



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 03:05 AM UTC

PDB ID : 7VD6 / pdb_00007vd6
EMDB ID : EMD-31906
Title : Structure of S1M1-type FCPH complex from diatom
Authors : Nagao, R.; Kato, K.; Akita, F.; Miyazaki, N.; Shen, J.R.
Deposited on : 2021-09-06
Resolution : 2.80 Å(reported)
Based on initial model : 6J40

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

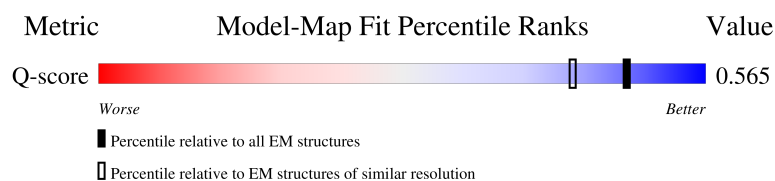
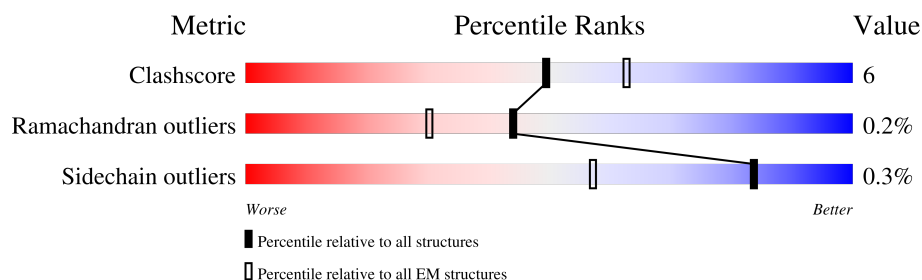
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 Å.

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



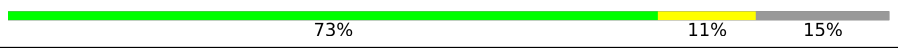
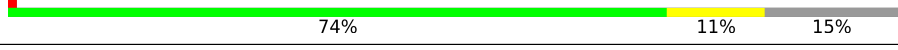
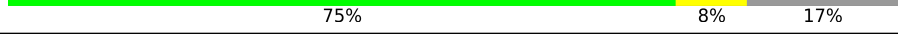
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	11	207	
1	13	207	
1	14	207	
1	15	207	

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Mol	Chain	Length	Quality of chain
1	18	207	
2	12	207	
3	16	210	
4	17	207	
5	19	271	
6	20	223	
7	21	195	

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
8	CLA	11	303	X	-	-	-
8	CLA	11	305	X	-	-	-
8	CLA	11	309	X	-	-	-
8	CLA	12	301	X	-	-	-
8	CLA	12	303	X	-	-	-
8	CLA	12	304	X	-	-	-
8	CLA	12	305	X	-	-	-
8	CLA	12	309	X	-	-	-
8	CLA	12	311	X	-	-	-
8	CLA	13	304	X	-	-	-
8	CLA	13	306	X	-	-	-
8	CLA	13	308	X	-	-	-
8	CLA	14	302	X	-	-	-
8	CLA	14	305	X	-	-	-
8	CLA	14	307	X	-	-	-
8	CLA	14	308	X	-	-	-
8	CLA	14	310	X	-	-	-
8	CLA	15	303	X	-	-	-
8	CLA	15	305	X	-	-	-
8	CLA	15	307	X	-	-	-
8	CLA	15	308	X	-	-	-
8	CLA	15	310	X	-	-	-
8	CLA	16	303	X	-	-	-
8	CLA	16	306	X	-	-	-
8	CLA	16	307	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	CLA	16	309	X	-	-	-
8	CLA	17	304	X	-	-	-
8	CLA	17	307	X	-	-	-
8	CLA	17	308	X	-	-	-
8	CLA	17	310	X	-	-	-
8	CLA	18	302	X	-	-	-
8	CLA	18	303	X	-	-	-
8	CLA	18	305	X	-	-	-
8	CLA	18	307	X	-	-	-
8	CLA	18	308	X	-	-	-
8	CLA	19	301	X	-	-	-
8	CLA	19	302	X	-	-	-
8	CLA	19	303	X	-	-	-
8	CLA	19	304	X	-	-	-
8	CLA	19	305	X	-	-	-
8	CLA	19	306	X	-	-	-
8	CLA	19	307	X	-	-	-
8	CLA	19	309	X	-	-	-
8	CLA	19	310	X	-	-	-
8	CLA	20	304	X	-	-	-
8	CLA	20	307	X	-	-	-
8	CLA	20	308	X	-	-	-
8	CLA	20	309	X	-	-	-
8	CLA	20	310	X	-	-	-
8	CLA	21	202	X	-	-	-
8	CLA	21	204	X	-	-	-
8	CLA	21	205	X	-	-	-
8	CLA	21	206	X	-	-	-
8	CLA	21	208	X	-	-	-
8	CLA	21	209	X	-	-	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 23937 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 Chlorophyll a/b-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	11	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
1	13	169	Total	C	N	O	S	0	0
			1296	823	220	246	7		
1	14	172	Total	C	N	O	S	0	0
			1319	838	223	251	7		
1	15	170	Total	C	N	O	S	0	0
			1307	832	221	247	7		
1	18	168	Total	C	N	O	S	0	0
			1289	818	219	245	7		

- Molecule 2 is a protein called Fcpb2, Fucoxanthin chlorophyll a/c-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	12	169	Total	C	N	O	S	0	0
			1302	828	222	244	8		

- Molecule 3 is a protein called Fcpb3, Fucoxanthin chlorophyll a/c-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	16	179	Total	C	N	O	S	0	0
			1386	891	233	256	6		

- Molecule 4 is a protein called Fcpb4, Fucoxanthin chlorophyll a/c-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	17	176	Total	C	N	O	S	0	0
			1353	862	227	258	6		

- Molecule 5 is a protein called Fcpb5, Fucoxanthin chlorophyll a/c-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	19	220	Total	C	N	O	S	0	0
			1690	1088	283	314	5		

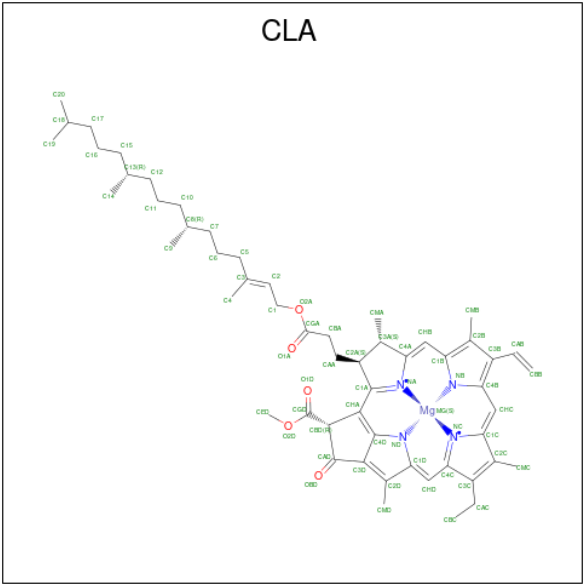
- Molecule 6 is a protein called Fcpb6, Fucoxanthin chlorophyll a/c-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	20	155	Total	C	N	O	S	0	0
			1198	773	202	215	8		

- Molecule 7 is a protein called Fcpb7, Fucoxanthin chlorophyll a/c-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	21	162	Total	C	N	O	S	0	0
			1262	822	206	229	5		

- Molecule 8 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
8	11	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	11	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
8	11	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
8	11	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
8	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	12	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
8	12	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
8	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
8	13	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	13	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	13	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
8	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
8	13	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
8	13	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
8	14	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	14	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	14	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
8	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
8	14	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
8	14	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
8	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
8	15	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	15	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
8	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
8	15	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
8	15	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
8	16	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	16	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
8	16	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	16	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
8	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
8	17	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	17	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
8	17	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
8	17	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	17	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	18	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	18	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	18	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
8	18	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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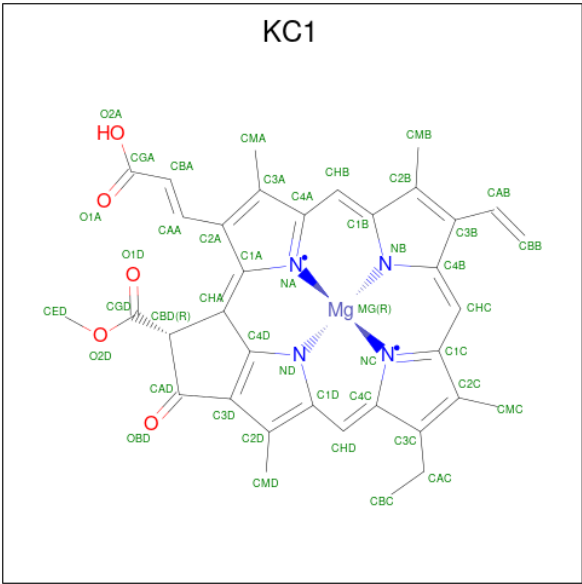
Mol	Chain	Residues	Atoms					AltConf
8	18	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
8	18	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	18	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
8	19	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	19	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	19	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	19	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
8	19	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
8	19	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	19	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	19	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
8	19	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	20	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
8	20	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
8	20	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
8	20	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
8	20	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
8	20	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
8	21	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
8	21	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
8	21	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
8	21	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	21	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	21	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
8	21	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 9 is Chlorophyll c1 (CCD ID: KC1) (formula: C₃₅H₃₀MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
9	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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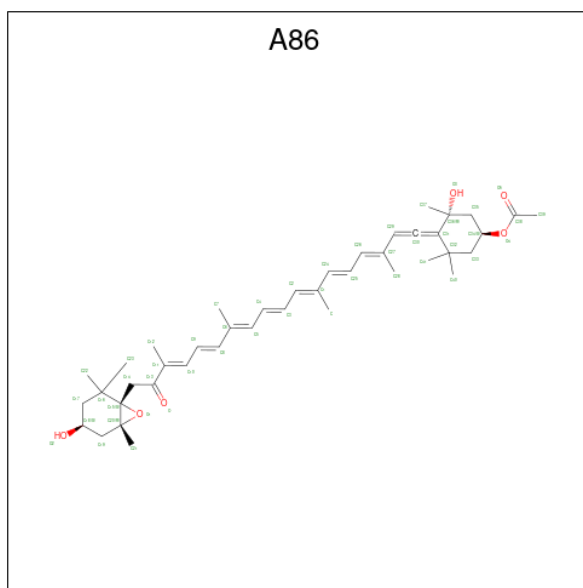
Mol	Chain	Residues	Atoms					AltConf
9	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
9	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
9	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
9	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
9	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
9	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
9	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
9	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
9	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
9	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
9	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
9	16	1	Total 45	C 35	Mg 1	N 4	O 5	0
9	16	1	Total 45	C 35	Mg 1	N 4	O 5	0
9	16	1	Total 45	C 35	Mg 1	N 4	O 5	0
9	16	1	Total 45	C 35	Mg 1	N 4	O 5	0
9	17	1	Total 45	C 35	Mg 1	N 4	O 5	0
9	17	1	Total 45	C 35	Mg 1	N 4	O 5	0
9	17	1	Total 45	C 35	Mg 1	N 4	O 5	0
9	17	1	Total 45	C 35	Mg 1	N 4	O 5	0
9	18	1	Total 45	C 35	Mg 1	N 4	O 5	0
9	18	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
9	18	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	19	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	20	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	20	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	20	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	21	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	21	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 10 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: $C_{42}H_{58}O_6$).



Mol	Chain	Residues	Atoms			AltConf
10	11	1	Total	C	O	0
			48	42	6	
10	11	1	Total	C	O	0
			48	42	6	
10	11	1	Total	C	O	0
			48	42	6	
10	11	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
10	11	1	Total	C	O	0
			48	42	6	
10	11	1	Total	C	O	0
			48	42	6	
10	12	1	Total	C	O	0
			48	42	6	
10	12	1	Total	C	O	0
			48	42	6	
10	12	1	Total	C	O	0
			48	42	6	
10	12	1	Total	C	O	0
			48	42	6	
10	12	1	Total	C	O	0
			48	42	6	
10	12	1	Total	C	O	0
			48	42	6	
10	13	1	Total	C	O	0
			48	42	6	
10	13	1	Total	C	O	0
			48	42	6	
10	13	1	Total	C	O	0
			48	42	6	
10	13	1	Total	C	O	0
			48	42	6	
10	13	1	Total	C	O	0
			48	42	6	
10	14	1	Total	C	O	0
			48	42	6	
10	14	1	Total	C	O	0
			48	42	6	
10	14	1	Total	C	O	0
			48	42	6	
10	14	1	Total	C	O	0
			48	42	6	
10	14	1	Total	C	O	0
			48	42	6	
10	15	1	Total	C	O	0
			48	42	6	

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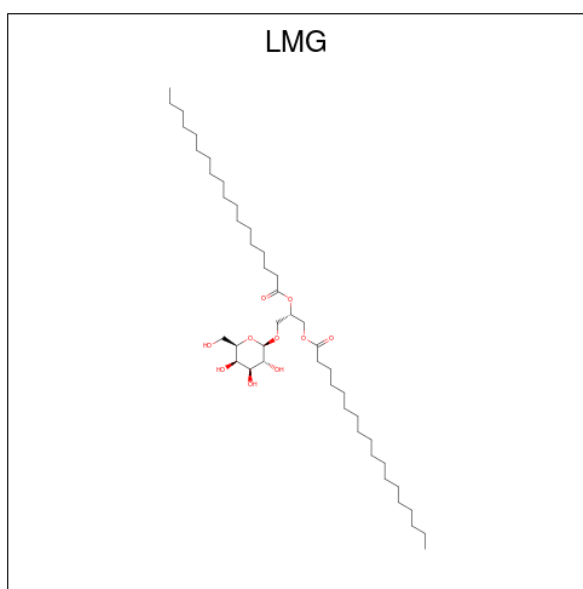
Mol	Chain	Residues	Atoms			AltConf
10	15	1	Total	C	O	0
			48	42	6	
10	15	1	Total	C	O	0
			48	42	6	
10	15	1	Total	C	O	0
			48	42	6	
10	15	1	Total	C	O	0
			48	42	6	
10	15	1	Total	C	O	0
			48	42	6	
10	16	1	Total	C	O	0
			48	42	6	
10	16	1	Total	C	O	0
			48	42	6	
10	16	1	Total	C	O	0
			48	42	6	
10	17	1	Total	C	O	0
			48	42	6	
10	17	1	Total	C	O	0
			48	42	6	
10	17	1	Total	C	O	0
			48	42	6	
10	17	1	Total	C	O	0
			48	42	6	
10	17	1	Total	C	O	0
			48	42	6	
10	17	1	Total	C	O	0
			48	42	6	
10	18	1	Total	C	O	0
			48	42	6	
10	18	1	Total	C	O	0
			48	42	6	
10	18	1	Total	C	O	0
			48	42	6	
10	18	1	Total	C	O	0
			48	42	6	
10	19	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
10	19	1	Total	C	O	0
			48	42	6	
10	20	1	Total	C	O	0
			48	42	6	
10	20	1	Total	C	O	0
			48	42	6	
10	20	1	Total	C	O	0
			48	42	6	
10	21	1	Total	C	O	0
			48	42	6	
10	21	1	Total	C	O	0
			48	42	6	
10	21	1	Total	C	O	0
			48	42	6	
10	21	1	Total	C	O	0
			48	42	6	

- Molecule 11 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
11	11	1	Total	C	O	0
			42	32	10	
11	11	1	Total	C	O	0
			32	22	10	
11	16	1	Total	C	O	0
			36	26	10	

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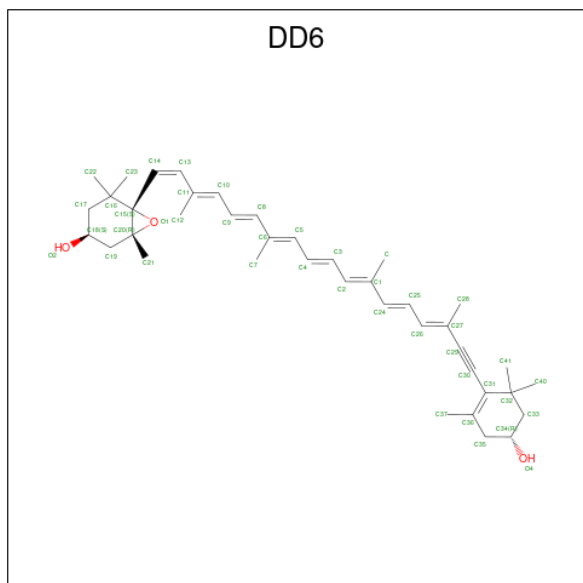
Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
11	17	1	Total	C	O	0
			37	27	10	

- Molecule 12 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

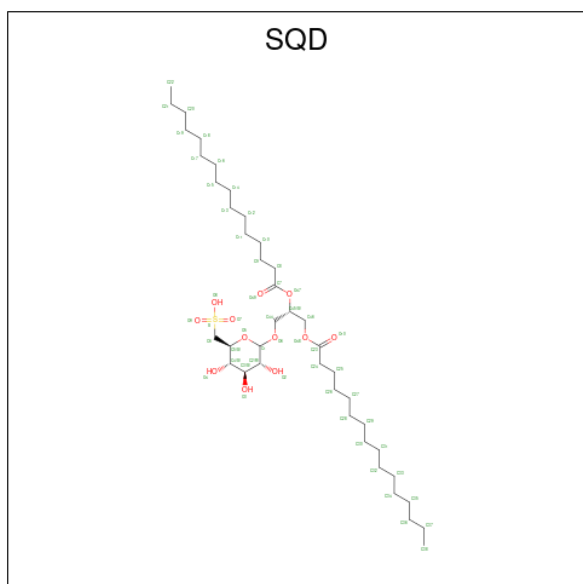
Mol	Chain	Residues	Atoms			AltConf
12	11	1	Total	C	O	0
			19	17	2	
12	12	2	Total	C	O	0
			34	32	2	
12	13	3	Total	C	O	0
			49	47	2	
12	14	1	Total	C		0
			16	16		
12	15	2	Total	C		0
			28	28		
12	16	2	Total	C		0
			24	24		
12	17	3	Total	C	O	0
			54	48	6	
12	18	4	Total	C		0
			58	58		
12	19	1	Total	C		0
			12	12		

- 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).



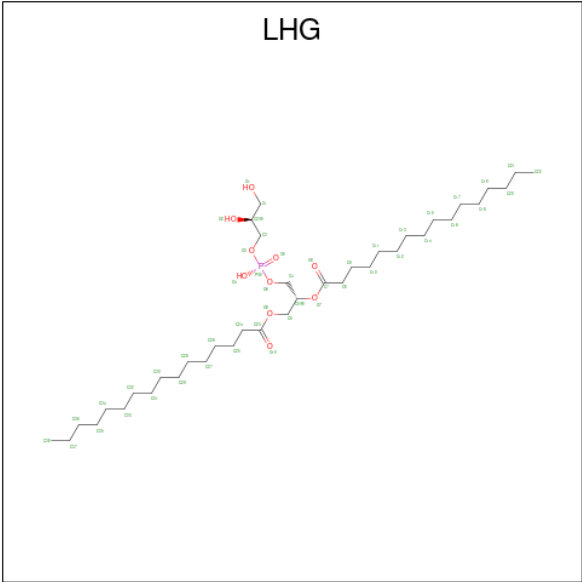
Mol	Chain	Residues	Atoms			AltConf
13	16	1	Total	C	O	0
			43	40	3	
13	19	1	Total	C	O	0
			43	40	3	
13	20	1	Total	C	O	0
			43	40	3	
13	20	1	Total	C	O	0
			43	40	3	
13	21	1	Total	C	O	0
			43	40	3	
13	21	1	Total	C	O	0
			43	40	3	

- Molecule 14 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



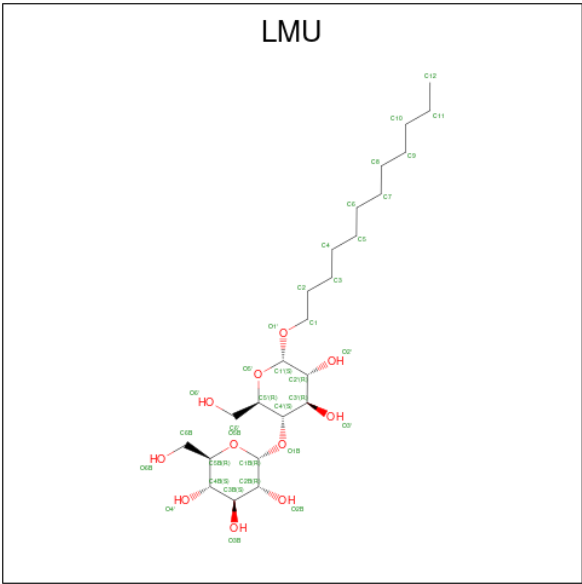
Mol	Chain	Residues	Atoms				AltConf
14	16	1	Total	C	O	S	0
			54	41	12	1	
14	17	1	Total	C	O	S	0
			49	36	12	1	

- Molecule 15 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
15	17	1	Total	C	O	P	0
			44	33	10	1	
15	19	1	Total	C	O	P	0
			49	38	10	1	
15	21	1	Total	C	O	P	0
			35	25	9	1	
15	21	1	Total	C	O	P	0
			45	34	10	1	

- Molecule 16 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
16	19	1	Total	C	O	0
			35	24	11	

- Molecule 17 is water.

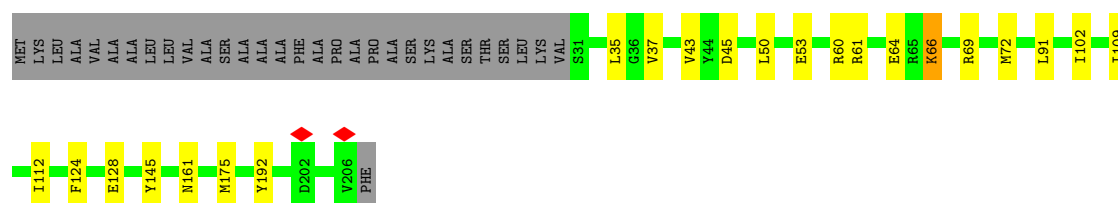
Mol	Chain	Residues	Atoms		AltConf
17	11	3	Total	O	0
			3	3	
17	12	1	Total	O	0
			1	1	
17	13	2	Total	O	0
			2	2	
17	14	1	Total	O	0
			1	1	
17	15	1	Total	O	0
			1	1	
17	16	1	Total	O	0
			1	1	
17	17	2	Total	O	0
			2	2	
17	18	1	Total	O	0
			1	1	
17	19	1	Total	O	0
			1	1	

3 Residue-property plots [i](#)

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

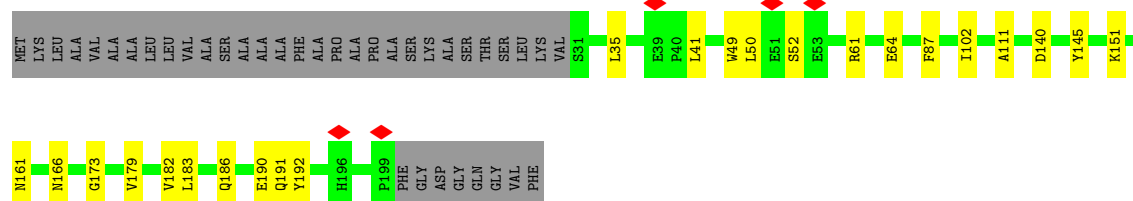
- Molecule 1: Chlorophyll a/b-binding protein

Chain 11: 



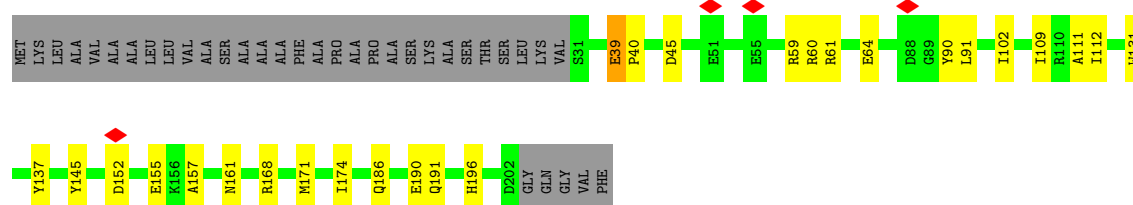
- Molecule 1: Chlorophyll a/b-binding protein

Chain 13: 



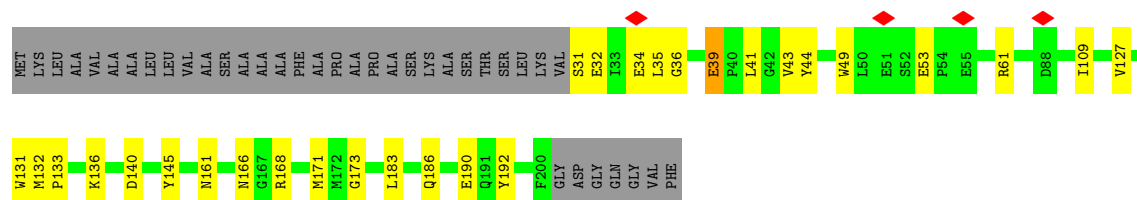
- Molecule 1: Chlorophyll a/b-binding protein

Chain 14: 

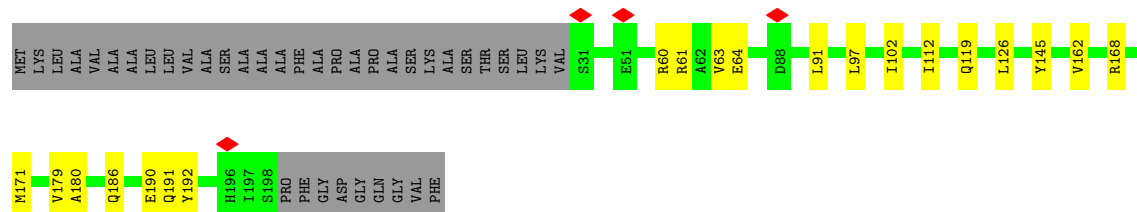


- Molecule 1: Chlorophyll a/b-binding protein

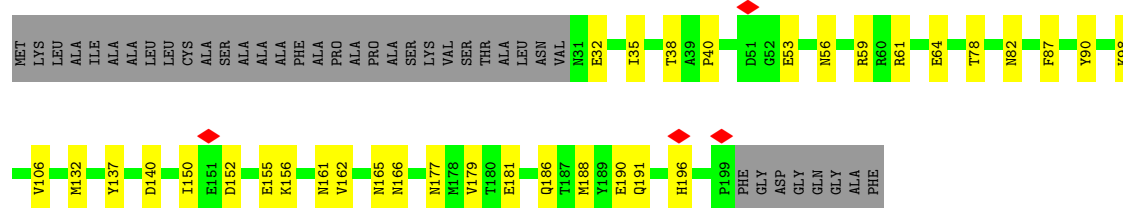
Chain 15: 



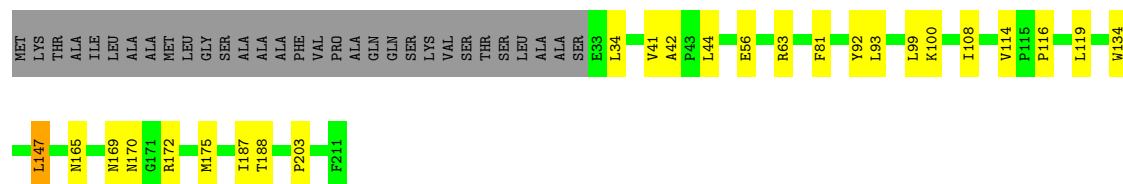
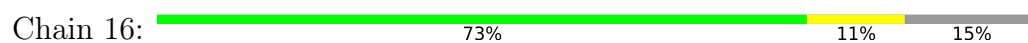
• Molecule 1: Chlorophyll a/b-binding protein



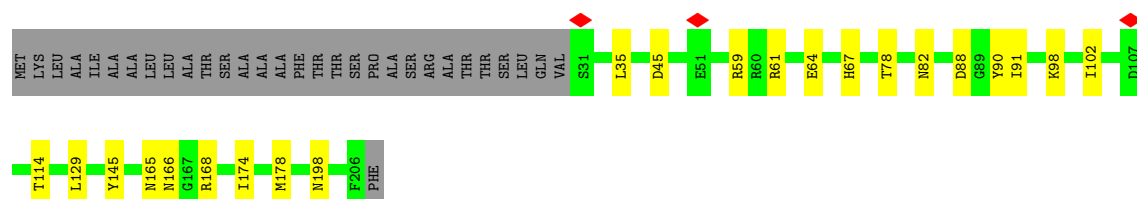
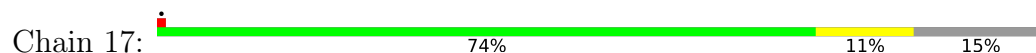
• Molecule 2: Fcpb2, Fucoxanthin chlorophyll a/c-binding protein



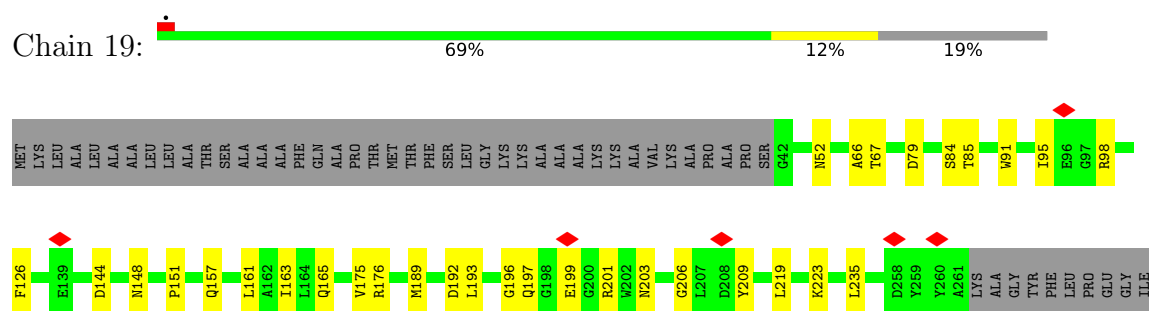
• Molecule 3: Fcpb3, Fucoxanthin chlorophyll a/c-binding protein



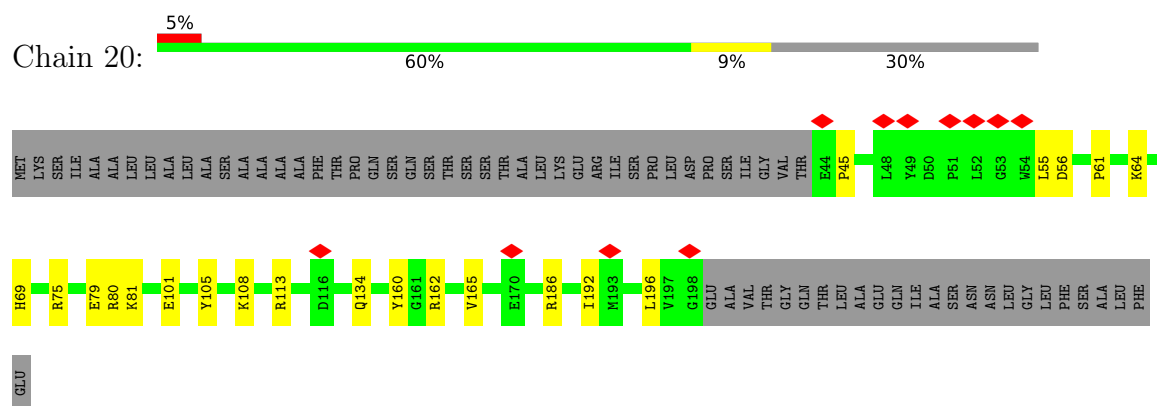
• Molecule 4: Fcpb4, Fucoxanthin chlorophyll a/c-binding protein



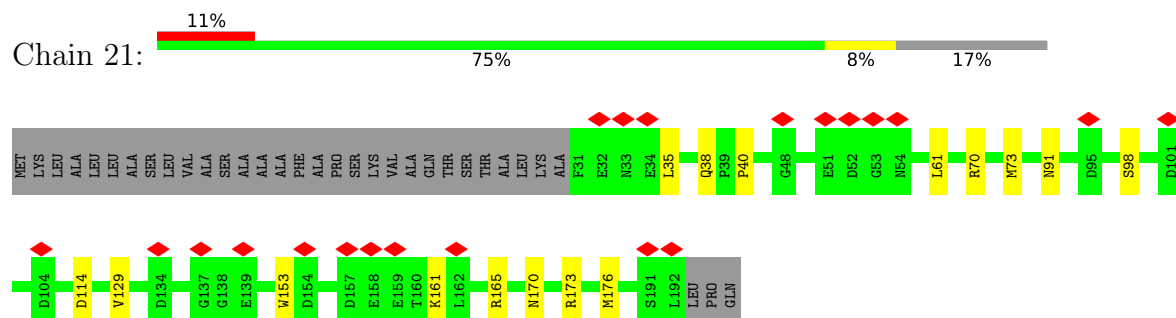
- Molecule 5: Fcpb5, Fucoxanthin chlorophyll a/c-binding protein



- Molecule 6: Fcpb6, Fucoxanthin chlorophyll a/c-binding protein



- Molecule 7: Fcpb7, Fucoxanthin chlorophyll a/c-binding protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	373897	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 ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.296	Depositor
Minimum map value	-0.107	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.055	Depositor
Map size (Å)	569.856, 569.856, 569.856	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.113, 1.113, 1.113	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: KC1, CLA, DD6, A86, SQD, UNL, LMG, LMU, 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	11	0.34	0/1373	0.48	0/1861
1	13	0.25	0/1325	0.43	0/1797
1	14	0.24	0/1349	0.41	0/1829
1	15	0.24	0/1337	0.49	0/1813
1	18	0.27	0/1317	0.46	0/1785
2	12	0.30	0/1334	0.46	0/1810
3	16	0.30	0/1425	0.45	0/1930
4	17	0.31	0/1386	0.48	0/1879
5	19	0.29	0/1737	0.47	0/2365
6	20	0.27	0/1229	0.56	0/1662
7	21	0.23	0/1290	0.50	0/1735
All	All	0.28	0/15102	0.47	0/20466

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
1	14	0	1
1	15	0	1
3	16	0	1
5	19	0	1
6	20	0	3
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	14	39	GLU	Peptide
1	15	39	GLU	Peptide
3	16	147	LEU	Peptide
5	19	196	GLY	Peptide
6	20	101	GLU	Peptide
6	20	55	LEU	Peptide
6	20	56	ASP	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	11	1343	0	1306	17	0
1	13	1296	0	1267	18	0
1	14	1319	0	1283	18	0
1	15	1307	0	1275	22	0
1	18	1289	0	1260	15	0
2	12	1302	0	1257	25	0
3	16	1386	0	1314	19	0
4	17	1353	0	1291	18	0
5	19	1690	0	1627	23	0
6	20	1198	0	1180	12	0
7	21	1262	0	1247	12	0
8	11	278	0	261	6	0
8	12	407	0	403	12	0
8	13	394	0	378	13	0
8	14	394	0	378	6	0
8	15	329	0	304	14	0
8	16	293	0	291	7	0
8	17	303	0	310	7	0
8	18	394	0	376	12	0
8	19	531	0	537	12	0
8	20	299	0	242	3	0
8	21	380	0	342	6	0
9	11	180	0	0	1	0
9	12	135	0	0	0	0
9	13	180	0	0	0	0
9	14	135	0	0	0	0
9	15	180	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	16	180	0	0	0	0
9	17	180	0	0	2	0
9	18	135	0	0	1	0
9	19	45	0	0	0	0
9	20	135	0	0	0	0
9	21	90	0	0	0	0
10	11	288	0	0	2	0
10	12	336	0	0	0	0
10	13	240	0	0	1	0
10	14	288	0	0	2	0
10	15	336	0	0	1	0
10	16	144	0	0	0	0
10	17	336	0	0	0	0
10	18	192	0	0	2	0
10	19	96	0	0	0	0
10	20	144	0	0	0	0
10	21	192	0	0	0	0
11	11	74	0	88	0	0
11	16	36	0	42	1	0
11	17	37	0	44	0	0
12	11	19	0	0	0	0
12	12	34	0	0	0	0
12	13	49	0	0	0	0
12	14	16	0	0	0	0
12	15	28	0	0	0	0
12	16	24	0	0	0	0
12	17	54	0	0	0	0
12	18	58	0	0	0	0
12	19	12	0	0	0	0
13	16	43	0	0	0	0
13	19	43	0	0	2	0
13	20	86	0	0	2	0
13	21	86	0	0	0	0
14	16	54	0	77	2	0
14	17	49	0	65	3	0
15	17	44	0	61	1	0
15	19	49	0	74	2	0
15	21	80	0	102	4	0
16	19	35	0	46	1	0
17	11	3	0	0	0	0
17	12	1	0	0	0	0
17	13	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	14	1	0	0	0	0
17	15	1	0	0	0	0
17	16	1	0	0	0	0
17	17	2	0	0	0	0
17	18	1	0	0	0	0
17	19	1	0	0	0	0
All	All	23937	0	18728	241	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (241) 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)
1:18:63:VAL:HG11	8:18:302:CLA:HAA2	1.79	0.65
8:19:302:CLA:H2	8:19:302:CLA:HED1	1.78	0.65
2:12:186:GLN:HB3	2:12:190:GLU:HB2	1.79	0.63
15:17:317:LHG:H121	5:19:175:VAL:HG22	1.81	0.62
1:18:145:TYR:HB2	8:18:307:CLA:HAA1	1.81	0.62
3:16:63:ARG:NH1	8:16:301:CLA:O1D	2.32	0.62
3:16:41:VAL:HG21	3:16:169:ASN:HD21	1.65	0.61
4:17:129:LEU:HD13	8:19:305:CLA:HBA1	1.81	0.61
6:20:162:ARG:HE	6:20:165:VAL:HG13	1.64	0.61
1:15:145:TYR:HB2	8:15:307:CLA:HAA1	1.82	0.61
5:19:176:ARG:NH2	5:19:193:LEU:O	2.34	0.60
2:12:191:GLN:HG3	2:12:196:HIS:HB2	1.84	0.60
4:17:61:ARG:NH1	4:17:64:GLU:OE2	2.35	0.59
2:12:152:ASP:HB3	2:12:155:GLU:HG2	1.84	0.59
7:21:153:TRP:O	7:21:161:LYS:NZ	2.35	0.58
1:14:61:ARG:NH1	1:14:64:GLU:OE2	2.36	0.58
2:12:53:GLU:HG3	2:12:56:ASN:HD22	1.69	0.58
1:11:61:ARG:NH1	1:11:64:GLU:OE2	2.36	0.58
1:11:35:LEU:O	1:11:161:ASN:ND2	2.37	0.58
5:19:203:ASN:ND2	5:19:206:GLY:O	2.36	0.57
2:12:61:ARG:NH2	2:12:64:GLU:OE2	2.38	0.57
1:11:69:ARG:HB3	8:11:307:CLA:HBC3	1.87	0.57
6:20:108:LYS:HG3	13:20:314:DD6:C37	2.36	0.56
2:12:166:ASN:ND2	8:13:301:CLA:OBD	2.38	0.56
1:15:127:VAL:HA	1:15:131:TRP:HB2	1.85	0.56
1:18:61:ARG:NH1	1:18:64:GLU:OE2	2.39	0.56
1:15:31:SER:N	1:15:34:GLU:OE2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:16:42:ALA:HB1	5:19:98:ARG:HB3	1.88	0.55
5:19:144:ASP:O	5:19:157:GLN:NE2	2.40	0.55
1:11:112:ILE:HD11	8:11:303:CLA:HAA2	1.88	0.55
2:12:78:THR:O	2:12:82:ASN:ND2	2.40	0.55
4:17:35:LEU:O	4:17:61:ARG:NH2	2.40	0.55
5:19:52:ASN:HB2	5:19:66:ALA:HB2	1.89	0.54
1:18:186:GLN:HB3	1:18:190:GLU:HB2	1.88	0.54
5:19:148:ASN:ND2	5:19:157:GLN:OE1	2.39	0.54
1:11:192:TYR:OH	10:11:310:A86:O2	2.25	0.54
2:12:179:VAL:HG21	8:12:311:CLA:HBC3	1.90	0.54
3:16:108:ILE:HG13	14:16:314:SQD:H441	1.90	0.53
4:17:78:THR:O	4:17:82:ASN:ND2	2.39	0.53
1:15:132:MET:HG3	8:18:308:CLA:H12	1.91	0.53
4:17:166:ASN:ND2	8:17:308:CLA:OBD	2.41	0.53
1:15:31:SER:OG	1:15:32:GLU:N	2.41	0.53
5:19:161:LEU:O	5:19:165:GLN:NE2	2.40	0.53
7:21:35:LEU:HD11	7:21:165:ARG:HH11	1.72	0.53
1:15:161:ASN:HB2	8:15:308:CLA:HED2	1.91	0.53
4:17:165:ASN:ND2	8:17:308:CLA:O1D	2.40	0.53
14:17:301:SQD:H241	14:17:301:SQD:H81	1.91	0.53
6:20:160:TYR:HB2	8:20:307:CLA:HAA1	1.91	0.53
4:17:88:ASP:HB2	14:17:301:SQD:H441	1.91	0.52
1:15:61:ARG:NH2	8:15:301:CLA:O1D	2.42	0.52
1:15:49:TRP:HZ3	8:15:301:CLA:H51	1.74	0.52
7:21:173:ARG:HA	7:21:176:MET:HE2	1.91	0.52
1:18:91:LEU:HD22	1:18:102:ILE:HD11	1.92	0.52
6:20:81:LYS:NZ	13:20:314:DD6:O2	2.42	0.52
1:14:145:TYR:HB2	8:14:307:CLA:HAA1	1.92	0.52
5:19:192:ASP:OD2	5:19:201:ARG:NH1	2.42	0.52
2:12:140:ASP:OD1	2:12:140:ASP:N	2.42	0.52
1:13:35:LEU:O	1:13:161:ASN:ND2	2.43	0.52
7:21:38:GLN:HB3	7:21:40:PRO:HD2	1.92	0.52
8:13:309:CLA:H12	1:14:131:TRP:HB3	1.91	0.51
1:11:72:MET:HE1	8:11:307:CLA:HHC	1.93	0.51
1:13:186:GLN:O	1:13:191:GLN:NE2	2.41	0.51
1:18:192:TYR:OH	10:18:311:A86:O2	2.27	0.51
3:16:116:PRO:HA	3:16:119:LEU:HB2	1.91	0.51
5:19:126:PHE:HB3	5:19:235:LEU:HD22	1.93	0.51
1:15:36:GLY:HA2	1:15:168:ARG:HH12	1.76	0.50
5:19:84:SER:HB3	8:19:301:CLA:HBA1	1.94	0.50
1:14:90:TYR:O	10:14:315:A86:O3	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:13:179:VAL:HG21	8:13:311:CLA:HBC3	1.94	0.50
1:14:186:GLN:HB3	1:14:190:GLU:HB2	1.94	0.50
1:18:119:GLN:OE1	9:18:304:KC1:C4D	2.48	0.50
5:19:67:THR:HG21	5:19:85:THR:HA	1.94	0.50
14:16:314:SQD:O49	6:20:134:GLN:NE2	2.45	0.49
1:14:168:ARG:HA	1:14:171:MET:HE3	1.93	0.49
1:18:180:ALA:O	1:18:191:GLN:NE2	2.45	0.49
6:20:69:HIS:O	6:20:75:ARG:NH1	2.46	0.49
1:14:91:LEU:HD22	1:14:102:ILE:HD11	1.94	0.49
1:13:61:ARG:NH1	1:13:64:GLU:OE2	2.46	0.49
1:11:45:ASP:N	1:11:45:ASP:OD1	2.45	0.49
1:11:66:LYS:HG2	9:11:306:KC1:C3D	2.43	0.49
1:14:45:ASP:N	1:14:45:ASP:OD1	2.45	0.48
1:14:112:ILE:HD11	8:14:303:CLA:H3A	1.94	0.48
1:14:59:ARG:NH1	1:14:137:TYR:OH	2.43	0.48
1:13:145:TYR:HB2	8:13:308:CLA:HAA1	1.94	0.48
1:15:168:ARG:HB3	8:15:301:CLA:HBC3	1.95	0.48
1:15:136:LYS:NZ	1:15:140:ASP:O	2.42	0.48
1:18:60:ARG:NH1	8:18:302:CLA:O1A	2.47	0.48
8:20:302:CLA:H61	8:20:302:CLA:H41	1.69	0.48
4:17:90:TYR:HA	4:17:98:LYS:HA	1.94	0.48
3:16:172:ARG:HA	3:16:175:MET:HE3	1.96	0.47
8:21:206:CLA:HAA2	15:21:217:LHG:H102	1.95	0.47
2:12:32:GLU:HA	2:12:35:ILE:HD12	1.97	0.47
1:14:59:ARG:NH2	8:14:302:CLA:OBD	2.46	0.47
3:16:34:LEU:HD12	3:16:56:GLU:HG2	1.96	0.47
1:18:168:ARG:HA	1:18:171:MET:HE3	1.96	0.47
8:19:302:CLA:H62	8:19:302:CLA:H41	1.75	0.47
7:21:91:ASN:H	7:21:98:SER:HA	1.79	0.47
7:21:129:VAL:HG22	15:21:217:LHG:H292	1.96	0.47
8:19:309:CLA:HBB2	15:19:314:LHG:H371	1.95	0.47
8:11:301:CLA:HBA2	8:11:301:CLA:H3A	1.68	0.47
3:16:93:LEU:HD21	3:16:114:VAL:HG13	1.95	0.47
3:16:187:ILE:HG13	3:16:188:THR:HG23	1.96	0.47
2:12:90:TYR:HA	2:12:98:LYS:HA	1.97	0.47
15:19:314:LHG:H281	15:19:314:LHG:H102	1.96	0.47
6:20:105:TYR:HA	6:20:113:ARG:HA	1.96	0.47
2:12:152:ASP:OD1	1:13:151:LYS:NZ	2.42	0.47
8:12:303:CLA:HBA2	8:12:303:CLA:H3A	1.67	0.46
1:13:179:VAL:HA	1:13:182:VAL:HG22	1.97	0.46
3:16:81:PHE:HB3	14:17:301:SQD:H131	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:18:179:VAL:HG21	8:18:310:CLA:HBC3	1.96	0.46
1:15:192:TYR:OH	10:15:311:A86:O2	2.33	0.46
4:17:168:ARG:HB3	8:17:302:CLA:HBC3	1.97	0.46
5:19:95:ILE:HA	5:19:98:ARG:HD2	1.97	0.46
5:19:151:PRO:O	13:19:312:DD6:O2	2.33	0.46
7:21:114:ASP:OD1	7:21:114:ASP:N	2.47	0.46
5:19:79:ASP:OD1	13:19:312:DD6:O4	2.33	0.46
4:17:145:TYR:HB2	8:17:307:CLA:HAA1	1.98	0.46
8:18:302:CLA:H11	8:18:302:CLA:H52	1.68	0.46
6:20:45:PRO:O	6:20:80:ARG:NH2	2.46	0.46
8:12:301:CLA:HHC	8:12:301:CLA:HBB1	1.98	0.46
8:13:309:CLA:H2	8:13:309:CLA:H61	1.68	0.46
3:16:170:ASN:ND2	8:16:307:CLA:OBD	2.49	0.45
8:19:310:CLA:H62	8:19:310:CLA:H41	1.68	0.45
1:13:192:TYR:OH	10:13:312:A86:O2	2.33	0.45
1:14:152:ASP:HB3	1:14:155:GLU:HB3	1.98	0.45
3:16:44:LEU:HD21	8:19:302:CLA:H43	1.98	0.45
8:16:301:CLA:H142	8:16:301:CLA:H112	1.84	0.45
2:12:35:ILE:O	2:12:161:ASN:ND2	2.50	0.45
1:15:35:LEU:O	1:15:161:ASN:ND2	2.49	0.45
8:13:301:CLA:H101	8:13:301:CLA:H62	1.76	0.45
1:15:173:GLY:HA2	8:15:310:CLA:HBB1	1.99	0.45
2:12:132:MET:HG3	8:12:301:CLA:H12	1.98	0.45
3:16:93:LEU:HD23	3:16:99:LEU:HD23	1.99	0.45
4:17:114:THR:HG21	5:19:163:ILE:HD12	1.97	0.45
2:12:177:ASN:ND2	2:12:188:MET:SD	2.90	0.45
1:13:186:GLN:NE2	1:13:190:GLU:O	2.50	0.45
8:11:301:CLA:H142	8:11:301:CLA:H112	1.87	0.45
3:16:169:ASN:ND2	8:16:307:CLA:O1D	2.46	0.45
8:12:301:CLA:H142	8:12:301:CLA:H111	1.78	0.45
8:19:306:CLA:H152	8:19:306:CLA:H112	1.64	0.44
8:12:307:CLA:H3A	8:12:307:CLA:HBA2	1.78	0.44
4:17:59:ARG:NH1	9:17:303:KC1:O2A	2.50	0.44
5:19:197:GLN:NE2	5:19:209:TYR:O	2.49	0.44
1:14:157:ALA:O	1:14:161:ASN:ND2	2.41	0.44
3:16:165:ASN:HB2	8:16:307:CLA:HED2	2.00	0.44
8:13:311:CLA:H3A	8:13:311:CLA:HBA2	1.80	0.44
1:15:168:ARG:HA	1:15:171:MET:HE3	2.00	0.44
1:11:124:PHE:O	1:11:128:GLU:HB2	2.17	0.44
1:14:60:ARG:HG2	8:14:301:CLA:HHB	2.00	0.44
6:20:192:ILE:HG23	6:20:196:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:15:301:CLA:H3A	8:15:301:CLA:HBA2	1.77	0.43
3:16:92:TYR:HA	3:16:100:LYS:HA	2.00	0.43
8:17:310:CLA:H61	8:17:310:CLA:H102	1.82	0.43
8:21:202:CLA:H3A	8:21:202:CLA:HBA2	1.73	0.43
2:12:59:ARG:NH1	8:12:304:CLA:O1A	2.51	0.43
1:13:182:VAL:HG23	1:13:183:LEU:HD12	2.00	0.43
1:15:61:ARG:HH22	8:15:301:CLA:HED3	1.82	0.43
1:13:87:PHE:HE2	8:13:304:CLA:H11	1.84	0.43
5:19:163:ILE:HG23	16:19:315:LMU:H123	2.00	0.43
7:21:61:LEU:HB3	8:21:202:CLA:HHB	1.99	0.43
1:11:53:GLU:OE1	1:11:60:ARG:NH1	2.45	0.43
2:12:106:VAL:HG13	2:12:181:GLU:HG2	1.99	0.43
4:17:174:ILE:HG13	4:17:178:MET:HE2	2.00	0.43
10:11:318:A86:O3	2:12:90:TYR:O	2.36	0.43
1:15:186:GLN:HB3	1:15:190:GLU:HB2	2.00	0.43
8:13:309:CLA:H92	8:13:309:CLA:H62	1.81	0.43
8:18:308:CLA:H61	8:18:308:CLA:H41	1.85	0.43
1:11:66:LYS:HE3	1:11:128:GLU:OE2	2.18	0.42
2:12:38:THR:HG23	2:12:40:PRO:HD2	2.00	0.42
1:13:102:ILE:HG23	1:13:111:ALA:HB3	2.02	0.42
1:13:173:GLY:HA2	8:13:311:CLA:HBB1	2.00	0.42
8:15:308:CLA:H12	3:16:134:TRP:NE1	2.34	0.42
4:17:165:ASN:OD1	4:17:168:ARG:NH2	2.42	0.42
8:17:308:CLA:H101	8:17:308:CLA:H62	1.81	0.42
2:12:87:PHE:HE2	8:12:305:CLA:H11	1.85	0.42
4:17:67:HIS:HE1	9:17:303:KC1:ND	2.17	0.42
5:19:219:LEU:HG	5:19:223:LYS:HE2	2.01	0.42
1:11:50:LEU:HD23	1:11:50:LEU:HA	1.90	0.42
1:11:91:LEU:HD22	1:11:102:ILE:HD11	2.01	0.42
1:11:37:VAL:HG11	1:11:43:VAL:HG22	2.00	0.42
1:15:132:MET:HA	1:15:133:PRO:HD3	1.93	0.42
8:15:308:CLA:H92	8:15:308:CLA:H41	2.01	0.42
2:12:162:VAL:HG12	8:12:309:CLA:HBB1	2.01	0.42
11:16:315:LMG:O5	11:16:315:LMG:O4	2.30	0.42
5:19:189:MET:HG3	5:19:192:ASP:HB2	2.01	0.42
1:15:109:ILE:HD11	8:15:303:CLA:HMB1	2.02	0.42
3:16:34:LEU:HD23	3:16:34:LEU:HA	1.87	0.42
1:14:102:ILE:HG23	1:14:111:ALA:HB3	2.02	0.42
1:14:191:GLN:HG3	1:14:196:HIS:HB3	2.01	0.42
1:15:166:ASN:ND2	8:15:308:CLA:OBD	2.53	0.42
5:19:199:GLU:O	5:19:201:ARG:N	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:17:91:ILE:HG21	4:17:102:ILE:HD11	2.01	0.42
2:12:38:THR:HB	2:12:165:ASN:HD21	1.84	0.41
1:13:50:LEU:HG	8:13:302:CLA:HBA1	2.01	0.41
4:17:198:ASN:HD22	7:21:114:ASP:HB3	1.85	0.41
8:12:305:CLA:HBD	8:12:305:CLA:HBA1	2.02	0.41
1:14:109:ILE:HD12	1:14:112:ILE:HD12	2.03	0.41
8:18:301:CLA:HBA2	8:18:301:CLA:H3A	1.71	0.41
8:14:301:CLA:H3A	8:14:301:CLA:HBA2	1.80	0.41
8:14:302:CLA:HBB1	10:14:314:A86:C4	2.51	0.41
1:15:41:LEU:HB3	1:15:44:TYR:HB2	2.02	0.41
1:15:183:LEU:HD23	1:15:183:LEU:HA	1.93	0.41
5:19:91:TRP:NE1	8:19:305:CLA:O1A	2.42	0.41
6:20:61:PRO:HA	6:20:64:LYS:HG3	2.02	0.41
1:14:174:ILE:HD12	1:14:174:ILE:HA	1.93	0.41
1:18:112:ILE:HD11	8:18:303:CLA:HAA2	2.02	0.41
8:13:302:CLA:H203	8:13:302:CLA:H162	1.87	0.41
6:20:79:GLU:OE1	8:20:302:CLA:NB	2.54	0.41
8:21:206:CLA:H11	15:21:217:LHG:H171	2.01	0.41
1:13:140:ASP:OD1	1:13:140:ASP:N	2.54	0.41
8:18:302:CLA:HBB1	10:18:313:A86:C4	2.51	0.41
8:19:304:CLA:H3A	8:19:304:CLA:HBA1	1.71	0.41
6:20:79:GLU:OE2	6:20:186:ARG:NE	2.41	0.41
8:21:206:CLA:HHB	15:21:217:LHG:H312	2.02	0.41
2:12:59:ARG:HG3	2:12:137:TYR:CZ	2.56	0.41
2:12:150:ILE:HB	2:12:156:LYS:HB2	2.02	0.41
8:15:301:CLA:H91	8:15:301:CLA:H111	1.92	0.41
1:18:162:VAL:HG12	8:18:307:CLA:HBB1	2.02	0.41
7:21:70:ARG:HA	7:21:73:MET:HE3	2.02	0.41
2:12:191:GLN:NE2	2:12:196:HIS:O	2.47	0.41
3:16:203:PRO:HD3	8:16:309:CLA:HBA1	2.02	0.41
8:17:308:CLA:HBC3	1:18:126:LEU:HD21	2.03	0.41
1:18:91:LEU:N	1:18:97:LEU:O	2.53	0.41
8:18:308:CLA:H193	8:18:308:CLA:H161	1.93	0.41
8:12:303:CLA:H142	8:12:303:CLA:H112	1.90	0.41
8:15:308:CLA:H41	8:15:308:CLA:H61	1.63	0.41
5:19:189:MET:HE3	5:19:189:MET:HB2	1.94	0.41
1:13:41:LEU:HD23	1:13:41:LEU:HA	1.94	0.40
8:19:301:CLA:H3A	8:19:301:CLA:HBA2	1.76	0.40
1:11:145:TYR:HB2	8:11:307:CLA:HAA1	2.04	0.40
8:16:306:CLA:H143	8:16:306:CLA:H111	1.88	0.40
4:17:45:ASP:OD1	4:17:45:ASP:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:19:307:CLA:H112	8:19:307:CLA:H72	1.87	0.40
1:11:175:MET:HE3	1:11:175:MET:HB3	1.97	0.40
8:12:303:CLA:H2	8:12:303:CLA:H61	1.80	0.40
1:13:49:TRP:HA	1:13:52:SER:HB2	2.03	0.40
1:11:109:ILE:HG22	1:11:112:ILE:HD12	2.02	0.40
7:21:176:MET:HE3	7:21:176:MET:HB2	1.82	0.40
1:13:166:ASN:ND2	8:13:309:CLA:OBD	2.54	0.40
7:21:170:ASN:HA	7:21:173:ARG:HB2	2.03	0.40
8:21:208:CLA:H142	8:21:208:CLA:H111	1.88	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	11	174/207 (84%)	166 (95%)	8 (5%)	0	100	100
1	13	167/207 (81%)	161 (96%)	6 (4%)	0	100	100
1	14	170/207 (82%)	162 (95%)	6 (4%)	2 (1%)	10	34
1	15	168/207 (81%)	148 (88%)	19 (11%)	1 (1%)	21	51
1	18	166/207 (80%)	155 (93%)	11 (7%)	0	100	100
2	12	167/207 (81%)	163 (98%)	4 (2%)	0	100	100
3	16	177/210 (84%)	171 (97%)	6 (3%)	0	100	100
4	17	174/207 (84%)	169 (97%)	5 (3%)	0	100	100
5	19	218/271 (80%)	208 (95%)	10 (5%)	0	100	100
6	20	153/223 (69%)	135 (88%)	18 (12%)	0	100	100
7	21	160/195 (82%)	142 (89%)	18 (11%)	0	100	100
All	All	1894/2348 (81%)	1780 (94%)	111 (6%)	3 (0%)	44	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	14	39	GLU
1	15	39	GLU
1	14	40	PRO

5.3.2 Protein sidechains [i](#)

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	11	138/158 (87%)	137 (99%)	1 (1%)	76	91
1	13	134/158 (85%)	134 (100%)	0	100	100
1	14	136/158 (86%)	136 (100%)	0	100	100
1	15	135/158 (85%)	133 (98%)	2 (2%)	57	84
1	18	133/158 (84%)	133 (100%)	0	100	100
2	12	133/156 (85%)	133 (100%)	0	100	100
3	16	137/158 (87%)	136 (99%)	1 (1%)	76	91
4	17	137/159 (86%)	137 (100%)	0	100	100
5	19	169/202 (84%)	169 (100%)	0	100	100
6	20	122/174 (70%)	122 (100%)	0	100	100
7	21	129/152 (85%)	129 (100%)	0	100	100
All	All	1503/1791 (84%)	1499 (100%)	4 (0%)	84	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	11	66	LYS
1	15	43	VAL
1	15	53	GLU
3	16	147	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	11	161	ASN
1	11	177	ASN
2	12	56	ASN
2	12	161	ASN
1	13	84	HIS
1	13	161	ASN
1	13	165	ASN
1	13	186	GLN
3	16	169	ASN
3	16	190	GLN
1	18	165	ASN
1	18	177	ASN
1	18	191	GLN
5	19	240	GLN
6	20	97	ASN
6	20	167	ASN
7	21	38	GLN
7	21	54	ASN
7	21	55	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 196 ligands modelled in this entry, 19 are unknown - leaving 177 for Mogul analysis.

