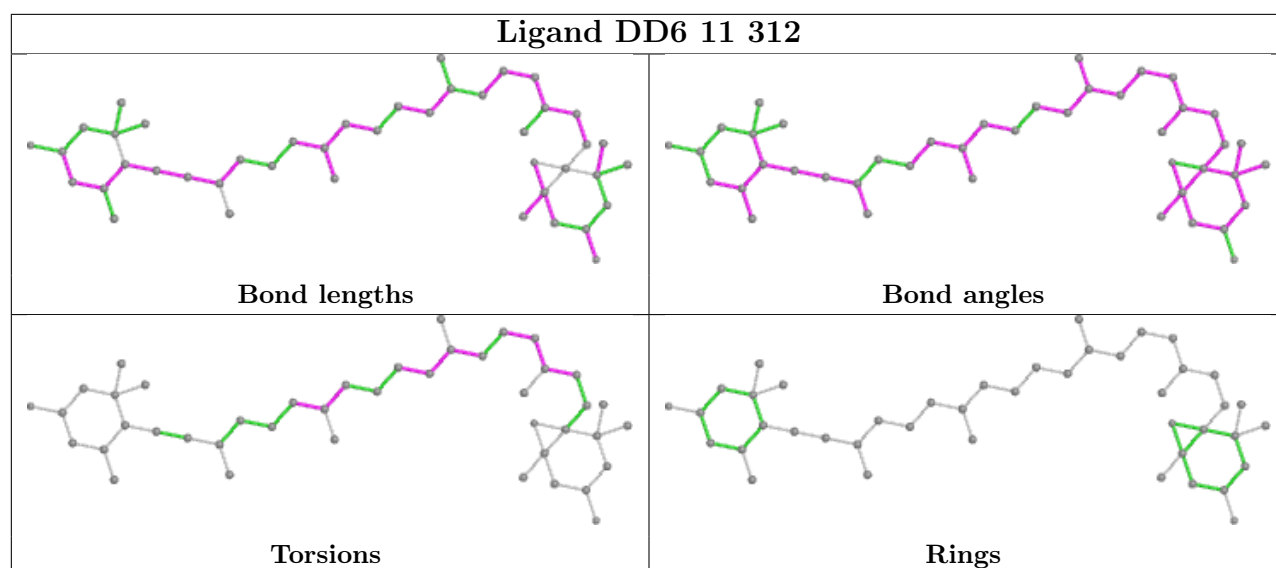


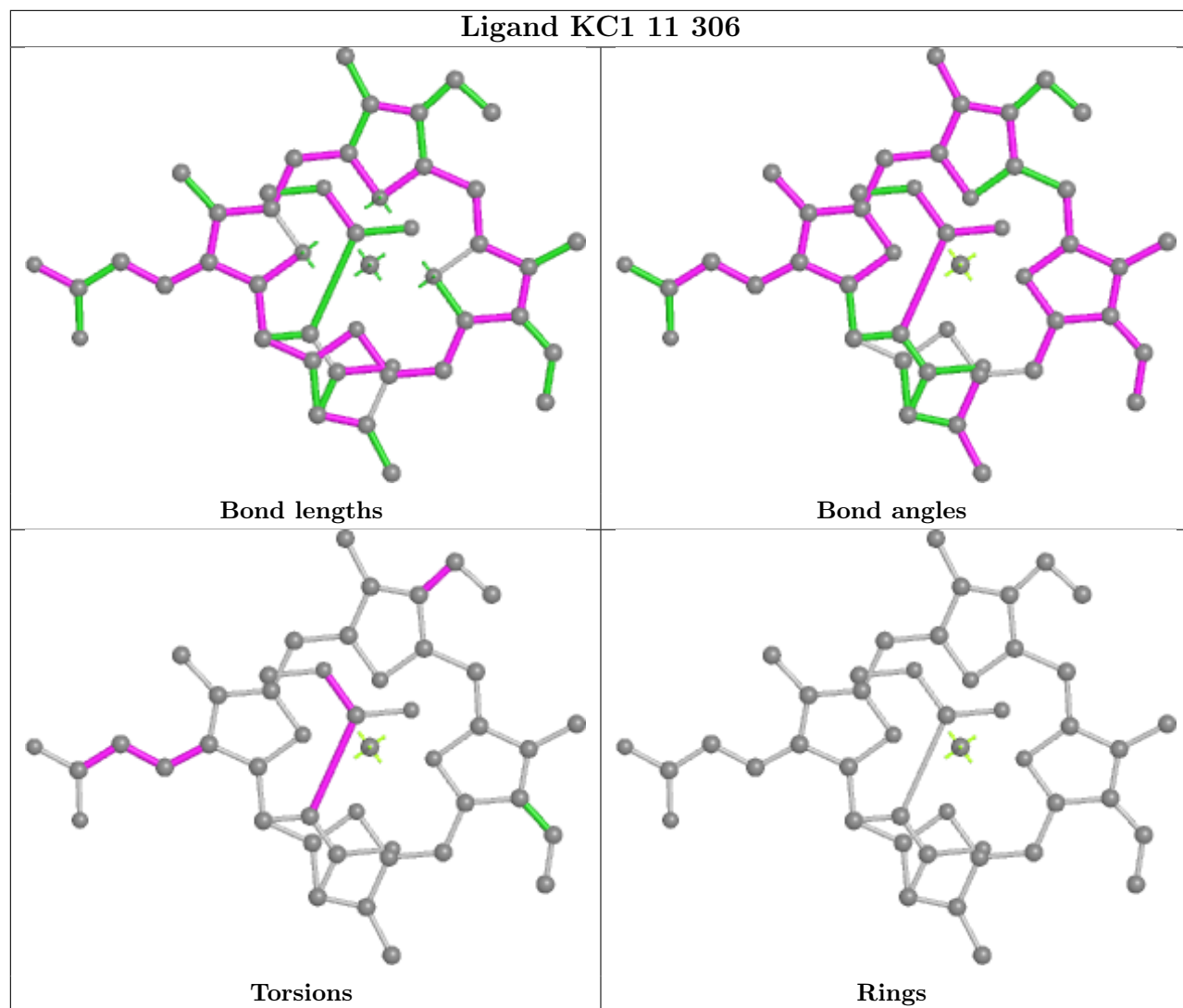
Torsions

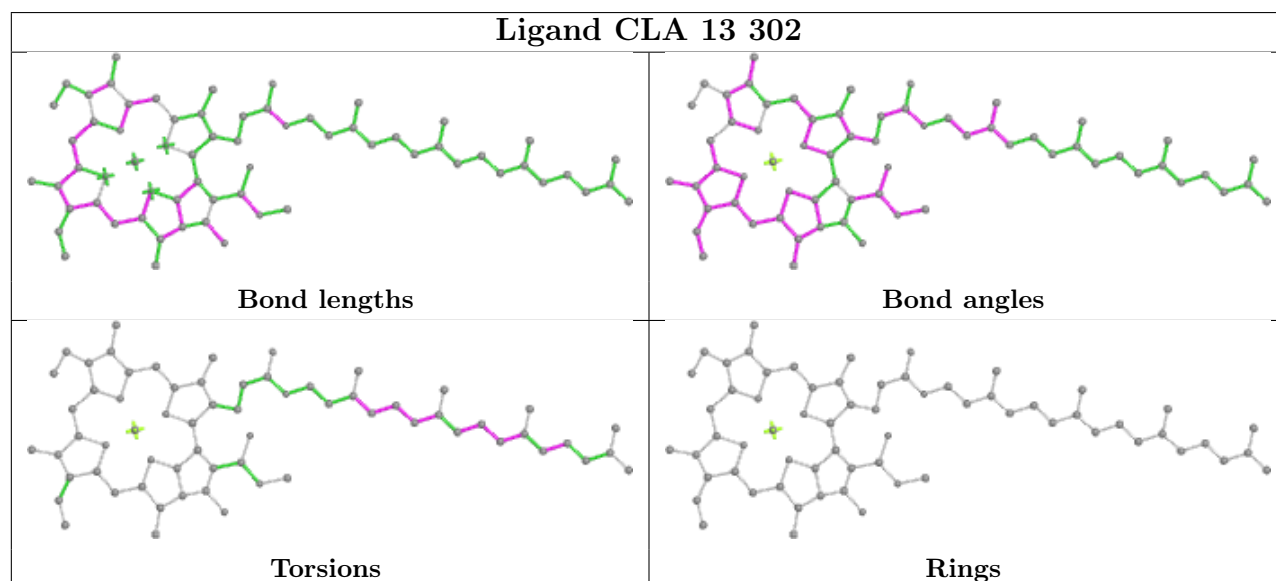
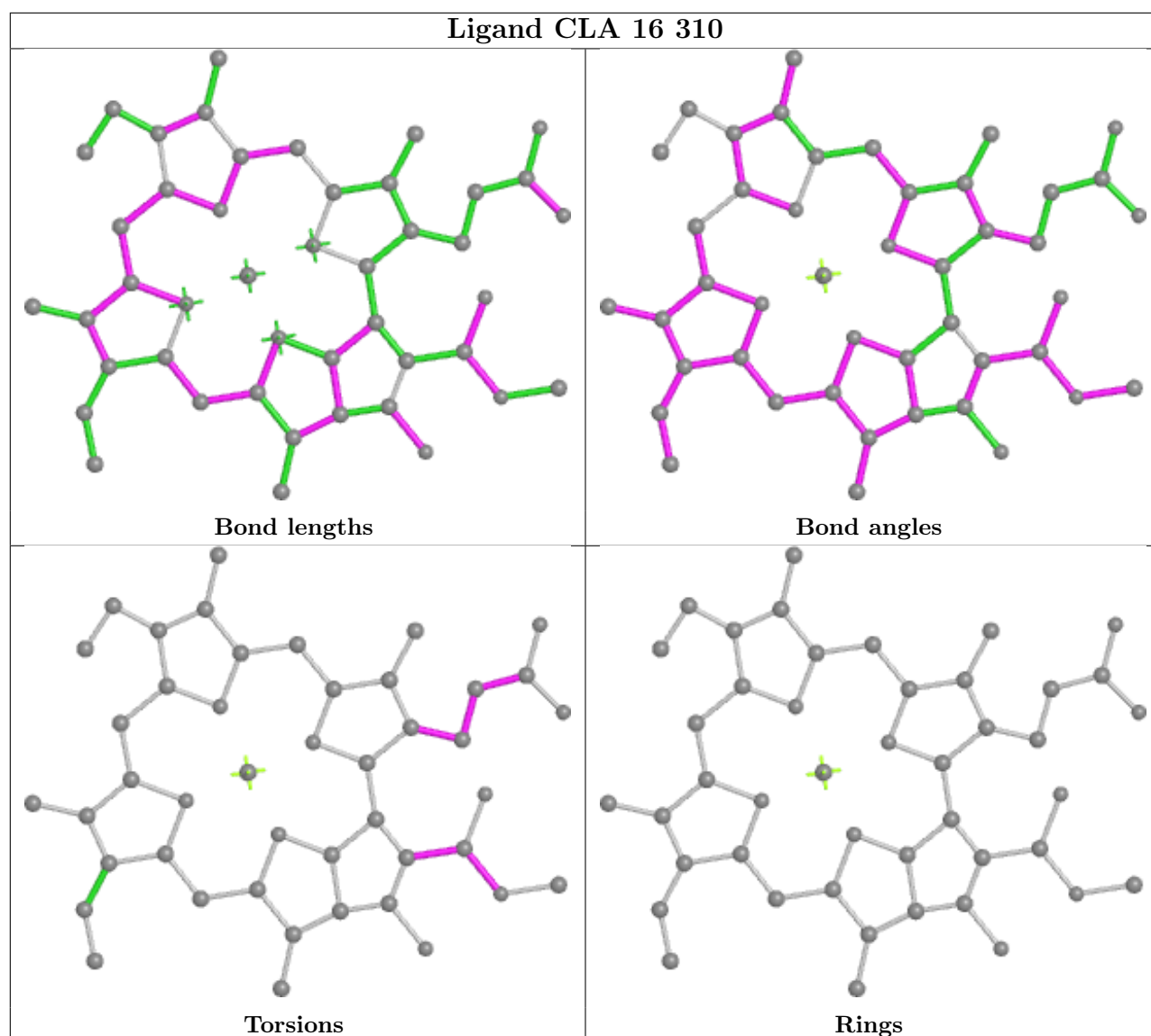


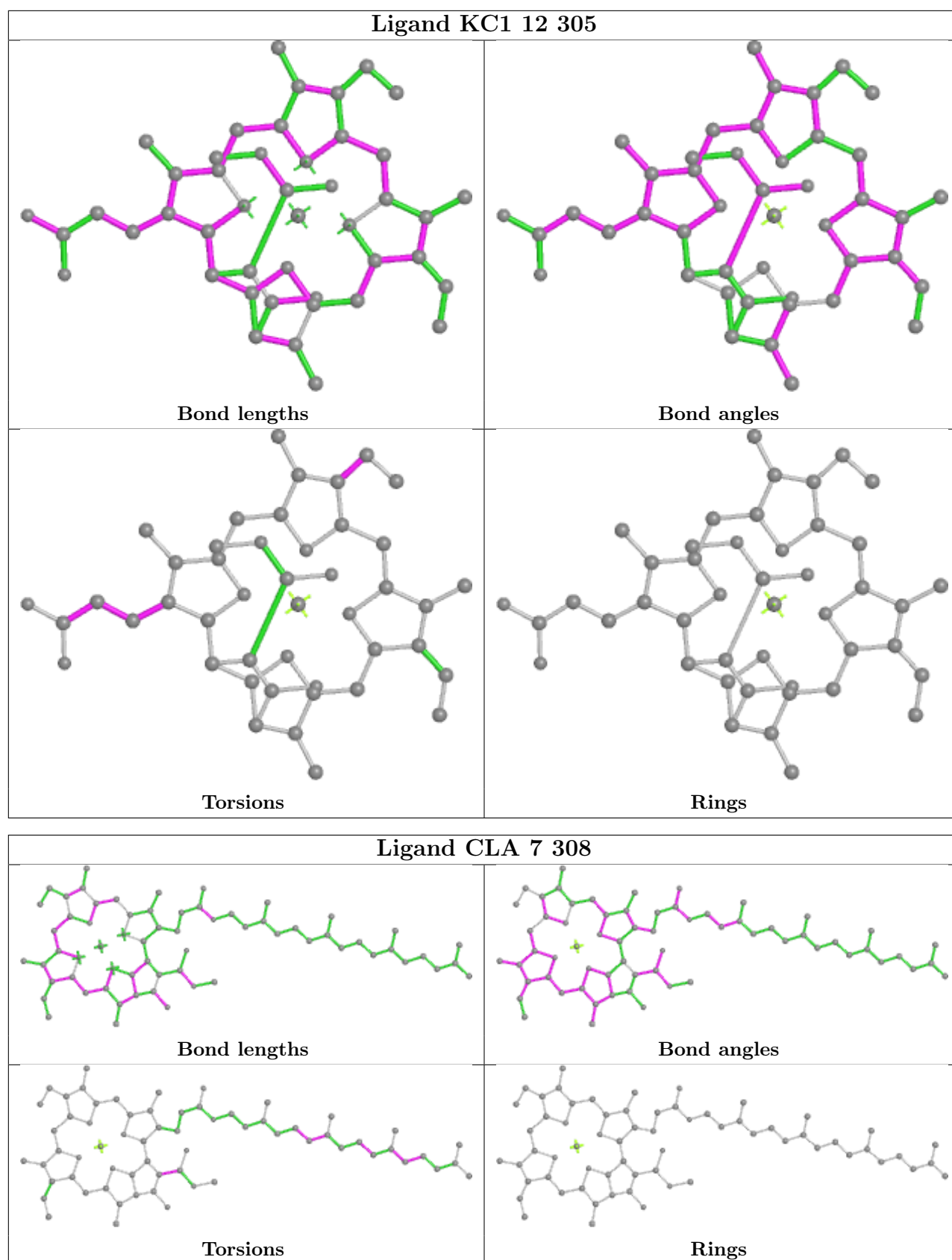
Rings

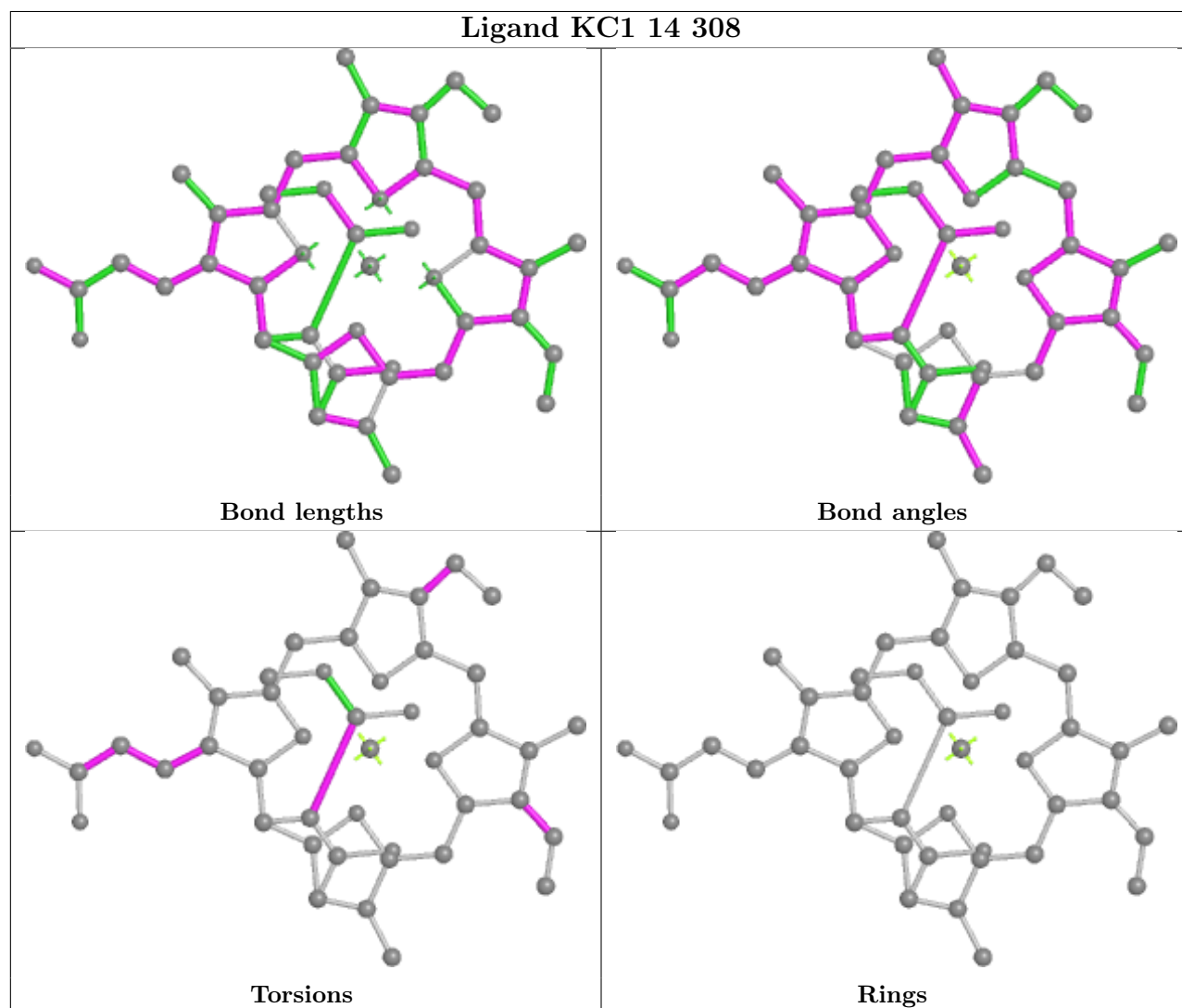
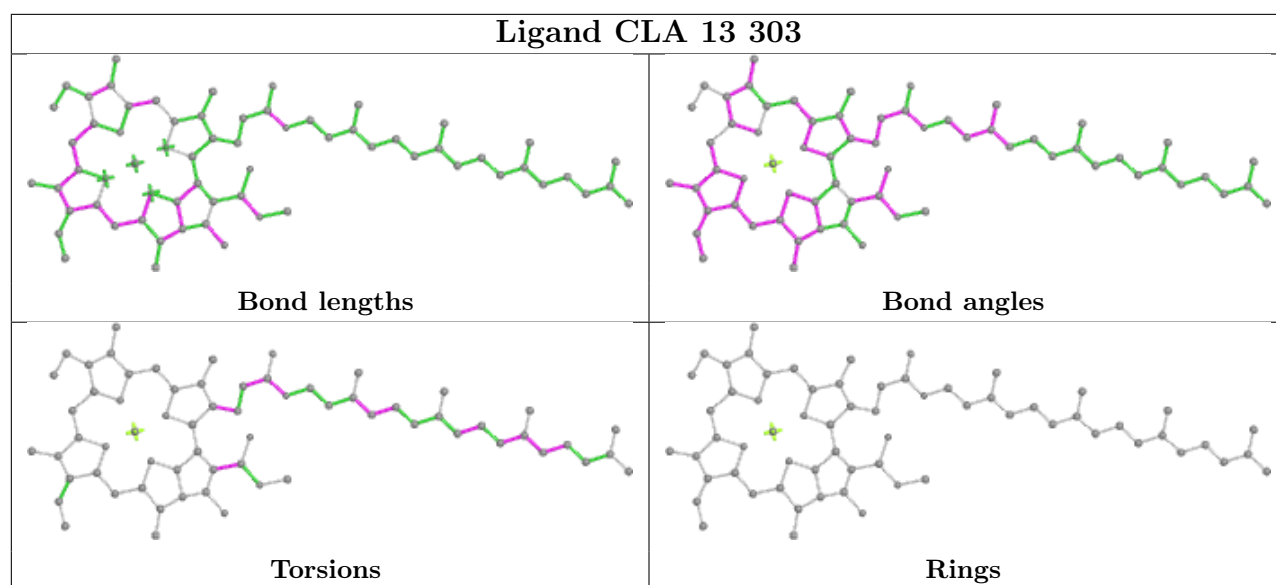


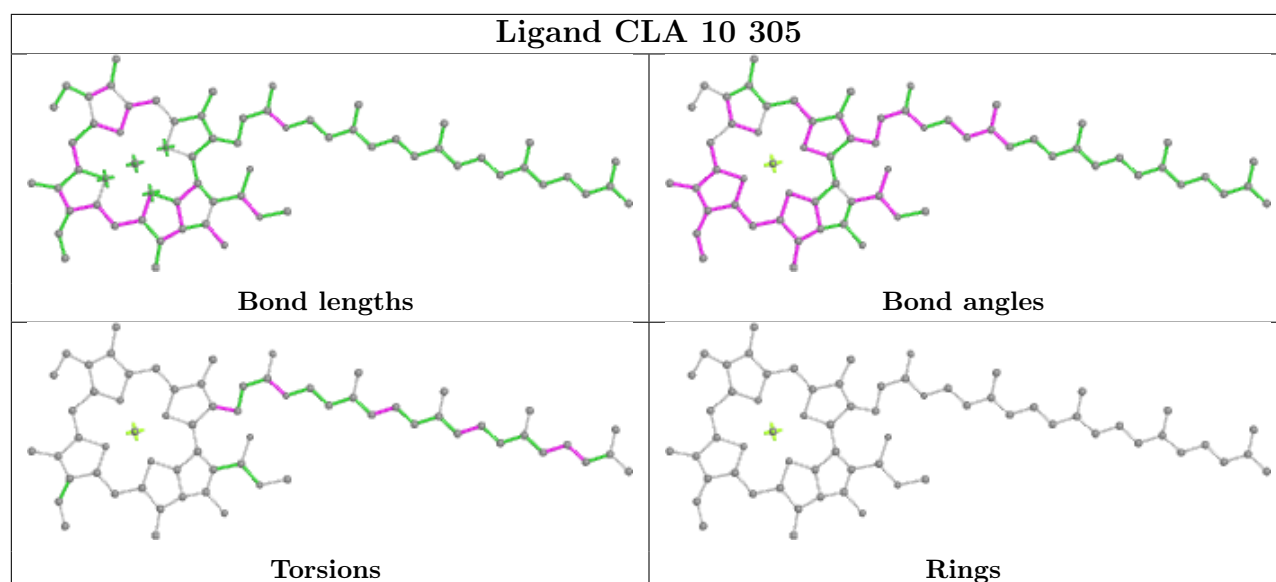
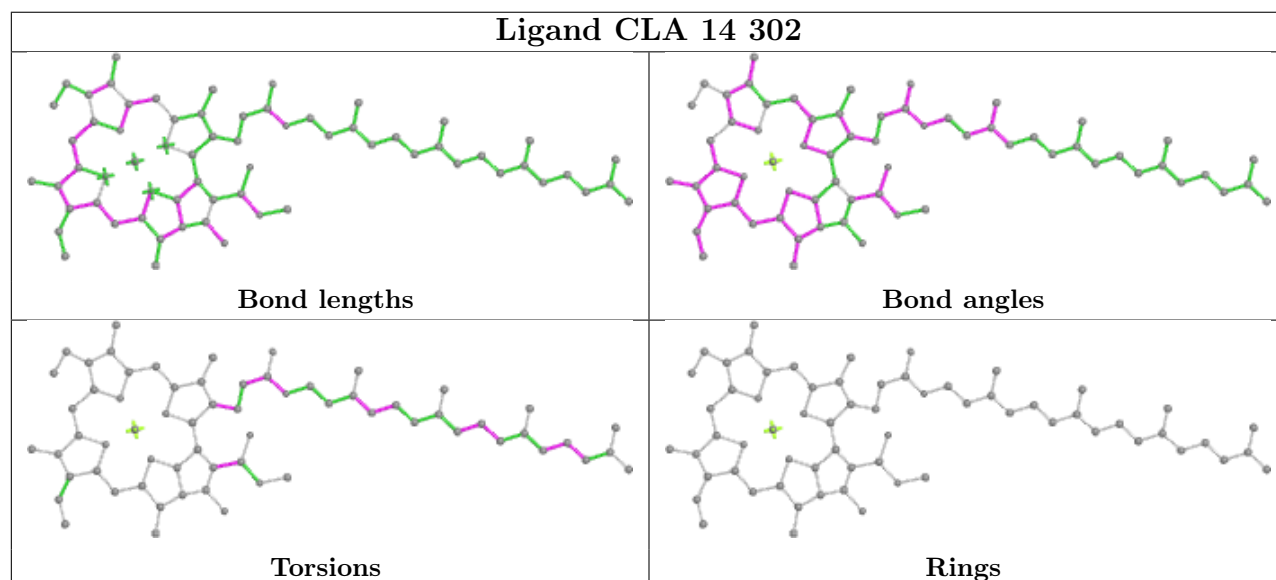
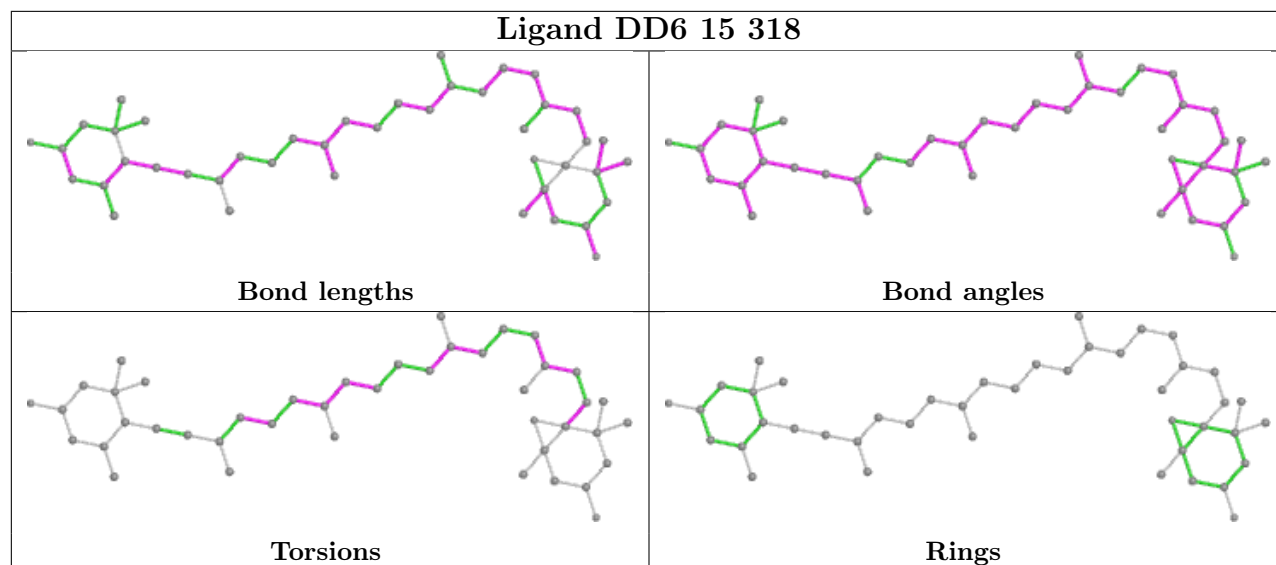


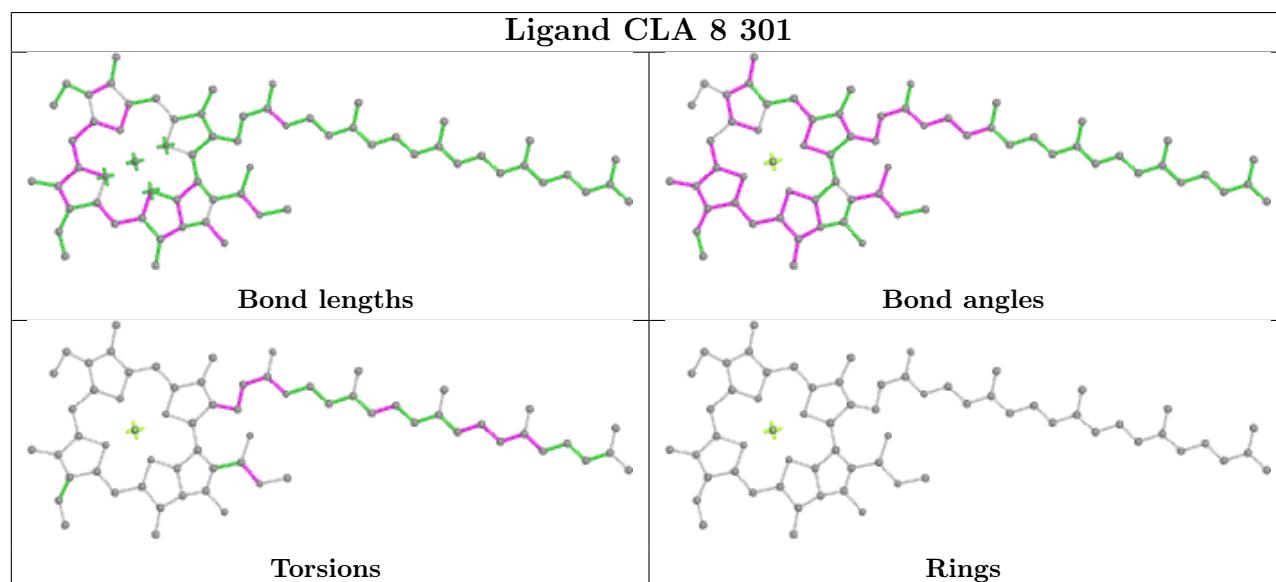
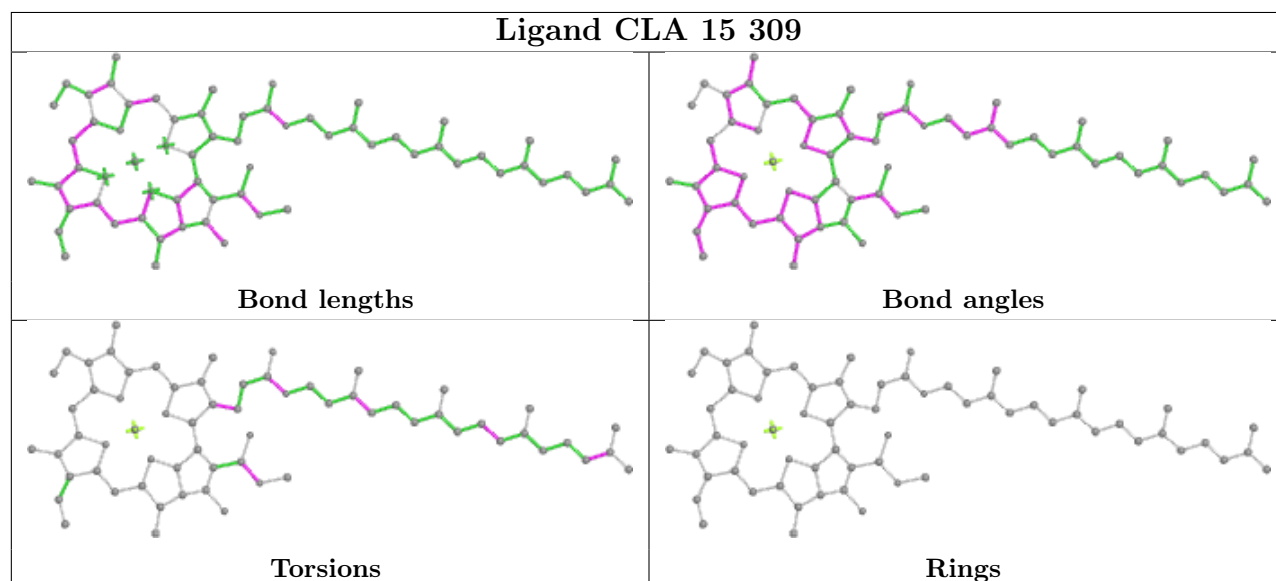
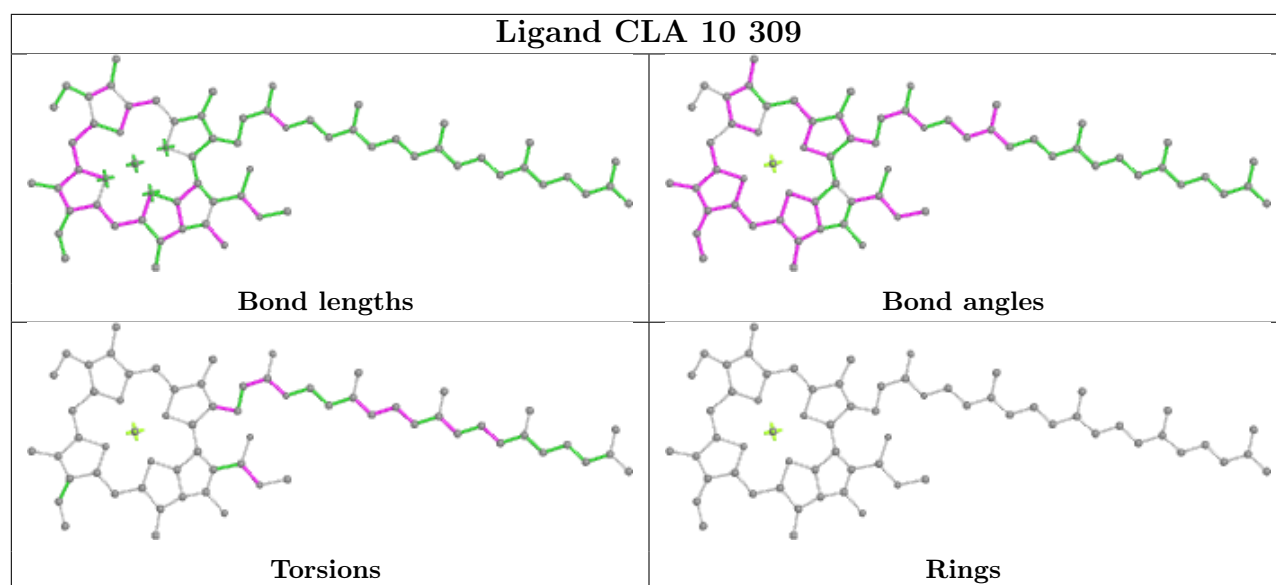


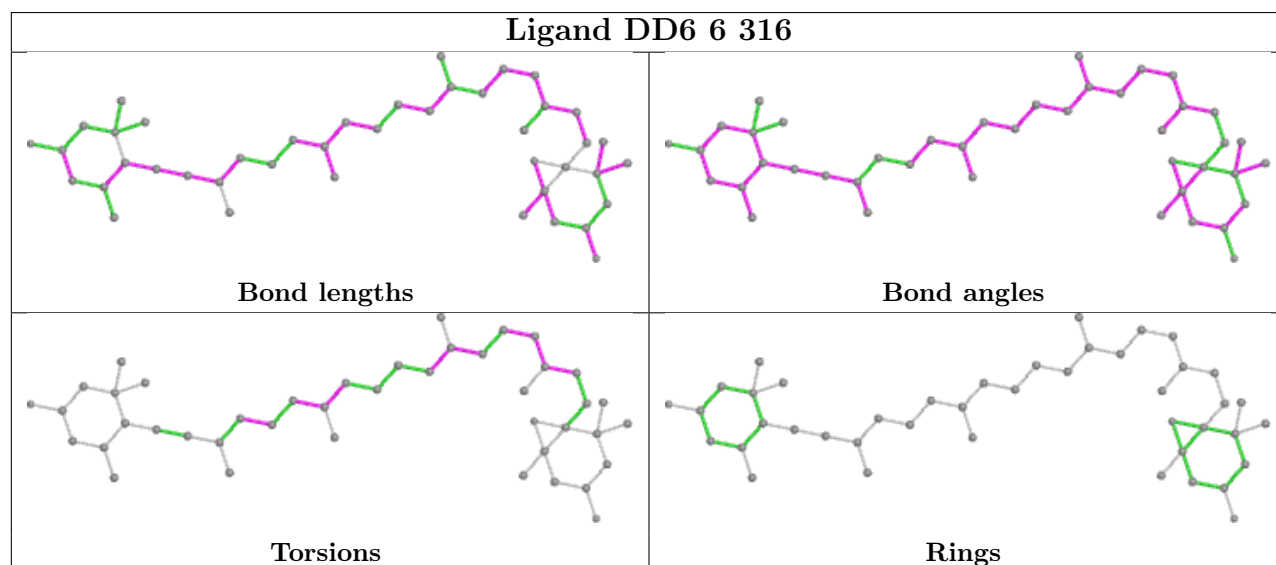
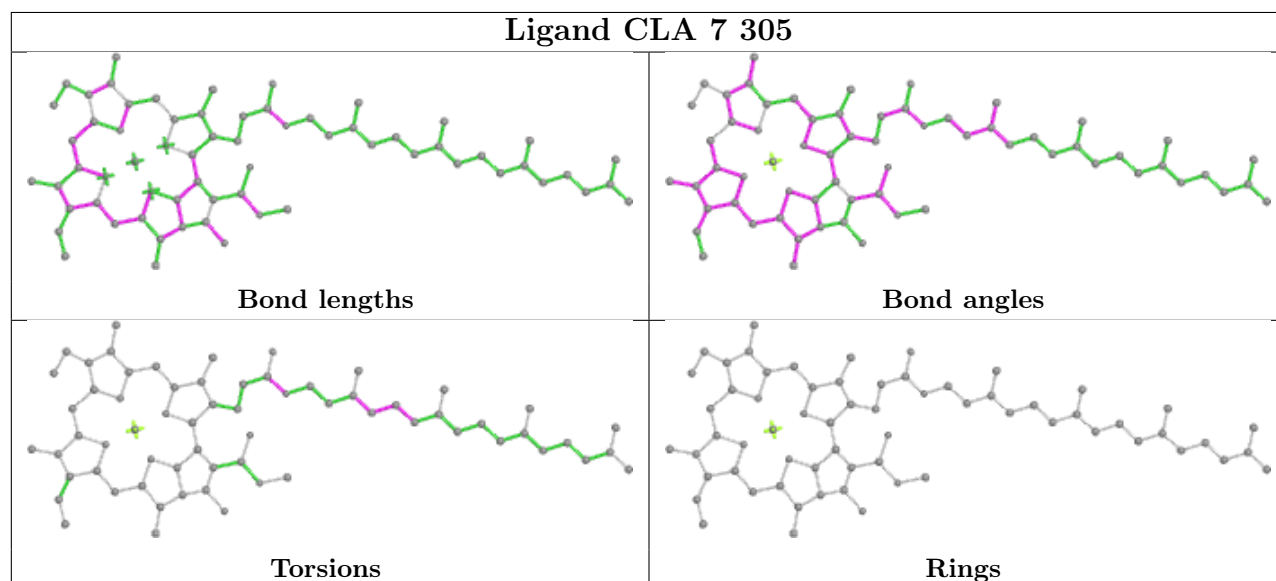
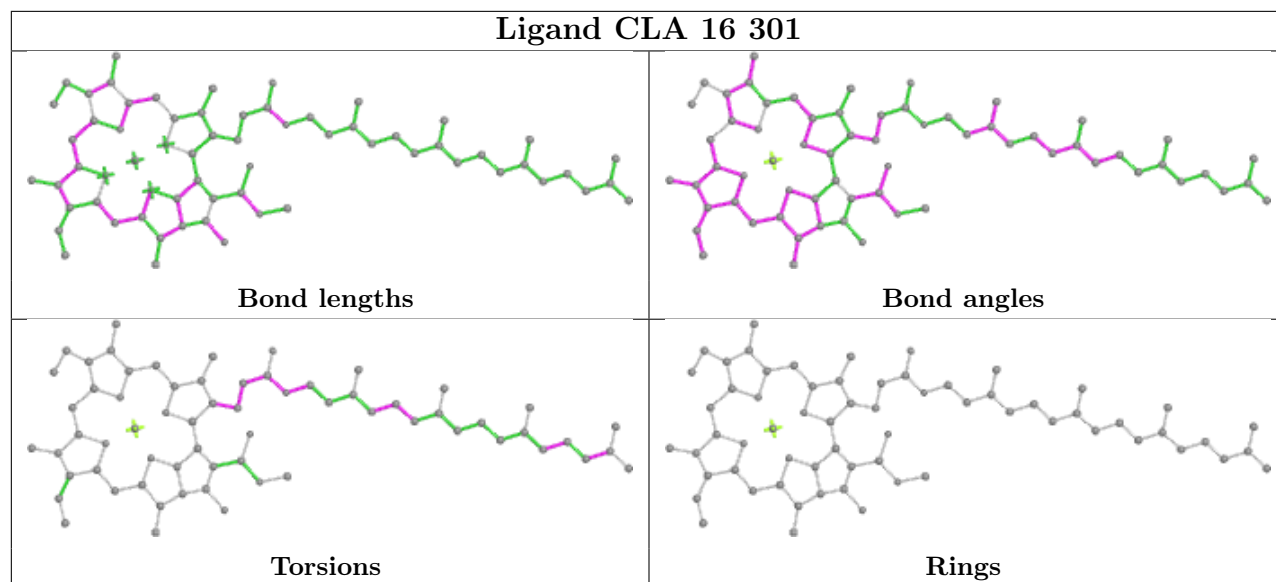