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	$\# Z > 2$
9	KC1	12	306	2	49,53,53	3.00	24 (48%)	61,89,89	3.91	32 (52%)
13	DD6	21	216	-	40,45,45	5.56	22 (55%)	51,67,67	6.17	28 (54%)
8	CLA	17	310	17	69,73,73	2.02	20 (28%)	82,113,113	2.82	36 (43%)
8	CLA	19	309	5	49,53,73	2.37	19 (38%)	58,89,113	2.98	28 (48%)
9	KC1	17	309	4	49,53,53	3.01	24 (48%)	61,89,89	3.74	36 (59%)
9	KC1	14	304	1	49,53,53	3.03	25 (51%)	61,89,89	3.96	33 (54%)
9	KC1	15	302	-	49,53,53	3.02	23 (46%)	61,89,89	3.81	36 (59%)
10	A86	15	319	-	47,50,50	4.15	24 (51%)	51,76,76	6.03	21 (41%)
8	CLA	20	302	6	60,64,73	2.16	20 (33%)	71,102,113	2.92	33 (46%)
9	KC1	11	308	1	49,53,53	2.99	23 (46%)	61,89,89	3.70	36 (59%)
8	CLA	14	308	17	69,73,73	1.98	20 (28%)	82,113,113	2.57	33 (40%)
10	A86	14	314	-	47,50,50	4.34	24 (51%)	51,76,76	7.02	20 (39%)
9	KC1	16	305	3	49,53,53	3.00	23 (46%)	61,89,89	3.74	34 (55%)
10	A86	19	311	-	47,50,50	4.12	23 (48%)	51,76,76	6.41	19 (37%)
8	CLA	13	309	17	69,73,73	2.00	20 (28%)	82,113,113	2.62	29 (35%)
8	CLA	12	309	2	56,60,73	2.19	21 (37%)	65,97,113	2.98	34 (52%)
10	A86	21	215	-	47,50,50	4.30	25 (53%)	51,76,76	6.51	17 (33%)
10	A86	17	311	-	47,50,50	4.22	24 (51%)	51,76,76	6.94	14 (27%)
8	CLA	12	301	17	69,73,73	1.97	19 (27%)	82,113,113	2.63	32 (39%)
8	CLA	17	307	4	56,60,73	2.20	19 (33%)	65,97,113	2.90	33 (50%)
9	KC1	14	306	1	49,53,53	3.00	22 (44%)	61,89,89	3.79	36 (59%)
10	A86	14	313	-	47,50,50	4.35	24 (51%)	51,76,76	6.19	17 (33%)
8	CLA	13	308	1	56,60,73	2.19	18 (32%)	65,97,113	2.87	34 (52%)
8	CLA	16	303	-	61,65,73	2.10	20 (32%)	72,103,113	2.89	34 (47%)
10	A86	13	314	-	47,50,50	4.38	24 (51%)	51,76,76	7.19	18 (35%)
10	A86	19	313	-	47,50,50	4.28	25 (53%)	51,76,76	7.27	20 (39%)
10	A86	18	314	-	47,50,50	4.23	24 (51%)	51,76,76	6.35	18 (35%)
13	DD6	16	312	-	40,45,45	5.56	23 (57%)	51,67,67	5.86	26 (50%)
9	KC1	11	304	1	49,53,53	3.03	23 (46%)	61,89,89	3.75	34 (55%)
9	KC1	12	310	2	49,53,53	3.01	24 (48%)	61,89,89	3.69	38 (62%)
9	KC1	15	304	1	49,53,53	3.03	23 (46%)	61,89,89	3.92	35 (57%)
10	A86	17	321	-	47,50,50	4.14	24 (51%)	51,76,76	6.42	19 (37%)
15	LHG	19	314	8	48,48,48	0.73	1 (2%)	51,54,54	1.24	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	A86	13	313	-	47,50,50	4.30	23 (48%)	51,76,76	6.60	17 (33%)
10	A86	16	311	-	47,50,50	4.04	23 (48%)	51,76,76	6.33	22 (43%)
9	KC1	18	309	1	49,53,53	3.00	25 (51%)	61,89,89	3.83	35 (57%)
8	CLA	15	308	17	69,73,73	1.97	21 (30%)	82,113,113	2.62	31 (37%)
10	A86	13	312	-	47,50,50	4.18	23 (48%)	51,76,76	6.61	20 (39%)
9	KC1	15	306	1	49,53,53	3.01	23 (46%)	61,89,89	3.78	37 (60%)
15	LHG	21	201	-	34,34,48	0.77	1 (2%)	37,39,54	1.42	5 (13%)
9	KC1	17	306	4	49,53,53	2.98	23 (46%)	61,89,89	3.67	36 (59%)
8	CLA	11	309	17	55,59,73	2.20	22 (40%)	64,96,113	2.91	29 (45%)
8	CLA	19	303	17	69,73,73	1.97	19 (27%)	82,113,113	2.75	33 (40%)
10	A86	18	312	-	47,50,50	4.28	24 (51%)	51,76,76	6.79	19 (37%)
8	CLA	17	308	17	69,73,73	1.99	19 (27%)	82,113,113	2.56	31 (37%)
8	CLA	19	305	5	55,59,73	2.19	19 (34%)	64,96,113	2.96	31 (48%)
8	CLA	20	310	6	49,53,73	2.39	20 (40%)	58,89,113	3.01	26 (44%)
11	LMG	11	316	-	32,32,55	0.98	1 (3%)	40,40,63	1.21	3 (7%)
9	KC1	13	303	-	49,53,53	3.05	24 (48%)	61,89,89	3.82	37 (60%)
10	A86	12	313	-	47,50,50	4.14	24 (51%)	51,76,76	6.54	17 (33%)
10	A86	16	313	-	47,50,50	3.98	21 (44%)	51,76,76	6.22	14 (27%)
10	A86	21	213	-	47,50,50	4.45	24 (51%)	51,76,76	6.76	16 (31%)
8	CLA	21	210	-	49,53,73	2.40	20 (40%)	58,89,113	3.12	27 (46%)
8	CLA	16	301	3	69,73,73	1.95	20 (28%)	82,113,113	2.67	27 (32%)
8	CLA	11	307	1	56,60,73	2.19	19 (33%)	65,97,113	2.98	31 (47%)
8	CLA	14	305	-	49,53,73	2.39	19 (38%)	58,89,113	3.05	28 (48%)
13	DD6	20	314	-	40,45,45	5.61	23 (57%)	51,67,67	6.05	28 (54%)
9	KC1	17	305	4	49,53,53	3.01	24 (48%)	61,89,89	3.74	33 (54%)
11	LMG	17	318	-	37,37,55	0.99	3 (8%)	45,45,63	1.27	5 (11%)
10	A86	12	302	-	47,50,50	4.13	22 (46%)	51,76,76	6.36	20 (39%)
8	CLA	21	209	7	49,53,73	2.41	19 (38%)	58,89,113	3.04	27 (46%)
8	CLA	13	304	-	61,65,73	2.12	19 (31%)	72,103,113	2.88	34 (47%)
9	KC1	17	303	-	49,53,53	3.03	22 (44%)	61,89,89	3.70	37 (60%)
9	KC1	20	305	6	49,53,53	3.03	24 (48%)	61,89,89	3.73	33 (54%)
9	KC1	18	306	1	49,53,53	3.01	24 (48%)	61,89,89	3.78	38 (62%)
10	A86	18	313	-	47,50,50	4.36	24 (51%)	51,76,76	6.84	19 (37%)
8	CLA	11	303	-	69,73,73	1.97	20 (28%)	82,113,113	2.75	34 (41%)
8	CLA	12	305	-	69,73,73	1.97	19 (27%)	82,113,113	2.74	34 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	CLA	11	301	1	69,73,73	1.97	19 (27%)	82,113,113	2.65	32 (39%)
8	CLA	18	303	-	60,64,73	2.12	20 (33%)	71,102,113	2.88	35 (49%)
8	CLA	11	305	17	49,53,73	2.35	19 (38%)	58,89,113	3.07	28 (48%)
10	A86	11	311	-	47,50,50	4.11	22 (46%)	51,76,76	6.54	22 (43%)
10	A86	12	319	-	47,50,50	4.08	21 (44%)	51,76,76	6.63	22 (43%)
13	DD6	19	312	-	40,45,45	5.35	23 (57%)	51,67,67	5.79	32 (62%)
10	A86	18	311	-	47,50,50	4.24	23 (48%)	51,76,76	6.79	18 (35%)
8	CLA	19	310	5	69,73,73	1.98	19 (27%)	82,113,113	2.55	31 (37%)
8	CLA	19	304	5	49,53,73	2.36	20 (40%)	58,89,113	3.06	25 (43%)
10	A86	11	312	-	47,50,50	4.27	22 (46%)	51,76,76	6.34	16 (31%)
10	A86	11	318	-	47,50,50	4.08	23 (48%)	51,76,76	6.19	20 (39%)
8	CLA	18	305	-	49,53,73	2.38	20 (40%)	58,89,113	3.06	28 (48%)
9	KC1	16	308	3	49,53,53	3.01	23 (46%)	61,89,89	3.68	34 (55%)
10	A86	14	311	-	47,50,50	4.16	20 (42%)	51,76,76	6.91	20 (39%)
8	CLA	12	304	-	69,73,73	1.98	18 (26%)	82,113,113	2.58	31 (37%)
8	CLA	16	306	3	69,73,73	1.95	18 (26%)	82,113,113	2.52	31 (37%)
8	CLA	14	307	1	56,60,73	2.18	18 (32%)	65,97,113	2.87	32 (49%)
11	LMG	11	315	-	42,42,55	1.07	3 (7%)	50,50,63	1.21	3 (6%)
10	A86	21	214	-	47,50,50	4.35	25 (53%)	51,76,76	6.94	18 (35%)
8	CLA	14	310	-	49,53,73	2.39	19 (38%)	58,89,113	3.05	26 (44%)
8	CLA	15	301	1	69,73,73	2.00	19 (27%)	82,113,113	2.66	26 (31%)
9	KC1	13	305	1	49,53,53	3.02	24 (48%)	61,89,89	3.80	35 (57%)
10	A86	11	313	-	47,50,50	4.20	23 (48%)	51,76,76	6.98	22 (43%)
8	CLA	14	302	-	69,73,73	2.00	18 (26%)	82,113,113	2.57	32 (39%)
8	CLA	21	205	7	49,53,73	2.36	20 (40%)	58,89,113	3.04	28 (48%)
15	LHG	21	217	-	44,44,48	0.64	0	47,50,54	1.25	4 (8%)
8	CLA	19	302	-	69,73,73	1.96	20 (28%)	82,113,113	2.72	30 (36%)
8	CLA	14	303	-	61,65,73	2.13	19 (31%)	72,103,113	3.00	36 (50%)
8	CLA	17	302	4	69,73,73	2.01	18 (26%)	82,113,113	2.59	26 (31%)
14	SQD	16	314	-	52,54,54	0.96	6 (11%)	62,65,65	1.55	11 (17%)
9	KC1	18	304	1	49,53,53	3.01	23 (46%)	61,89,89	3.76	35 (57%)
10	A86	17	312	-	47,50,50	4.14	23 (48%)	51,76,76	6.32	19 (37%)
10	A86	16	310	-	47,50,50	3.99	21 (44%)	51,76,76	6.30	18 (35%)
10	A86	21	211	-	47,50,50	4.36	25 (53%)	51,76,76	6.86	12 (23%)
8	CLA	13	302	1	69,73,73	2.01	19 (27%)	82,113,113	2.63	31 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	CLA	15	307	1	56,60,73	2.20	19 (33%)	65,97,113	2.96	33 (50%)
8	CLA	20	308	6	49,53,73	2.42	20 (40%)	58,89,113	3.04	28 (48%)
10	A86	17	316	-	47,50,50	4.18	22 (46%)	51,76,76	6.40	19 (37%)
10	A86	15	314	-	47,50,50	4.45	24 (51%)	51,76,76	6.87	18 (35%)
8	CLA	18	308	17	69,73,73	1.97	20 (28%)	82,113,113	2.57	31 (37%)
9	KC1	21	207	7	49,53,53	3.01	25 (51%)	61,89,89	4.01	37 (60%)
10	A86	11	314	-	47,50,50	4.13	23 (48%)	51,76,76	6.36	20 (39%)
8	CLA	20	304	-	60,64,73	2.09	19 (31%)	71,102,113	3.03	36 (50%)
10	A86	13	315	-	47,50,50	4.40	24 (51%)	51,76,76	7.16	17 (33%)
8	CLA	21	206	7	69,73,73	1.97	19 (27%)	82,113,113	2.65	31 (37%)
10	A86	17	314	-	47,50,50	4.25	23 (48%)	51,76,76	6.96	20 (39%)
8	CLA	17	304	-	60,64,73	2.13	20 (33%)	71,102,113	2.94	35 (49%)
8	CLA	13	306	-	49,53,73	2.43	20 (40%)	58,89,113	3.04	27 (46%)
9	KC1	11	302	-	49,53,53	3.02	21 (42%)	61,89,89	3.73	33 (54%)
10	A86	12	314	-	47,50,50	4.36	23 (48%)	51,76,76	6.73	14 (27%)
10	A86	12	316	-	47,50,50	4.23	24 (51%)	51,76,76	6.20	20 (39%)
8	CLA	18	301	1	69,73,73	1.97	19 (27%)	82,113,113	2.65	31 (37%)
10	A86	11	310	-	47,50,50	4.11	22 (46%)	51,76,76	6.23	16 (31%)
9	KC1	12	308	2	49,53,53	2.99	22 (44%)	61,89,89	3.68	35 (57%)
10	A86	20	301	-	47,50,50	4.32	23 (48%)	51,76,76	7.08	20 (39%)
8	CLA	19	301	5	69,73,73	1.96	19 (27%)	82,113,113	2.64	31 (37%)
8	CLA	21	202	7	61,65,73	2.13	20 (32%)	72,103,113	2.82	31 (43%)
8	CLA	18	307	-	57,61,73	2.18	19 (33%)	67,98,113	2.86	31 (46%)
16	LMU	19	315	-	36,36,36	1.14	2 (5%)	47,47,47	1.02	2 (4%)
8	CLA	15	310	-	49,53,73	2.38	19 (38%)	58,89,113	3.11	28 (48%)
9	KC1	16	302	-	49,53,53	3.01	25 (51%)	61,89,89	3.59	35 (57%)
8	CLA	20	307	6	54,58,73	2.24	19 (35%)	64,95,113	2.91	31 (48%)
8	CLA	21	204	-	62,66,73	2.13	18 (29%)	73,104,113	2.93	35 (47%)
9	KC1	13	310	1	49,53,53	3.01	23 (46%)	61,89,89	3.75	36 (59%)
9	KC1	15	309	1	49,53,53	2.98	21 (42%)	61,89,89	3.68	36 (59%)
8	CLA	15	303	-	61,65,73	2.12	19 (31%)	72,103,113	2.88	35 (48%)
10	A86	14	316	-	47,50,50	4.18	23 (48%)	51,76,76	6.16	20 (39%)
8	CLA	18	310	-	49,53,73	2.44	19 (38%)	58,89,113	3.05	28 (48%)
8	CLA	19	307	15	69,73,73	1.98	20 (28%)	82,113,113	2.62	31 (37%)
8	CLA	20	309	-	51,55,73	2.31	19 (37%)	60,91,113	2.97	30 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	CLA	12	311	-	49,53,73	2.39	21 (42%)	58,89,113	3.09	29 (50%)
10	A86	12	312	-	47,50,50	4.22	23 (48%)	51,76,76	6.75	21 (41%)
10	A86	15	315	-	47,50,50	4.21	24 (51%)	51,76,76	6.44	18 (35%)
13	DD6	20	312	-	40,45,45	5.46	24 (60%)	51,67,67	6.43	25 (49%)
8	CLA	18	302	-	69,73,73	2.00	18 (26%)	82,113,113	2.62	32 (39%)
10	A86	17	315	-	47,50,50	4.10	22 (46%)	51,76,76	7.21	16 (31%)
8	CLA	15	305	-	49,53,73	2.41	20 (40%)	58,89,113	3.06	28 (48%)
10	A86	13	316	-	47,50,50	4.28	24 (51%)	51,76,76	6.33	17 (33%)
8	CLA	16	307	17	65,69,73	2.02	18 (27%)	77,108,113	2.64	29 (37%)
10	A86	15	311	-	47,50,50	4.17	23 (48%)	51,76,76	6.62	14 (27%)
10	A86	20	311	-	47,50,50	4.32	23 (48%)	51,76,76	7.06	14 (27%)
9	KC1	19	308	-	49,53,53	2.98	23 (46%)	61,89,89	3.91	37 (60%)
8	CLA	16	309	-	49,53,73	2.35	20 (40%)	58,89,113	3.17	29 (50%)
10	A86	15	312	-	47,50,50	4.23	23 (48%)	51,76,76	6.38	17 (33%)
10	A86	14	315	-	47,50,50	4.16	23 (48%)	51,76,76	6.58	17 (33%)
8	CLA	14	301	1	69,73,73	1.97	18 (26%)	82,113,113	2.65	29 (35%)
9	KC1	20	306	6	49,53,53	3.03	24 (48%)	61,89,89	3.77	34 (55%)
8	CLA	21	208	-	69,73,73	2.04	21 (30%)	82,113,113	2.60	31 (37%)
9	KC1	13	307	1	49,53,53	3.00	23 (46%)	61,89,89	3.83	35 (57%)
10	A86	20	313	-	47,50,50	4.37	24 (51%)	51,76,76	7.21	14 (27%)
10	A86	15	316	-	47,50,50	4.24	24 (51%)	51,76,76	6.38	20 (39%)
8	CLA	19	306	5	69,73,73	1.94	20 (28%)	82,113,113	2.64	31 (37%)
15	LHG	17	317	-	43,43,48	0.65	0	46,49,54	1.32	6 (13%)
8	CLA	13	301	17	69,73,73	1.99	20 (28%)	82,113,113	2.60	31 (37%)
10	A86	12	315	-	47,50,50	4.29	23 (48%)	51,76,76	6.91	19 (37%)
11	LMG	16	315	-	36,36,55	0.96	1 (2%)	44,44,63	1.24	6 (13%)
8	CLA	13	311	-	49,53,73	2.42	20 (40%)	58,89,113	3.10	29 (50%)
13	DD6	21	212	-	40,45,45	5.47	23 (57%)	51,67,67	6.18	32 (62%)
8	CLA	12	303	2	69,73,73	1.96	19 (27%)	82,113,113	2.60	29 (35%)
9	KC1	16	304	3	49,53,53	3.01	23 (46%)	61,89,89	3.88	33 (54%)
9	KC1	14	309	1	49,53,53	2.97	22 (44%)	61,89,89	3.74	36 (59%)
10	A86	15	313	-	47,50,50	4.30	23 (48%)	51,76,76	6.26	14 (27%)
9	KC1	11	306	1	49,53,53	2.97	22 (44%)	61,89,89	3.80	33 (54%)
8	CLA	12	307	17	54,58,73	2.27	19 (35%)	64,95,113	3.02	32 (50%)
9	KC1	20	303	-	49,53,53	3.00	22 (44%)	61,89,89	4.06	37 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	SQD	17	301	-	47,49,54	1.00	5 (10%)	57,60,65	1.48	11 (19%)
9	KC1	21	203	-	49,53,53	3.04	24 (48%)	61,89,89	3.83	35 (57%)
10	A86	14	312	-	47,50,50	4.20	23 (48%)	51,76,76	6.65	22 (43%)
10	A86	17	313	-	47,50,50	4.19	23 (48%)	51,76,76	6.00	19 (37%)

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
9	KC1	12	306	2	-	6/15/71/71	-
13	DD6	21	216	-	-	15/26/80/80	0/3/3/3
8	CLA	17	310	17	1/1/15/20	9/39/115/115	-
8	CLA	19	309	5	1/1/11/20	4/15/91/115	-
9	KC1	17	309	4	-	6/15/71/71	-
9	KC1	14	304	1	-	4/15/71/71	-
9	KC1	15	302	-	-	6/15/71/71	-
10	A86	15	319	-	-	8/34/90/90	0/3/3/3
8	CLA	20	302	6	-	13/29/105/115	-
9	KC1	11	308	1	-	8/15/71/71	-
8	CLA	14	308	17	1/1/15/20	11/39/115/115	-
10	A86	14	314	-	-	14/34/90/90	0/3/3/3
9	KC1	16	305	3	-	6/15/71/71	-
10	A86	19	311	-	-	6/34/90/90	0/3/3/3
8	CLA	13	309	17	-	8/39/115/115	-
8	CLA	12	309	2	1/1/12/20	13/24/100/115	-
10	A86	21	215	-	-	7/34/90/90	0/3/3/3
10	A86	17	311	-	-	9/34/90/90	0/3/3/3
8	CLA	12	301	17	1/1/15/20	13/39/115/115	-
8	CLA	17	307	4	1/1/12/20	11/24/100/115	-
9	KC1	14	306	1	-	6/15/71/71	-
10	A86	14	313	-	-	12/34/90/90	0/3/3/3
8	CLA	13	308	1	1/1/12/20	13/24/100/115	-
8	CLA	16	303	-	1/1/13/20	9/30/106/115	-
10	A86	13	314	-	-	19/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	A86	19	313	-	-	7/34/90/90	0/3/3/3
10	A86	18	314	-	-	13/34/90/90	0/3/3/3
13	DD6	16	312	-	-	11/26/80/80	0/3/3/3
9	KC1	11	304	1	-	4/15/71/71	-
9	KC1	12	310	2	-	8/15/71/71	-
9	KC1	15	304	1	-	6/15/71/71	-
10	A86	17	321	-	-	7/34/90/90	0/3/3/3
15	LHG	19	314	8	-	26/53/53/53	-
10	A86	13	313	-	-	8/34/90/90	0/3/3/3
10	A86	16	311	-	-	7/34/90/90	0/3/3/3
9	KC1	18	309	1	-	6/15/71/71	-
8	CLA	15	308	17	1/1/15/20	10/39/115/115	-
10	A86	13	312	-	-	5/34/90/90	0/3/3/3
9	KC1	15	306	1	-	7/15/71/71	-
15	LHG	21	201	-	-	18/38/38/53	-
9	KC1	17	306	4	-	10/15/71/71	-
8	CLA	11	309	17	1/1/12/20	8/23/99/115	-
8	CLA	19	303	17	1/1/15/20	15/39/115/115	-
10	A86	18	312	-	-	9/34/90/90	0/3/3/3
8	CLA	17	308	17	1/1/15/20	8/39/115/115	-
8	CLA	19	305	5	1/1/12/20	7/23/99/115	-
8	CLA	20	310	6	1/1/11/20	4/15/91/115	-
11	LMG	11	316	-	-	13/27/47/70	0/1/1/1
9	KC1	13	303	-	-	5/15/71/71	-
10	A86	12	313	-	-	3/34/90/90	0/3/3/3
10	A86	16	313	-	-	8/34/90/90	0/3/3/3
10	A86	21	213	-	-	8/34/90/90	0/3/3/3
8	CLA	21	210	-	-	6/15/91/115	-
8	CLA	16	301	3	-	12/39/115/115	-
8	CLA	11	307	1	-	9/24/100/115	-
8	CLA	14	305	-	1/1/11/20	3/15/91/115	-
13	DD6	20	314	-	-	12/26/80/80	0/3/3/3
9	KC1	17	305	4	-	6/15/71/71	-
11	LMG	17	318	-	-	13/32/52/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	A86	12	302	-	-	13/34/90/90	0/3/3/3
8	CLA	21	209	7	1/1/11/20	7/15/91/115	-
8	CLA	13	304	-	1/1/13/20	12/30/106/115	-
9	KC1	17	303	-	-	6/15/71/71	-
9	KC1	20	305	6	-	6/15/71/71	-
9	KC1	18	306	1	-	5/15/71/71	-
10	A86	18	313	-	-	12/34/90/90	0/3/3/3
8	CLA	11	303	-	1/1/15/20	9/39/115/115	-
8	CLA	12	305	-	1/1/15/20	11/39/115/115	-
8	CLA	11	301	1	-	11/39/115/115	-
8	CLA	18	303	-	1/1/13/20	7/29/105/115	-
8	CLA	11	305	17	1/1/11/20	5/15/91/115	-
10	A86	11	311	-	-	6/34/90/90	0/3/3/3
10	A86	12	319	-	-	9/34/90/90	0/3/3/3
13	DD6	19	312	-	-	12/26/80/80	0/3/3/3
10	A86	18	311	-	-	6/34/90/90	0/3/3/3
8	CLA	19	310	5	1/1/15/20	9/39/115/115	-
8	CLA	19	304	5	1/1/11/20	5/15/91/115	-
10	A86	11	312	-	-	9/34/90/90	0/3/3/3
10	A86	11	318	-	-	7/34/90/90	0/3/3/3
8	CLA	18	305	-	1/1/11/20	6/15/91/115	-
9	KC1	16	308	3	-	5/15/71/71	-
10	A86	14	311	-	-	4/34/90/90	0/3/3/3
8	CLA	12	304	-	1/1/15/20	7/39/115/115	-
8	CLA	16	306	3	1/1/15/20	13/39/115/115	-
8	CLA	14	307	1	1/1/12/20	14/24/100/115	-
11	LMG	11	315	-	-	19/37/57/70	0/1/1/1
10	A86	21	214	-	-	5/34/90/90	0/3/3/3
8	CLA	14	310	-	1/1/11/20	4/15/91/115	-
8	CLA	15	301	1	-	7/39/115/115	-
9	KC1	13	305	1	-	7/15/71/71	-
10	A86	11	313	-	-	10/34/90/90	0/3/3/3
8	CLA	14	302	-	1/1/15/20	19/39/115/115	-
8	CLA	21	205	7	1/1/11/20	9/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	LHG	21	217	-	-	27/49/49/53	-
8	CLA	19	302	-	1/1/15/20	11/39/115/115	-
8	CLA	14	303	-	-	6/30/106/115	-
8	CLA	17	302	4	-	13/39/115/115	-
14	SQD	16	314	-	-	22/49/69/69	0/1/1/1
9	KC1	18	304	1	-	7/15/71/71	-
10	A86	17	312	-	-	8/34/90/90	0/3/3/3
10	A86	16	310	-	-	5/34/90/90	0/3/3/3
10	A86	21	211	-	-	9/34/90/90	0/3/3/3
8	CLA	15	307	1	1/1/12/20	13/24/100/115	-
8	CLA	13	302	1	-	13/39/115/115	-
8	CLA	20	308	6	1/1/11/20	8/15/91/115	-
10	A86	17	316	-	-	13/34/90/90	0/3/3/3
10	A86	15	314	-	-	13/34/90/90	0/3/3/3
8	CLA	18	308	17	1/1/15/20	8/39/115/115	-
9	KC1	21	207	7	-	7/15/71/71	-
10	A86	11	314	-	-	6/34/90/90	0/3/3/3
8	CLA	20	304	-	1/1/13/20	10/29/105/115	-
10	A86	13	315	-	-	9/34/90/90	0/3/3/3
8	CLA	21	206	7	1/1/15/20	15/39/115/115	-
10	A86	17	314	-	-	7/34/90/90	0/3/3/3
8	CLA	17	304	-	1/1/13/20	8/29/105/115	-
8	CLA	13	306	-	1/1/11/20	4/15/91/115	-
9	KC1	11	302	-	-	2/15/71/71	-
10	A86	12	314	-	-	12/34/90/90	0/3/3/3
10	A86	12	316	-	-	13/34/90/90	0/3/3/3
8	CLA	18	301	1	-	15/39/115/115	-
10	A86	11	310	-	-	6/34/90/90	0/3/3/3
9	KC1	12	308	2	-	6/15/71/71	-
10	A86	20	301	-	-	13/34/90/90	0/3/3/3
8	CLA	19	301	5	1/1/15/20	10/39/115/115	-
8	CLA	21	202	7	1/1/13/20	9/30/106/115	-
8	CLA	18	307	-	1/1/12/20	12/25/101/115	-
16	LMU	19	315	-	-	6/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	CLA	15	310	-	1/1/11/20	4/15/91/115	-
9	KC1	16	302	-	-	2/15/71/71	-
8	CLA	20	307	6	1/1/12/20	6/21/97/115	-
8	CLA	21	204	-	1/1/13/20	8/31/107/115	-
9	KC1	13	310	1	-	6/15/71/71	-
9	KC1	15	309	1	-	8/15/71/71	-
8	CLA	15	303	-	1/1/13/20	7/30/106/115	-
10	A86	14	316	-	-	13/34/90/90	0/3/3/3
8	CLA	19	307	15	1/1/15/20	8/39/115/115	-
8	CLA	20	309	-	1/1/11/20	4/18/94/115	-
8	CLA	18	310	-	-	5/15/91/115	-
8	CLA	12	311	-	1/1/11/20	8/15/91/115	-
10	A86	12	312	-	-	5/34/90/90	0/3/3/3
10	A86	15	315	-	-	8/34/90/90	0/3/3/3
13	DD6	20	312	-	-	14/26/80/80	0/3/3/3
8	CLA	18	302	-	1/1/15/20	9/39/115/115	-
10	A86	17	315	-	-	9/34/90/90	0/3/3/3
8	CLA	15	305	-	1/1/11/20	5/15/91/115	-
10	A86	13	316	-	-	11/34/90/90	0/3/3/3
8	CLA	16	307	17	1/1/14/20	14/35/111/115	-
10	A86	15	311	-	-	6/34/90/90	0/3/3/3
10	A86	20	311	-	-	5/34/90/90	0/3/3/3
9	KC1	19	308	-	-	4/15/71/71	-
8	CLA	16	309	-	1/1/11/20	6/15/91/115	-
10	A86	15	312	-	-	9/34/90/90	0/3/3/3
10	A86	14	315	-	-	6/34/90/90	0/3/3/3
8	CLA	14	301	1	-	14/39/115/115	-
9	KC1	20	306	6	-	11/15/71/71	-
8	CLA	21	208	-	1/1/15/20	12/39/115/115	-
9	KC1	13	307	1	-	5/15/71/71	-
10	A86	20	313	-	-	15/34/90/90	0/3/3/3
10	A86	15	316	-	-	13/34/90/90	0/3/3/3
8	CLA	19	306	5	1/1/15/20	8/39/115/115	-
15	LHG	17	317	-	-	26/48/48/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	CLA	13	301	17	-	10/39/115/115	-
10	A86	12	315	-	-	9/34/90/90	0/3/3/3
11	LMG	16	315	-	-	14/31/51/70	0/1/1/1
8	CLA	13	311	-	-	2/15/91/115	-
13	DD6	21	212	-	-	13/26/80/80	0/3/3/3
8	CLA	12	303	2	1/1/15/20	14/39/115/115	-
9	KC1	16	304	3	-	6/15/71/71	-
9	KC1	14	309	1	-	6/15/71/71	-
10	A86	15	313	-	-	9/34/90/90	0/3/3/3
9	KC1	11	306	1	-	7/15/71/71	-
8	CLA	12	307	17	-	2/21/97/115	-
9	KC1	20	303	-	-	6/15/71/71	-
14	SQD	17	301	-	-	24/44/64/69	0/1/1/1
9	KC1	21	203	-	-	2/15/71/71	-
10	A86	14	312	-	-	6/34/90/90	0/3/3/3
10	A86	17	313	-	-	6/34/90/90	0/3/3/3