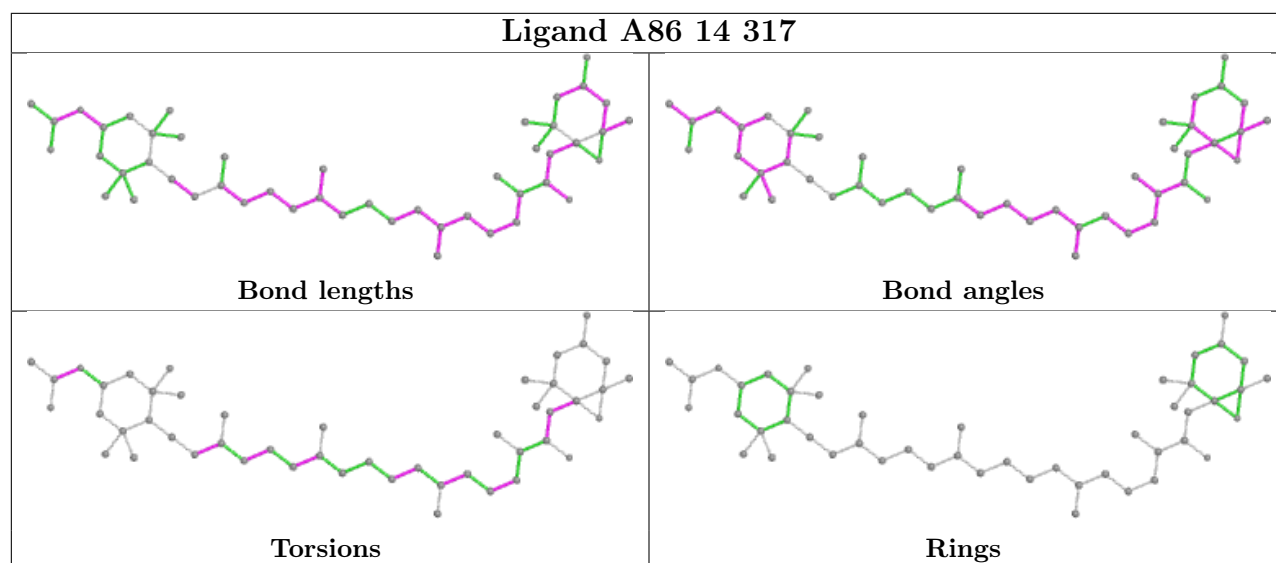
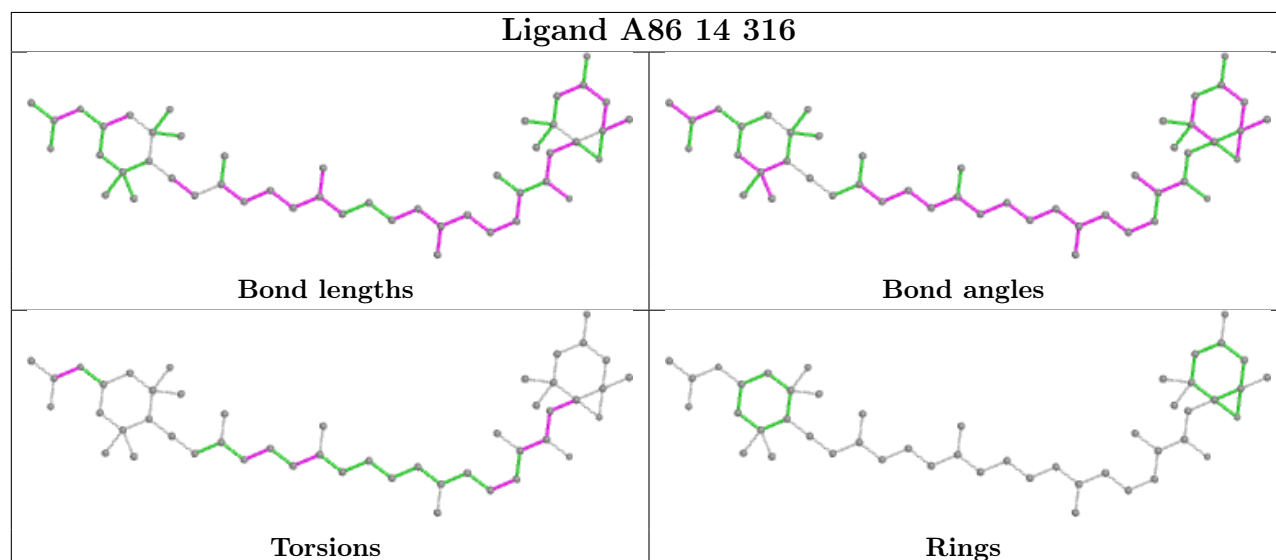
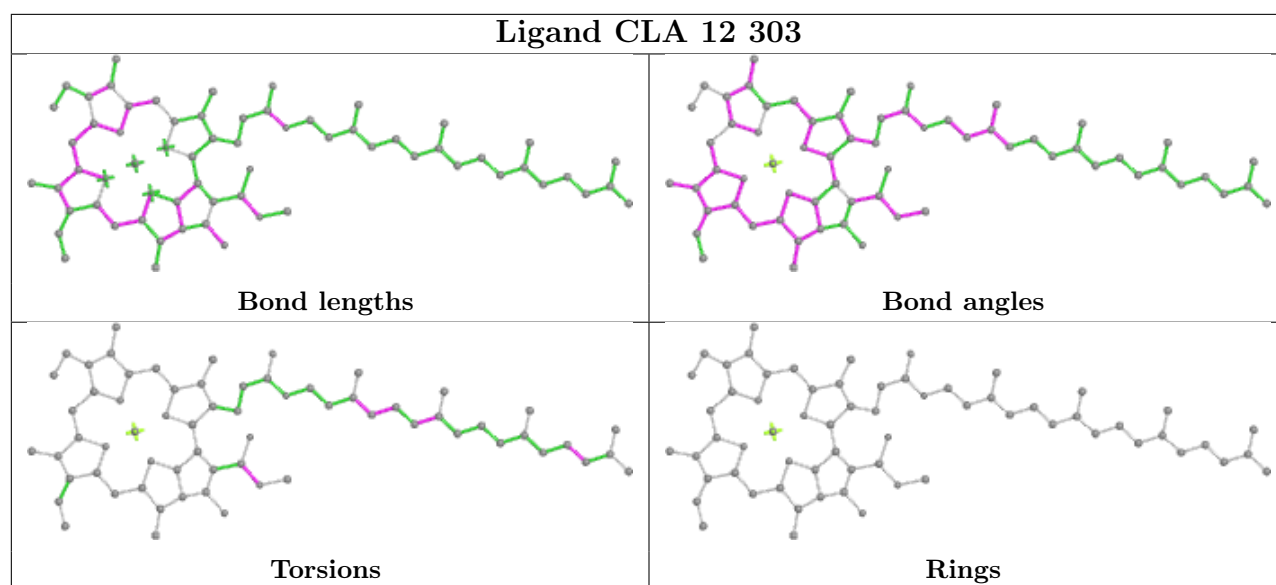




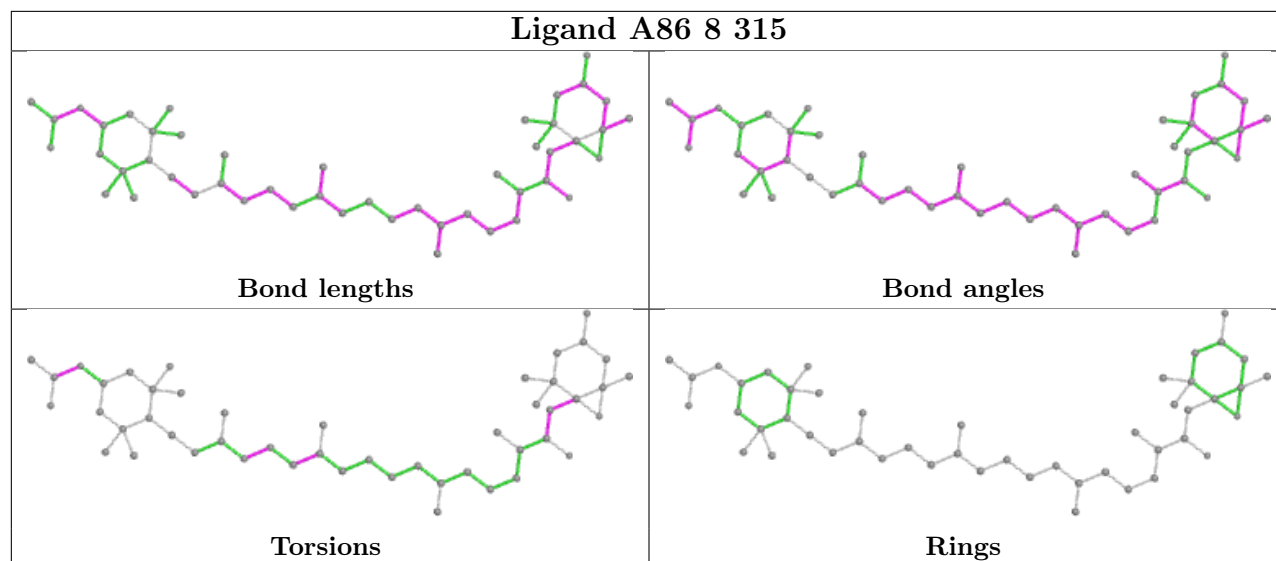




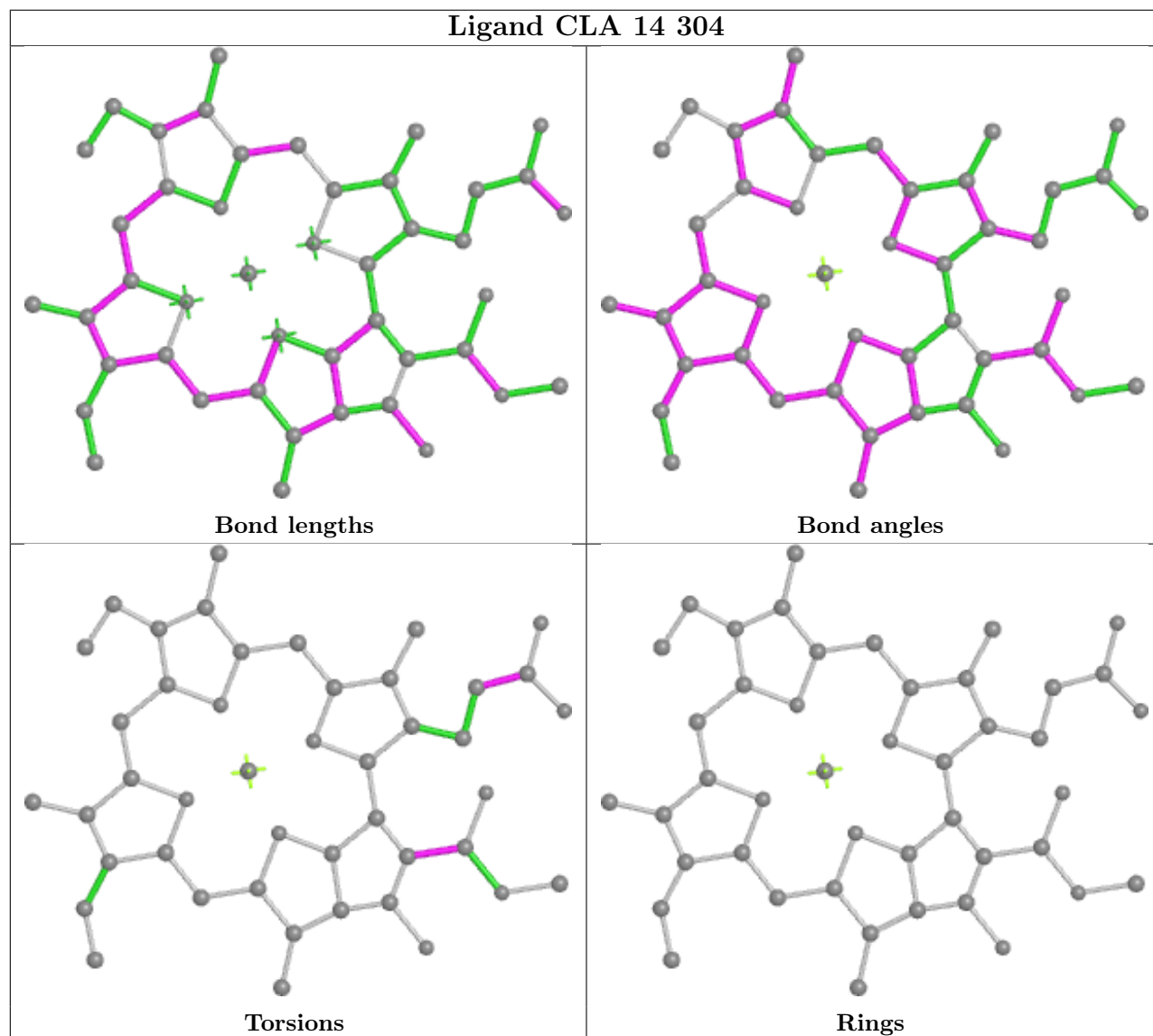


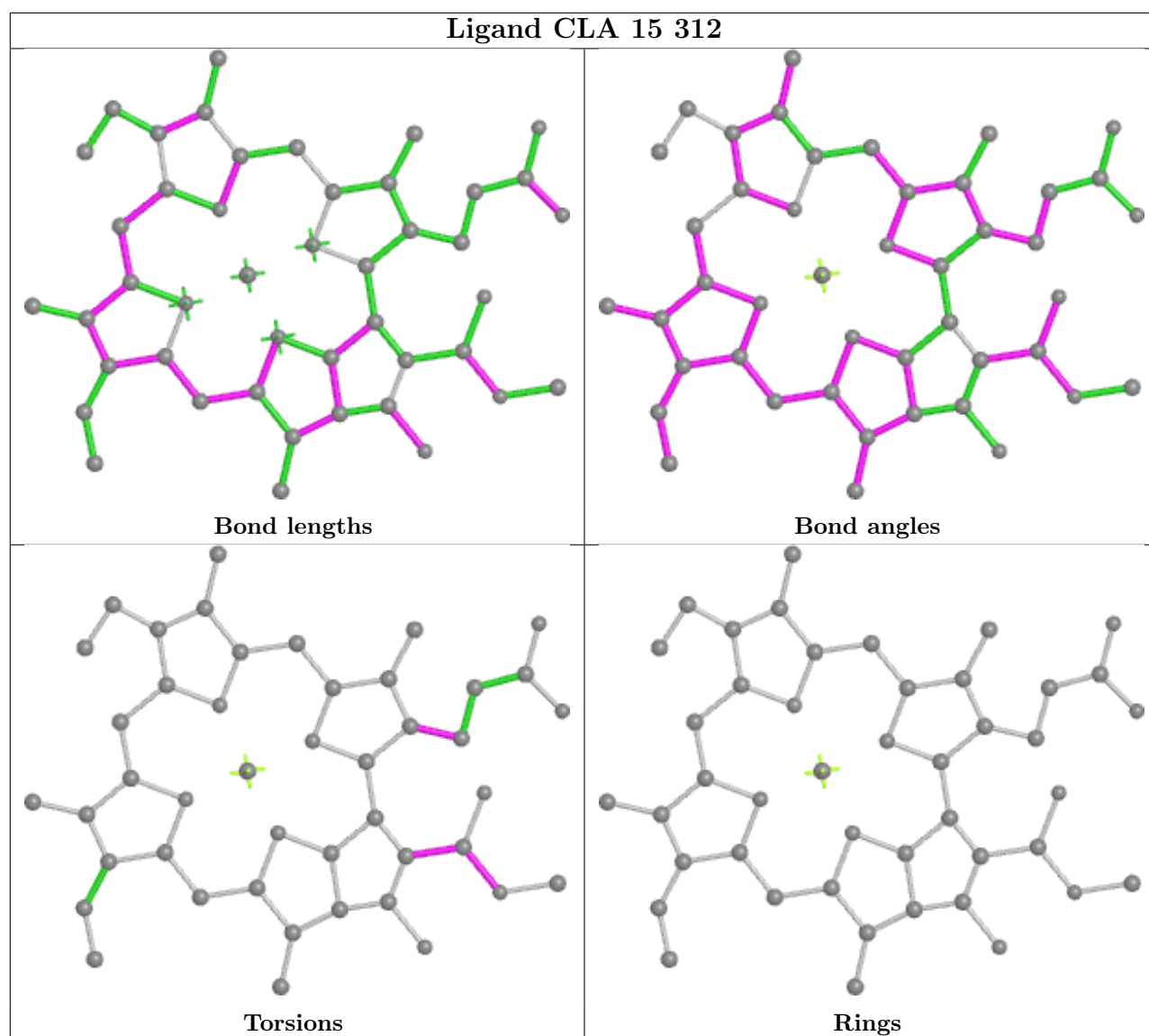


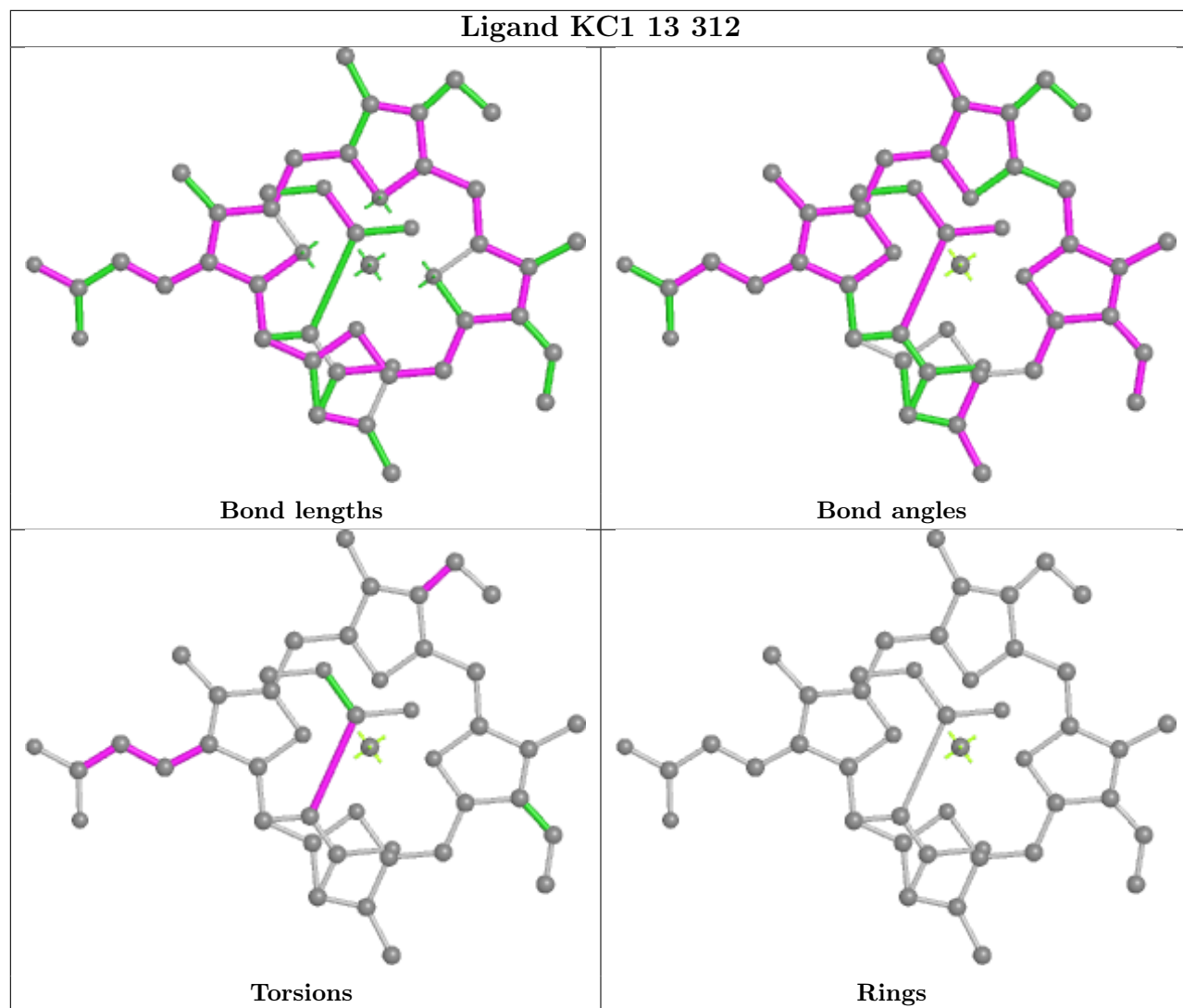
Ligand A86 8 315



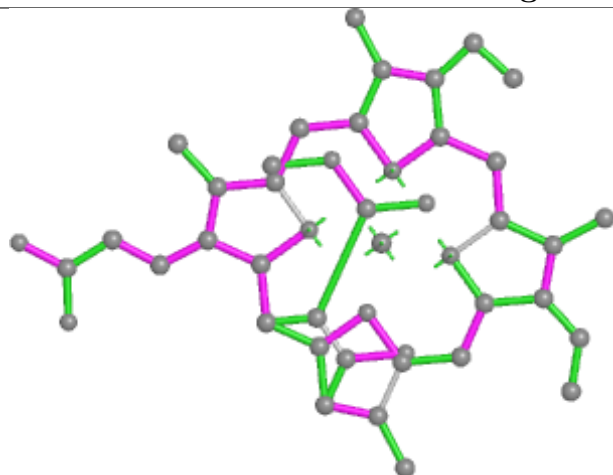
Ligand CLA 14 304



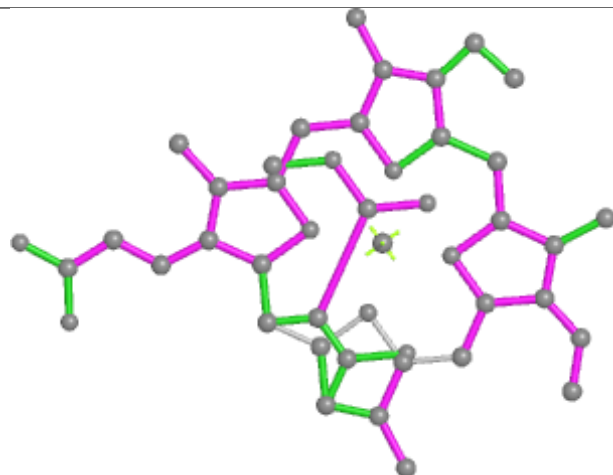




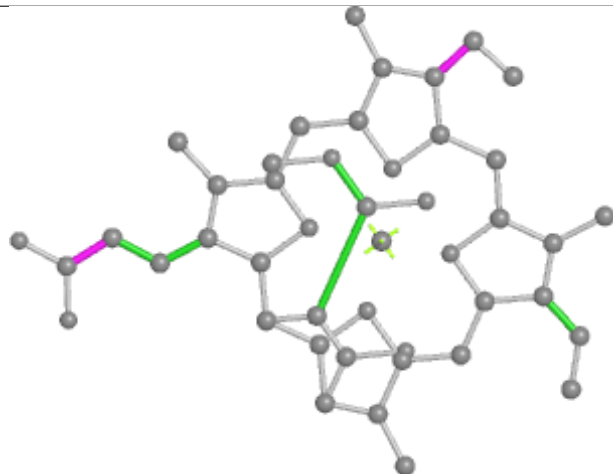
Ligand KC1 7 312



Bond lengths



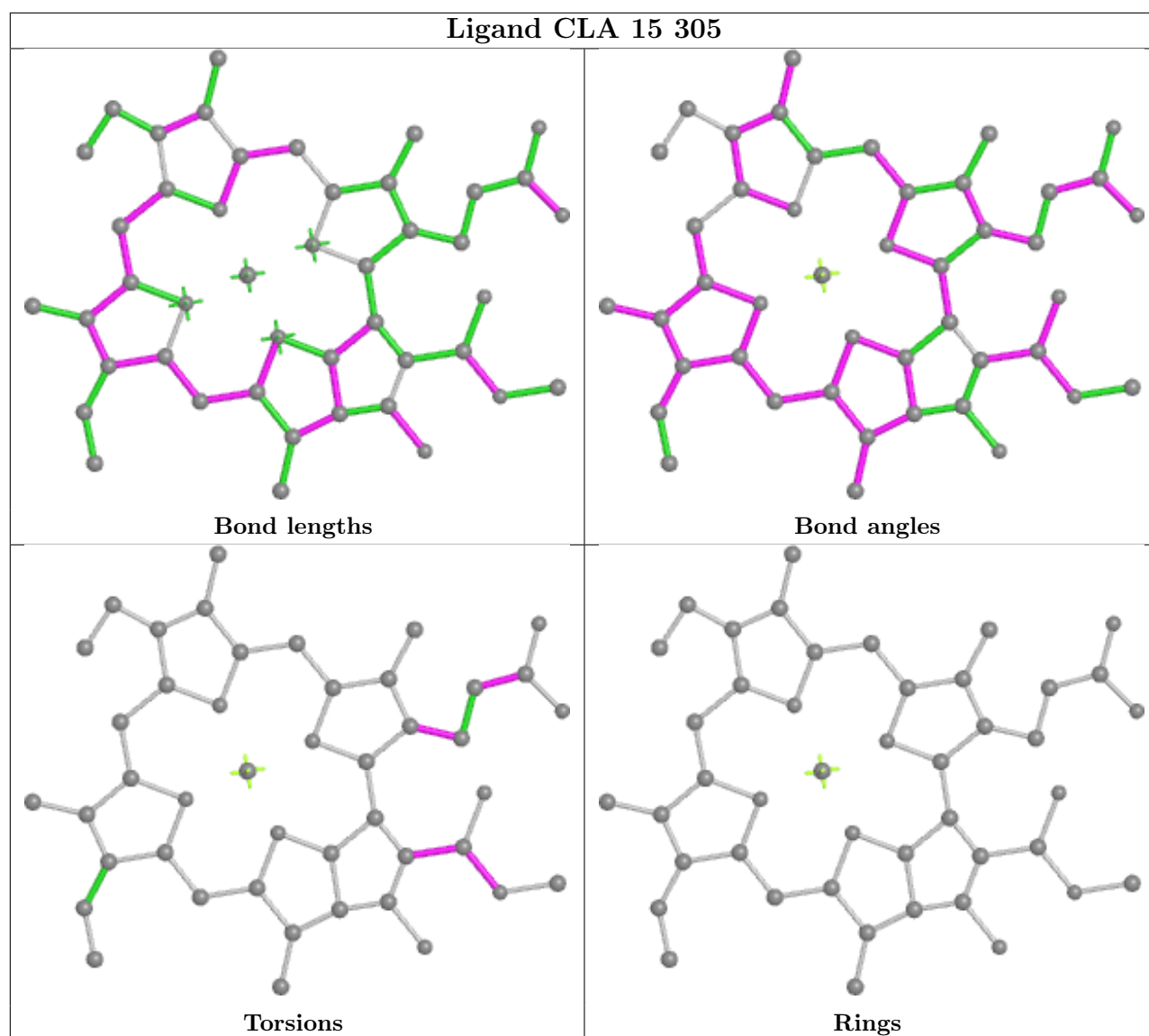
Bond angles

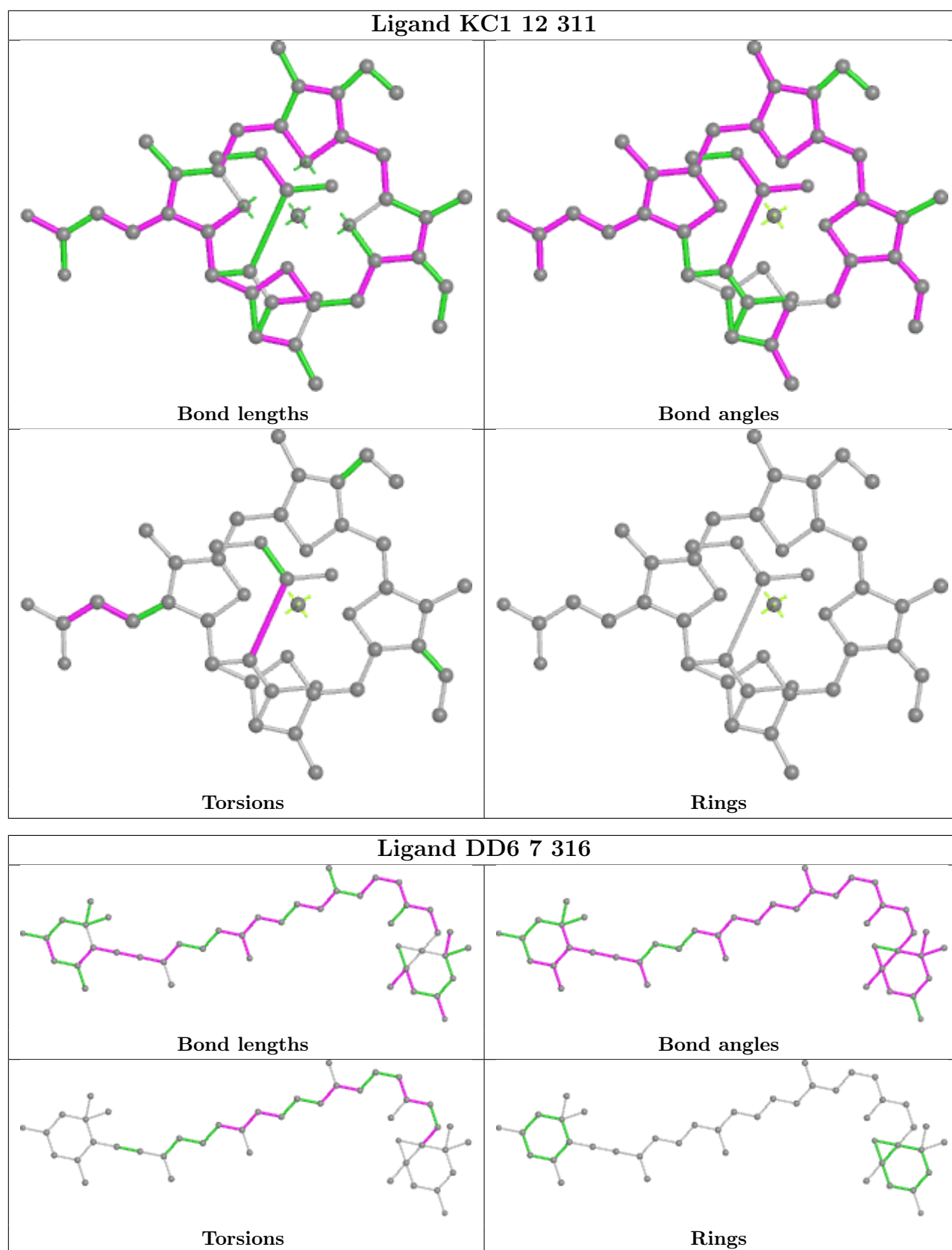


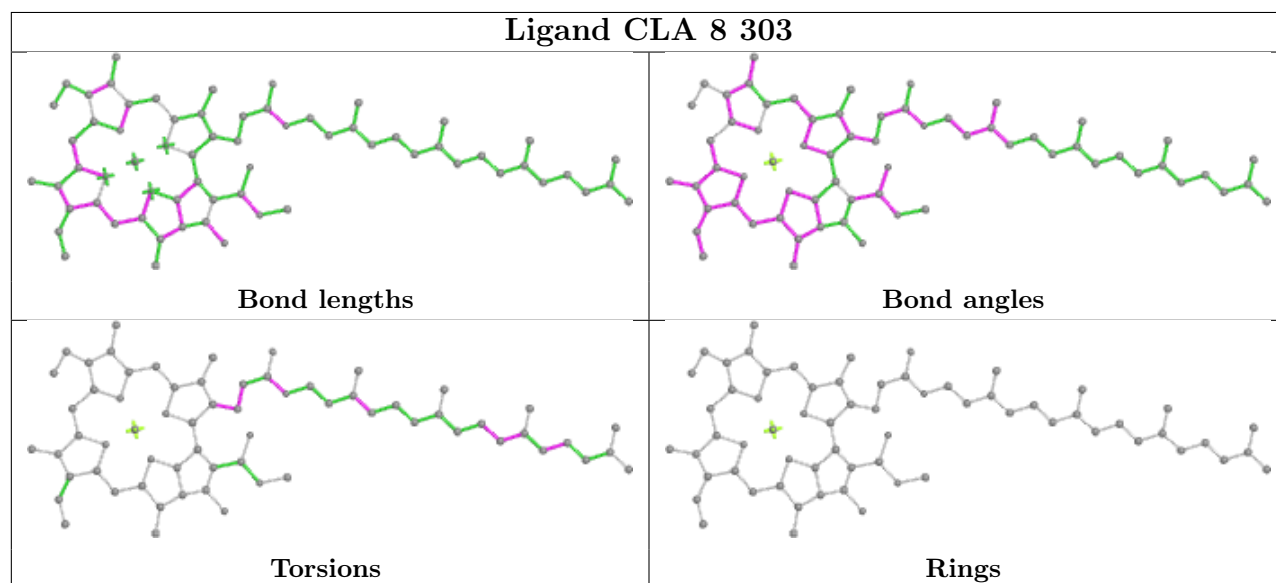
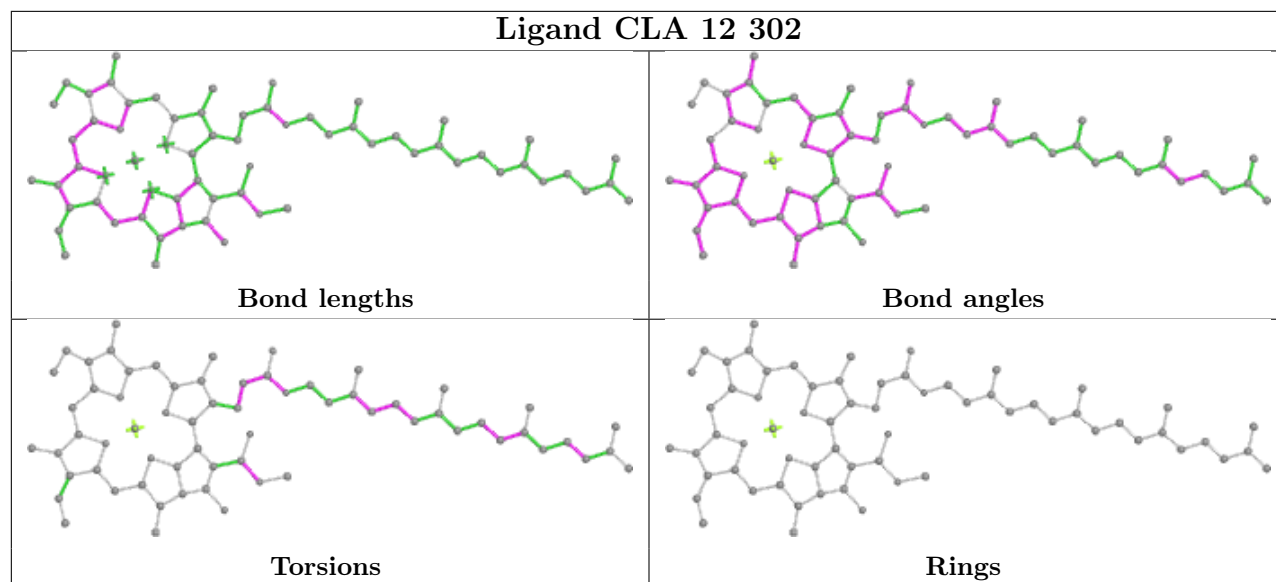
Torsions

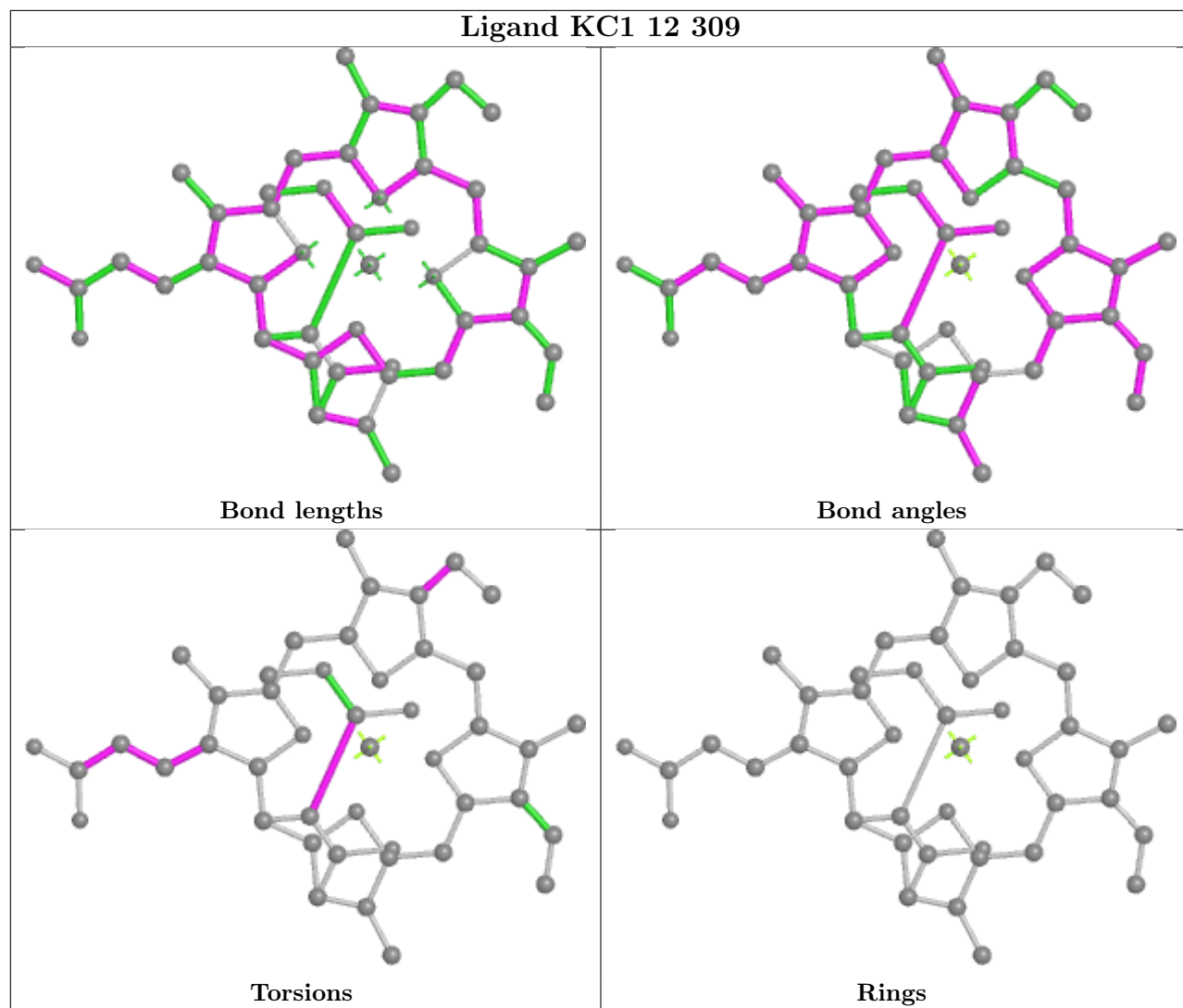


Rings

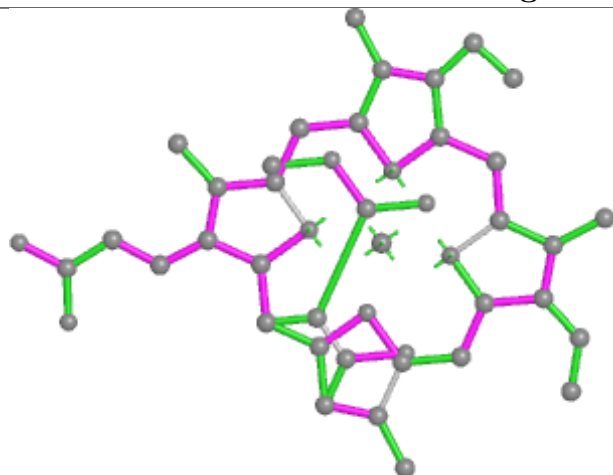




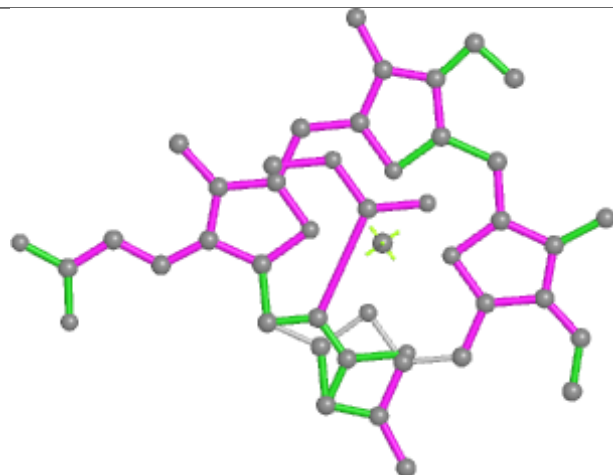




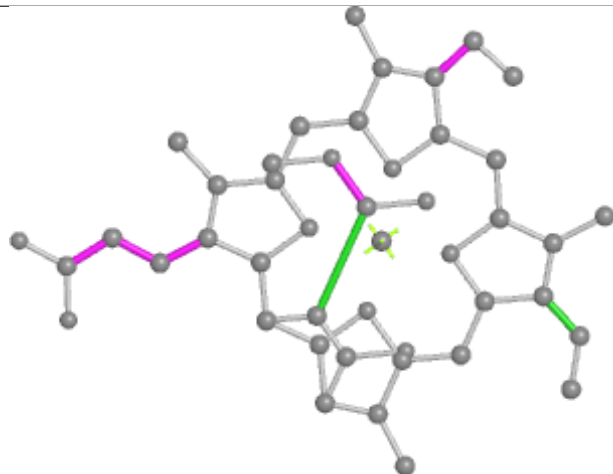
Ligand KC1 8 311



Bond lengths



Bond angles

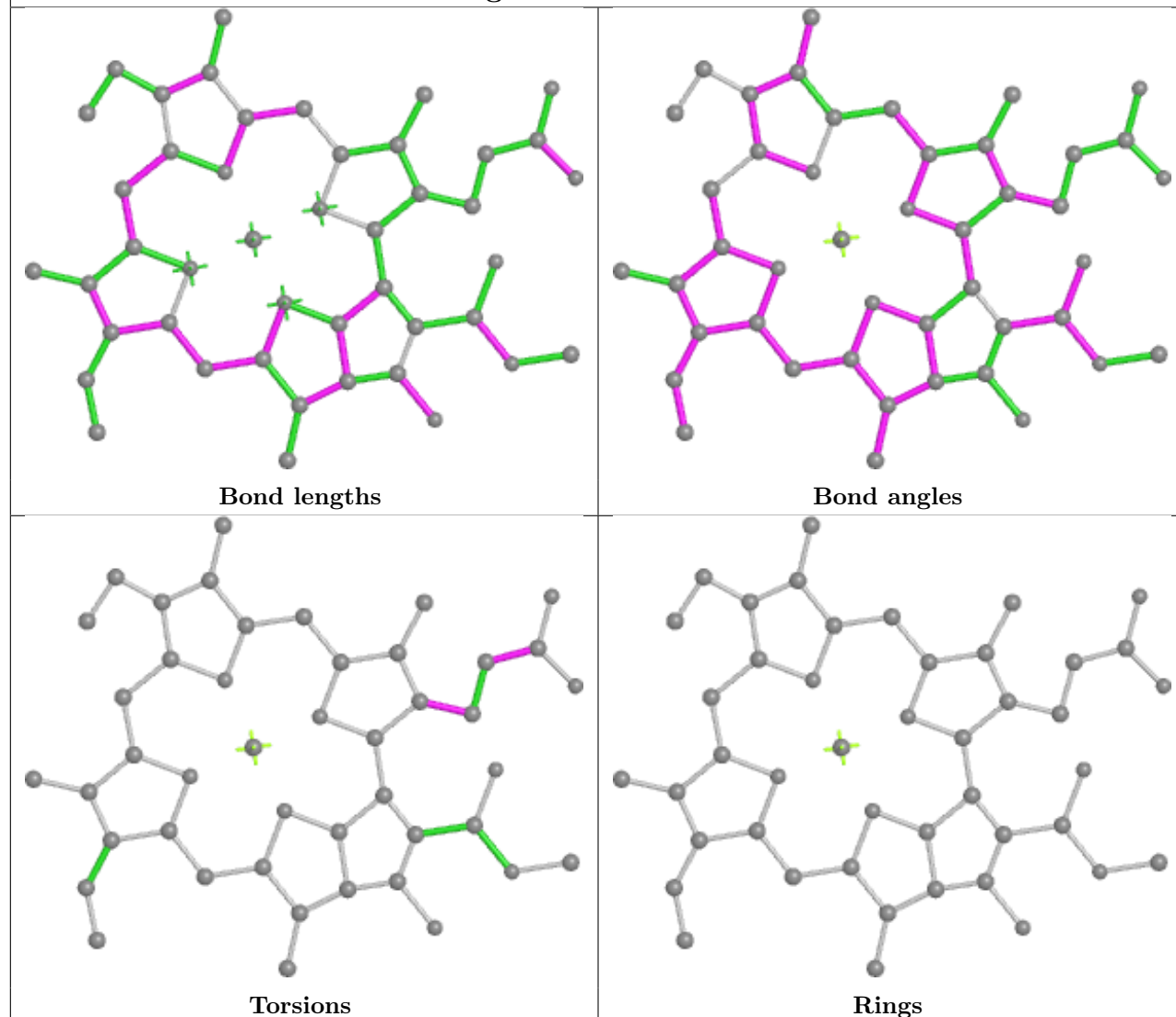


Torsions

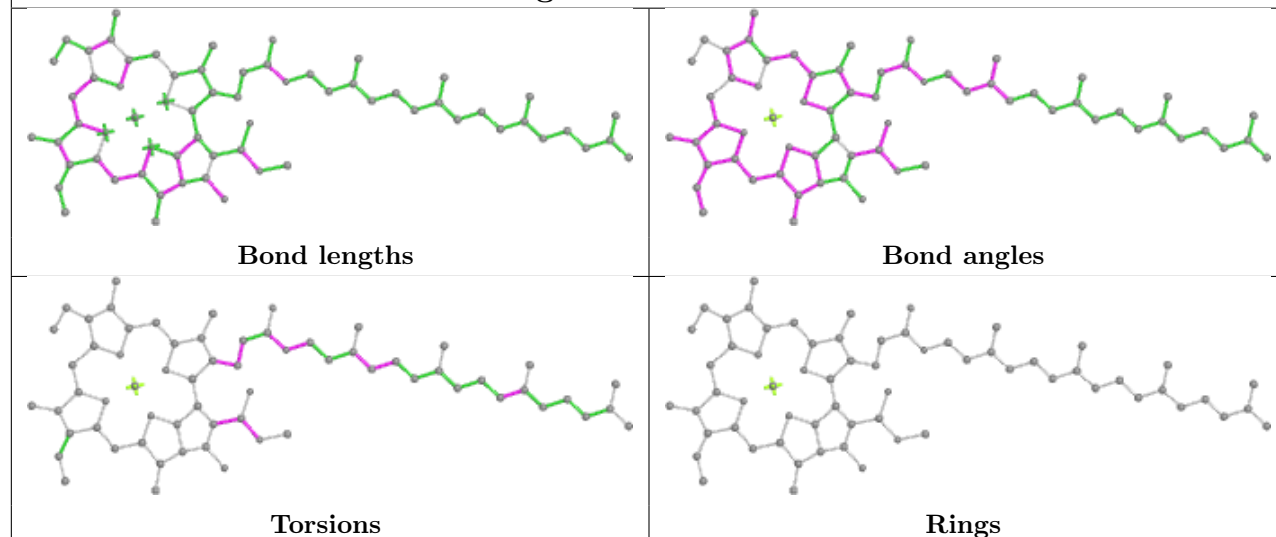


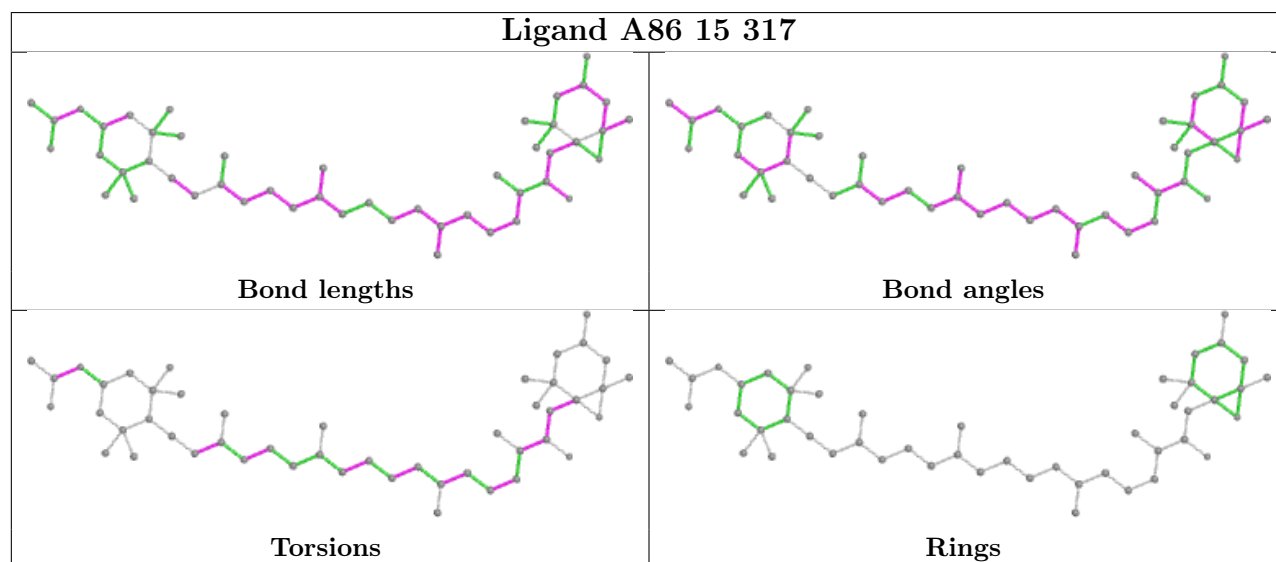
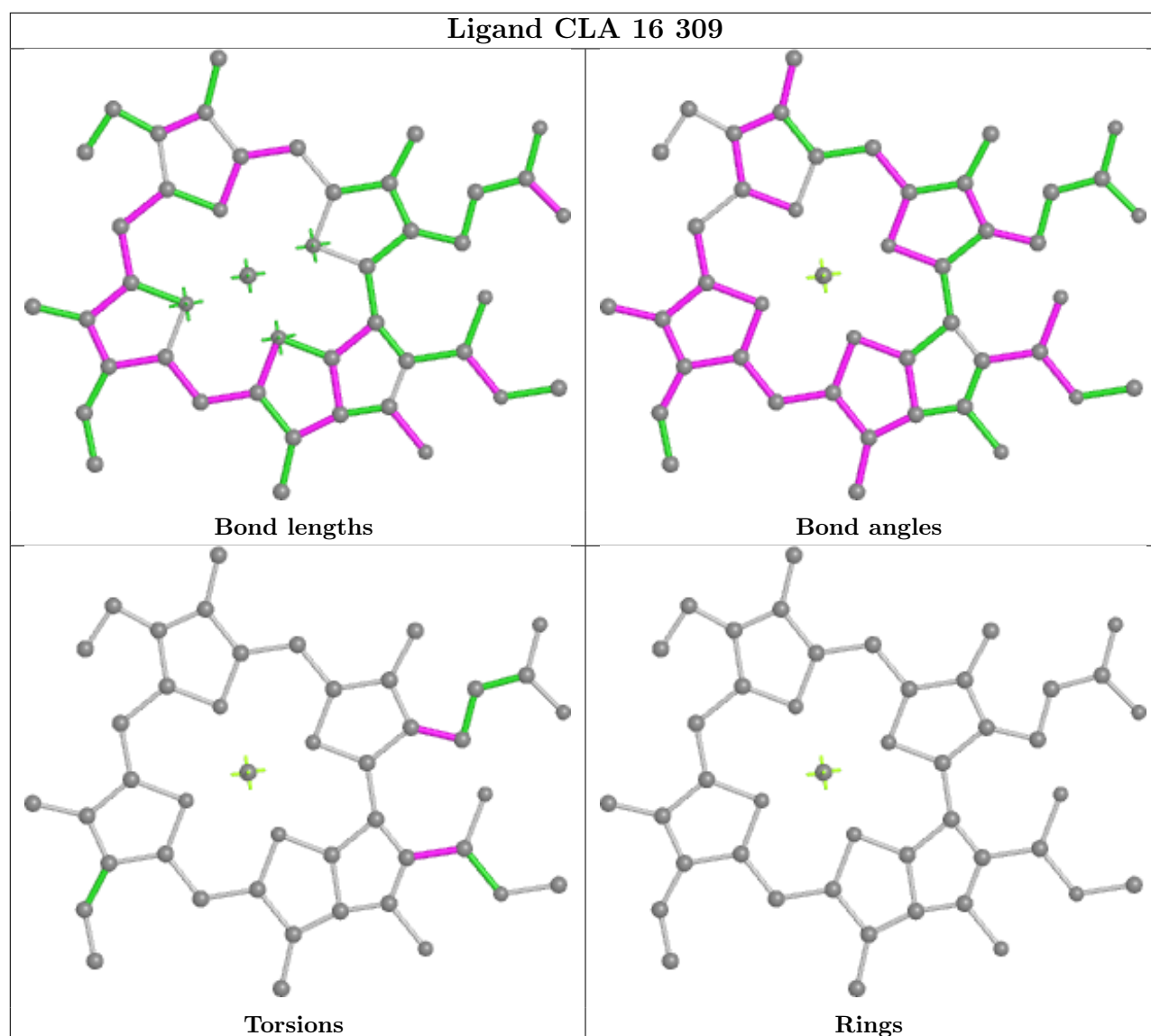
Rings

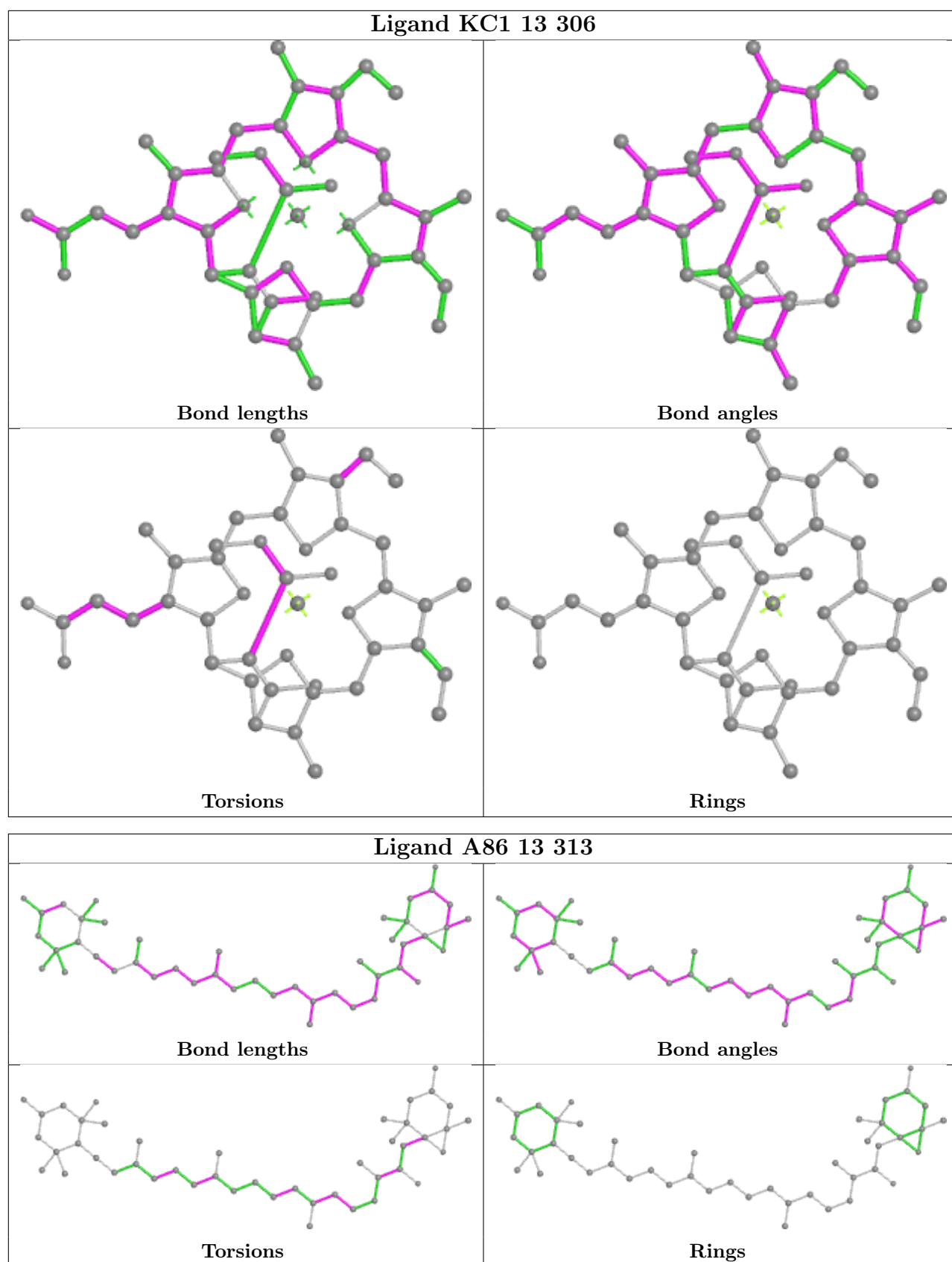
Ligand CLA 14 309

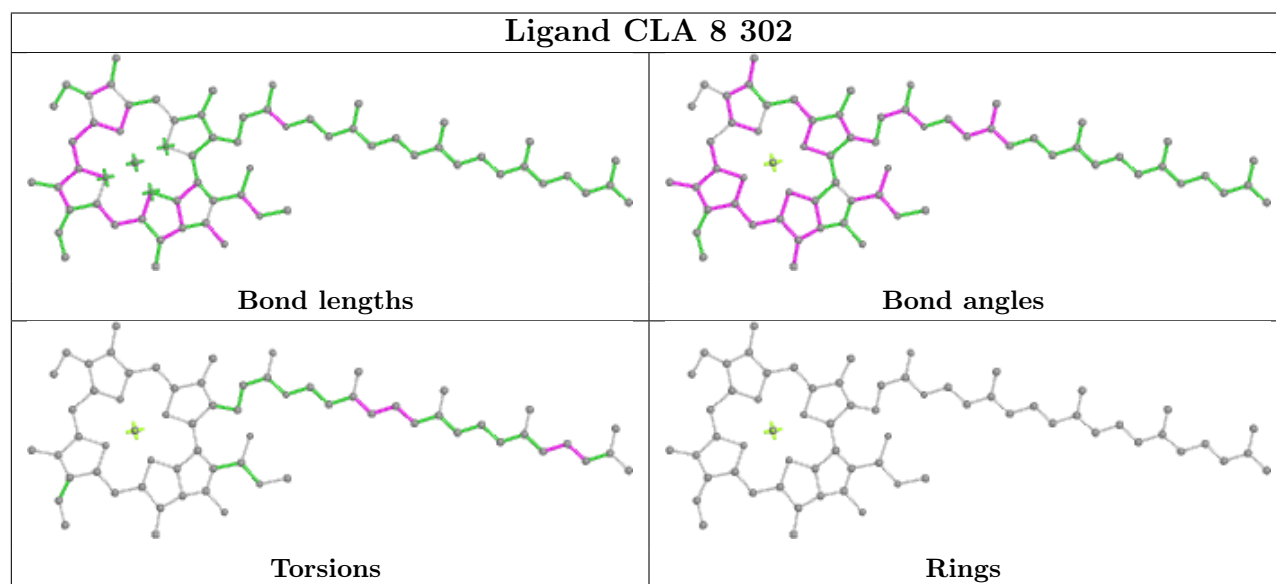
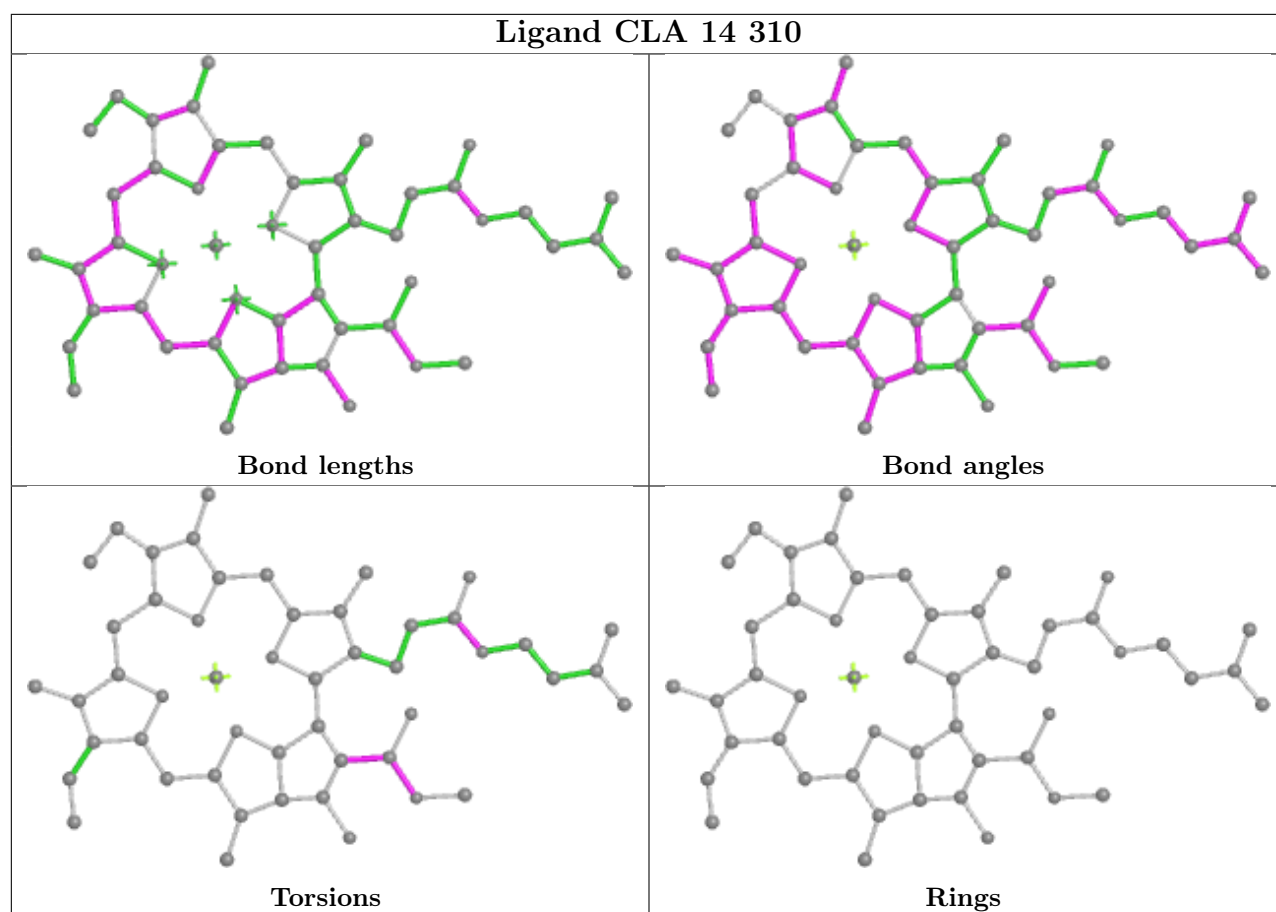


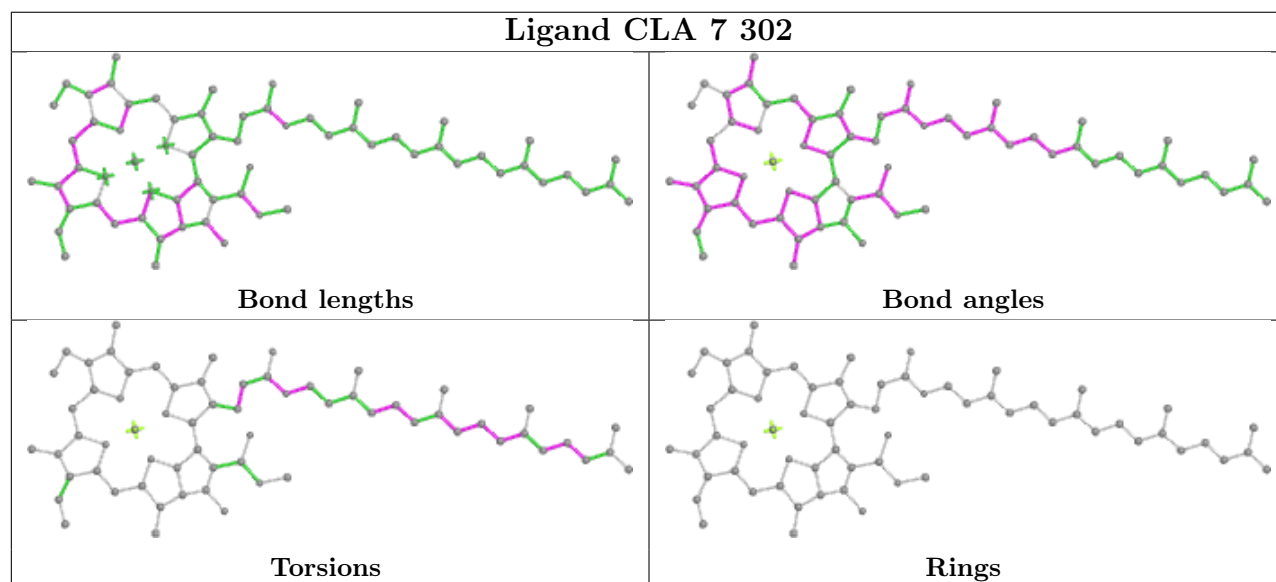
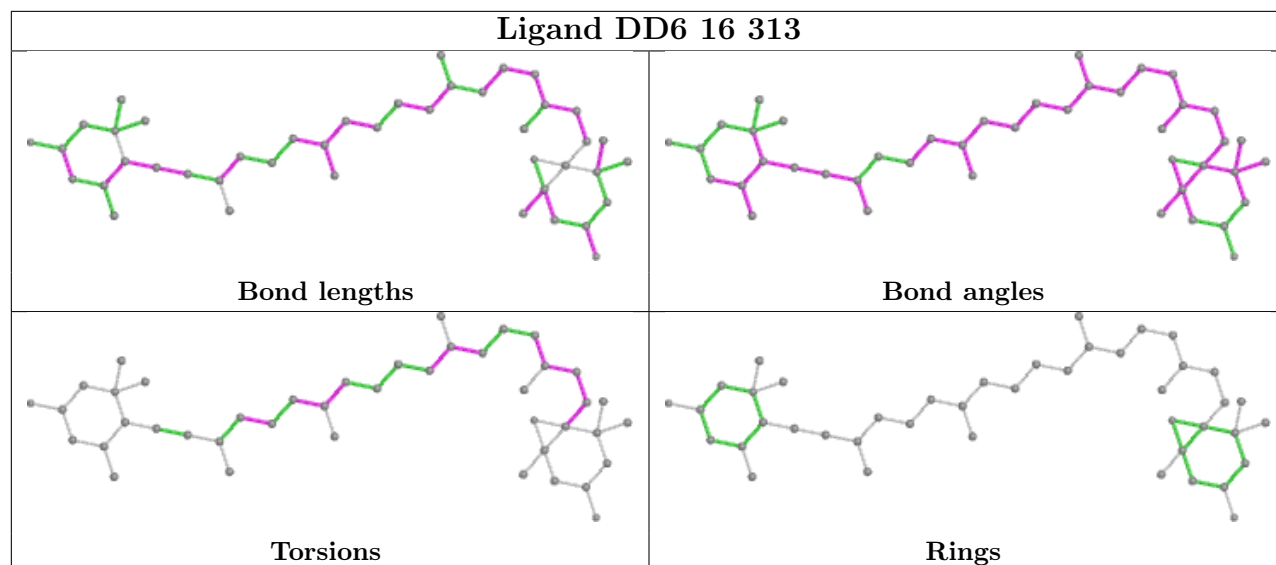
Ligand CLA 6 311

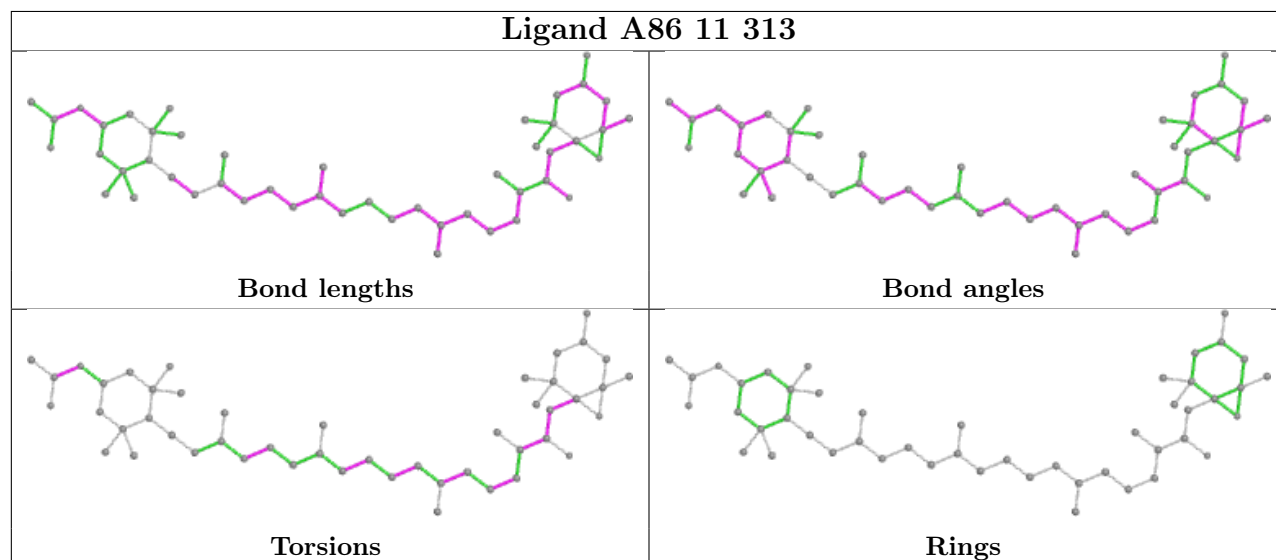
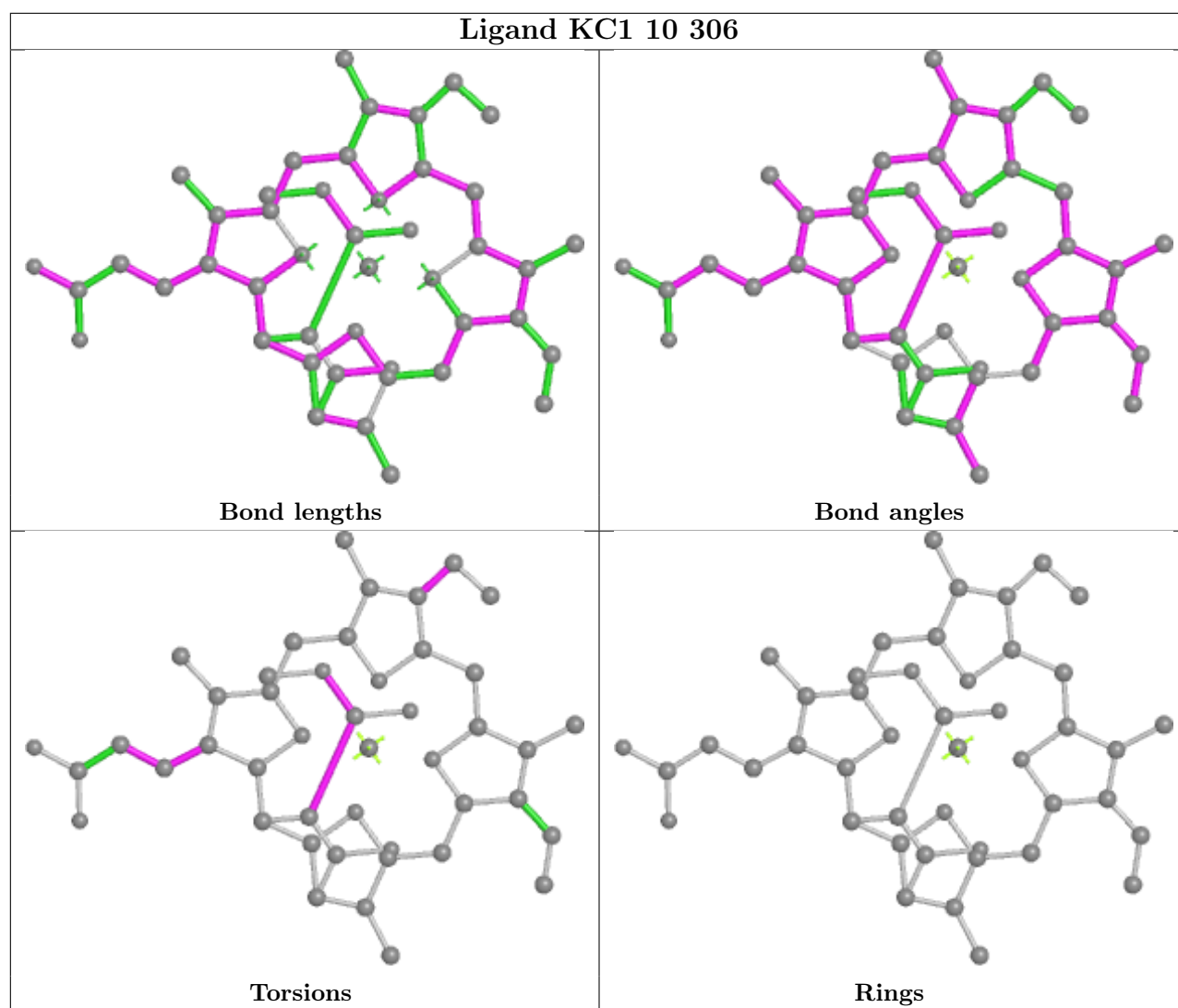


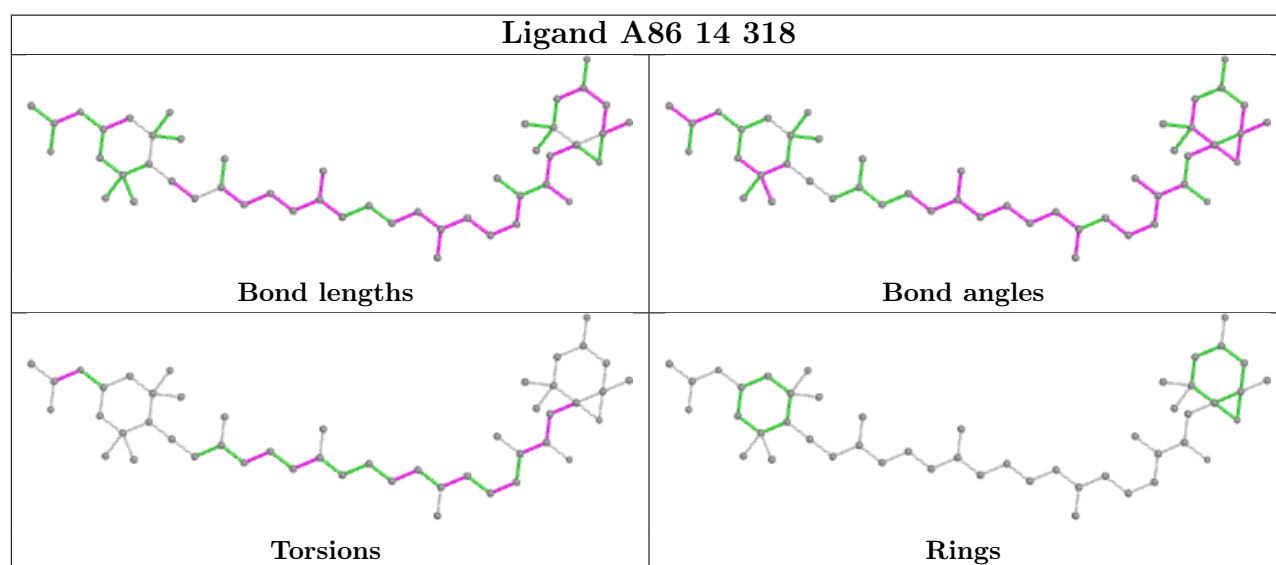
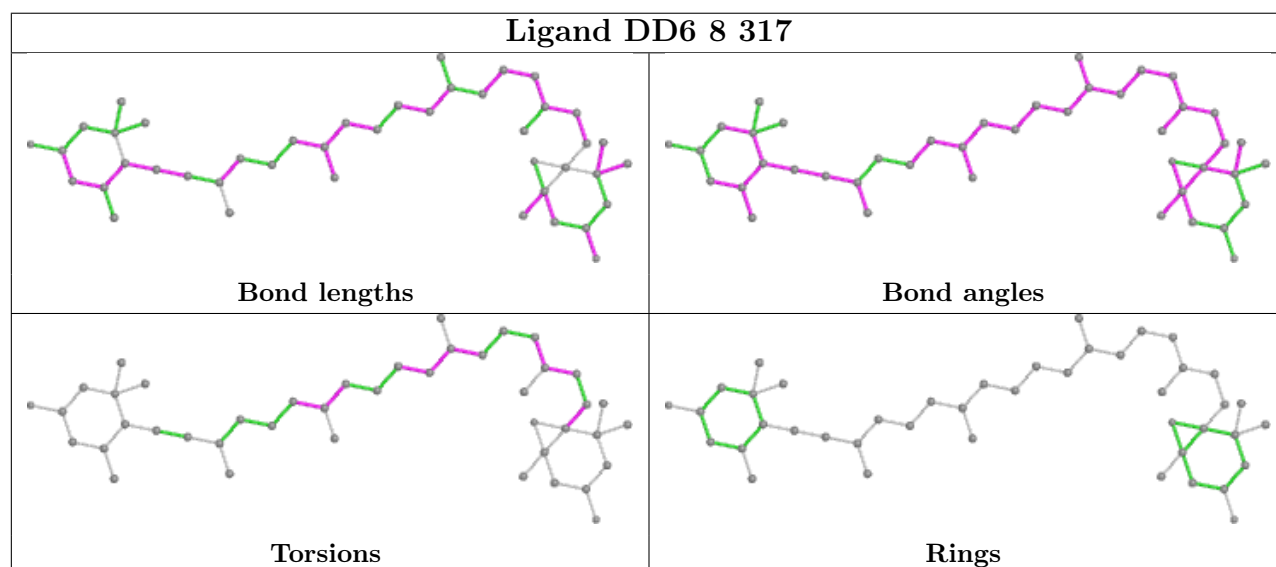
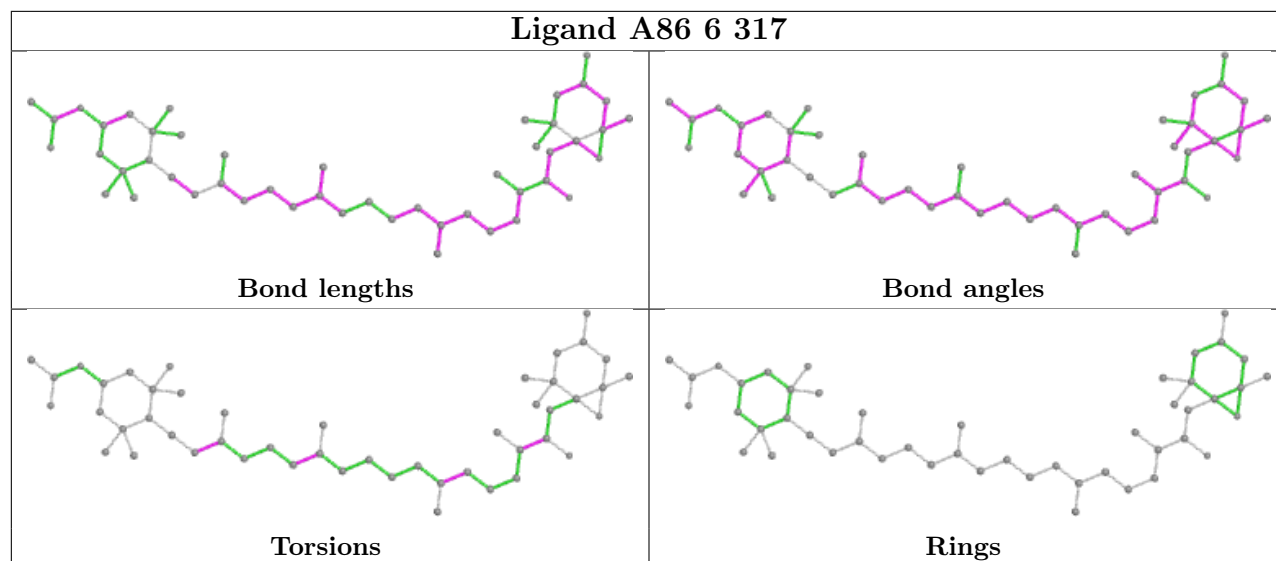