All (3602) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	20	313	A86	C14-C13	15.94	1.69	1.51
10	15	314	A86	C14-C13	15.67	1.68	1.51
10	14	314	A86	C14-C13	15.65	1.68	1.51
10	20	311	A86	C14-C13	15.58	1.68	1.51
10	21	214	A86	C14-C13	15.56	1.68	1.51
10	19	313	A86	C14-C13	15.56	1.68	1.51
10	21	213	A86	C14-C13	15.53	1.68	1.51
10	21	211	A86	C14-C13	15.51	1.68	1.51
10	12	319	A86	C14-C13	15.49	1.68	1.51
10	18	313	A86	C14-C13	15.47	1.68	1.51
10	15	319	A86	C14-C13	15.39	1.68	1.51
10	15	315	A86	C14-C13	15.39	1.68	1.51
10	17	314	A86	C14-C13	15.37	1.68	1.51
10	12	315	A86	C14-C13	15.35	1.68	1.51
10	17	311	A86	C14-C13	15.32	1.68	1.51
10	14	312	A86	C14-C13	15.32	1.68	1.51
10	11	314	A86	C14-C13	15.31	1.68	1.51
10	14	315	A86	C14-C13	15.30	1.68	1.51
10	13	315	A86	C14-C13	15.28	1.68	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	18	312	A86	C14-C13	15.27	1.68	1.51
10	11	312	A86	C14-C13	15.25	1.68	1.51
10	13	316	A86	C14-C13	15.24	1.68	1.51
10	12	312	A86	C14-C13	15.23	1.68	1.51
10	13	314	A86	C14-C13	15.23	1.68	1.51
10	14	311	A86	C14-C13	15.23	1.68	1.51
10	13	312	A86	C14-C13	15.19	1.68	1.51
10	12	316	A86	C14-C13	15.18	1.68	1.51
10	17	321	A86	C14-C13	15.17	1.68	1.51
10	13	313	A86	C14-C13	15.10	1.68	1.51
10	16	311	A86	C14-C13	15.08	1.68	1.51
10	11	313	A86	C14-C13	15.05	1.68	1.51
10	12	302	A86	C14-C13	15.05	1.68	1.51
10	11	318	A86	C14-C13	15.04	1.68	1.51
10	15	311	A86	C14-C13	15.03	1.68	1.51
10	19	311	A86	C14-C13	15.01	1.68	1.51
10	17	313	A86	C14-C13	14.99	1.68	1.51
10	14	316	A86	C14-C13	14.90	1.67	1.51
10	11	310	A86	C14-C13	14.88	1.67	1.51
10	17	316	A86	C14-C13	14.86	1.67	1.51
10	11	311	A86	C14-C13	14.85	1.67	1.51
10	20	301	A86	C14-C13	14.81	1.67	1.51
10	15	312	A86	C14-C13	14.80	1.67	1.51
10	14	313	A86	C14-C13	14.78	1.67	1.51
10	18	311	A86	C14-C13	14.77	1.67	1.51
10	15	316	A86	C14-C13	14.72	1.67	1.51
10	16	310	A86	C14-C13	14.68	1.67	1.51
10	21	215	A86	C14-C13	14.67	1.67	1.51
10	12	314	A86	C14-C13	14.63	1.67	1.51
10	17	315	A86	C14-C13	14.59	1.67	1.51
10	17	312	A86	C14-C13	14.59	1.67	1.51
13	20	314	DD6	C10-C11	14.58	1.69	1.35
13	21	212	DD6	C10-C11	14.54	1.69	1.35
10	12	313	A86	C14-C13	14.54	1.67	1.51
13	21	216	DD6	C10-C11	14.52	1.69	1.35
10	18	314	A86	C14-C13	14.47	1.67	1.51
13	19	312	DD6	C10-C11	14.47	1.69	1.35
13	20	312	DD6	C10-C11	14.46	1.69	1.35
13	16	312	DD6	C10-C11	14.40	1.69	1.35
13	20	314	DD6	C36-C31	14.35	1.50	1.35
10	16	313	A86	C14-C13	14.07	1.66	1.51
10	15	313	A86	C14-C13	13.98	1.66	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	16	312	DD6	C36-C31	13.84	1.50	1.35
13	20	312	DD6	C36-C31	13.45	1.49	1.35
13	21	212	DD6	C36-C31	13.44	1.49	1.35
13	21	216	DD6	C36-C31	13.42	1.49	1.35
13	19	312	DD6	C36-C31	12.75	1.49	1.35
10	20	301	A86	C30-C31	11.93	1.44	1.30
10	21	213	A86	C30-C31	11.87	1.44	1.30
10	15	313	A86	C30-C31	11.80	1.44	1.30
10	12	314	A86	C30-C31	11.75	1.44	1.30
10	15	314	A86	C30-C31	11.68	1.44	1.30
10	14	313	A86	C30-C31	11.66	1.44	1.30
10	13	315	A86	C30-C31	11.60	1.44	1.30
10	13	314	A86	C30-C31	11.58	1.44	1.30
10	21	215	A86	C30-C31	11.55	1.44	1.30
10	11	312	A86	C30-C31	11.54	1.44	1.30
13	16	312	DD6	C28-C27	11.47	1.58	1.50
10	13	313	A86	C30-C31	11.28	1.43	1.30
10	18	314	A86	C30-C31	11.28	1.43	1.30
10	21	214	A86	C30-C31	11.23	1.43	1.30
10	18	313	A86	C30-C31	11.18	1.43	1.30
10	15	316	A86	C30-C31	11.12	1.43	1.30
10	21	211	A86	C30-C31	11.11	1.43	1.30
10	18	311	A86	C30-C31	11.00	1.43	1.30
10	14	314	A86	C30-C31	11.00	1.43	1.30
10	12	316	A86	C30-C31	10.99	1.43	1.30
10	12	315	A86	C30-C31	10.99	1.43	1.30
10	13	316	A86	C30-C31	10.97	1.43	1.30
10	14	312	A86	C30-C31	10.96	1.43	1.30
13	20	312	DD6	C28-C27	10.95	1.58	1.50
10	18	312	A86	C30-C31	10.90	1.43	1.30
13	20	314	DD6	C28-C27	10.87	1.58	1.50
10	14	311	A86	C30-C31	10.87	1.43	1.30
10	17	313	A86	C30-C31	10.84	1.43	1.30
10	20	311	A86	C30-C31	10.83	1.43	1.30
10	12	312	A86	C30-C31	10.83	1.43	1.30
10	14	316	A86	C30-C31	10.81	1.43	1.30
13	19	312	DD6	C28-C27	10.77	1.58	1.50
13	21	216	DD6	C28-C27	10.74	1.58	1.50
10	17	311	A86	C30-C31	10.72	1.43	1.30
10	17	312	A86	C30-C31	10.70	1.43	1.30
10	13	312	A86	C30-C31	10.68	1.43	1.30
10	11	311	A86	C30-C31	10.67	1.43	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	17	314	A86	C30-C31	10.65	1.43	1.30
10	15	312	A86	C30-C31	10.64	1.43	1.30
10	19	313	A86	C30-C31	10.61	1.43	1.30
10	12	313	A86	C30-C31	10.61	1.43	1.30
10	20	313	A86	C30-C31	10.56	1.42	1.30
10	15	311	A86	C30-C31	10.55	1.42	1.30
10	11	313	A86	C30-C31	10.50	1.42	1.30
10	17	316	A86	C30-C31	10.49	1.42	1.30
10	11	314	A86	C30-C31	10.48	1.42	1.30
10	11	310	A86	C30-C31	10.47	1.42	1.30
10	15	319	A86	C30-C31	10.47	1.42	1.30
10	15	315	A86	C30-C31	10.40	1.42	1.30
10	16	313	A86	C30-C31	10.31	1.42	1.30
10	12	302	A86	C30-C31	10.13	1.42	1.30
10	17	315	A86	C30-C31	10.11	1.42	1.30
10	17	321	A86	C30-C31	10.11	1.42	1.30
13	21	212	DD6	C28-C27	10.11	1.57	1.50
10	14	315	A86	C30-C31	10.08	1.42	1.30
10	19	311	A86	C30-C31	10.03	1.42	1.30
13	21	216	DD6	C5-C6	9.99	1.58	1.35
13	20	314	DD6	C5-C6	9.93	1.58	1.35
10	11	318	A86	C30-C31	9.86	1.42	1.30
13	21	212	DD6	C5-C6	9.86	1.58	1.35
10	16	311	A86	C30-C31	9.82	1.42	1.30
13	20	312	DD6	C5-C6	9.79	1.58	1.35
13	16	312	DD6	C5-C6	9.77	1.58	1.35
10	16	310	A86	C30-C31	9.64	1.41	1.30
13	19	312	DD6	C5-C6	9.60	1.58	1.35
10	21	213	A86	C30-C29	9.59	1.47	1.31
10	12	319	A86	C30-C31	9.57	1.41	1.30
10	15	313	A86	C30-C29	9.55	1.47	1.31
10	20	301	A86	C30-C29	9.51	1.47	1.31
10	15	314	A86	C30-C29	9.47	1.47	1.31
10	13	314	A86	C30-C29	9.43	1.47	1.31
10	12	314	A86	C30-C29	9.40	1.47	1.31
10	14	313	A86	C30-C29	9.37	1.47	1.31
10	13	315	A86	C30-C29	9.34	1.47	1.31
10	21	215	A86	C30-C29	9.34	1.47	1.31
10	11	312	A86	C30-C29	9.24	1.46	1.31
13	16	312	DD6	C13-C11	-9.13	1.26	1.46
10	18	314	A86	C30-C29	9.11	1.46	1.31
10	18	313	A86	C30-C29	9.10	1.46	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	21	214	A86	C30-C29	9.10	1.46	1.31
10	12	315	A86	C30-C29	9.10	1.46	1.31
10	21	211	A86	C30-C29	9.07	1.46	1.31
10	13	313	A86	C30-C29	9.06	1.46	1.31
10	15	316	A86	C30-C29	9.03	1.46	1.31
10	14	314	A86	C30-C29	9.00	1.46	1.31
13	20	314	DD6	C23-C16	8.99	1.71	1.53
13	21	216	DD6	C23-C16	8.96	1.70	1.53
10	18	311	A86	C30-C29	8.95	1.46	1.31
10	13	316	A86	C30-C29	8.94	1.46	1.31
10	20	311	A86	C30-C29	8.94	1.46	1.31
10	12	316	A86	C30-C29	8.84	1.46	1.31
10	17	311	A86	C30-C29	8.83	1.46	1.31
10	12	312	A86	C30-C29	8.83	1.46	1.31
10	17	313	A86	C30-C29	8.82	1.46	1.31
10	17	314	A86	C30-C29	8.81	1.46	1.31
10	18	312	A86	C30-C29	8.80	1.46	1.31
10	11	313	A86	C30-C29	8.77	1.46	1.31
10	12	313	A86	C30-C29	8.76	1.46	1.31
10	15	312	A86	C30-C29	8.75	1.46	1.31
10	15	319	A86	C30-C29	8.74	1.46	1.31
10	14	312	A86	C30-C29	8.73	1.46	1.31
13	20	312	DD6	C23-C16	8.73	1.70	1.53
10	14	311	A86	C30-C29	8.73	1.46	1.31
10	15	311	A86	C30-C29	8.72	1.46	1.31
10	14	316	A86	C30-C29	8.72	1.46	1.31
10	11	314	A86	C30-C29	8.70	1.46	1.31
10	13	312	A86	C30-C29	8.68	1.46	1.31
10	20	313	A86	C30-C29	8.64	1.45	1.31
10	17	312	A86	C30-C29	8.61	1.45	1.31
10	19	313	A86	C30-C29	8.59	1.45	1.31
10	11	311	A86	C30-C29	8.59	1.45	1.31
10	17	316	A86	C30-C29	8.56	1.45	1.31
10	11	310	A86	C30-C29	8.55	1.45	1.31
10	15	315	A86	C30-C29	8.54	1.45	1.31
10	16	313	A86	C30-C29	8.49	1.45	1.31
10	17	321	A86	C30-C29	8.49	1.45	1.31
13	20	314	DD6	C13-C11	-8.47	1.27	1.46
13	21	212	DD6	C13-C11	-8.36	1.28	1.46
10	17	315	A86	C30-C29	8.35	1.45	1.31
10	12	302	A86	C30-C29	8.33	1.45	1.31
10	14	315	A86	C30-C29	8.33	1.45	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	21	216	DD6	C13-C11	-8.33	1.28	1.46
13	19	312	DD6	C13-C11	-8.27	1.28	1.46
13	21	212	DD6	C23-C16	8.26	1.69	1.53
10	19	311	A86	C30-C29	8.19	1.45	1.31
13	16	312	DD6	C23-C16	8.18	1.69	1.53
10	11	318	A86	C30-C29	8.17	1.45	1.31
13	20	312	DD6	C13-C11	-8.14	1.28	1.46
10	16	310	A86	C30-C29	8.06	1.45	1.31
10	12	319	A86	C30-C29	8.05	1.45	1.31
10	16	311	A86	C30-C29	8.02	1.44	1.31
13	21	216	DD6	C19-C20	8.02	1.63	1.52
13	21	212	DD6	C19-C20	7.98	1.63	1.52
9	16	302	KC1	C2A-C3A	7.94	1.53	1.37
9	16	308	KC1	C2A-C3A	7.90	1.53	1.37
9	17	303	KC1	C2A-C3A	7.87	1.53	1.37
10	18	312	A86	C19-C20	7.87	1.63	1.52
9	12	310	KC1	C2A-C3A	7.84	1.53	1.37
13	19	312	DD6	C23-C16	7.81	1.68	1.53
9	17	306	KC1	C2A-C3A	7.79	1.53	1.37
10	20	301	A86	C4-C5	7.75	1.67	1.43
9	14	306	KC1	C2A-C3A	7.75	1.52	1.37
9	17	309	KC1	C2A-C3A	7.75	1.52	1.37
9	11	308	KC1	C2A-C3A	7.71	1.52	1.37
9	18	306	KC1	C2A-C3A	7.70	1.52	1.37
10	20	313	A86	C4-C5	7.66	1.66	1.43
10	12	316	A86	C4-C5	7.65	1.66	1.43
10	13	314	A86	C4-C5	7.65	1.66	1.43
9	15	309	KC1	C2A-C3A	7.65	1.52	1.37
9	13	310	KC1	C2A-C3A	7.65	1.52	1.37
9	21	203	KC1	C2A-C3A	7.65	1.52	1.37
10	21	213	A86	C4-C5	7.64	1.66	1.43
9	11	304	KC1	C2A-C3A	7.64	1.52	1.37
10	14	313	A86	C4-C5	7.63	1.66	1.43
13	20	314	DD6	C9-C10	7.62	1.66	1.43
10	18	314	A86	C4-C5	7.62	1.66	1.43
10	15	314	A86	C4-C5	7.61	1.66	1.43
10	13	315	A86	C4-C5	7.61	1.66	1.43
13	19	312	DD6	C19-C20	7.61	1.62	1.52
9	17	305	KC1	C2A-C3A	7.61	1.52	1.37
10	21	211	A86	C4-C5	7.60	1.66	1.43
9	11	302	KC1	C2A-C3A	7.60	1.52	1.37
13	21	216	DD6	C9-C10	7.59	1.66	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	14	316	A86	C4-C5	7.59	1.66	1.43
10	15	313	A86	C4-C5	7.58	1.66	1.43
10	15	316	A86	C4-C5	7.58	1.66	1.43
9	16	305	KC1	C2A-C3A	7.57	1.52	1.37
10	12	314	A86	C4-C5	7.57	1.66	1.43
13	16	312	DD6	C19-C20	7.56	1.62	1.52
9	13	307	KC1	C2A-C3A	7.56	1.52	1.37
9	20	306	KC1	C2A-C3A	7.56	1.52	1.37
9	12	308	KC1	C2A-C3A	7.56	1.52	1.37
10	13	315	A86	C8-C6	7.55	1.62	1.46
9	11	306	KC1	C2A-C3A	7.54	1.52	1.37
10	21	215	A86	C4-C5	7.53	1.66	1.43
10	13	316	A86	C4-C5	7.53	1.66	1.43
10	15	312	A86	C4-C5	7.52	1.66	1.43
10	14	314	A86	C4-C5	7.52	1.66	1.43
9	20	305	KC1	C2A-C3A	7.51	1.52	1.37
9	14	309	KC1	C2A-C3A	7.51	1.52	1.37
10	17	316	A86	C4-C5	7.51	1.66	1.43
13	19	312	DD6	C9-C10	7.50	1.66	1.43
10	19	313	A86	C4-C5	7.50	1.66	1.43
13	20	312	DD6	C9-C10	7.50	1.66	1.43
9	18	309	KC1	C2A-C3A	7.49	1.52	1.37
13	16	312	DD6	C9-C10	7.49	1.66	1.43
10	20	313	A86	C8-C6	7.49	1.62	1.46
10	13	314	A86	C8-C6	7.49	1.62	1.46
13	21	212	DD6	C9-C10	7.48	1.66	1.43
9	15	306	KC1	C2A-C3A	7.47	1.52	1.37
10	18	313	A86	C4-C5	7.47	1.66	1.43
10	15	314	A86	C19-C20	7.46	1.62	1.52
10	13	313	A86	C4-C5	7.45	1.66	1.43
10	21	214	A86	C4-C5	7.44	1.66	1.43
10	20	311	A86	C4-C5	7.44	1.66	1.43
9	13	303	KC1	C2A-C3A	7.44	1.52	1.37
10	20	311	A86	C19-C20	7.43	1.62	1.52
10	14	313	A86	C8-C6	7.42	1.61	1.46
9	15	302	KC1	C2A-C3A	7.42	1.52	1.37
10	18	314	A86	C8-C6	7.41	1.61	1.46
10	15	314	A86	C8-C6	7.40	1.61	1.46
10	13	316	A86	C8-C6	7.40	1.61	1.46
10	18	311	A86	C8-C6	7.40	1.61	1.46
10	11	310	A86	C4-C5	7.38	1.66	1.43
10	14	314	A86	C19-C20	7.37	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	12	315	A86	C4-C5	7.37	1.66	1.43
10	21	213	A86	C8-C6	7.37	1.61	1.46
13	20	314	DD6	C19-C20	7.36	1.62	1.52
10	15	311	A86	C4-C5	7.36	1.66	1.43
10	11	312	A86	C4-C5	7.36	1.66	1.43
10	14	315	A86	C4-C5	7.36	1.66	1.43
10	15	313	A86	C8-C6	7.35	1.61	1.46
9	20	303	KC1	C2A-C3A	7.35	1.52	1.37
10	18	313	A86	C19-C20	7.35	1.62	1.52
10	18	311	A86	C4-C5	7.34	1.65	1.43
10	12	302	A86	C4-C5	7.34	1.65	1.43
10	12	316	A86	C8-C6	7.33	1.61	1.46
10	20	313	A86	C19-C20	7.33	1.62	1.52
9	18	304	KC1	C2A-C3A	7.33	1.52	1.37
10	17	313	A86	C4-C5	7.32	1.65	1.43
10	17	312	A86	C4-C5	7.32	1.65	1.43
10	21	211	A86	C8-C6	7.32	1.61	1.46
10	15	315	A86	C19-C20	7.31	1.62	1.52
9	12	306	KC1	C2A-C3A	7.31	1.52	1.37
10	11	313	A86	C4-C5	7.31	1.65	1.43
10	21	215	A86	C8-C6	7.31	1.61	1.46
10	13	315	A86	C19-C20	7.31	1.62	1.52
10	13	312	A86	C4-C5	7.31	1.65	1.43
10	17	316	A86	C8-C6	7.30	1.61	1.46
10	12	312	A86	C4-C5	7.30	1.65	1.43
10	19	313	A86	C19-C20	7.30	1.62	1.52
10	19	313	A86	C8-C6	7.29	1.61	1.46
10	12	314	A86	C8-C6	7.29	1.61	1.46
10	17	314	A86	C4-C5	7.29	1.65	1.43
10	19	311	A86	C4-C5	7.28	1.65	1.43
10	20	311	A86	C8-C6	7.28	1.61	1.46
10	21	211	A86	C19-C20	7.28	1.62	1.52
10	15	316	A86	C8-C6	7.27	1.61	1.46
10	15	319	A86	C4-C5	7.26	1.65	1.43
9	16	304	KC1	C2A-C3A	7.26	1.51	1.37
10	15	315	A86	C4-C5	7.26	1.65	1.43
10	17	311	A86	C4-C5	7.26	1.65	1.43
10	17	315	A86	C4-C5	7.25	1.65	1.43
10	17	321	A86	C4-C5	7.25	1.65	1.43
10	14	316	A86	C8-C6	7.25	1.61	1.46
9	13	305	KC1	C2A-C3A	7.25	1.51	1.37
9	19	308	KC1	C2A-C3A	7.23	1.51	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	21	214	A86	C19-C20	7.23	1.62	1.52
13	20	312	DD6	C19-C20	7.22	1.62	1.52
10	21	214	A86	C8-C6	7.22	1.61	1.46
10	17	314	A86	C19-C20	7.21	1.62	1.52
10	11	318	A86	C4-C5	7.21	1.65	1.43
10	16	310	A86	C4-C5	7.20	1.65	1.43
10	14	314	A86	C8-C6	7.20	1.61	1.46
10	16	313	A86	C4-C5	7.20	1.65	1.43
10	18	313	A86	C8-C6	7.20	1.61	1.46
10	11	311	A86	C4-C5	7.19	1.65	1.43
10	14	312	A86	C4-C5	7.19	1.65	1.43
10	12	313	A86	C4-C5	7.19	1.65	1.43
10	20	301	A86	C8-C6	7.18	1.61	1.46
10	11	314	A86	C4-C5	7.16	1.65	1.43
10	18	312	A86	C4-C5	7.15	1.65	1.43
9	15	304	KC1	C2A-C3A	7.14	1.51	1.37
10	12	315	A86	C19-C20	7.13	1.62	1.52
10	12	314	A86	C19-C20	7.13	1.62	1.52
10	13	313	A86	C8-C6	7.13	1.61	1.46
13	21	216	DD6	C30-C29	7.12	1.40	1.20
9	21	207	KC1	C2A-C3A	7.12	1.51	1.37
10	12	302	A86	C8-C6	7.12	1.61	1.46
10	14	311	A86	C4-C5	7.11	1.65	1.43
10	15	312	A86	C8-C6	7.11	1.61	1.46
10	11	313	A86	C19-C20	7.10	1.62	1.52
13	21	212	DD6	C24-C1	7.10	1.61	1.46
10	16	311	A86	C4-C5	7.10	1.65	1.43
13	16	312	DD6	C30-C31	7.09	1.55	1.42
13	21	212	DD6	C30-C29	7.09	1.40	1.20
13	16	312	DD6	C30-C29	7.08	1.40	1.20
13	19	312	DD6	C21-C20	-7.07	1.41	1.51
13	21	212	DD6	C30-C31	7.06	1.55	1.42
9	14	304	KC1	C2A-C3A	7.06	1.51	1.37
10	12	315	A86	C8-C6	7.05	1.61	1.46
10	12	319	A86	C4-C5	7.04	1.65	1.43
10	19	311	A86	C8-C6	7.04	1.61	1.46
10	17	315	A86	C19-C20	7.04	1.62	1.52
10	17	313	A86	C8-C6	7.02	1.61	1.46
10	15	313	A86	C25-C26	7.02	1.64	1.43
13	20	314	DD6	C24-C1	7.01	1.61	1.46
10	15	312	A86	C25-C26	7.00	1.64	1.43
10	11	312	A86	C25-C26	7.00	1.64	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	15	315	A86	C8-C6	7.00	1.60	1.46
10	11	312	A86	C8-C6	6.99	1.60	1.46
10	13	313	A86	C25-C26	6.99	1.64	1.43
10	21	213	A86	C25-C26	6.99	1.64	1.43
10	14	313	A86	C25-C26	6.99	1.64	1.43
10	13	312	A86	C8-C6	6.99	1.60	1.46
10	12	312	A86	C8-C6	6.99	1.60	1.46
10	12	313	A86	C25-C26	6.98	1.64	1.43
10	17	314	A86	C8-C6	6.98	1.60	1.46
13	20	314	DD6	C30-C29	6.97	1.39	1.20
10	12	314	A86	C25-C26	6.97	1.64	1.43
13	20	314	DD6	C30-C31	6.97	1.55	1.42
10	17	315	A86	C8-C6	6.96	1.60	1.46
10	16	313	A86	C8-C6	6.96	1.60	1.46
10	11	313	A86	C8-C6	6.96	1.60	1.46
10	14	315	A86	C8-C6	6.94	1.60	1.46
10	13	314	A86	C25-C26	6.93	1.64	1.43
10	21	213	A86	C19-C20	6.93	1.61	1.52
10	18	312	A86	C8-C6	6.91	1.60	1.46
10	14	312	A86	C8-C6	6.91	1.60	1.46
10	17	321	A86	C8-C6	6.90	1.60	1.46
13	21	216	DD6	C30-C31	6.89	1.55	1.42
10	13	315	A86	C25-C26	6.88	1.64	1.43
10	17	311	A86	C19-C20	6.88	1.61	1.52
10	17	311	A86	C8-C6	6.88	1.60	1.46
10	17	313	A86	C25-C26	6.88	1.64	1.43
10	17	312	A86	C25-C26	6.88	1.64	1.43
10	13	314	A86	C19-C20	6.86	1.61	1.52
10	12	312	A86	C19-C20	6.86	1.61	1.52
10	11	311	A86	C8-C6	6.86	1.60	1.46
10	11	310	A86	C8-C6	6.85	1.60	1.46
10	13	313	A86	C19-C20	6.85	1.61	1.52
10	15	319	A86	C8-C6	6.85	1.60	1.46
10	15	311	A86	C8-C6	6.85	1.60	1.46
13	20	312	DD6	C24-C1	6.85	1.60	1.46
10	17	312	A86	C8-C6	6.84	1.60	1.46
10	18	311	A86	C19-C20	6.83	1.61	1.52
13	20	314	DD6	C21-C20	-6.82	1.41	1.51
10	20	313	A86	C25-C26	6.82	1.64	1.43
13	20	312	DD6	C30-C29	6.82	1.39	1.20
13	21	216	DD6	C24-C1	6.81	1.60	1.46
10	15	314	A86	C25-C26	6.81	1.64	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	21	215	A86	C19-C20	6.80	1.61	1.52
10	11	318	A86	C25-C26	6.80	1.64	1.43
10	15	312	A86	C19-C20	6.79	1.61	1.52
10	15	311	A86	C25-C26	6.79	1.64	1.43
10	21	214	A86	C25-C26	6.79	1.64	1.43
10	18	313	A86	C25-C26	6.79	1.64	1.43
10	16	311	A86	C8-C6	6.78	1.60	1.46
10	21	215	A86	C25-C26	6.78	1.64	1.43
10	11	314	A86	C25-C26	6.78	1.64	1.43
10	12	313	A86	C19-C20	6.78	1.61	1.52
10	11	318	A86	C8-C6	6.78	1.60	1.46
13	16	312	DD6	C24-C1	6.78	1.60	1.46
10	16	310	A86	C8-C6	6.78	1.60	1.46
10	20	301	A86	C19-C20	6.78	1.61	1.52
10	15	316	A86	C25-C26	6.77	1.64	1.43
10	18	314	A86	C25-C26	6.77	1.64	1.43
9	13	305	KC1	CBA-CAA	6.76	1.53	1.33
10	14	314	A86	C25-C26	6.76	1.64	1.43
9	20	306	KC1	CBA-CAA	6.76	1.53	1.33
13	16	312	DD6	C21-C20	-6.75	1.41	1.51
10	18	311	A86	C25-C26	6.75	1.64	1.43
10	11	311	A86	C25-C26	6.75	1.64	1.43
10	14	311	A86	C8-C6	6.74	1.60	1.46
10	14	315	A86	C19-C20	6.74	1.61	1.52
10	20	301	A86	C25-C26	6.73	1.64	1.43
10	14	311	A86	C19-C20	6.73	1.61	1.52
10	21	211	A86	C25-C26	6.73	1.64	1.43
13	19	312	DD6	C30-C29	6.72	1.39	1.20
10	12	313	A86	C8-C6	6.71	1.60	1.46
10	12	316	A86	C25-C26	6.71	1.64	1.43
10	12	315	A86	C25-C26	6.71	1.64	1.43
10	17	316	A86	C25-C26	6.70	1.64	1.43
10	14	312	A86	C19-C20	6.69	1.61	1.52
9	18	306	KC1	CBA-CAA	6.69	1.53	1.33
9	11	304	KC1	CBA-CAA	6.68	1.53	1.33
10	11	310	A86	C25-C26	6.68	1.63	1.43
10	16	311	A86	C25-C26	6.68	1.63	1.43
10	12	319	A86	C19-C20	6.67	1.61	1.52
10	12	319	A86	C8-C6	6.67	1.60	1.46
9	16	308	KC1	CBA-CAA	6.67	1.53	1.33
10	13	316	A86	C25-C26	6.67	1.63	1.43
9	17	309	KC1	CBA-CAA	6.67	1.52	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	17	314	A86	C25-C26	6.67	1.63	1.43
9	17	305	KC1	CBA-CAA	6.66	1.52	1.33
9	12	306	KC1	CBA-CAA	6.66	1.52	1.33
10	17	321	A86	C19-C20	6.65	1.61	1.52
9	14	306	KC1	CBA-CAA	6.65	1.52	1.33
10	14	315	A86	C25-C26	6.65	1.63	1.43
10	11	314	A86	C8-C6	6.65	1.60	1.46
10	14	316	A86	C25-C26	6.65	1.63	1.43
9	20	305	KC1	CBA-CAA	6.64	1.52	1.33
9	14	304	KC1	CBA-CAA	6.64	1.52	1.33
9	18	309	KC1	CBA-CAA	6.63	1.52	1.33
10	19	313	A86	C25-C26	6.63	1.63	1.43
10	19	311	A86	C25-C26	6.63	1.63	1.43
9	11	302	KC1	CBA-CAA	6.63	1.52	1.33
9	16	304	KC1	CBA-CAA	6.63	1.52	1.33
9	15	304	KC1	CBA-CAA	6.62	1.52	1.33
9	13	307	KC1	CBA-CAA	6.62	1.52	1.33
13	21	216	DD6	C21-C20	-6.62	1.41	1.51
13	19	312	DD6	C24-C1	6.61	1.60	1.46
9	15	302	KC1	CBA-CAA	6.61	1.52	1.33
9	17	303	KC1	CBA-CAA	6.60	1.52	1.33
10	15	319	A86	C25-C26	6.60	1.63	1.43
9	21	207	KC1	CBA-CAA	6.59	1.52	1.33
13	20	312	DD6	C21-C20	-6.59	1.42	1.51
10	11	313	A86	C25-C26	6.59	1.63	1.43
10	14	312	A86	C25-C26	6.59	1.63	1.43
9	12	308	KC1	CBA-CAA	6.59	1.52	1.33
9	12	310	KC1	CBA-CAA	6.58	1.52	1.33
9	16	302	KC1	CBA-CAA	6.58	1.52	1.33
10	20	311	A86	C25-C26	6.58	1.63	1.43
10	19	311	A86	C19-C20	6.57	1.61	1.52
9	16	305	KC1	CBA-CAA	6.57	1.52	1.33
9	19	308	KC1	CBA-CAA	6.57	1.52	1.33
9	15	306	KC1	CBA-CAA	6.56	1.52	1.33
10	18	312	A86	C25-C26	6.56	1.63	1.43
9	17	306	KC1	CBA-CAA	6.56	1.52	1.33
9	13	303	KC1	CBA-CAA	6.55	1.52	1.33
10	13	312	A86	C19-C20	6.54	1.61	1.52
9	18	304	KC1	CBA-CAA	6.54	1.52	1.33
10	15	315	A86	C25-C26	6.53	1.63	1.43
9	11	306	KC1	CBA-CAA	6.53	1.52	1.33
9	21	203	KC1	CBA-CAA	6.53	1.52	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	15	309	KC1	CBA-CAA	6.52	1.52	1.33
10	17	312	A86	C19-C20	6.52	1.61	1.52
9	13	310	KC1	CBA-CAA	6.52	1.52	1.33
10	15	313	A86	C19-C20	6.51	1.61	1.52
10	14	313	A86	C19-C20	6.51	1.61	1.52
10	13	312	A86	C25-C26	6.51	1.63	1.43
9	20	303	KC1	CBA-CAA	6.51	1.52	1.33
10	17	311	A86	C25-C26	6.50	1.63	1.43
10	12	312	A86	C25-C26	6.48	1.63	1.43
10	17	321	A86	C25-C26	6.48	1.63	1.43
9	11	308	KC1	CBA-CAA	6.48	1.52	1.33
9	14	309	KC1	CBA-CAA	6.47	1.52	1.33
13	21	212	DD6	C21-C20	-6.46	1.42	1.51
13	20	312	DD6	C30-C31	6.45	1.54	1.42
10	14	311	A86	C25-C26	6.44	1.63	1.43
10	13	316	A86	C19-C20	6.43	1.61	1.52
10	12	302	A86	C25-C26	6.42	1.63	1.43
10	16	313	A86	C25-C26	6.41	1.63	1.43
10	15	311	A86	C19-C20	6.40	1.61	1.52
10	11	311	A86	C19-C20	6.39	1.61	1.52
10	12	319	A86	C25-C26	6.38	1.63	1.43
10	15	316	A86	C19-C20	6.38	1.61	1.52
10	12	302	A86	C19-C20	6.37	1.61	1.52
10	17	315	A86	C25-C26	6.36	1.62	1.43
10	16	310	A86	C25-C26	6.33	1.62	1.43
10	16	310	A86	C19-C20	6.31	1.61	1.52
10	17	316	A86	C19-C20	6.30	1.61	1.52
10	17	313	A86	C19-C20	6.22	1.60	1.52
10	11	318	A86	C19-C20	6.18	1.60	1.52
13	19	312	DD6	C30-C31	6.16	1.54	1.42
10	16	311	A86	C19-C20	6.15	1.60	1.52
10	18	314	A86	C19-C20	6.08	1.60	1.52
10	14	316	A86	C19-C20	6.08	1.60	1.52
9	15	304	KC1	O2A-CGA	6.05	1.45	1.30
10	11	310	A86	C19-C20	6.00	1.60	1.52
9	20	305	KC1	O2A-CGA	6.00	1.45	1.30
10	12	316	A86	C19-C20	5.98	1.60	1.52
10	11	314	A86	C19-C20	5.97	1.60	1.52
9	13	305	KC1	O2A-CGA	5.95	1.45	1.30
9	13	307	KC1	O2A-CGA	5.94	1.45	1.30
9	15	302	KC1	O2A-CGA	5.94	1.45	1.30
9	13	303	KC1	O2A-CGA	5.94	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	21	207	KC1	O2A-CGA	5.94	1.45	1.30
10	15	319	A86	C19-C20	5.93	1.60	1.52
9	14	304	KC1	O2A-CGA	5.93	1.45	1.30
9	20	303	KC1	O2A-CGA	5.92	1.45	1.30
9	21	203	KC1	O2A-CGA	5.92	1.45	1.30
9	21	203	KC1	C3B-C2B	5.90	1.49	1.37
9	15	306	KC1	O2A-CGA	5.89	1.45	1.30
9	14	306	KC1	O2A-CGA	5.87	1.45	1.30
9	17	309	KC1	O2A-CGA	5.87	1.45	1.30
9	17	303	KC1	O2A-CGA	5.87	1.45	1.30
9	19	308	KC1	O2A-CGA	5.86	1.45	1.30
13	21	216	DD6	C13-C14	5.85	1.45	1.32
9	18	304	KC1	O2A-CGA	5.85	1.45	1.30
9	12	308	KC1	O2A-CGA	5.84	1.45	1.30
9	16	304	KC1	O2A-CGA	5.83	1.45	1.30
9	18	306	KC1	O2A-CGA	5.82	1.45	1.30
9	16	302	KC1	O2A-CGA	5.82	1.45	1.30
9	13	310	KC1	O2A-CGA	5.82	1.45	1.30
9	11	306	KC1	O2A-CGA	5.82	1.45	1.30
9	12	306	KC1	O2A-CGA	5.81	1.45	1.30
9	20	306	KC1	O2A-CGA	5.81	1.45	1.30
9	15	309	KC1	O2A-CGA	5.80	1.45	1.30
9	11	302	KC1	C3B-C2B	5.79	1.48	1.37
9	18	309	KC1	O2A-CGA	5.78	1.45	1.30
9	12	310	KC1	O2A-CGA	5.78	1.45	1.30
9	11	308	KC1	O2A-CGA	5.78	1.45	1.30
9	17	306	KC1	O2A-CGA	5.78	1.45	1.30
9	16	305	KC1	O2A-CGA	5.78	1.45	1.30
9	11	302	KC1	O2A-CGA	5.78	1.45	1.30
9	11	304	KC1	O2A-CGA	5.77	1.45	1.30
9	16	308	KC1	O2A-CGA	5.76	1.45	1.30
10	11	312	A86	C19-C20	5.76	1.60	1.52
9	17	305	KC1	O2A-CGA	5.71	1.45	1.30
13	20	314	DD6	C13-C14	5.67	1.45	1.32
10	16	313	A86	C19-C20	5.67	1.60	1.52
9	14	309	KC1	O2A-CGA	5.62	1.44	1.30
9	12	306	KC1	C3C-C2C	5.53	1.48	1.36
9	20	306	KC1	C3C-C2C	5.53	1.48	1.36
9	15	304	KC1	C3B-C2B	5.51	1.48	1.37
8	18	310	CLA	C3C-C2C	5.50	1.48	1.36
9	14	304	KC1	C3B-C2B	5.50	1.48	1.37
9	16	304	KC1	C3B-C2B	5.48	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	11	307	CLA	C3C-C2C	5.47	1.48	1.36
9	19	308	KC1	C3B-C2B	5.46	1.48	1.37
9	13	310	KC1	C3B-C2B	5.45	1.48	1.37
9	18	304	KC1	C3B-C2B	5.44	1.48	1.37
9	17	303	KC1	C3B-C2B	5.42	1.48	1.37
9	20	305	KC1	C3B-C2B	5.42	1.48	1.37
9	18	309	KC1	C3B-C2B	5.38	1.48	1.37
9	11	304	KC1	C3B-C2B	5.36	1.48	1.37
13	20	314	DD6	C3-C2	5.34	1.59	1.43
9	13	305	KC1	C3B-C2B	5.34	1.48	1.37
9	20	306	KC1	C3B-C2B	5.34	1.48	1.37
9	18	306	KC1	C3B-C2B	5.34	1.48	1.37
9	13	307	KC1	C3B-C2B	5.33	1.48	1.37
8	13	311	CLA	C3C-C2C	5.33	1.48	1.36
9	13	303	KC1	C3B-C2B	5.32	1.48	1.37
9	12	306	KC1	C3B-C2B	5.31	1.47	1.37
13	19	312	DD6	C13-C14	5.29	1.44	1.32
9	15	306	KC1	C3B-C2B	5.29	1.47	1.37
9	12	310	KC1	C3B-C2B	5.29	1.47	1.37
13	21	216	DD6	C3-C2	5.28	1.59	1.43
8	17	302	CLA	C3C-C2C	5.28	1.48	1.36
9	14	306	KC1	C3B-C2B	5.28	1.47	1.37
9	20	303	KC1	C3B-C2B	5.28	1.47	1.37
9	17	309	KC1	C3B-C2B	5.27	1.47	1.37
9	15	309	KC1	C3B-C2B	5.26	1.47	1.37
9	17	306	KC1	C3C-C2C	5.24	1.48	1.36
9	17	306	KC1	C3B-C2B	5.24	1.47	1.37
9	11	306	KC1	C3B-C2B	5.22	1.47	1.37
9	14	309	KC1	C3B-C2B	5.22	1.47	1.37
9	11	306	KC1	C3C-C2C	5.21	1.48	1.36
8	20	308	CLA	O2D-CGD	5.20	1.46	1.33
9	15	302	KC1	C3B-C2B	5.19	1.47	1.37
8	13	306	CLA	C3C-C2C	5.18	1.47	1.36
8	20	310	CLA	C3C-C2C	5.17	1.47	1.36
8	12	311	CLA	C3C-C2C	5.17	1.47	1.36
8	17	310	CLA	C3C-C2C	5.17	1.47	1.36
8	21	208	CLA	C3C-C2C	5.17	1.47	1.36
9	21	207	KC1	C3B-C2B	5.17	1.47	1.37
9	17	305	KC1	C3B-C2B	5.16	1.47	1.37
8	21	209	CLA	C3C-C2C	5.16	1.47	1.36
8	20	308	CLA	C3C-C2C	5.16	1.47	1.36
8	15	310	CLA	C3C-C2C	5.16	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	20	310	CLA	O2D-CGD	5.15	1.45	1.33
8	19	304	CLA	C3C-C2C	5.14	1.47	1.36
8	12	307	CLA	C3C-C2C	5.14	1.47	1.36
8	15	305	CLA	C3C-C2C	5.14	1.47	1.36
8	15	301	CLA	C3C-C2C	5.13	1.47	1.36
8	14	310	CLA	C3C-C2C	5.13	1.47	1.36
8	21	210	CLA	C3C-C2C	5.13	1.47	1.36
13	21	212	DD6	C13-C14	5.13	1.44	1.32
9	11	308	KC1	C3B-C2B	5.12	1.47	1.37
9	14	304	KC1	C3C-C2C	5.12	1.47	1.36
8	14	303	CLA	C3C-C2C	5.12	1.47	1.36
13	20	312	DD6	C3-C2	5.11	1.59	1.43
9	16	308	KC1	C3B-C2B	5.11	1.47	1.37
8	18	302	CLA	C3C-C2C	5.10	1.47	1.36
8	21	208	CLA	O2D-CGD	5.09	1.45	1.33
13	16	312	DD6	C13-C14	5.09	1.43	1.32
9	16	305	KC1	C3C-C2C	5.09	1.47	1.36
8	13	308	CLA	O2D-CGD	5.09	1.45	1.33
9	21	207	KC1	O2D-CGD	5.08	1.45	1.33
13	20	312	DD6	C13-C14	5.08	1.43	1.32
8	21	204	CLA	C3C-C2C	5.08	1.47	1.36
9	19	308	KC1	C3C-C2C	5.08	1.47	1.36
8	18	308	CLA	C3C-C2C	5.07	1.47	1.36
8	17	310	CLA	O2D-CGD	5.07	1.45	1.33
8	21	209	CLA	O2D-CGD	5.07	1.45	1.33
8	21	210	CLA	O2D-CGD	5.06	1.45	1.33
8	13	309	CLA	C3C-C2C	5.06	1.47	1.36
8	15	303	CLA	C3C-C2C	5.06	1.47	1.36
8	16	309	CLA	C3C-C2C	5.05	1.47	1.36
8	11	309	CLA	C3C-C2C	5.05	1.47	1.36
13	16	312	DD6	C3-C2	5.05	1.58	1.43
8	14	305	CLA	C3C-C2C	5.05	1.47	1.36
9	12	308	KC1	C3B-C2B	5.05	1.47	1.37
8	21	205	CLA	C3C-C2C	5.05	1.47	1.36
10	12	302	A86	C17-C18	-5.04	1.45	1.52
8	14	305	CLA	O2D-CGD	5.04	1.45	1.33
8	18	305	CLA	C3C-C2C	5.04	1.47	1.36
8	13	306	CLA	O2D-CGD	5.04	1.45	1.33
9	16	304	KC1	C3C-C2C	5.03	1.47	1.36
8	19	310	CLA	C3C-C2C	5.03	1.47	1.36
9	21	207	KC1	C3C-C2C	5.03	1.47	1.36
8	15	305	CLA	O2D-CGD	5.02	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	21	212	DD6	C3-C2	5.02	1.58	1.43
8	20	302	CLA	C3C-C2C	5.02	1.47	1.36
9	13	305	KC1	C3C-C2C	5.02	1.47	1.36
8	19	307	CLA	C3C-C2C	5.01	1.47	1.36
8	11	303	CLA	C3C-C2C	5.01	1.47	1.36
9	13	303	KC1	C3C-C2C	5.01	1.47	1.36
9	16	305	KC1	C3B-C2B	5.01	1.47	1.37
8	20	309	CLA	O2D-CGD	5.00	1.45	1.33
8	14	302	CLA	O2D-CGD	5.00	1.45	1.33
9	20	303	KC1	C3C-C2C	5.00	1.47	1.36
8	15	308	CLA	O2D-CGD	4.99	1.45	1.33
8	21	206	CLA	O2D-CGD	4.99	1.45	1.33
9	21	203	KC1	C3C-C2C	4.99	1.47	1.36
8	13	302	CLA	C3C-C2C	4.99	1.47	1.36
8	20	309	CLA	C3C-C2C	4.99	1.47	1.36
8	14	302	CLA	C3C-C2C	4.99	1.47	1.36
8	18	310	CLA	O2D-CGD	4.99	1.45	1.33
8	21	206	CLA	C3C-C2C	4.99	1.47	1.36
9	15	302	KC1	C3C-C2C	4.98	1.47	1.36
8	19	309	CLA	C3C-C2C	4.98	1.47	1.36
10	13	314	A86	C9-C8	4.98	1.47	1.34
9	14	306	KC1	C3C-C2C	4.98	1.47	1.36
9	12	308	KC1	C3C-C2C	4.98	1.47	1.36
9	18	304	KC1	C3C-C2C	4.98	1.47	1.36
8	13	309	CLA	O2D-CGD	4.97	1.45	1.33
8	16	303	CLA	C3C-C2C	4.97	1.47	1.36
9	18	304	KC1	O2D-CGD	4.97	1.45	1.33
9	13	303	KC1	O2D-CGD	4.97	1.45	1.33
8	19	302	CLA	C3C-C2C	4.97	1.47	1.36
9	11	304	KC1	C3C-C2C	4.97	1.47	1.36
8	12	304	CLA	C3C-C2C	4.97	1.47	1.36
8	11	305	CLA	C3C-C2C	4.97	1.47	1.36
8	17	302	CLA	O2D-CGD	4.96	1.45	1.33
8	21	202	CLA	C1D-ND	4.96	1.44	1.37
8	19	307	CLA	O2D-CGD	4.96	1.45	1.33
9	15	304	KC1	C3C-C2C	4.96	1.47	1.36
8	13	302	CLA	O2D-CGD	4.96	1.45	1.33
8	14	310	CLA	O2D-CGD	4.95	1.45	1.33
8	18	308	CLA	O2D-CGD	4.95	1.45	1.33
9	11	308	KC1	C3C-C2C	4.95	1.47	1.36
9	20	303	KC1	O2D-CGD	4.95	1.45	1.33
9	13	305	KC1	O2D-CGD	4.95	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	18	302	CLA	O2D-CGD	4.95	1.45	1.33
8	20	302	CLA	O2D-CGD	4.95	1.45	1.33
8	13	311	CLA	O2D-CGD	4.94	1.45	1.33
8	12	307	CLA	O2D-CGD	4.94	1.45	1.33
8	21	202	CLA	O2D-CGD	4.94	1.45	1.33
9	15	304	KC1	O2D-CGD	4.94	1.45	1.33
8	18	305	CLA	O2D-CGD	4.94	1.45	1.33
9	11	302	KC1	C3C-C2C	4.94	1.47	1.36
8	20	304	CLA	O2D-CGD	4.93	1.45	1.33
8	11	305	CLA	O2D-CGD	4.93	1.45	1.33
8	21	205	CLA	O2D-CGD	4.93	1.45	1.33
9	15	302	KC1	O2D-CGD	4.93	1.45	1.33
9	19	308	KC1	O2D-CGD	4.93	1.45	1.33
8	15	310	CLA	O2D-CGD	4.93	1.45	1.33
8	17	304	CLA	C3C-C2C	4.93	1.47	1.36
8	13	301	CLA	O2D-CGD	4.92	1.45	1.33
8	15	301	CLA	O2D-CGD	4.92	1.45	1.33
8	21	202	CLA	C3C-C2C	4.92	1.47	1.36
8	12	309	CLA	C3C-C2C	4.92	1.47	1.36
9	15	306	KC1	C3C-C2C	4.92	1.47	1.36
9	18	306	KC1	C3C-C2C	4.92	1.47	1.36
10	15	314	A86	C9-C8	4.92	1.47	1.34
8	16	307	CLA	C3C-C2C	4.92	1.47	1.36
8	18	303	CLA	O2D-CGD	4.91	1.45	1.33
9	17	305	KC1	C3C-C2C	4.91	1.47	1.36
9	12	308	KC1	O2D-CGD	4.91	1.45	1.33
8	13	306	CLA	C1D-ND	4.90	1.44	1.37
8	18	301	CLA	CHC-C1C	4.90	1.48	1.38
9	13	310	KC1	C3C-C2C	4.90	1.47	1.36
8	14	308	CLA	O2D-CGD	4.90	1.45	1.33
10	21	213	A86	O4-C38	4.90	1.46	1.35
8	13	304	CLA	C3C-C2C	4.90	1.47	1.36
8	13	304	CLA	O2D-CGD	4.90	1.45	1.33
9	14	304	KC1	O2D-CGD	4.89	1.45	1.33
8	19	301	CLA	CHC-C1C	4.89	1.48	1.38
10	20	313	A86	C9-C8	4.89	1.47	1.34
8	11	301	CLA	CHC-C1C	4.89	1.48	1.38
8	17	308	CLA	C3C-C2C	4.89	1.47	1.36
10	13	315	A86	C9-C8	4.89	1.47	1.34
8	12	303	CLA	O2D-CGD	4.89	1.45	1.33
9	15	309	KC1	O2D-CGD	4.89	1.45	1.33
9	15	306	KC1	O2D-CGD	4.88	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	14	303	CLA	O2D-CGD	4.88	1.45	1.33
9	16	308	KC1	C3C-C2C	4.88	1.47	1.36
8	17	308	CLA	O2D-CGD	4.88	1.45	1.33
9	15	309	KC1	C3C-C2C	4.88	1.47	1.36
8	15	303	CLA	O2D-CGD	4.88	1.45	1.33
9	15	304	KC1	CHD-C4C	4.88	1.48	1.38
8	20	307	CLA	O2D-CGD	4.87	1.45	1.33
8	12	304	CLA	O2D-CGD	4.87	1.45	1.33
8	19	304	CLA	O2D-CGD	4.87	1.45	1.33
8	16	301	CLA	O2D-CGD	4.87	1.45	1.33
10	14	313	A86	C9-C8	4.87	1.47	1.34
10	18	311	A86	C9-C8	4.87	1.47	1.34
9	15	302	KC1	CHD-C4C	4.87	1.48	1.38
10	21	213	A86	C9-C8	4.87	1.47	1.34
9	16	304	KC1	O2D-CGD	4.87	1.45	1.33
8	13	301	CLA	C3C-C2C	4.86	1.47	1.36
9	18	306	KC1	O2D-CGD	4.86	1.45	1.33
8	14	308	CLA	C3C-C2C	4.86	1.47	1.36
10	13	316	A86	C9-C8	4.86	1.47	1.34
8	12	305	CLA	C3C-C2C	4.86	1.47	1.36
8	19	306	CLA	CHC-C1C	4.86	1.48	1.38
8	19	301	CLA	C3C-C2C	4.86	1.47	1.36
8	14	301	CLA	O2D-CGD	4.86	1.45	1.33
8	20	307	CLA	C3C-C2C	4.86	1.47	1.36
8	12	301	CLA	O2D-CGD	4.86	1.45	1.33
9	20	305	KC1	C3C-C2C	4.86	1.47	1.36
8	19	303	CLA	C3C-C2C	4.85	1.47	1.36
8	18	301	CLA	O2D-CGD	4.85	1.45	1.33
9	18	309	KC1	C3C-C2C	4.85	1.47	1.36
10	13	316	A86	C17-C18	-4.85	1.45	1.52
9	20	305	KC1	O2D-CGD	4.84	1.45	1.33
8	11	307	CLA	O2D-CGD	4.84	1.45	1.33
9	11	304	KC1	O2D-CGD	4.84	1.45	1.33
8	19	309	CLA	O2D-CGD	4.84	1.45	1.33
8	13	308	CLA	C3C-C2C	4.84	1.47	1.36
9	16	302	KC1	C3C-C2C	4.84	1.47	1.36
8	18	310	CLA	C1D-ND	4.83	1.44	1.37
8	14	307	CLA	O2D-CGD	4.83	1.45	1.33
8	18	307	CLA	O2D-CGD	4.83	1.45	1.33
8	19	305	CLA	C3C-C2C	4.83	1.47	1.36
8	16	307	CLA	O2D-CGD	4.83	1.45	1.33
8	17	307	CLA	C3C-C2C	4.83	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	12	311	CLA	O2D-CGD	4.83	1.45	1.33
10	18	313	A86	C9-C8	4.82	1.47	1.34
8	18	307	CLA	C3C-C2C	4.82	1.47	1.36
8	16	306	CLA	O2D-CGD	4.82	1.45	1.33
9	13	307	KC1	O2D-CGD	4.82	1.45	1.33
9	17	305	KC1	O2D-CGD	4.82	1.45	1.33
13	19	312	DD6	C3-C2	4.82	1.58	1.43
8	21	208	CLA	C1D-ND	4.82	1.44	1.37
10	15	313	A86	C9-C8	4.82	1.47	1.34
10	18	311	A86	C17-C18	-4.82	1.45	1.52
9	13	307	KC1	C3C-C2C	4.81	1.47	1.36
8	19	306	CLA	O2D-CGD	4.81	1.45	1.33
8	15	305	CLA	C1D-ND	4.81	1.44	1.37
8	21	204	CLA	O2D-CGD	4.81	1.45	1.33
8	16	306	CLA	CHC-C1C	4.81	1.48	1.38
9	21	203	KC1	O2D-CGD	4.81	1.45	1.33
9	13	310	KC1	O2D-CGD	4.81	1.45	1.33
9	17	303	KC1	CHD-C4C	4.81	1.48	1.38
8	12	301	CLA	C3C-C2C	4.81	1.47	1.36
8	14	301	CLA	CHC-C1C	4.81	1.48	1.38
10	18	314	A86	C9-C8	4.81	1.47	1.34
8	19	303	CLA	CHC-C1C	4.81	1.48	1.38
8	11	303	CLA	O2D-CGD	4.80	1.45	1.33
9	16	302	KC1	O2D-CGD	4.80	1.45	1.33
8	18	303	CLA	C3C-C2C	4.80	1.47	1.36
9	13	303	KC1	CHD-C4C	4.80	1.48	1.38
9	16	302	KC1	C3B-C2B	4.80	1.46	1.37
9	12	306	KC1	O2D-CGD	4.80	1.45	1.33
8	16	303	CLA	O2D-CGD	4.80	1.45	1.33
8	21	210	CLA	C1D-ND	4.80	1.44	1.37
8	15	307	CLA	C3C-C2C	4.80	1.47	1.36
9	18	309	KC1	O2D-CGD	4.79	1.45	1.33
8	20	302	CLA	C1D-ND	4.79	1.44	1.37
8	15	307	CLA	CHC-C1C	4.79	1.48	1.38
9	21	203	KC1	CHD-C4C	4.79	1.48	1.38
9	17	309	KC1	C3C-C2C	4.79	1.47	1.36
8	21	210	CLA	CHC-C1C	4.79	1.48	1.38
10	19	313	A86	C9-C8	4.79	1.47	1.34
10	12	313	A86	C17-C18	-4.79	1.45	1.52
10	11	310	A86	C17-C18	-4.79	1.45	1.52
8	16	306	CLA	C3C-C2C	4.79	1.47	1.36
8	19	305	CLA	O2D-CGD	4.79	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	17	307	CLA	O2D-CGD	4.79	1.45	1.33
8	20	304	CLA	C3C-C2C	4.79	1.47	1.36
9	17	303	KC1	C3C-C2C	4.79	1.47	1.36
8	14	307	CLA	C3C-C2C	4.78	1.47	1.36
9	16	305	KC1	O2D-CGD	4.78	1.45	1.33
9	21	207	KC1	CHD-C4C	4.78	1.48	1.38
10	13	314	A86	O4-C38	4.78	1.45	1.35
10	14	313	A86	O4-C38	4.78	1.45	1.35
9	14	309	KC1	C3C-C2C	4.78	1.47	1.36
9	14	304	KC1	CHD-C4C	4.78	1.48	1.38
9	17	305	KC1	CHD-C4C	4.78	1.48	1.38
8	11	301	CLA	C3C-C2C	4.78	1.47	1.36
9	14	309	KC1	O2D-CGD	4.77	1.45	1.33
10	11	312	A86	O4-C38	4.77	1.45	1.35
8	21	209	CLA	C1D-ND	4.77	1.44	1.37
8	12	305	CLA	O2D-CGD	4.77	1.44	1.33
8	18	301	CLA	C3C-C2C	4.77	1.47	1.36
9	17	303	KC1	O2D-CGD	4.76	1.44	1.33
8	17	304	CLA	O2D-CGD	4.76	1.44	1.33
9	20	305	KC1	CHD-C4C	4.76	1.48	1.38
9	11	304	KC1	CHD-C4C	4.76	1.48	1.38
9	12	310	KC1	C3C-C2C	4.76	1.47	1.36
9	16	308	KC1	O2D-CGD	4.76	1.44	1.33
8	15	308	CLA	C3C-C2C	4.75	1.47	1.36
9	11	308	KC1	O2D-CGD	4.75	1.44	1.33
10	12	314	A86	C9-C8	4.75	1.47	1.34
8	15	307	CLA	O2D-CGD	4.75	1.44	1.33
9	20	305	KC1	C1D-ND	4.75	1.44	1.37
8	20	302	CLA	CHC-C1C	4.74	1.48	1.38
9	13	310	KC1	CHD-C4C	4.73	1.48	1.38
10	17	316	A86	C17-C18	-4.73	1.45	1.52
8	14	301	CLA	C3C-C2C	4.73	1.47	1.36
8	15	310	CLA	C1D-ND	4.73	1.44	1.37
10	11	312	A86	C17-C18	-4.73	1.45	1.52
13	20	314	DD6	C2-C1	4.73	1.46	1.35
8	11	301	CLA	O2D-CGD	4.73	1.44	1.33
9	11	302	KC1	CHD-C4C	4.72	1.47	1.38
8	13	311	CLA	C1D-ND	4.72	1.44	1.37
9	13	303	KC1	C1D-ND	4.72	1.44	1.37
8	11	309	CLA	O2D-CGD	4.72	1.44	1.33
10	21	215	A86	C9-C8	4.72	1.47	1.34
8	20	308	CLA	C1D-ND	4.72	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	15	305	CLA	CHC-C1C	4.71	1.47	1.38
10	15	313	A86	O4-C38	4.71	1.45	1.35
8	12	309	CLA	O2D-CGD	4.71	1.44	1.33
9	16	302	KC1	CHD-C4C	4.71	1.47	1.38
9	18	304	KC1	CHD-C4C	4.70	1.47	1.38
10	15	316	A86	C9-C8	4.70	1.47	1.34
8	19	310	CLA	O2D-CGD	4.70	1.44	1.33
8	16	301	CLA	CHC-C1C	4.70	1.47	1.38
8	13	306	CLA	CHC-C1C	4.70	1.47	1.38
9	21	207	KC1	CHC-C4B	4.70	1.47	1.38
9	12	310	KC1	O2D-CGD	4.70	1.44	1.33
8	21	206	CLA	CHC-C1C	4.70	1.47	1.38
9	19	308	KC1	CHC-C4B	4.69	1.47	1.38
8	13	302	CLA	CHC-C1C	4.69	1.47	1.38
9	17	309	KC1	O2D-CGD	4.69	1.44	1.33
8	12	311	CLA	CHC-C1C	4.69	1.47	1.38
10	17	316	A86	C9-C8	4.69	1.46	1.34
10	15	316	A86	C17-C18	-4.69	1.45	1.52
8	20	307	CLA	CHC-C1C	4.69	1.47	1.38
8	19	306	CLA	C3C-C2C	4.69	1.46	1.36
9	14	306	KC1	O2D-CGD	4.68	1.44	1.33
8	21	208	CLA	CHC-C1C	4.68	1.47	1.38
8	18	303	CLA	CHC-C1C	4.67	1.47	1.38
9	20	303	KC1	CHD-C4C	4.67	1.47	1.38
8	16	309	CLA	O2D-CGD	4.67	1.44	1.33
8	15	301	CLA	CHC-C1C	4.67	1.47	1.38
8	14	302	CLA	CHC-C1C	4.67	1.47	1.38
9	15	304	KC1	C1D-ND	4.67	1.44	1.37
10	20	301	A86	C9-C8	4.67	1.46	1.34
9	11	302	KC1	O2D-CGD	4.66	1.44	1.33
8	20	310	CLA	C1D-ND	4.66	1.44	1.37
10	17	312	A86	C17-C18	-4.66	1.45	1.52
10	12	316	A86	C9-C8	4.66	1.46	1.34
8	11	301	CLA	C1D-ND	4.66	1.44	1.37
8	14	301	CLA	C1D-ND	4.66	1.44	1.37
10	20	311	A86	C9-C8	4.66	1.46	1.34
10	11	318	A86	C17-C18	-4.65	1.45	1.52
10	17	315	A86	C17-C18	-4.65	1.45	1.52
8	20	309	CLA	C1D-ND	4.65	1.44	1.37
8	19	301	CLA	O2D-CGD	4.65	1.44	1.33
10	14	314	A86	C9-C8	4.65	1.46	1.34
9	13	307	KC1	CHD-C4C	4.65	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	17	313	A86	C17-C18	-4.65	1.45	1.52
8	13	302	CLA	C1D-ND	4.65	1.44	1.37
9	15	306	KC1	CHD-C4C	4.65	1.47	1.38
9	20	306	KC1	CHD-C4C	4.65	1.47	1.38
8	18	305	CLA	C1D-ND	4.65	1.44	1.37
8	13	309	CLA	C1D-ND	4.65	1.44	1.37
13	21	212	DD6	C2-C1	4.65	1.46	1.35
10	21	214	A86	C9-C8	4.65	1.46	1.34
10	12	314	A86	O4-C38	4.64	1.45	1.35
8	17	302	CLA	CHC-C1C	4.64	1.47	1.38
9	11	308	KC1	CHD-C4C	4.64	1.47	1.38
8	14	307	CLA	CHC-C1C	4.64	1.47	1.38
9	13	305	KC1	CHD-C4C	4.64	1.47	1.38
10	17	311	A86	O4-C38	4.63	1.45	1.35
8	14	305	CLA	C1D-ND	4.63	1.43	1.37
9	16	308	KC1	CHD-C4C	4.63	1.47	1.38
10	15	312	A86	C17-C18	-4.63	1.45	1.52
8	19	304	CLA	O2A-CGA	4.62	1.46	1.30
9	20	303	KC1	C1D-ND	4.62	1.43	1.37
8	20	308	CLA	O2A-CGA	4.62	1.46	1.30
10	12	302	A86	C9-C8	4.62	1.46	1.34
8	14	310	CLA	C1D-ND	4.61	1.43	1.37
9	11	308	KC1	C1D-ND	4.61	1.43	1.37
9	16	302	KC1	C1D-ND	4.61	1.43	1.37
10	12	316	A86	C17-C18	-4.61	1.45	1.52
9	13	305	KC1	C1D-ND	4.61	1.43	1.37
8	21	204	CLA	CHC-C1C	4.61	1.47	1.38
10	17	311	A86	C9-C8	4.61	1.46	1.34
8	18	305	CLA	O2A-CGA	4.61	1.46	1.30
8	20	308	CLA	CHC-C1C	4.61	1.47	1.38
9	12	310	KC1	CHD-C4C	4.60	1.47	1.38
8	12	311	CLA	C1D-ND	4.60	1.43	1.37
8	12	309	CLA	CHC-C1C	4.60	1.47	1.38
8	21	206	CLA	C1D-ND	4.60	1.43	1.37
9	17	306	KC1	C1A-CHA	4.60	1.52	1.40
13	21	216	DD6	C2-C1	4.59	1.46	1.35
8	13	306	CLA	O2A-CGA	4.59	1.46	1.30
8	12	311	CLA	O2A-CGA	4.59	1.46	1.30
10	21	211	A86	C9-C8	4.59	1.46	1.34
9	18	309	KC1	CHD-C4C	4.59	1.47	1.38
10	13	313	A86	C9-C8	4.59	1.46	1.34
9	16	304	KC1	CHD-C4C	4.59	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	11	314	A86	C17-C18	-4.59	1.45	1.52
8	12	303	CLA	CHC-C1C	4.59	1.47	1.38
8	20	310	CLA	CHC-C1C	4.59	1.47	1.38
10	15	311	A86	O4-C38	4.59	1.45	1.35
10	11	312	A86	C9-C8	4.59	1.46	1.34
8	19	302	CLA	O2D-CGD	4.59	1.44	1.33
8	21	204	CLA	C1D-ND	4.58	1.43	1.37
9	11	306	KC1	CHC-C4B	4.58	1.47	1.38
9	17	309	KC1	CHD-C4C	4.58	1.47	1.38
8	15	305	CLA	O2A-CGA	4.58	1.45	1.30
10	19	313	A86	O4-C38	4.57	1.45	1.35
8	21	209	CLA	O2A-CGA	4.57	1.45	1.30
9	12	306	KC1	CHC-C4B	4.57	1.47	1.38
10	14	315	A86	C9-C8	4.57	1.46	1.34
8	19	309	CLA	O2A-CGA	4.57	1.45	1.30
9	19	308	KC1	C1A-NA	-4.57	1.28	1.38
8	19	304	CLA	CHC-C1C	4.57	1.47	1.38
9	14	304	KC1	C1A-NA	-4.57	1.28	1.38
9	15	304	KC1	C1A-NA	-4.57	1.28	1.38
9	14	304	KC1	CHC-C4B	4.57	1.47	1.38
9	12	310	KC1	CHC-C4B	4.56	1.47	1.38
10	17	313	A86	O4-C38	4.56	1.45	1.35
9	14	309	KC1	CHD-C4C	4.56	1.47	1.38
9	16	304	KC1	C1A-NA	-4.56	1.28	1.38
8	19	309	CLA	CHC-C1C	4.56	1.47	1.38
8	18	302	CLA	CHC-C1C	4.56	1.47	1.38
9	15	306	KC1	C1D-ND	4.56	1.43	1.37
8	18	310	CLA	O2A-CGA	4.56	1.45	1.30
9	11	306	KC1	O2D-CGD	4.55	1.44	1.33
8	14	310	CLA	O2A-CGA	4.55	1.45	1.30
8	13	311	CLA	CHC-C1C	4.55	1.47	1.38
9	16	305	KC1	CHD-C4C	4.55	1.47	1.38
8	21	210	CLA	O2A-CGA	4.55	1.45	1.30
9	17	306	KC1	O2D-CGD	4.55	1.44	1.33
8	21	205	CLA	C1D-ND	4.55	1.43	1.37
10	17	313	A86	C9-C8	4.55	1.46	1.34
9	14	304	KC1	C1D-ND	4.55	1.43	1.37
8	13	311	CLA	O2A-CGA	4.54	1.45	1.30
8	12	307	CLA	CHC-C1C	4.54	1.47	1.38
9	13	303	KC1	CHC-C4B	4.54	1.47	1.38
10	14	316	A86	C9-C8	4.54	1.46	1.34
8	18	301	CLA	C1D-ND	4.54	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	17	308	CLA	CHC-C1C	4.53	1.47	1.38
10	15	315	A86	C9-C8	4.53	1.46	1.34
8	21	205	CLA	O2A-CGA	4.53	1.45	1.30
9	14	309	KC1	CHC-C4B	4.53	1.47	1.38
8	18	302	CLA	C1D-ND	4.53	1.43	1.37
8	21	209	CLA	CHC-C1C	4.53	1.47	1.38
10	15	311	A86	C17-C18	-4.53	1.45	1.52
9	21	207	KC1	C1D-ND	4.52	1.43	1.37
10	15	312	A86	C9-C8	4.52	1.46	1.34
10	17	314	A86	C9-C8	4.52	1.46	1.34
10	14	313	A86	C17-C18	-4.52	1.45	1.52
8	18	305	CLA	CHC-C1C	4.52	1.47	1.38
8	20	304	CLA	CHC-C1C	4.52	1.47	1.38
9	12	306	KC1	C1A-NA	-4.52	1.28	1.38
9	18	309	KC1	C1D-ND	4.52	1.43	1.37
8	16	301	CLA	C3C-C2C	4.52	1.46	1.36
8	20	310	CLA	O2A-CGA	4.52	1.45	1.30
10	16	311	A86	C17-C18	-4.51	1.45	1.52
8	14	305	CLA	O2A-CGA	4.51	1.45	1.30
8	15	301	CLA	C1D-ND	4.51	1.43	1.37
10	12	319	A86	C17-C18	-4.51	1.45	1.52
8	17	310	CLA	C1D-ND	4.51	1.43	1.37
8	12	305	CLA	CHC-C1C	4.51	1.47	1.38
10	19	311	A86	O4-C38	4.51	1.45	1.35
13	16	312	DD6	C2-C1	4.51	1.46	1.35
8	13	301	CLA	C1D-ND	4.51	1.43	1.37
9	17	309	KC1	C1D-ND	4.50	1.43	1.37
10	21	215	A86	C17-C18	-4.50	1.45	1.52
9	16	305	KC1	C1D-ND	4.50	1.43	1.37
9	15	302	KC1	C1D-ND	4.50	1.43	1.37
8	16	306	CLA	C1B-NB	-4.50	1.31	1.37
8	19	303	CLA	O2D-CGD	4.50	1.44	1.33
8	14	303	CLA	CHC-C1C	4.50	1.47	1.38
8	15	310	CLA	O2A-CGA	4.50	1.45	1.30
10	16	310	A86	C17-C18	-4.50	1.45	1.52
10	12	302	A86	O4-C38	4.49	1.45	1.35
9	13	303	KC1	C1A-NA	-4.49	1.28	1.38
10	11	310	A86	O4-C38	4.49	1.45	1.35
10	17	321	A86	C9-C8	4.49	1.46	1.34
8	18	310	CLA	CHC-C1C	4.49	1.47	1.38
9	19	308	KC1	CHD-C4C	4.49	1.47	1.38
9	17	305	KC1	C1A-NA	-4.49	1.28	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	19	302	CLA	CHC-C1C	4.49	1.47	1.38
8	18	307	CLA	C1D-ND	4.49	1.43	1.37
9	17	303	KC1	C1D-ND	4.49	1.43	1.37
10	12	315	A86	C9-C8	4.48	1.46	1.34
10	12	312	A86	C9-C8	4.48	1.46	1.34
10	13	312	A86	C17-C18	-4.48	1.46	1.52
10	21	215	A86	O4-C38	4.48	1.45	1.35
9	16	304	KC1	CHC-C4B	4.48	1.47	1.38
8	12	303	CLA	C1D-ND	4.48	1.43	1.37
9	11	306	KC1	CHD-C4C	4.48	1.47	1.38
10	15	314	A86	C7-C6	4.48	1.59	1.50
9	11	304	KC1	C1D-ND	4.48	1.43	1.37
8	17	308	CLA	C1D-ND	4.48	1.43	1.37
10	17	315	A86	C9-C8	4.48	1.46	1.34
10	13	312	A86	C9-C8	4.47	1.46	1.34
10	15	313	A86	C17-C18	-4.47	1.46	1.52
8	19	305	CLA	CHC-C1C	4.47	1.47	1.38
8	17	310	CLA	CHC-C1C	4.47	1.47	1.38
9	17	305	KC1	C1D-ND	4.47	1.43	1.37
8	11	305	CLA	O2A-CGA	4.47	1.45	1.30
8	19	302	CLA	C1D-ND	4.47	1.43	1.37
8	15	308	CLA	C1D-ND	4.46	1.43	1.37
9	15	302	KC1	C1A-NA	-4.46	1.28	1.38
10	17	321	A86	C17-C18	-4.46	1.46	1.52
9	12	308	KC1	CHD-C4C	4.46	1.47	1.38
8	12	307	CLA	C1D-ND	4.46	1.43	1.37
8	16	309	CLA	O2A-CGA	4.46	1.45	1.30
10	13	313	A86	C17-C18	-4.46	1.46	1.52
8	14	305	CLA	CHC-C1C	4.46	1.47	1.38
9	13	305	KC1	CHC-C4B	4.46	1.47	1.38
10	19	311	A86	C9-C8	4.46	1.46	1.34
9	18	304	KC1	C1D-ND	4.45	1.43	1.37
10	14	311	A86	C9-C8	4.45	1.46	1.34
9	18	306	KC1	CHD-C4C	4.45	1.47	1.38
8	17	307	CLA	CHC-C1C	4.45	1.47	1.38
8	12	301	CLA	C1D-ND	4.45	1.43	1.37
8	15	303	CLA	CHC-C1C	4.45	1.47	1.38
9	16	304	KC1	C1D-ND	4.45	1.43	1.37
9	17	306	KC1	CHD-C4C	4.45	1.47	1.38
9	15	306	KC1	CHC-C4B	4.45	1.47	1.38
8	14	303	CLA	C1D-ND	4.45	1.43	1.37
9	15	309	KC1	CHD-C4C	4.44	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	18	306	KC1	C1A-CHA	4.44	1.51	1.40
10	12	319	A86	C9-C8	4.44	1.46	1.34
9	14	306	KC1	CHC-C4B	4.44	1.47	1.38
8	18	307	CLA	CHC-C1C	4.44	1.47	1.38
10	18	312	A86	C9-C8	4.44	1.46	1.34
10	13	316	A86	O4-C38	4.44	1.45	1.35
9	11	304	KC1	C1A-NA	-4.44	1.28	1.38
8	12	303	CLA	C3C-C2C	4.43	1.46	1.36
8	11	305	CLA	C1D-ND	4.43	1.43	1.37
9	13	307	KC1	CHB-C1B	4.43	1.47	1.38
8	15	310	CLA	CHC-C1C	4.43	1.47	1.38
9	11	306	KC1	C1D-ND	4.43	1.43	1.37
9	11	302	KC1	C1A-NA	-4.43	1.28	1.38
9	18	304	KC1	CHC-C4B	4.43	1.47	1.38
9	20	305	KC1	C1A-NA	-4.43	1.28	1.38
9	17	306	KC1	CHB-C1B	4.43	1.47	1.38
10	14	312	A86	C9-C8	4.42	1.46	1.34
8	13	304	CLA	C1D-ND	4.42	1.43	1.37
8	14	308	CLA	C1D-ND	4.42	1.43	1.37
8	15	307	CLA	C1D-ND	4.42	1.43	1.37
9	13	310	KC1	C1D-ND	4.42	1.43	1.37
8	21	204	CLA	CHD-C1D	4.42	1.47	1.38
10	15	316	A86	O4-C38	4.42	1.45	1.35
9	20	303	KC1	C1A-NA	-4.42	1.28	1.38
10	21	211	A86	O4-C38	4.42	1.45	1.35
10	13	315	A86	O4-C38	4.42	1.45	1.35
10	15	319	A86	C9-C8	4.42	1.46	1.34
10	12	314	A86	C17-C18	-4.42	1.46	1.52
9	18	306	KC1	CHB-C1B	4.42	1.47	1.38
10	11	318	A86	O4-C38	4.42	1.45	1.35
9	18	306	KC1	CHC-C4B	4.42	1.47	1.38
10	11	310	A86	C9-C8	4.42	1.46	1.34
8	20	304	CLA	O2A-CGA	4.42	1.46	1.33
9	18	304	KC1	C1A-NA	-4.41	1.28	1.38
9	12	308	KC1	CHC-C4B	4.41	1.47	1.38
8	17	302	CLA	C1D-ND	4.41	1.43	1.37
9	16	305	KC1	C1A-CHA	4.41	1.51	1.40
10	18	313	A86	O4-C38	4.41	1.44	1.35
10	21	214	A86	O4-C38	4.41	1.44	1.35
10	13	315	A86	C7-C6	4.41	1.59	1.50
9	21	207	KC1	C1A-NA	-4.41	1.28	1.38
10	15	314	A86	C21-C20	4.41	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	11	306	KC1	C1A-CHA	4.41	1.51	1.40
10	11	313	A86	C9-C8	4.41	1.46	1.34
8	20	304	CLA	C1D-ND	4.41	1.43	1.37
10	15	311	A86	C9-C8	4.41	1.46	1.34
9	12	310	KC1	C1D-ND	4.40	1.43	1.37
9	15	304	KC1	CHC-C4B	4.40	1.47	1.38
9	15	306	KC1	C1A-NA	-4.40	1.28	1.38
9	14	309	KC1	C1D-ND	4.40	1.43	1.37
8	14	308	CLA	CHC-C1C	4.40	1.47	1.38
9	21	203	KC1	C1A-NA	-4.40	1.28	1.38
8	16	307	CLA	CHC-C1C	4.40	1.47	1.38
10	19	313	A86	C10-C11	4.40	1.46	1.34
10	17	314	A86	C17-C18	-4.40	1.46	1.52
8	16	303	CLA	C1D-ND	4.40	1.43	1.37
10	12	315	A86	O4-C38	4.40	1.44	1.35
9	14	306	KC1	C1A-CHA	4.39	1.51	1.40
8	18	310	CLA	CHD-C1D	4.39	1.47	1.38
9	13	305	KC1	CHB-C1B	4.39	1.47	1.38
9	16	302	KC1	C1A-CHA	4.39	1.51	1.40
10	21	211	A86	C10-C11	4.39	1.46	1.34
10	12	315	A86	C7-C6	4.38	1.59	1.50
9	15	309	KC1	C1A-CHA	4.38	1.51	1.40
8	21	204	CLA	O2A-CGA	4.38	1.46	1.33
10	20	313	A86	C7-C6	4.38	1.59	1.50
8	16	303	CLA	CHC-C1C	4.38	1.47	1.38
10	20	311	A86	O4-C38	4.38	1.44	1.35
9	13	307	KC1	C1D-ND	4.38	1.43	1.37
13	20	312	DD6	C2-C1	4.38	1.45	1.35
8	16	309	CLA	C1D-ND	4.38	1.43	1.37
10	20	313	A86	O4-C38	4.38	1.44	1.35
10	12	316	A86	O4-C38	4.38	1.44	1.35
9	21	203	KC1	C1D-ND	4.38	1.43	1.37
10	14	316	A86	O4-C38	4.37	1.44	1.35
9	13	310	KC1	CHC-C4B	4.37	1.47	1.38
9	17	305	KC1	CHC-C4B	4.37	1.47	1.38
8	19	307	CLA	CHC-C1C	4.37	1.47	1.38
8	19	307	CLA	C1D-ND	4.37	1.43	1.37
9	20	306	KC1	O2D-CGD	4.37	1.44	1.33
10	17	316	A86	O4-C38	4.37	1.44	1.35
8	12	304	CLA	C1D-ND	4.37	1.43	1.37
10	11	313	A86	O4-C38	4.37	1.44	1.35
8	14	302	CLA	C1D-ND	4.37	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	21	205	CLA	CHC-C1C	4.37	1.47	1.38
10	20	301	A86	O4-C38	4.37	1.44	1.35
8	11	307	CLA	CHC-C1C	4.37	1.47	1.38
9	14	306	KC1	CHB-C1B	4.37	1.46	1.38
10	15	315	A86	O4-C38	4.37	1.44	1.35
9	11	304	KC1	CHC-C4B	4.37	1.46	1.38
10	16	313	A86	C9-C8	4.37	1.46	1.34
8	14	307	CLA	C1B-NB	-4.37	1.32	1.37
8	17	304	CLA	O2A-CGA	4.36	1.46	1.33
9	18	309	KC1	CHC-C4B	4.36	1.46	1.38
8	15	303	CLA	C1D-ND	4.36	1.43	1.37
8	18	308	CLA	C1D-ND	4.36	1.43	1.37
10	17	314	A86	O4-C38	4.36	1.44	1.35
8	16	309	CLA	CHC-C1C	4.36	1.47	1.38
9	12	306	KC1	CHD-C4C	4.36	1.47	1.38
9	17	303	KC1	C1A-CHA	4.36	1.51	1.40
10	20	311	A86	C21-C20	4.36	1.58	1.51
10	14	312	A86	O4-C38	4.35	1.44	1.35
9	16	308	KC1	C1D-ND	4.35	1.43	1.37
8	18	303	CLA	O2A-CGA	4.35	1.46	1.33
9	15	309	KC1	CHC-C4B	4.35	1.46	1.38
8	12	305	CLA	O2A-CGA	4.35	1.46	1.33
8	19	303	CLA	C1D-ND	4.35	1.43	1.37
9	11	306	KC1	CHB-C1B	4.35	1.46	1.38
9	11	308	KC1	C1A-CHA	4.35	1.51	1.40
10	14	311	A86	C17-C18	-4.35	1.46	1.52
9	16	305	KC1	CHC-C4B	4.35	1.46	1.38
10	14	314	A86	C7-C6	4.35	1.59	1.50
8	13	302	CLA	O2A-CGA	4.34	1.46	1.33
9	14	306	KC1	CHD-C4C	4.34	1.47	1.38
10	11	318	A86	C9-C8	4.34	1.46	1.34
8	13	304	CLA	CHC-C1C	4.34	1.47	1.38
10	21	214	A86	C7-C6	4.34	1.59	1.50
10	13	312	A86	O4-C38	4.34	1.44	1.35
10	21	213	A86	C17-C18	-4.34	1.46	1.52
10	16	311	A86	C9-C8	4.34	1.46	1.34
9	17	309	KC1	C1A-CHA	4.34	1.51	1.40
8	11	309	CLA	CHC-C1C	4.34	1.47	1.38
8	19	310	CLA	CHC-C1C	4.34	1.47	1.38
10	14	313	A86	C7-C6	4.34	1.59	1.50
8	11	309	CLA	C1D-ND	4.33	1.43	1.37
8	17	304	CLA	C1B-NB	-4.33	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	11	302	KC1	C1A-CHA	4.33	1.51	1.40
9	13	305	KC1	C1A-NA	-4.33	1.28	1.38
8	21	202	CLA	CHC-C1C	4.33	1.47	1.38
9	20	303	KC1	CHC-C4B	4.33	1.46	1.38
9	11	302	KC1	C1D-ND	4.33	1.43	1.37
10	18	312	A86	O4-C38	4.33	1.44	1.35
8	14	302	CLA	O2A-CGA	4.33	1.46	1.33
10	17	316	A86	C7-C6	4.33	1.59	1.50
9	14	306	KC1	C1D-ND	4.33	1.43	1.37
10	18	314	A86	C7-C6	4.33	1.59	1.50
9	13	307	KC1	CHC-C4B	4.33	1.46	1.38
10	20	313	A86	C21-C20	4.33	1.58	1.51
9	15	302	KC1	CHC-C4B	4.33	1.46	1.38
10	13	314	A86	C7-C6	4.33	1.59	1.50
10	12	312	A86	O4-C38	4.32	1.44	1.35
10	17	315	A86	C21-C20	4.32	1.58	1.51
8	20	302	CLA	CHD-C1D	4.32	1.46	1.38
9	20	306	KC1	C1D-ND	4.32	1.43	1.37
10	17	314	A86	C7-C6	4.32	1.59	1.50
10	16	310	A86	C9-C8	4.32	1.46	1.34
10	12	312	A86	C7-C6	4.32	1.59	1.50
8	11	303	CLA	C1D-ND	4.32	1.43	1.37
9	13	307	KC1	C1A-CHA	4.32	1.51	1.40
10	19	311	A86	C17-C18	-4.32	1.46	1.52
8	13	301	CLA	CHC-C1C	4.32	1.47	1.38
10	20	311	A86	C10-C11	4.32	1.46	1.34
9	17	309	KC1	CHC-C4B	4.32	1.46	1.38
9	12	308	KC1	C1A-NA	-4.31	1.29	1.38
8	20	309	CLA	O2A-CGA	4.31	1.45	1.33
8	17	310	CLA	CHD-C1D	4.31	1.46	1.38
8	15	303	CLA	O2A-CGA	4.31	1.45	1.33
8	14	310	CLA	CHC-C1C	4.31	1.47	1.38
10	15	314	A86	C10-C11	4.31	1.46	1.34
8	13	304	CLA	O2A-CGA	4.31	1.45	1.33
9	18	306	KC1	C1D-ND	4.31	1.43	1.37
8	15	307	CLA	O2A-CGA	4.31	1.45	1.33
8	13	309	CLA	CHC-C1C	4.31	1.47	1.38
9	13	310	KC1	C1A-NA	-4.31	1.29	1.38
9	15	306	KC1	CHB-C1B	4.31	1.46	1.38
10	21	215	A86	C7-C6	4.31	1.59	1.50
10	15	319	A86	O4-C38	4.31	1.44	1.35
8	11	305	CLA	CHC-C1C	4.31	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	14	316	A86	C17-C18	-4.31	1.46	1.52
9	16	305	KC1	C1A-NA	-4.30	1.29	1.38
8	13	309	CLA	O2A-CGA	4.30	1.45	1.33
8	17	307	CLA	C1B-NB	-4.30	1.32	1.37
9	18	309	KC1	C1A-NA	-4.30	1.29	1.38
10	12	319	A86	C21-C20	4.30	1.58	1.51
10	18	312	A86	C7-C6	4.30	1.59	1.50
8	13	311	CLA	CHD-C1D	4.30	1.46	1.38
8	13	306	CLA	CHD-C1D	4.30	1.46	1.38
8	21	202	CLA	CHD-C1D	4.30	1.46	1.38
8	17	304	CLA	CHC-C1C	4.30	1.47	1.38
9	20	305	KC1	CHB-C1B	4.30	1.46	1.38
8	14	305	CLA	CHD-C1D	4.30	1.46	1.38
8	21	208	CLA	CHD-C1D	4.30	1.46	1.38
8	21	209	CLA	CHD-C1D	4.30	1.46	1.38
9	12	308	KC1	C1A-CHA	4.29	1.51	1.40
8	18	308	CLA	CHC-C1C	4.29	1.47	1.38
9	14	309	KC1	C1A-CHA	4.29	1.51	1.40
8	12	304	CLA	O2A-CGA	4.29	1.45	1.33
9	16	308	KC1	C1A-CHA	4.29	1.51	1.40
10	14	315	A86	C21-C20	4.29	1.58	1.51
10	18	313	A86	C7-C6	4.29	1.59	1.50
8	19	303	CLA	O2A-CGA	4.28	1.45	1.33
10	19	313	A86	C19-C18	4.28	1.58	1.52
8	21	208	CLA	O2A-CGA	4.28	1.45	1.33
9	18	309	KC1	C1A-CHA	4.28	1.51	1.40
9	16	308	KC1	C1A-NA	-4.28	1.29	1.38
10	20	311	A86	C7-C6	4.28	1.59	1.50
10	12	313	A86	O4-C38	4.28	1.44	1.35
8	13	304	CLA	CHD-C1D	4.28	1.46	1.38
8	14	303	CLA	CHD-C1D	4.28	1.46	1.38
8	12	311	CLA	CHD-C1D	4.28	1.46	1.38
10	15	312	A86	C7-C6	4.27	1.59	1.50
8	12	309	CLA	C1B-NB	-4.27	1.32	1.37
10	11	314	A86	C9-C8	4.27	1.45	1.34
10	11	313	A86	C17-C18	-4.27	1.46	1.52
8	12	304	CLA	CHC-C1C	4.27	1.47	1.38
10	11	313	A86	C7-C6	4.27	1.59	1.50
8	11	303	CLA	O2A-CGA	4.27	1.45	1.33
10	17	312	A86	C9-C8	4.27	1.45	1.34
10	11	314	A86	C7-C6	4.27	1.59	1.50
10	12	312	A86	C21-C20	4.27	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	15	301	CLA	O2A-CGA	4.27	1.45	1.33
10	12	314	A86	C7-C6	4.27	1.59	1.50
8	12	301	CLA	CHC-C1C	4.27	1.47	1.38
9	20	305	KC1	CHC-C4B	4.27	1.46	1.38
9	15	306	KC1	C1A-CHA	4.27	1.51	1.40
10	11	311	A86	C9-C8	4.27	1.45	1.34
8	19	307	CLA	O2A-CGA	4.27	1.45	1.33
9	11	306	KC1	C1A-NA	-4.26	1.29	1.38
9	17	309	KC1	C1A-NA	-4.26	1.29	1.38
8	20	309	CLA	CHC-C1C	4.26	1.47	1.38
8	18	308	CLA	O2A-CGA	4.26	1.45	1.33
10	13	313	A86	O4-C38	4.26	1.44	1.35
10	15	314	A86	O4-C38	4.26	1.44	1.35
10	12	315	A86	C17-C18	-4.26	1.46	1.52
9	13	307	KC1	C1A-NA	-4.26	1.29	1.38
8	18	302	CLA	O2A-CGA	4.26	1.45	1.33
8	13	308	CLA	O2A-CGA	4.26	1.45	1.33
10	16	313	A86	C7-C6	4.26	1.59	1.50
9	16	308	KC1	C1B-NB	-4.26	1.32	1.37
8	14	310	CLA	CHD-C1D	4.26	1.46	1.38
8	16	303	CLA	O2A-CGA	4.26	1.45	1.33
9	20	306	KC1	C1A-CHA	4.26	1.51	1.40
10	15	313	A86	C7-C6	4.26	1.59	1.50
10	18	311	A86	C21-C20	4.25	1.58	1.51
8	15	307	CLA	C1B-NB	-4.25	1.32	1.37
9	13	305	KC1	C1A-CHA	4.25	1.51	1.40
8	12	307	CLA	O2A-CGA	4.25	1.45	1.33
8	17	304	CLA	CHD-C1D	4.25	1.46	1.38
8	14	301	CLA	O2A-CGA	4.25	1.45	1.33
10	12	313	A86	C9-C8	4.25	1.45	1.34
10	11	311	A86	C7-C6	4.25	1.59	1.50
10	15	315	A86	C7-C6	4.25	1.59	1.50
10	14	311	A86	O4-C38	4.25	1.44	1.35
10	14	312	A86	C7-C6	4.25	1.59	1.50
10	14	311	A86	C21-C20	4.25	1.58	1.51
10	20	301	A86	C10-C11	4.25	1.46	1.34
9	20	303	KC1	C1A-CHA	4.25	1.51	1.40
8	16	301	CLA	C1D-ND	4.25	1.43	1.37
9	11	304	KC1	CHB-C1B	4.25	1.46	1.38
9	17	303	KC1	C1A-NA	-4.25	1.29	1.38
9	17	306	KC1	C1D-ND	4.25	1.43	1.37
8	15	305	CLA	CHD-C1D	4.25	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	20	306	KC1	CHB-C1B	4.25	1.46	1.38
10	13	313	A86	C7-C6	4.25	1.59	1.50
9	12	310	KC1	C1A-NA	-4.24	1.29	1.38
10	17	321	A86	O4-C38	4.24	1.44	1.35
9	20	306	KC1	C1A-NA	-4.24	1.29	1.38
9	20	306	KC1	CHC-C4B	4.24	1.46	1.38
10	15	316	A86	C21-C20	4.24	1.58	1.51
10	21	211	A86	C7-C6	4.24	1.59	1.50
10	16	313	A86	O4-C38	4.24	1.44	1.35
9	15	304	KC1	CHB-C1B	4.24	1.46	1.38
10	13	316	A86	C7-C6	4.24	1.59	1.50
10	12	319	A86	O4-C38	4.24	1.44	1.35
10	13	315	A86	C21-C20	4.23	1.58	1.51
8	14	303	CLA	O2A-CGA	4.23	1.45	1.33
9	17	303	KC1	CHB-C1B	4.23	1.46	1.38
10	14	314	A86	O4-C38	4.23	1.44	1.35
10	14	315	A86	C17-C18	-4.23	1.46	1.52
10	19	311	A86	C21-C20	4.23	1.58	1.51
10	12	302	A86	C7-C6	4.23	1.59	1.50
8	16	303	CLA	CHD-C1D	4.23	1.46	1.38
10	13	316	A86	C21-C20	4.23	1.58	1.51
10	17	311	A86	C21-C20	4.23	1.58	1.51
10	17	313	A86	C7-C6	4.23	1.59	1.50
8	15	310	CLA	CHD-C1D	4.23	1.46	1.38
8	15	308	CLA	O2A-CGA	4.23	1.45	1.33
9	15	309	KC1	C1D-ND	4.23	1.43	1.37
10	12	312	A86	C17-C18	-4.23	1.46	1.52
8	12	307	CLA	CHD-C1D	4.22	1.46	1.38
9	17	303	KC1	C1B-NB	-4.22	1.32	1.37
10	14	311	A86	C7-C6	4.22	1.59	1.50
8	17	307	CLA	O2A-CGA	4.22	1.45	1.33
10	13	312	A86	C7-C6	4.22	1.59	1.50
10	18	311	A86	C7-C6	4.22	1.59	1.50
9	20	305	KC1	C1A-CHA	4.22	1.51	1.40
8	11	307	CLA	C1B-NB	-4.22	1.32	1.37
9	12	306	KC1	C1B-NB	-4.22	1.32	1.37
10	17	315	A86	C7-C6	4.22	1.59	1.50
10	11	312	A86	C7-C6	4.22	1.59	1.50
8	19	302	CLA	O2A-CGA	4.22	1.45	1.33
9	11	308	KC1	CHC-C4B	4.22	1.46	1.38
8	18	307	CLA	O2A-CGA	4.22	1.45	1.33
8	13	308	CLA	CHC-C1C	4.21	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	17	321	A86	C7-C6	4.21	1.59	1.50
9	12	308	KC1	CHB-C1B	4.21	1.46	1.38
10	15	316	A86	C7-C6	4.21	1.59	1.50
10	15	319	A86	C7-C6	4.21	1.59	1.50
9	11	304	KC1	C1A-CHA	4.21	1.51	1.40
8	13	309	CLA	CHD-C1D	4.21	1.46	1.38
8	20	302	CLA	O2A-CGA	4.21	1.45	1.33
9	15	302	KC1	CHB-C1B	4.21	1.46	1.38
8	20	307	CLA	C1D-ND	4.21	1.43	1.37
8	17	302	CLA	CHD-C1D	4.21	1.46	1.38
9	12	306	KC1	CHB-C1B	4.21	1.46	1.38
10	18	312	A86	C21-C20	4.21	1.58	1.51
8	19	301	CLA	O2A-CGA	4.21	1.45	1.33
10	13	315	A86	C10-C11	4.20	1.46	1.34
10	20	301	A86	C7-C6	4.20	1.59	1.50
8	13	308	CLA	C1D-ND	4.20	1.43	1.37
10	17	321	A86	C21-C20	4.20	1.58	1.51
8	21	202	CLA	O2A-CGA	4.20	1.45	1.33
13	19	312	DD6	C2-C1	4.20	1.45	1.35
8	19	309	CLA	C1D-ND	4.20	1.43	1.37
9	12	310	KC1	C1B-NB	-4.20	1.32	1.37
10	18	314	A86	C21-C20	4.20	1.58	1.51
8	16	307	CLA	O2A-CGA	4.20	1.45	1.33
10	19	313	A86	C9-C10	4.20	1.56	1.43
10	12	315	A86	C21-C20	4.20	1.58	1.51
8	20	308	CLA	CHD-C1D	4.20	1.46	1.38
10	14	313	A86	C10-C11	4.20	1.46	1.34
9	19	308	KC1	CHB-C1B	4.20	1.46	1.38
9	18	304	KC1	CHB-C1B	4.19	1.46	1.38
9	11	308	KC1	C1A-NA	-4.19	1.29	1.38
8	11	303	CLA	CHC-C1C	4.19	1.46	1.38
8	19	305	CLA	O2A-CGA	4.19	1.45	1.33
10	17	311	A86	C7-C6	4.19	1.59	1.50
8	13	301	CLA	CHD-C1D	4.19	1.46	1.38
8	20	310	CLA	CHD-C1D	4.19	1.46	1.38
9	16	304	KC1	C1A-CHA	4.19	1.51	1.40
9	19	308	KC1	C1D-ND	4.19	1.43	1.37
10	21	214	A86	C17-C18	-4.19	1.46	1.52
9	21	203	KC1	C1B-NB	-4.19	1.32	1.37
8	21	210	CLA	CHD-C1D	4.19	1.46	1.38
10	21	213	A86	C21-C20	4.18	1.58	1.51
9	14	304	KC1	CHB-C1B	4.18	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	16	304	KC1	CHB-C1B	4.18	1.46	1.38
8	20	307	CLA	O2A-CGA	4.18	1.45	1.33
9	12	308	KC1	C1D-ND	4.18	1.43	1.37
10	20	313	A86	C10-C11	4.18	1.46	1.34
10	18	313	A86	C21-C20	4.18	1.58	1.51
8	19	310	CLA	O2A-CGA	4.18	1.45	1.33
9	12	306	KC1	C1A-CHA	4.18	1.51	1.40
10	15	312	A86	O4-C38	4.18	1.44	1.35
8	15	303	CLA	CHD-C1D	4.18	1.46	1.38
10	16	311	A86	C7-C6	4.18	1.59	1.50
9	12	310	KC1	C1A-CHA	4.17	1.51	1.40
10	19	311	A86	C7-C6	4.17	1.59	1.50
10	21	213	A86	C10-C11	4.17	1.45	1.34
10	18	313	A86	C17-C18	-4.17	1.46	1.52
8	12	301	CLA	CHD-C1D	4.17	1.46	1.38
8	17	307	CLA	C1D-ND	4.17	1.43	1.37
9	16	302	KC1	C1B-NB	-4.17	1.32	1.37
8	16	307	CLA	C1D-ND	4.17	1.43	1.37
8	13	302	CLA	CHD-C1D	4.16	1.46	1.38
9	21	203	KC1	CHC-C4B	4.16	1.46	1.38
10	14	316	A86	C21-C20	4.16	1.58	1.51
10	18	313	A86	C10-C11	4.16	1.45	1.34
8	12	305	CLA	C1D-ND	4.16	1.43	1.37
8	11	303	CLA	CHD-C1D	4.16	1.46	1.38
8	14	308	CLA	CHD-C1D	4.16	1.46	1.38
10	16	310	A86	C7-C6	4.16	1.59	1.50
9	13	310	KC1	C1A-CHA	4.16	1.51	1.40
10	15	311	A86	C7-C6	4.16	1.59	1.50
10	17	316	A86	C21-C20	4.16	1.58	1.51
10	21	211	A86	C21-C20	4.15	1.58	1.51
10	18	314	A86	O4-C38	4.15	1.44	1.35
10	15	313	A86	C10-C11	4.15	1.45	1.34
8	15	308	CLA	CHC-C1C	4.15	1.46	1.38
8	19	301	CLA	C1D-ND	4.15	1.43	1.37
10	11	318	A86	C21-C20	4.15	1.58	1.51
8	12	309	CLA	O2A-CGA	4.15	1.45	1.33
9	21	207	KC1	C1A-CHA	4.15	1.51	1.40
10	13	312	A86	C21-C20	4.15	1.58	1.51
10	12	319	A86	C7-C6	4.15	1.59	1.50
10	15	311	A86	C21-C20	4.15	1.58	1.51
10	17	314	A86	C21-C20	4.15	1.58	1.51
8	19	310	CLA	C1D-ND	4.14	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	16	308	KC1	CHC-C4B	4.14	1.46	1.38
10	18	312	A86	C19-C18	4.14	1.58	1.52
8	18	305	CLA	CHD-C1D	4.14	1.46	1.38
8	19	310	CLA	CHD-C1D	4.14	1.46	1.38
9	14	309	KC1	C1A-NA	-4.14	1.29	1.38
9	13	303	KC1	C1A-CHA	4.14	1.51	1.40
10	18	311	A86	C10-C11	4.14	1.45	1.34
8	14	302	CLA	CHD-C1D	4.14	1.46	1.38
8	17	304	CLA	C1D-ND	4.14	1.43	1.37
9	14	304	KC1	C1A-CHA	4.14	1.50	1.40
8	19	309	CLA	CHD-C1D	4.13	1.46	1.38
8	17	302	CLA	O2A-CGA	4.13	1.45	1.33
10	16	310	A86	C21-C20	4.13	1.58	1.51
8	18	302	CLA	CHD-C1D	4.13	1.46	1.38
8	16	301	CLA	O2A-CGA	4.13	1.45	1.33
10	13	314	A86	C10-C11	4.13	1.45	1.34
10	15	314	A86	C9-C10	4.13	1.56	1.43
10	14	315	A86	C7-C6	4.13	1.59	1.50
10	21	215	A86	C21-C20	4.12	1.58	1.51
8	17	308	CLA	O2A-CGA	4.12	1.45	1.33
10	13	316	A86	C10-C11	4.12	1.45	1.34
10	20	301	A86	C19-C18	4.12	1.58	1.52
8	12	309	CLA	C1D-ND	4.12	1.43	1.37
9	21	203	KC1	C1A-CHA	4.12	1.50	1.40
9	18	304	KC1	C1A-CHA	4.12	1.50	1.40
10	21	213	A86	C7-C6	4.12	1.59	1.50
9	14	309	KC1	C1B-NB	-4.12	1.32	1.37
9	11	302	KC1	CHB-C1B	4.12	1.46	1.38
10	14	314	A86	C17-C18	-4.12	1.46	1.52
9	14	306	KC1	C1A-NA	-4.12	1.29	1.38
10	15	319	A86	C17-C18	-4.12	1.46	1.52
10	14	315	A86	O4-C38	4.12	1.44	1.35
9	16	302	KC1	CHB-C1B	4.12	1.46	1.38
8	21	206	CLA	O2A-CGA	4.12	1.45	1.33
9	16	302	KC1	CHC-C4B	4.11	1.46	1.38
8	11	307	CLA	O2A-CGA	4.11	1.45	1.33
8	19	305	CLA	C1D-ND	4.11	1.43	1.37
10	12	314	A86	C10-C11	4.11	1.45	1.34
10	15	315	A86	C17-C18	-4.11	1.46	1.52
10	11	311	A86	O4-C38	4.11	1.44	1.35
8	11	309	CLA	O2A-CGA	4.11	1.45	1.33
8	16	306	CLA	O2A-CGA	4.11	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	13	301	CLA	O2A-CGA	4.10	1.45	1.33
10	17	316	A86	C10-C11	4.10	1.45	1.34
8	14	308	CLA	O2A-CGA	4.10	1.45	1.33
8	11	305	CLA	CHD-C1D	4.10	1.46	1.38
9	17	305	KC1	CHB-C1B	4.10	1.46	1.38
10	20	313	A86	C17-C18	-4.09	1.46	1.52
10	15	314	A86	C17-C18	-4.09	1.46	1.52
9	17	309	KC1	C1B-NB	-4.09	1.32	1.37
10	17	312	A86	C7-C6	4.09	1.59	1.50
8	18	310	CLA	CHD-C4C	4.09	1.48	1.39
10	12	313	A86	C7-C6	4.09	1.59	1.50
10	12	316	A86	C7-C6	4.09	1.59	1.50
10	11	318	A86	C7-C6	4.09	1.59	1.50
9	15	302	KC1	C1A-CHA	4.09	1.50	1.40
10	13	313	A86	C21-C20	4.09	1.57	1.51
8	21	204	CLA	CHD-C4C	4.08	1.48	1.39
8	11	307	CLA	C1D-ND	4.08	1.43	1.37
10	11	314	A86	O4-C38	4.08	1.44	1.35
10	20	301	A86	C9-C10	4.08	1.55	1.43
10	18	314	A86	C17-C18	-4.08	1.46	1.52
8	12	304	CLA	CHD-C1D	4.08	1.46	1.38
8	16	309	CLA	CHD-C1D	4.08	1.46	1.38
10	21	214	A86	C21-C20	4.08	1.57	1.51
8	14	307	CLA	O2A-CGA	4.08	1.45	1.33
9	11	302	KC1	C1B-NB	-4.08	1.32	1.37
8	17	310	CLA	O2A-CGA	4.08	1.45	1.33
9	15	304	KC1	C1A-CHA	4.08	1.50	1.40
10	20	311	A86	C9-C10	4.07	1.55	1.43
10	17	311	A86	C10-C11	4.07	1.45	1.34
10	15	315	A86	C21-C20	4.07	1.57	1.51
8	17	308	CLA	CHD-C1D	4.07	1.46	1.38
8	13	308	CLA	CHD-C1D	4.07	1.46	1.38
8	13	304	CLA	CHD-C4C	4.07	1.48	1.39
10	14	316	A86	C7-C6	4.07	1.59	1.50
8	12	309	CLA	CHD-C1D	4.07	1.46	1.38
10	17	311	A86	C17-C18	-4.07	1.46	1.52
10	13	315	A86	C9-C10	4.07	1.55	1.43
9	11	302	KC1	CHC-C4B	4.07	1.46	1.38
10	13	316	A86	C9-C10	4.06	1.55	1.43
10	17	315	A86	O4-C38	4.06	1.44	1.35
10	16	313	A86	C21-C20	4.06	1.57	1.51
10	13	314	A86	C9-C10	4.06	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	15	319	A86	C21-C20	4.06	1.57	1.51
10	11	314	A86	C21-C20	4.06	1.57	1.51
8	16	307	CLA	C1B-NB	-4.06	1.32	1.37
10	18	311	A86	O4-C38	4.06	1.44	1.35
8	19	306	CLA	O2A-CGA	4.06	1.45	1.33
10	20	301	A86	C21-C20	4.06	1.57	1.51
9	20	303	KC1	C1B-NB	-4.05	1.32	1.37
8	18	303	CLA	C1D-ND	4.05	1.43	1.37
9	11	308	KC1	C1B-NB	-4.05	1.32	1.37
9	18	306	KC1	C1A-NA	-4.05	1.29	1.38
8	14	307	CLA	C1D-ND	4.05	1.43	1.37
10	11	313	A86	C21-C20	4.05	1.57	1.51
10	16	311	A86	C21-C20	4.04	1.57	1.51
9	15	309	KC1	C1A-NA	-4.04	1.29	1.38
8	21	208	CLA	CHD-C4C	4.04	1.48	1.39
8	18	301	CLA	O2A-CGA	4.04	1.45	1.33
8	20	309	CLA	CHD-C1D	4.04	1.46	1.38
9	16	302	KC1	C1A-NA	-4.04	1.29	1.38
10	12	302	A86	C21-C20	4.04	1.57	1.51
10	21	211	A86	C9-C10	4.04	1.55	1.43
10	20	313	A86	C9-C10	4.04	1.55	1.43
10	13	315	A86	C17-C18	-4.04	1.46	1.52
8	13	306	CLA	CHD-C4C	4.03	1.48	1.39
10	11	310	A86	C7-C6	4.03	1.59	1.50
8	18	302	CLA	C1B-NB	-4.03	1.32	1.37
9	17	305	KC1	C1A-CHA	4.03	1.50	1.40
8	19	302	CLA	CHD-C1D	4.03	1.46	1.38
9	16	305	KC1	CHB-C1B	4.03	1.46	1.38
8	21	202	CLA	CHD-C4C	4.02	1.48	1.39
8	19	304	CLA	C1D-ND	4.02	1.43	1.37
8	12	304	CLA	C1B-NB	-4.02	1.32	1.37
9	17	306	KC1	C1B-NB	-4.02	1.32	1.37
8	15	301	CLA	CHD-C1D	4.02	1.46	1.38
10	21	211	A86	C17-C18	-4.02	1.46	1.52
9	13	303	KC1	CHB-C1B	4.02	1.46	1.38
10	12	314	A86	C21-C20	4.02	1.57	1.51
10	15	312	A86	C21-C20	4.02	1.57	1.51
8	20	307	CLA	CHD-C1D	4.01	1.46	1.38
8	21	209	CLA	CHD-C4C	4.01	1.48	1.39
8	15	307	CLA	CHD-C1D	4.01	1.46	1.38
8	18	303	CLA	C1B-NB	-4.01	1.32	1.37
10	18	314	A86	C10-C11	4.01	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	19	307	CLA	CHD-C1D	4.01	1.46	1.38
8	12	303	CLA	O2A-CGA	4.01	1.45	1.33
9	11	304	KC1	C1B-NB	-4.01	1.32	1.37
9	21	207	KC1	CHB-C1B	4.01	1.46	1.38
9	13	303	KC1	C1B-NB	-4.01	1.32	1.37
8	13	308	CLA	C1B-NB	-4.00	1.32	1.37
9	15	309	KC1	C1B-NB	-4.00	1.32	1.37
8	15	305	CLA	CHD-C4C	4.00	1.48	1.39
8	19	304	CLA	CHD-C4C	4.00	1.48	1.39
8	14	305	CLA	CHD-C4C	4.00	1.48	1.39
8	21	205	CLA	CHD-C1D	3.99	1.46	1.38
10	17	312	A86	O4-C38	3.99	1.44	1.35
8	14	310	CLA	CHD-C4C	3.99	1.48	1.39
10	18	314	A86	C9-C10	3.99	1.55	1.43
9	13	310	KC1	C1B-NB	-3.99	1.32	1.37
8	18	307	CLA	CHD-C1D	3.99	1.46	1.38
10	21	215	A86	C10-C11	3.99	1.45	1.34
9	12	306	KC1	C1D-ND	3.99	1.43	1.37
10	15	313	A86	C21-C20	3.99	1.57	1.51
10	11	310	A86	C21-C20	3.99	1.57	1.51
10	12	302	A86	C10-C11	3.99	1.45	1.34
9	17	306	KC1	C1A-NA	-3.98	1.29	1.38
8	18	307	CLA	C1B-NB	-3.98	1.32	1.37
9	18	309	KC1	C1B-NB	-3.98	1.32	1.37
10	17	313	A86	C10-C11	3.98	1.45	1.34
10	16	310	A86	O4-C38	3.98	1.44	1.35
8	21	206	CLA	CHD-C1D	3.98	1.46	1.38
8	13	311	CLA	CHD-C4C	3.98	1.48	1.39
8	17	304	CLA	CHD-C4C	3.98	1.48	1.39
10	14	312	A86	C19-C18	3.98	1.57	1.52
9	21	207	KC1	CHC-C1C	3.98	1.48	1.39
10	17	315	A86	C10-C11	3.98	1.45	1.34
10	18	313	A86	C9-C10	3.97	1.55	1.43
10	17	316	A86	C9-C10	3.97	1.55	1.43
8	19	306	CLA	C1D-ND	3.97	1.43	1.37
8	14	307	CLA	CHD-C1D	3.97	1.46	1.38
8	19	303	CLA	CHD-C1D	3.97	1.46	1.38
10	20	311	A86	C17-C18	-3.97	1.46	1.52
8	19	305	CLA	CHD-C1D	3.97	1.46	1.38
10	15	312	A86	C10-C11	3.97	1.45	1.34
8	20	302	CLA	CHD-C4C	3.96	1.48	1.39
10	12	314	A86	C9-C10	3.96	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	12	316	A86	C9-C10	3.96	1.55	1.43
8	16	307	CLA	CHD-C1D	3.96	1.46	1.38
10	19	313	A86	C7-C6	3.96	1.58	1.50
8	12	305	CLA	CHD-C1D	3.96	1.46	1.38
8	21	210	CLA	CHD-C4C	3.95	1.48	1.39
10	21	214	A86	C10-C11	3.95	1.45	1.34
8	12	303	CLA	CHD-C1D	3.95	1.46	1.38
10	11	311	A86	C21-C20	3.95	1.57	1.51
8	17	307	CLA	CHD-C1D	3.95	1.46	1.38
8	12	307	CLA	CHD-C4C	3.95	1.48	1.39
8	15	310	CLA	CHD-C4C	3.95	1.48	1.39
10	14	312	A86	C21-C20	3.95	1.57	1.51
9	12	308	KC1	C1B-NB	-3.95	1.32	1.37
10	21	213	A86	C9-C10	3.95	1.55	1.43
9	17	303	KC1	CHC-C4B	3.95	1.46	1.38
10	14	313	A86	C9-C10	3.94	1.55	1.43
8	18	303	CLA	CHD-C1D	3.94	1.46	1.38
10	17	312	A86	C21-C20	3.94	1.57	1.51
10	15	316	A86	C9-C10	3.94	1.55	1.43
10	14	314	A86	C10-C11	3.94	1.45	1.34
8	11	309	CLA	CHD-C1D	3.93	1.46	1.38
8	12	311	CLA	CHD-C4C	3.93	1.48	1.39
8	12	301	CLA	O2A-CGA	3.93	1.44	1.33
10	13	313	A86	C10-C11	3.93	1.45	1.34
8	17	310	CLA	CHD-C4C	3.93	1.48	1.39
8	20	308	CLA	CHD-C4C	3.93	1.48	1.39
9	20	306	KC1	C1B-NB	-3.93	1.32	1.37
8	11	301	CLA	CHD-C1D	3.93	1.46	1.38
9	17	305	KC1	C1B-NB	-3.92	1.32	1.37
8	18	301	CLA	CHD-C1D	3.92	1.46	1.38
10	20	311	A86	C19-C18	3.91	1.57	1.52
8	14	302	CLA	CHD-C4C	3.91	1.48	1.39
9	18	309	KC1	CHB-C1B	3.91	1.46	1.38
8	16	303	CLA	CHD-C4C	3.90	1.48	1.39
8	18	302	CLA	CHD-C4C	3.90	1.48	1.39
10	17	315	A86	C9-C10	3.90	1.55	1.43
10	20	313	A86	C19-C18	3.90	1.57	1.52
8	17	308	CLA	C1B-NB	-3.90	1.32	1.37
10	14	315	A86	C10-C11	3.90	1.45	1.34
8	18	305	CLA	CHD-C4C	3.90	1.48	1.39
8	17	302	CLA	CHD-C4C	3.90	1.48	1.39
10	11	310	A86	C10-C11	3.90	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	14	303	CLA	CHD-C4C	3.90	1.48	1.39
10	17	321	A86	C10-C11	3.89	1.45	1.34
8	11	305	CLA	CHD-C4C	3.89	1.48	1.39
10	15	316	A86	C10-C11	3.89	1.45	1.34
10	18	312	A86	C10-C11	3.89	1.45	1.34
10	17	311	A86	C19-C18	3.89	1.57	1.52
8	15	308	CLA	CHD-C1D	3.89	1.46	1.38
10	18	312	A86	C17-C18	-3.89	1.46	1.52
8	19	309	CLA	CHD-C4C	3.89	1.48	1.39
9	21	203	KC1	CHB-C1B	3.89	1.46	1.38
10	12	312	A86	C10-C11	3.88	1.45	1.34
10	11	312	A86	C10-C11	3.88	1.45	1.34
10	15	313	A86	C9-C10	3.88	1.55	1.43
10	13	312	A86	C10-C11	3.88	1.45	1.34
10	14	314	A86	C19-C18	3.88	1.57	1.52
10	12	316	A86	C21-C20	3.88	1.57	1.51
8	14	301	CLA	CHD-C1D	3.88	1.46	1.38
9	19	308	KC1	C1A-CHA	3.88	1.50	1.40
10	14	316	A86	C9-C10	3.88	1.55	1.43
8	13	302	CLA	CHD-C4C	3.87	1.48	1.39
10	14	316	A86	C10-C11	3.87	1.45	1.34
8	15	303	CLA	C1B-NB	-3.86	1.32	1.37
8	16	309	CLA	C1B-NB	-3.86	1.32	1.37
8	13	309	CLA	CHD-C4C	3.86	1.48	1.39
8	11	303	CLA	CHD-C4C	3.86	1.48	1.39
9	16	305	KC1	C1B-NB	-3.85	1.32	1.37
10	21	215	A86	C9-C10	3.85	1.55	1.43
8	21	205	CLA	CHD-C4C	3.85	1.48	1.39
8	13	301	CLA	CHD-C4C	3.85	1.48	1.39
8	14	303	CLA	C3D-C2D	3.84	1.49	1.39
8	12	301	CLA	C1B-NB	-3.84	1.32	1.37
10	15	311	A86	C10-C11	3.84	1.45	1.34
10	13	314	A86	C21-C20	3.84	1.57	1.51
8	11	301	CLA	O2A-CGA	3.84	1.44	1.33
8	21	210	CLA	C3D-C2D	3.84	1.49	1.39
10	12	302	A86	C9-C10	3.84	1.55	1.43
8	18	308	CLA	CHD-C1D	3.84	1.45	1.38
9	20	303	KC1	CHB-C1B	3.84	1.45	1.38
10	14	314	A86	C21-C20	3.83	1.57	1.51
10	19	311	A86	C10-C11	3.83	1.45	1.34
8	20	310	CLA	CHD-C4C	3.83	1.47	1.39
10	15	314	A86	C19-C18	3.83	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	17	308	CLA	CHD-C4C	3.83	1.47	1.39
13	21	216	DD6	C35-C34	3.83	1.58	1.52
8	15	303	CLA	CHD-C4C	3.83	1.47	1.39
8	12	305	CLA	C1B-NB	-3.83	1.32	1.37
8	11	307	CLA	CHD-C1D	3.82	1.45	1.38
8	19	310	CLA	C1B-NB	-3.82	1.32	1.37
8	17	304	CLA	C3D-C2D	3.82	1.49	1.39
8	15	301	CLA	CHD-C4C	3.82	1.47	1.39
8	20	309	CLA	CHD-C4C	3.82	1.47	1.39
8	17	302	CLA	C1B-NB	-3.82	1.32	1.37
10	21	214	A86	C9-C10	3.82	1.55	1.43
10	14	315	A86	C9-C10	3.82	1.55	1.43
10	14	314	A86	C9-C10	3.81	1.55	1.43
10	16	313	A86	C17-C18	-3.81	1.46	1.52
10	12	313	A86	C21-C20	3.81	1.57	1.51
10	13	313	A86	C9-C10	3.81	1.55	1.43
8	11	309	CLA	C1B-NB	-3.81	1.32	1.37
8	19	302	CLA	C1B-NB	-3.81	1.32	1.37
8	12	301	CLA	CHD-C4C	3.81	1.47	1.39
8	19	301	CLA	C1B-NB	-3.80	1.32	1.37
9	17	309	KC1	CHB-C1B	3.80	1.45	1.38
9	13	310	KC1	CHB-C1B	3.80	1.45	1.38
8	16	309	CLA	CHD-C4C	3.80	1.47	1.39
10	14	313	A86	C21-C20	3.80	1.57	1.51
10	15	312	A86	C9-C10	3.80	1.55	1.43
10	12	315	A86	C9-C10	3.80	1.55	1.43
8	16	306	CLA	CHD-C1D	3.80	1.45	1.38
10	12	316	A86	C10-C11	3.79	1.44	1.34
9	16	308	KC1	CHB-C1B	3.79	1.45	1.38
10	17	313	A86	C21-C20	3.79	1.57	1.51
9	15	309	KC1	CHB-C1B	3.79	1.45	1.38
8	14	302	CLA	C1B-NB	-3.79	1.32	1.37
8	19	310	CLA	CHD-C4C	3.79	1.47	1.39
8	21	206	CLA	CHD-C4C	3.79	1.47	1.39
8	13	304	CLA	C3D-C2D	3.79	1.49	1.39
10	18	311	A86	C9-C10	3.79	1.54	1.43
10	11	311	A86	C19-C18	3.79	1.57	1.52
8	14	308	CLA	CHD-C4C	3.79	1.47	1.39
8	18	310	CLA	C3D-C2D	3.79	1.49	1.39
10	13	312	A86	C9-C10	3.79	1.54	1.43
8	20	307	CLA	CHD-C4C	3.79	1.47	1.39
9	17	306	KC1	CHC-C4B	3.79	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	13	308	CLA	C3D-C2D	3.78	1.49	1.39
8	11	303	CLA	C1B-NB	-3.78	1.32	1.37
10	16	311	A86	O4-C38	3.78	1.43	1.35
8	12	304	CLA	CHD-C4C	3.78	1.47	1.39
9	14	306	KC1	C1B-NB	-3.78	1.32	1.37
9	14	304	KC1	CHC-C1C	3.78	1.47	1.39
9	12	310	KC1	CHB-C1B	3.78	1.45	1.38
9	14	309	KC1	CHB-C1B	3.78	1.45	1.38
10	14	311	A86	C10-C11	3.78	1.44	1.34
10	18	313	A86	C19-C18	3.77	1.57	1.52
8	19	303	CLA	CHD-C4C	3.77	1.47	1.39
8	16	303	CLA	C1B-NB	-3.77	1.32	1.37
10	18	312	A86	C9-C10	3.77	1.54	1.43
8	20	304	CLA	C1B-NB	-3.77	1.32	1.37
8	12	303	CLA	CHD-C4C	3.77	1.47	1.39
8	17	307	CLA	C3D-C2D	3.77	1.49	1.39
8	19	307	CLA	C1B-NB	-3.77	1.32	1.37
8	17	307	CLA	CHD-C4C	3.77	1.47	1.39
10	15	315	A86	C19-C18	3.77	1.57	1.52
13	20	312	DD6	C35-C34	3.77	1.58	1.52
8	15	305	CLA	C3D-C2D	3.77	1.49	1.39
8	19	306	CLA	C1B-NB	-3.76	1.32	1.37
10	15	315	A86	C10-C11	3.76	1.44	1.34
8	13	308	CLA	CHD-C4C	3.76	1.47	1.39
10	21	214	A86	C19-C18	3.76	1.57	1.52
8	20	307	CLA	C1B-NB	-3.76	1.32	1.37
8	20	304	CLA	CHD-C1D	3.76	1.45	1.38
9	15	302	KC1	C1B-NB	-3.76	1.32	1.37
8	14	302	CLA	C3D-C2D	3.76	1.49	1.39
10	17	314	A86	C10-C11	3.76	1.44	1.34
8	19	305	CLA	C3D-C2D	3.76	1.49	1.39
8	11	303	CLA	C4B-NB	-3.75	1.32	1.37
9	18	304	KC1	C1B-NB	-3.75	1.32	1.37
8	15	307	CLA	CHD-C4C	3.75	1.47	1.39
8	12	303	CLA	C1B-NB	-3.75	1.32	1.37
9	16	304	KC1	C1B-NB	-3.75	1.32	1.37
8	14	301	CLA	CHC-C4B	3.75	1.47	1.39
8	16	303	CLA	C3D-C2D	3.75	1.49	1.39
8	19	301	CLA	CHD-C1D	3.75	1.45	1.38
10	16	310	A86	C10-C11	3.75	1.44	1.34
10	12	312	A86	C9-C10	3.75	1.54	1.43
8	20	308	CLA	C3D-C2D	3.75	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	17	311	A86	C9-C10	3.75	1.54	1.43
8	19	306	CLA	CHC-C4B	3.75	1.47	1.39
8	19	309	CLA	C1B-NB	-3.74	1.32	1.37
8	21	209	CLA	C3D-C2D	3.74	1.49	1.39
8	19	301	CLA	C3D-C2D	3.74	1.49	1.39
10	12	315	A86	C10-C11	3.74	1.44	1.34
8	18	307	CLA	C3D-C2D	3.74	1.49	1.39
8	13	304	CLA	C4B-NB	-3.74	1.33	1.37
8	19	302	CLA	CHD-C4C	3.74	1.47	1.39
8	21	204	CLA	C3D-C2D	3.74	1.49	1.39
8	11	307	CLA	C4B-NB	-3.73	1.33	1.37
8	12	311	CLA	C3D-C2D	3.73	1.49	1.39
13	16	312	DD6	C35-C34	3.73	1.58	1.52
8	18	310	CLA	OBD-CAD	3.73	1.28	1.22
8	14	301	CLA	CHD-C4C	3.73	1.47	1.39
9	19	308	KC1	C1B-NB	-3.73	1.33	1.37