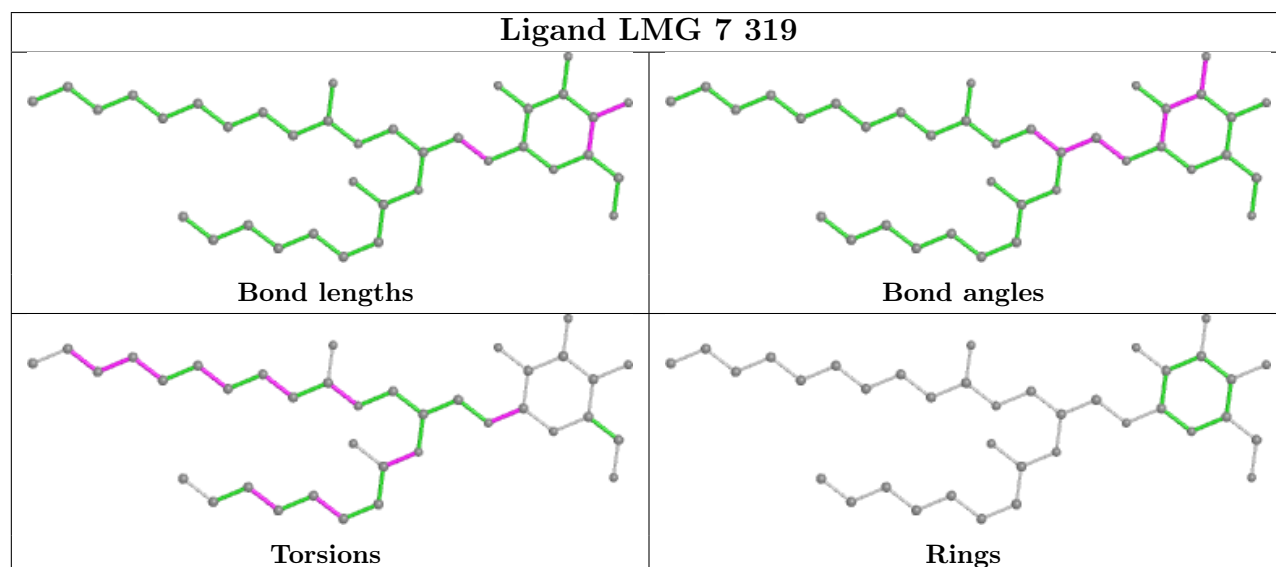
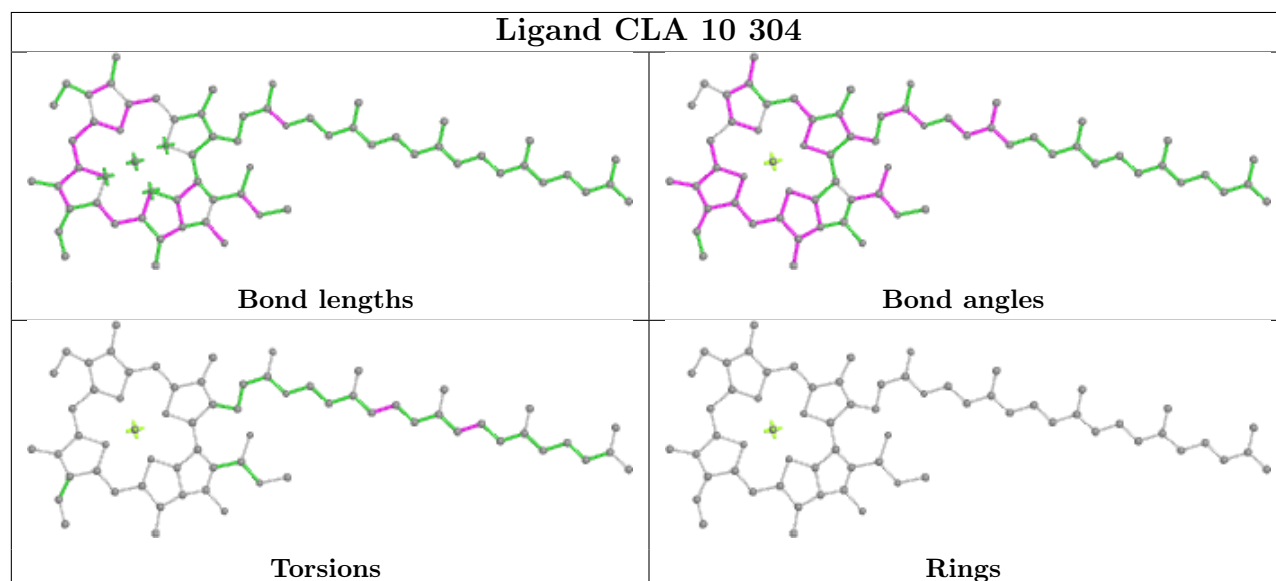
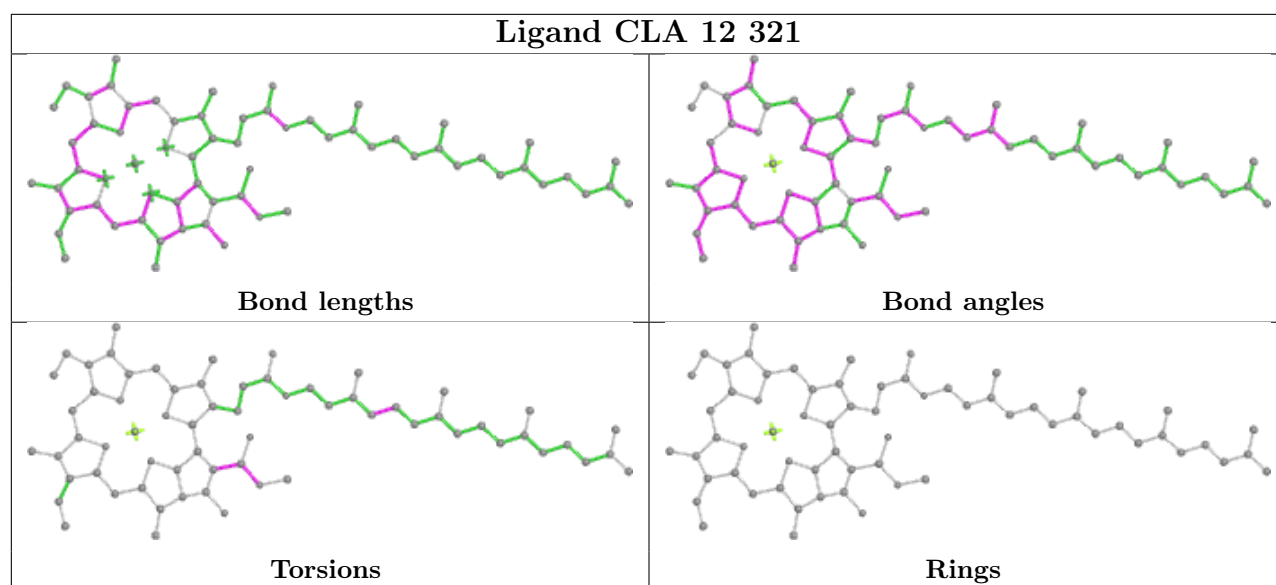


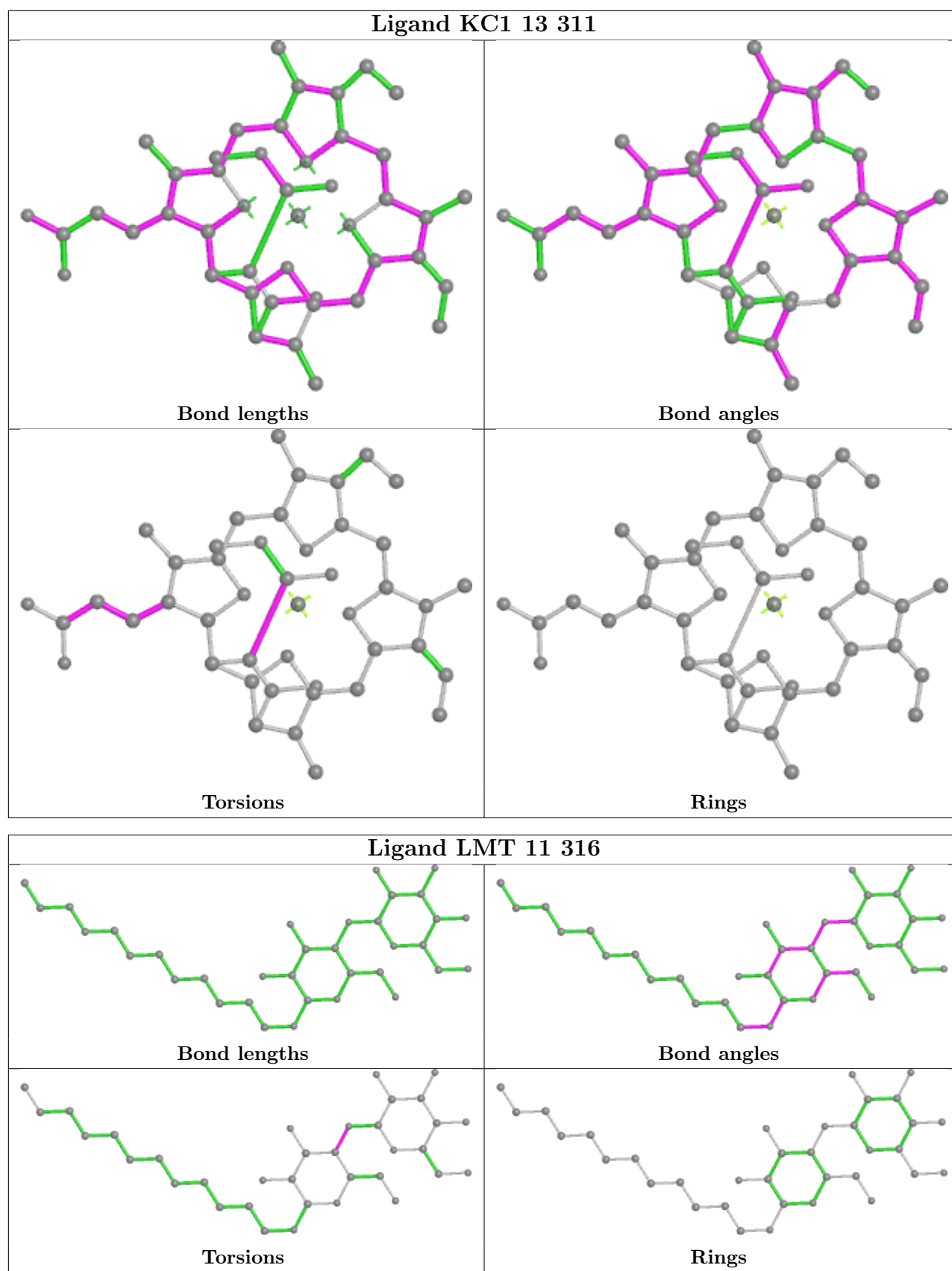


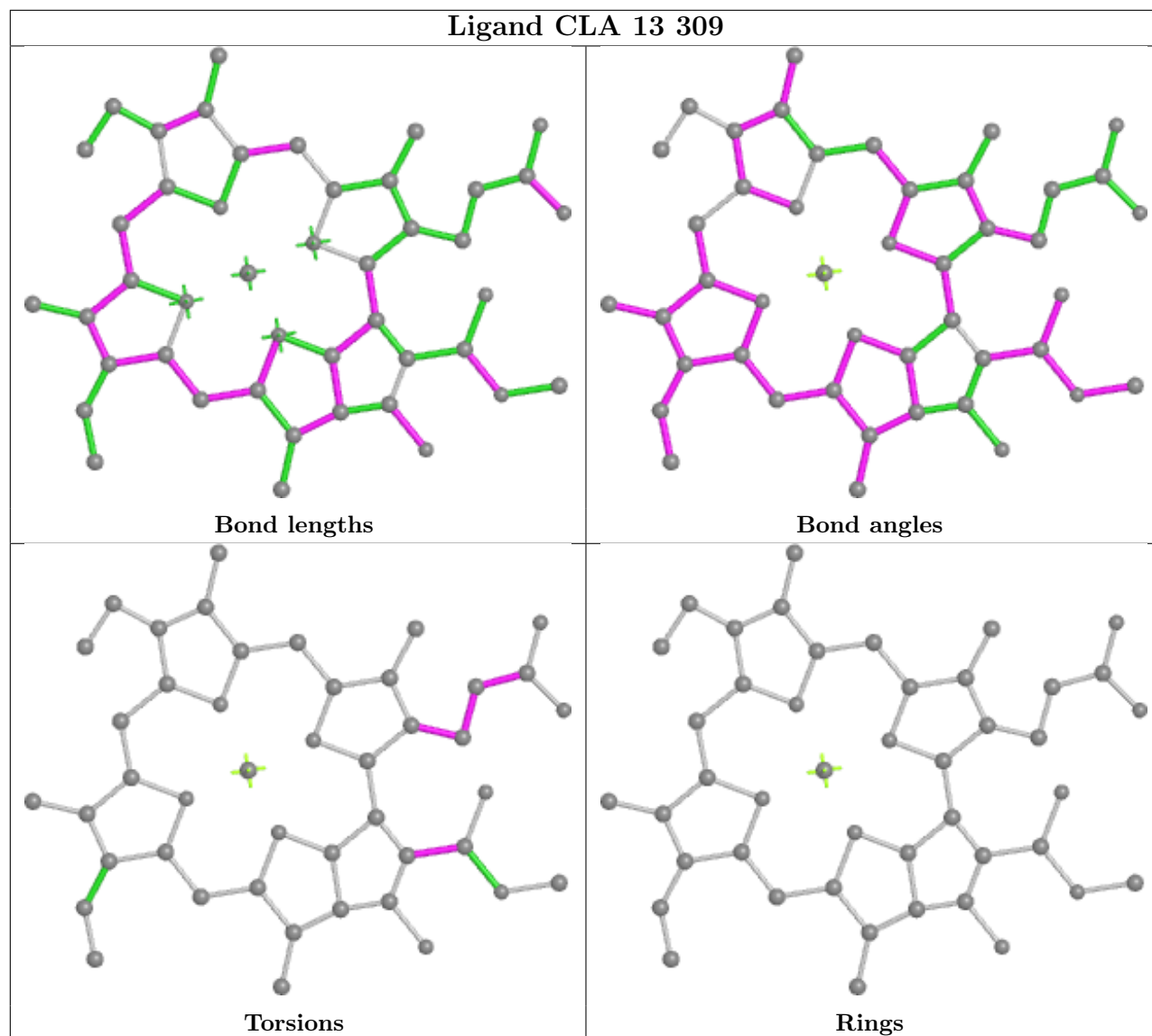


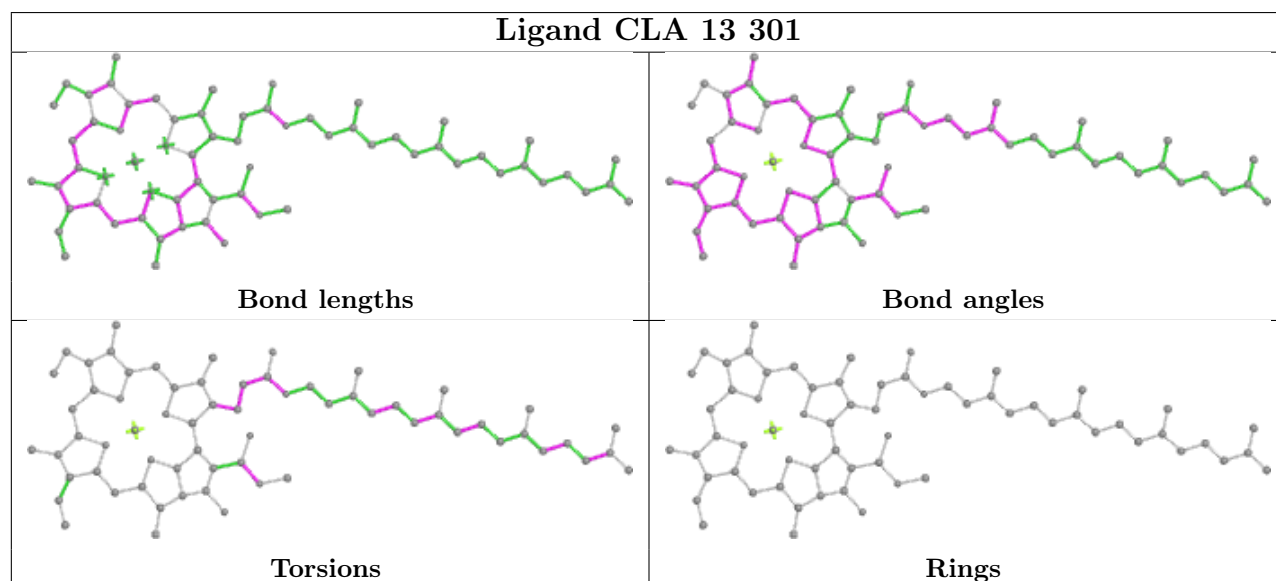
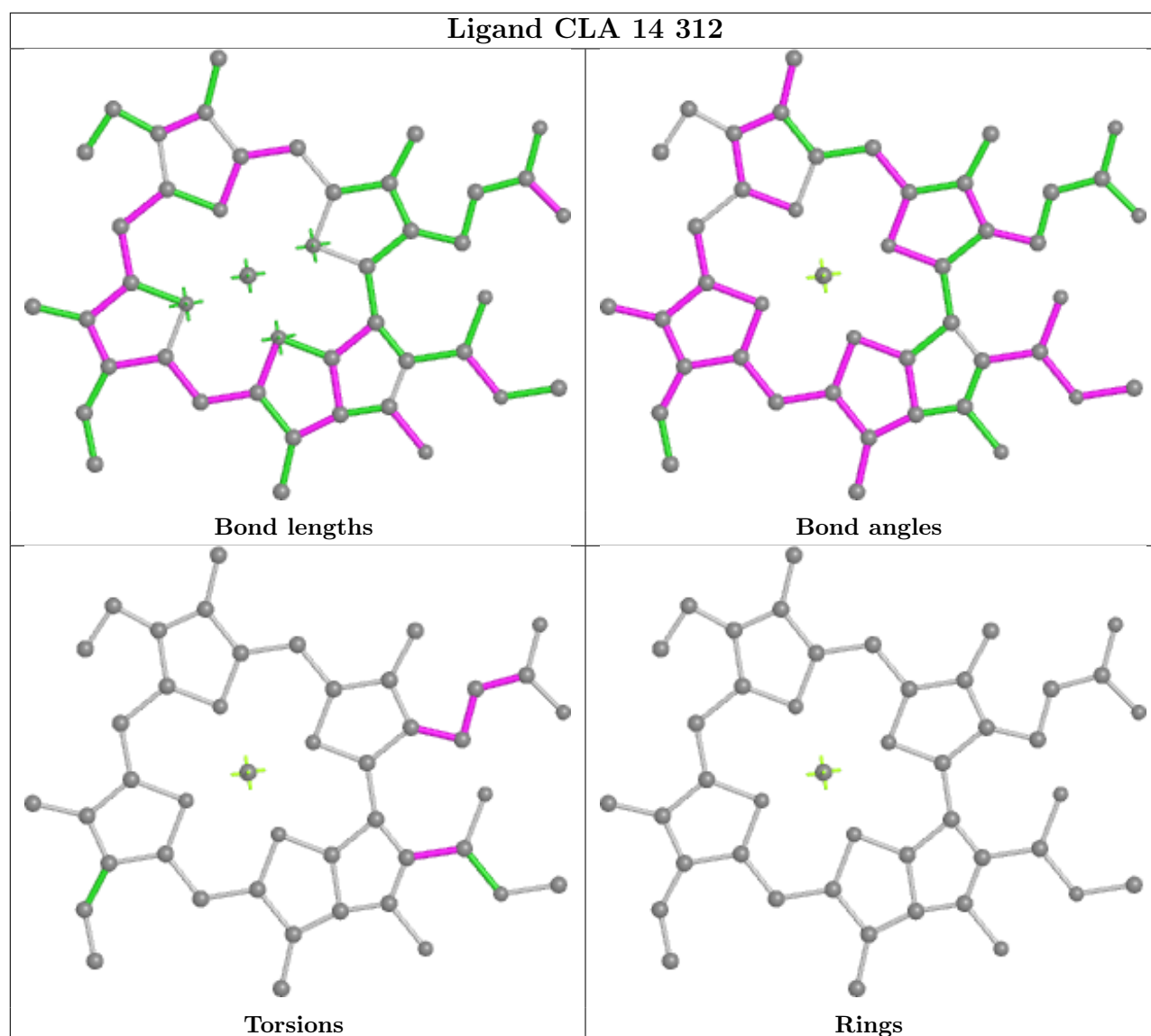