9	18	306	KC1	C1B-NB	-3.73	1.33	1.37
8	11	301	CLA	CHD-C4C	3.73	1.47	1.39
8	16	301	CLA	CHD-C1D	3.72	1.45	1.38
8	15	305	CLA	OBD-CAD	3.72	1.28	1.22
8	12	309	CLA	CHD-C4C	3.72	1.47	1.39
8	13	311	CLA	C3D-C2D	3.72	1.49	1.39
9	11	308	KC1	CHB-C1B	3.72	1.45	1.38
8	18	303	CLA	CHD-C4C	3.72	1.47	1.39
10	15	315	A86	C9-C10	3.72	1.54	1.43
10	17	314	A86	C19-C18	3.72	1.57	1.52
8	12	305	CLA	CHD-C4C	3.72	1.47	1.39
8	18	301	CLA	CHC-C4B	3.72	1.47	1.39
10	17	321	A86	C9-C10	3.72	1.54	1.43
10	11	318	A86	C10-C11	3.72	1.44	1.34
10	14	312	A86	C10-C11	3.72	1.44	1.34
8	19	307	CLA	CHD-C4C	3.72	1.47	1.39
9	20	305	KC1	C1B-NB	-3.72	1.33	1.37
8	12	307	CLA	C1B-NB	-3.71	1.33	1.37
8	15	303	CLA	C3D-C2D	3.71	1.49	1.39
8	21	208	CLA	C3D-C2D	3.71	1.49	1.39
8	14	307	CLA	C3D-C2D	3.71	1.49	1.39
9	13	307	KC1	C1B-NB	-3.71	1.33	1.37
10	15	311	A86	C9-C10	3.71	1.54	1.43
8	13	306	CLA	C3D-C2D	3.71	1.49	1.39
8	12	309	CLA	C3D-C2D	3.70	1.49	1.39
8	19	310	CLA	C3D-C2D	3.70	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	20	302	CLA	C3D-C2D	3.70	1.49	1.39
8	20	307	CLA	C3D-C2D	3.70	1.49	1.39
8	11	305	CLA	C1B-NB	-3.70	1.33	1.37
10	17	314	A86	C9-C10	3.70	1.54	1.43
8	18	301	CLA	CHD-C4C	3.70	1.47	1.39
10	19	311	A86	C9-C10	3.70	1.54	1.43
8	20	308	CLA	OBD-CAD	3.70	1.28	1.22
10	14	312	A86	C9-C10	3.70	1.54	1.43
8	21	202	CLA	C3D-C2D	3.70	1.49	1.39
10	16	311	A86	C10-C11	3.69	1.44	1.34
10	11	311	A86	C17-C18	-3.69	1.47	1.52
8	15	308	CLA	CHD-C4C	3.69	1.47	1.39
8	18	305	CLA	C3D-C2D	3.69	1.49	1.39
8	13	306	CLA	OBD-CAD	3.69	1.28	1.22
8	19	305	CLA	C1B-NB	-3.69	1.33	1.37
10	15	319	A86	C10-C11	3.69	1.44	1.34
8	18	308	CLA	C1B-NB	-3.69	1.33	1.37
10	11	313	A86	C19-C18	3.68	1.57	1.52
8	19	304	CLA	CHD-C1D	3.68	1.45	1.38
9	13	305	KC1	CHC-C1C	3.68	1.47	1.39
8	14	307	CLA	CHD-C4C	3.68	1.47	1.39
8	19	301	CLA	CHC-C4B	3.68	1.47	1.39
8	15	301	CLA	CHC-C4B	3.68	1.47	1.39
8	20	310	CLA	OBD-CAD	3.68	1.28	1.22
10	11	313	A86	C10-C11	3.68	1.44	1.34
8	13	304	CLA	C1B-NB	-3.68	1.33	1.37
8	13	306	CLA	CHC-C4B	3.68	1.47	1.39
8	11	301	CLA	C1B-NB	-3.67	1.33	1.37
8	19	305	CLA	CHD-C4C	3.67	1.47	1.39
9	12	310	KC1	CHC-C1C	3.67	1.47	1.39
10	19	313	A86	C21-C20	3.67	1.57	1.51
8	21	208	CLA	OBD-CAD	3.67	1.28	1.22
10	11	313	A86	C9-C10	3.67	1.54	1.43
10	13	315	A86	C19-C18	3.67	1.57	1.52
8	18	307	CLA	CHD-C4C	3.67	1.47	1.39
8	21	210	CLA	CHC-C4B	3.67	1.47	1.39
8	13	302	CLA	C3D-C2D	3.67	1.49	1.39
8	14	305	CLA	C3D-C2D	3.67	1.49	1.39
8	15	307	CLA	C3D-C2D	3.67	1.49	1.39
10	17	313	A86	C9-C10	3.67	1.54	1.43
8	12	307	CLA	C3D-C2D	3.67	1.49	1.39
9	14	304	KC1	C1B-NB	-3.67	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	18	305	CLA	OBD-CAD	3.66	1.28	1.22
8	16	301	CLA	C3D-C2D	3.66	1.49	1.39
8	14	308	CLA	C3D-C2D	3.66	1.49	1.39
10	11	314	A86	C10-C11	3.66	1.44	1.34
8	15	310	CLA	C3D-C2D	3.66	1.49	1.39
9	17	309	KC1	CHC-C1C	3.66	1.47	1.39
9	16	305	KC1	CHC-C1C	3.66	1.47	1.39
8	11	301	CLA	CHC-C4B	3.66	1.47	1.39
8	13	301	CLA	C3D-C2D	3.65	1.49	1.39
8	13	301	CLA	C1B-NB	-3.65	1.33	1.37
9	14	309	KC1	CHC-C1C	3.65	1.47	1.39
10	15	319	A86	C9-C10	3.65	1.54	1.43
10	11	311	A86	C10-C11	3.65	1.44	1.34
8	20	302	CLA	CHC-C4B	3.65	1.47	1.39
8	17	304	CLA	C4B-NB	-3.64	1.33	1.37
8	12	304	CLA	C3D-C2D	3.64	1.48	1.39
8	14	310	CLA	OBD-CAD	3.64	1.28	1.22
10	11	312	A86	C9-C10	3.64	1.54	1.43
8	15	310	CLA	C1B-NB	-3.64	1.33	1.37
8	18	303	CLA	C3D-C2D	3.64	1.48	1.39
8	21	209	CLA	OBD-CAD	3.64	1.28	1.22
8	11	309	CLA	CHD-C4C	3.64	1.47	1.39
10	16	311	A86	C9-C10	3.64	1.54	1.43
8	15	308	CLA	C1B-NB	-3.64	1.33	1.37
10	17	312	A86	C10-C11	3.63	1.44	1.34
10	12	313	A86	C10-C11	3.63	1.44	1.34
8	16	307	CLA	CHD-C4C	3.63	1.47	1.39
8	16	306	CLA	C1D-ND	3.63	1.42	1.37
8	14	310	CLA	C1B-NB	-3.63	1.33	1.37
8	12	303	CLA	C3D-C2D	3.63	1.48	1.39
10	11	318	A86	C9-C10	3.63	1.54	1.43
8	20	309	CLA	C3D-C2D	3.63	1.48	1.39
8	21	210	CLA	OBD-CAD	3.63	1.28	1.22
8	12	305	CLA	C3D-C2D	3.62	1.48	1.39
8	19	306	CLA	C3D-C2D	3.62	1.48	1.39
10	21	211	A86	C19-C18	3.62	1.57	1.52
8	11	303	CLA	C3D-C2D	3.62	1.48	1.39
8	11	305	CLA	C3D-C2D	3.62	1.48	1.39
8	15	305	CLA	CHC-C4B	3.62	1.47	1.39
8	18	308	CLA	OBD-CAD	3.62	1.28	1.22
8	14	303	CLA	C4B-NB	-3.62	1.33	1.37
8	20	310	CLA	C3D-C2D	3.62	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	14	305	CLA	OBD-CAD	3.62	1.28	1.22
8	15	301	CLA	C3D-C2D	3.62	1.48	1.39
8	14	310	CLA	C3D-C2D	3.62	1.48	1.39
8	18	308	CLA	CHD-C4C	3.62	1.47	1.39
8	11	307	CLA	C3D-C2D	3.62	1.48	1.39
13	21	212	DD6	C35-C34	3.62	1.58	1.52
9	16	304	KC1	CHC-C1C	3.62	1.47	1.39
8	12	311	CLA	C1B-NB	-3.62	1.33	1.37
8	19	304	CLA	C1B-NB	-3.62	1.33	1.37
10	11	310	A86	C9-C10	3.62	1.54	1.43
8	19	306	CLA	CHD-C1D	3.61	1.45	1.38
8	13	308	CLA	C4B-NB	-3.61	1.33	1.37
8	18	308	CLA	C3D-C2D	3.61	1.48	1.39
8	21	209	CLA	CHC-C4B	3.61	1.47	1.39
8	16	306	CLA	CHD-C4C	3.61	1.47	1.39
8	12	311	CLA	OBD-CAD	3.61	1.28	1.22
9	19	308	KC1	CHC-C1C	3.60	1.47	1.39
10	12	319	A86	C10-C11	3.60	1.44	1.34
9	11	306	KC1	CHC-C1C	3.60	1.47	1.39
9	21	207	KC1	C1B-NB	-3.60	1.33	1.37
8	13	311	CLA	OBD-CAD	3.60	1.28	1.22
9	15	306	KC1	C1B-NB	-3.60	1.33	1.37
9	18	306	KC1	OBD-CAD	3.60	1.28	1.22
8	19	309	CLA	C3D-C2D	3.60	1.48	1.39
8	17	310	CLA	C3D-C2D	3.60	1.48	1.39
9	11	306	KC1	C1B-NB	-3.60	1.33	1.37
8	19	309	CLA	OBD-CAD	3.60	1.28	1.22
8	14	303	CLA	C1B-NB	-3.60	1.33	1.37
8	21	206	CLA	C3D-C2D	3.60	1.48	1.39
8	13	302	CLA	C1B-NB	-3.59	1.33	1.37
8	17	302	CLA	C3D-C2D	3.59	1.48	1.39
8	12	307	CLA	OBD-CAD	3.59	1.28	1.22
9	14	304	KC1	OBD-CAD	3.59	1.28	1.22
9	17	305	KC1	CHC-C1C	3.59	1.47	1.39
10	12	313	A86	C9-C10	3.59	1.54	1.43
10	12	315	A86	C19-C18	3.59	1.57	1.52
8	16	309	CLA	CHC-C4B	3.59	1.47	1.39
10	14	311	A86	C9-C10	3.58	1.54	1.43
8	21	202	CLA	C1B-NB	-3.58	1.33	1.37
8	21	206	CLA	C1B-NB	-3.58	1.33	1.37
9	15	306	KC1	CHC-C1C	3.58	1.47	1.39
8	15	310	CLA	OBD-CAD	3.58	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	11	309	CLA	OBD-CAD	3.58	1.28	1.22
8	19	301	CLA	CHD-C4C	3.58	1.47	1.39
8	20	308	CLA	CHC-C4B	3.58	1.47	1.39
8	17	307	CLA	C4B-NB	-3.58	1.33	1.37
9	13	305	KC1	C1B-NB	-3.58	1.33	1.37
9	12	306	KC1	CHC-C1C	3.58	1.47	1.39
8	18	302	CLA	C3D-C2D	3.58	1.48	1.39
8	14	301	CLA	C3D-C2D	3.58	1.48	1.39
8	17	310	CLA	OBD-CAD	3.58	1.28	1.22
8	14	308	CLA	C1B-NB	-3.58	1.33	1.37
8	19	303	CLA	CHC-C4B	3.57	1.47	1.39
8	12	311	CLA	CHC-C4B	3.57	1.47	1.39
8	13	302	CLA	OBD-CAD	3.57	1.28	1.22
8	21	205	CLA	C3D-C2D	3.57	1.48	1.39
9	13	303	KC1	OBD-CAD	3.57	1.28	1.22
8	17	308	CLA	C3D-C2D	3.57	1.48	1.39
8	15	307	CLA	CHC-C4B	3.57	1.47	1.39
9	18	304	KC1	CHC-C1C	3.57	1.47	1.39
8	21	208	CLA	CHC-C4B	3.57	1.47	1.39
8	16	307	CLA	C3D-C2D	3.57	1.48	1.39
10	20	301	A86	C17-C18	-3.57	1.47	1.52
8	11	301	CLA	C3D-C2D	3.57	1.48	1.39
8	11	309	CLA	C3D-C2D	3.57	1.48	1.39
8	14	307	CLA	C4B-NB	-3.57	1.33	1.37
10	11	314	A86	C9-C10	3.57	1.54	1.43
8	14	305	CLA	C1B-NB	-3.57	1.33	1.37
8	19	302	CLA	C3D-C2D	3.57	1.48	1.39
10	21	213	A86	C19-C18	3.57	1.57	1.52
10	11	311	A86	C9-C10	3.56	1.54	1.43
8	13	311	CLA	CHC-C4B	3.56	1.47	1.39
8	16	301	CLA	CHD-C4C	3.56	1.47	1.39
8	18	301	CLA	C1B-NB	-3.56	1.33	1.37
8	16	306	CLA	C3D-C2D	3.56	1.48	1.39
13	20	314	DD6	C-C1	3.56	1.58	1.50
9	20	303	KC1	CHC-C1C	3.56	1.47	1.39
8	19	304	CLA	CHC-C4B	3.56	1.47	1.39
9	15	302	KC1	CHC-C1C	3.56	1.47	1.39
10	13	314	A86	C17-C18	-3.55	1.47	1.52
8	15	301	CLA	OBD-CAD	3.55	1.28	1.22
8	16	301	CLA	C1B-NB	-3.55	1.33	1.37
8	20	310	CLA	CHC-C4B	3.55	1.47	1.39
8	20	304	CLA	CHD-C4C	3.55	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	19	304	CLA	C3D-C2D	3.55	1.48	1.39
9	21	203	KC1	CHC-C1C	3.55	1.47	1.39
8	19	307	CLA	C3D-C2D	3.55	1.48	1.39
9	13	303	KC1	CHC-C1C	3.55	1.47	1.39
10	13	314	A86	C19-C18	3.55	1.57	1.52
8	11	307	CLA	CHD-C4C	3.54	1.47	1.39
9	15	304	KC1	CHC-C1C	3.54	1.47	1.39
8	20	309	CLA	OBD-CAD	3.54	1.28	1.22
8	12	301	CLA	C3D-C2D	3.54	1.48	1.39
8	16	309	CLA	C3D-C2D	3.54	1.48	1.39
10	17	312	A86	C9-C10	3.54	1.54	1.43
8	17	308	CLA	OBD-CAD	3.54	1.28	1.22
9	14	306	KC1	OBD-CAD	3.54	1.28	1.22
8	15	303	CLA	CHC-C4B	3.54	1.47	1.39
9	15	309	KC1	CHC-C1C	3.54	1.47	1.39
8	17	310	CLA	C1B-NB	-3.54	1.33	1.37
8	21	205	CLA	C1B-NB	-3.54	1.33	1.37
8	21	206	CLA	CHC-C4B	3.54	1.47	1.39
9	15	304	KC1	OBD-CAD	3.53	1.28	1.22
9	11	304	KC1	CHC-C1C	3.53	1.47	1.39
8	17	307	CLA	OBD-CAD	3.53	1.28	1.22
8	19	303	CLA	C3D-C2D	3.53	1.48	1.39
8	20	310	CLA	C1B-NB	-3.53	1.33	1.37
8	13	302	CLA	CHC-C4B	3.53	1.47	1.39
8	18	303	CLA	CHC-C4B	3.52	1.47	1.39
8	18	302	CLA	OBD-CAD	3.52	1.28	1.22
10	16	313	A86	C10-C11	3.52	1.44	1.34
9	21	207	KC1	OBD-CAD	3.52	1.28	1.22
8	13	311	CLA	C1B-NB	-3.52	1.33	1.37
9	15	302	KC1	OBD-CAD	3.52	1.28	1.22
8	21	209	CLA	C1B-NB	-3.52	1.33	1.37
9	15	304	KC1	C1B-NB	-3.51	1.33	1.37
9	16	305	KC1	OBD-CAD	3.51	1.28	1.22
10	12	319	A86	C9-C10	3.51	1.54	1.43
8	17	310	CLA	CHC-C4B	3.51	1.47	1.39
9	12	308	KC1	CHC-C1C	3.51	1.47	1.39
8	19	310	CLA	C4B-NB	-3.51	1.33	1.37
13	21	216	DD6	O2-C18	3.51	1.53	1.43
8	18	301	CLA	C3D-C2D	3.51	1.48	1.39
8	20	307	CLA	OBD-CAD	3.51	1.28	1.22
8	19	303	CLA	OBD-CAD	3.50	1.28	1.22
8	16	301	CLA	CHC-C4B	3.50	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	17	303	KC1	C4B-NB	-3.50	1.33	1.37
8	12	301	CLA	CHC-C4B	3.50	1.47	1.39
8	18	308	CLA	CHC-C4B	3.50	1.47	1.39
8	16	306	CLA	CHC-C4B	3.50	1.47	1.39
8	15	308	CLA	C3D-C2D	3.50	1.48	1.39
8	11	305	CLA	OBD-CAD	3.49	1.28	1.22
8	14	301	CLA	OBD-CAD	3.49	1.28	1.22
8	15	308	CLA	CHB-C1B	3.49	1.47	1.39
9	20	303	KC1	OBD-CAD	3.49	1.28	1.22
8	13	301	CLA	OBD-CAD	3.49	1.28	1.22
8	16	307	CLA	OBD-CAD	3.49	1.28	1.22
8	17	302	CLA	C4B-NB	-3.49	1.33	1.37
8	21	204	CLA	C1B-NB	-3.49	1.33	1.37
8	14	302	CLA	OBD-CAD	3.49	1.28	1.22
13	21	212	DD6	O2-C18	3.48	1.53	1.43
8	20	307	CLA	CHC-C4B	3.48	1.47	1.39
10	12	314	A86	C19-C18	3.48	1.57	1.52
8	18	305	CLA	CHC-C4B	3.48	1.47	1.39
9	13	307	KC1	CHC-C1C	3.48	1.47	1.39
8	19	302	CLA	CHC-C4B	3.48	1.47	1.39
10	16	313	A86	C9-C10	3.47	1.54	1.43
8	21	204	CLA	OBD-CAD	3.47	1.28	1.22
8	18	305	CLA	C1B-NB	-3.47	1.33	1.37
8	13	309	CLA	C3D-C2D	3.47	1.48	1.39
9	16	304	KC1	OBD-CAD	3.47	1.28	1.22
9	11	302	KC1	C4B-NB	-3.47	1.33	1.37
8	12	304	CLA	OBD-CAD	3.47	1.28	1.22
8	13	309	CLA	CHB-C1B	3.47	1.47	1.39
8	19	303	CLA	CHB-C1B	3.47	1.47	1.39
8	19	310	CLA	CHC-C4B	3.47	1.47	1.39
8	12	307	CLA	CHC-C4B	3.47	1.47	1.39
9	16	302	KC1	OBD-CAD	3.47	1.28	1.22
8	11	309	CLA	CHC-C4B	3.46	1.47	1.39
8	16	301	CLA	C4B-NB	-3.46	1.33	1.37
8	19	305	CLA	CHC-C4B	3.46	1.47	1.39
8	18	307	CLA	OBD-CAD	3.46	1.28	1.22
8	12	304	CLA	CHC-C4B	3.46	1.47	1.39
9	11	308	KC1	C4B-NB	-3.46	1.33	1.37
9	11	302	KC1	CHC-C1C	3.45	1.47	1.39
9	14	306	KC1	CHC-C1C	3.45	1.47	1.39
10	12	312	A86	C19-C18	3.45	1.57	1.52
9	13	310	KC1	CHC-C1C	3.45	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	21	202	CLA	OBD-CAD	3.45	1.28	1.22
10	19	311	A86	C19-C18	3.45	1.57	1.52
8	12	309	CLA	C4B-NB	-3.44	1.33	1.37
8	21	204	CLA	C4B-NB	-3.44	1.33	1.37
8	18	301	CLA	OBD-CAD	3.44	1.28	1.22
8	19	303	CLA	C1B-NB	-3.44	1.33	1.37
8	16	307	CLA	CHC-C4B	3.44	1.47	1.39
8	14	305	CLA	CHC-C4B	3.44	1.47	1.39
10	16	310	A86	C9-C10	3.44	1.53	1.43
9	17	303	KC1	OBD-CAD	3.44	1.28	1.22
8	19	310	CLA	OBD-CAD	3.43	1.28	1.22
8	14	302	CLA	CHC-C4B	3.43	1.47	1.39
8	14	308	CLA	CHB-C1B	3.43	1.47	1.39
8	21	204	CLA	CHC-C4B	3.43	1.47	1.39
8	13	309	CLA	C1B-NB	-3.43	1.33	1.37
8	19	309	CLA	CHC-C4B	3.43	1.47	1.39
9	18	306	KC1	CHC-C1C	3.43	1.47	1.39
8	15	301	CLA	CHB-C1B	3.43	1.47	1.39
13	16	312	DD6	O2-C18	3.43	1.53	1.43
8	20	309	CLA	C1B-NB	-3.43	1.33	1.37
8	14	308	CLA	CHC-C4B	3.43	1.47	1.39
9	18	309	KC1	CHC-C1C	3.43	1.47	1.39
8	13	309	CLA	CHC-C4B	3.42	1.47	1.39
8	19	307	CLA	CHC-C4B	3.42	1.47	1.39
8	14	303	CLA	OBD-CAD	3.42	1.28	1.22
8	17	302	CLA	OBD-CAD	3.42	1.28	1.22
9	13	307	KC1	OBD-CAD	3.42	1.28	1.22
8	20	309	CLA	CHB-C1B	3.42	1.47	1.39
9	11	302	KC1	OBD-CAD	3.42	1.28	1.22
8	19	306	CLA	CHD-C4C	3.42	1.47	1.39
8	18	307	CLA	C4B-NB	-3.42	1.33	1.37
8	12	309	CLA	OBD-CAD	3.42	1.28	1.22
8	12	303	CLA	CHC-C4B	3.42	1.47	1.39
8	20	304	CLA	C3D-C2D	3.42	1.48	1.39
8	18	310	CLA	CHC-C4B	3.42	1.47	1.39
8	18	302	CLA	CHC-C4B	3.41	1.47	1.39
9	18	304	KC1	OBD-CAD	3.41	1.28	1.22
8	14	310	CLA	CHC-C4B	3.41	1.47	1.39
8	20	308	CLA	C1B-NB	-3.41	1.33	1.37
8	18	308	CLA	CHB-C1B	3.40	1.47	1.39
9	11	308	KC1	CHC-C1C	3.40	1.46	1.39
9	13	310	KC1	OBD-CAD	3.40	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	12	303	CLA	OBD-CAD	3.40	1.28	1.22
8	12	305	CLA	C4B-NB	-3.40	1.33	1.37
8	17	302	CLA	CHC-C4B	3.40	1.47	1.39
8	14	308	CLA	OBD-CAD	3.40	1.28	1.22
9	15	309	KC1	OBD-CAD	3.40	1.28	1.22
8	13	306	CLA	C1B-NB	-3.39	1.33	1.37
8	20	304	CLA	C4B-NB	-3.39	1.33	1.37
8	13	301	CLA	CHB-C1B	3.39	1.47	1.39
9	20	306	KC1	OBD-CAD	3.39	1.28	1.22
8	20	308	CLA	CHB-C1B	3.39	1.47	1.39
8	12	305	CLA	CHC-C4B	3.39	1.47	1.39
8	11	305	CLA	C4B-NB	-3.39	1.33	1.37
8	14	301	CLA	C1B-NB	-3.39	1.33	1.37
8	21	208	CLA	C1B-NB	-3.39	1.33	1.37
8	17	308	CLA	CHC-C4B	3.39	1.47	1.39
8	11	307	CLA	OBD-CAD	3.38	1.28	1.22
8	21	209	CLA	CHB-C1B	3.38	1.47	1.39
10	14	312	A86	C17-C18	-3.38	1.47	1.52
9	21	203	KC1	C4B-NB	-3.38	1.33	1.37
9	17	305	KC1	OBD-CAD	3.38	1.28	1.22
16	19	315	LMU	O5B-C1B	3.37	1.50	1.41
9	15	306	KC1	OBD-CAD	3.37	1.28	1.22
8	21	205	CLA	CHC-C4B	3.37	1.47	1.39
9	20	305	KC1	OBD-CAD	3.37	1.28	1.22
13	16	312	DD6	C-C1	3.37	1.57	1.50
10	17	315	A86	C19-C18	3.37	1.57	1.52
13	20	312	DD6	O2-C18	3.37	1.53	1.43
8	20	304	CLA	CHC-C4B	3.36	1.47	1.39
9	13	305	KC1	OBD-CAD	3.36	1.28	1.22
8	11	301	CLA	OBD-CAD	3.36	1.28	1.22
13	20	314	DD6	O2-C18	3.36	1.53	1.43
8	14	307	CLA	OBD-CAD	3.36	1.28	1.22
8	20	302	CLA	OBD-CAD	3.36	1.28	1.22
9	20	306	KC1	CHC-C1C	3.36	1.46	1.39
9	12	306	KC1	OBD-CAD	3.36	1.28	1.22
8	15	310	CLA	CHC-C4B	3.36	1.46	1.39
8	18	303	CLA	OBD-CAD	3.36	1.28	1.22
9	20	305	KC1	CHC-C1C	3.36	1.46	1.39
9	11	304	KC1	OBD-CAD	3.35	1.28	1.22
8	12	309	CLA	CHC-C4B	3.35	1.46	1.39
8	19	307	CLA	OBD-CAD	3.35	1.28	1.22
13	20	314	DD6	C35-C34	3.35	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	13	313	A86	C19-C18	3.35	1.57	1.52
10	18	311	A86	C19-C18	3.35	1.57	1.52
8	12	301	CLA	OBD-CAD	3.35	1.28	1.22
8	21	205	CLA	OBD-CAD	3.34	1.28	1.22
8	18	310	CLA	C1B-NB	-3.34	1.33	1.37
8	13	301	CLA	CHC-C4B	3.34	1.46	1.39
8	17	307	CLA	CHC-C4B	3.34	1.46	1.39
8	19	306	CLA	OBD-CAD	3.34	1.28	1.22
8	21	202	CLA	C4B-NB	-3.34	1.33	1.37
8	13	309	CLA	OBD-CAD	3.34	1.28	1.22
9	17	305	KC1	C4B-NB	-3.34	1.33	1.37
8	19	304	CLA	C4B-NB	-3.34	1.33	1.37
8	21	210	CLA	C1B-NB	-3.34	1.33	1.37
9	16	308	KC1	CHC-C1C	3.33	1.46	1.39
8	20	309	CLA	CHC-C4B	3.33	1.46	1.39
8	18	307	CLA	CHC-C4B	3.33	1.46	1.39
16	19	315	LMU	O5'-C1'	3.33	1.50	1.41
10	14	311	A86	C19-C18	3.33	1.57	1.52
8	11	305	CLA	CHC-C4B	3.32	1.46	1.39
8	20	302	CLA	CHB-C1B	3.32	1.46	1.39
8	15	301	CLA	C1B-NB	-3.32	1.33	1.37
9	20	306	KC1	CHD-C1D	3.32	1.46	1.39
8	15	305	CLA	C1B-NB	-3.32	1.33	1.37
8	14	307	CLA	CHC-C4B	3.32	1.46	1.39
8	20	307	CLA	C4B-NB	-3.32	1.33	1.37
8	16	303	CLA	C4B-NB	-3.32	1.33	1.37
8	19	305	CLA	OBD-CAD	3.32	1.28	1.22
8	16	309	CLA	OBD-CAD	3.31	1.28	1.22
8	20	304	CLA	CHB-C1B	3.31	1.46	1.39
8	21	205	CLA	CHB-C1B	3.31	1.46	1.39
9	21	203	KC1	OBD-CAD	3.31	1.28	1.22
13	21	216	DD6	C-C1	3.31	1.57	1.50
8	19	305	CLA	C4B-NB	-3.31	1.33	1.37
8	15	308	CLA	CHC-C4B	3.31	1.46	1.39
9	17	303	KC1	CHC-C1C	3.30	1.46	1.39
9	17	306	KC1	C4B-NB	-3.30	1.33	1.37
9	18	309	KC1	OBD-CAD	3.29	1.28	1.22
9	20	305	KC1	C4B-NB	-3.29	1.33	1.37
9	15	304	KC1	CHD-C1D	3.29	1.46	1.39
8	19	302	CLA	C4B-NB	-3.29	1.33	1.37
8	21	202	CLA	CHB-C1B	3.29	1.46	1.39
8	18	310	CLA	CHB-C1B	3.28	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	13	303	KC1	CHD-C1D	3.28	1.46	1.39
10	14	313	A86	C25-C24	3.28	1.43	1.34
8	15	308	CLA	OBD-CAD	3.28	1.28	1.22
8	11	307	CLA	CHC-C4B	3.28	1.46	1.39
9	13	310	KC1	CHD-C1D	3.28	1.46	1.39
8	20	310	CLA	CHB-C1B	3.27	1.46	1.39
8	14	301	CLA	CHB-C1B	3.27	1.46	1.39
9	15	309	KC1	C4B-NB	-3.27	1.33	1.37
8	13	308	CLA	OBD-CAD	3.27	1.28	1.22
8	18	301	CLA	CHB-C1B	3.27	1.46	1.39
8	12	303	CLA	C4B-NB	-3.26	1.33	1.37
13	20	312	DD6	C-C1	3.26	1.57	1.50
8	18	305	CLA	CHB-C1B	3.26	1.46	1.39
8	21	210	CLA	CHB-C1B	3.26	1.46	1.39
8	14	310	CLA	CHB-C1B	3.26	1.46	1.39
10	11	312	A86	C21-C20	3.26	1.56	1.51
8	13	306	CLA	CHB-C1B	3.26	1.46	1.39
9	12	308	KC1	OBD-CAD	3.26	1.28	1.22
9	15	302	KC1	CHD-C1D	3.25	1.46	1.39
9	16	308	KC1	C4B-NB	-3.25	1.33	1.37
8	16	306	CLA	OBD-CAD	3.25	1.28	1.22
8	15	305	CLA	CHB-C1B	3.25	1.46	1.39
8	15	303	CLA	OBD-CAD	3.25	1.28	1.22
9	20	306	KC1	C4B-NB	-3.25	1.33	1.37
8	19	301	CLA	OBD-CAD	3.24	1.28	1.22
8	13	302	CLA	C4B-NB	-3.24	1.33	1.37
8	20	309	CLA	C4B-NB	-3.24	1.33	1.37
9	16	304	KC1	C4B-NB	-3.24	1.33	1.37
8	15	307	CLA	OBD-CAD	3.24	1.28	1.22
9	19	308	KC1	OBD-CAD	3.24	1.28	1.22
8	15	308	CLA	C4B-NB	-3.24	1.33	1.37
10	18	312	A86	O-C13	-3.24	1.16	1.23
9	16	302	KC1	CHC-C1C	3.24	1.46	1.39
8	17	310	CLA	C4B-NB	-3.23	1.33	1.37
9	15	304	KC1	C4B-NB	-3.23	1.33	1.37
9	18	304	KC1	CHD-C1D	3.23	1.46	1.39
9	17	306	KC1	CHC-C1C	3.23	1.46	1.39
8	14	305	CLA	CHB-C1B	3.22	1.46	1.39
8	12	305	CLA	OBD-CAD	3.22	1.28	1.22
9	21	203	KC1	CHD-C1D	3.22	1.46	1.39
9	13	305	KC1	C4B-NB	-3.22	1.33	1.37
8	20	302	CLA	C1B-NB	-3.22	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	19	304	CLA	OBD-CAD	3.22	1.28	1.22
8	19	304	CLA	CHB-C1B	3.21	1.46	1.39
9	15	306	KC1	C4B-NB	-3.21	1.33	1.37
9	11	304	KC1	CHD-C1D	3.21	1.46	1.39
9	17	306	KC1	OBD-CAD	3.21	1.28	1.22
10	21	215	A86	C19-C18	3.21	1.56	1.52
8	12	305	CLA	CHB-C1B	3.21	1.46	1.39
8	16	301	CLA	CHB-C1B	3.21	1.46	1.39
9	18	309	KC1	C4B-NB	-3.20	1.33	1.37
8	14	308	CLA	C4B-NB	-3.20	1.33	1.37
8	21	208	CLA	CHB-C1B	3.20	1.46	1.39
8	16	309	CLA	C4B-NB	-3.20	1.33	1.37
8	19	309	CLA	CHB-C1B	3.20	1.46	1.39
8	13	311	CLA	CHB-C1B	3.20	1.46	1.39
8	21	204	CLA	CHB-C1B	3.20	1.46	1.39
8	19	302	CLA	CHB-C1B	3.20	1.46	1.39
9	20	305	KC1	CHD-C1D	3.20	1.46	1.39
8	19	301	CLA	CHB-C1B	3.20	1.46	1.39
8	11	309	CLA	C4B-NB	-3.20	1.33	1.37
8	13	304	CLA	OBD-CAD	3.19	1.28	1.22
8	16	301	CLA	OBD-CAD	3.19	1.28	1.22
8	14	303	CLA	CHC-C4B	3.19	1.46	1.39
9	16	308	KC1	OBD-CAD	3.19	1.28	1.22
8	16	303	CLA	CHB-C1B	3.19	1.46	1.39
10	12	313	A86	C19-C18	3.19	1.56	1.52
10	18	314	A86	C19-C18	3.19	1.56	1.52
10	12	319	A86	C19-C18	3.19	1.56	1.52
8	12	304	CLA	CHB-C1B	3.19	1.46	1.39
8	12	307	CLA	CHB-C1B	3.18	1.46	1.39
9	12	310	KC1	C4B-NB	-3.18	1.33	1.37
9	16	302	KC1	CHD-C1D	3.17	1.46	1.39
8	19	309	CLA	C4B-NB	-3.17	1.33	1.37
8	13	308	CLA	CHC-C4B	3.17	1.46	1.39
10	17	312	A86	O-C13	-3.17	1.16	1.23
9	17	309	KC1	C4B-NB	-3.17	1.33	1.37
8	18	307	CLA	CHB-C1B	3.17	1.46	1.39
8	15	301	CLA	C4B-NB	-3.17	1.33	1.37
9	14	304	KC1	CHD-C1D	3.17	1.46	1.39
13	19	312	DD6	O2-C18	3.17	1.52	1.43
8	12	303	CLA	CHB-C1B	3.17	1.46	1.39
10	15	313	A86	C25-C24	3.17	1.42	1.34
8	19	305	CLA	CHB-C1B	3.16	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	11	308	KC1	CHD-C1D	3.16	1.46	1.39
8	16	303	CLA	CHC-C4B	3.16	1.46	1.39
8	17	302	CLA	CHB-C1B	3.16	1.46	1.39
10	16	313	A86	C19-C18	3.16	1.56	1.52
10	11	312	A86	C25-C24	3.16	1.42	1.34
8	11	301	CLA	C4B-NB	-3.16	1.33	1.37
8	11	309	CLA	CHB-C1B	3.15	1.46	1.39
8	12	307	CLA	C4B-NB	-3.15	1.33	1.37
8	14	302	CLA	C4B-NB	-3.15	1.33	1.37
9	12	308	KC1	C4B-NB	-3.15	1.33	1.37
9	17	305	KC1	CHD-C1D	3.15	1.46	1.39
8	17	308	CLA	CHB-C1B	3.14	1.46	1.39
9	17	303	KC1	CHD-C1D	3.14	1.46	1.39
8	12	301	CLA	CHB-C1B	3.14	1.46	1.39
14	16	314	SQD	O48-C23	3.14	1.42	1.33
8	15	310	CLA	CHB-C1B	3.14	1.46	1.39
8	17	304	CLA	OBD-CAD	3.14	1.27	1.22
8	15	310	CLA	C4B-NB	-3.14	1.33	1.37
8	16	307	CLA	C4B-NB	-3.14	1.33	1.37
13	19	312	DD6	C26-C27	-3.13	1.30	1.37
8	19	306	CLA	CHB-C1B	3.13	1.46	1.39
8	14	302	CLA	CHB-C1B	3.13	1.46	1.39
9	16	308	KC1	CHD-C1D	3.13	1.46	1.39
8	20	302	CLA	C4B-NB	-3.13	1.33	1.37
8	21	206	CLA	CHB-C1B	3.13	1.46	1.39
8	13	301	CLA	C4B-NB	-3.13	1.33	1.37
9	13	310	KC1	C4B-NB	-3.13	1.33	1.37
8	13	304	CLA	CHB-C1B	3.12	1.46	1.39
10	15	313	A86	C19-C18	3.12	1.56	1.52
9	17	306	KC1	CHD-C1D	3.12	1.46	1.39
9	16	304	KC1	CHD-C1D	3.12	1.46	1.39
8	17	308	CLA	C4B-NB	-3.12	1.33	1.37
8	18	303	CLA	C4B-NB	-3.12	1.33	1.37
10	13	314	A86	C25-C24	3.12	1.42	1.34
8	21	205	CLA	C4B-NB	-3.11	1.33	1.37
10	19	313	A86	C17-C18	-3.11	1.47	1.52
9	15	306	KC1	CHD-C1D	3.11	1.46	1.39
8	19	307	CLA	CHB-C1B	3.11	1.46	1.39
8	15	303	CLA	CHB-C1B	3.10	1.46	1.39
9	18	304	KC1	C4B-NB	-3.10	1.33	1.37
9	13	305	KC1	CHD-C1D	3.10	1.46	1.39
8	17	310	CLA	CHB-C1B	3.10	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	21	213	A86	C25-C24	3.10	1.42	1.34
8	14	301	CLA	C4B-NB	-3.10	1.33	1.37
10	12	314	A86	C25-C24	3.09	1.42	1.34
8	20	307	CLA	CHB-C1B	3.09	1.46	1.39
10	14	314	A86	C14-C15	3.09	1.58	1.52
8	16	306	CLA	C4B-NB	-3.09	1.33	1.37
10	15	312	A86	C19-C18	3.09	1.56	1.52
8	11	303	CLA	CHB-C1B	3.09	1.46	1.39
10	17	312	A86	C19-C18	3.09	1.56	1.52
10	15	312	A86	O-C13	-3.08	1.16	1.23
8	19	306	CLA	C4B-NB	-3.08	1.33	1.37
10	17	321	A86	C19-C18	3.08	1.56	1.52
9	12	306	KC1	C4B-NB	-3.08	1.33	1.37
10	13	315	A86	C25-C24	3.08	1.42	1.34
10	20	313	A86	C25-C24	3.08	1.42	1.34
9	11	304	KC1	C4B-NB	-3.08	1.33	1.37
8	15	303	CLA	C4B-NB	-3.08	1.33	1.37
9	17	309	KC1	OBD-CAD	3.07	1.27	1.22
10	12	313	A86	C25-C24	3.07	1.42	1.34
8	18	303	CLA	CHB-C1B	3.07	1.46	1.39
8	15	307	CLA	C4B-NB	-3.07	1.33	1.37
8	11	305	CLA	CHB-C1B	3.07	1.46	1.39
9	19	308	KC1	C4B-NB	-3.07	1.33	1.37
8	14	305	CLA	C4B-NB	-3.07	1.33	1.37
8	13	304	CLA	CHC-C4B	3.07	1.46	1.39
9	14	306	KC1	C4B-NB	-3.06	1.33	1.37
9	18	309	KC1	CHD-C1D	3.06	1.46	1.39
9	14	309	KC1	C4B-NB	-3.06	1.33	1.37
10	14	316	A86	C19-C18	3.06	1.56	1.52
10	13	312	A86	C19-C18	3.06	1.56	1.52
8	19	307	CLA	C4B-NB	-3.06	1.33	1.37
8	19	310	CLA	CHB-C1B	3.05	1.46	1.39
9	12	310	KC1	CHD-C1D	3.05	1.46	1.39
8	16	307	CLA	CHB-C1B	3.05	1.46	1.39
8	12	301	CLA	C4B-NB	-3.05	1.33	1.37
9	14	304	KC1	C4B-NB	-3.05	1.33	1.37
8	11	303	CLA	CHC-C4B	3.05	1.46	1.39
9	12	310	KC1	OBD-CAD	3.05	1.27	1.22
8	16	309	CLA	CHB-C1B	3.04	1.46	1.39
9	11	302	KC1	CHD-C1D	3.04	1.46	1.39
9	11	306	KC1	OBD-CAD	3.04	1.27	1.22
8	18	302	CLA	C4B-NB	-3.04	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	11	308	KC1	OBD-CAD	3.04	1.27	1.22
9	16	305	KC1	CHD-C1D	3.04	1.46	1.39
8	13	309	CLA	C4B-NB	-3.04	1.33	1.37
8	16	303	CLA	OBD-CAD	3.04	1.27	1.22
14	17	301	SQD	O48-C23	3.04	1.42	1.33
9	16	305	KC1	C4B-NB	-3.04	1.33	1.37
10	14	315	A86	C19-C18	3.04	1.56	1.52
9	14	309	KC1	OBD-CAD	3.03	1.27	1.22
9	16	302	KC1	C2A-C1A	3.03	1.54	1.44
8	11	301	CLA	CHB-C1B	3.03	1.46	1.39
8	12	311	CLA	CHB-C1B	3.03	1.46	1.39
10	15	312	A86	C26-C27	3.03	1.42	1.35
10	15	319	A86	C19-C18	3.02	1.56	1.52
10	20	301	A86	C25-C24	3.02	1.42	1.34
10	17	312	A86	C26-C27	3.02	1.42	1.35
8	21	206	CLA	OBD-CAD	3.02	1.27	1.22
8	14	303	CLA	CHB-C1B	3.01	1.46	1.39
9	15	302	KC1	C4B-NB	-3.01	1.33	1.37
10	15	314	A86	C25-C24	3.01	1.42	1.34
9	21	207	KC1	CHD-C1D	3.01	1.46	1.39
8	12	304	CLA	C4B-NB	-3.01	1.33	1.37
10	15	316	A86	C19-C18	3.00	1.56	1.52
13	19	312	DD6	C-C1	3.00	1.56	1.50
8	17	304	CLA	CHC-C4B	3.00	1.46	1.39
8	18	310	CLA	C4B-NB	-3.00	1.33	1.37
10	18	313	A86	C25-C24	3.00	1.42	1.34
9	11	306	KC1	CHD-C1D	2.99	1.46	1.39
9	20	303	KC1	C4B-NB	-2.99	1.33	1.37
8	20	310	CLA	C4B-NB	-2.99	1.33	1.37
8	19	301	CLA	C4B-NB	-2.99	1.33	1.37
8	18	302	CLA	CHB-C1B	2.98	1.46	1.39
8	16	306	CLA	CHB-C1B	2.98	1.46	1.39
9	17	309	KC1	CHD-C1D	2.98	1.46	1.39
8	13	311	CLA	C4B-NB	-2.98	1.33	1.37
9	14	309	KC1	CHD-C1D	2.98	1.46	1.39
8	20	308	CLA	C4B-NB	-2.98	1.33	1.37
8	13	302	CLA	CHB-C1B	2.98	1.46	1.39
10	19	313	A86	C14-C15	2.98	1.58	1.52
9	18	306	KC1	CHD-C1D	2.97	1.46	1.39
8	18	308	CLA	C4B-NB	-2.97	1.34	1.37
8	21	210	CLA	C4B-NB	-2.97	1.34	1.37
8	14	310	CLA	C4B-NB	-2.97	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	21	214	A86	C25-C24	2.97	1.42	1.34
9	20	303	KC1	CHD-C1D	2.97	1.46	1.39
8	11	303	CLA	OBD-CAD	2.97	1.27	1.22
8	19	303	CLA	C4B-NB	-2.96	1.34	1.37
9	19	308	KC1	CHD-C1D	2.96	1.46	1.39
10	21	213	A86	C14-C15	2.96	1.58	1.52
8	18	305	CLA	C4B-NB	-2.96	1.34	1.37
10	15	311	A86	C19-C18	2.96	1.56	1.52
10	12	314	A86	O-C13	-2.95	1.17	1.23
10	13	313	A86	C26-C27	2.95	1.42	1.35
9	12	308	KC1	CHD-C1D	2.95	1.46	1.39
9	15	309	KC1	CHD-C1D	2.95	1.46	1.39
10	15	314	A86	C14-C15	2.95	1.58	1.52
10	16	311	A86	C19-C18	2.94	1.56	1.52
10	16	310	A86	C19-C18	2.93	1.56	1.52
10	15	312	A86	C25-C24	2.93	1.42	1.34
10	21	213	A86	C26-C27	2.93	1.42	1.35
10	21	213	A86	C24-C1	2.92	1.52	1.46
10	17	315	A86	O-C13	-2.92	1.17	1.23
10	14	312	A86	C14-C15	2.92	1.58	1.52
10	14	313	A86	C19-C18	2.92	1.56	1.52
8	18	301	CLA	C4B-NB	-2.91	1.34	1.37
10	15	315	A86	C14-C15	2.91	1.58	1.52
10	16	311	A86	C25-C24	2.91	1.42	1.34
9	21	207	KC1	C4B-NB	-2.91	1.34	1.37
9	11	306	KC1	C4B-NB	-2.91	1.34	1.37
8	21	206	CLA	C4B-NB	-2.91	1.34	1.37
8	21	202	CLA	CHC-C4B	2.90	1.45	1.39
8	13	308	CLA	CHB-C1B	2.90	1.45	1.39
10	17	313	A86	C19-C18	2.90	1.56	1.52
10	17	313	A86	C25-C24	2.90	1.42	1.34
10	16	310	A86	O-C13	-2.89	1.17	1.23
13	21	216	DD6	C26-C27	-2.89	1.31	1.37
10	18	314	A86	C25-C24	2.89	1.42	1.34
10	14	314	A86	C25-C24	2.89	1.42	1.34
13	21	212	DD6	C-C1	2.89	1.56	1.50
8	13	306	CLA	C4B-NB	-2.89	1.34	1.37
9	13	307	KC1	C4B-NB	-2.88	1.34	1.37
10	18	313	A86	C14-C15	2.88	1.58	1.52
10	17	314	A86	O-C13	-2.88	1.17	1.23
15	19	314	LHG	O7-C5	-2.88	1.39	1.46
10	15	313	A86	C26-C27	2.88	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	16	308	KC1	CHB-C4A	-2.88	1.32	1.39
10	11	311	A86	O-C13	-2.87	1.17	1.23
10	20	313	A86	C14-C15	2.87	1.58	1.52
9	14	306	KC1	CHD-C1D	2.87	1.45	1.39
8	15	305	CLA	C4B-NB	-2.87	1.34	1.37
10	12	313	A86	O-C13	-2.87	1.17	1.23
9	18	306	KC1	C4B-NB	-2.86	1.34	1.37
10	12	315	A86	C25-C24	2.86	1.42	1.34
9	17	303	KC1	C2A-C1A	2.86	1.53	1.44
10	21	211	A86	C14-C15	2.86	1.58	1.52
10	14	313	A86	C14-C15	2.86	1.58	1.52
10	14	313	A86	C24-C1	2.86	1.52	1.46
10	15	316	A86	C25-C24	2.86	1.42	1.34
10	13	314	A86	C24-C1	2.86	1.52	1.46
10	12	314	A86	C26-C27	2.86	1.42	1.35
10	15	311	A86	O-C13	-2.85	1.17	1.23
10	15	313	A86	C24-C1	2.85	1.52	1.46
9	14	309	KC1	CHB-C4A	-2.85	1.32	1.39
8	12	311	CLA	C4D-CHA	2.84	1.48	1.38
13	20	314	DD6	C9-C8	2.84	1.42	1.34
8	21	208	CLA	C4B-NB	-2.84	1.34	1.37
8	17	304	CLA	CHB-C1B	2.84	1.45	1.39
10	17	321	A86	O-C13	-2.84	1.17	1.23
10	13	316	A86	C25-C24	2.84	1.42	1.34
10	13	316	A86	C19-C18	2.84	1.56	1.52
10	11	313	A86	C25-C24	2.84	1.42	1.34
10	12	314	A86	C24-C1	2.84	1.52	1.46
10	17	311	A86	O-C13	-2.84	1.17	1.23
13	21	216	DD6	C9-C8	2.83	1.42	1.34
10	11	318	A86	C19-C18	2.83	1.56	1.52
9	11	308	KC1	CHB-C4A	-2.83	1.32	1.39
10	15	314	A86	C26-C27	2.83	1.42	1.35
10	13	313	A86	C25-C24	2.83	1.42	1.34
10	18	311	A86	C25-C24	2.83	1.42	1.34
10	15	314	A86	C-C1	2.82	1.56	1.50
10	13	315	A86	C26-C27	2.82	1.42	1.35
8	21	209	CLA	C4B-NB	-2.82	1.34	1.37
9	21	207	KC1	CHB-C4A	-2.82	1.32	1.39
10	13	315	A86	C-C1	2.82	1.56	1.50
10	21	211	A86	C25-C24	2.82	1.42	1.34
10	14	314	A86	C-C1	2.82	1.56	1.50
10	13	314	A86	C26-C27	2.82	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	19	302	CLA	C3D-C4D	-2.81	1.37	1.44
9	16	302	KC1	C4B-NB	-2.81	1.34	1.37
10	20	311	A86	C25-C24	2.81	1.42	1.34
10	12	316	A86	C25-C24	2.81	1.42	1.34
10	17	316	A86	C19-C18	2.81	1.56	1.52
10	15	313	A86	O-C13	-2.81	1.17	1.23
10	17	316	A86	C25-C24	2.81	1.42	1.34
10	17	314	A86	C25-C24	2.81	1.42	1.34
9	13	303	KC1	C4B-NB	-2.81	1.34	1.37
10	11	312	A86	C14-C15	2.81	1.58	1.52
10	16	311	A86	O4-C34	-2.81	1.40	1.46
10	19	313	A86	O-C13	-2.81	1.17	1.23
8	12	311	CLA	C4B-NB	-2.80	1.34	1.37
10	21	215	A86	C25-C24	2.80	1.42	1.34
10	11	318	A86	C26-C27	2.80	1.42	1.35
9	21	203	KC1	CHB-C4A	-2.80	1.32	1.39
10	17	313	A86	C14-C15	2.80	1.58	1.52
10	15	313	A86	C-C1	2.80	1.56	1.50
10	15	319	A86	C-C1	2.80	1.56	1.50
9	17	309	KC1	CHB-C4A	-2.80	1.32	1.39
10	13	315	A86	C24-C1	2.79	1.51	1.46
8	14	302	CLA	C4D-CHA	2.79	1.47	1.38
9	12	310	KC1	CHB-C4A	-2.79	1.32	1.39
10	11	314	A86	C14-C15	2.79	1.58	1.52
13	21	212	DD6	C9-C8	2.78	1.41	1.34
10	15	315	A86	O-C13	-2.78	1.17	1.23
10	12	313	A86	C26-C27	2.78	1.42	1.35
8	18	302	CLA	C4D-CHA	2.77	1.47	1.38
13	20	312	DD6	C26-C27	-2.77	1.31	1.37
10	11	310	A86	O-C13	-2.77	1.17	1.23
10	14	313	A86	C-C1	2.77	1.56	1.50
10	21	215	A86	C24-C1	2.77	1.51	1.46
10	11	311	A86	C25-C24	2.77	1.41	1.34
11	11	315	LMG	C4-C5	2.77	1.58	1.53
10	12	314	A86	C14-C15	2.76	1.58	1.52
10	21	214	A86	C14-C15	2.76	1.58	1.52
8	17	307	CLA	CHB-C1B	2.76	1.45	1.39
10	13	313	A86	O-C13	-2.76	1.17	1.23
10	12	314	A86	C-C1	2.76	1.56	1.50
10	15	319	A86	C14-C15	2.76	1.58	1.52
8	17	307	CLA	C4D-CHA	2.76	1.47	1.38
9	20	306	KC1	C4C-C3C	2.76	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	15	319	A86	C25-C24	2.75	1.41	1.34
9	15	309	KC1	CHB-C4A	-2.75	1.32	1.39
8	13	308	CLA	C4D-CHA	2.75	1.47	1.38
10	19	311	A86	O-C13	-2.75	1.17	1.23
8	15	307	CLA	CHB-C1B	2.75	1.45	1.39
10	13	314	A86	C-C1	2.75	1.56	1.50
10	17	313	A86	C26-C27	2.75	1.42	1.35
9	18	304	KC1	CHB-C4A	-2.74	1.32	1.39
8	13	306	CLA	C4D-CHA	2.74	1.47	1.38
10	14	312	A86	O-C13	-2.74	1.17	1.23
10	15	315	A86	C25-C24	2.74	1.41	1.34
8	15	305	CLA	C4D-CHA	2.74	1.47	1.38
10	12	302	A86	C19-C18	2.74	1.56	1.52
10	21	215	A86	C-C1	2.74	1.56	1.50
8	18	310	CLA	C4D-CHA	2.74	1.47	1.38
8	19	304	CLA	C4C-C3C	2.74	1.49	1.45
9	13	303	KC1	CHB-C4A	-2.74	1.33	1.39
8	12	304	CLA	C4D-CHA	2.74	1.47	1.38
10	11	318	A86	O-C13	-2.73	1.17	1.23
10	11	312	A86	C24-C1	2.73	1.51	1.46
10	14	313	A86	C26-C27	2.73	1.42	1.35
10	13	312	A86	O-C13	-2.73	1.17	1.23
10	18	312	A86	C25-C24	2.73	1.41	1.34
10	21	213	A86	C-C1	2.73	1.56	1.50
9	20	303	KC1	CHB-C4A	-2.73	1.33	1.39
8	15	310	CLA	C4D-CHA	2.73	1.47	1.38
8	20	304	CLA	C3D-C4D	-2.73	1.38	1.44
9	16	305	KC1	CHB-C4A	-2.73	1.33	1.39
9	12	306	KC1	CHD-C1D	2.73	1.45	1.39
10	18	313	A86	C-C1	2.73	1.56	1.50
9	17	306	KC1	C2A-C1A	2.73	1.53	1.44
9	12	308	KC1	CHB-C4A	-2.73	1.33	1.39
8	21	208	CLA	C4D-CHA	2.72	1.47	1.38
9	13	310	KC1	CHB-C4A	-2.72	1.33	1.39
10	11	313	A86	O-C13	-2.72	1.17	1.23
9	11	302	KC1	C2A-C1A	2.72	1.53	1.44
13	21	212	DD6	O1-C20	2.72	1.49	1.46
8	20	304	CLA	C4D-CHA	2.72	1.47	1.38
8	18	310	CLA	C4C-C3C	2.72	1.49	1.45
10	18	314	A86	C26-C27	2.72	1.42	1.35
10	21	211	A86	C26-C27	2.72	1.42	1.35
10	12	316	A86	C19-C18	2.72	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	12	306	KC1	CHB-C4A	-2.72	1.33	1.39
9	13	307	KC1	CHD-C1D	2.71	1.45	1.39
8	18	308	CLA	C4D-CHA	2.71	1.47	1.38
10	12	316	A86	O-C13	-2.71	1.17	1.23
8	12	309	CLA	C4D-CHA	2.71	1.47	1.38
10	15	313	A86	C14-C15	2.71	1.58	1.52
8	14	307	CLA	C4D-CHA	2.71	1.47	1.38
10	20	313	A86	C24-C1	2.70	1.51	1.46
9	14	304	KC1	CHB-C4A	-2.70	1.33	1.39
10	16	311	A86	O-C13	-2.70	1.17	1.23
10	20	313	A86	C-C1	2.70	1.56	1.50
8	15	307	CLA	C4D-CHA	2.70	1.47	1.38
8	19	307	CLA	C4D-CHA	2.70	1.47	1.38
8	21	206	CLA	C4D-CHA	2.70	1.47	1.38
8	12	303	CLA	C4D-CHA	2.70	1.47	1.38
8	11	301	CLA	C4D-CHA	2.70	1.47	1.38
10	17	312	A86	C25-C24	2.70	1.41	1.34
10	16	313	A86	C-C1	2.70	1.56	1.50
8	14	303	CLA	C4D-CHA	2.69	1.47	1.38
9	16	308	KC1	C4A-C3A	2.69	1.50	1.44
13	21	216	DD6	C35-C36	2.69	1.55	1.51
10	19	311	A86	C14-C15	2.69	1.58	1.52
9	15	309	KC1	C2A-C1A	2.69	1.53	1.44
10	17	321	A86	C14-C15	2.69	1.58	1.52
10	11	314	A86	C19-C18	2.69	1.56	1.52
10	14	314	A86	C26-C27	2.69	1.42	1.35
10	11	312	A86	C26-C27	2.69	1.42	1.35
10	13	312	A86	C25-C24	2.69	1.41	1.34
8	20	309	CLA	C4D-CHA	2.69	1.47	1.38
8	14	310	CLA	C4D-CHA	2.69	1.47	1.38
8	13	302	CLA	C4D-CHA	2.69	1.47	1.38
8	13	311	CLA	C4D-CHA	2.69	1.47	1.38
10	12	315	A86	C-C1	2.69	1.56	1.50
8	18	305	CLA	C4D-CHA	2.68	1.47	1.38
9	18	309	KC1	CHB-C4A	-2.68	1.33	1.39
10	11	312	A86	O-C13	-2.68	1.17	1.23
8	14	305	CLA	C4D-CHA	2.68	1.47	1.38
9	19	308	KC1	CHB-C4A	-2.68	1.33	1.39
10	14	314	A86	O-C13	-2.68	1.17	1.23
8	14	308	CLA	C4D-CHA	2.68	1.47	1.38
10	12	312	A86	O-C13	-2.68	1.17	1.23
10	20	311	A86	C14-C15	2.68	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	11	313	A86	C-C1	2.68	1.56	1.50
10	14	312	A86	C-C1	2.68	1.56	1.50
10	14	316	A86	C25-C24	2.67	1.41	1.34
10	19	313	A86	C-C1	2.67	1.56	1.50
9	18	309	KC1	C2A-C1A	2.67	1.52	1.44
13	16	312	DD6	C35-C36	2.67	1.55	1.51
10	21	214	A86	C-C1	2.67	1.56	1.50
13	20	312	DD6	C9-C8	2.67	1.41	1.34
14	17	301	SQD	O47-C7	2.67	1.41	1.34
8	11	307	CLA	CHB-C1B	2.67	1.45	1.39
10	14	312	A86	C25-C24	2.67	1.41	1.34
9	21	203	KC1	C2A-C1A	2.67	1.52	1.44
8	12	309	CLA	CHB-C1B	2.67	1.45	1.39
10	11	310	A86	C26-C27	2.67	1.42	1.35
9	13	310	KC1	C2A-C1A	2.67	1.52	1.44
10	15	311	A86	C26-C27	2.67	1.42	1.35
9	11	308	KC1	C2A-C1A	2.67	1.52	1.44
9	16	308	KC1	C2A-C1A	2.67	1.52	1.44
10	11	312	A86	C-C1	2.67	1.56	1.50
10	18	314	A86	C-C1	2.67	1.56	1.50
10	17	314	A86	C-C1	2.66	1.56	1.50
10	15	314	A86	C24-C1	2.66	1.51	1.46
8	11	303	CLA	C4D-CHA	2.66	1.47	1.38
8	20	308	CLA	C4D-CHA	2.66	1.47	1.38
8	21	209	CLA	C4D-CHA	2.66	1.47	1.38
10	14	316	A86	C-C1	2.66	1.56	1.50
8	17	308	CLA	C4D-CHA	2.66	1.47	1.38
10	11	314	A86	C25-C24	2.66	1.41	1.34
10	13	312	A86	C14-C15	2.66	1.57	1.52
8	21	202	CLA	C4D-CHA	2.66	1.47	1.38
8	13	301	CLA	C4D-CHA	2.66	1.47	1.38
10	14	313	A86	O-C13	-2.66	1.17	1.23
9	14	309	KC1	C2A-C1A	2.65	1.52	1.44
9	17	309	KC1	C2A-C1A	2.65	1.52	1.44
13	19	312	DD6	C9-C8	2.65	1.41	1.34
9	17	305	KC1	CHB-C4A	-2.65	1.33	1.39
8	18	301	CLA	C4D-CHA	2.65	1.47	1.38
10	18	313	A86	C26-C27	2.65	1.41	1.35
8	21	205	CLA	C4D-CHA	2.65	1.47	1.38
8	12	301	CLA	C4D-CHA	2.65	1.47	1.38
10	13	313	A86	C14-C15	2.65	1.57	1.52
8	18	307	CLA	C4D-CHA	2.65	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	12	315	A86	C14-C15	2.64	1.57	1.52
10	17	314	A86	C14-C15	2.64	1.57	1.52
8	20	307	CLA	C4D-CHA	2.64	1.47	1.38
9	18	306	KC1	C2A-C1A	2.64	1.52	1.44
8	15	308	CLA	C4D-CHA	2.64	1.47	1.38
8	19	310	CLA	C4D-CHA	2.64	1.47	1.38
10	14	316	A86	O-C13	-2.64	1.17	1.23
10	17	313	A86	O-C13	-2.64	1.17	1.23
10	13	313	A86	C-C1	2.64	1.56	1.50
13	19	312	DD6	C35-C34	2.64	1.56	1.52
10	17	316	A86	C-C1	2.64	1.56	1.50
9	16	302	KC1	CHB-C4A	-2.64	1.33	1.39
9	20	305	KC1	C4A-C3A	2.64	1.49	1.44
10	12	312	A86	C25-C24	2.64	1.41	1.34
9	14	306	KC1	C2A-C1A	2.64	1.52	1.44
13	20	312	DD6	C35-C36	2.64	1.55	1.51
9	12	310	KC1	C2A-C1A	2.64	1.52	1.44
10	11	318	A86	C14-C15	2.64	1.57	1.52
10	11	314	A86	C26-C27	2.64	1.41	1.35
10	18	312	A86	C14-C15	2.64	1.57	1.52
10	15	319	A86	O-C13	-2.64	1.17	1.23
10	18	313	A86	O-C13	-2.64	1.17	1.23
10	21	213	A86	O-C13	-2.64	1.17	1.23
8	19	309	CLA	C4D-CHA	2.63	1.47	1.38
10	12	315	A86	O-C13	-2.63	1.17	1.23
10	11	314	A86	O-C13	-2.63	1.17	1.23
10	15	316	A86	C-C1	2.63	1.56	1.50
10	15	311	A86	C25-C24	2.63	1.41	1.34
9	15	302	KC1	CHB-C4A	-2.63	1.33	1.39
10	12	302	A86	O-C13	-2.63	1.17	1.23
10	19	311	A86	C26-C27	2.63	1.41	1.35
10	17	311	A86	C25-C24	2.63	1.41	1.34
8	17	310	CLA	C4D-CHA	2.62	1.47	1.38
9	13	303	KC1	C3B-C4B	2.62	1.50	1.46
9	16	305	KC1	C2A-C1A	2.62	1.52	1.44
10	14	315	A86	C26-C27	2.62	1.41	1.35
8	11	307	CLA	C4D-CHA	2.62	1.47	1.38
10	14	315	A86	C14-C15	2.62	1.57	1.52
8	11	305	CLA	C4D-CHA	2.62	1.47	1.38
8	21	210	CLA	C4D-CHA	2.62	1.47	1.38
10	11	310	A86	C14-C15	2.62	1.57	1.52
10	11	311	A86	C14-C15	2.62	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	21	214	A86	O-C13	-2.62	1.17	1.23
8	13	309	CLA	C4D-CHA	2.62	1.47	1.38
10	21	214	A86	C24-C1	2.62	1.51	1.46
8	11	303	CLA	C3D-C4D	-2.62	1.38	1.44
9	15	306	KC1	CHB-C4A	-2.61	1.33	1.39
10	12	319	A86	O-C13	-2.61	1.17	1.23
8	15	303	CLA	C4D-CHA	2.61	1.47	1.38
10	15	312	A86	C-C1	2.61	1.56	1.50
13	20	312	DD6	O1-C20	2.61	1.49	1.46
10	14	311	A86	O-C13	-2.61	1.17	1.23
10	14	315	A86	C25-C24	2.61	1.41	1.34
10	15	316	A86	C26-C27	2.61	1.41	1.35
10	15	312	A86	C14-C15	2.61	1.57	1.52
10	18	314	A86	C24-C1	2.61	1.51	1.46
8	13	304	CLA	C4D-CHA	2.61	1.47	1.38
8	12	305	CLA	C4D-CHA	2.61	1.47	1.38
10	17	321	A86	C25-C24	2.61	1.41	1.34
9	13	303	KC1	C2A-C1A	2.61	1.52	1.44
8	16	303	CLA	C4D-CHA	2.61	1.47	1.38
10	11	313	A86	C14-C15	2.61	1.57	1.52
14	16	314	SQD	O47-C7	2.61	1.41	1.34
8	16	309	CLA	C4D-CHA	2.60	1.47	1.38
10	14	313	A86	C2-C1	2.60	1.41	1.35
10	16	310	A86	O4-C34	-2.60	1.40	1.46
10	14	315	A86	O-C13	-2.60	1.17	1.23
10	15	316	A86	C24-C1	2.60	1.51	1.46
8	16	306	CLA	C3D-C4D	-2.60	1.38	1.44
9	15	304	KC1	CHB-C4A	-2.60	1.33	1.39
13	16	312	DD6	C9-C8	2.60	1.41	1.34
8	17	304	CLA	C4D-CHA	2.60	1.47	1.38
10	13	316	A86	C-C1	2.60	1.56	1.50
9	11	302	KC1	CHB-C4A	-2.60	1.33	1.39
10	12	319	A86	C14-C15	2.60	1.57	1.52
10	19	313	A86	C25-C24	2.59	1.41	1.34
9	17	303	KC1	CHB-C4A	-2.59	1.33	1.39
8	17	302	CLA	C4D-CHA	2.59	1.47	1.38
10	12	316	A86	C-C1	2.59	1.56	1.50
10	13	315	A86	C2-C1	2.59	1.41	1.35
9	20	306	KC1	CHB-C4A	-2.59	1.33	1.39
9	11	304	KC1	CHB-C4A	-2.59	1.33	1.39
8	14	301	CLA	C4D-CHA	2.59	1.47	1.38
8	11	309	CLA	C4D-CHA	2.59	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	13	315	A86	C14-C15	2.59	1.57	1.52
10	17	316	A86	O-C13	-2.59	1.17	1.23
10	14	315	A86	C-C1	2.59	1.56	1.50
10	17	312	A86	O4-C34	-2.59	1.40	1.46
9	13	305	KC1	C2A-C1A	2.59	1.52	1.44
8	17	304	CLA	C3D-C4D	-2.59	1.38	1.44
8	21	204	CLA	C4D-CHA	2.58	1.47	1.38
10	12	319	A86	C25-C24	2.58	1.41	1.34
10	17	313	A86	C-C1	2.58	1.56	1.50
8	16	309	CLA	C3D-C4D	-2.58	1.38	1.44
9	16	304	KC1	CHB-C4A	-2.58	1.33	1.39
13	16	312	DD6	C26-C27	-2.58	1.31	1.37
10	13	316	A86	O-C13	-2.58	1.17	1.23
10	12	302	A86	C-C1	2.58	1.56	1.50
10	13	316	A86	C26-C27	2.58	1.41	1.35
10	16	311	A86	C14-C15	2.58	1.57	1.52
8	17	310	CLA	C3D-C4D	-2.58	1.38	1.44
10	21	214	A86	C26-C27	2.58	1.41	1.35
8	17	302	CLA	C3D-C4D	-2.58	1.38	1.44
9	13	305	KC1	CHB-C4A	-2.57	1.33	1.39
10	17	312	A86	C14-C15	2.57	1.57	1.52
10	12	313	A86	C-C1	2.57	1.56	1.50
8	21	202	CLA	C1B-C2B	2.57	1.49	1.43
8	20	302	CLA	C3D-C4D	-2.57	1.38	1.44
8	21	209	CLA	C3B-C4B	2.57	1.50	1.42
8	16	307	CLA	C4D-CHA	2.57	1.47	1.38
8	12	301	CLA	C3B-C4B	2.57	1.50	1.42
8	12	305	CLA	C3D-C4D	-2.57	1.38	1.44
10	17	321	A86	C-C1	2.57	1.56	1.50
8	19	303	CLA	C3D-C4D	-2.57	1.38	1.44
9	15	302	KC1	C2A-C1A	2.56	1.52	1.44
10	12	302	A86	C25-C24	2.56	1.41	1.34
8	19	304	CLA	C4D-CHA	2.56	1.47	1.38
10	15	312	A86	C24-C1	2.56	1.51	1.46
8	19	302	CLA	C4D-CHA	2.56	1.47	1.38
11	11	315	LMG	C3-C2	2.56	1.59	1.52
8	12	307	CLA	C4D-CHA	2.56	1.47	1.38
9	20	305	KC1	CHB-C4A	-2.56	1.33	1.39
8	19	304	CLA	C3D-C4D	-2.56	1.38	1.44
10	21	215	A86	C26-C27	2.56	1.41	1.35
10	18	312	A86	C-C1	2.56	1.56	1.50
8	19	305	CLA	C4D-CHA	2.55	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	16	303	CLA	C3D-C4D	-2.55	1.38	1.44
9	20	306	KC1	C2A-C1A	2.55	1.52	1.44
10	12	316	A86	C26-C27	2.55	1.41	1.35
10	12	315	A86	C26-C27	2.55	1.41	1.35
9	13	307	KC1	CHB-C4A	-2.55	1.33	1.39
9	12	308	KC1	C2A-C1A	2.55	1.52	1.44
11	16	315	LMG	C4-C5	2.55	1.58	1.53
10	13	314	A86	C2-C1	2.55	1.41	1.35
8	13	309	CLA	C4C-C3C	2.55	1.49	1.45
10	15	316	A86	O-C13	-2.55	1.17	1.23
8	19	307	CLA	C3D-C4D	-2.54	1.38	1.44
8	18	303	CLA	C4D-CHA	2.54	1.47	1.38
9	12	310	KC1	C4A-C3A	2.54	1.49	1.44
8	15	301	CLA	C4D-CHA	2.54	1.47	1.38
9	12	306	KC1	C2A-C1A	2.54	1.52	1.44
10	20	301	A86	O-C13	-2.54	1.18	1.23
9	15	309	KC1	C4A-C3A	2.54	1.49	1.44
10	21	211	A86	C24-C1	2.54	1.51	1.46
8	15	301	CLA	C1B-C2B	2.54	1.49	1.43
10	20	313	A86	C2-C1	2.54	1.41	1.35
9	20	305	KC1	C2A-C1A	2.54	1.52	1.44
8	13	308	CLA	C3D-C4D	-2.54	1.38	1.44
10	14	315	A86	O4-C34	-2.54	1.40	1.46
10	12	314	A86	C2-C1	2.54	1.41	1.35
10	13	314	A86	O-C13	-2.53	1.18	1.23
13	19	312	DD6	C22-C16	-2.53	1.49	1.53
10	21	215	A86	O-C13	-2.53	1.18	1.23
8	19	301	CLA	C4D-CHA	2.53	1.47	1.38
9	11	304	KC1	C2A-C1A	2.53	1.52	1.44
10	12	312	A86	C14-C15	2.53	1.57	1.52
8	11	307	CLA	C3D-C4D	-2.53	1.38	1.44
13	21	216	DD6	C4-C5	2.53	1.51	1.43
9	17	309	KC1	C4A-C3A	2.52	1.49	1.44
10	17	314	A86	C26-C27	2.52	1.41	1.35
10	18	311	A86	O-C13	-2.52	1.18	1.23
9	13	307	KC1	C2A-C1A	2.52	1.52	1.44
8	18	310	CLA	C1B-C2B	2.52	1.49	1.43
8	21	202	CLA	C4C-C3C	2.52	1.49	1.45
10	15	315	A86	C-C1	2.52	1.55	1.50
10	15	312	A86	C2-C1	2.52	1.41	1.35
8	20	302	CLA	C4D-CHA	2.52	1.47	1.38
8	13	309	CLA	C1B-C2B	2.52	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	21	213	A86	C2-C1	2.52	1.41	1.35
10	14	314	A86	C24-C1	2.51	1.51	1.46
10	18	313	A86	C24-C1	2.51	1.51	1.46
8	19	309	CLA	C3D-C4D	-2.51	1.38	1.44
8	15	303	CLA	C3B-C4B	2.51	1.50	1.42
8	18	303	CLA	C3D-C4D	-2.51	1.38	1.44
10	21	211	A86	C2-C1	2.51	1.41	1.35
10	11	318	A86	C-C1	2.51	1.55	1.50
8	13	304	CLA	C3D-C4D	-2.51	1.38	1.44
10	11	310	A86	C25-C24	2.51	1.41	1.34
9	17	303	KC1	C4A-C3A	2.51	1.49	1.44
10	13	313	A86	C24-C1	2.51	1.51	1.46
8	14	307	CLA	CHB-C1B	2.50	1.45	1.39
8	16	301	CLA	C4D-CHA	2.50	1.47	1.38
8	13	311	CLA	C4C-C3C	2.50	1.49	1.45
8	14	307	CLA	C3D-C4D	-2.50	1.38	1.44
10	15	313	A86	C2-C1	2.50	1.41	1.35
9	11	304	KC1	C4A-C3A	2.49	1.49	1.44
8	15	308	CLA	C1B-C2B	2.49	1.49	1.43
9	13	307	KC1	C4A-C3A	2.49	1.49	1.44
10	21	211	A86	O-C13	-2.49	1.18	1.23
8	12	311	CLA	C3B-C4B	2.49	1.50	1.42
10	17	316	A86	C26-C27	2.49	1.41	1.35
10	16	310	A86	C14-C15	2.49	1.57	1.52
10	20	301	A86	C26-C27	2.49	1.41	1.35
9	16	302	KC1	CAA-C2A	2.49	1.53	1.46
8	21	208	CLA	C4C-C3C	2.49	1.49	1.45
8	20	309	CLA	C1B-C2B	2.49	1.49	1.43
9	12	308	KC1	C4A-C3A	2.49	1.49	1.44
8	15	303	CLA	C3D-C4D	-2.49	1.38	1.44
10	15	314	A86	O-C13	-2.48	1.18	1.23
8	16	306	CLA	C4D-CHA	2.48	1.46	1.38
8	12	304	CLA	C3B-C4B	2.48	1.50	1.42
9	13	303	KC1	C4A-C3A	2.48	1.49	1.44
8	13	306	CLA	C3B-C4B	2.48	1.50	1.42
8	21	208	CLA	C3B-C4B	2.48	1.50	1.42
8	18	301	CLA	C3B-C4B	2.48	1.50	1.42
8	20	308	CLA	C1B-C2B	2.48	1.48	1.43
10	17	315	A86	C-C1	2.48	1.55	1.50
11	17	318	LMG	O8-C9	-2.48	1.39	1.45
8	20	308	CLA	C3B-C4B	2.48	1.49	1.42
10	18	311	A86	C26-C27	2.48	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	18	306	KC1	CHB-C4A	-2.48	1.33	1.39
10	13	312	A86	C-C1	2.48	1.55	1.50
8	14	310	CLA	C3D-C4D	-2.48	1.38	1.44
9	14	309	KC1	C4A-C3A	2.48	1.49	1.44
10	17	315	A86	C14-C15	2.48	1.57	1.52
9	20	303	KC1	C2A-C1A	2.47	1.52	1.44
10	12	312	A86	O4-C34	-2.47	1.40	1.46
10	18	314	A86	O-C13	-2.47	1.18	1.23
8	12	304	CLA	C3D-C4D	-2.47	1.38	1.44
10	15	311	A86	C14-C15	2.47	1.57	1.52
8	20	310	CLA	C4D-CHA	2.47	1.46	1.38
13	20	314	DD6	C4-C5	2.47	1.50	1.43
8	19	306	CLA	C3D-C4D	-2.47	1.38	1.44
10	15	314	A86	C2-C1	2.47	1.41	1.35
8	20	310	CLA	C3D-C4D	-2.47	1.38	1.44
10	21	215	A86	C2-C1	2.47	1.41	1.35
10	17	315	A86	O4-C34	-2.46	1.40	1.46
9	17	305	KC1	C2A-C1A	2.46	1.52	1.44
10	13	313	A86	C2-C1	2.46	1.41	1.35
10	18	313	A86	C2-C1	2.46	1.41	1.35
8	16	301	CLA	C3D-C4D	-2.46	1.38	1.44
10	17	311	A86	C14-C15	2.46	1.57	1.52
10	14	314	A86	C2-C1	2.46	1.41	1.35
8	13	311	CLA	C3B-C4B	2.46	1.49	1.42
9	11	308	KC1	C4A-C3A	2.46	1.49	1.44
8	21	205	CLA	C4C-C3C	2.45	1.49	1.45
8	21	205	CLA	C1B-C2B	2.45	1.48	1.43
10	12	319	A86	C-C1	2.45	1.55	1.50
9	21	207	KC1	CAA-C2A	2.45	1.53	1.46
9	13	305	KC1	C4A-C3A	2.45	1.49	1.44
10	17	315	A86	C25-C24	2.45	1.41	1.34
9	16	302	KC1	C4A-C3A	2.45	1.49	1.44
8	15	307	CLA	C3D-C4D	-2.45	1.38	1.44
8	18	308	CLA	C1B-C2B	2.45	1.48	1.43
10	21	211	A86	C-C1	2.45	1.55	1.50
10	16	313	A86	C25-C24	2.45	1.41	1.34
8	19	303	CLA	C4D-CHA	2.45	1.46	1.38
8	19	307	CLA	C3B-C4B	2.45	1.49	1.42
8	19	306	CLA	C4D-CHA	2.45	1.46	1.38
10	20	313	A86	O-C13	-2.45	1.18	1.23
8	13	301	CLA	C1B-C2B	2.45	1.48	1.43
8	15	307	CLA	C3B-C4B	2.45	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	13	316	A86	C24-C1	2.44	1.51	1.46
8	21	204	CLA	C3D-C4D	-2.44	1.38	1.44
8	15	305	CLA	C3B-C4B	2.44	1.49	1.42
10	20	313	A86	C26-C27	2.44	1.41	1.35
8	16	307	CLA	C3D-C4D	-2.44	1.38	1.44
10	16	313	A86	O-C13	-2.44	1.18	1.23
9	11	306	KC1	C2A-C1A	2.44	1.52	1.44
8	16	309	CLA	C3B-C4B	2.44	1.49	1.42
8	19	306	CLA	C3B-C4B	2.44	1.49	1.42
9	13	310	KC1	C4A-C3A	2.44	1.49	1.44
8	12	307	CLA	C3D-C4D	-2.44	1.38	1.44
10	11	310	A86	C19-C18	2.44	1.55	1.52
10	14	316	A86	C26-C27	2.43	1.41	1.35
9	16	305	KC1	C4A-C3A	2.43	1.49	1.44
9	18	306	KC1	C4A-C3A	2.43	1.49	1.44
8	16	306	CLA	C3B-C4B	2.43	1.49	1.42
8	20	307	CLA	C3D-C4D	-2.43	1.38	1.44
10	17	316	A86	C24-C1	2.43	1.51	1.46
10	11	318	A86	C25-C24	2.43	1.41	1.34
9	18	304	KC1	C2A-C1A	2.43	1.52	1.44
9	11	306	KC1	CHB-C4A	-2.43	1.33	1.39
8	14	310	CLA	C1B-C2B	2.43	1.48	1.43
13	21	212	DD6	C26-C27	-2.43	1.32	1.37
9	14	304	KC1	C2A-C1A	2.43	1.52	1.44
9	18	309	KC1	C4A-C3A	2.43	1.49	1.44
8	20	310	CLA	C3B-C4B	2.43	1.49	1.42
8	12	309	CLA	C3D-C4D	-2.43	1.38	1.44
8	13	309	CLA	C3D-C4D	-2.43	1.38	1.44
8	21	206	CLA	C3D-C4D	-2.43	1.38	1.44
13	20	312	DD6	C4-C5	2.43	1.50	1.43
9	14	306	KC1	C4A-C3A	2.42	1.49	1.44
10	12	319	A86	O4-C34	-2.42	1.40	1.46
8	21	210	CLA	C1B-C2B	2.42	1.48	1.43
10	20	311	A86	O-C13	-2.42	1.18	1.23
9	14	306	KC1	CHB-C4A	-2.42	1.33	1.39
10	11	314	A86	O4-C34	-2.42	1.40	1.46
8	11	305	CLA	C3D-C4D	-2.42	1.38	1.44
9	16	304	KC1	C2A-C1A	2.42	1.52	1.44
8	18	301	CLA	C3D-C4D	-2.42	1.38	1.44
9	17	306	KC1	C4A-C3A	2.42	1.49	1.44
9	15	302	KC1	C4A-C3A	2.42	1.49	1.44
8	18	305	CLA	C1B-C2B	2.42	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	21	209	CLA	C1B-C2B	2.42	1.48	1.43
9	18	304	KC1	C4A-C3A	2.41	1.49	1.44
13	21	212	DD6	C4-C5	2.41	1.50	1.43
8	19	310	CLA	C3D-C4D	-2.41	1.38	1.44
10	14	311	A86	C-C1	2.41	1.55	1.50
8	14	308	CLA	C3D-C4D	-2.41	1.38	1.44
10	12	312	A86	C-C1	2.41	1.55	1.50
8	15	308	CLA	C3D-C4D	-2.41	1.38	1.44
10	18	311	A86	C-C1	2.41	1.55	1.50
8	13	306	CLA	C1B-C2B	2.41	1.48	1.43
9	11	302	KC1	C4A-C3A	2.41	1.49	1.44
8	15	301	CLA	C3D-C4D	-2.41	1.38	1.44
8	21	208	CLA	C1B-C2B	2.41	1.48	1.43
13	20	314	DD6	C35-C36	2.41	1.54	1.51
10	17	311	A86	C-C1	2.40	1.55	1.50
10	13	316	A86	C14-C15	2.40	1.57	1.52
10	11	313	A86	C26-C27	2.40	1.41	1.35
10	12	316	A86	C2-C1	2.40	1.41	1.35
8	15	310	CLA	C3B-C4B	2.40	1.49	1.42
8	18	302	CLA	C3D-C4D	-2.40	1.38	1.44
10	19	311	A86	C25-C24	2.40	1.40	1.34
10	18	311	A86	C14-C15	2.40	1.57	1.52
10	17	313	A86	C24-C1	2.40	1.51	1.46
10	18	314	A86	C2-C1	2.40	1.41	1.35
8	17	307	CLA	C3D-C4D	-2.40	1.38	1.44
8	15	305	CLA	C1B-C2B	2.40	1.48	1.43
15	21	201	LHG	O7-C5	-2.39	1.41	1.46
8	17	310	CLA	C3B-C4B	2.39	1.49	1.42
10	17	312	A86	C-C1	2.39	1.55	1.50
10	18	311	A86	O4-C34	-2.39	1.41	1.46
8	14	303	CLA	C3D-C4D	-2.39	1.38	1.44
9	12	306	KC1	C4A-C3A	2.39	1.49	1.44
8	17	308	CLA	C3D-C4D	-2.39	1.38	1.44
10	11	311	A86	O4-C34	-2.39	1.41	1.46
8	18	305	CLA	C3B-C4B	2.39	1.49	1.42
10	15	312	A86	O4-C34	-2.39	1.41	1.46
8	13	304	CLA	C4C-C3C	2.39	1.49	1.45
8	14	305	CLA	C3D-C4D	-2.39	1.38	1.44
8	19	305	CLA	C3D-C4D	-2.39	1.38	1.44
10	13	316	A86	C2-C1	2.39	1.41	1.35
10	18	311	A86	C24-C1	2.39	1.51	1.46
9	13	303	KC1	C4C-C3C	2.38	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	20	301	A86	C-C1	2.38	1.55	1.50
10	11	318	A86	O4-C34	-2.38	1.41	1.46
10	18	312	A86	C26-C27	2.38	1.41	1.35
10	16	313	A86	O4-C34	-2.38	1.41	1.46
10	15	319	A86	C24-C1	2.38	1.51	1.46
8	14	308	CLA	C1B-C2B	2.38	1.48	1.43
9	21	203	KC1	C4A-C3A	2.38	1.49	1.44
9	20	303	KC1	C3B-C4B	2.38	1.50	1.46
10	12	315	A86	C24-C1	2.38	1.51	1.46
8	21	206	CLA	C1B-C2B	2.37	1.48	1.43
9	15	306	KC1	C2A-C1A	2.37	1.51	1.44
8	13	311	CLA	C1B-C2B	2.37	1.48	1.43
8	11	301	CLA	C3B-C4B	2.37	1.49	1.42
10	12	313	A86	O4-C34	-2.37	1.41	1.46
10	21	214	A86	C2-C1	2.37	1.41	1.35
8	21	204	CLA	C1B-C2B	2.37	1.48	1.43
9	15	306	KC1	C4A-C3A	2.37	1.49	1.44
8	18	307	CLA	C3D-C4D	-2.37	1.38	1.44
10	11	314	A86	C-C1	2.36	1.55	1.50
9	20	306	KC1	C4A-C3A	2.36	1.49	1.44
8	18	303	CLA	C3B-C4B	2.36	1.49	1.42
8	21	210	CLA	C3B-C4B	2.36	1.49	1.42
9	17	305	KC1	C4A-C3A	2.36	1.49	1.44
9	17	306	KC1	C4C-C3C	2.36	1.49	1.45
8	20	302	CLA	C1B-C2B	2.36	1.48	1.43
8	13	301	CLA	C3D-C4D	-2.36	1.38	1.44
10	16	311	A86	C-C1	2.36	1.55	1.50
10	14	311	A86	C25-C24	2.36	1.40	1.34
10	13	312	A86	O4-C34	-2.35	1.41	1.46
8	16	303	CLA	C1B-C2B	2.35	1.48	1.43
8	11	309	CLA	C3D-C4D	-2.35	1.38	1.44
13	20	314	DD6	C26-C27	-2.35	1.32	1.37
10	12	316	A86	C24-C1	2.35	1.51	1.46
10	15	314	A86	O4-C34	-2.35	1.41	1.46
10	12	313	A86	C14-C15	2.35	1.57	1.52
8	21	205	CLA	C3D-C4D	-2.35	1.38	1.44
10	15	319	A86	C26-C27	2.35	1.41	1.35
10	17	314	A86	C2-C1	2.35	1.41	1.35
11	11	315	LMG	O7-C8	-2.35	1.41	1.46
8	20	308	CLA	C4C-C3C	2.35	1.49	1.45
8	17	308	CLA	C3B-C4B	2.35	1.49	1.42
8	11	305	CLA	C1B-C2B	2.35	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	18	308	CLA	C3B-C4B	2.34	1.49	1.42
8	19	305	CLA	C1B-C2B	2.34	1.48	1.43
10	14	315	A86	C2-C1	2.34	1.41	1.35
8	12	303	CLA	C1B-C2B	2.34	1.48	1.43
10	20	301	A86	C24-C1	2.34	1.51	1.46
8	19	302	CLA	OBD-CAD	2.34	1.26	1.22
8	19	301	CLA	C3D-C4D	-2.34	1.38	1.44
9	15	304	KC1	C2A-C1A	2.34	1.51	1.44
8	13	306	CLA	C4C-C3C	2.34	1.49	1.45
9	14	304	KC1	C1D-C2D	2.33	1.48	1.43
13	16	312	DD6	C22-C16	-2.33	1.49	1.53
10	12	316	A86	C14-C15	2.33	1.57	1.52
9	15	304	KC1	C1D-C2D	2.33	1.48	1.43
13	21	212	DD6	C35-C36	2.33	1.54	1.51
8	13	304	CLA	C1B-C2B	2.33	1.48	1.43
8	19	303	CLA	C1B-C2B	2.33	1.48	1.43
8	21	206	CLA	C3B-C4B	2.33	1.49	1.42
10	15	315	A86	O4-C34	-2.33	1.41	1.46
8	19	301	CLA	C3B-C4B	2.33	1.49	1.42
10	11	313	A86	C2-C1	2.33	1.41	1.35
10	20	311	A86	C26-C27	2.33	1.41	1.35
10	18	311	A86	C2-C1	2.33	1.41	1.35
10	13	313	A86	O4-C34	-2.33	1.41	1.46
8	14	310	CLA	C3B-C4B	2.33	1.49	1.42
8	19	309	CLA	C3B-C4B	2.33	1.49	1.42
8	12	311	CLA	C1B-C2B	2.33	1.48	1.43
8	14	301	CLA	C1B-C2B	2.33	1.48	1.43
8	13	311	CLA	C3D-C4D	-2.32	1.39	1.44
10	14	314	A86	O4-C34	-2.32	1.41	1.46
10	15	316	A86	C2-C1	2.32	1.41	1.35
8	14	305	CLA	C3B-C4B	2.32	1.49	1.42
8	13	302	CLA	C3D-C4D	-2.32	1.39	1.44
10	13	312	A86	C26-C27	2.32	1.41	1.35
8	12	301	CLA	C3D-C4D	-2.32	1.39	1.44
8	20	309	CLA	C3D-C4D	-2.32	1.39	1.44
8	15	305	CLA	C4C-C3C	2.32	1.49	1.45
10	21	215	A86	C14-C15	2.32	1.57	1.52
8	18	310	CLA	C3D-C4D	-2.32	1.39	1.44
10	16	311	A86	C26-C27	2.32	1.41	1.35
8	19	304	CLA	C1B-C2B	2.32	1.48	1.43
10	20	311	A86	C2-C1	2.32	1.41	1.35
10	19	313	A86	C2-C1	2.31	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	12	307	CLA	C3B-C4B	2.31	1.49	1.42
8	18	302	CLA	C3B-C4B	2.31	1.49	1.42
8	15	310	CLA	C3D-C4D	-2.31	1.39	1.44
8	14	305	CLA	C1B-C2B	2.31	1.48	1.43
10	17	321	A86	O4-C34	-2.31	1.41	1.46
8	20	304	CLA	C1B-C2B	2.31	1.48	1.43
10	15	311	A86	C-C1	2.31	1.55	1.50
9	16	304	KC1	C4A-C3A	2.31	1.49	1.44
9	20	305	KC1	C4C-C3C	2.31	1.49	1.45
10	21	215	A86	O4-C34	-2.31	1.41	1.46
10	14	316	A86	C24-C1	2.31	1.50	1.46
8	21	202	CLA	C3D-C4D	-2.31	1.39	1.44
9	13	303	KC1	C1D-C2D	2.31	1.48	1.43
8	20	308	CLA	C3D-C4D	-2.30	1.39	1.44
8	18	310	CLA	C3B-C4B	2.30	1.49	1.42
8	14	302	CLA	C3D-C4D	-2.30	1.39	1.44
8	14	301	CLA	C3B-C4B	2.30	1.49	1.42
8	16	301	CLA	C1B-C2B	2.30	1.48	1.43
8	16	307	CLA	C3B-C4B	2.30	1.49	1.42
10	11	311	A86	C26-C27	2.30	1.41	1.35
8	21	209	CLA	C4C-C3C	2.30	1.48	1.45
8	17	302	CLA	C1B-C2B	2.30	1.48	1.43
8	14	310	CLA	C4C-C3C	2.30	1.48	1.45
13	20	314	DD6	C22-C16	-2.30	1.49	1.53
10	14	316	A86	C2-C1	2.30	1.41	1.35
10	11	310	A86	O4-C34	-2.30	1.41	1.46
8	20	309	CLA	C4C-C3C	2.30	1.48	1.45
9	17	306	KC1	CHB-C4A	-2.29	1.34	1.39
10	11	318	A86	C39-C38	2.29	1.57	1.49
10	20	311	A86	C-C1	2.29	1.55	1.50
9	17	309	KC1	CBD-CAD	-2.29	1.46	1.56
8	19	304	CLA	C3B-C4B	2.29	1.49	1.42
8	20	304	CLA	OBD-CAD	2.29	1.26	1.22
10	11	313	A86	C24-C1	2.29	1.50	1.46
8	12	307	CLA	C1B-C2B	2.29	1.48	1.43
8	13	309	CLA	C3B-C4B	2.29	1.49	1.42
10	19	313	A86	C22-C16	2.29	1.58	1.53
8	20	307	CLA	C1B-C2B	2.29	1.48	1.43
8	15	310	CLA	C1B-C2B	2.29	1.48	1.43
8	19	309	CLA	C1B-C2B	2.29	1.48	1.43
9	19	308	KC1	CAA-C2A	2.29	1.53	1.46
8	21	204	CLA	C4C-C3C	2.29	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	14	301	CLA	C3D-C4D	-2.29	1.39	1.44
10	18	314	A86	O4-C34	-2.29	1.41	1.46
10	17	312	A86	C2-C1	2.28	1.41	1.35
9	21	207	KC1	C2A-C1A	2.28	1.51	1.44
8	11	301	CLA	C3D-C4D	-2.28	1.39	1.44
8	12	303	CLA	C3D-C4D	-2.28	1.39	1.44
8	13	301	CLA	C4C-C3C	2.28	1.48	1.45
10	14	311	A86	C14-C15	2.28	1.57	1.52
10	20	313	A86	O4-C34	-2.28	1.41	1.46
8	16	301	CLA	C1C-NC	-2.28	1.34	1.37
8	13	308	CLA	C1B-C2B	2.28	1.48	1.43
8	11	309	CLA	C3B-C4B	2.28	1.49	1.42
9	11	306	KC1	C4A-C3A	2.28	1.49	1.44
10	17	314	A86	C24-C1	2.27	1.50	1.46
9	17	303	KC1	CAA-C2A	2.27	1.53	1.46
10	15	319	A86	O4-C34	-2.27	1.41	1.46
8	11	305	CLA	C3B-C4B	2.27	1.49	1.42
8	13	302	CLA	C3B-C4B	2.27	1.49	1.42
10	12	302	A86	C26-C27	2.27	1.41	1.35
8	13	306	CLA	C3D-C4D	-2.27	1.39	1.44
10	18	314	A86	C14-C15	2.27	1.57	1.52
8	18	305	CLA	C3D-C4D	-2.27	1.39	1.44
9	19	308	KC1	C3B-C4B	2.27	1.50	1.46
9	15	304	KC1	C4A-C3A	2.27	1.49	1.44
8	19	309	CLA	C4C-C3C	2.27	1.48	1.45
10	11	312	A86	C19-C18	2.26	1.55	1.52
8	14	303	CLA	C4C-C3C	2.26	1.48	1.45
8	17	308	CLA	C4C-C3C	2.26	1.48	1.45
10	17	316	A86	C2-C1	2.26	1.41	1.35
14	16	314	SQD	O47-C45	-2.26	1.41	1.46
9	14	304	KC1	CAA-C2A	2.26	1.53	1.46
10	12	312	A86	C26-C27	2.26	1.41	1.35
8	20	304	CLA	C1C-C2C	2.26	1.49	1.44
8	19	302	CLA	CBD-CAD	-2.26	1.46	1.56
9	21	203	KC1	C4C-C3C	2.26	1.48	1.45
8	12	311	CLA	C4C-C3C	2.25	1.48	1.45
8	15	301	CLA	C3B-C4B	2.25	1.49	1.42
10	13	315	A86	O4-C34	-2.25	1.41	1.46
10	12	312	A86	C24-C1	2.25	1.50	1.46
8	12	303	CLA	C3B-C4B	2.25	1.49	1.42
9	11	308	KC1	C4C-C3C	2.25	1.48	1.45
10	14	311	A86	O4-C34	-2.25	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	14	312	A86	C26-C27	2.25	1.41	1.35
8	14	308	CLA	C3B-C4B	2.25	1.49	1.42
10	12	316	A86	O4-C34	-2.25	1.41	1.46
8	20	310	CLA	C1B-C2B	2.25	1.48	1.43
9	21	207	KC1	C1D-C2D	2.25	1.48	1.43
8	21	210	CLA	C3D-C4D	-2.25	1.39	1.44
10	19	313	A86	C26-C27	2.25	1.41	1.35
10	14	312	A86	C24-C1	2.25	1.50	1.46
9	21	207	KC1	C1C-C2C	2.25	1.49	1.44
10	19	313	A86	O4-C34	-2.25	1.41	1.46
8	19	302	CLA	C3B-C4B	2.24	1.49	1.42
10	21	214	A86	O4-C34	-2.24	1.41	1.46
8	13	302	CLA	C1B-C2B	2.24	1.48	1.43
10	15	311	A86	C2-C1	2.24	1.41	1.35
10	18	313	A86	O4-C34	-2.24	1.41	1.46
8	19	303	CLA	C3B-C4B	2.24	1.49	1.42
10	13	316	A86	O4-C34	-2.24	1.41	1.46
8	12	309	CLA	C3B-C4B	2.24	1.49	1.42
10	12	315	A86	O4-C34	-2.24	1.41	1.46
10	14	316	A86	O4-C34	-2.24	1.41	1.46
10	14	312	A86	O4-C34	-2.24	1.41	1.46
10	17	313	A86	C2-C1	2.24	1.41	1.35
10	14	316	A86	C14-C15	2.24	1.57	1.52
10	18	312	A86	O4-C34	-2.24	1.41	1.46
13	16	312	DD6	C4-C5	2.24	1.50	1.43
8	21	202	CLA	C1C-NC	-2.23	1.34	1.37
8	12	305	CLA	C1B-C2B	2.23	1.48	1.43
9	20	306	KC1	C1D-C2D	2.23	1.48	1.43
8	21	209	CLA	C3D-C4D	-2.23	1.39	1.44
8	18	305	CLA	C4C-C3C	2.23	1.48	1.45
10	11	311	A86	C-C1	2.23	1.55	1.50
9	18	304	KC1	C4C-C3C	2.23	1.48	1.45
9	19	308	KC1	C2A-C1A	2.23	1.51	1.44
10	11	311	A86	C2-C1	2.23	1.41	1.35
9	16	304	KC1	C1D-C2D	2.23	1.48	1.43
9	17	305	KC1	C4C-C3C	2.23	1.48	1.45
9	11	304	KC1	CAA-C2A	2.23	1.53	1.46
10	20	301	A86	C2-C1	2.23	1.41	1.35
8	14	305	CLA	C4C-C3C	2.23	1.48	1.45
8	13	311	CLA	C3B-C2B	2.23	1.48	1.41
10	21	211	A86	C5-C6	2.23	1.40	1.35
8	17	310	CLA	C1B-C2B	2.22	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	17	311	A86	O4-C34	-2.22	1.41	1.46
9	17	305	KC1	CAA-C2A	2.22	1.53	1.46
8	12	311	CLA	C3D-C4D	-2.22	1.39	1.44
13	20	312	DD6	C22-C16	-2.22	1.49	1.53
8	15	308	CLA	C4C-C3C	2.22	1.48	1.45
9	17	305	KC1	C1D-C2D	2.22	1.48	1.43
9	19	308	KC1	C4A-C3A	2.22	1.49	1.44
9	18	304	KC1	C1D-C2D	2.22	1.48	1.43
10	15	311	A86	O4-C34	-2.22	1.41	1.46
8	21	204	CLA	C3B-C2B	2.22	1.48	1.41
10	20	311	A86	C24-C1	2.22	1.50	1.46
9	15	304	KC1	C4C-C3C	2.22	1.48	1.45
8	11	303	CLA	C1B-C2B	2.22	1.48	1.43
8	14	302	CLA	C1B-C2B	2.22	1.48	1.43
9	14	304	KC1	C4C-C3C	2.22	1.48	1.45
8	13	306	CLA	C1C-C2C	2.22	1.49	1.44
10	15	315	A86	C24-C1	2.22	1.50	1.46
8	15	305	CLA	C3D-C4D	-2.21	1.39	1.44
10	12	315	A86	C2-C1	2.21	1.40	1.35
10	19	313	A86	C24-C1	2.21	1.50	1.46
10	15	319	A86	C2-C1	2.21	1.40	1.35
9	15	302	KC1	C4C-C3C	2.21	1.48	1.45
9	12	308	KC1	CAA-C2A	2.21	1.53	1.46
8	16	303	CLA	C4C-C3C	2.21	1.48	1.45
10	20	313	A86	C5-C6	2.21	1.40	1.35
8	20	310	CLA	C3B-C2B	2.21	1.48	1.41
8	11	309	CLA	C1B-C2B	2.21	1.48	1.43
9	16	308	KC1	C4C-C3C	2.21	1.48	1.45
10	15	315	A86	C26-C27	2.20	1.40	1.35
8	15	301	CLA	C1C-C2C	2.20	1.49	1.44
9	11	308	KC1	CBD-CAD	-2.20	1.46	1.56
8	21	205	CLA	C3B-C4B	2.20	1.49	1.42
9	15	302	KC1	C1D-C2D	2.20	1.48	1.43
9	21	207	KC1	C4A-C3A	2.20	1.49	1.44
8	12	309	CLA	CHB-C4A	-2.20	1.32	1.37
8	20	310	CLA	C4C-C3C	2.20	1.48	1.45
10	11	313	A86	O4-C34	-2.20	1.41	1.46
8	17	302	CLA	C1C-NC	-2.20	1.34	1.37
10	13	312	A86	C24-C1	2.20	1.50	1.46
8	13	301	CLA	C3B-C4B	2.20	1.49	1.42
8	14	302	CLA	C3B-C4B	2.20	1.49	1.42
8	14	303	CLA	C1B-C2B	2.20	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	11	312	A86	C2-C1	2.20	1.40	1.35
10	14	313	A86	C5-C6	2.19	1.40	1.35
9	14	304	KC1	C4A-C3A	2.19	1.49	1.44
8	21	210	CLA	C4C-C3C	2.19	1.48	1.45
10	14	315	A86	C24-C1	2.19	1.50	1.46
8	11	303	CLA	C4C-C3C	2.19	1.48	1.45
8	19	302	CLA	C1C-NC	-2.19	1.34	1.37
8	19	307	CLA	C1C-NC	-2.19	1.34	1.37
8	18	310	CLA	C3B-C2B	2.19	1.48	1.41
9	15	304	KC1	CAA-C2A	2.19	1.53	1.46
9	13	310	KC1	C4C-C3C	2.19	1.48	1.45
9	20	305	KC1	C1D-C2D	2.19	1.48	1.43
10	17	314	A86	O4-C34	-2.19	1.41	1.46
8	16	307	CLA	C1C-NC	-2.19	1.34	1.37
8	21	208	CLA	C3D-C4D	-2.19	1.39	1.44
9	16	308	KC1	CBD-CAD	-2.19	1.46	1.56
8	20	302	CLA	C4C-C3C	2.19	1.48	1.45
8	17	308	CLA	C1B-C2B	2.19	1.48	1.43
8	16	306	CLA	C1C-C2C	2.18	1.49	1.44
8	17	310	CLA	C4C-C3C	2.18	1.48	1.45
8	12	304	CLA	C1B-C2B	2.18	1.48	1.43
9	15	306	KC1	C1D-C2D	2.18	1.48	1.43
8	13	306	CLA	C3B-C2B	2.18	1.48	1.41
10	18	312	A86	C24-C1	2.18	1.50	1.46
8	15	310	CLA	C4C-C3C	2.18	1.48	1.45
8	18	302	CLA	C4C-C3C	2.18	1.48	1.45
8	17	310	CLA	C1C-NC	-2.18	1.34	1.37
8	11	307	CLA	C1C-NC	-2.17	1.34	1.37
10	19	311	A86	C2-C1	2.17	1.40	1.35
9	20	305	KC1	CAA-C2A	2.17	1.52	1.46
8	14	310	CLA	C3B-C2B	2.17	1.48	1.41
9	11	304	KC1	C1D-C2D	2.17	1.48	1.43
10	15	315	A86	C2-C1	2.17	1.40	1.35
10	12	312	A86	C2-C1	2.17	1.40	1.35
10	15	314	A86	C5-C6	2.17	1.40	1.35
10	15	316	A86	C14-C15	2.17	1.57	1.52
10	20	301	A86	C14-C15	2.17	1.57	1.52
10	21	213	A86	C5-C6	2.17	1.40	1.35
9	14	309	KC1	CBD-CAD	-2.17	1.46	1.56
10	16	310	A86	C25-C24	2.17	1.40	1.34
9	18	306	KC1	CAA-C2A	2.17	1.52	1.46
8	12	301	CLA	C1C-NC	-2.17	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	17	311	A86	C26-C27	2.17	1.40	1.35
8	17	304	CLA	C3B-C2B	2.17	1.48	1.41
8	15	305	CLA	C3B-C2B	2.17	1.48	1.41
9	11	308	KC1	C1D-C2D	2.17	1.48	1.43
9	11	304	KC1	C4C-C3C	2.16	1.48	1.45
10	17	311	A86	C24-C1	2.16	1.50	1.46
10	13	314	A86	C14-C15	2.16	1.57	1.52
8	18	307	CLA	C1B-C2B	2.16	1.48	1.43
8	15	308	CLA	C3B-C4B	2.16	1.49	1.42
8	12	301	CLA	C4C-C3C	2.16	1.48	1.45
8	19	303	CLA	C1C-C2C	2.16	1.48	1.44
10	13	315	A86	C5-C6	2.16	1.40	1.35
8	15	305	CLA	C1C-C2C	2.16	1.48	1.44
9	21	203	KC1	C1D-C2D	2.16	1.48	1.43
8	14	302	CLA	C4C-C3C	2.16	1.48	1.45
10	17	316	A86	O4-C34	-2.16	1.41	1.46
8	18	301	CLA	C1C-C2C	2.16	1.48	1.44
8	20	307	CLA	C3B-C4B	2.16	1.49	1.42
10	17	311	A86	C15-C16	-2.16	1.52	1.55
8	21	210	CLA	C1C-C2C	2.16	1.48	1.44
9	13	305	KC1	CAA-C2A	2.16	1.52	1.46
8	18	308	CLA	C3D-C4D	-2.16	1.39	1.44
10	13	314	A86	C5-C6	2.16	1.40	1.35
10	11	314	A86	C2-C1	2.16	1.40	1.35
10	11	314	A86	C24-C1	2.16	1.50	1.46
13	19	312	DD6	C4-C5	2.16	1.49	1.43
8	19	307	CLA	C1B-C2B	2.16	1.48	1.43
10	11	318	A86	C2-C1	2.15	1.40	1.35
8	19	301	CLA	C1B-C2B	2.15	1.48	1.43
10	21	215	A86	C5-C6	2.15	1.40	1.35
10	16	310	A86	C2-C1	2.15	1.40	1.35
9	18	306	KC1	C4C-C3C	2.15	1.48	1.45
8	15	307	CLA	CHB-C4A	-2.15	1.32	1.37
8	18	303	CLA	C3B-C2B	2.15	1.48	1.41
10	13	312	A86	C2-C1	2.15	1.40	1.35
9	16	305	KC1	C4C-C3C	2.15	1.48	1.45
8	18	301	CLA	C1B-C2B	2.15	1.48	1.43
8	15	303	CLA	C3B-C2B	2.15	1.48	1.41
8	17	307	CLA	C3B-C4B	2.15	1.49	1.42
10	19	311	A86	C39-C38	2.15	1.56	1.49
8	12	311	CLA	C1C-C2C	2.15	1.48	1.44
8	14	307	CLA	CHB-C4A	-2.14	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	19	302	CLA	C1B-C2B	2.14	1.48	1.43
8	18	307	CLA	C3B-C2B	2.14	1.48	1.41
9	12	306	KC1	C1C-C2C	2.14	1.48	1.44
9	15	302	KC1	CAA-C2A	2.14	1.52	1.46
9	16	302	KC1	C4C-C3C	2.14	1.48	1.45
9	16	304	KC1	C4C-C3C	2.14	1.48	1.45
8	13	308	CLA	C1C-NC	-2.14	1.34	1.37
10	20	301	A86	O4-C34	-2.14	1.41	1.46
9	21	207	KC1	C3B-C4B	2.14	1.49	1.46
8	12	303	CLA	C1C-C2C	2.14	1.48	1.44
10	18	312	A86	C2-C1	2.14	1.40	1.35
9	12	310	KC1	CBD-CAD	-2.14	1.46	1.56
10	20	311	A86	O4-C34	-2.14	1.41	1.46
11	17	318	LMG	O7-C8	-2.14	1.41	1.46
9	16	305	KC1	CAA-C2A	2.13	1.52	1.46
10	12	314	A86	C5-C6	2.13	1.40	1.35
8	16	309	CLA	C1C-NC	-2.13	1.34	1.37
8	21	208	CLA	C3B-C2B	2.13	1.48	1.41
8	20	308	CLA	C3B-C2B	2.13	1.48	1.41
8	11	303	CLA	CBD-CAD	-2.13	1.46	1.56
10	17	321	A86	C24-C1	2.13	1.50	1.46
10	11	310	A86	C-C1	2.13	1.55	1.50
9	18	309	KC1	CBD-CAD	-2.13	1.46	1.56
9	16	305	KC1	C1D-C2D	2.13	1.48	1.43
8	11	305	CLA	C1C-NC	-2.13	1.34	1.37
9	17	309	KC1	C3B-C4B	2.13	1.49	1.46
8	17	304	CLA	C4C-C3C	2.13	1.48	1.45
8	16	306	CLA	CHB-C4A	-2.13	1.32	1.37
10	18	313	A86	C5-C6	2.13	1.40	1.35
8	19	306	CLA	C1C-C2C	2.13	1.48	1.44
8	20	302	CLA	C3B-C4B	2.13	1.48	1.42
8	21	202	CLA	C3B-C4B	2.12	1.48	1.42
8	12	305	CLA	CBD-CAD	-2.12	1.47	1.56
8	12	304	CLA	C4C-C3C	2.12	1.48	1.45
8	11	307	CLA	C3B-C4B	2.12	1.48	1.42
8	11	301	CLA	C1C-C2C	2.12	1.48	1.44
10	15	313	A86	C5-C6	2.12	1.40	1.35
10	15	316	A86	O4-C34	-2.12	1.41	1.46
8	11	309	CLA	C1C-NC	-2.12	1.34	1.37
9	15	306	KC1	CAA-C2A	2.12	1.52	1.46
8	20	304	CLA	C3B-C2B	2.12	1.48	1.41
8	15	308	CLA	C3B-C2B	2.12	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	16	313	A86	C14-C15	2.12	1.56	1.52
9	20	306	KC1	CAA-C2A	2.12	1.52	1.46
9	11	302	KC1	CAA-C2A	2.12	1.52	1.46
10	11	310	A86	C2-C1	2.12	1.40	1.35
8	21	205	CLA	C3B-C2B	2.12	1.48	1.41
9	20	303	KC1	C4A-C3A	2.12	1.48	1.44
8	18	305	CLA	C3B-C2B	2.12	1.48	1.41
14	16	314	SQD	O4-C4	-2.12	1.37	1.43
8	21	209	CLA	C3B-C2B	2.12	1.48	1.41
8	19	310	CLA	C4C-C3C	2.12	1.48	1.45
8	15	310	CLA	C3B-C2B	2.11	1.48	1.41
9	13	307	KC1	CAA-C2A	2.11	1.52	1.46
8	17	307	CLA	CHB-C4A	-2.11	1.32	1.37
8	12	301	CLA	C1B-C2B	2.11	1.48	1.43
10	19	313	A86	C15-C16	-2.11	1.52	1.55
8	14	301	CLA	C1C-C2C	2.11	1.48	1.44
10	12	319	A86	C39-C38	2.11	1.56	1.49
8	17	307	CLA	C1C-C2C	2.11	1.48	1.44
8	15	308	CLA	CBD-CAD	-2.11	1.47	1.56
10	17	321	A86	C26-C27	2.11	1.40	1.35
9	14	306	KC1	CAA-C2A	2.11	1.52	1.46
8	21	206	CLA	C3B-C2B	2.11	1.48	1.41
8	19	310	CLA	C3B-C2B	2.11	1.48	1.41
9	20	306	KC1	CBD-CAD	-2.11	1.47	1.56
8	15	303	CLA	C4C-C3C	2.11	1.48	1.45
9	18	306	KC1	C3B-C4B	2.11	1.49	1.46
10	21	214	A86	C5-C6	2.11	1.40	1.35
9	18	309	KC1	CAA-C2A	2.11	1.52	1.46
8	20	302	CLA	C1C-C2C	2.11	1.48	1.44
8	20	309	CLA	C3B-C2B	2.11	1.48	1.41
8	14	308	CLA	C3B-C2B	2.11	1.48	1.41
8	12	305	CLA	C3B-C2B	2.11	1.48	1.41
8	19	310	CLA	C1B-C2B	2.11	1.48	1.43
8	20	308	CLA	C1C-C2C	2.11	1.48	1.44
8	13	301	CLA	C3B-C2B	2.10	1.48	1.41
8	19	305	CLA	C3B-C4B	2.10	1.48	1.42
8	18	303	CLA	C1C-NC	-2.10	1.34	1.37
14	17	301	SQD	O47-C45	-2.10	1.41	1.46
8	13	311	CLA	C1C-C2C	2.10	1.48	1.44
9	14	306	KC1	C1C-C2C	2.10	1.48	1.44
10	15	311	A86	C24-C1	2.10	1.50	1.46
9	13	310	KC1	C1D-C2D	2.10	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	21	208	CLA	C1C-C2C	2.10	1.48	1.44
8	19	305	CLA	CBD-CAD	-2.10	1.47	1.56
8	15	308	CLA	C1C-NC	-2.09	1.34	1.37
10	17	312	A86	C24-C1	2.09	1.50	1.46
8	15	301	CLA	C3B-C2B	2.09	1.48	1.41
10	17	311	A86	C2-C1	2.09	1.40	1.35
8	14	308	CLA	C4C-C3C	2.09	1.48	1.45
10	12	313	A86	C2-C1	2.09	1.40	1.35
9	12	306	KC1	CAA-C2A	2.09	1.52	1.46
9	13	305	KC1	C1D-C2D	2.09	1.48	1.43
8	11	307	CLA	C1C-C2C	2.09	1.48	1.44
8	15	307	CLA	C1C-C2C	2.09	1.48	1.44
8	21	206	CLA	C1C-C2C	2.09	1.48	1.44
14	16	314	SQD	O2-C2	-2.09	1.37	1.43
9	18	309	KC1	C4C-C3C	2.09	1.48	1.45
9	14	309	KC1	C3B-C4B	2.09	1.49	1.46
10	16	311	A86	C24-C1	2.09	1.50	1.46
8	17	307	CLA	C3B-C2B	2.09	1.48	1.41
8	11	309	CLA	C1C-C2C	2.09	1.48	1.44
8	21	202	CLA	C3B-C2B	2.09	1.48	1.41
11	17	318	LMG	C4-C5	2.09	1.57	1.53
10	18	314	A86	C5-C6	2.08	1.40	1.35
9	13	303	KC1	CAA-C2A	2.08	1.52	1.46
9	12	310	KC1	C3B-C4B	2.08	1.49	1.46
8	17	310	CLA	C3B-C2B	2.08	1.48	1.41
10	16	310	A86	C26-C27	2.08	1.40	1.35
8	18	307	CLA	C1C-NC	-2.08	1.34	1.37
8	20	304	CLA	CBD-CAD	-2.08	1.47	1.56
8	18	303	CLA	C1C-C2C	2.08	1.48	1.44
10	19	311	A86	C-C1	2.08	1.55	1.50
8	18	307	CLA	C1C-C2C	2.08	1.48	1.44
10	16	311	A86	C2-C1	2.08	1.40	1.35
8	20	307	CLA	C4C-C3C	2.08	1.48	1.45
8	11	301	CLA	C1B-C2B	2.08	1.48	1.43
9	12	310	KC1	C1D-C2D	2.08	1.48	1.43
8	17	304	CLA	C1C-NC	-2.08	1.34	1.37
8	21	205	CLA	C1C-NC	-2.08	1.34	1.37
8	18	308	CLA	C3B-C2B	2.08	1.48	1.41
10	12	302	A86	C2-C1	2.08	1.40	1.35
10	12	302	A86	O4-C34	-2.08	1.41	1.46
8	13	309	CLA	C3B-C2B	2.08	1.48	1.41
10	17	321	A86	C2-C1	2.08	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	11	316	LMG	O7-C8	-2.08	1.41	1.46
8	11	309	CLA	C3B-C2B	2.08	1.48	1.41
8	14	305	CLA	C3B-C2B	2.07	1.48	1.41
9	16	302	KC1	C1D-C2D	2.07	1.48	1.43
10	21	211	A86	O4-C34	-2.07	1.41	1.46
8	16	301	CLA	C3B-C4B	2.07	1.48	1.42
10	14	314	A86	C5-C6	2.07	1.40	1.35
8	19	304	CLA	C3B-C2B	2.07	1.48	1.41
10	14	313	A86	C39-C38	2.07	1.56	1.49
8	18	302	CLA	C1B-C2B	2.07	1.48	1.43
14	17	301	SQD	O2-C2	-2.07	1.37	1.43
8	15	303	CLA	C1C-NC	-2.07	1.34	1.37
9	21	207	KC1	C4C-C3C	2.07	1.48	1.45
9	18	309	KC1	C3B-C4B	2.07	1.49	1.46
8	19	304	CLA	C1C-NC	-2.07	1.34	1.37
9	12	308	KC1	CBD-CAD	-2.07	1.47	1.56
9	12	310	KC1	C1C-C2C	2.06	1.48	1.44
8	11	305	CLA	C4C-C3C	2.06	1.48	1.45
9	11	306	KC1	CBD-CAD	-2.06	1.47	1.56
9	21	203	KC1	CAA-C2A	2.06	1.52	1.46
8	17	304	CLA	CHB-C4A	-2.06	1.32	1.37
8	16	301	CLA	C1C-C2C	2.06	1.48	1.44
8	19	302	CLA	C3B-C2B	2.06	1.48	1.41
8	14	307	CLA	C3B-C4B	2.06	1.48	1.42
8	12	307	CLA	C4C-C3C	2.06	1.48	1.45
10	12	313	A86	C24-C1	2.06	1.50	1.46
9	17	309	KC1	C1D-C2D	2.06	1.48	1.43
8	19	301	CLA	C1C-C2C	2.06	1.48	1.44
8	16	301	CLA	CBD-CAD	-2.06	1.47	1.56
8	11	303	CLA	C1C-NC	-2.06	1.34	1.37
10	12	302	A86	C24-C1	2.06	1.50	1.46
8	19	307	CLA	C3B-C2B	2.06	1.48	1.41
9	17	305	KC1	CBD-CAD	-2.06	1.47	1.56
9	17	303	KC1	C1D-C2D	2.06	1.48	1.43
9	14	304	KC1	C3B-C4B	2.06	1.49	1.46
8	17	304	CLA	CBD-CAD	-2.05	1.47	1.56
10	16	313	A86	C26-C27	2.05	1.40	1.35
8	18	305	CLA	C1C-C2C	2.05	1.48	1.44
9	16	302	KC1	C3B-C4B	2.05	1.49	1.46
8	21	210	CLA	C3B-C2B	2.05	1.48	1.41
10	21	214	A86	C15-C16	-2.05	1.52	1.55
10	21	215	A86	C39-C38	2.05	1.56	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	14	312	A86	C2-C1	2.05	1.40	1.35
10	17	321	A86	C39-C38	2.05	1.56	1.49
9	18	306	KC1	C1C-C2C	2.05	1.48	1.44
10	15	319	A86	C39-C38	2.05	1.56	1.49
8	12	311	CLA	C3B-C2B	2.05	1.48	1.41
9	20	303	KC1	C1D-C2D	2.05	1.47	1.43
10	19	311	A86	O4-C34	-2.05	1.41	1.46
10	15	316	A86	C5-C6	2.05	1.40	1.35
9	15	306	KC1	C1C-C2C	2.05	1.48	1.44
8	19	306	CLA	C1C-NC	-2.05	1.34	1.37
8	19	309	CLA	C1C-NC	-2.05	1.34	1.37
8	19	310	CLA	C1C-NC	-2.05	1.34	1.37
8	21	208	CLA	C1A-CHA	2.04	1.51	1.43
8	13	304	CLA	C3B-C2B	2.04	1.48	1.41
10	13	314	A86	C39-C38	2.04	1.56	1.49
14	16	314	SQD	O3-C3	-2.04	1.37	1.43
10	12	313	A86	C15-C16	-2.04	1.52	1.55
8	14	307	CLA	CBD-CAD	-2.04	1.47	1.56
8	19	305	CLA	C1C-NC	-2.04	1.34	1.37
9	16	304	KC1	CAA-C2A	2.04	1.52	1.46
8	15	307	CLA	C3B-C2B	2.04	1.48	1.41
9	13	307	KC1	CBD-CAD	-2.04	1.47	1.56
9	13	305	KC1	C1C-C2C	2.04	1.48	1.44
8	16	309	CLA	C3B-C2B	2.04	1.48	1.41
9	15	309	KC1	C1C-C2C	2.04	1.48	1.44
8	20	309	CLA	C3B-C4B	2.04	1.48	1.42
9	20	305	KC1	CBD-CAD	-2.04	1.47	1.56
13	19	312	DD6	C41-C32	-2.04	1.49	1.53
10	21	213	A86	C39-C38	2.03	1.56	1.49
8	20	307	CLA	C3B-C2B	2.03	1.48	1.41
8	16	309	CLA	CHB-C4A	-2.03	1.32	1.37
8	12	309	CLA	C3B-C2B	2.03	1.48	1.41
8	19	306	CLA	CBD-CAD	-2.03	1.47	1.56
9	16	302	KC1	CBD-CAD	-2.03	1.47	1.56
8	16	303	CLA	C1C-NC	-2.03	1.34	1.37
8	13	309	CLA	C1C-NC	-2.03	1.34	1.37
9	17	306	KC1	CBD-CAD	-2.03	1.47	1.56
8	19	301	CLA	CBD-CAD	-2.03	1.47	1.56
9	18	304	KC1	CAA-C2A	2.03	1.52	1.46
8	19	307	CLA	C4C-C3C	2.03	1.48	1.45
9	19	308	KC1	CBD-CAD	-2.03	1.47	1.56
9	12	306	KC1	C3B-C4B	2.03	1.49	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	12	309	CLA	C1C-NC	-2.03	1.34	1.37
8	18	303	CLA	CHB-C4A	-2.03	1.32	1.37
8	18	308	CLA	C4C-C3C	2.03	1.48	1.45
8	16	309	CLA	C4C-C3C	2.03	1.48	1.45
8	12	303	CLA	C3B-C2B	2.03	1.48	1.41
8	20	302	CLA	C3B-C2B	2.03	1.48	1.41
10	12	316	A86	C5-C6	2.03	1.40	1.35
8	11	307	CLA	CHB-C4A	-2.03	1.32	1.37
8	11	301	CLA	C1A-CHA	2.03	1.51	1.43
10	15	315	A86	C39-C38	2.03	1.56	1.49
8	16	307	CLA	CBD-CAD	-2.03	1.47	1.56
8	19	306	CLA	C1B-C2B	2.03	1.47	1.43
9	12	306	KC1	CBD-CAD	-2.02	1.47	1.56
8	18	308	CLA	C1A-CHA	2.02	1.51	1.43
8	13	302	CLA	C1C-C2C	2.02	1.48	1.44
9	13	310	KC1	C3B-C4B	2.02	1.49	1.46
10	13	316	A86	C5-C6	2.02	1.40	1.35
10	18	312	A86	C15-C16	-2.02	1.52	1.55
8	12	307	CLA	C3B-C2B	2.02	1.48	1.41
10	13	315	A86	O-C13	-2.02	1.19	1.23
8	12	309	CLA	C1C-C2C	2.02	1.48	1.44
8	17	308	CLA	C1C-C2C	2.02	1.48	1.44
8	19	303	CLA	C3B-C2B	2.02	1.48	1.41
8	18	301	CLA	C3B-C2B	2.02	1.48	1.41
9	17	309	KC1	CAA-C2A	2.02	1.52	1.46
8	13	304	CLA	C1C-NC	-2.02	1.34	1.37
9	11	306	KC1	C1C-C2C	2.02	1.48	1.44
8	11	309	CLA	C4C-C3C	2.02	1.48	1.45
8	14	303	CLA	C1C-NC	-2.02	1.34	1.37
8	14	303	CLA	C3B-C2B	2.02	1.48	1.41
8	16	303	CLA	C3B-C2B	2.02	1.48	1.41
9	14	304	KC1	C1C-C2C	2.02	1.48	1.44
14	17	301	SQD	O4-C4	-2.02	1.38	1.43
9	16	308	KC1	C1D-C2D	2.02	1.47	1.43
9	17	306	KC1	CAA-C2A	2.02	1.52	1.46
8	13	301	CLA	C1C-NC	-2.01	1.34	1.37
8	16	303	CLA	CBD-CAD	-2.01	1.47	1.56
10	17	313	A86	C39-C38	2.01	1.56	1.49
8	11	303	CLA	C3B-C2B	2.01	1.48	1.41
8	13	308	CLA	C3B-C2B	2.01	1.48	1.41
10	17	315	A86	C2-C1	2.01	1.40	1.35
8	14	308	CLA	CBD-CAD	-2.01	1.47	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	13	305	KC1	C4C-C3C	2.01	1.48	1.45
10	21	211	A86	C39-C38	2.01	1.56	1.49
8	13	302	CLA	C4C-C3C	2.01	1.48	1.45
9	21	203	KC1	C1C-C2C	2.01	1.48	1.44
9	18	309	KC1	C1D-C2D	2.01	1.47	1.43
8	12	305	CLA	C4C-C3C	2.00	1.48	1.45
8	17	302	CLA	C3B-C4B	2.00	1.48	1.42
8	12	311	CLA	C1A-CHA	2.00	1.51	1.43
8	11	309	CLA	CBD-CAD	-2.00	1.47	1.56
10	17	315	A86	C24-C1	2.00	1.50	1.46
8	12	309	CLA	CBD-CAD	-2.00	1.47	1.56
8	20	310	CLA	C1C-C2C	2.00	1.48	1.44
9	13	307	KC1	C1C-C2C	2.00	1.48	1.44