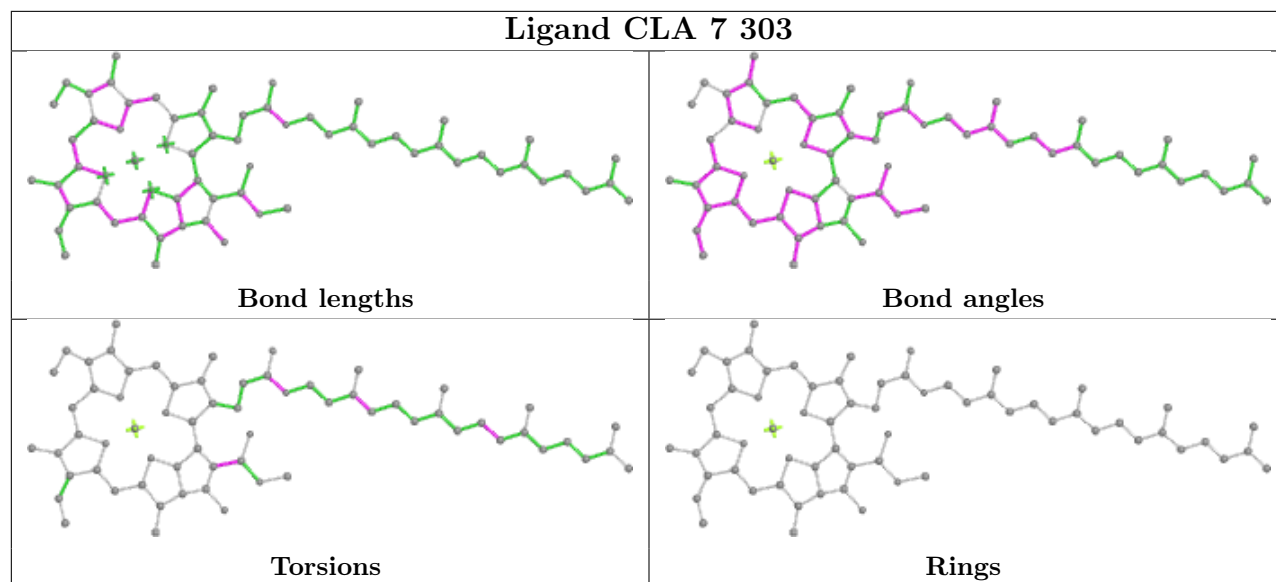




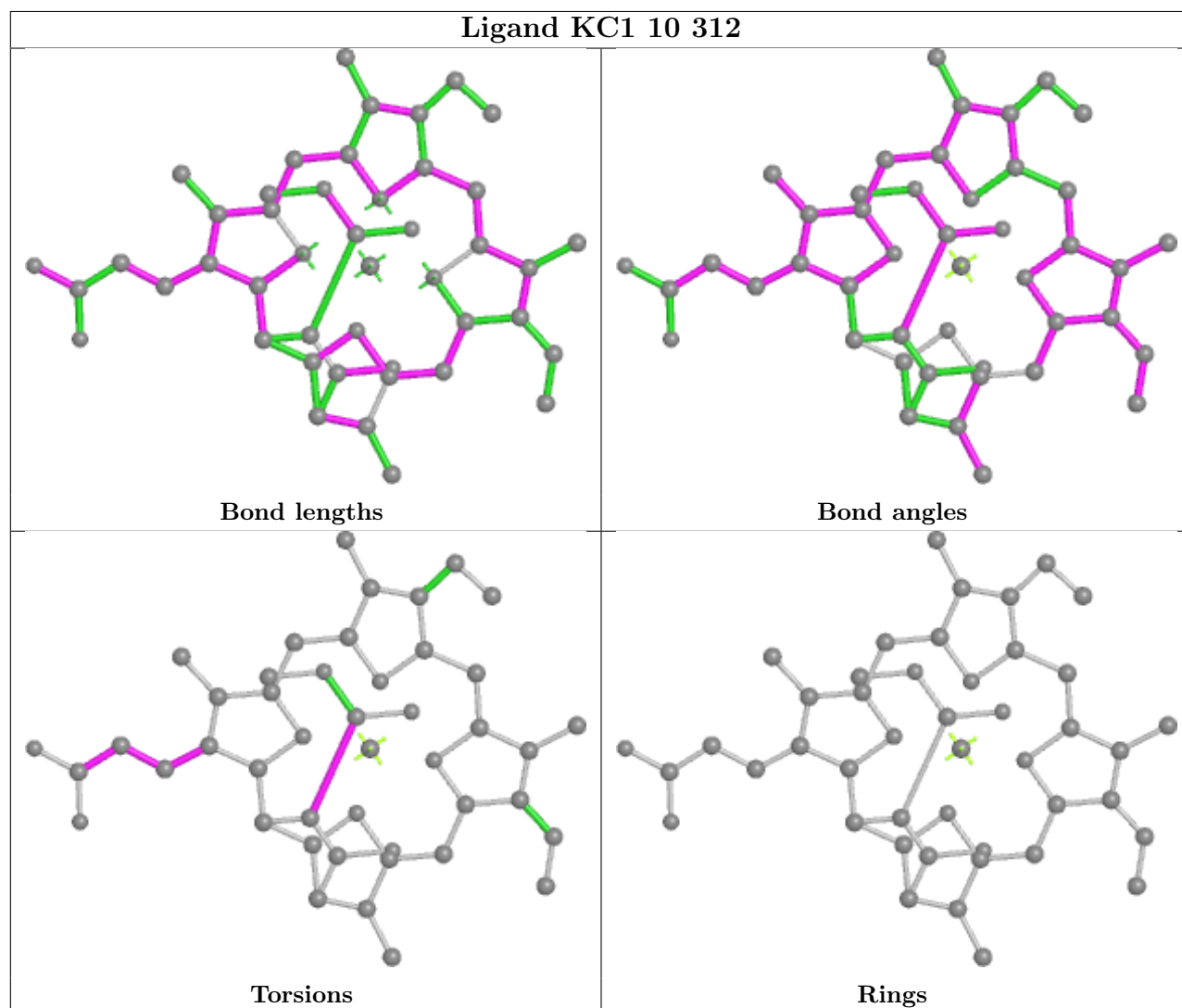




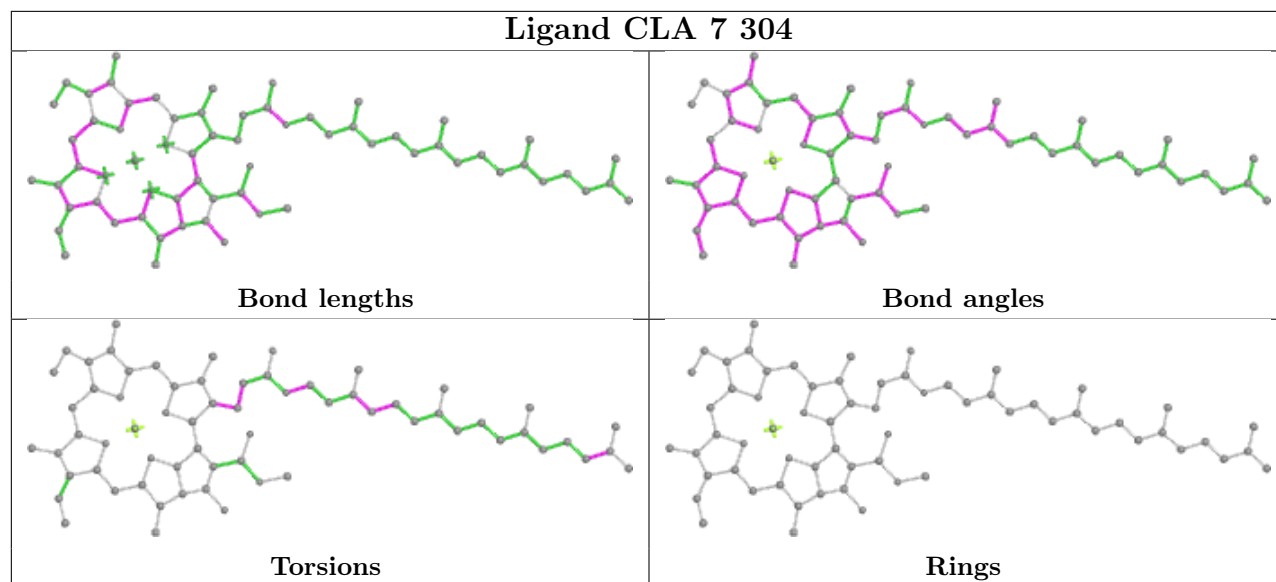
Ligand CLA 7 303



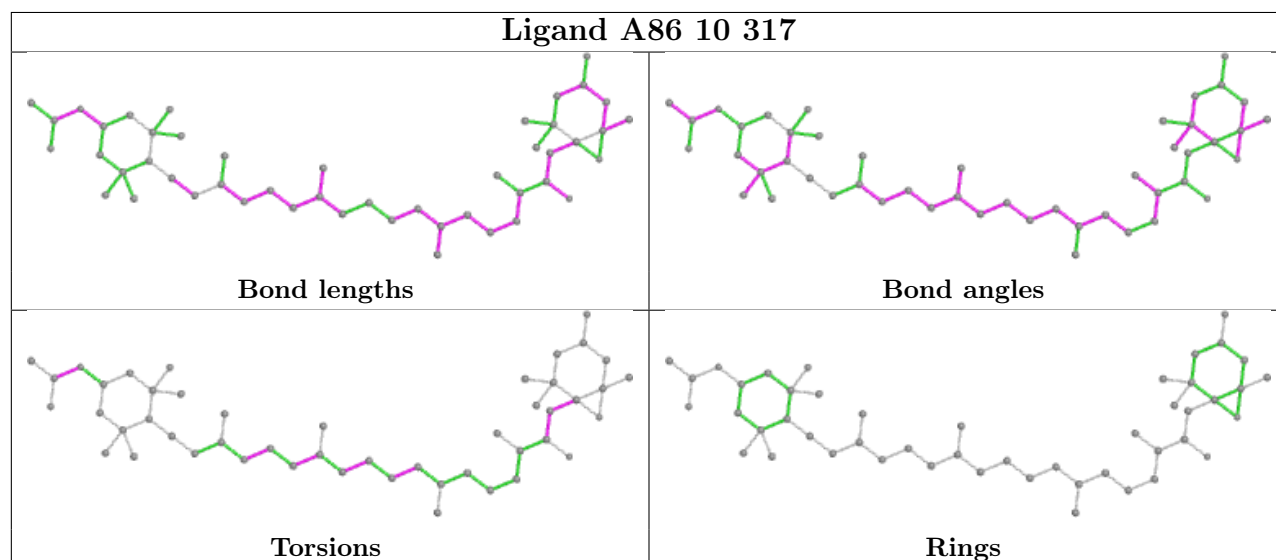
Ligand KC1 10 312



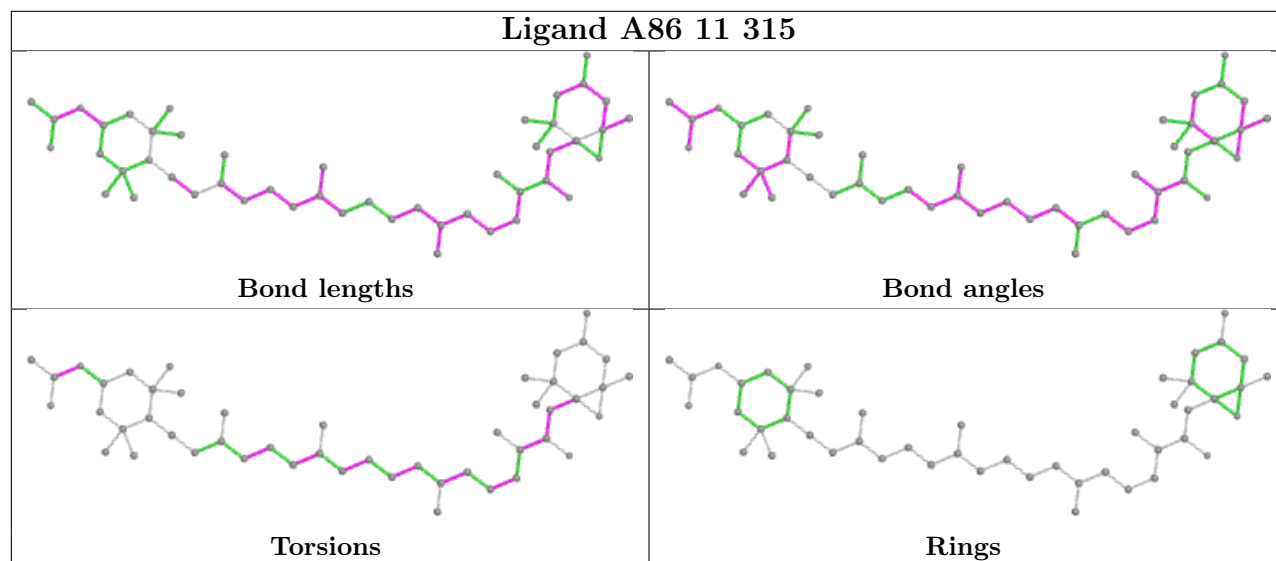
Ligand CLA 7 304

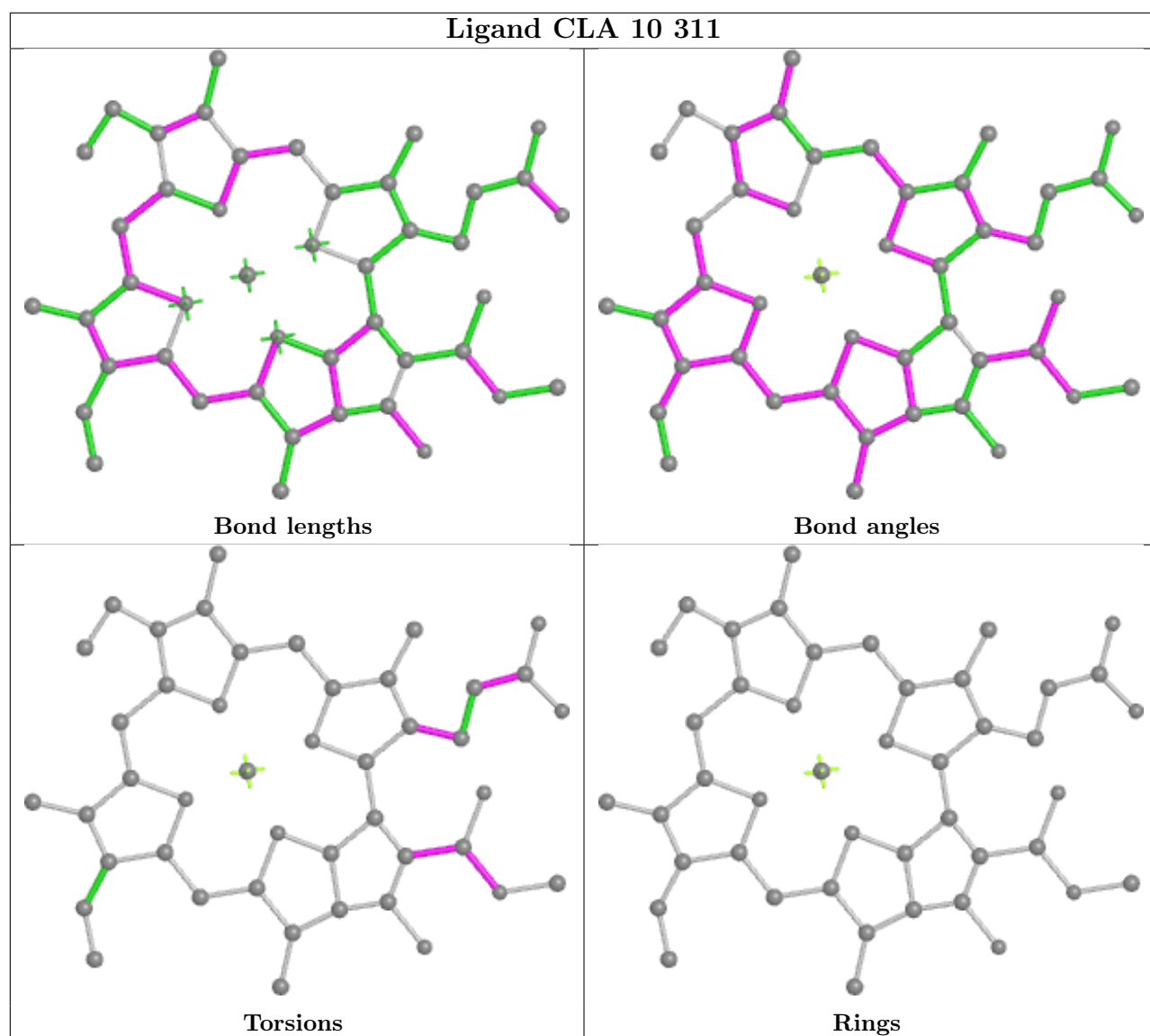


Ligand A86 10 317

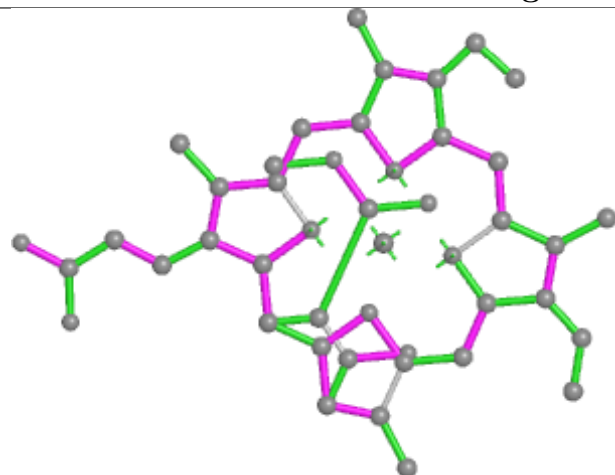


Ligand A86 11 315

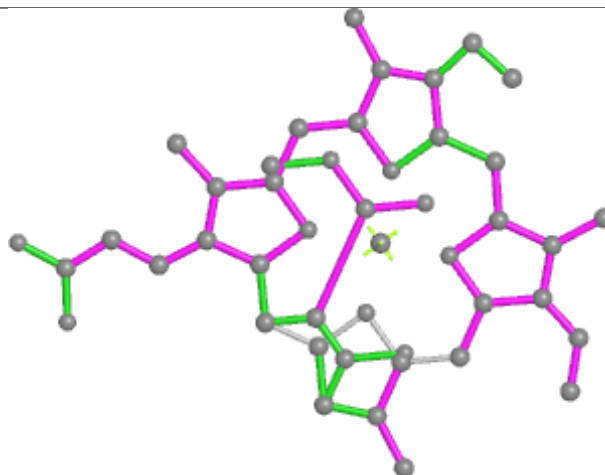




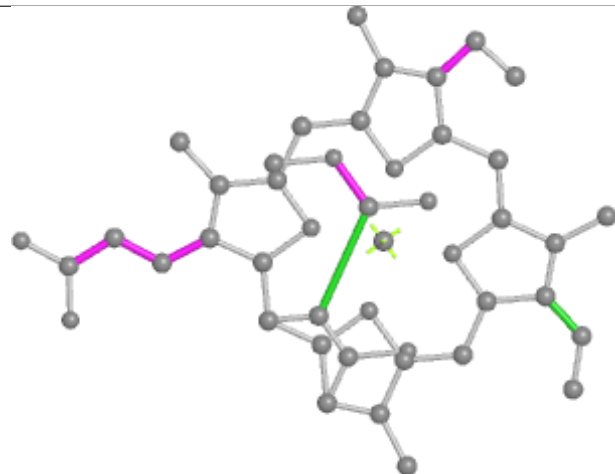
Ligand KC1 8 307



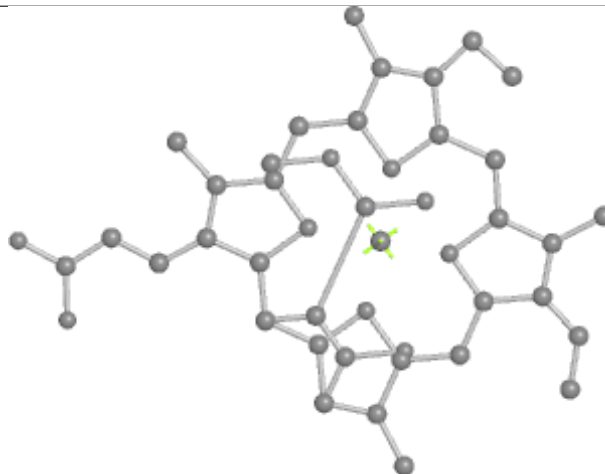
Bond lengths



Bond angles

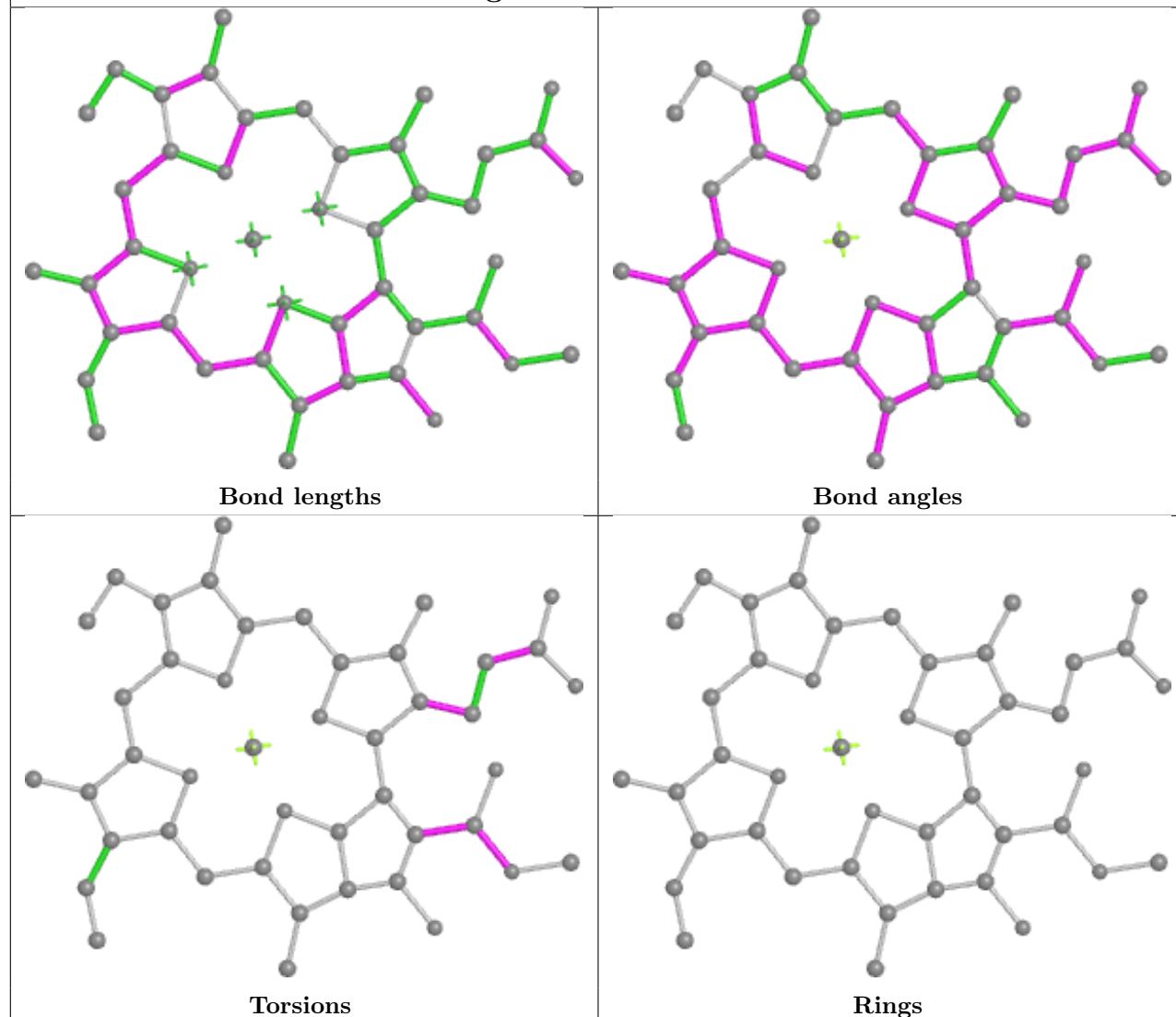


Torsions

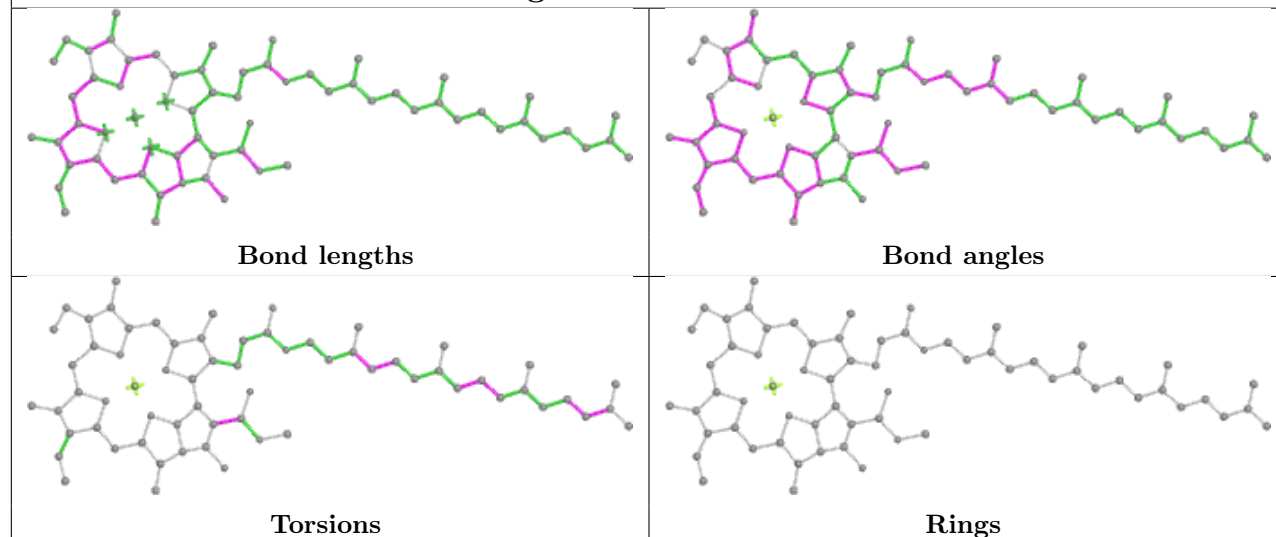


Rings

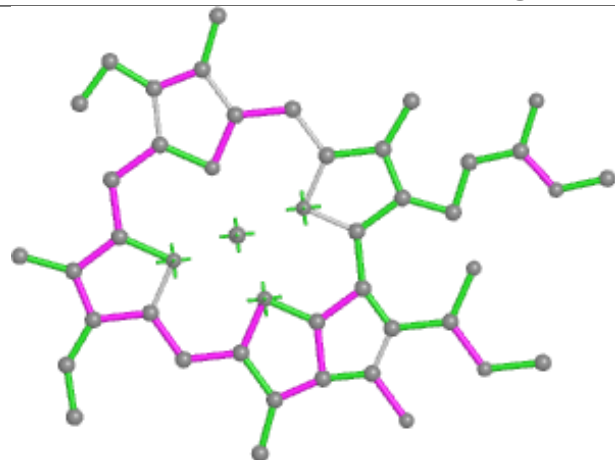
Ligand CLA 15 308



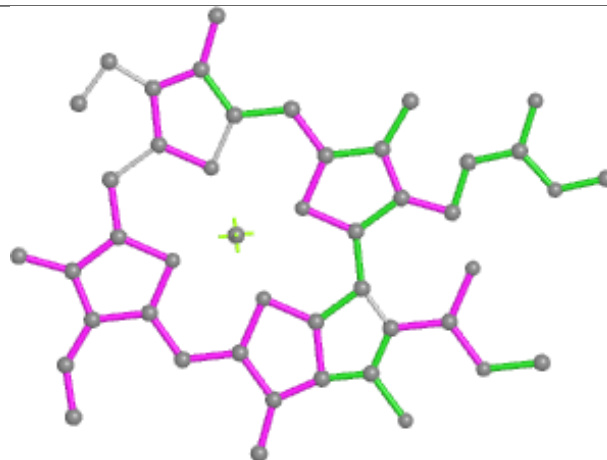
Ligand CLA 16 302



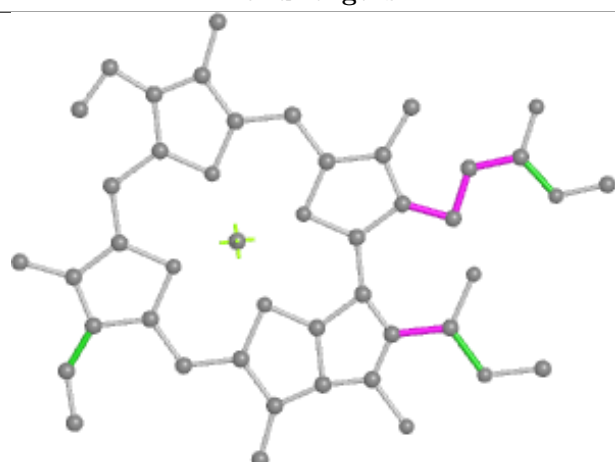
Ligand CLA 16 307



Bond lengths



Bond angles

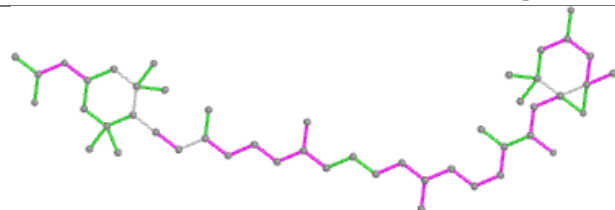


Torsions

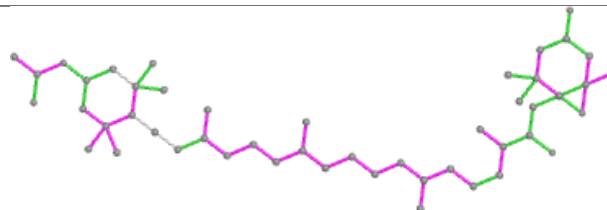


Rings

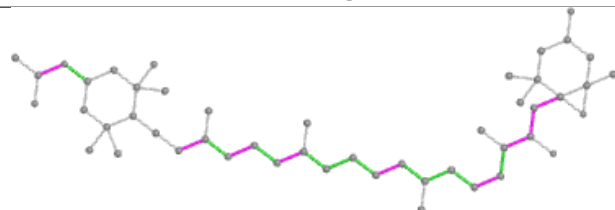
Ligand A86 13 315



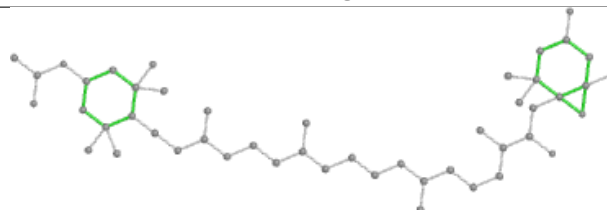
Bond lengths



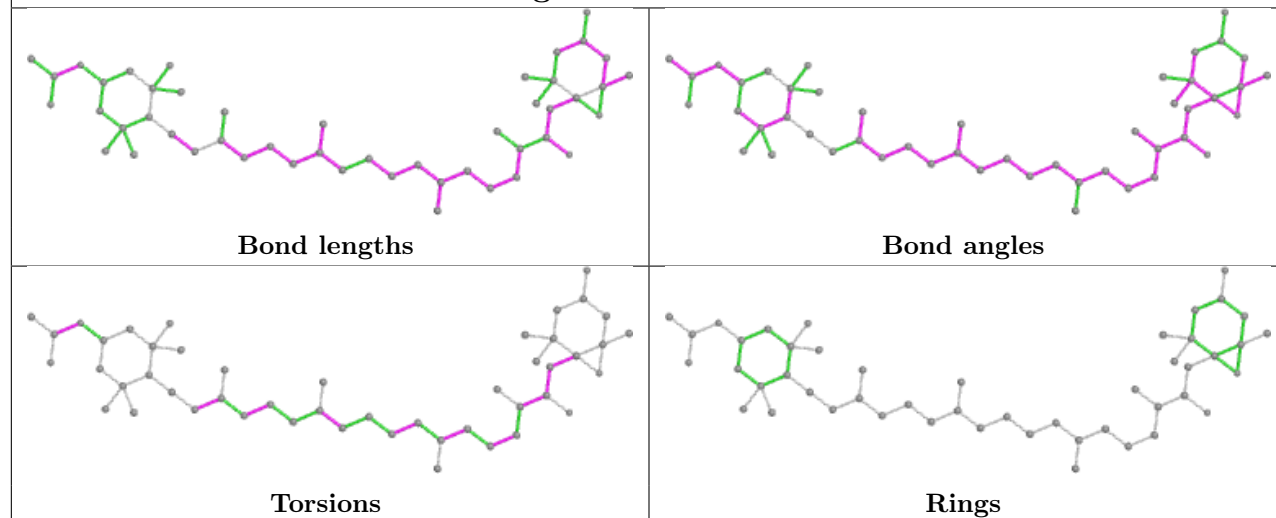
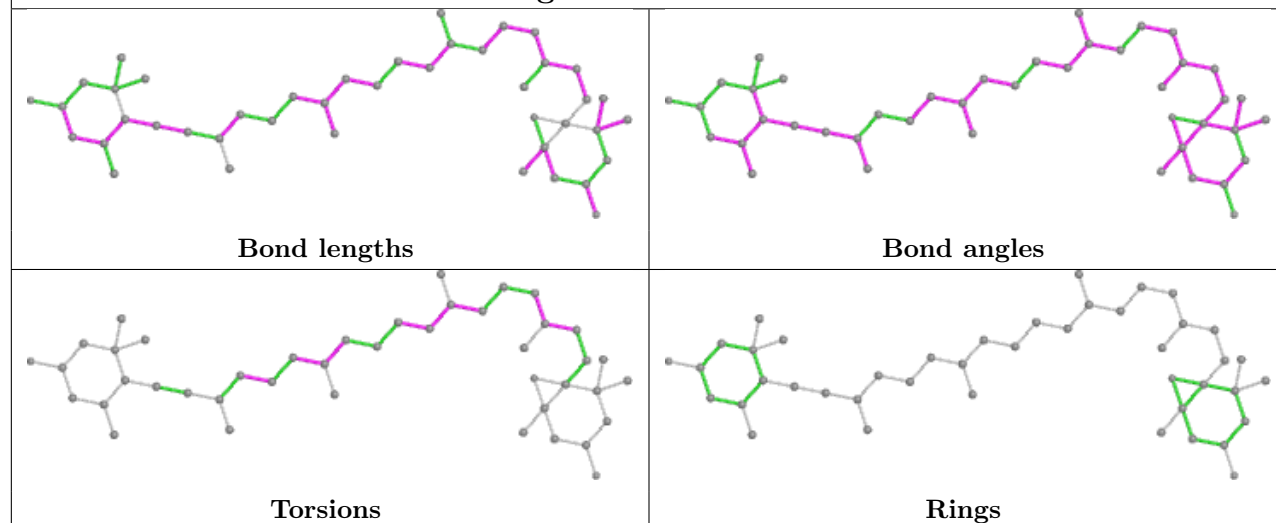
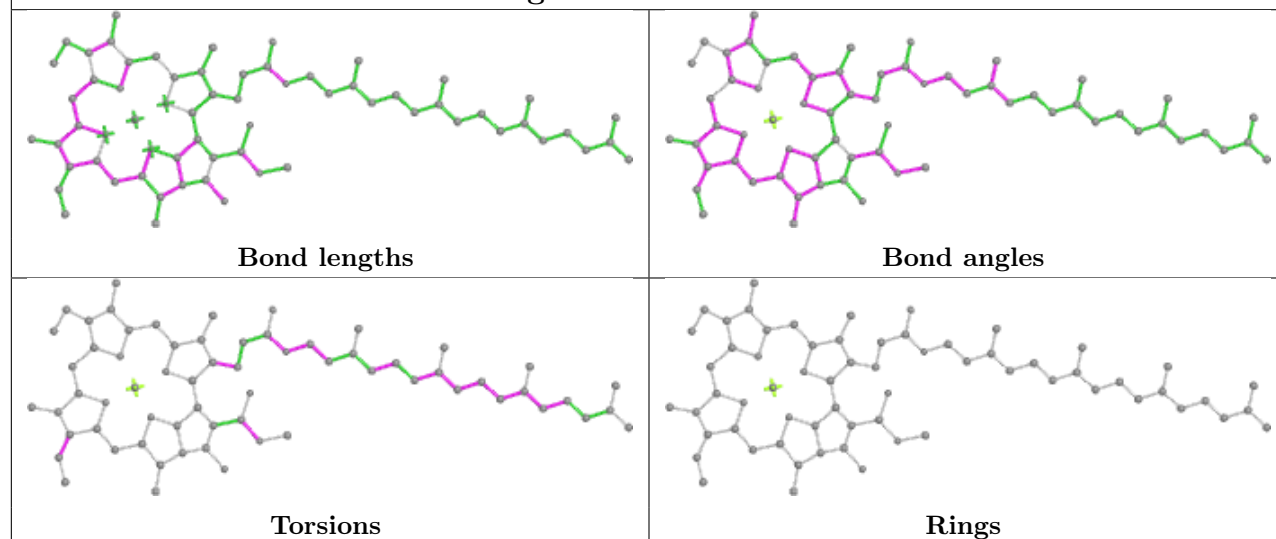
Bond angles

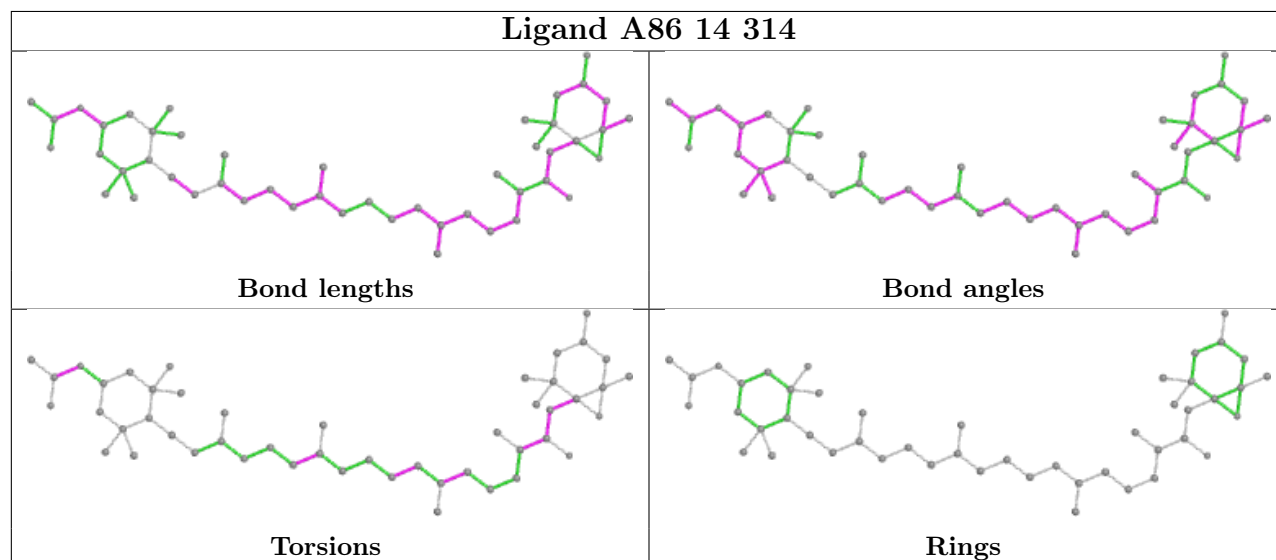
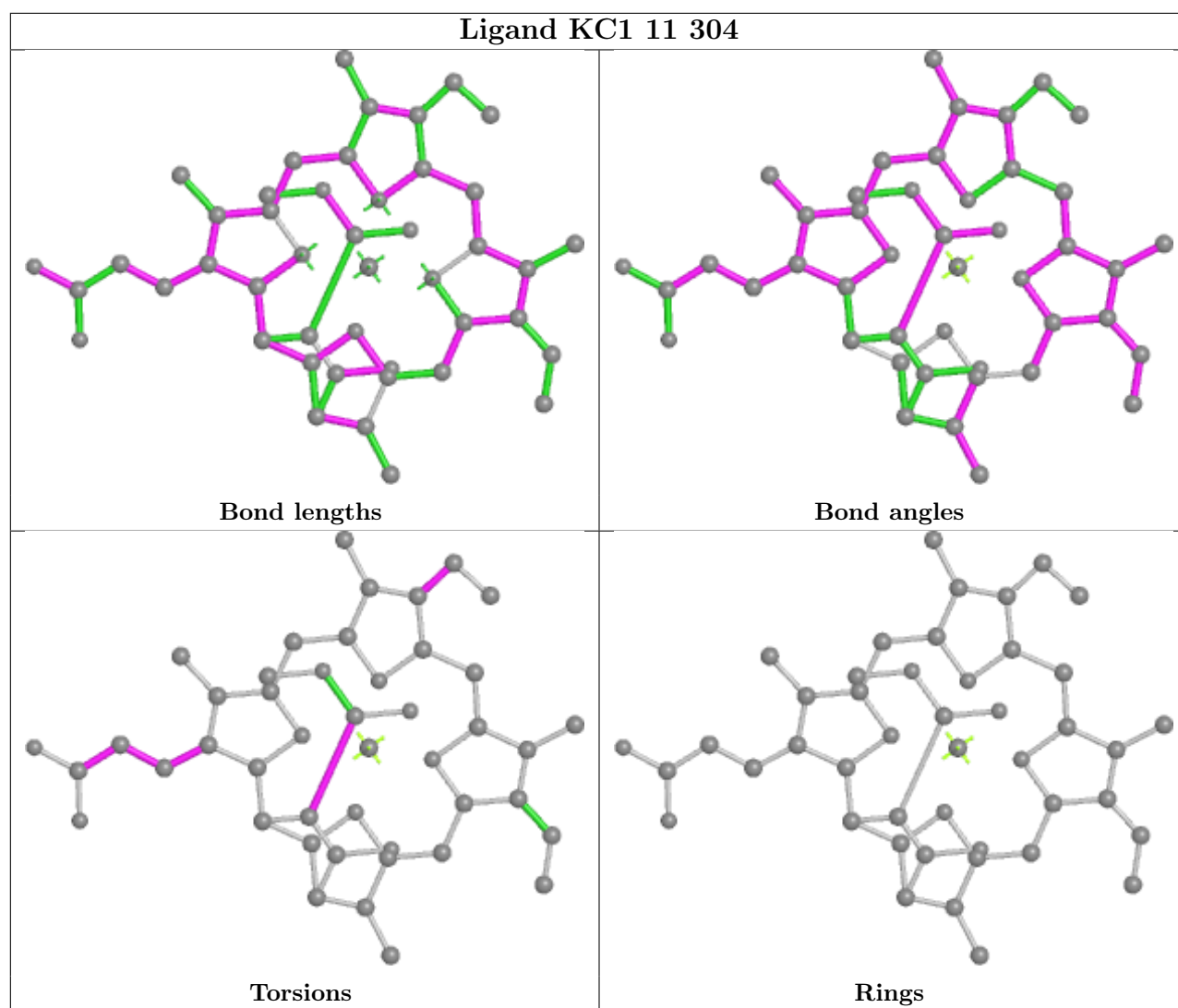


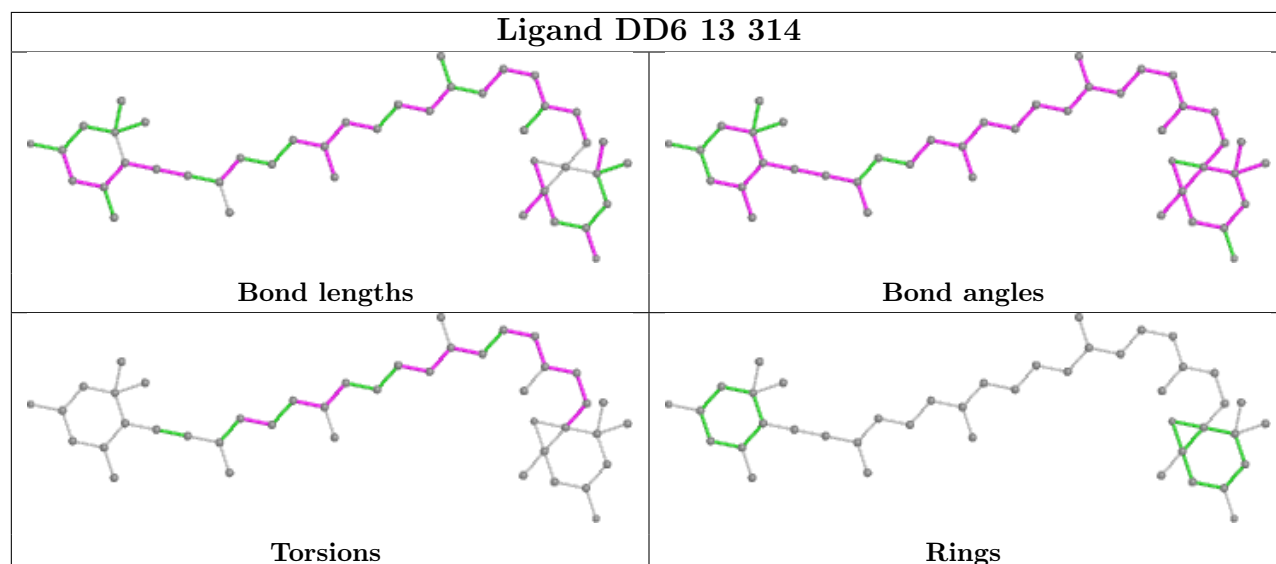
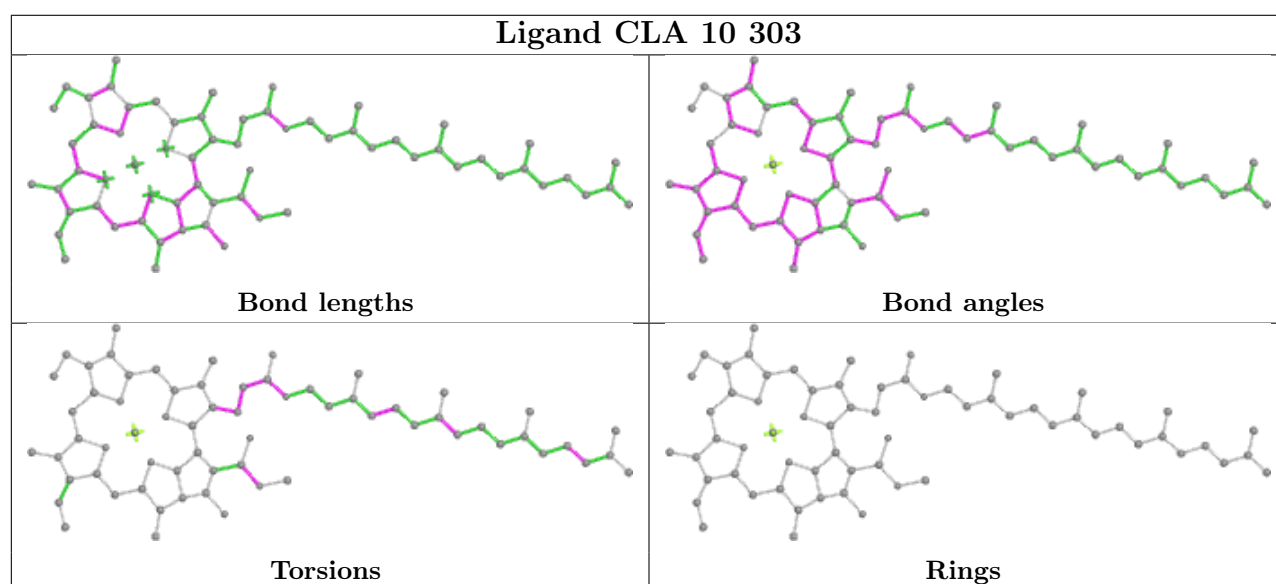
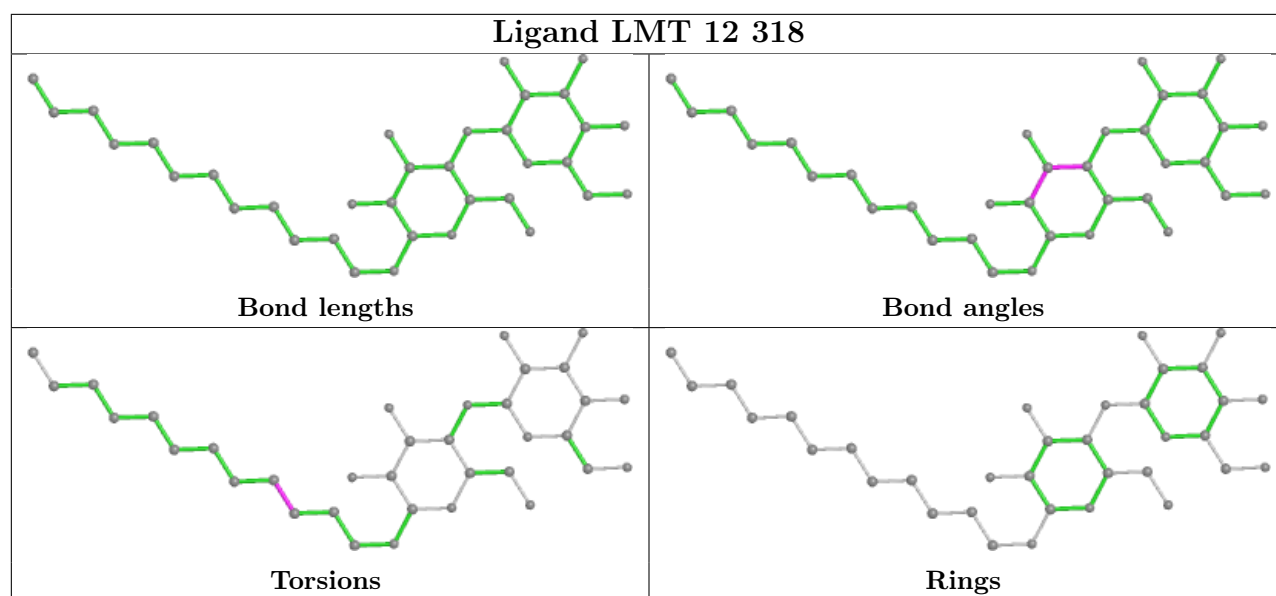
Torsions

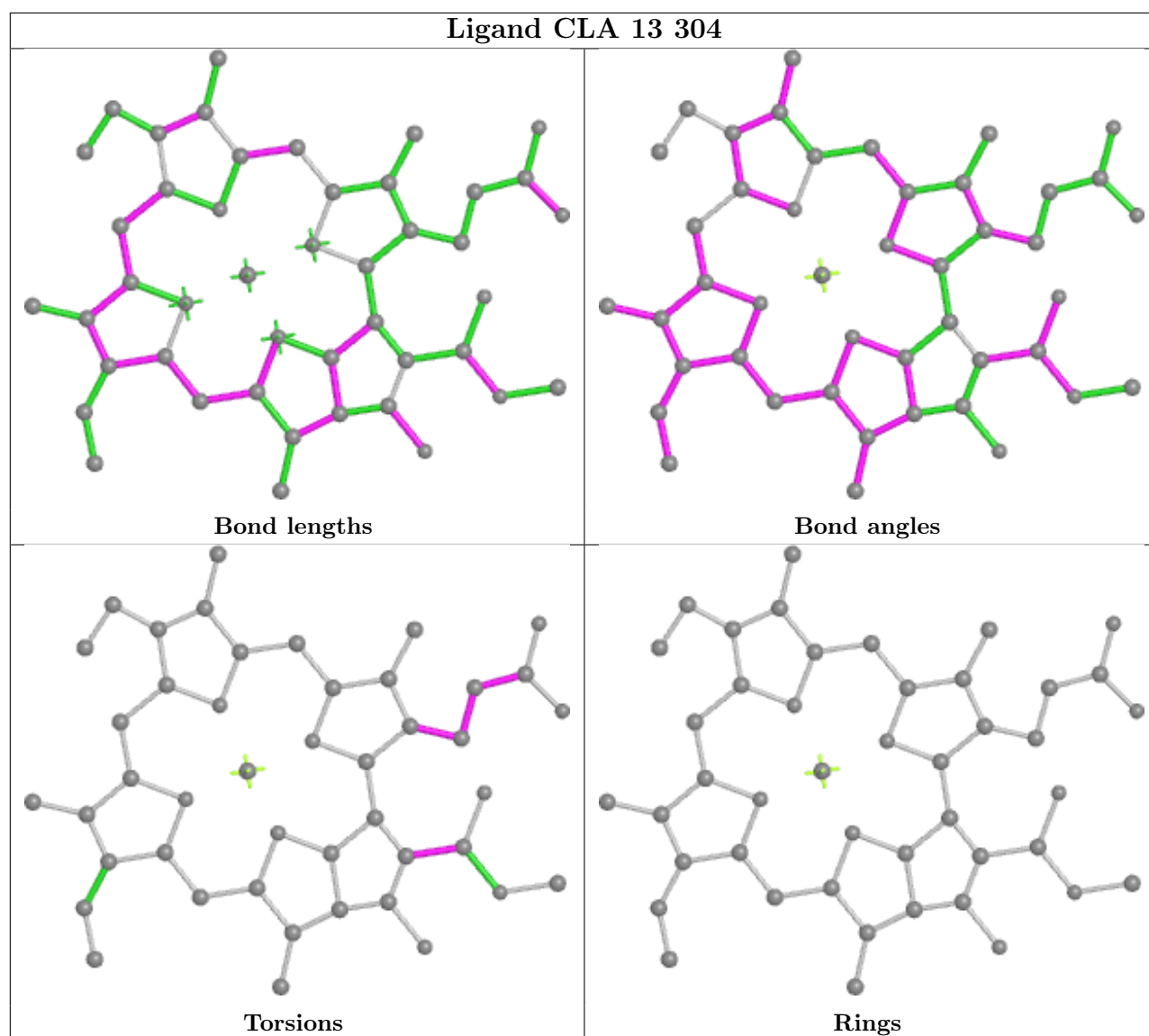


Rings

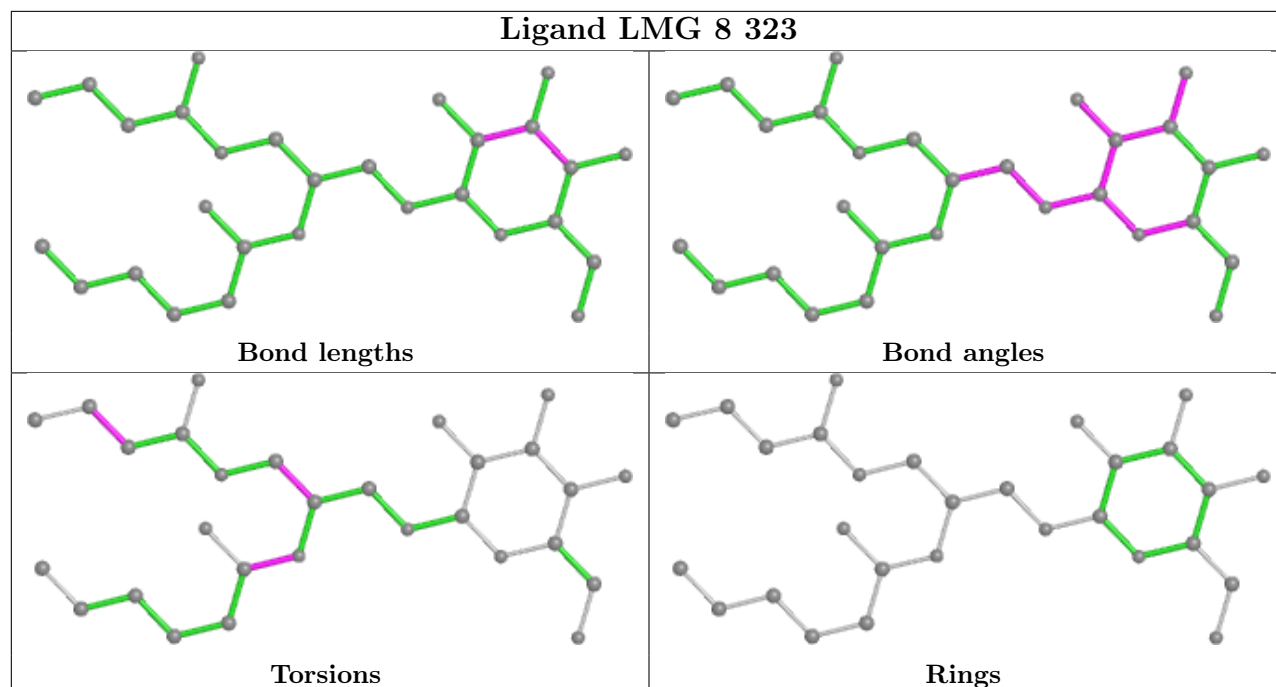
Ligand A86 15 322**Ligand DD6 7 301****Ligand CLA 15 304**