All (4624) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	17	315	A86	O1-C20-C19	46.30	156.89	113.49
10	20	313	A86	O1-C20-C19	45.76	156.38	113.49
10	19	313	A86	O1-C20-C19	45.41	156.05	113.49
10	13	314	A86	O1-C20-C19	45.15	155.81	113.49
10	20	311	A86	O1-C20-C19	45.12	155.78	113.49
10	13	315	A86	O1-C20-C19	45.02	155.68	113.49
10	14	314	A86	O1-C20-C19	44.49	155.19	113.49
10	21	214	A86	O1-C20-C19	44.34	155.04	113.49
10	21	211	A86	O1-C20-C19	43.86	154.60	113.49
10	17	311	A86	O1-C20-C19	43.85	154.59	113.49
10	11	313	A86	O1-C20-C19	43.61	154.37	113.49
10	17	314	A86	O1-C20-C19	43.56	154.32	113.49
10	14	311	A86	O1-C20-C19	43.53	154.29	113.49
10	15	314	A86	O1-C20-C19	43.46	154.23	113.49
10	20	301	A86	O1-C20-C19	43.42	154.19	113.49
10	18	313	A86	O1-C20-C19	43.35	154.12	113.49
10	18	311	A86	O1-C20-C19	43.29	154.07	113.49
10	12	315	A86	O1-C20-C19	43.13	153.92	113.49
10	12	314	A86	O1-C20-C19	42.93	153.72	113.49
10	12	312	A86	O1-C20-C19	42.82	153.62	113.49
10	21	213	A86	O1-C20-C19	42.78	153.58	113.49
10	14	315	A86	O1-C20-C19	42.25	153.09	113.49
10	18	312	A86	O1-C20-C19	42.06	152.91	113.49
10	13	313	A86	O1-C20-C19	41.96	152.82	113.49
10	15	311	A86	O1-C20-C19	41.88	152.75	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	13	312	A86	O1-C20-C19	41.73	152.60	113.49
10	12	319	A86	O1-C20-C19	41.72	152.59	113.49
10	21	215	A86	O1-C20-C19	41.64	152.52	113.49
10	14	312	A86	O1-C20-C19	41.58	152.46	113.49
10	12	313	A86	O1-C20-C19	41.40	152.30	113.49
10	11	311	A86	O1-C20-C19	40.78	151.71	113.49
10	15	315	A86	O1-C20-C19	40.74	151.67	113.49
10	19	311	A86	O1-C20-C19	40.60	151.55	113.49
10	15	312	A86	O1-C20-C19	40.51	151.46	113.49
10	17	321	A86	O1-C20-C19	40.43	151.39	113.49
10	17	316	A86	O1-C20-C19	40.41	151.37	113.49
10	11	314	A86	O1-C20-C19	40.21	151.17	113.49
10	15	316	A86	O1-C20-C19	39.85	150.84	113.49
10	18	314	A86	O1-C20-C19	39.85	150.84	113.49
10	17	312	A86	O1-C20-C19	39.82	150.81	113.49
10	12	302	A86	O1-C20-C19	39.80	150.79	113.49
10	13	316	A86	O1-C20-C19	39.62	150.62	113.49
10	15	313	A86	O1-C20-C19	39.58	150.58	113.49
10	16	311	A86	O1-C20-C19	39.39	150.41	113.49
10	11	310	A86	O1-C20-C19	39.25	150.28	113.49
10	11	312	A86	O1-C20-C19	39.23	150.26	113.49
10	11	318	A86	O1-C20-C19	39.12	150.16	113.49
10	16	310	A86	O1-C20-C19	39.02	150.06	113.49
10	14	313	A86	O1-C20-C19	38.94	149.98	113.49
10	16	313	A86	O1-C20-C19	38.80	149.86	113.49
10	12	316	A86	O1-C20-C19	38.61	149.67	113.49
10	14	316	A86	O1-C20-C19	38.40	149.48	113.49
10	15	319	A86	O1-C20-C19	38.13	149.23	113.49
10	17	313	A86	O1-C20-C19	37.98	149.09	113.49
13	21	212	DD6	O1-C20-C19	25.98	137.84	113.49
13	20	312	DD6	O1-C20-C19	25.70	137.58	113.49
13	21	216	DD6	O1-C20-C19	25.15	137.06	113.49
13	20	314	DD6	O1-C20-C19	23.43	135.45	113.49
13	16	312	DD6	O1-C20-C19	20.94	133.12	113.49
13	19	312	DD6	O1-C20-C19	19.59	131.85	113.49
13	20	312	DD6	C29-C30-C31	-17.99	133.59	175.48
13	19	312	DD6	C29-C30-C31	-16.53	136.98	175.48
13	21	212	DD6	C29-C30-C31	-16.19	137.78	175.48
13	20	314	DD6	C29-C30-C31	-15.81	138.66	175.48
13	16	312	DD6	C29-C30-C31	-15.13	140.24	175.48
10	20	313	A86	O1-C20-C21	-14.02	99.38	115.05
10	19	313	A86	O1-C20-C21	-13.35	100.13	115.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	21	216	DD6	C29-C30-C31	-13.23	144.67	175.48
10	20	311	A86	O1-C20-C21	-12.80	100.74	115.05
10	14	314	A86	O1-C20-C21	-12.71	100.84	115.05
13	20	312	DD6	C3-C2-C1	-12.42	109.86	127.28
10	13	314	A86	C21-C20-C19	-12.36	100.35	114.24
10	11	313	A86	O1-C20-C21	-12.32	101.28	115.05
10	21	214	A86	O1-C20-C21	-12.22	101.40	115.05
9	20	303	KC1	CMA-C3A-C4A	-12.10	106.12	125.03
10	17	315	A86	C21-C20-C19	-12.09	100.66	114.24
10	13	315	A86	C21-C20-C19	-12.05	100.70	114.24
10	18	313	A86	O1-C20-C21	-11.93	101.72	115.05
10	17	314	A86	O1-C20-C21	-11.88	101.77	115.05
10	12	315	A86	O1-C20-C21	-11.85	101.81	115.05
10	21	211	A86	O1-C20-C21	-11.77	101.89	115.05
10	15	314	A86	O1-C20-C21	-11.74	101.93	115.05
10	17	315	A86	O1-C20-C21	-11.73	101.94	115.05
10	18	312	A86	O1-C20-C21	-11.71	101.96	115.05
10	12	314	A86	O1-C20-C21	-11.68	101.99	115.05
9	14	304	KC1	CMA-C3A-C4A	-11.56	106.97	125.03
9	21	207	KC1	CMA-C3A-C4A	-11.55	106.99	125.03
10	17	311	A86	O1-C20-C21	-11.48	102.22	115.05
10	21	213	A86	O1-C20-C21	-11.38	102.33	115.05
10	18	311	A86	O1-C20-C21	-11.28	102.44	115.05
13	21	216	DD6	C9-C10-C11	-11.27	111.48	127.28
10	13	315	A86	O1-C20-C21	-11.27	102.46	115.05
9	14	309	KC1	C2A-C3A-C4A	-11.24	97.97	106.41
10	11	310	A86	C21-C20-C19	-11.22	101.64	114.24
9	15	309	KC1	C2A-C3A-C4A	-11.19	98.01	106.41
10	11	312	A86	C21-C20-C19	-11.18	101.68	114.24
10	12	313	A86	O1-C20-C21	-11.18	102.55	115.05
9	15	304	KC1	CMA-C3A-C4A	-11.16	107.60	125.03
10	12	312	A86	O1-C20-C21	-11.11	102.64	115.05
10	13	313	A86	O1-C20-C21	-11.08	102.66	115.05
10	20	301	A86	O1-C20-C21	-11.07	102.68	115.05
9	17	309	KC1	C2A-C3A-C4A	-11.05	98.11	106.41
10	12	302	A86	C21-C20-C19	-11.04	101.84	114.24
10	13	316	A86	C21-C20-C19	-11.04	101.84	114.24
13	20	314	DD6	C3-C2-C1	-11.03	111.80	127.28
10	14	311	A86	C21-C20-C19	-10.97	101.92	114.24
9	18	309	KC1	C2A-C3A-C4A	-10.97	98.18	106.41
10	14	311	A86	O1-C20-C21	-10.93	102.84	115.05
10	21	215	A86	O1-C20-C21	-10.90	102.87	115.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	19	308	KC1	CMA-C3A-C4A	-10.87	108.04	125.03
13	20	312	DD6	C4-C5-C6	-10.87	112.04	127.28
9	16	304	KC1	CMA-C3A-C4A	-10.77	108.20	125.03
13	20	312	DD6	C9-C10-C11	-10.77	112.18	127.28
10	17	311	A86	C21-C20-C19	-10.75	102.16	114.24
9	11	308	KC1	C2A-C3A-C4A	-10.74	98.35	106.41
10	14	315	A86	O1-C20-C21	-10.72	103.07	115.05
10	12	319	A86	O1-C20-C21	-10.67	103.13	115.05
10	13	314	A86	O1-C20-C21	-10.66	103.13	115.05
10	14	312	A86	O1-C20-C21	-10.66	103.14	115.05
10	11	311	A86	O1-C20-C21	-10.63	103.17	115.05
10	11	312	A86	C33-C32-C31	10.55	119.47	109.21
10	17	316	A86	C21-C20-C19	-10.55	102.39	114.24
10	20	301	A86	C21-C20-C19	-10.51	102.44	114.24
10	13	312	A86	C21-C20-C19	-10.49	102.45	114.24
10	14	315	A86	C21-C20-C19	-10.47	102.48	114.24
10	15	311	A86	C21-C20-C19	-10.46	102.49	114.24
10	18	311	A86	C21-C20-C19	-10.45	102.50	114.24
10	21	211	A86	C21-C20-C19	-10.43	102.53	114.24
10	15	311	A86	O1-C20-C21	-10.39	103.44	115.05
10	21	214	A86	C21-C20-C19	-10.37	102.59	114.24
9	16	308	KC1	C2A-C3A-C4A	-10.36	98.63	106.41
10	12	312	A86	C21-C20-C19	-10.35	102.62	114.24
10	15	314	A86	C21-C20-C19	-10.31	102.67	114.24
10	17	314	A86	C33-C32-C31	10.30	119.22	109.21
8	15	301	CLA	C1D-ND-C4D	-10.29	99.09	106.31
10	13	312	A86	O1-C20-C21	-10.27	103.57	115.05
10	18	314	A86	C21-C20-C19	-10.24	102.74	114.24
10	15	315	A86	C21-C20-C19	-10.24	102.74	114.24
9	15	302	KC1	CMA-C3A-C4A	-10.24	109.04	125.03
10	20	311	A86	C21-C20-C19	-10.20	102.78	114.24
9	13	310	KC1	C2A-C3A-C4A	-10.19	98.76	106.41
10	21	213	A86	C21-C20-C19	-10.18	102.80	114.24
10	17	314	A86	C21-C20-C19	-10.17	102.81	114.24
10	19	313	A86	C21-C20-C19	-10.15	102.84	114.24
10	17	321	A86	O1-C20-C21	-10.15	103.70	115.05
10	19	311	A86	O1-C20-C21	-10.11	103.75	115.05
13	20	314	DD6	C9-C10-C11	-10.11	113.11	127.28
10	15	312	A86	O1-C20-C21	-10.10	103.76	115.05
10	14	314	A86	C21-C20-C19	-10.07	102.92	114.24
10	12	314	A86	C21-C20-C19	-10.06	102.95	114.24
9	20	303	KC1	C2A-C3A-C4A	-10.05	98.86	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	19	311	A86	C21-C20-C19	-10.05	102.95	114.24
10	15	313	A86	C21-C20-C19	-10.04	102.97	114.24
10	15	316	A86	C21-C20-C19	-10.02	102.99	114.24
10	15	315	A86	O1-C20-C21	-10.02	103.86	115.05
10	17	312	A86	C21-C20-C19	-10.00	103.01	114.24
10	11	314	A86	O1-C20-C21	-9.96	103.91	115.05
10	12	319	A86	C21-C20-C19	-9.96	103.06	114.24
10	18	313	A86	C21-C20-C19	-9.96	103.06	114.24
9	21	203	KC1	C2A-C3A-C4A	-9.94	98.94	106.41
9	12	310	KC1	C2A-C3A-C4A	-9.93	98.95	106.41
10	21	215	A86	C21-C20-C19	-9.92	103.09	114.24
10	14	313	A86	C21-C20-C19	-9.91	103.10	114.24
9	12	306	KC1	CMA-C3A-C4A	-9.91	109.55	125.03
10	12	315	A86	C21-C20-C19	-9.90	103.12	114.24
9	12	306	KC1	C2A-C3A-C4A	-9.87	99.00	106.41
10	14	316	A86	C21-C20-C19	-9.87	103.16	114.24
10	15	312	A86	C21-C20-C19	-9.86	103.17	114.24
13	16	312	DD6	C3-C2-C1	-9.86	113.46	127.28
9	11	304	KC1	C2A-C3A-C4A	-9.85	99.02	106.41
13	20	314	DD6	C4-C5-C6	-9.82	113.50	127.28
10	16	311	A86	O1-C20-C21	-9.82	104.07	115.05
13	21	216	DD6	C3-C2-C1	-9.81	113.53	127.28
8	16	301	CLA	C1D-ND-C4D	-9.80	99.44	106.31
9	20	305	KC1	C2A-C3A-C4A	-9.80	99.05	106.41
10	13	313	A86	C21-C20-C19	-9.80	103.24	114.24
8	18	301	CLA	C1D-ND-C4D	-9.79	99.44	106.31
10	14	312	A86	C21-C20-C19	-9.78	103.25	114.24
10	11	313	A86	C21-C20-C19	-9.77	103.27	114.24
8	19	306	CLA	C1D-ND-C4D	-9.76	99.46	106.31
10	12	316	A86	C21-C20-C19	-9.75	103.29	114.24
10	17	321	A86	C21-C20-C19	-9.72	103.32	114.24
13	19	312	DD6	C9-C10-C11	-9.71	113.66	127.28
13	21	212	DD6	C9-C10-C11	-9.70	113.68	127.28
8	19	303	CLA	C1D-ND-C4D	-9.68	99.52	106.31
8	14	301	CLA	C1D-ND-C4D	-9.67	99.52	106.31
9	16	304	KC1	C2A-C3A-C4A	-9.67	99.15	106.41
10	16	310	A86	O1-C20-C21	-9.67	104.24	115.05
8	19	304	CLA	C1D-ND-C4D	-9.67	99.53	106.31
8	21	210	CLA	C1D-ND-C4D	-9.65	99.54	106.31
9	13	303	KC1	C2A-C3A-C4A	-9.64	99.17	106.41
9	15	304	KC1	C2A-C3A-C4A	-9.64	99.17	106.41
8	20	302	CLA	C1D-ND-C4D	-9.62	99.56	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	11	318	A86	C21-C20-C19	-9.62	103.44	114.24
9	13	305	KC1	C2A-C3A-C4A	-9.61	99.19	106.41
9	16	305	KC1	C2A-C3A-C4A	-9.61	99.19	106.41
9	14	304	KC1	C2A-C3A-C4A	-9.60	99.20	106.41
9	16	302	KC1	C2A-C3A-C4A	-9.59	99.21	106.41
9	18	304	KC1	C2A-C3A-C4A	-9.59	99.21	106.41
13	21	212	DD6	C4-C5-C6	-9.58	113.84	127.28
13	21	216	DD6	C4-C5-C6	-9.58	113.84	127.28
9	13	307	KC1	C1D-ND-C4D	-9.55	99.61	106.31
9	14	306	KC1	CMA-C3A-C4A	-9.55	110.12	125.03
8	11	301	CLA	C1D-ND-C4D	-9.54	99.62	106.31
9	18	306	KC1	C2A-C3A-C4A	-9.54	99.25	106.41
9	11	306	KC1	CMA-C3A-C4A	-9.54	110.13	125.03
10	18	312	A86	C21-C20-C19	-9.52	103.54	114.24
8	19	301	CLA	C1D-ND-C4D	-9.51	99.64	106.31
10	15	319	A86	O1-C20-C21	-9.51	104.42	115.05
13	16	312	DD6	C13-C11-C10	-9.50	104.06	119.01
13	16	312	DD6	C9-C10-C11	-9.50	113.96	127.28
8	19	305	CLA	C1D-ND-C4D	-9.49	99.66	106.31
9	21	207	KC1	C1D-ND-C4D	-9.48	99.66	106.31
9	21	207	KC1	C2A-C3A-C4A	-9.47	99.30	106.41
9	14	306	KC1	C2A-C3A-C4A	-9.47	99.30	106.41
10	15	316	A86	C4-C5-C6	-9.47	114.00	127.28
10	17	312	A86	O1-C20-C21	-9.46	104.47	115.05
9	11	302	KC1	C2A-C3A-C4A	-9.46	99.31	106.41
10	18	312	A86	C33-C32-C31	9.45	118.40	109.21
9	13	303	KC1	CMA-C3A-C4A	-9.45	110.26	125.03
10	12	313	A86	C21-C20-C19	-9.44	103.64	114.24
9	11	306	KC1	C2A-C3A-C4A	-9.43	99.33	106.41
10	17	313	A86	C21-C20-C19	-9.43	103.64	114.24
9	17	305	KC1	C2A-C3A-C4A	-9.43	99.33	106.41
8	13	309	CLA	C1D-ND-C4D	-9.42	99.70	106.31
9	17	303	KC1	C2A-C3A-C4A	-9.41	99.34	106.41
8	12	301	CLA	C1D-ND-C4D	-9.41	99.71	106.31
13	21	216	DD6	C12-C11-C10	-9.40	107.58	122.82
10	12	315	A86	C33-C32-C31	9.40	118.34	109.21
8	12	307	CLA	C1D-ND-C4D	-9.39	99.72	106.31
8	17	302	CLA	C1D-ND-C4D	-9.39	99.72	106.31
9	12	308	KC1	C2A-C3A-C4A	-9.37	99.38	106.41
9	15	306	KC1	C2A-C3A-C4A	-9.36	99.38	106.41
8	15	308	CLA	C1D-ND-C4D	-9.35	99.75	106.31
8	11	309	CLA	C1D-ND-C4D	-9.35	99.75	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	20	313	A86	C21-C20-C19	-9.34	103.75	114.24
9	20	306	KC1	C2A-C3A-C4A	-9.32	99.41	106.41
9	11	304	KC1	CMA-C3A-C4A	-9.31	110.49	125.03
9	13	307	KC1	CMA-C3A-C4A	-9.29	110.51	125.03
13	20	312	DD6	C12-C11-C10	-9.29	107.77	122.82
9	13	307	KC1	C2A-C3A-C4A	-9.29	99.44	106.41
13	21	212	DD6	C13-C11-C10	-9.29	104.40	119.01
13	19	312	DD6	C4-C5-C6	-9.28	114.26	127.28
9	15	302	KC1	C2A-C3A-C4A	-9.28	99.45	106.41
8	21	206	CLA	C1D-ND-C4D	-9.27	99.81	106.31
9	21	203	KC1	CMA-C3A-C4A	-9.27	110.55	125.03
10	20	301	A86	C33-C32-C31	9.25	118.20	109.21
8	18	308	CLA	C1D-ND-C4D	-9.24	99.83	106.31
10	11	314	A86	C21-C20-C19	-9.23	103.87	114.24
10	11	311	A86	C21-C20-C19	-9.23	103.87	114.24
10	15	313	A86	O1-C20-C21	-9.23	104.73	115.05
10	15	316	A86	O1-C20-C21	-9.23	104.73	115.05
10	16	313	A86	C21-C20-C19	-9.23	103.88	114.24
8	21	205	CLA	C1D-ND-C4D	-9.19	99.86	106.31
10	11	318	A86	O1-C20-C21	-9.19	104.78	115.05
9	17	306	KC1	C2A-C3A-C4A	-9.19	99.51	106.41
8	13	302	CLA	C1D-ND-C4D	-9.17	99.87	106.31
8	13	311	CLA	C1D-ND-C4D	-9.17	99.88	106.31
9	13	305	KC1	CMA-C3A-C4A	-9.15	110.74	125.03
8	15	305	CLA	C1D-ND-C4D	-9.14	99.90	106.31
8	13	301	CLA	C1D-ND-C4D	-9.13	99.91	106.31
8	13	306	CLA	C1D-ND-C4D	-9.10	99.92	106.31
8	17	308	CLA	C1D-ND-C4D	-9.10	99.92	106.31
10	17	316	A86	O1-C20-C21	-9.10	104.88	115.05
9	19	308	KC1	C2A-C3A-C4A	-9.09	99.58	106.41
8	16	307	CLA	C1D-ND-C4D	-9.09	99.94	106.31
8	21	208	CLA	C1D-ND-C4D	-9.08	99.94	106.31
8	18	305	CLA	C1D-ND-C4D	-9.07	99.95	106.31
8	18	310	CLA	C1D-ND-C4D	-9.06	99.96	106.31
10	11	313	A86	C33-C32-C31	9.05	118.01	109.21
10	16	310	A86	C21-C20-C19	-9.05	104.08	114.24
10	12	316	A86	C4-C5-C6	-9.04	114.60	127.28
8	19	307	CLA	C1D-ND-C4D	-9.03	99.97	106.31
8	21	209	CLA	C1D-ND-C4D	-9.02	99.98	106.31
9	20	303	KC1	C1D-ND-C4D	-9.02	99.98	106.31
10	14	313	A86	O1-C20-C21	-9.02	104.97	115.05
8	14	305	CLA	C1D-ND-C4D	-9.01	99.99	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	16	311	A86	C21-C20-C19	-9.01	104.12	114.24
8	15	310	CLA	C1D-ND-C4D	-9.01	99.99	106.31
8	16	309	CLA	C1D-ND-C4D	-9.00	100.00	106.31
9	19	308	KC1	C1D-ND-C4D	-9.00	100.00	106.31
8	21	204	CLA	C1D-ND-C4D	-8.99	100.01	106.31
8	14	310	CLA	C1D-ND-C4D	-8.98	100.01	106.31
8	17	310	CLA	C1D-ND-C4D	-8.98	100.01	106.31
13	20	312	DD6	C13-C11-C10	-8.97	104.89	119.01
8	21	202	CLA	C1D-ND-C4D	-8.97	100.02	106.31
8	11	307	CLA	C1D-ND-C4D	-8.96	100.03	106.31
8	20	308	CLA	C1D-ND-C4D	-8.96	100.03	106.31
8	18	303	CLA	C1D-ND-C4D	-8.96	100.03	106.31
8	15	303	CLA	C1D-ND-C4D	-8.95	100.03	106.31
8	11	305	CLA	C1D-ND-C4D	-8.95	100.03	106.31
10	14	316	A86	C4-C5-C6	-8.94	114.73	127.28
9	14	306	KC1	C1D-ND-C4D	-8.94	100.04	106.31
9	15	306	KC1	CMA-C3A-C4A	-8.94	111.06	125.03
8	18	307	CLA	C1D-ND-C4D	-8.94	100.04	106.31
13	19	312	DD6	C37-C36-C31	-8.93	107.46	124.16
9	17	305	KC1	C1D-ND-C4D	-8.91	100.06	106.31
8	16	303	CLA	C1D-ND-C4D	-8.87	100.08	106.31
9	12	306	KC1	C1D-ND-C4D	-8.87	100.08	106.31
13	21	212	DD6	C12-C11-C10	-8.86	108.45	122.82
9	20	306	KC1	CMA-C3A-C4A	-8.85	111.21	125.03
13	20	314	DD6	C12-C11-C10	-8.84	108.49	122.82
10	18	314	A86	C4-C5-C6	-8.83	114.89	127.28
9	16	305	KC1	CMA-C3A-C4A	-8.83	111.23	125.03
9	11	302	KC1	CMA-C3A-C4A	-8.82	111.25	125.03
9	18	304	KC1	C1D-ND-C4D	-8.82	100.12	106.31
13	19	312	DD6	C3-C2-C1	-8.80	114.93	127.28
9	17	305	KC1	CMA-C3A-C4A	-8.80	111.28	125.03
13	16	312	DD6	C4-C5-C6	-8.80	114.94	127.28
9	13	305	KC1	C1D-ND-C4D	-8.80	100.14	106.31
8	19	302	CLA	C1D-ND-C4D	-8.79	100.14	106.31
8	12	303	CLA	C1D-ND-C4D	-8.78	100.15	106.31
8	20	309	CLA	C1D-ND-C4D	-8.77	100.16	106.31
9	17	306	KC1	CMA-C3A-C4A	-8.77	111.33	125.03
8	12	305	CLA	C1D-ND-C4D	-8.77	100.16	106.31
9	14	304	KC1	C1D-ND-C4D	-8.74	100.18	106.31
8	20	307	CLA	C1D-ND-C4D	-8.72	100.19	106.31
13	16	312	DD6	C37-C36-C31	-8.71	107.87	124.16
9	17	309	KC1	C1D-ND-C4D	-8.68	100.22	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	18	306	KC1	CMA-C3A-C4A	-8.67	111.48	125.03
10	16	313	A86	O1-C20-C21	-8.67	105.36	115.05
8	14	308	CLA	C1D-ND-C4D	-8.67	100.23	106.31
9	14	309	KC1	C1D-ND-C4D	-8.66	100.24	106.31
9	11	306	KC1	C1D-ND-C4D	-8.65	100.24	106.31
10	20	301	A86	C4-C5-C6	-8.65	115.14	127.28
9	18	304	KC1	CMA-C3A-C4A	-8.64	111.53	125.03
9	15	306	KC1	C1D-ND-C4D	-8.64	100.25	106.31
10	12	312	A86	C33-C32-C31	8.64	117.61	109.21
10	13	315	A86	C33-C32-C31	8.64	117.61	109.21
8	14	303	CLA	C1D-ND-C4D	-8.62	100.26	106.31
8	19	309	CLA	C1D-ND-C4D	-8.62	100.26	106.31
9	16	304	KC1	C1D-ND-C4D	-8.62	100.27	106.31
13	21	212	DD6	C7-C6-C5	-8.61	108.87	122.82
8	12	311	CLA	C1D-ND-C4D	-8.61	100.27	106.31
8	16	306	CLA	C1D-ND-C4D	-8.61	100.27	106.31
10	18	314	A86	O1-C20-C21	-8.61	105.43	115.05
9	20	305	KC1	C1D-ND-C4D	-8.61	100.27	106.31
10	12	316	A86	O1-C20-C21	-8.60	105.44	115.05
8	20	310	CLA	C1D-ND-C4D	-8.59	100.28	106.31
13	16	312	DD6	C12-C11-C10	-8.57	108.93	122.82
9	15	302	KC1	C1D-ND-C4D	-8.55	100.31	106.31
8	15	307	CLA	C1D-ND-C4D	-8.54	100.32	106.31
10	17	311	A86	C33-C32-C31	8.54	117.51	109.21
10	16	311	A86	C33-C32-C31	8.53	117.50	109.21
10	17	313	A86	O1-C20-C21	-8.53	105.52	115.05
10	15	319	A86	C21-C20-C19	-8.53	104.66	114.24
13	20	314	DD6	C37-C36-C31	-8.52	108.23	124.16
9	12	308	KC1	C1D-ND-C4D	-8.52	100.33	106.31
10	13	314	A86	C33-C32-C31	8.51	117.49	109.21
8	20	304	CLA	C1D-ND-C4D	-8.51	100.34	106.31
9	12	308	KC1	CMA-C3A-C4A	-8.49	111.76	125.03
9	15	304	KC1	C1D-ND-C4D	-8.49	100.35	106.31
9	13	303	KC1	C1D-ND-C4D	-8.47	100.37	106.31
8	12	304	CLA	C1D-ND-C4D	-8.46	100.38	106.31
8	13	304	CLA	C1D-ND-C4D	-8.46	100.38	106.31
9	18	309	KC1	C1D-ND-C4D	-8.45	100.38	106.31
8	19	310	CLA	C1D-ND-C4D	-8.44	100.39	106.31
9	15	309	KC1	C1D-ND-C4D	-8.43	100.40	106.31
8	11	303	CLA	C1D-ND-C4D	-8.42	100.41	106.31
9	12	310	KC1	C1D-ND-C4D	-8.39	100.42	106.31
13	20	312	DD6	C37-C36-C31	-8.39	108.47	124.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	14	302	CLA	C1D-ND-C4D	-8.39	100.42	106.31
10	16	310	A86	C33-C32-C31	8.38	117.36	109.21
10	19	313	A86	C33-C32-C31	8.38	117.36	109.21
10	19	313	A86	C4-C5-C6	-8.36	115.55	127.28
8	12	309	CLA	C1D-ND-C4D	-8.35	100.45	106.31
13	19	312	DD6	C8-C6-C5	-8.34	105.89	119.01
9	11	302	KC1	C1D-ND-C4D	-8.34	100.46	106.31
8	17	304	CLA	C1D-ND-C4D	-8.32	100.47	106.31
10	20	313	A86	C33-C32-C31	8.32	117.30	109.21
13	20	312	DD6	C-C1-C2	-8.31	109.35	122.82
9	16	305	KC1	C1D-ND-C4D	-8.29	100.49	106.31
13	21	216	DD6	C28-C27-C26	-8.29	108.08	124.18
10	12	302	A86	O1-C20-C21	-8.29	105.78	115.05
10	16	313	A86	C4-C5-C6	-8.28	115.67	127.28
9	18	306	KC1	C1D-ND-C4D	-8.28	100.50	106.31
13	19	312	DD6	C12-C11-C10	-8.26	109.43	122.82
8	17	307	CLA	C1D-ND-C4D	-8.26	100.52	106.31
8	18	302	CLA	C1D-ND-C4D	-8.25	100.52	106.31
9	17	303	KC1	CMA-C3A-C4A	-8.24	112.16	125.03
10	15	311	A86	C33-C32-C31	8.24	117.22	109.21
13	21	216	DD6	C7-C6-C5	-8.23	109.48	122.82
9	11	308	KC1	C1D-ND-C4D	-8.22	100.55	106.31
13	21	216	DD6	C37-C36-C31	-8.20	108.83	124.16
9	14	304	KC1	CMA-C3A-C2A	-8.19	108.60	128.43
10	14	312	A86	C33-C32-C31	8.19	117.17	109.21
13	21	212	DD6	C-C1-C2	-8.18	109.56	122.82
9	16	302	KC1	C1D-ND-C4D	-8.17	100.58	106.31
9	16	308	KC1	C1D-ND-C4D	-8.15	100.59	106.31
9	13	310	KC1	C1D-ND-C4D	-8.14	100.60	106.31
9	13	310	KC1	CMA-C3A-C4A	-8.13	112.33	125.03
8	13	308	CLA	C1D-ND-C4D	-8.13	100.61	106.31
10	13	316	A86	O1-C20-C21	-8.12	105.98	115.05
9	17	305	KC1	CMD-C2D-C1D	8.10	137.76	125.42
13	21	216	DD6	C-C1-C24	-8.10	105.71	118.09
13	19	312	DD6	O1-C15-C14	-8.10	93.68	116.88
10	14	311	A86	C33-C32-C31	8.09	117.08	109.21
8	14	303	CLA	CAA-C2A-C3A	-8.09	91.14	113.00
10	14	316	A86	O1-C20-C21	-8.08	106.02	115.05
8	14	307	CLA	C1D-ND-C4D	-8.08	100.64	106.31
9	17	303	KC1	C1D-ND-C4D	-8.06	100.65	106.31
9	11	304	KC1	C1D-ND-C4D	-8.06	100.66	106.31
10	12	302	A86	C4-C5-C6	-8.05	115.98	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	18	313	A86	C33-C32-C31	8.04	117.02	109.21
13	16	312	DD6	C8-C6-C5	-8.03	106.39	119.01
9	18	309	KC1	CMA-C3A-C4A	-7.96	112.60	125.03
10	11	312	A86	O1-C20-C21	-7.95	106.17	115.05
13	20	312	DD6	C7-C6-C5	-7.92	109.98	122.82
10	18	311	A86	C33-C32-C31	7.91	116.90	109.21
10	11	311	A86	C3-C2-C1	-7.90	116.19	127.28
9	21	203	KC1	C1D-ND-C4D	-7.88	100.79	106.31
13	21	212	DD6	C3-C2-C1	-7.86	116.25	127.28
13	21	212	DD6	C37-C36-C31	-7.86	109.46	124.16
13	20	314	DD6	C7-C6-C5	-7.85	110.10	122.82
10	11	310	A86	O1-C20-C21	-7.85	106.28	115.05
9	20	305	KC1	CMD-C2D-C1D	7.75	137.22	125.42
9	15	304	KC1	CMA-C3A-C2A	-7.72	109.75	128.43
10	11	311	A86	C33-C32-C31	7.70	116.70	109.21
9	21	207	KC1	CMA-C3A-C2A	-7.60	110.04	128.43
9	17	306	KC1	C1D-ND-C4D	-7.60	100.98	106.31
9	20	306	KC1	C1D-ND-C4D	-7.58	100.99	106.31
10	15	312	A86	C3-C2-C1	-7.58	116.64	127.28
9	16	308	KC1	CMD-C2D-C1D	7.58	136.96	125.42
9	20	303	KC1	CMA-C3A-C2A	-7.55	110.16	128.43
9	11	308	KC1	CMD-C2D-C1D	7.54	136.90	125.42
10	21	213	A86	C33-C32-C31	7.53	116.53	109.21
10	13	316	A86	C4-C5-C6	-7.51	116.75	127.28
13	19	312	DD6	C7-C6-C5	-7.51	110.65	122.82
9	20	306	KC1	CMD-C2D-C1D	7.51	136.85	125.42
9	19	308	KC1	CMA-C3A-C2A	-7.50	110.27	128.43
13	16	312	DD6	C7-C6-C5	-7.50	110.67	122.82
13	16	312	DD6	C-C1-C24	-7.48	106.66	118.09
13	21	216	DD6	C13-C11-C10	-7.45	107.30	119.01
13	21	216	DD6	C-C1-C2	-7.44	110.76	122.82
13	19	312	DD6	C13-C11-C10	-7.43	107.32	119.01
8	19	302	CLA	O2D-CGD-CBD	7.42	124.20	111.23
10	21	211	A86	C33-C32-C31	7.41	116.42	109.21
9	16	304	KC1	CMD-C2D-C1D	7.41	136.70	125.42
13	20	314	DD6	C28-C27-C26	-7.41	109.79	124.18
13	20	312	DD6	C8-C6-C5	-7.40	107.37	119.01
9	13	305	KC1	CMA-C3A-C2A	-7.39	110.55	128.43
10	14	313	A86	C33-C32-C31	7.38	116.38	109.21
13	16	312	DD6	C28-C27-C26	-7.35	109.90	124.18
13	20	314	DD6	C-C1-C24	-7.34	106.88	118.09
10	13	314	A86	C4-C5-C6	-7.32	117.02	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	16	312	DD6	C12-C11-C13	-7.31	106.92	118.09
9	15	304	KC1	CMD-C2D-C1D	7.30	136.54	125.42
9	14	309	KC1	CHB-C4A-C3A	-7.30	113.51	125.03
9	17	309	KC1	CHB-C4A-C3A	-7.28	113.54	125.03
9	11	304	KC1	CMD-C2D-C1D	7.27	136.50	125.42
9	18	309	KC1	CHB-C4A-C3A	-7.27	113.55	125.03
10	16	311	A86	C3-C2-C1	-7.26	117.09	127.28
9	16	304	KC1	CMA-C3A-C2A	-7.26	110.86	128.43
9	20	305	KC1	CMA-C3A-C4A	-7.24	113.72	125.03
9	21	207	KC1	CMD-C2D-C1D	7.24	136.44	125.42
9	15	309	KC1	CHB-C4A-C3A	-7.24	113.61	125.03
10	17	316	A86	C4-C5-C6	-7.23	117.14	127.28
13	19	312	DD6	C28-C27-C26	-7.22	110.16	124.18
8	20	304	CLA	CMD-C2D-C1D	7.22	137.44	124.73
10	13	312	A86	C33-C32-C31	7.20	116.20	109.21
9	11	308	KC1	CHB-C4A-C3A	-7.19	113.67	125.03
13	20	314	DD6	C-C1-C2	-7.19	111.16	122.82
13	16	312	DD6	C-C1-C2	-7.16	111.21	122.82
9	20	303	KC1	CMD-C2D-C1D	7.14	136.29	125.42
9	13	310	KC1	CHB-C4A-C3A	-7.12	113.78	125.03
9	13	303	KC1	CMD-C2D-C1D	7.12	136.26	125.42
13	19	312	DD6	C24-C1-C2	-7.11	107.82	119.01
10	11	310	A86	C33-C32-C31	7.11	116.12	109.21
9	14	309	KC1	CMD-C2D-C1D	7.10	136.23	125.42
9	20	303	KC1	CHB-C4A-C3A	-7.10	113.82	125.03
9	20	306	KC1	O2D-CGD-CBD	7.10	123.64	111.23
13	20	312	DD6	C28-C27-C26	-7.09	110.40	124.18
10	21	214	A86	C33-C32-C31	7.08	116.09	109.21
10	15	314	A86	C33-C32-C31	7.05	116.06	109.21
10	17	312	A86	C33-C32-C31	7.04	116.06	109.21
9	15	302	KC1	CMD-C2D-C1D	7.04	136.14	125.42
10	14	314	A86	C33-C32-C31	7.02	116.04	109.21
10	11	318	A86	C3-C2-C1	-7.02	117.43	127.28
13	20	314	DD6	C8-C6-C5	-7.02	107.97	119.01
8	20	302	CLA	CMD-C2D-C1D	7.02	137.09	124.73
8	14	310	CLA	CMD-C2D-C1D	7.00	137.06	124.73
9	18	304	KC1	CMD-C2D-C1D	7.00	136.07	125.42
9	18	306	KC1	O2D-CGD-CBD	6.99	123.46	111.23
9	16	305	KC1	CHB-C4A-C3A	-6.99	114.00	125.03
8	13	309	CLA	CMD-C2D-C1D	6.98	137.02	124.73
9	14	304	KC1	CMD-C2D-C1D	6.98	136.05	125.42
9	12	310	KC1	CHB-C4A-C3A	-6.98	114.01	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	17	306	KC1	O2D-CGD-CBD	6.98	123.43	111.23
9	12	310	KC1	CMD-C2D-C1D	6.98	136.04	125.42
9	17	309	KC1	CMA-C3A-C4A	-6.98	114.13	125.03
8	21	205	CLA	CMD-C2D-C1D	6.97	137.00	124.73
8	18	301	CLA	CMD-C2D-C1D	6.97	137.00	124.73
8	21	206	CLA	CMD-C2D-C1D	6.97	137.00	124.73
10	20	311	A86	C33-C32-C31	6.94	115.96	109.21
9	13	310	KC1	CMD-C2D-C1D	6.94	135.98	125.42
9	13	305	KC1	CMD-C2D-C1D	6.93	135.98	125.42
9	16	308	KC1	CMA-C3A-C4A	-6.93	114.21	125.03
9	16	305	KC1	CMD-C2D-C1D	6.92	135.96	125.42
9	21	207	KC1	CHB-C4A-C3A	-6.91	114.13	125.03
9	14	304	KC1	CHB-C4A-C3A	-6.90	114.13	125.03
9	17	309	KC1	CMD-C2D-C1D	6.90	135.92	125.42
13	20	314	DD6	O1-C15-C14	-6.90	97.12	116.88
9	13	303	KC1	CHB-C4A-C3A	-6.89	114.16	125.03
9	15	306	KC1	CMD-C2D-C1D	6.88	135.89	125.42
8	21	204	CLA	CMD-C2D-C1D	6.87	136.83	124.73
9	16	302	KC1	CMD-C2D-C1D	6.86	135.87	125.42
9	11	306	KC1	CMD-C2D-C1D	6.86	135.86	125.42
9	12	310	KC1	CMA-C3A-C4A	-6.85	114.33	125.03
8	20	310	CLA	CMD-C2D-C1D	6.85	136.79	124.73
8	13	306	CLA	CMD-C2D-C1D	6.85	136.78	124.73
9	18	309	KC1	CMD-C2D-C1D	6.83	135.81	125.42
10	15	314	A86	C25-C26-C27	-6.83	117.70	127.28
8	21	208	CLA	CMD-C2D-C1D	6.82	136.74	124.73
9	18	304	KC1	CHB-C4A-C3A	-6.81	114.27	125.03
8	15	310	CLA	CMD-C2D-C1D	6.81	136.72	124.73
9	18	306	KC1	CHB-C4A-C3A	-6.80	114.29	125.03
9	12	306	KC1	CMA-C3A-C2A	-6.80	111.97	128.43
8	18	302	CLA	CMD-C2D-C1D	6.80	136.70	124.73
10	18	314	A86	C33-C32-C31	6.80	115.82	109.21
9	11	302	KC1	CHB-C4A-C3A	-6.80	114.30	125.03
9	16	308	KC1	CHB-C4A-C3A	-6.80	114.30	125.03
9	16	302	KC1	CHB-C4A-C3A	-6.79	114.31	125.03
8	17	310	CLA	CMD-C2D-C1D	6.79	136.69	124.73
9	18	309	KC1	O2D-CGD-CBD	6.79	123.09	111.23
8	14	305	CLA	CMD-C2D-C1D	6.79	136.68	124.73
8	13	302	CLA	CMD-C2D-C1D	6.78	136.66	124.73
8	18	310	CLA	CMD-C2D-C1D	6.78	136.66	124.73
9	21	203	KC1	CHB-C4A-C3A	-6.77	114.33	125.03
8	15	308	CLA	CMD-C2D-C1D	6.77	136.65	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	11	306	KC1	CHB-C4A-C3A	-6.76	114.35	125.03
9	16	302	KC1	CMA-C3A-C4A	-6.76	114.47	125.03
8	21	202	CLA	CMD-C2D-C1D	6.76	136.63	124.73
9	17	305	KC1	CHB-C4A-C3A	-6.76	114.36	125.03
9	13	307	KC1	CMD-C2D-C1D	6.75	135.70	125.42
9	14	306	KC1	CHB-C4A-C3A	-6.75	114.37	125.03
9	15	302	KC1	CHB-C4A-C3A	-6.75	114.37	125.03
9	15	304	KC1	CHB-C4A-C3A	-6.75	114.38	125.03
9	20	306	KC1	CHB-C4A-C3A	-6.74	114.38	125.03
9	17	303	KC1	CHB-C4A-C3A	-6.74	114.38	125.03
8	12	307	CLA	CMD-C2D-C1D	6.73	136.59	124.73
8	13	311	CLA	CMD-C2D-C1D	6.73	136.58	124.73
10	17	312	A86	C3-C2-C1	-6.72	117.85	127.28
8	12	311	CLA	O2D-CGD-CBD	6.72	122.98	111.23
13	20	314	DD6	C13-C11-C10	-6.72	108.44	119.01
8	15	301	CLA	CMD-C2D-C1D	6.71	136.54	124.73
9	16	304	KC1	CHB-C4A-C3A	-6.70	114.46	125.03
9	13	305	KC1	CHB-C4A-C3A	-6.68	114.48	125.03
8	11	305	CLA	CMD-C2D-C1D	6.68	136.49	124.73
8	20	308	CLA	CMD-C2D-C1D	6.68	136.49	124.73
10	13	313	A86	C3-C2-C1	-6.68	117.91	127.28
8	11	309	CLA	CMD-C2D-C1D	6.68	136.49	124.73
8	17	302	CLA	CMD-C2D-C1D	6.68	136.48	124.73
13	20	312	DD6	C-C1-C24	-6.67	107.90	118.09
8	19	303	CLA	CMD-C2D-C1D	6.67	136.47	124.73
8	15	305	CLA	CMD-C2D-C1D	6.67	136.47	124.73
9	11	304	KC1	CHB-C4A-C3A	-6.67	114.50	125.03
9	14	306	KC1	O2D-CGD-CBD	6.66	122.88	111.23
9	20	305	KC1	CHB-C4A-C3A	-6.66	114.51	125.03
9	21	203	KC1	C2B-C1B-NB	6.66	116.71	110.13
8	17	310	CLA	O2D-CGD-CBD	6.65	122.85	111.23
8	16	309	CLA	CMD-C2D-C1D	6.65	136.43	124.73
9	15	306	KC1	CHB-C4A-C3A	-6.64	114.54	125.03
8	14	301	CLA	CMD-C2D-C1D	6.64	136.42	124.73
8	21	209	CLA	CMD-C2D-C1D	6.63	136.40	124.73
8	11	303	CLA	CMD-C2D-C1D	6.62	136.38	124.73
8	12	301	CLA	CMD-C2D-C1D	6.61	136.37	124.73
10	13	316	A86	C33-C32-C31	6.60	115.63	109.21
9	17	306	KC1	CMD-C2D-C1D	6.60	135.47	125.42
9	17	303	KC1	CMD-C2D-C1D	6.60	135.47	125.42
9	12	306	KC1	CHB-C4A-C3A	-6.59	114.62	125.03
13	21	216	DD6	C8-C6-C5	-6.59	108.65	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	15	313	A86	C33-C32-C31	6.59	115.61	109.21
9	17	306	KC1	CHB-C4A-C3A	-6.58	114.63	125.03
13	20	314	DD6	C12-C11-C13	-6.58	108.03	118.09
10	17	321	A86	C33-C32-C31	6.58	115.61	109.21
13	19	312	DD6	C-C1-C2	-6.58	112.16	122.82
9	11	306	KC1	O2D-CGD-CBD	6.57	122.72	111.23
8	11	301	CLA	CMD-C2D-C1D	6.57	136.30	124.73
9	12	308	KC1	CHB-C4A-C3A	-6.57	114.65	125.03
8	12	305	CLA	CMD-C2D-C1D	6.57	136.30	124.73
8	17	308	CLA	CMD-C2D-C1D	6.56	136.28	124.73
8	16	301	CLA	C2D-C1D-ND	6.56	116.62	110.13
8	18	305	CLA	CMD-C2D-C1D	6.56	136.28	124.73
9	19	308	KC1	CHB-C4A-C3A	-6.56	114.67	125.03
10	13	313	A86	C33-C32-C31	6.56	115.59	109.21
9	16	308	KC1	O2D-CGD-CBD	6.55	122.68	111.23
10	11	318	A86	O4-C38-C39	6.54	122.75	111.09
9	12	306	KC1	CMD-C2D-C1D	6.54	135.38	125.42
9	21	203	KC1	CMD-C2D-C1D	6.53	135.37	125.42
8	19	301	CLA	C2D-C1D-ND	6.53	116.59	110.13