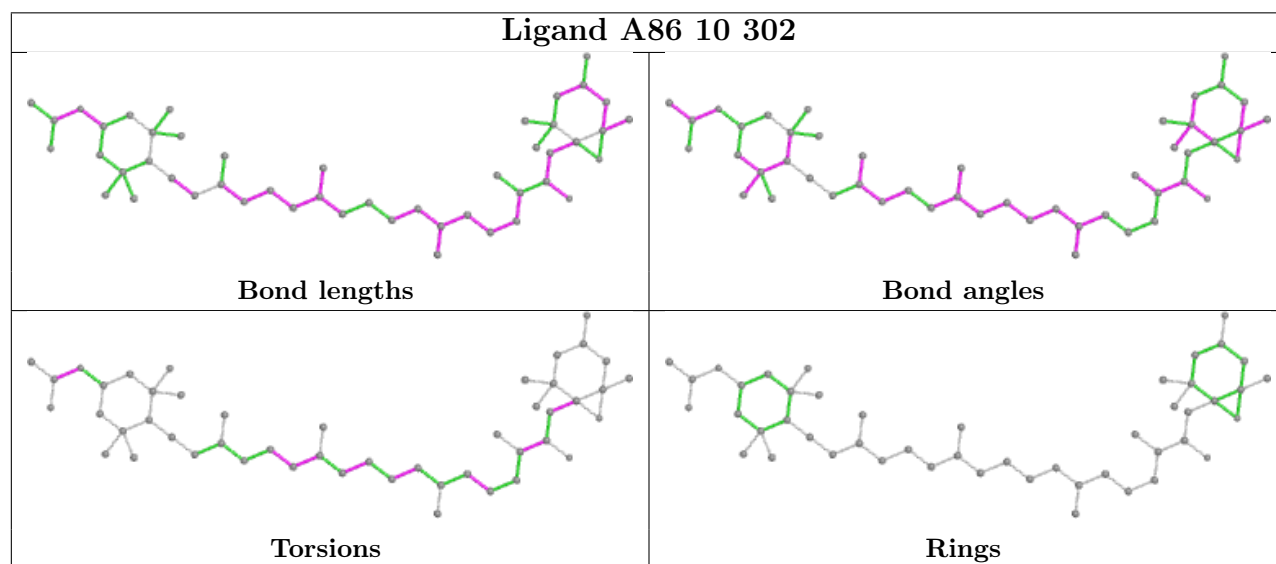




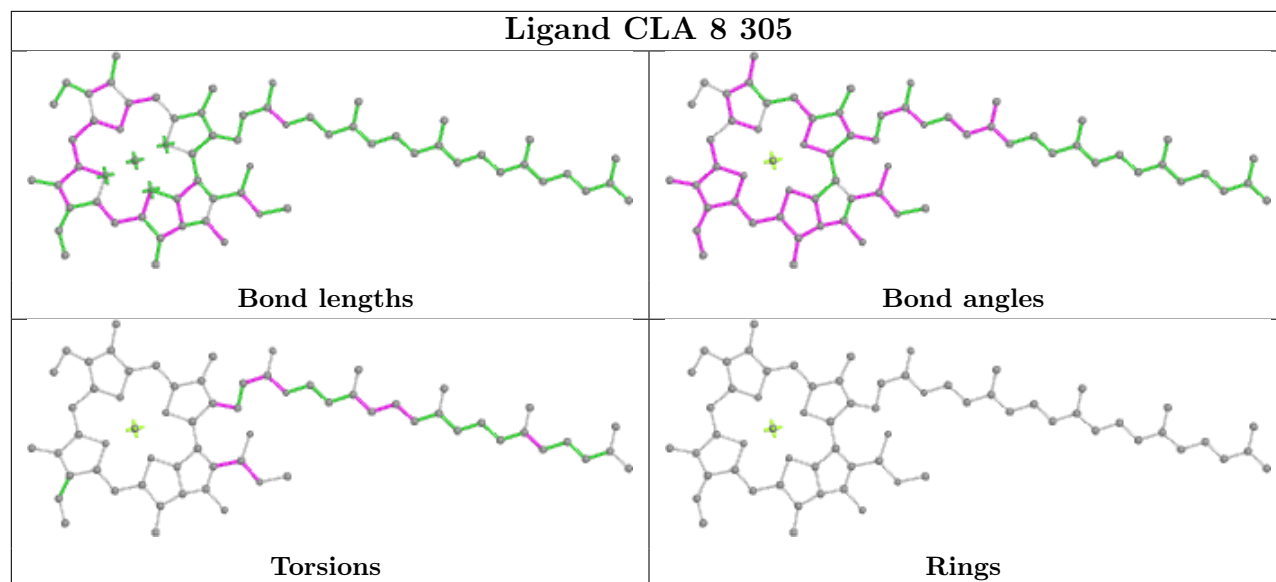
Ligand LMG 8 323



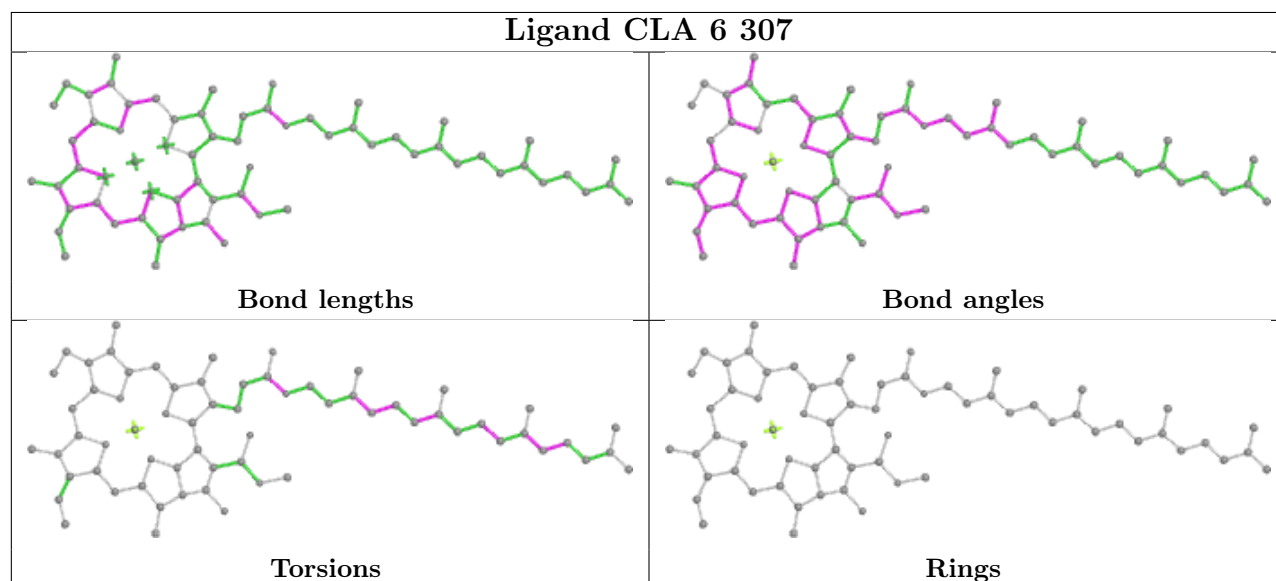
Ligand A86 10 302



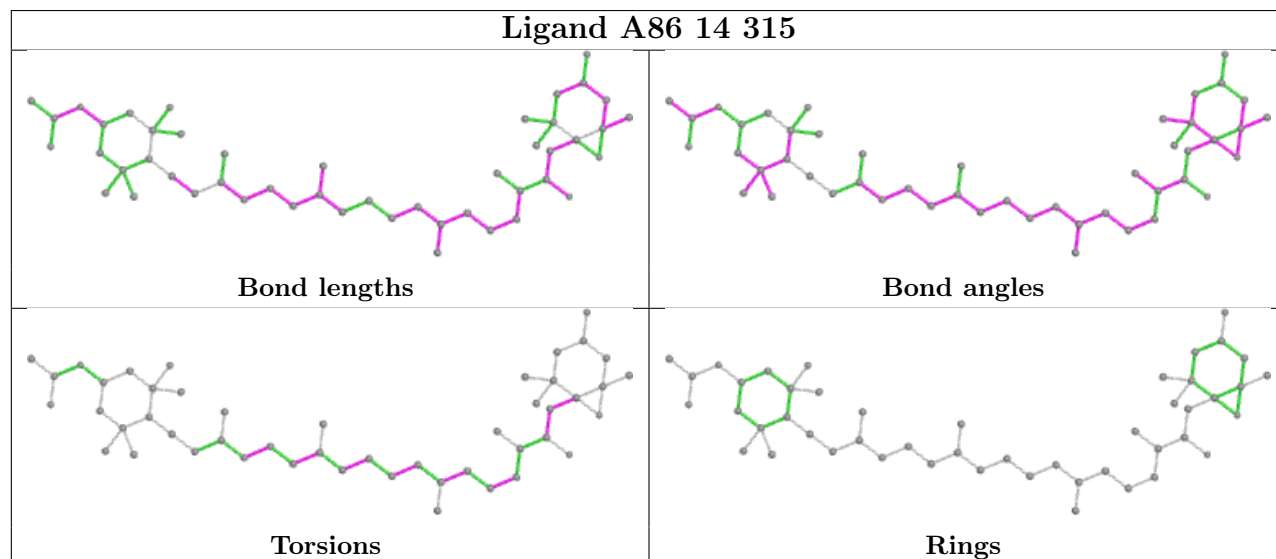
Ligand CLA 8 305



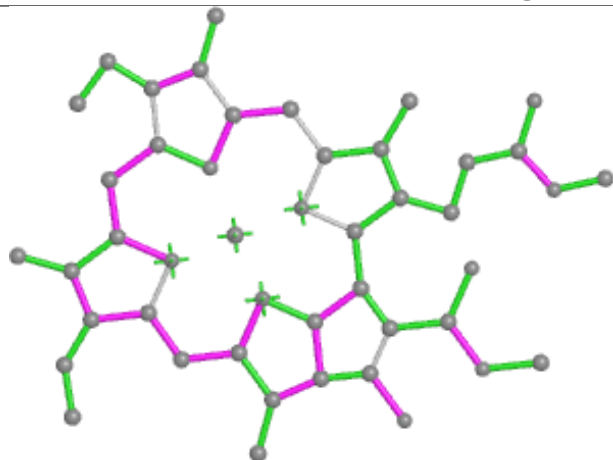
Ligand CLA 6 307



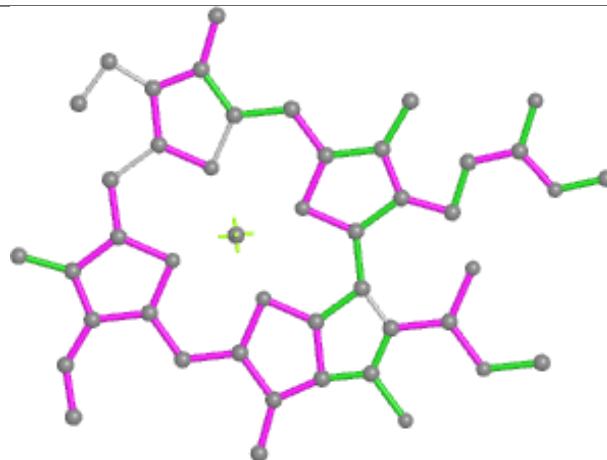
Ligand A86 14 315



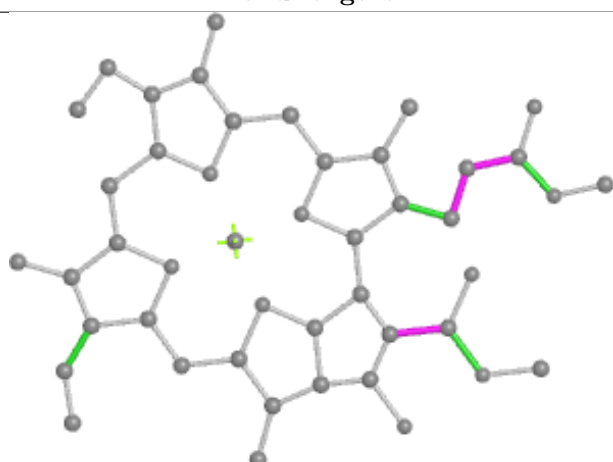
Ligand CLA 7 311



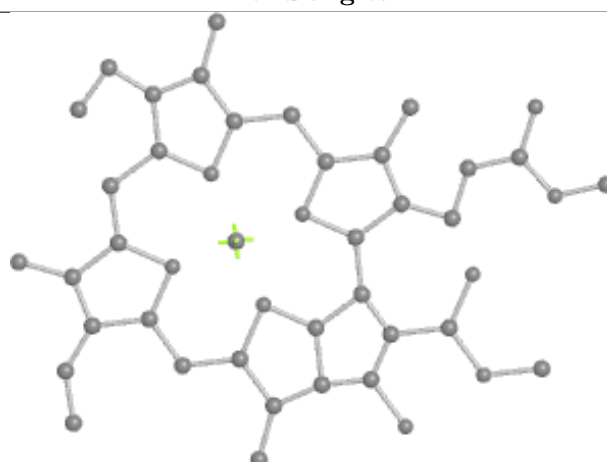
Bond lengths



Bond angles

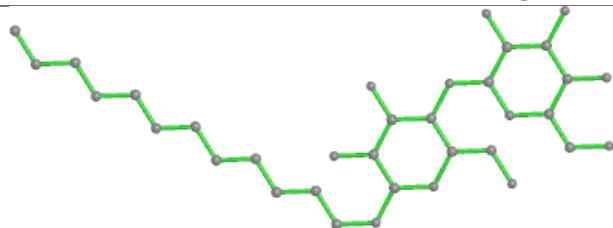


Torsions

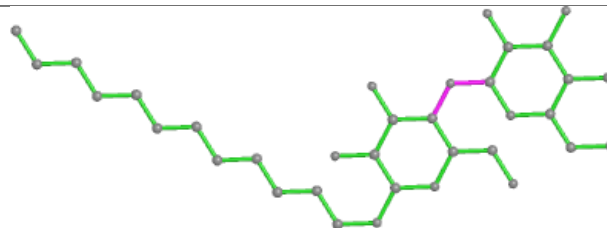


Rings

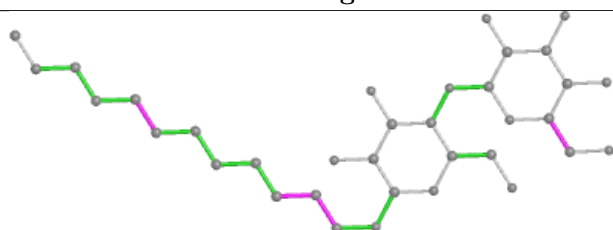
Ligand LMT 7 320



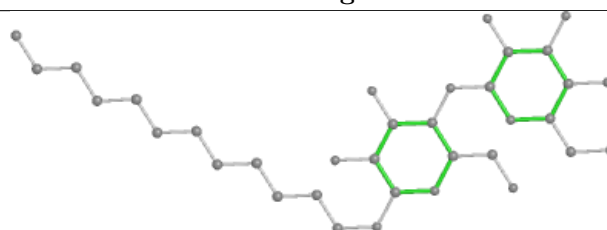
Bond lengths



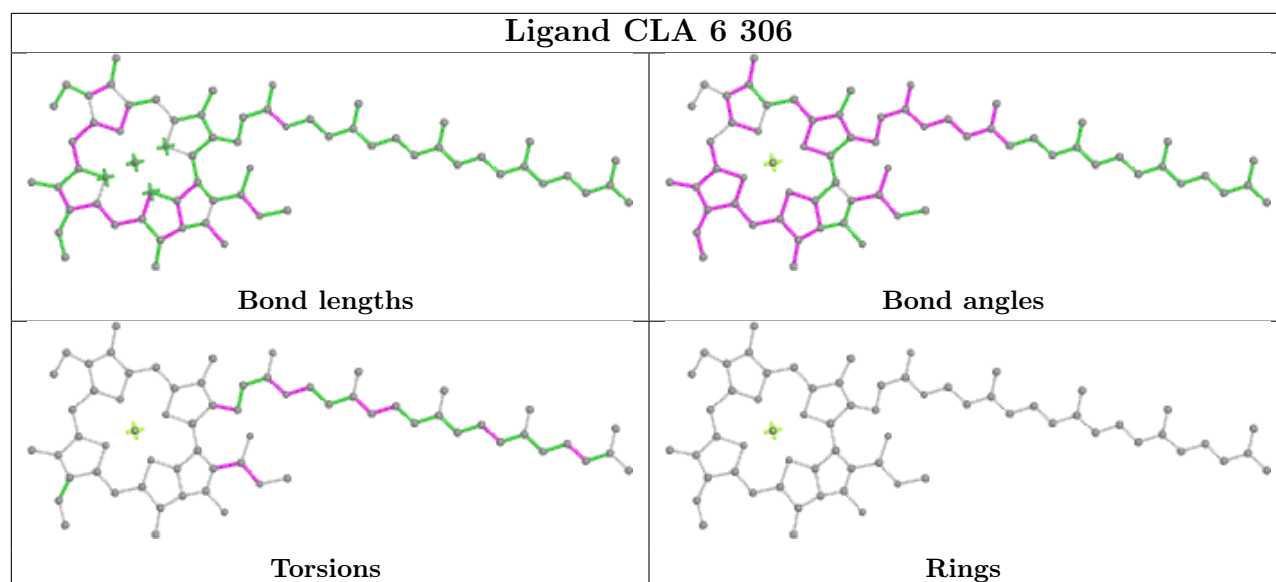
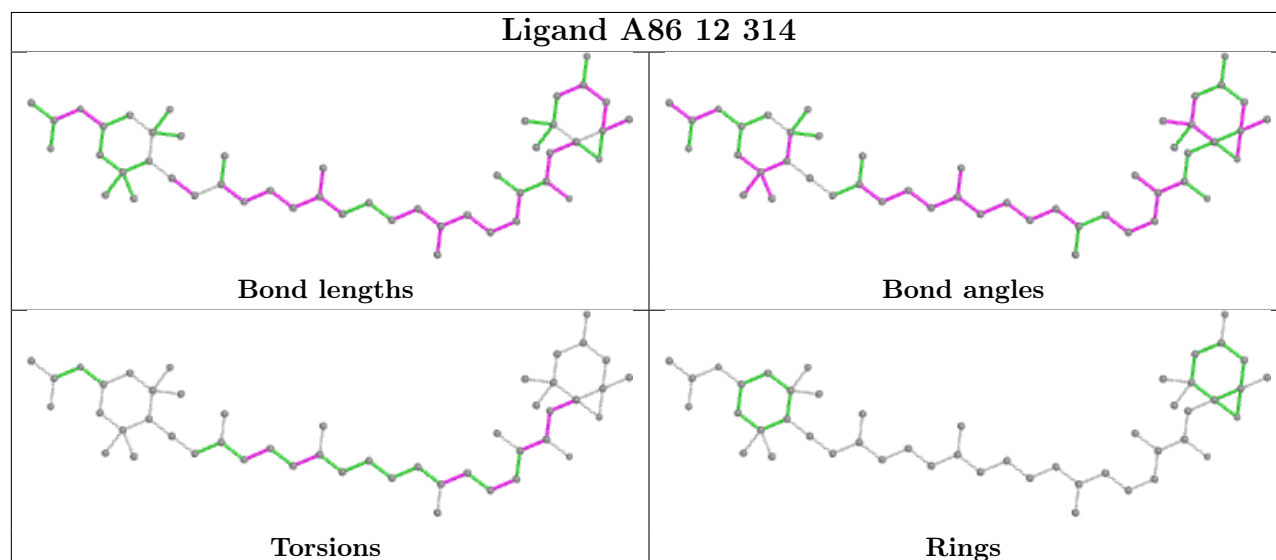
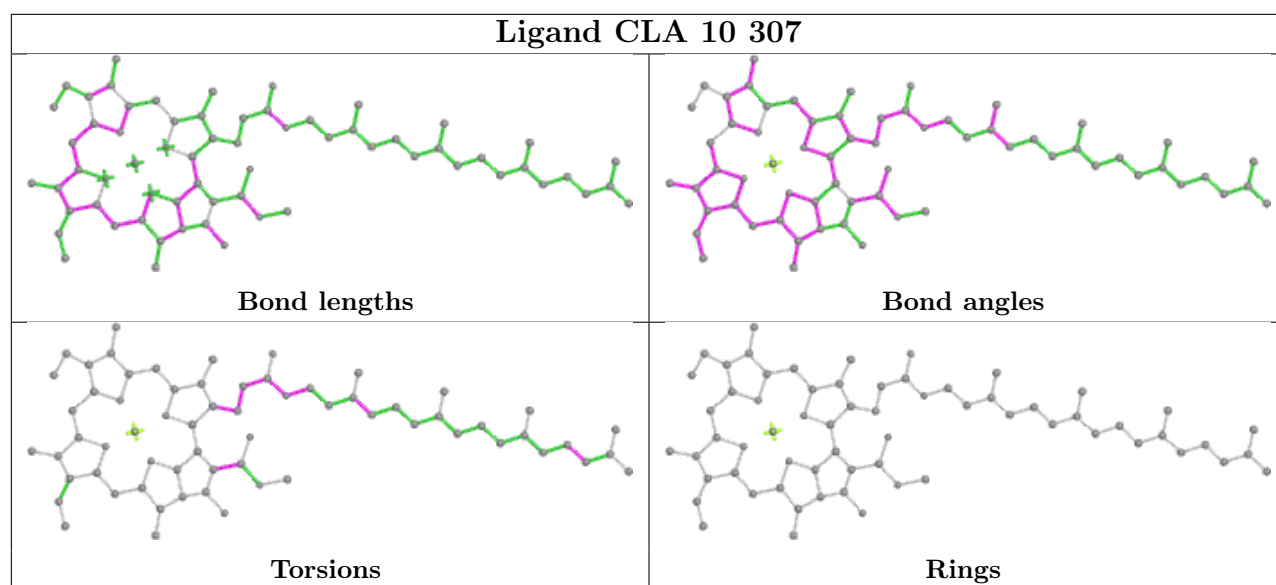
Bond angles

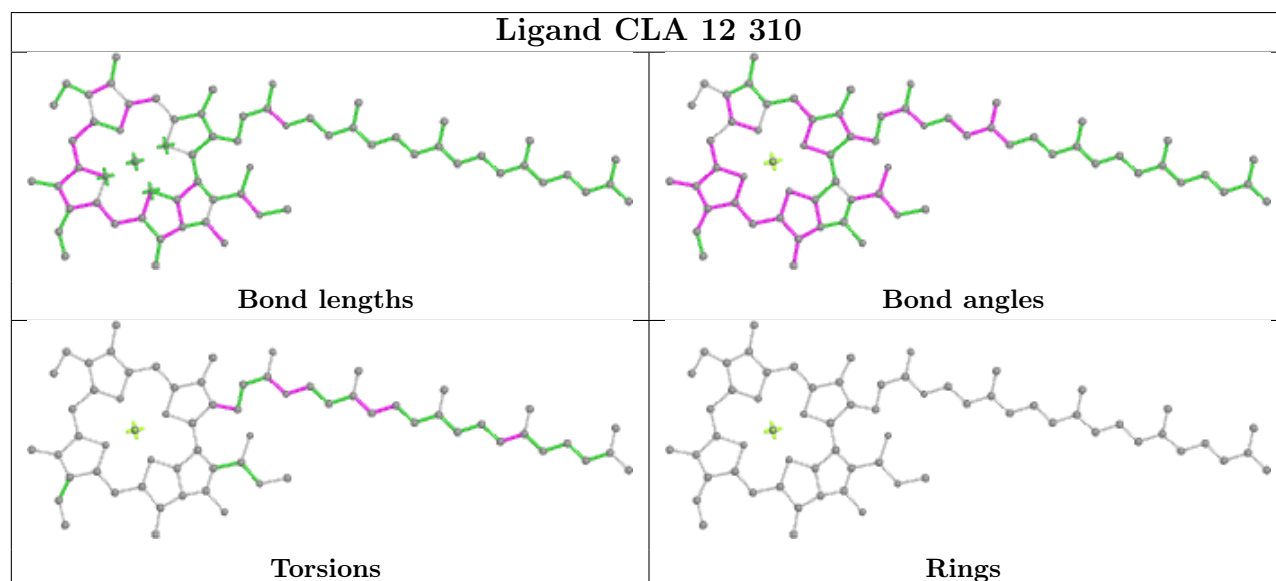
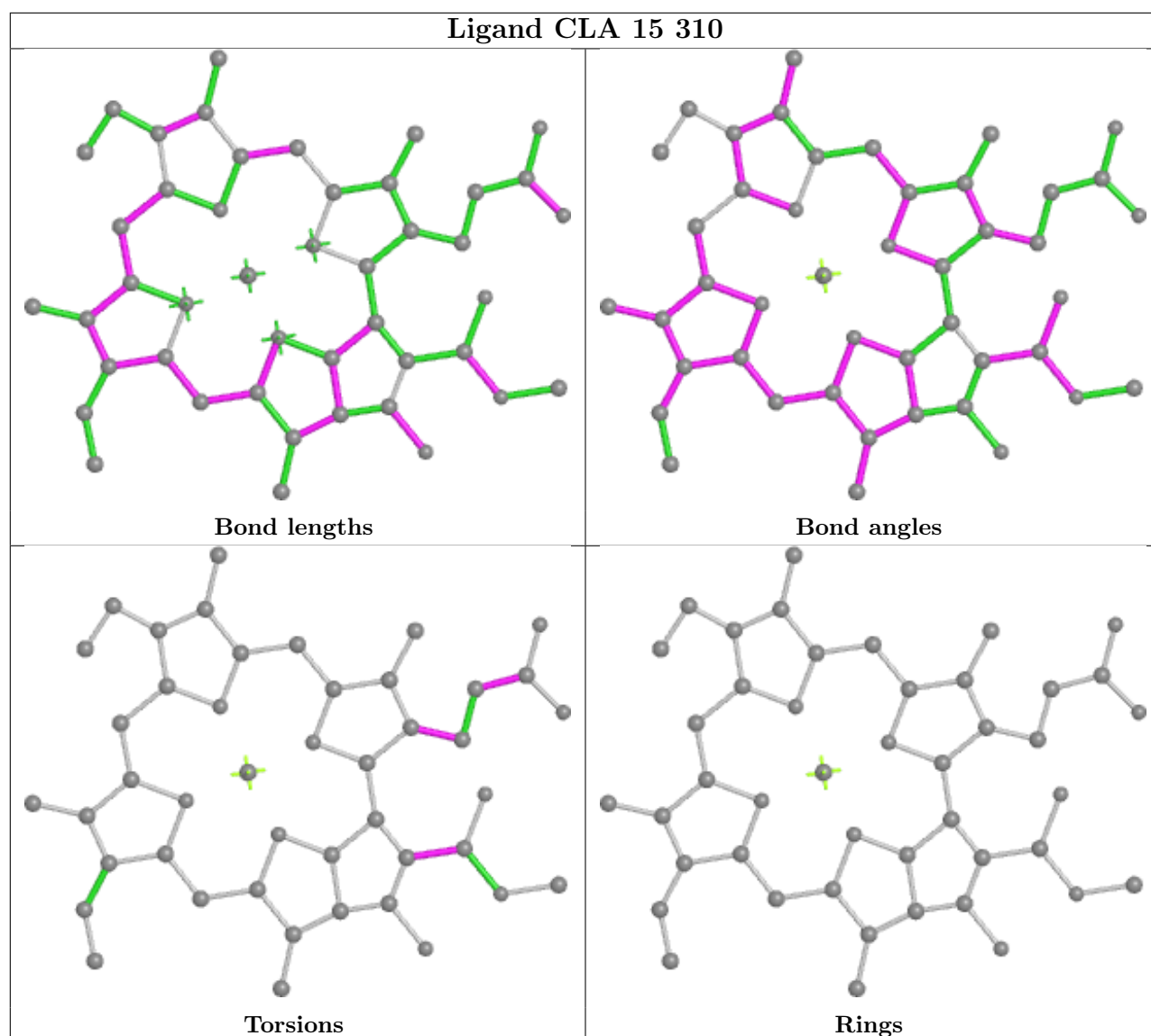


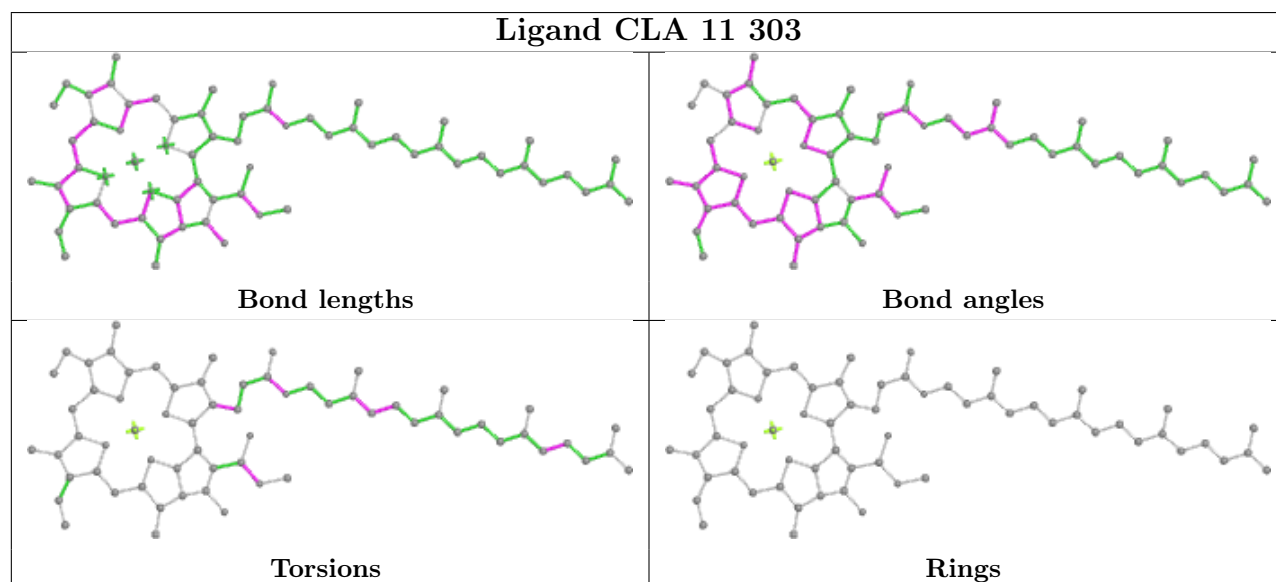
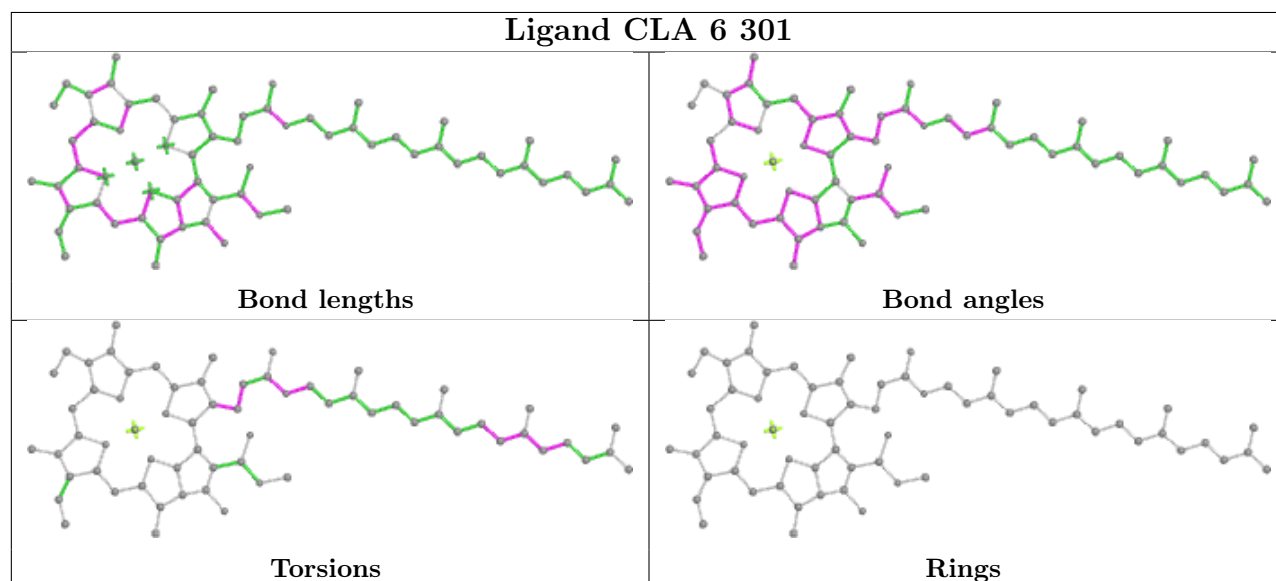
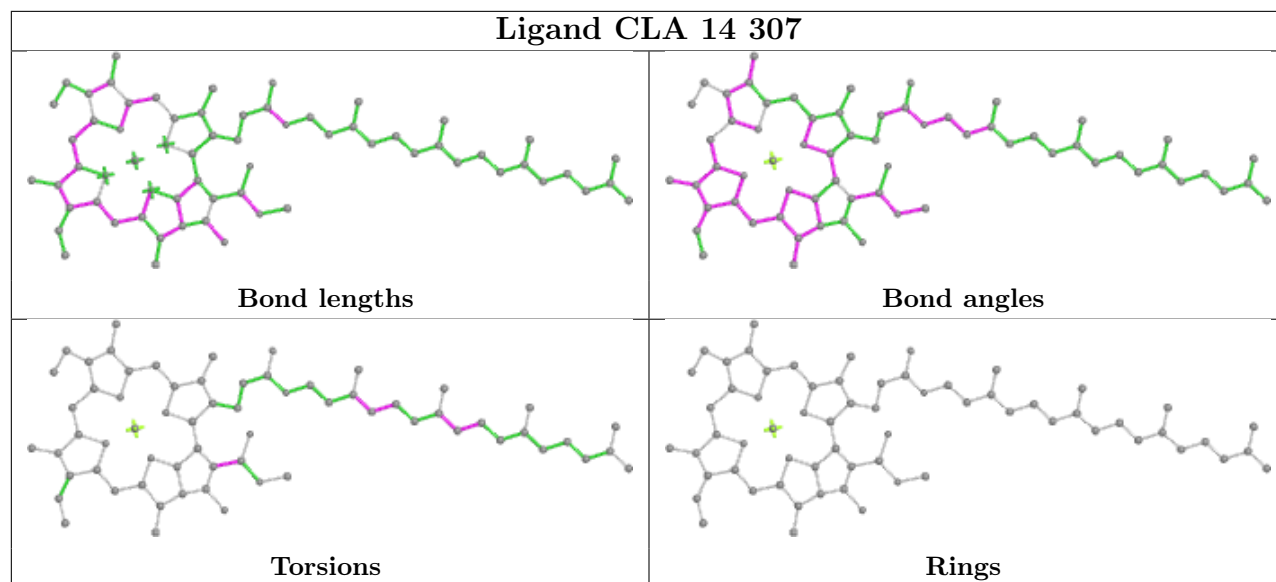
Torsions



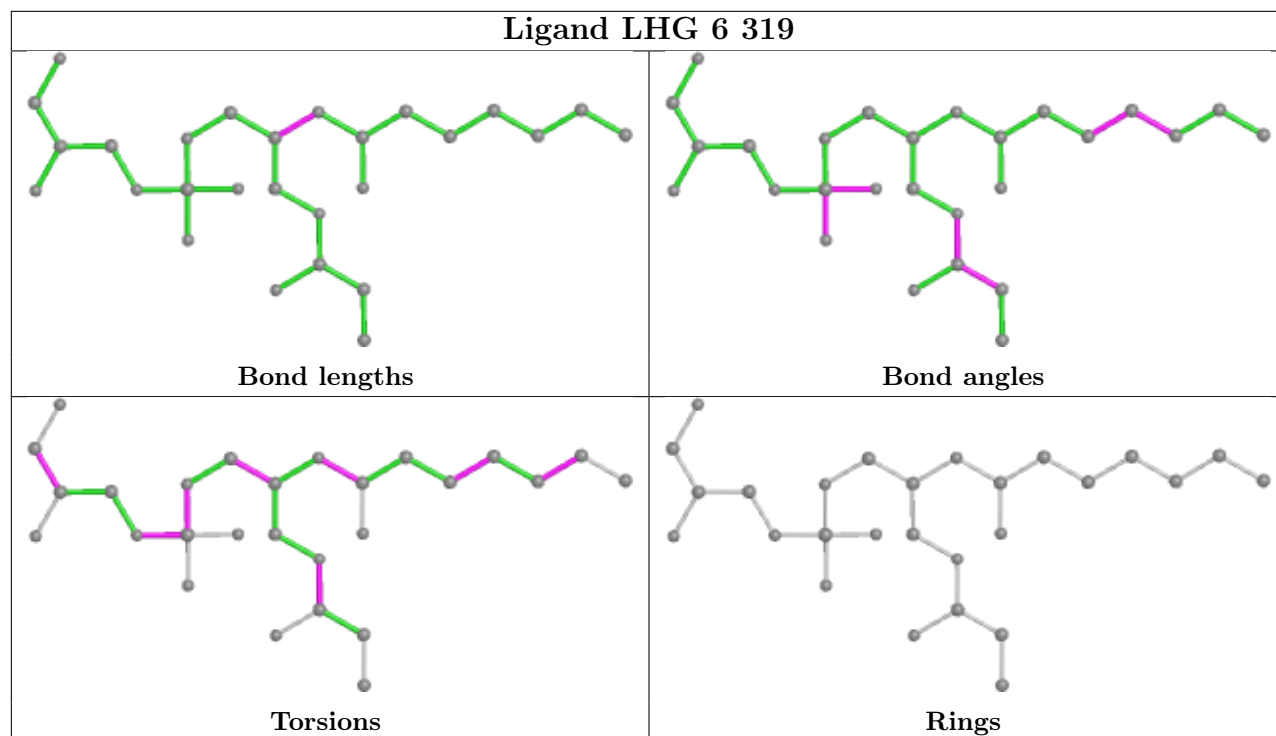
Rings



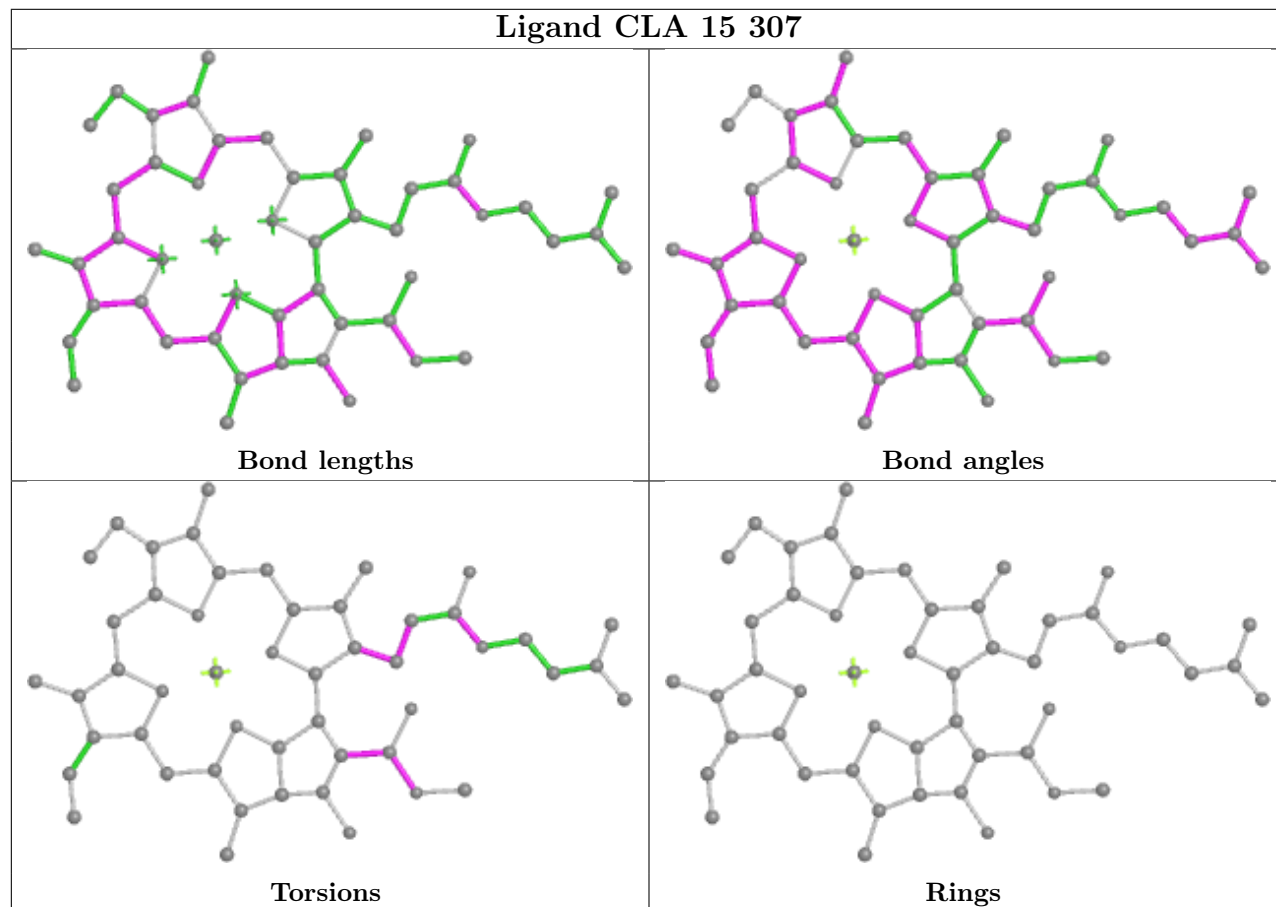


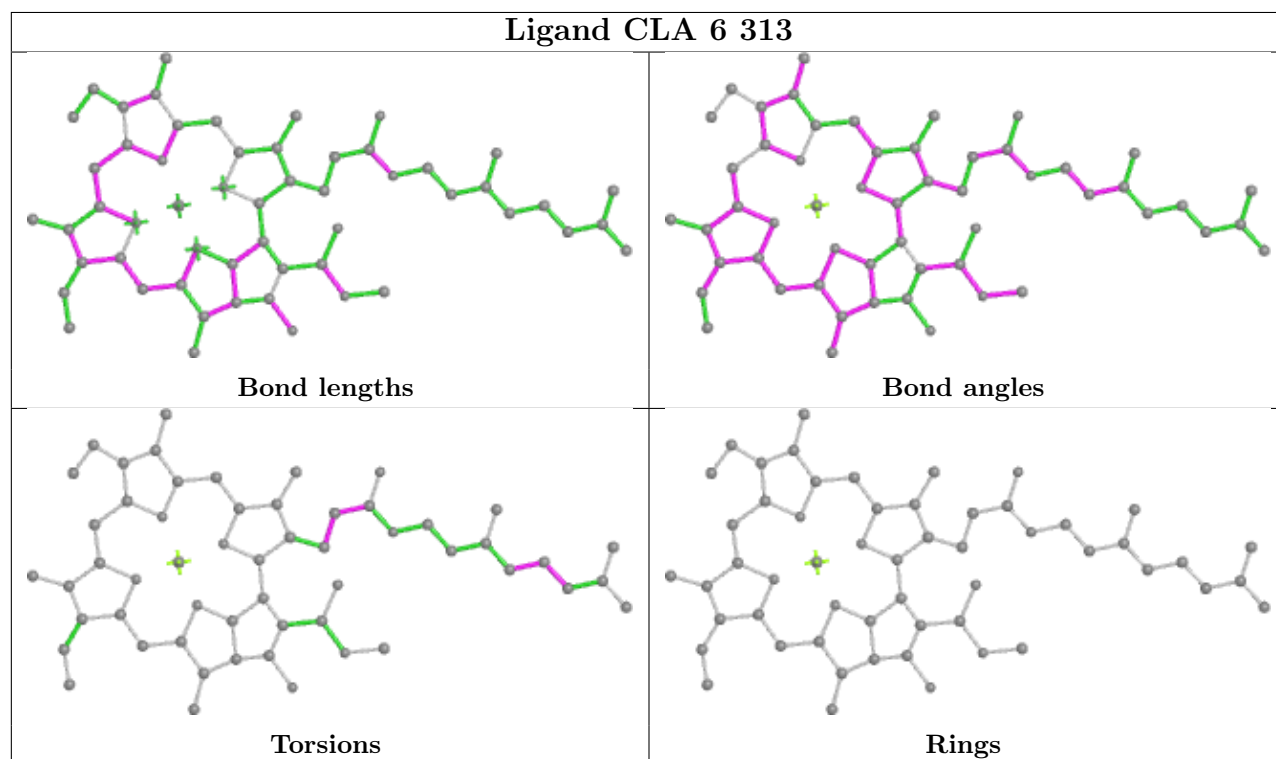
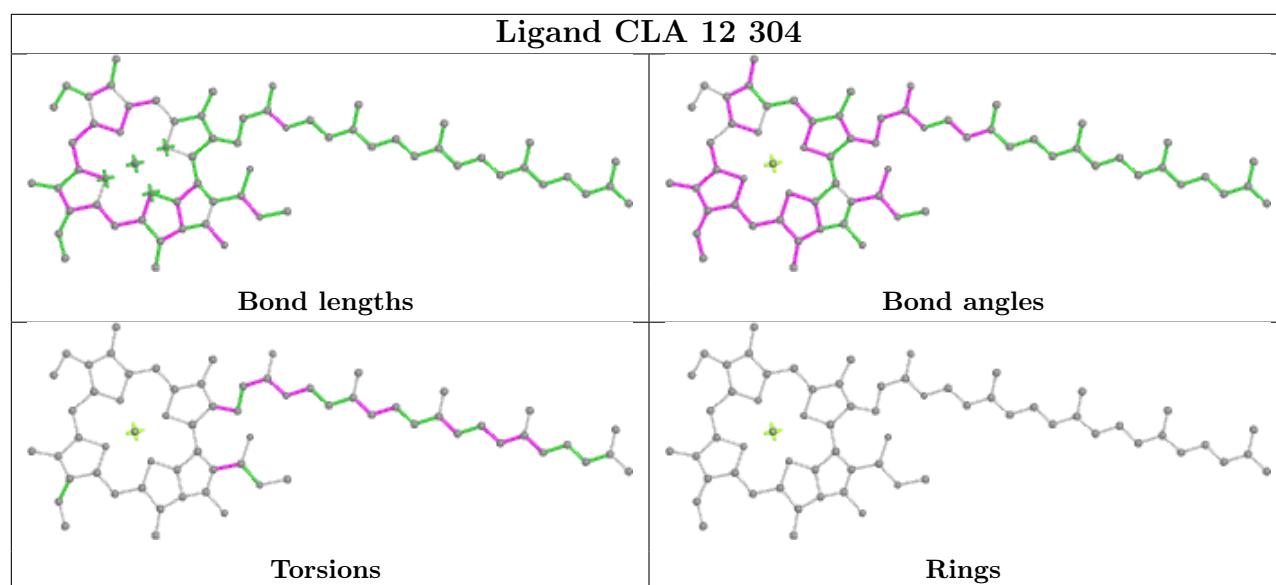


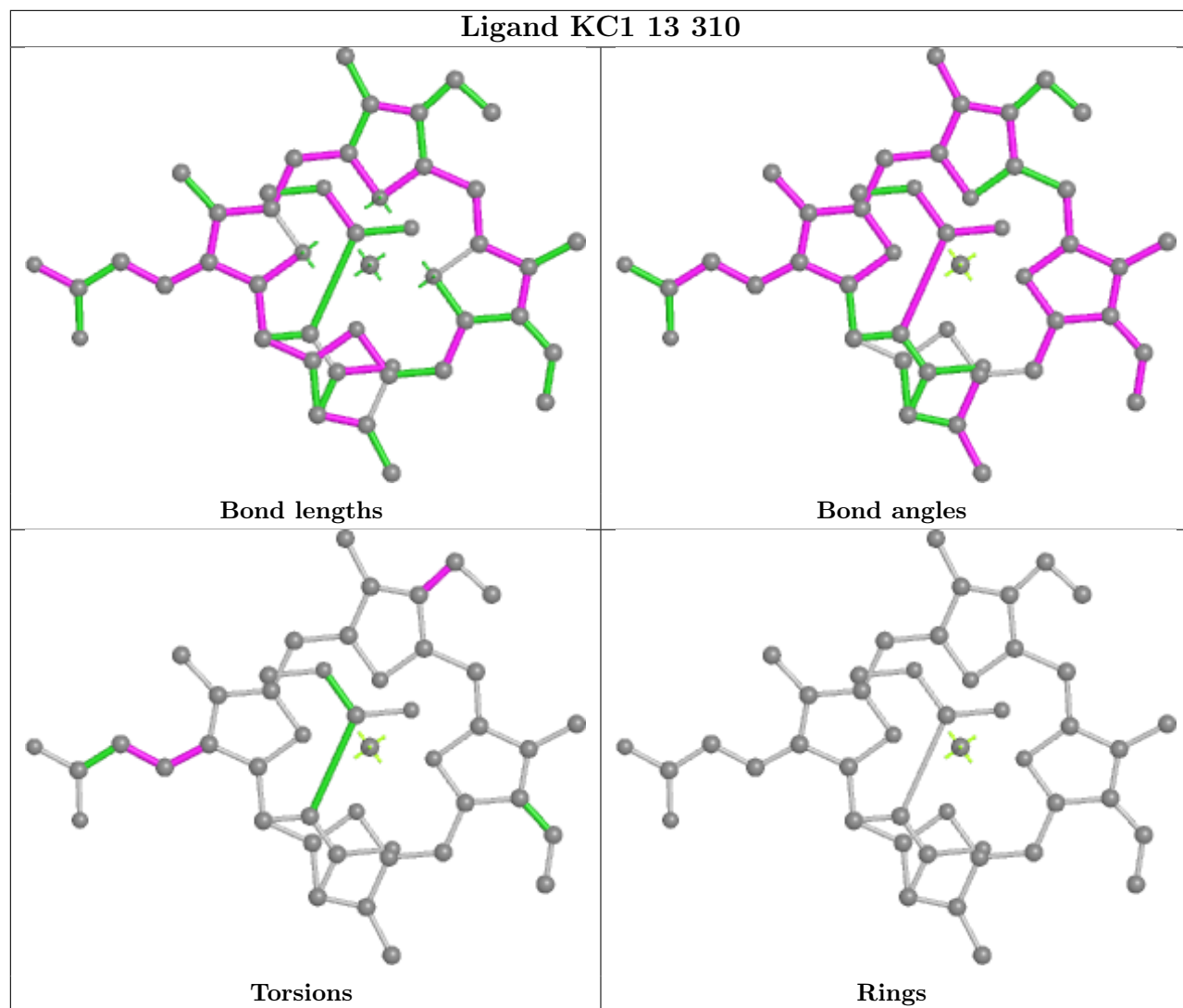
Ligand LHG 6 319

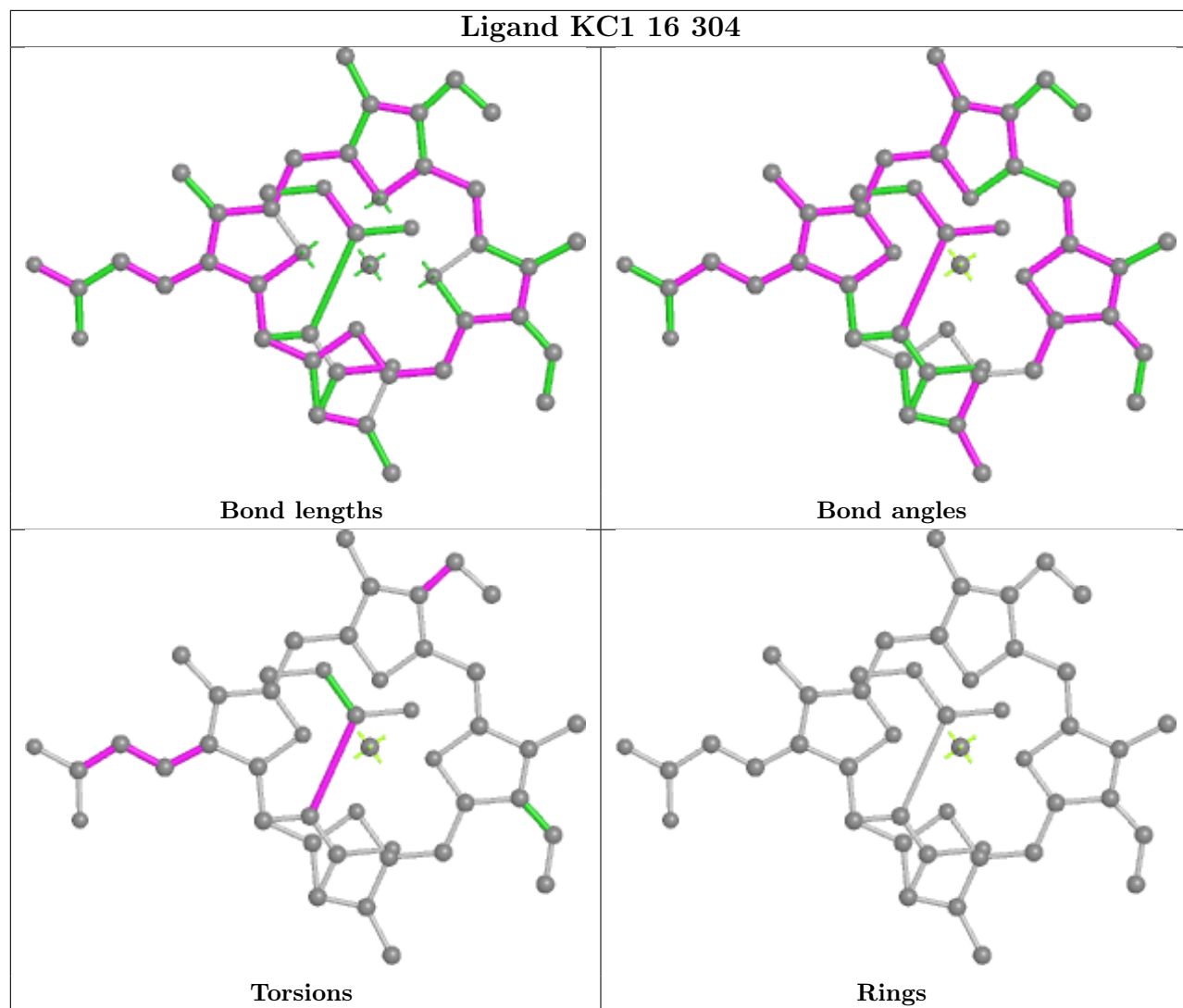


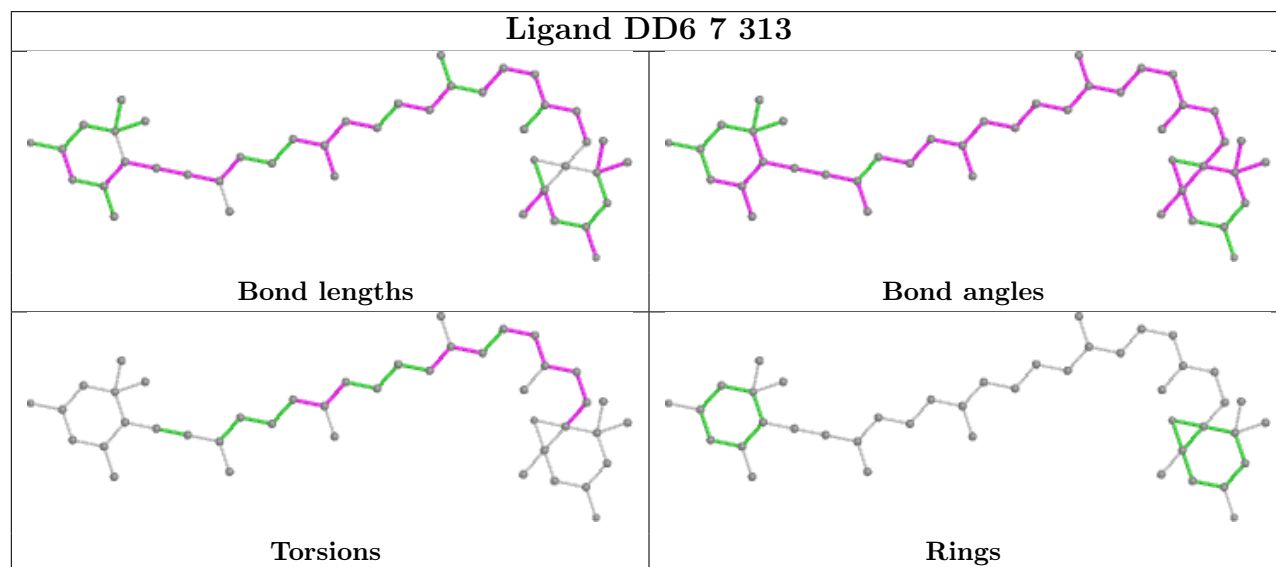
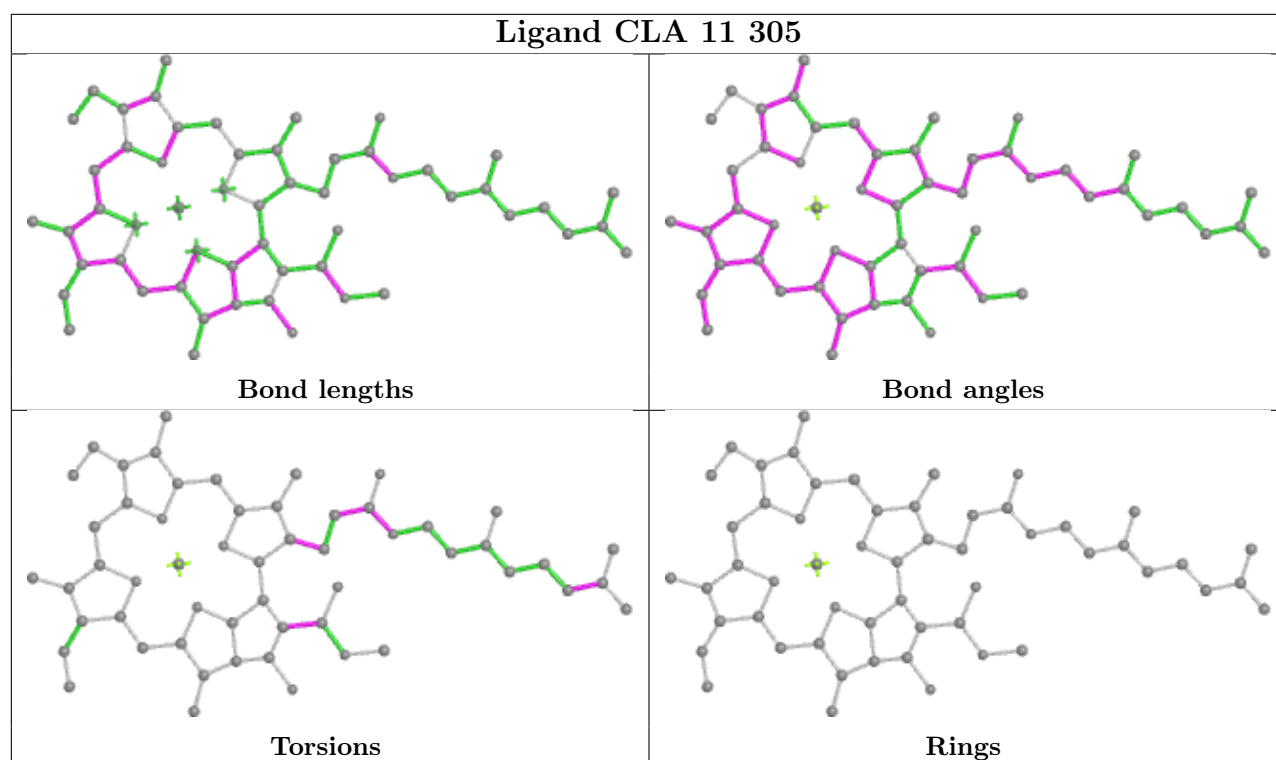
Ligand CLA 15 307

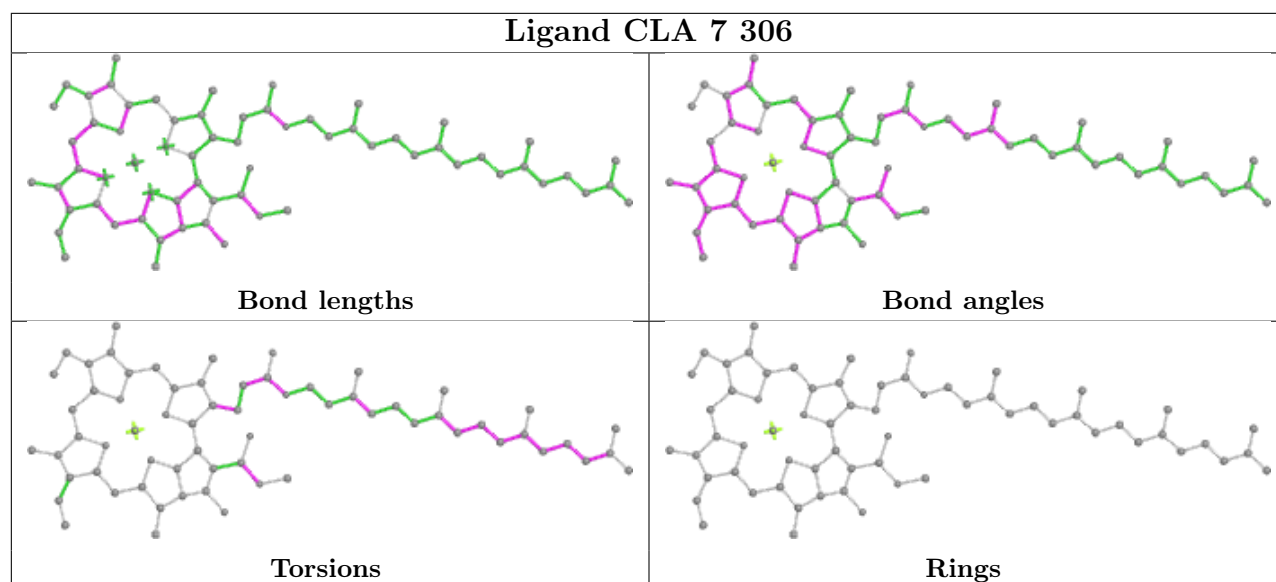
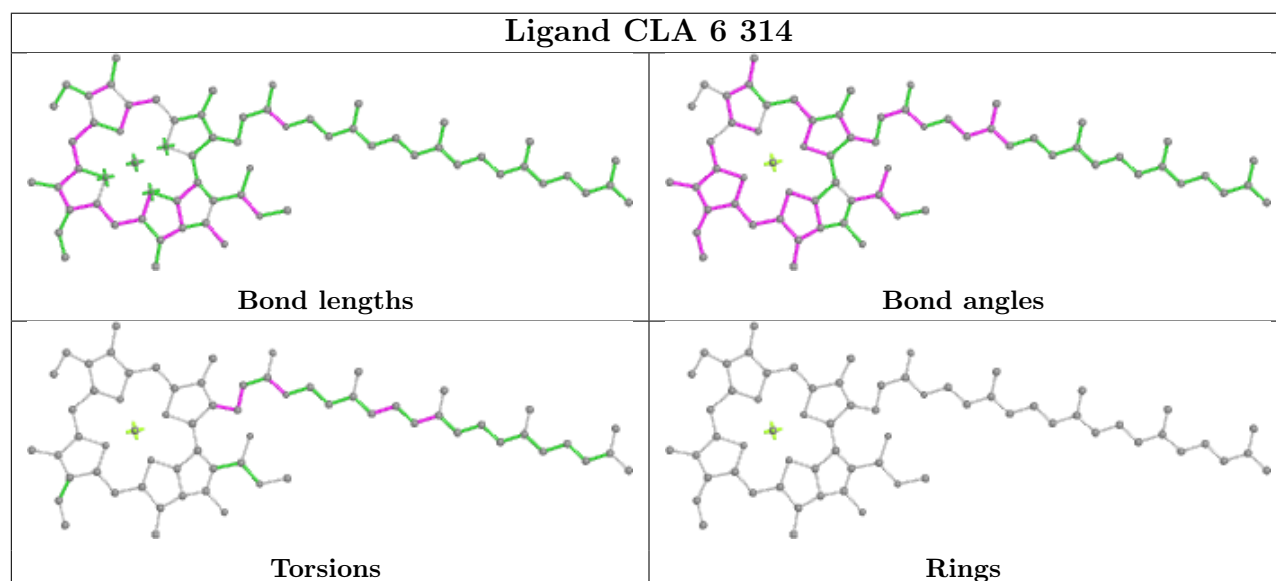
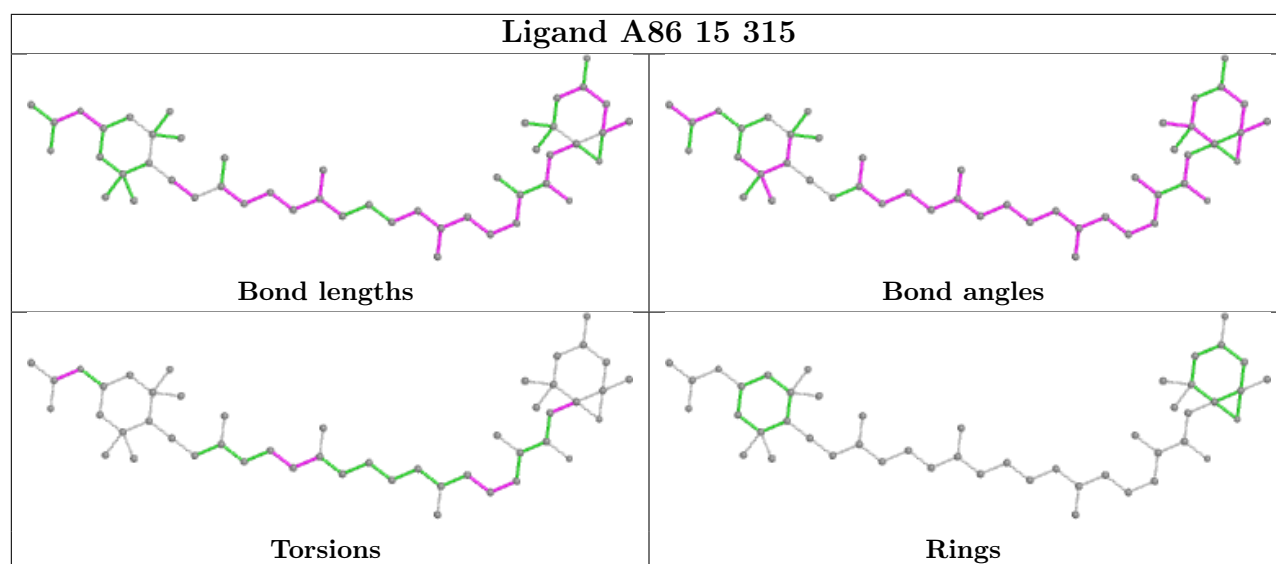




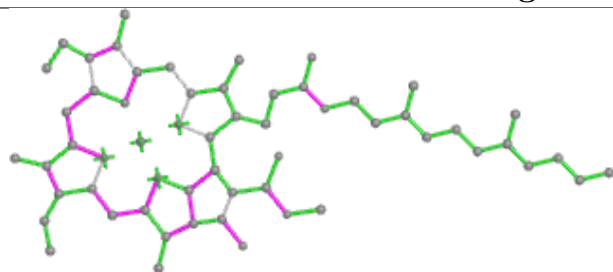




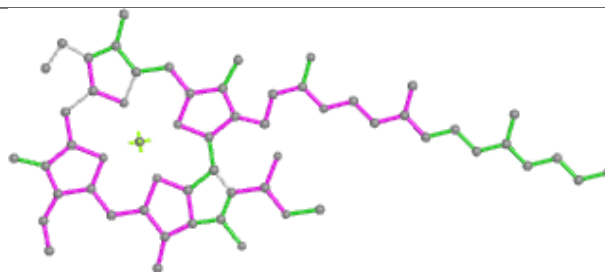




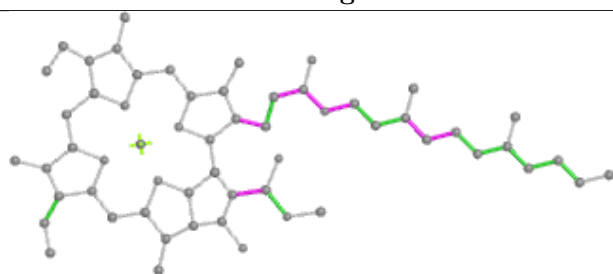
Ligand CLA 8 304



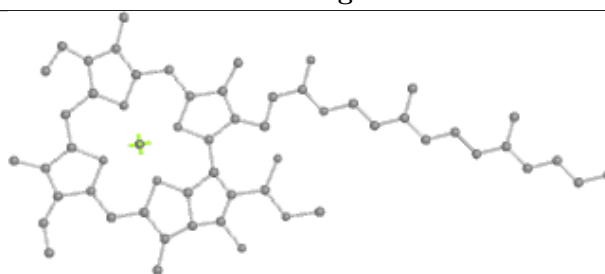
Bond lengths



Bond angles

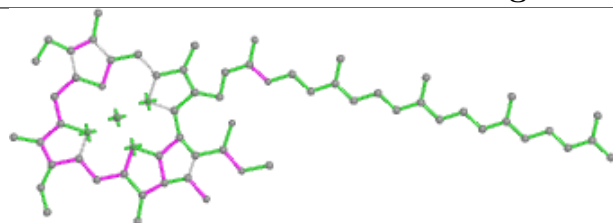


Torsions

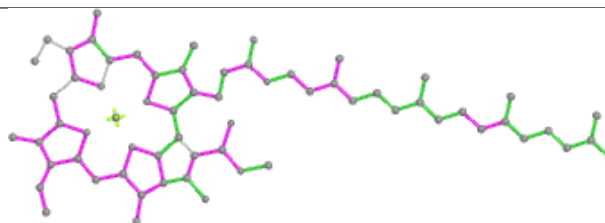


Rings

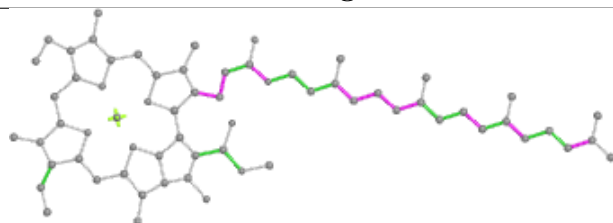
Ligand CLA 15 302



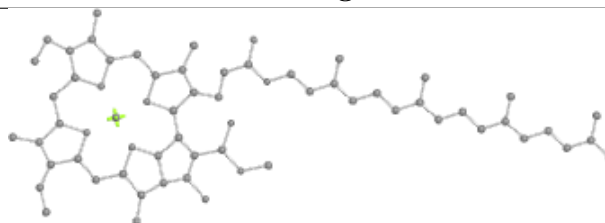
Bond lengths



Bond angles

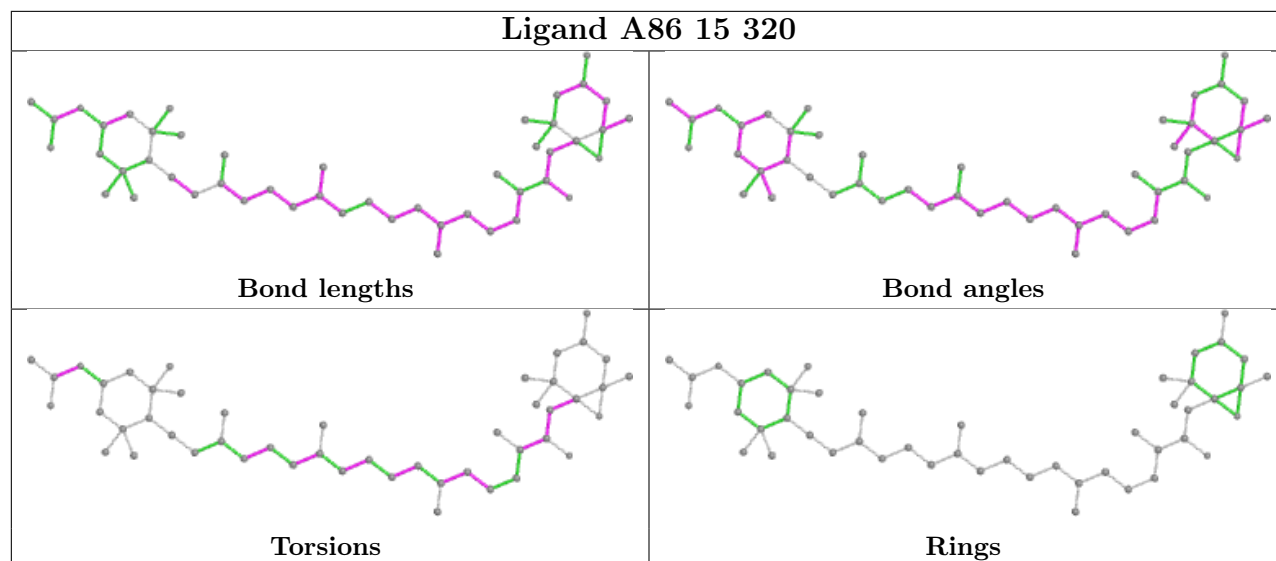


Torsions

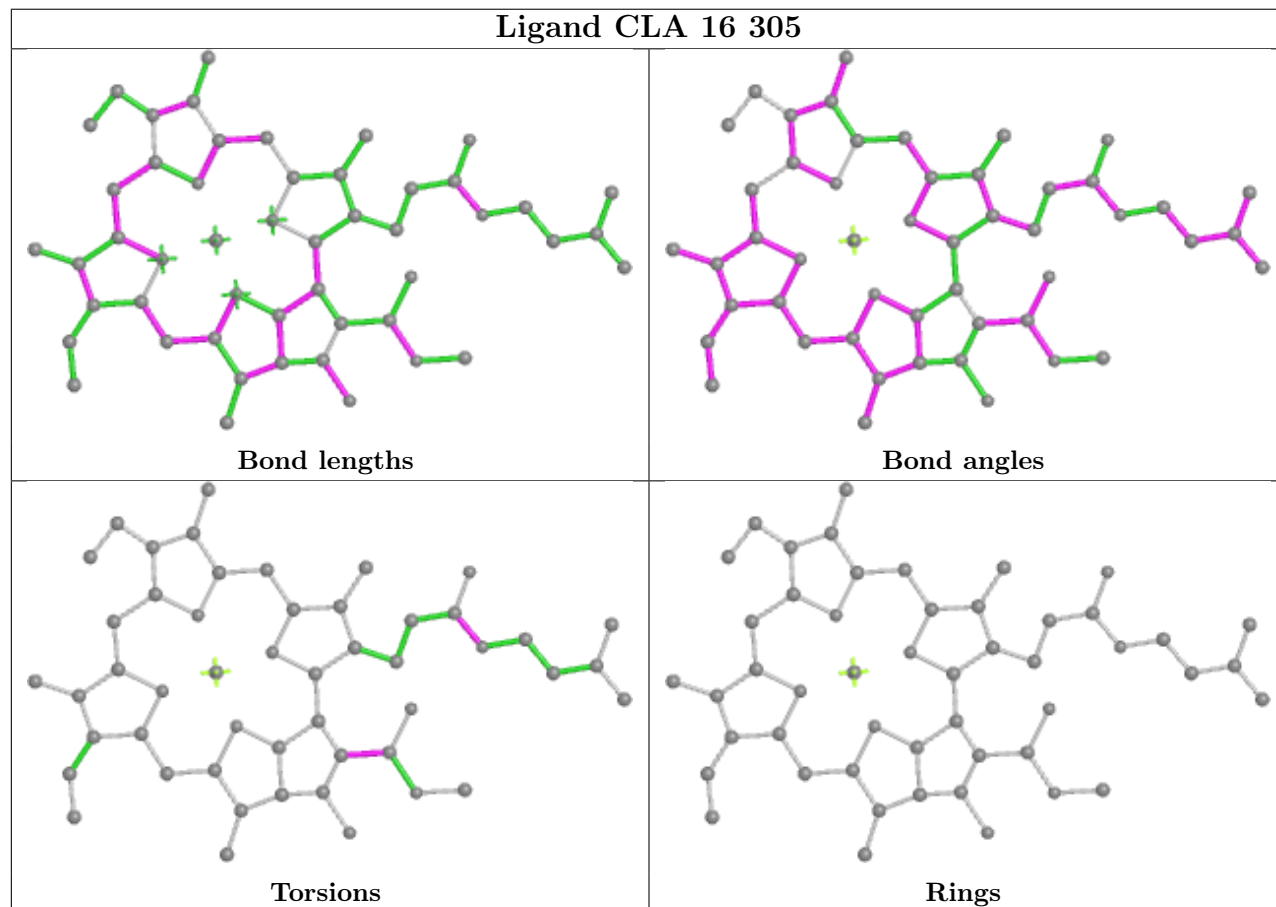


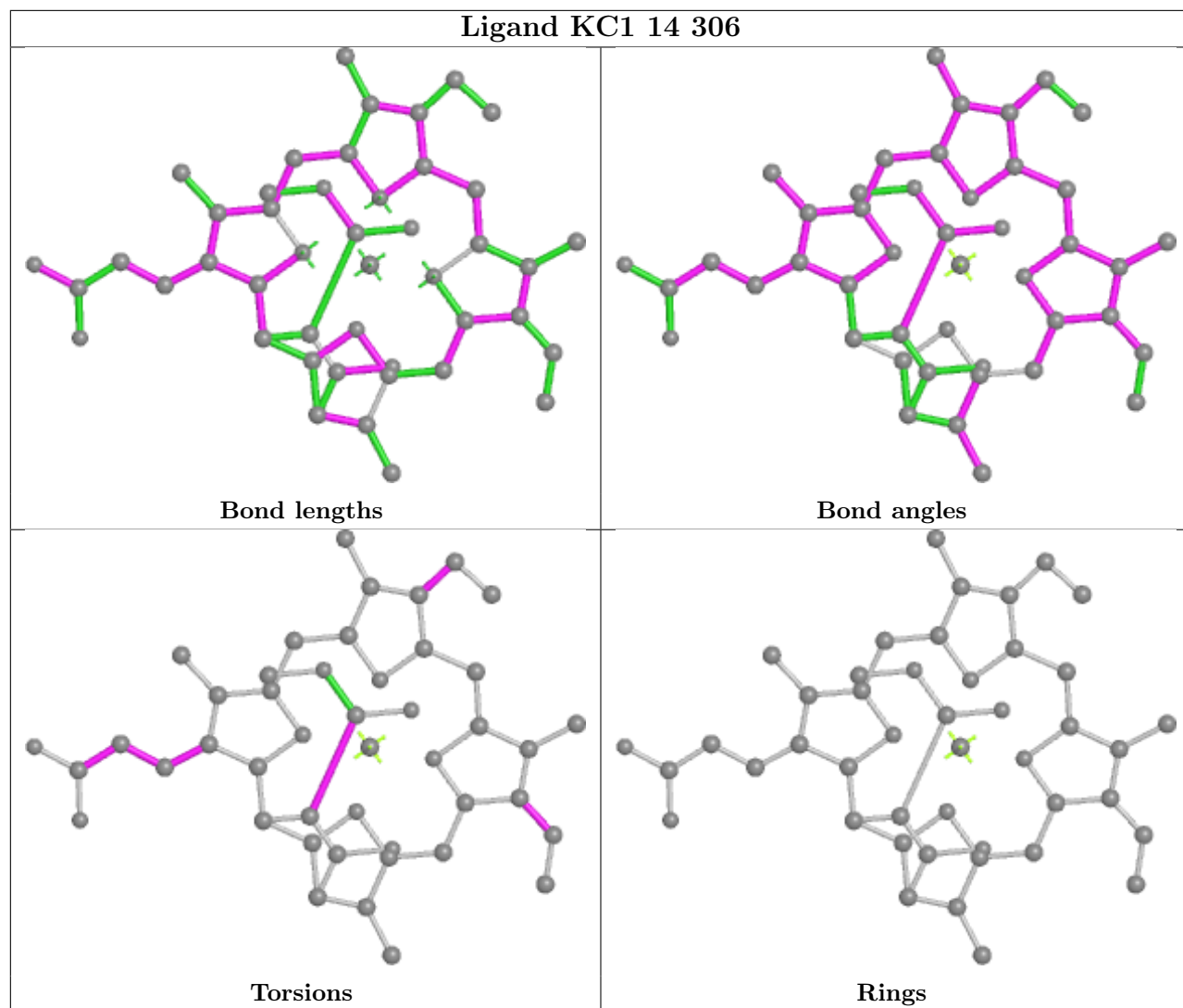
Rings

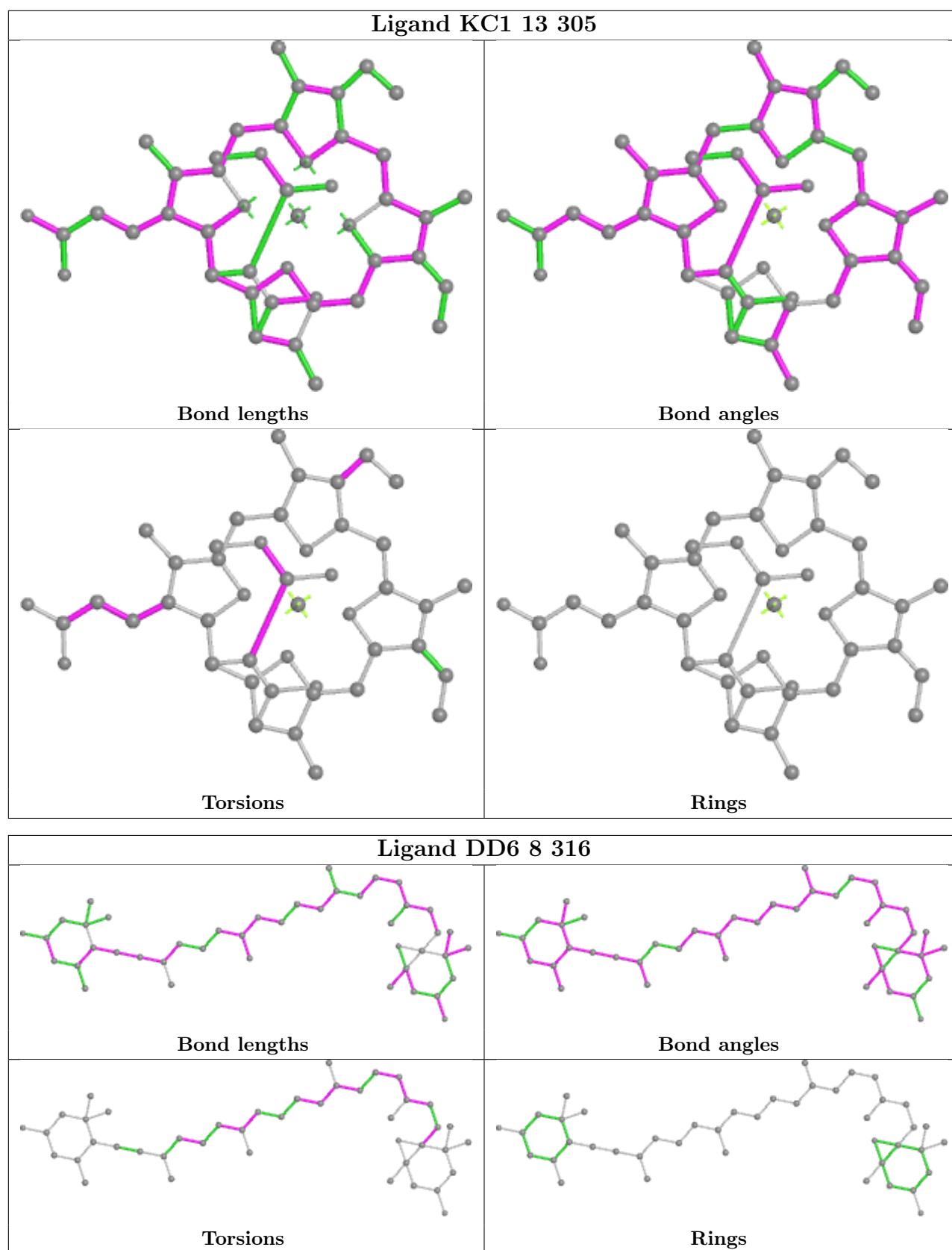
Ligand A86 15 320



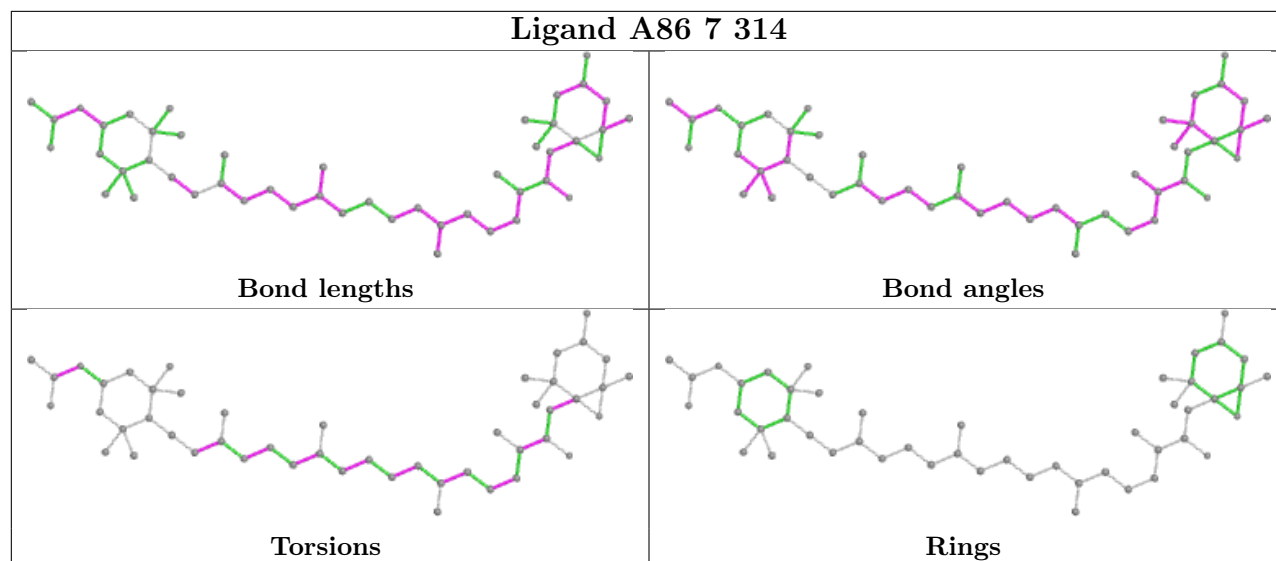
Ligand CLA 16 305



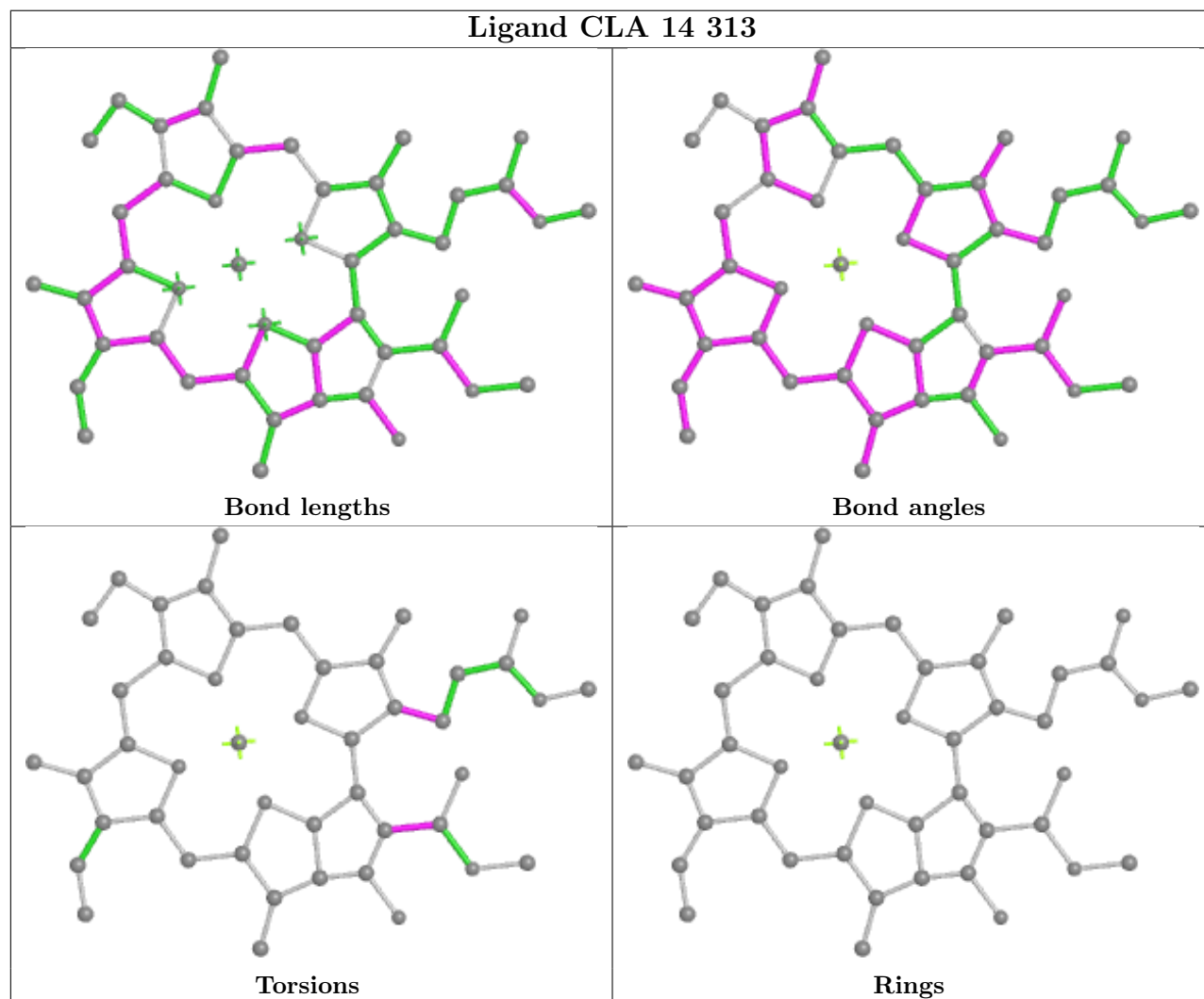


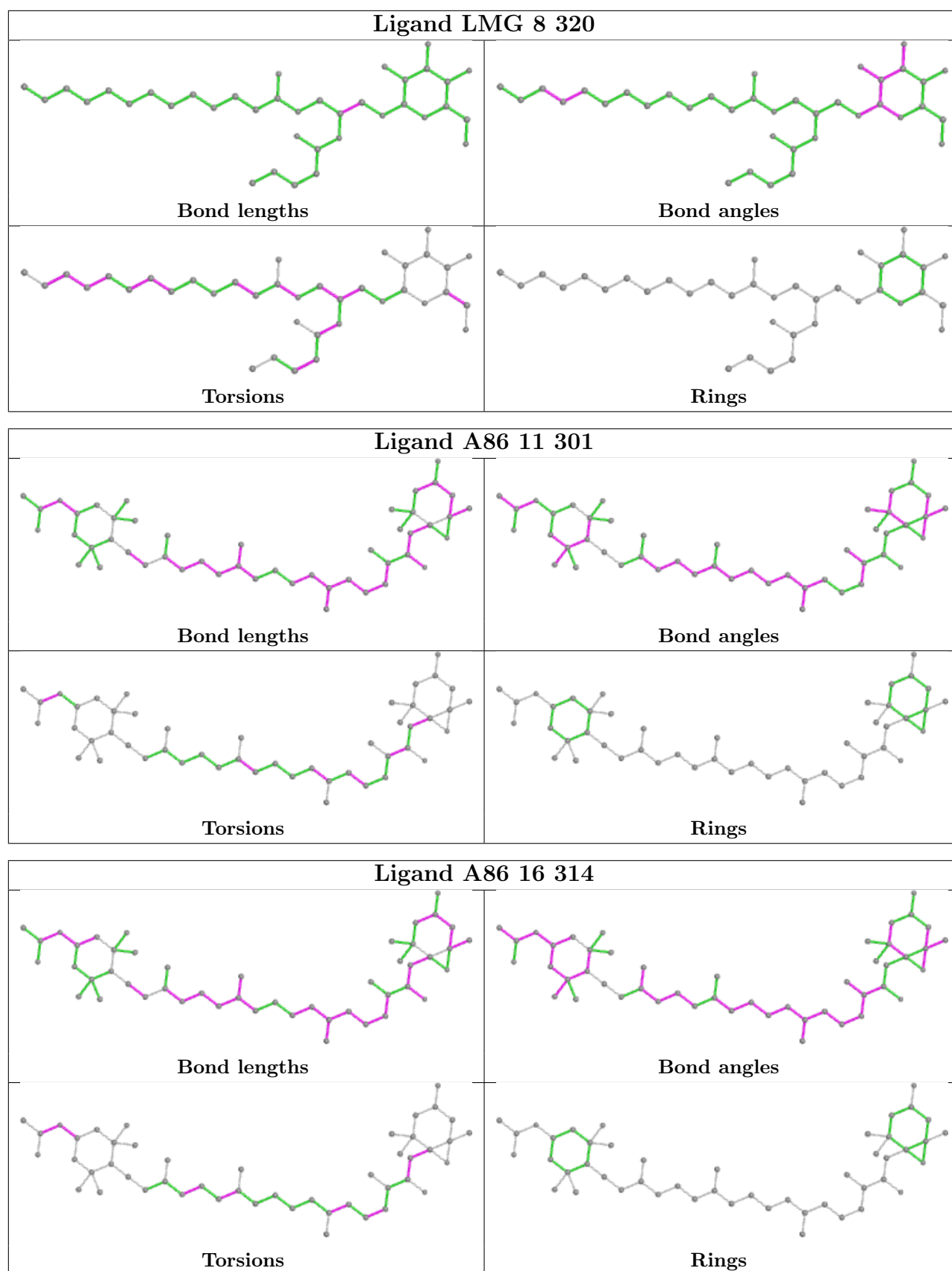


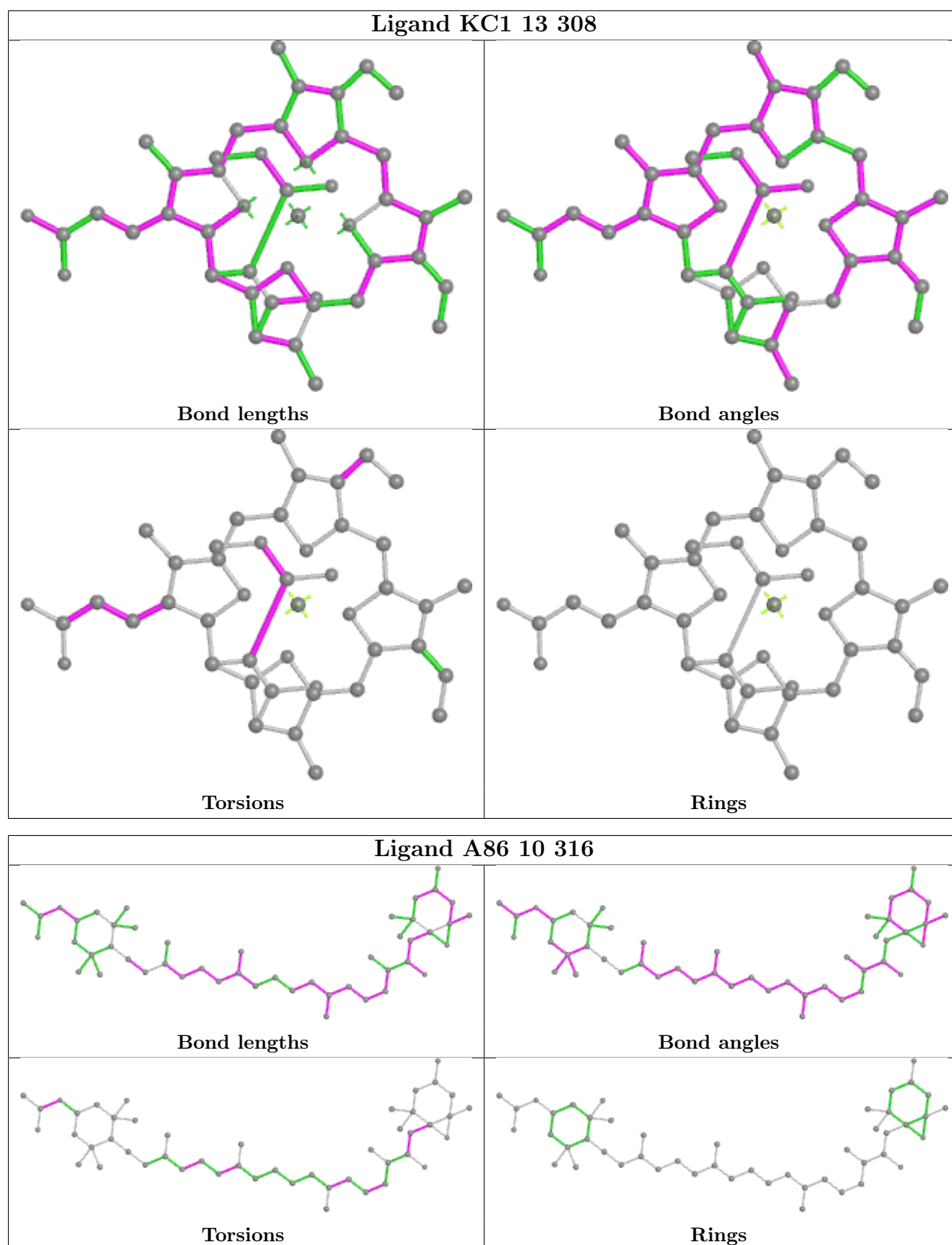
Ligand A86 7 314

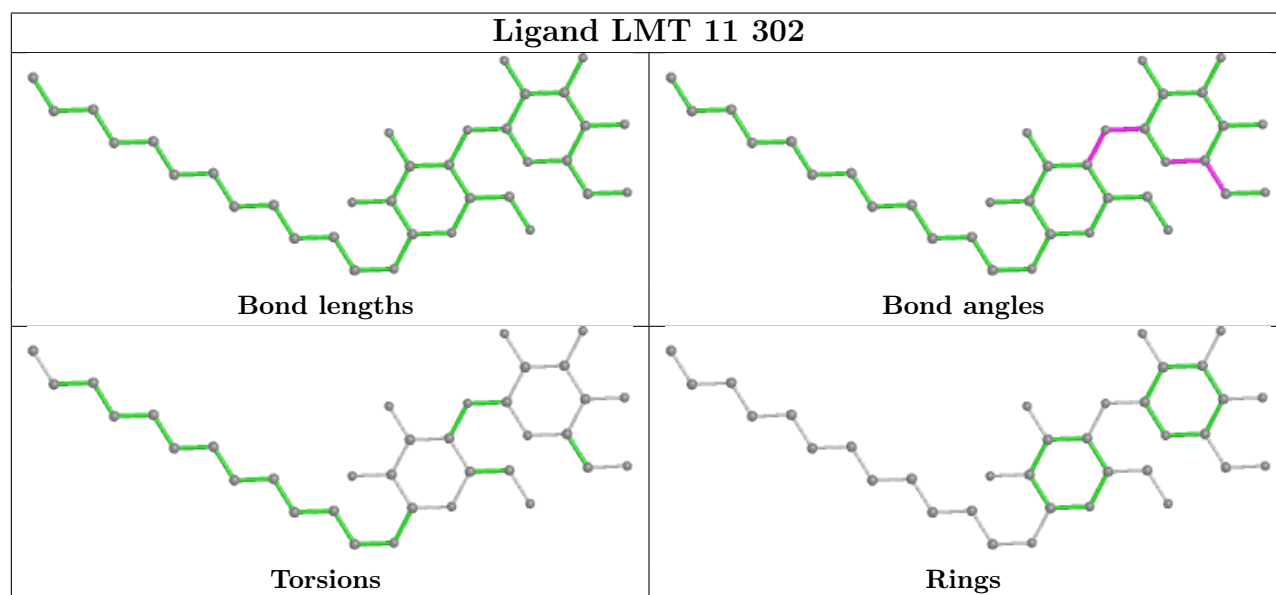
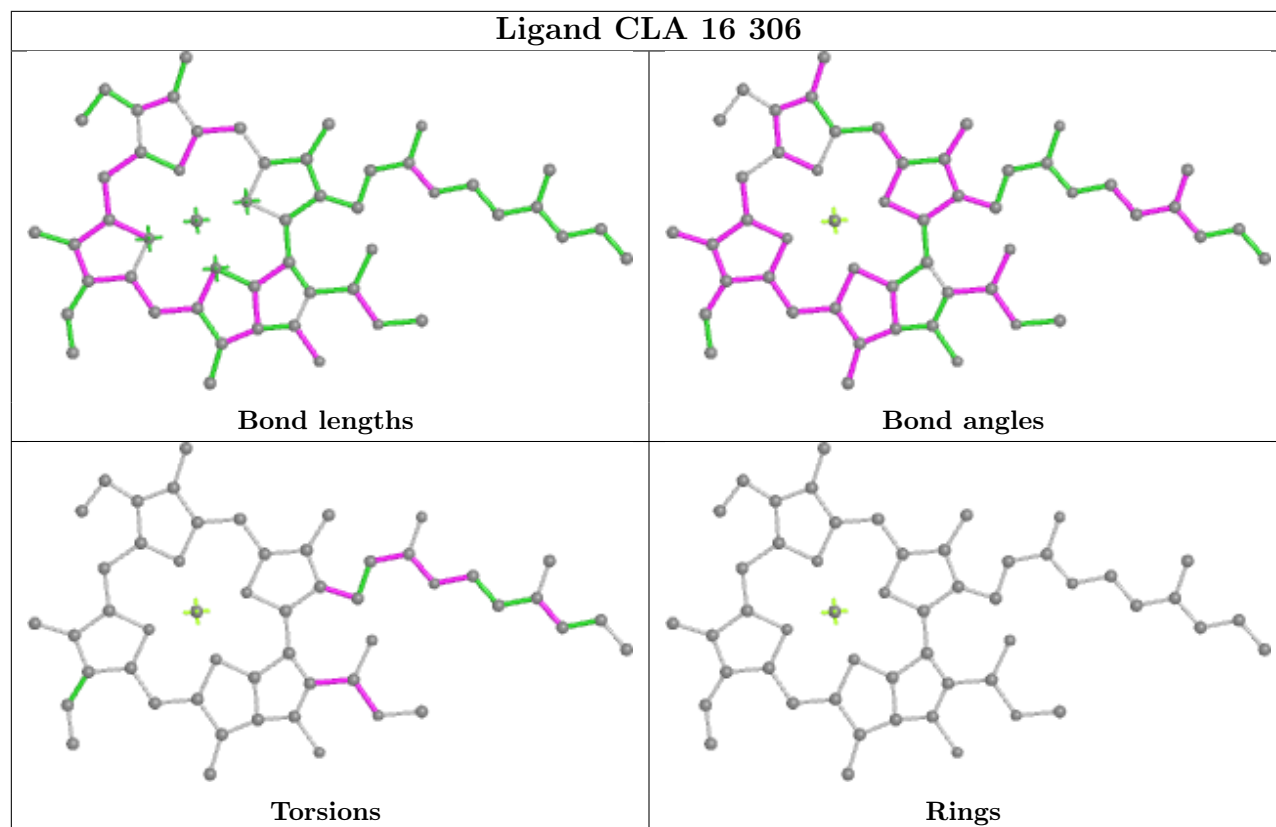


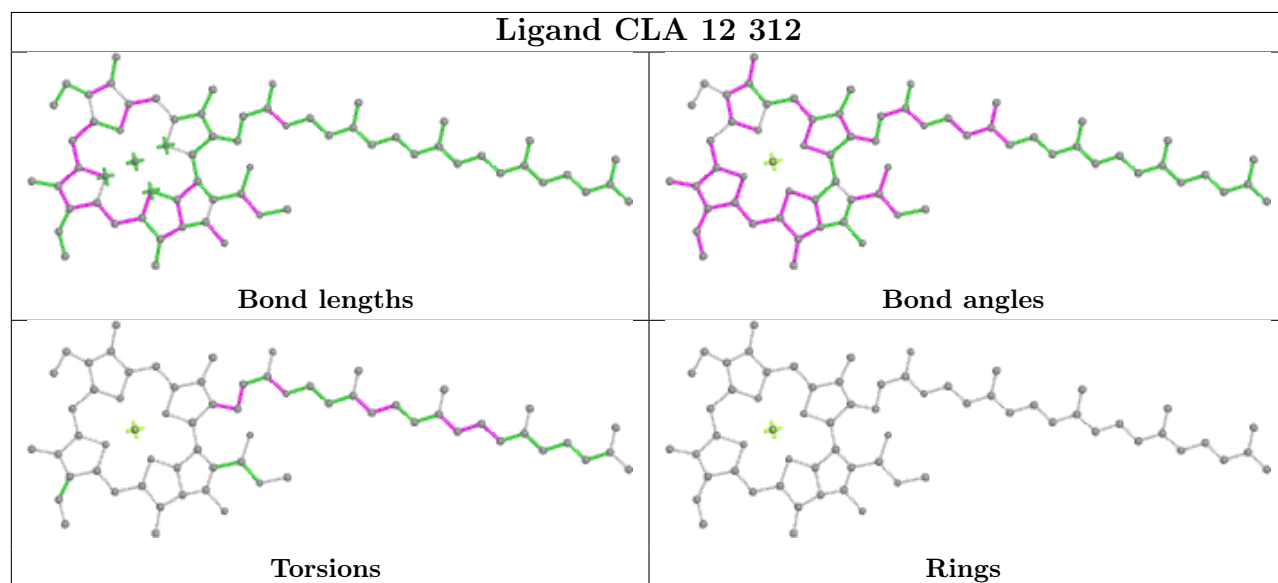
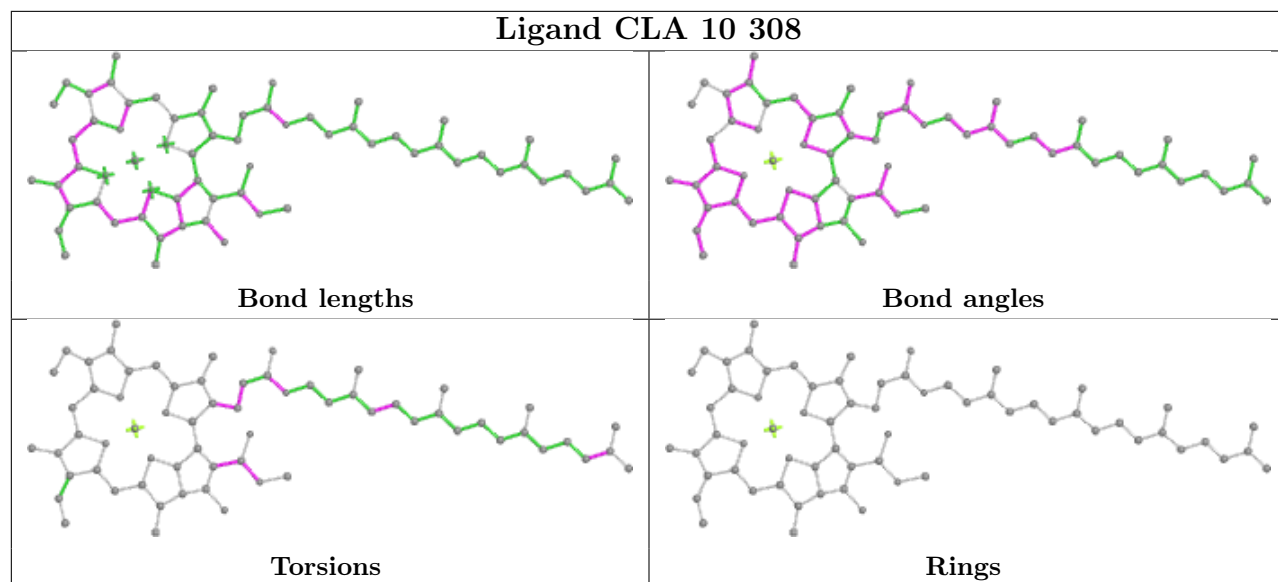
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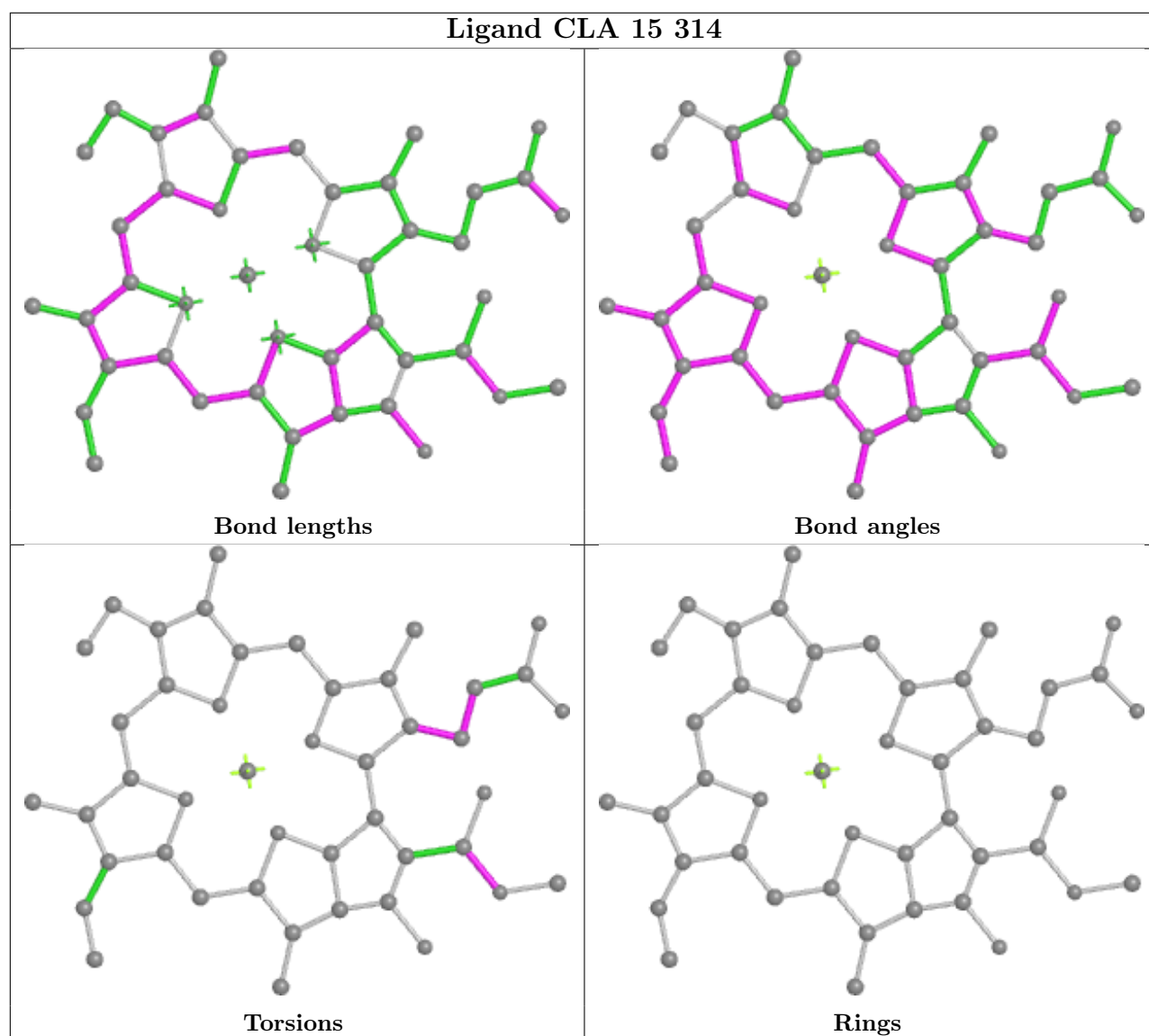




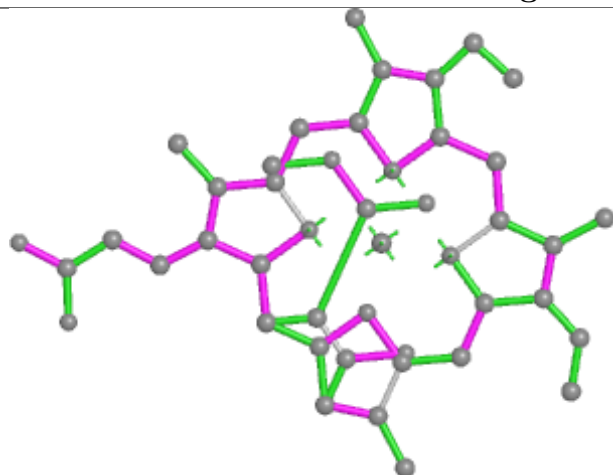




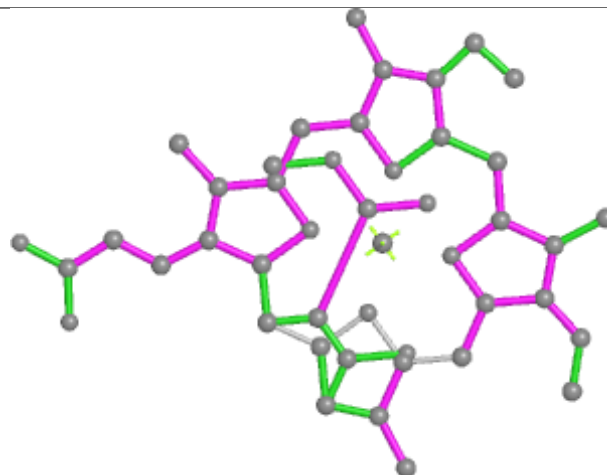




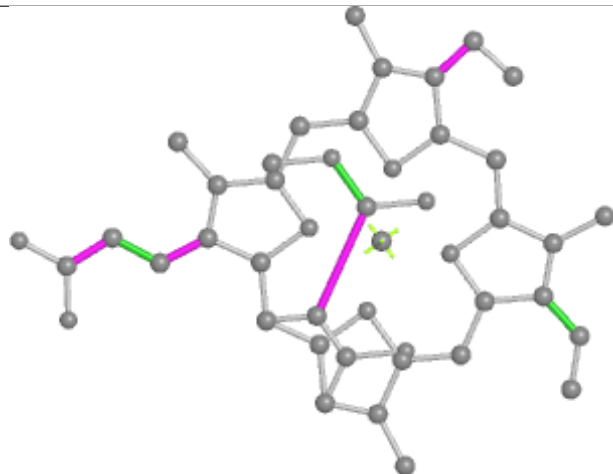
Ligand KC1 8 310



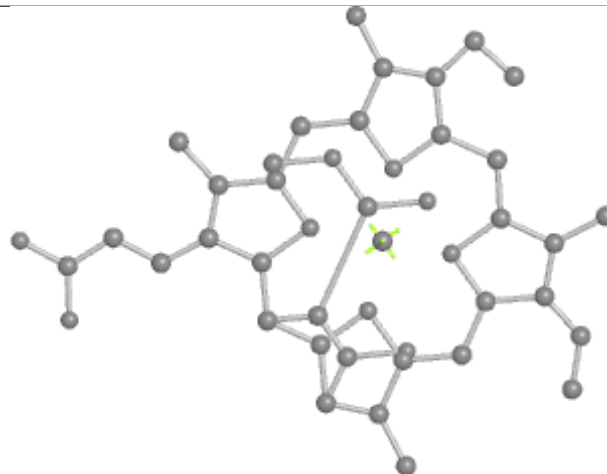
Bond lengths



Bond angles

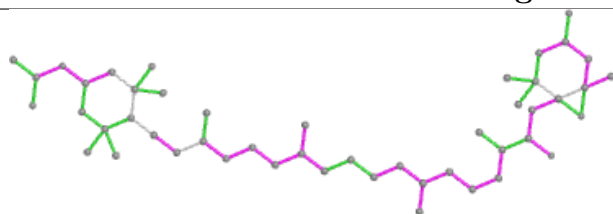


Torsions

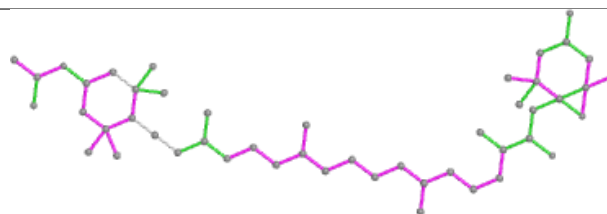


Rings

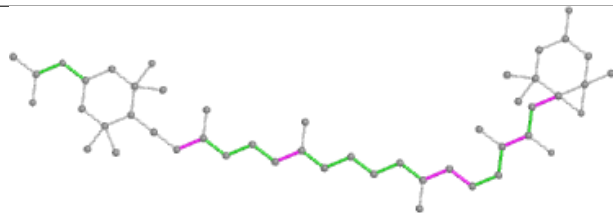
Ligand A86 16 312



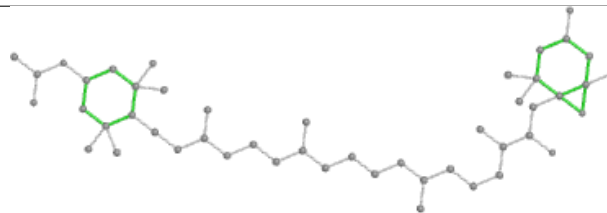
Bond lengths



Bond angles

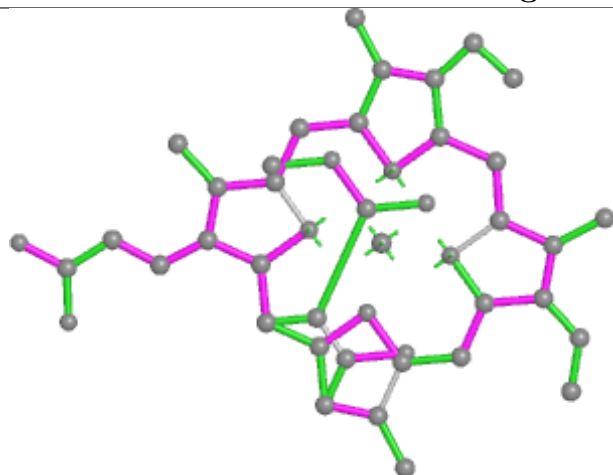


Torsions

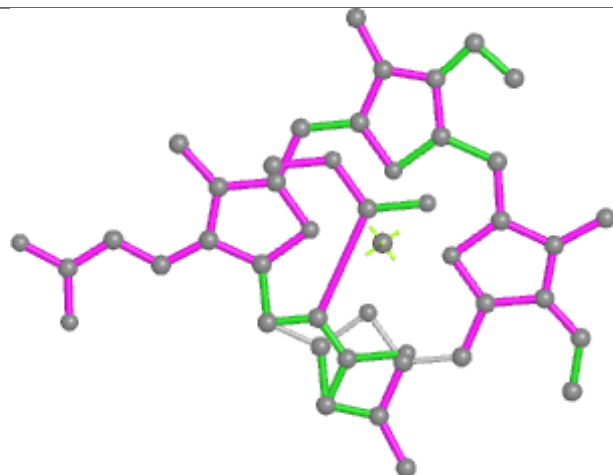


Rings

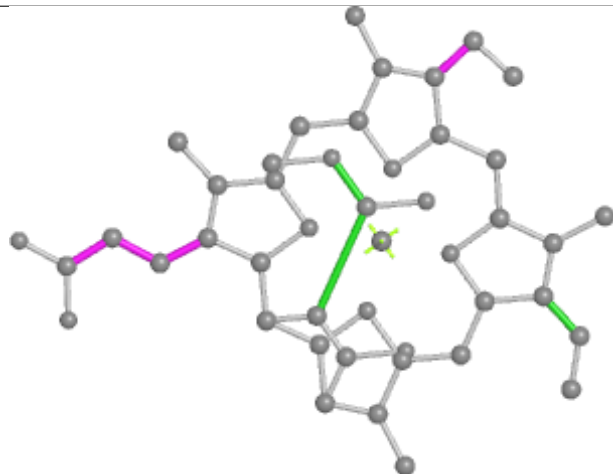
Ligand KC1 8 312



Bond lengths



Bond angles

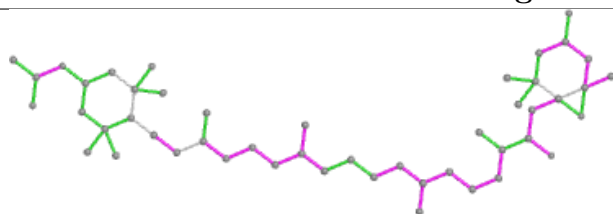


Torsions

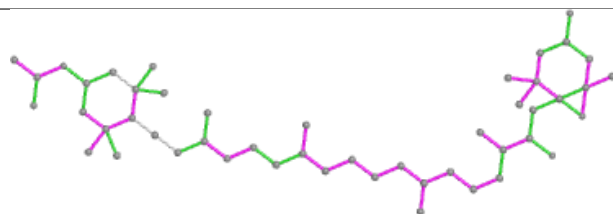


Rings

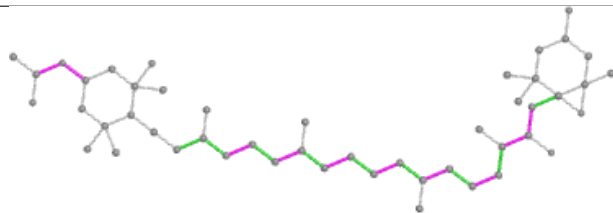
Ligand A86 10 315



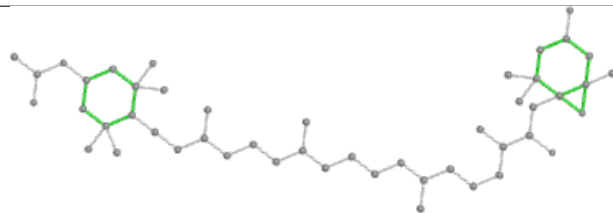
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0834. 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.