10	11	313	A86	C40-C32-C31	-6.53	104.63	110.47
9	15	302	KC1	CMA-C3A-C2A	-6.53	112.63	128.43
8	19	306	CLA	CHD-C4C-C3C	-6.52	115.27	124.77
9	13	307	KC1	CHB-C4A-C3A	-6.52	114.74	125.03
9	15	309	KC1	CMA-C3A-C4A	-6.51	114.86	125.03
10	12	313	A86	C33-C32-C31	6.50	115.53	109.21
13	21	216	DD6	O1-C15-C14	-6.50	98.25	116.88
10	15	313	A86	C4-C5-C6	-6.50	118.16	127.28
8	17	304	CLA	CMD-C2D-C1D	6.50	136.17	124.73
8	12	309	CLA	O2D-CGD-CBD	6.50	122.59	111.23
9	21	203	KC1	C3B-C2B-C1B	-6.49	100.90	107.05
8	19	304	CLA	CMD-C2D-C1D	6.49	136.16	124.73
8	19	307	CLA	CMD-C2D-C1D	6.49	136.16	124.73
8	19	309	CLA	CMD-C2D-C1D	6.49	136.16	124.73
8	15	301	CLA	C2D-C1D-ND	6.49	116.55	110.13
9	15	309	KC1	CMD-C2D-C1D	6.49	135.29	125.42
8	13	301	CLA	CMD-C2D-C1D	6.48	136.14	124.73
10	15	314	A86	C3-C2-C1	-6.48	118.19	127.28
8	20	309	CLA	CMD-C2D-C1D	6.47	136.12	124.73
9	21	203	KC1	C3A-C4A-NA	6.47	118.45	110.45
8	12	303	CLA	CMD-C2D-C1D	6.46	136.10	124.73
8	12	311	CLA	CMD-C2D-C1D	6.45	136.09	124.73
8	14	301	CLA	CHD-C4C-C3C	-6.45	115.37	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	18	301	CLA	C2D-C1D-ND	6.45	116.51	110.13
8	11	303	CLA	O2D-CGD-CBD	6.43	122.47	111.23
8	19	305	CLA	C2D-C1D-ND	6.42	116.48	110.13
8	19	302	CLA	CMD-C2D-C1D	6.42	136.03	124.73
9	18	309	KC1	C3A-C4A-NA	6.41	118.39	110.45
9	11	302	KC1	CMD-C2D-C1D	6.40	135.16	125.42
8	12	304	CLA	CMD-C2D-C1D	6.39	135.99	124.73
8	11	307	CLA	CHD-C4C-C3C	-6.39	115.45	124.77
8	21	210	CLA	CMD-C2D-C1D	6.39	135.98	124.73
13	20	312	DD6	C7-C6-C8	-6.39	108.33	118.09
9	20	303	KC1	C3A-C4A-NA	6.39	118.36	110.45
8	11	301	CLA	CHD-C4C-C3C	-6.37	115.48	124.77
8	19	306	CLA	C2D-C1D-ND	6.37	116.43	110.13
13	21	216	DD6	C12-C11-C13	-6.37	108.35	118.09
9	14	306	KC1	CMD-C2D-C1D	6.37	135.12	125.42
9	12	308	KC1	CMD-C2D-C1D	6.35	135.09	125.42
8	16	303	CLA	CMD-C2D-C1D	6.34	135.90	124.73
8	19	301	CLA	CHD-C4C-C3C	-6.34	115.52	124.77
10	16	310	A86	C3-C2-C1	-6.34	118.39	127.28
8	13	304	CLA	CMD-C2D-C1D	6.33	135.87	124.73
8	19	304	CLA	C2D-C1D-ND	6.33	116.39	110.13
10	20	313	A86	C4-C5-C6	-6.32	118.41	127.28
8	15	303	CLA	CMD-C2D-C1D	6.32	135.86	124.73
9	14	309	KC1	CMA-C3A-C4A	-6.32	115.16	125.03
9	13	310	KC1	C3A-C4A-NA	6.32	118.27	110.45
9	21	207	KC1	C3B-C2B-C1B	-6.32	101.07	107.05
8	14	301	CLA	C2D-C1D-ND	6.31	116.37	110.13
9	18	306	KC1	CMD-C2D-C1D	6.31	135.03	125.42
9	14	309	KC1	C3A-C4A-NA	6.31	118.26	110.45
8	15	307	CLA	O2D-CGD-CBD	6.28	122.21	111.23
9	20	303	KC1	C2B-C1B-NB	6.28	116.34	110.13
8	14	308	CLA	CMD-C2D-C1D	6.28	135.79	124.73
10	16	310	A86	C41-C32-C31	-6.28	104.85	110.47
9	19	308	KC1	CMD-C2D-C1D	6.27	134.97	125.42
13	21	216	DD6	C7-C6-C8	-6.27	108.51	118.09
8	16	301	CLA	CHD-C4C-C3C	-6.27	115.63	124.77
8	19	303	CLA	CAA-C2A-C3A	-6.26	96.07	113.00
9	13	303	KC1	CMA-C3A-C2A	-6.26	113.27	128.43
8	16	309	CLA	CAA-C2A-C3A	-6.26	96.08	113.00
10	17	311	A86	O4-C38-C39	6.26	122.25	111.09
9	11	302	KC1	C3B-C2B-C1B	-6.26	101.12	107.05
8	16	307	CLA	CMD-C2D-C1D	6.25	135.74	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	14	316	A86	O4-C38-C39	6.23	122.21	111.09
10	19	313	A86	O4-C38-C39	6.23	122.20	111.09
8	20	304	CLA	CHD-C4C-C3C	-6.22	115.70	124.77
9	15	309	KC1	C3B-C2B-C1B	-6.22	101.16	107.05
8	11	301	CLA	C2D-C1D-ND	6.22	116.28	110.13
9	19	308	KC1	C1A-C2A-C3A	-6.22	101.57	107.28
8	18	301	CLA	CHD-C4C-C3C	-6.21	115.71	124.77
8	21	206	CLA	CHD-C4C-C3C	-6.21	115.71	124.77
9	13	303	KC1	C3A-C4A-NA	6.20	118.12	110.45
9	14	304	KC1	C3A-C4A-NA	6.20	118.12	110.45
9	12	310	KC1	C3B-C2B-C1B	-6.20	101.18	107.05
9	17	309	KC1	C3A-C4A-NA	6.19	118.12	110.45
8	14	302	CLA	CMD-C2D-C1D	6.19	135.63	124.73
8	18	308	CLA	C2D-C1D-ND	6.19	116.25	110.13
9	11	308	KC1	C3B-C2B-C1B	-6.18	101.19	107.05
10	13	315	A86	C3-C2-C1	-6.18	118.61	127.28
9	17	309	KC1	C2B-C1B-NB	6.18	116.24	110.13
10	12	316	A86	O4-C38-C39	6.17	122.09	111.09
8	16	306	CLA	CHD-C4C-C3C	-6.17	115.78	124.77
8	15	308	CLA	C2D-C1D-ND	6.16	116.22	110.13
8	21	205	CLA	C2D-C1D-ND	6.16	116.22	110.13
9	12	306	KC1	C3A-C4A-NA	6.16	118.07	110.45
9	14	309	KC1	C3B-C2B-C1B	-6.16	101.22	107.05
9	12	310	KC1	C2B-C1B-NB	6.16	116.22	110.13
9	15	306	KC1	CMA-C3A-C2A	-6.15	113.53	128.43
13	21	212	DD6	C8-C6-C5	-6.15	109.33	119.01
8	12	309	CLA	C2B-C1B-NB	6.14	116.70	110.33
9	15	309	KC1	C3A-C4A-NA	6.14	118.05	110.45
9	15	306	KC1	C3B-C2B-C1B	-6.14	101.23	107.05
10	18	312	A86	C4-C5-C6	-6.14	118.67	127.28
9	16	305	KC1	C3A-C4A-NA	6.14	118.05	110.45
10	12	302	A86	C3-C2-C1	-6.14	118.67	127.28
8	19	303	CLA	CHD-C4C-C3C	-6.13	115.83	124.77
9	12	306	KC1	C3C-C4C-NC	6.13	116.47	109.90
9	12	310	KC1	O2D-CGD-CBD	6.13	121.94	111.23
9	11	304	KC1	C3A-C4A-NA	6.12	118.03	110.45
8	19	310	CLA	CMD-C2D-C1D	6.12	135.51	124.73
9	17	309	KC1	C3B-C2B-C1B	-6.10	101.27	107.05
10	12	319	A86	C4-C5-C6	-6.10	118.72	127.28
8	21	206	CLA	C2D-C1D-ND	6.09	116.15	110.13
8	20	304	CLA	CAA-C2A-C3A	-6.09	96.54	113.00
10	13	315	A86	C25-C26-C27	-6.09	118.74	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	13	307	KC1	C2D-C1D-ND	6.08	116.64	110.33
9	16	308	KC1	C3A-C4A-NA	6.08	117.97	110.45
9	12	310	KC1	C3A-C4A-NA	6.07	117.96	110.45
10	17	321	A86	C4-C5-C6	-6.07	118.77	127.28
8	12	301	CLA	C2D-C1D-ND	6.07	116.13	110.13
8	14	303	CLA	CMD-C2D-C1D	6.07	135.41	124.73
8	15	307	CLA	CHD-C4C-C3C	-6.06	115.93	124.77
10	11	310	A86	O4-C38-C39	6.06	121.90	111.09
10	14	314	A86	C3-C2-C1	-6.06	118.78	127.28
8	16	301	CLA	CMD-C2D-C1D	6.06	135.40	124.73
8	14	307	CLA	C2B-C1B-NB	6.06	116.61	110.33
9	13	310	KC1	C2B-C1B-NB	6.05	116.12	110.13
9	11	308	KC1	C3A-C4A-NA	6.05	117.94	110.45
8	11	307	CLA	C2D-C1D-ND	6.05	116.11	110.13
8	20	304	CLA	C2D-C1D-ND	6.05	116.11	110.13
8	21	210	CLA	C2D-C1D-ND	6.05	116.11	110.13
9	21	207	KC1	C2B-C1B-NB	6.04	116.10	110.13
9	13	307	KC1	CMA-C3A-C2A	-6.04	113.82	128.43
9	13	310	KC1	C3B-C2B-C1B	-6.04	101.33	107.05
8	15	310	CLA	O2D-CGD-CBD	6.03	121.78	111.23
9	17	305	KC1	C1A-C2A-C3A	-6.03	101.73	107.28
9	17	303	KC1	C1A-C2A-C3A	-6.02	101.75	107.28
9	18	304	KC1	C3A-C4A-NA	6.02	117.90	110.45
9	21	207	KC1	C3A-C4A-NA	6.02	117.90	110.45
10	20	311	A86	C4-C5-C6	-6.01	118.84	127.28
10	15	311	A86	O4-C38-C39	6.01	121.81	111.09
10	17	315	A86	C4-C5-C6	-6.01	118.85	127.28
9	15	304	KC1	C3B-C2B-C1B	-6.01	101.36	107.05
9	18	304	KC1	CMA-C3A-C2A	-6.01	113.89	128.43
9	14	309	KC1	C2B-C1B-NB	6.01	116.07	110.13
8	19	301	CLA	CMD-C2D-C1D	6.01	135.31	124.73
10	11	314	A86	C3-C2-C1	-6.01	118.86	127.28
8	20	307	CLA	CMD-C2D-C1D	6.00	135.29	124.73
9	11	308	KC1	O2D-CGD-CBD	6.00	121.72	111.23
9	15	304	KC1	C3A-C4A-NA	6.00	117.87	110.45
9	11	306	KC1	CMA-C3A-C2A	-5.99	113.93	128.43
8	15	301	CLA	CHD-C4C-C3C	-5.99	116.04	124.77
8	19	303	CLA	C2D-C1D-ND	5.99	116.05	110.13
9	16	304	KC1	C3A-C4A-NA	5.99	117.86	110.45
9	15	302	KC1	C1A-C2A-C3A	-5.99	101.78	107.28
8	12	309	CLA	CMD-C2D-C1D	5.99	135.27	124.73
8	11	307	CLA	C2B-C1B-NB	5.98	116.53	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	12	315	A86	C3-C2-C1	-5.98	118.89	127.28
8	15	307	CLA	C2B-C1B-NB	5.98	116.53	110.33
8	15	303	CLA	O2D-CGD-CBD	5.98	121.68	111.23
13	21	212	DD6	C28-C27-C26	-5.98	112.57	124.18
9	18	306	KC1	C3A-C4A-NA	5.98	117.85	110.45
10	12	313	A86	C3-C2-C1	-5.97	118.90	127.28
10	13	316	A86	O4-C38-C39	5.97	121.74	111.09
10	19	311	A86	C3-C2-C1	-5.97	118.91	127.28
8	12	303	CLA	CHD-C4C-C3C	-5.97	116.07	124.77
9	11	302	KC1	C3A-C4A-NA	5.97	117.83	110.45
8	18	307	CLA	CMD-C2D-C1D	5.96	135.23	124.73
8	18	303	CLA	CHD-C4C-C3C	-5.96	116.08	124.77
10	12	314	A86	C33-C32-C31	5.96	115.00	109.21
10	20	301	A86	C3-C2-C1	-5.96	118.92	127.28
9	13	305	KC1	C3A-C4A-NA	5.96	117.82	110.45
8	18	307	CLA	CHD-C4C-C3C	-5.95	116.09	124.77
8	11	309	CLA	C2D-C1D-ND	5.95	116.02	110.13
9	12	306	KC1	CHD-C4C-C3C	-5.95	114.26	125.23
9	18	309	KC1	C3B-C2B-C1B	-5.95	101.42	107.05
9	20	306	KC1	C3A-C4A-NA	5.94	117.80	110.45
8	15	307	CLA	CMD-C2D-C1D	5.94	135.19	124.73
9	17	305	KC1	C3A-C4A-NA	5.94	117.80	110.45
9	15	302	KC1	C3A-C4A-NA	5.93	117.80	110.45
9	17	303	KC1	C3A-C4A-NA	5.92	117.78	110.45
9	16	302	KC1	C1A-C2A-C3A	-5.92	101.84	107.28
8	17	307	CLA	CHD-C4C-C3C	-5.92	116.14	124.77
9	14	306	KC1	C2D-C1D-ND	5.92	116.47	110.33
10	15	315	A86	C33-C32-C31	5.92	114.96	109.21
9	12	308	KC1	C3A-C4A-NA	5.91	117.77	110.45
9	14	304	KC1	C3B-C2B-C1B	-5.91	101.45	107.05
9	11	302	KC1	C1A-C2A-C3A	-5.91	101.85	107.28
9	18	309	KC1	C2B-C1B-NB	5.91	115.97	110.13
8	17	304	CLA	O2D-CGD-CBD	5.91	121.56	111.23
8	21	204	CLA	O2D-CGD-CBD	5.91	121.56	111.23
8	19	305	CLA	CMD-C2D-C1D	5.91	135.13	124.73
8	13	311	CLA	O2D-CGD-CBD	5.90	121.54	111.23
8	14	302	CLA	CHD-C4C-C3C	-5.90	116.17	124.77
10	16	313	A86	C3-C2-C1	-5.90	119.01	127.28
9	16	304	KC1	C3B-C2B-C1B	-5.89	101.47	107.05
8	12	303	CLA	C2D-C1D-ND	5.89	115.96	110.13
8	16	307	CLA	CHD-C4C-C3C	-5.89	116.19	124.77
9	13	303	KC1	C1A-C2A-C3A	-5.89	101.87	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	19	307	CLA	C2D-C1D-ND	5.89	115.95	110.13
9	20	303	KC1	C3B-C2B-C1B	-5.88	101.48	107.05
9	21	203	KC1	C1A-C2A-C3A	-5.88	101.87	107.28
8	13	302	CLA	C2D-C1D-ND	5.88	115.95	110.13
9	12	310	KC1	C1A-C2A-C3A	-5.88	101.88	107.28
9	15	309	KC1	C2B-C1B-NB	5.88	115.94	110.13
9	20	305	KC1	C3A-C4A-NA	5.88	117.72	110.45
9	11	308	KC1	C2B-C1B-NB	5.87	115.94	110.13
8	16	303	CLA	O2D-CGD-CBD	5.87	121.50	111.23
8	18	307	CLA	C2D-C1D-ND	5.87	115.93	110.13
8	18	308	CLA	CHD-C4C-C3C	-5.87	116.22	124.77
8	20	310	CLA	CHD-C4C-C3C	-5.86	116.22	124.77
8	13	302	CLA	CHD-C4C-C3C	-5.86	116.23	124.77
9	13	307	KC1	C1A-C2A-C3A	-5.86	101.90	107.28
9	16	302	KC1	C3A-C4A-NA	5.86	117.70	110.45
9	17	303	KC1	C3B-C2B-C1B	-5.85	101.51	107.05
9	11	302	KC1	C2B-C1B-NB	5.85	115.92	110.13
9	13	307	KC1	C3A-C4A-NA	5.85	117.69	110.45
9	21	203	KC1	O2D-CGD-CBD	5.85	121.46	111.23
9	12	308	KC1	C1A-C2A-C3A	-5.85	101.91	107.28
8	14	307	CLA	CHD-C4C-C3C	-5.84	116.25	124.77
9	20	306	KC1	CMA-C3A-C2A	-5.84	114.29	128.43
8	18	308	CLA	CMD-C2D-C1D	5.84	135.01	124.73
9	19	308	KC1	C3A-C4A-NA	5.84	117.68	110.45
9	13	305	KC1	C3B-C2B-C1B	-5.84	101.52	107.05
8	11	307	CLA	CMD-C2D-C1D	5.84	135.01	124.73
8	13	309	CLA	C2D-C1D-ND	5.84	115.90	110.13
9	20	305	KC1	C3B-C2B-C1B	-5.83	101.53	107.05
9	20	305	KC1	CMA-C3A-C2A	-5.83	114.31	128.43
13	16	312	DD6	O1-C15-C14	-5.83	100.19	116.88
8	11	309	CLA	CHD-C4C-C3C	-5.82	116.28	124.77
8	17	307	CLA	O2D-CGD-CBD	5.82	121.41	111.23
9	11	306	KC1	C3B-C2B-C1B	-5.82	101.54	107.05
8	12	305	CLA	CHD-C4C-C3C	-5.82	116.29	124.77
10	15	316	A86	O4-C38-C39	5.82	121.46	111.09
8	15	307	CLA	C2D-C1D-ND	5.81	115.88	110.13
10	15	311	A86	C41-C32-C31	-5.81	105.27	110.47
9	18	304	KC1	C3B-C2B-C1B	-5.81	101.55	107.05
10	19	311	A86	O4-C38-C39	5.80	121.44	111.09
9	20	306	KC1	C1A-C2A-C3A	-5.80	101.95	107.28
8	12	307	CLA	C2D-C1D-ND	5.80	115.86	110.13
9	11	308	KC1	CMA-C3A-C4A	-5.80	115.98	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	14	309	KC1	CBA-CAA-C2A	-5.79	102.21	125.45
8	13	301	CLA	C2D-C1D-ND	5.79	115.86	110.13
9	19	308	KC1	C3B-C2B-C1B	-5.79	101.57	107.05
8	12	305	CLA	O2D-CGD-CBD	5.79	121.34	111.23
8	18	305	CLA	C2D-C1D-ND	5.78	115.85	110.13
8	14	302	CLA	C2D-C1D-ND	5.78	115.85	110.13
8	19	307	CLA	CHD-C4C-C3C	-5.78	116.35	124.77
9	20	306	KC1	C3B-C2B-C1B	-5.78	101.58	107.05
8	12	311	CLA	CHD-C4C-C3C	-5.78	116.35	124.77
8	15	305	CLA	C2D-C1D-ND	5.77	115.84	110.13
9	17	306	KC1	C3A-C4A-NA	5.77	117.59	110.45
8	19	305	CLA	CHD-C4C-C3C	-5.77	116.36	124.77
9	17	305	KC1	C3B-C2B-C1B	-5.77	101.59	107.05
9	15	306	KC1	C3A-C4A-NA	5.76	117.58	110.45
10	17	313	A86	C33-C32-C31	5.76	114.81	109.21
10	21	213	A86	C25-C26-C27	-5.75	119.21	127.28
9	11	304	KC1	CMA-C3A-C2A	-5.75	114.51	128.43
8	18	302	CLA	CHD-C4C-C3C	-5.75	116.39	124.77
8	21	208	CLA	C2D-C1D-ND	5.75	115.81	110.13
8	20	302	CLA	C2D-C1D-ND	5.75	115.81	110.13
8	17	308	CLA	C2D-C1D-ND	5.75	115.81	110.13
8	20	309	CLA	C2D-C1D-ND	5.74	115.81	110.13
9	14	306	KC1	C3A-C4A-NA	5.74	117.55	110.45
8	16	306	CLA	CMD-C2D-C1D	5.73	134.83	124.73
8	11	307	CLA	O2D-CGD-CBD	5.73	121.25	111.23
9	16	308	KC1	C2B-C1B-NB	5.73	115.80	110.13
8	17	307	CLA	C2D-C1D-ND	5.73	115.80	110.13
8	20	307	CLA	C2D-C1D-ND	5.73	115.80	110.13
9	11	306	KC1	C3A-C4A-NA	5.73	117.54	110.45
8	20	302	CLA	CHD-C4C-C3C	-5.72	116.43	124.77
10	17	316	A86	C3-C2-C1	-5.72	119.26	127.28
9	16	305	KC1	C1A-C2A-C3A	-5.72	102.03	107.28
10	21	215	A86	O4-C38-C39	5.71	121.27	111.09
9	12	306	KC1	C2D-C1D-ND	5.71	116.25	110.33
8	18	305	CLA	CHD-C4C-C3C	-5.71	116.45	124.77
10	14	313	A86	O4-C38-C39	5.71	121.27	111.09
9	16	308	KC1	C3B-C2B-C1B	-5.71	101.65	107.05
8	12	309	CLA	CHD-C4C-C3C	-5.70	116.45	124.77
8	21	210	CLA	CHD-C4C-C3C	-5.70	116.46	124.77
9	17	309	KC1	O2D-CGD-CBD	5.70	121.19	111.23
8	17	307	CLA	C2B-C1B-NB	5.70	116.23	110.33
8	16	309	CLA	C2D-C1D-ND	5.69	115.76	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	20	308	CLA	C2D-C1D-ND	5.69	115.76	110.13
8	21	202	CLA	C2D-C1D-ND	5.69	115.76	110.13
8	21	209	CLA	C2D-C1D-ND	5.69	115.76	110.13
8	14	303	CLA	O2D-CGD-CBD	5.69	121.18	111.23
9	21	207	KC1	O2D-CGD-CBD	5.69	121.18	111.23
8	11	305	CLA	C2D-C1D-ND	5.69	115.76	110.13
8	13	306	CLA	C2D-C1D-ND	5.69	115.76	110.13
10	12	315	A86	C25-C26-C27	-5.69	119.30	127.28
8	19	302	CLA	CHD-C4C-C3C	-5.69	116.48	124.77
9	15	306	KC1	C1A-C2A-C3A	-5.69	102.05	107.28
10	19	311	A86	C33-C32-C31	5.68	114.73	109.21
8	21	210	CLA	O2D-CGD-CBD	5.68	121.16	111.23
8	14	308	CLA	CHD-C4C-C3C	-5.68	116.49	124.77
8	20	307	CLA	CHD-C4C-C3C	-5.68	116.49	124.77
8	12	304	CLA	CHD-C4C-C3C	-5.68	116.49	124.77
10	18	313	A86	C3-C2-C1	-5.68	119.31	127.28
8	17	310	CLA	CAA-C2A-C3A	-5.68	97.66	113.00
8	16	307	CLA	C2D-C1D-ND	5.68	115.74	110.13
9	14	304	KC1	C1A-C2A-C3A	-5.68	102.06	107.28
9	17	306	KC1	C1A-C2A-C3A	-5.68	102.06	107.28
8	13	308	CLA	C2D-C1D-ND	5.67	115.74	110.13
8	17	302	CLA	C2D-C1D-ND	5.67	115.74	110.13
8	12	311	CLA	C2D-C1D-ND	5.67	115.74	110.13
8	18	303	CLA	C2D-C1D-ND	5.67	115.74	110.13
9	14	304	KC1	C2B-C1B-NB	5.67	115.74	110.13
9	11	306	KC1	C2D-C1D-ND	5.67	116.20	110.33
8	12	304	CLA	C2D-C1D-ND	5.67	115.73	110.13
8	17	304	CLA	C2B-C1B-NB	5.66	116.20	110.33
8	12	305	CLA	C2D-C1D-ND	5.66	115.73	110.13
10	14	315	A86	C3-C2-C1	-5.66	119.34	127.28
8	11	307	CLA	C3B-C2B-C1B	-5.66	100.50	107.17
10	12	313	A86	C4-C5-C6	-5.66	119.35	127.28
9	13	307	KC1	C3B-C2B-C1B	-5.65	101.70	107.05
8	13	311	CLA	C2D-C1D-ND	5.65	115.72	110.13
10	11	310	A86	C3-C4-C5	-5.65	111.97	123.52
9	11	304	KC1	C3B-C2B-C1B	-5.64	101.70	107.05
8	13	308	CLA	CHD-C4C-C3C	-5.63	116.56	124.77
9	17	306	KC1	CHC-C1C-C2C	-5.63	116.13	125.03
9	11	304	KC1	C1A-C2A-C3A	-5.63	102.10	107.28
8	18	303	CLA	CMD-C2D-C1D	5.63	134.64	124.73
10	15	315	A86	O4-C38-C39	5.63	121.13	111.09
8	19	310	CLA	CHD-C4C-C3C	-5.63	116.57	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	13	303	KC1	C2B-C1B-NB	5.62	115.69	110.13
10	17	315	A86	C25-C26-C27	-5.62	119.40	127.28
8	12	307	CLA	CHD-C4C-C3C	-5.62	116.58	124.77
8	12	309	CLA	C2D-C1D-ND	5.62	115.69	110.13
8	14	305	CLA	C2D-C1D-ND	5.62	115.68	110.13
8	14	305	CLA	O2D-CGD-CBD	5.61	121.04	111.23
8	20	309	CLA	CHD-C4C-C3C	-5.61	116.59	124.77
9	18	304	KC1	C1A-C2A-C3A	-5.61	102.12	107.28
8	15	303	CLA	C2D-C1D-ND	5.61	115.68	110.13
8	20	308	CLA	CHD-C4C-C3C	-5.61	116.59	124.77
9	21	207	KC1	C2D-C1D-ND	5.60	116.14	110.33
8	15	305	CLA	CHD-C4C-C3C	-5.59	116.62	124.77
10	11	313	A86	C3-C2-C1	-5.59	119.44	127.28
9	12	308	KC1	C3B-C2B-C1B	-5.59	101.76	107.05
9	21	207	KC1	C1A-C2A-C3A	-5.58	102.15	107.28
8	13	304	CLA	C3B-C2B-C1B	-5.58	100.59	107.17
8	15	310	CLA	C2D-C1D-ND	5.58	115.65	110.13
9	13	310	KC1	O2D-CGD-CBD	5.58	120.98	111.23
13	21	212	DD6	C26-C25-C24	5.58	139.37	123.20
8	14	307	CLA	C3B-C2B-C1B	-5.58	100.59	107.17
8	13	306	CLA	CHD-C4C-C3C	-5.58	116.64	124.77
9	16	305	KC1	C3B-C2B-C1B	-5.57	101.77	107.05
10	13	314	A86	O4-C38-C39	5.56	121.01	111.09
9	16	308	KC1	C1A-C2A-C3A	-5.56	102.17	107.28
13	21	212	DD6	C21-C20-C19	-5.56	108.00	114.24
9	14	309	KC1	O2D-CGD-CBD	5.56	120.95	111.23
8	14	303	CLA	C2D-C1D-ND	5.56	115.63	110.13
10	15	312	A86	C33-C32-C31	5.55	114.61	109.21
9	14	306	KC1	CMA-C3A-C2A	-5.55	114.99	128.43
9	18	306	KC1	CMA-C3A-C2A	-5.55	114.99	128.43
8	16	309	CLA	CHD-C4C-C3C	-5.55	116.68	124.77
8	14	303	CLA	C2B-C1B-NB	5.54	116.08	110.33
8	13	311	CLA	C2B-C1B-NB	5.54	116.07	110.33
10	14	312	A86	C25-C26-C27	-5.54	119.51	127.28
8	11	305	CLA	CHD-C4C-C3C	-5.54	116.70	124.77
8	14	303	CLA	C3B-C2B-C1B	-5.54	100.64	107.17
10	17	321	A86	O4-C38-C39	5.54	120.96	111.09
9	14	306	KC1	C3B-C2B-C1B	-5.54	101.81	107.05
10	20	301	A86	C26-C25-C24	-5.53	107.17	123.20
8	19	302	CLA	C2D-C1D-ND	5.53	115.60	110.13
9	11	308	KC1	CBA-CAA-C2A	-5.53	103.27	125.45
8	18	310	CLA	C2D-C1D-ND	5.53	115.59	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	16	306	CLA	C2D-C1D-ND	5.52	115.59	110.13
13	21	212	DD6	C7-C6-C8	-5.52	109.65	118.09
8	13	308	CLA	C2B-C1B-NB	5.52	116.05	110.33
9	15	309	KC1	O2D-CGD-CBD	5.52	120.88	111.23
8	15	303	CLA	CHD-C4C-C3C	-5.52	116.73	124.77
9	18	309	KC1	CBA-CAA-C2A	-5.51	103.32	125.45
10	16	313	A86	O4-C38-C39	5.51	120.92	111.09
9	15	304	KC1	C2B-C1B-NB	5.51	115.58	110.13
8	19	310	CLA	C2D-C1D-ND	5.51	115.58	110.13
8	14	310	CLA	C2D-C1D-ND	5.50	115.57	110.13
8	17	307	CLA	CMD-C2D-C1D	5.50	134.41	124.73
9	19	308	KC1	C2B-C1B-NB	5.50	115.57	110.13
9	20	306	KC1	C3C-C4C-NC	5.50	115.79	109.90
10	11	314	A86	O4-C38-C39	5.50	120.89	111.09
9	15	304	KC1	C1A-C2A-C3A	-5.49	102.23	107.28
8	17	302	CLA	CHD-C4C-C3C	-5.49	116.77	124.77
9	16	304	KC1	C1A-C2A-C3A	-5.49	102.23	107.28
8	19	302	CLA	C4A-NA-C1A	-5.48	104.18	106.68
10	12	319	A86	C3-C2-C1	-5.48	119.59	127.28
8	17	310	CLA	C2D-C1D-ND	5.48	115.55	110.13
9	13	307	KC1	C2B-C1B-NB	5.48	115.55	110.13
8	14	308	CLA	C2D-C1D-ND	5.48	115.55	110.13
8	16	303	CLA	C2D-C1D-ND	5.48	115.55	110.13
8	18	310	CLA	O2D-CGD-CBD	5.48	120.81	111.23
8	18	303	CLA	O2D-CGD-CBD	5.48	120.81	111.23
8	14	305	CLA	CHD-C4C-C3C	-5.48	116.79	124.77
8	12	311	CLA	C2B-C1B-NB	5.48	116.00	110.33
8	13	302	CLA	C2B-C1B-NB	5.48	116.00	110.33
8	18	302	CLA	C2B-C1B-NB	5.48	116.00	110.33
8	18	303	CLA	C2B-C1B-NB	5.48	116.00	110.33
8	14	308	CLA	C2C-C1C-NC	5.47	115.73	109.98
9	13	305	KC1	C2D-C1D-ND	5.47	116.00	110.33
9	18	306	KC1	C1A-C2A-C3A	-5.47	102.25	107.28
8	21	208	CLA	C2B-C1B-NB	5.47	116.00	110.33
13	20	314	DD6	C7-C6-C8	-5.47	109.73	118.09
9	16	304	KC1	C2B-C1B-NB	5.47	115.54	110.13
8	11	303	CLA	C2D-C1D-ND	5.46	115.53	110.13
8	15	310	CLA	CHD-C4C-C3C	-5.46	116.81	124.77
9	20	303	KC1	C2D-C1D-ND	5.46	115.98	110.33
9	16	305	KC1	O2D-CGD-CBD	5.46	120.77	111.23
9	13	310	KC1	C1A-C2A-C3A	-5.45	102.27	107.28
8	12	303	CLA	C2B-C1B-NB	5.45	115.98	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	11	312	A86	O4-C38-C39	5.45	120.81	111.09
9	20	305	KC1	C1A-C2A-C3A	-5.45	102.27	107.28
9	20	305	KC1	O2D-CGD-CBD	5.45	120.76	111.23
8	14	307	CLA	C2D-C1D-ND	5.45	115.52	110.13
8	18	305	CLA	O2D-CGD-CBD	5.45	120.75	111.23
10	11	314	A86	C33-C32-C31	5.45	114.50	109.21
8	21	209	CLA	CHD-C4C-C3C	-5.44	116.83	124.77
8	21	204	CLA	C3B-C2B-C1B	-5.44	100.75	107.17
13	16	312	DD6	C24-C1-C2	-5.44	110.45	119.01
8	21	204	CLA	C2D-C1D-ND	5.44	115.51	110.13
8	16	309	CLA	C4A-NA-C1A	-5.44	104.20	106.68
8	17	310	CLA	CHD-C4C-C3C	-5.44	116.85	124.77
8	13	308	CLA	C3B-C2B-C1B	-5.44	100.76	107.17
8	14	303	CLA	C4A-NA-C1A	-5.44	104.20	106.68
8	13	304	CLA	O2D-CGD-CBD	5.43	120.73	111.23
8	18	302	CLA	C2D-C1D-ND	5.43	115.50	110.13
9	12	306	KC1	C1A-C2A-C3A	-5.43	102.29	107.28
8	14	303	CLA	CHD-C4C-C3C	-5.43	116.86	124.77
8	12	309	CLA	C3B-C2B-C1B	-5.43	100.77	107.17
9	16	305	KC1	C2B-C1B-NB	5.43	115.50	110.13
8	13	308	CLA	CMD-C2D-C1D	5.42	134.28	124.73
8	14	310	CLA	CHD-C4C-C3C	-5.42	116.87	124.77
9	19	308	KC1	O2D-CGD-CBD	5.42	120.70	111.23
10	12	314	A86	C3-C2-C1	-5.42	119.68	127.28
8	20	304	CLA	O2D-CGD-CBD	5.42	120.70	111.23
10	21	211	A86	O4-C38-C39	5.41	120.74	111.09
10	17	313	A86	C4-C5-C6	-5.41	119.69	127.28
8	19	306	CLA	CMD-C2D-C1D	5.41	134.25	124.73
10	21	213	A86	C3-C2-C1	-5.41	119.69	127.28
9	12	306	KC1	O2D-CGD-CBD	5.41	120.68	111.23
9	18	304	KC1	C2B-C1B-NB	5.41	115.48	110.13
8	13	306	CLA	C2B-C1B-NB	5.40	115.93	110.33
9	12	308	KC1	CMA-C3A-C2A	-5.40	115.35	128.43
9	17	309	KC1	C2D-C1D-ND	5.40	115.93	110.33
8	14	307	CLA	CMD-C2D-C1D	5.40	134.24	124.73
8	15	308	CLA	C2C-C1C-NC	5.40	115.65	109.98
10	14	313	A86	C4-C5-C6	-5.40	119.71	127.28
8	15	310	CLA	C2B-C1B-NB	5.40	115.92	110.33
9	19	308	KC1	C2D-C1D-ND	5.40	115.92	110.33
9	17	303	KC1	C2B-C1B-NB	5.39	115.46	110.13
9	18	306	KC1	C3B-C2B-C1B	-5.39	101.95	107.05
9	15	306	KC1	O2D-CGD-CBD	5.39	120.64	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	15	302	KC1	C3B-C2B-C1B	-5.38	101.96	107.05
13	16	312	DD6	C21-C20-C15	-5.38	113.45	122.30
9	20	306	KC1	C2B-C1B-NB	5.37	115.44	110.13
9	15	309	KC1	C2D-C1D-ND	5.37	115.90	110.33
8	15	305	CLA	O2D-CGD-CBD	5.37	120.62	111.23
8	20	304	CLA	C3D-C2D-C1D	-5.37	98.50	105.83
8	21	210	CLA	C2B-C1B-NB	5.37	115.89	110.33
9	15	306	KC1	C2D-C1D-ND	5.37	115.89	110.33
8	13	302	CLA	C3B-C2B-C1B	-5.37	100.84	107.17
9	11	306	KC1	C1A-C2A-C3A	-5.36	102.35	107.28
8	15	308	CLA	CHD-C4C-C3C	-5.36	116.96	124.77
9	17	309	KC1	CBA-CAA-C2A	-5.36	103.95	125.45
9	12	308	KC1	C2D-C1D-ND	5.36	115.88	110.33
9	16	305	KC1	C3C-C4C-NC	5.35	115.63	109.90
9	14	309	KC1	C2D-C1D-ND	5.35	115.87	110.33
9	18	306	KC1	C3C-C4C-NC	5.35	115.63	109.90
9	14	306	KC1	C1A-C2A-C3A	-5.34	102.37	107.28
9	11	304	KC1	O2D-CGD-CBD	5.34	120.57	111.23
10	12	319	A86	O4-C38-C39	5.34	120.61	111.09
9	15	309	KC1	CBA-CAA-C2A	-5.34	104.02	125.45
10	15	319	A86	O4-C38-C39	5.34	120.60	111.09
8	11	303	CLA	C3B-C2B-C1B	-5.33	100.88	107.17
8	17	304	CLA	C2D-C1D-ND	5.33	115.40	110.13
8	13	311	CLA	CHD-C4C-C3C	-5.33	117.00	124.77
9	18	306	KC1	C2D-C1D-ND	5.33	115.85	110.33
8	21	204	CLA	C2B-C1B-NB	5.33	115.85	110.33
8	19	309	CLA	CHD-C4C-C3C	-5.33	117.01	124.77
9	20	306	KC1	CHC-C1C-C2C	-5.33	116.62	125.03
9	15	306	KC1	C2B-C1B-NB	5.32	115.39	110.13
8	17	308	CLA	CHD-C4C-C3C	-5.32	117.02	124.77
8	19	307	CLA	C2B-C1B-NB	5.32	115.84	110.33
9	14	306	KC1	C2B-C1B-NB	5.32	115.39	110.13
8	18	310	CLA	C2B-C1B-NB	5.32	115.84	110.33
8	19	310	CLA	C2C-C1C-NC	5.31	115.56	109.98
8	13	304	CLA	C2D-C1D-ND	5.31	115.39	110.13
8	21	204	CLA	CHD-C4C-C3C	-5.31	117.03	124.77
9	20	303	KC1	C1A-C2A-C3A	-5.31	102.40	107.28
8	11	301	CLA	C2B-C1B-NB	5.31	115.83	110.33
8	20	307	CLA	O2D-CGD-CBD	5.30	120.50	111.23
8	12	303	CLA	C3B-C2B-C1B	-5.30	100.92	107.17
9	12	308	KC1	O2D-CGD-CBD	5.29	120.49	111.23
8	18	310	CLA	C2C-C1C-NC	5.29	115.54	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	11	306	KC1	C2B-C1B-NB	5.29	115.36	110.13
9	17	305	KC1	C2B-C1B-NB	5.29	115.36	110.13
8	12	307	CLA	C2B-C1B-NB	5.29	115.81	110.33
8	17	304	CLA	C3B-C2B-C1B	-5.29	100.94	107.17
8	18	303	CLA	C4A-NA-C1A	-5.29	104.27	106.68
8	21	209	CLA	O2D-CGD-CBD	5.28	120.47	111.23
9	11	306	KC1	CHD-C4C-C3C	-5.28	115.49	125.23
10	14	312	A86	O4-C38-C39	5.28	120.50	111.09
8	16	309	CLA	C2B-C1B-NB	5.27	115.79	110.33
8	13	301	CLA	CHD-C4C-C3C	-5.27	117.09	124.77
9	13	305	KC1	C1A-C2A-C3A	-5.27	102.44	107.28
9	16	305	KC1	C2D-C1D-ND	5.27	115.79	110.33
9	18	304	KC1	C2D-C1D-ND	5.27	115.79	110.33
8	15	305	CLA	C2B-C1B-NB	5.27	115.79	110.33
10	17	311	A86	C4-C5-C6	-5.27	119.89	127.28
9	16	304	KC1	O2D-CGD-CBD	5.27	120.44	111.23
10	14	311	A86	C41-C32-C31	-5.27	105.76	110.47
8	16	303	CLA	CHD-C4C-C3C	-5.26	117.10	124.77
10	17	314	A86	C3-C2-C1	-5.26	119.90	127.28
10	12	319	A86	C12-C11-C13	5.26	124.53	116.00
8	13	301	CLA	C2C-C1C-NC	5.26	115.51	109.98
8	14	307	CLA	O2D-CGD-CBD	5.26	120.43	111.23
8	18	305	CLA	C2B-C1B-NB	5.26	115.78	110.33
8	11	305	CLA	C2B-C1B-NB	5.26	115.78	110.33
9	16	302	KC1	CHC-C1C-C2C	-5.26	116.73	125.03
8	17	302	CLA	C3B-C2B-C1B	-5.26	100.97	107.17
9	12	306	KC1	C3B-C2B-C1B	-5.26	102.07	107.05
9	11	302	KC1	O2D-CGD-CBD	5.25	120.41	111.23
9	16	304	KC1	C2D-C1D-ND	5.24	115.76	110.33
8	17	307	CLA	C3B-C2B-C1B	-5.24	100.99	107.17
8	11	303	CLA	CHD-C4C-C3C	-5.24	117.14	124.77
8	20	307	CLA	C2B-C1B-NB	5.24	115.76	110.33
8	17	304	CLA	C4A-NA-C1A	-5.23	104.29	106.68
9	11	302	KC1	C2D-C1D-ND	5.23	115.75	110.33
8	12	301	CLA	CHD-C4C-C3C	-5.23	117.15	124.77
8	21	205	CLA	CHD-C4C-C3C	-5.22	117.16	124.77
8	18	301	CLA	C2B-C1B-NB	5.22	115.74	110.33
9	18	304	KC1	O2D-CGD-CBD	5.22	120.36	111.23
8	19	304	CLA	O2D-CGD-CBD	5.22	120.36	111.23
8	21	206	CLA	C2B-C1B-NB	5.21	115.73	110.33
8	20	307	CLA	C3B-C2B-C1B	-5.21	101.03	107.17
10	11	313	A86	O4-C38-C39	5.21	120.38	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	20	302	CLA	C3B-C2B-C1B	-5.21	101.03	107.17
10	14	311	A86	O4-C38-C39	5.21	120.37	111.09
10	17	314	A86	O4-C38-C39	5.20	120.37	111.09
9	14	304	KC1	C2D-C1D-ND	5.20	115.72	110.33
9	11	304	KC1	C2B-C1B-NB	5.20	115.27	110.13
10	15	315	A86	C4-C5-C6	-5.20	119.99	127.28
9	18	306	KC1	C2B-C1B-NB	5.19	115.27	110.13
9	20	305	KC1	C2B-C1B-NB	5.19	115.27	110.13
8	15	303	CLA	C2B-C1B-NB	5.19	115.71	110.33
8	21	202	CLA	O2D-CGD-CBD	5.19	120.31	111.23
8	21	204	CLA	CAA-C2A-C3A	-5.19	98.97	113.00
8	20	310	CLA	C2D-C1D-ND	5.19	115.26	110.13
10	13	314	A86	C3-C2-C1	-5.19	120.00	127.28
8	13	309	CLA	C2C-C1C-NC	5.19	115.43	109.98
10	13	313	A86	O4-C38-C39	5.18	120.33	111.09
8	13	309	CLA	CHD-C4C-C3C	-5.18	117.22	124.77
8	11	305	CLA	O2D-CGD-CBD	5.18	120.29	111.23
8	13	304	CLA	CHD-C4C-C3C	-5.18	117.22	124.77
9	17	303	KC1	O2D-CGD-CBD	5.18	120.28	111.23
9	18	309	KC1	C2D-C1D-ND	5.18	115.69	110.33
10	17	313	A86	O4-C38-C39	5.17	120.32	111.09
10	15	312	A86	O4-C38-C39	5.17	120.31	111.09
8	19	310	CLA	C3B-C2B-C1B	-5.17	101.07	107.17
8	19	309	CLA	C2D-C1D-ND	5.17	115.24	110.13
9	13	307	KC1	O2D-CGD-CBD	5.17	120.27	111.23
10	18	313	A86	O4-C38-C39	5.17	120.31	111.09
9	13	303	KC1	C3B-C2B-C1B	-5.17	102.16	107.05
8	16	301	CLA	C3B-C2B-C1B	-5.17	101.08	107.17
8	21	202	CLA	CHD-C4C-C3C	-5.17	117.24	124.77
9	15	302	KC1	C2B-C1B-NB	5.16	115.23	110.13
10	11	311	A86	O4-C38-C39	5.16	120.29	111.09
8	17	304	CLA	CHD-C4C-C3C	-5.16	117.25	124.77
8	14	305	CLA	C2B-C1B-NB	5.16	115.67	110.33
9	15	302	KC1	C2D-C1D-ND	5.16	115.67	110.33
9	13	305	KC1	C2B-C1B-NB	5.16	115.23	110.13
9	16	302	KC1	C2B-C1B-NB	5.16	115.23	110.13
8	12	301	CLA	C2B-C1B-NB	5.15	115.67	110.33
8	12	304	CLA	C2C-C1C-NC	5.15	115.39	109.98
8	21	202	CLA	C2C-C1C-NC	5.15	115.39	109.98
9	16	308	KC1	C2D-C1D-ND	5.15	115.66	110.33
10	14	311	A86	C25-C26-C27	-5.15	120.06	127.28
9	17	306	KC1	CMA-C3A-C2A	-5.14	115.98	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	21	210	CLA	C3B-C2B-C1B	-5.14	101.11	107.17
8	17	304	CLA	CAA-C2A-C3A	-5.14	99.10	113.00
9	12	310	KC1	C2D-C1D-ND	5.14	115.66	110.33
8	19	309	CLA	C2B-C1B-NB	5.14	115.66	110.33
9	21	203	KC1	CMA-C3A-C2A	-5.14	116.00	128.43
10	17	316	A86	O4-C38-C39	5.14	120.25	111.09
8	13	306	CLA	O2D-CGD-CBD	5.14	120.21	111.23
10	12	315	A86	O4-C38-C39	5.13	120.24	111.09
8	14	310	CLA	C2B-C1B-NB	5.13	115.65	110.33
10	13	315	A86	O4-C38-C39	5.13	120.24	111.09
10	18	314	A86	O4-C38-C39	5.13	120.23	111.09
8	20	309	CLA	C2C-C1C-NC	5.13	115.37	109.98
8	15	303	CLA	C4A-NA-C1A	-5.13	104.34	106.68
9	12	306	KC1	C2B-C1B-NB	5.12	115.20	110.13
8	14	302	CLA	C2B-C1B-NB	5.12	115.64	110.33
8	16	309	CLA	O2D-CGD-CBD	5.12	120.18	111.23
8	12	304	CLA	O2D-CGD-CBD	5.12	120.18	111.23
8	18	310	CLA	CHD-C4C-C3C	-5.12	117.31	124.77
9	17	306	KC1	C3C-C4C-NC	5.12	115.38	109.90
10	20	313	A86	C25-C26-C27	-5.12	120.10	127.28
8	11	309	CLA	C2B-C1B-NB	5.11	115.63	110.33
10	20	301	A86	O4-C38-C39	5.11	120.20	111.09
10	15	311	A86	C3-C4-C5	-5.11	113.06	123.52
8	11	303	CLA	C2B-C1B-NB	5.11	115.62	110.33
8	13	304	CLA	C2B-C1B-NB	5.11	115.62	110.33
8	21	208	CLA	CHD-C4C-C3C	-5.11	117.33	124.77
9	16	302	KC1	C2D-C1D-ND	5.10	115.62	110.33
9	14	309	KC1	CHD-C4C-C3C	-5.10	115.82	125.23
8	16	306	CLA	C4A-NA-C1A	-5.10	104.35	106.68
8	19	304	CLA	C3B-C2B-C1B	-5.10	101.16	107.17
8	12	305	CLA	C3B-C2B-C1B	-5.10	101.16	107.17
9	17	303	KC1	C2D-C1D-ND	5.09	115.61	110.33
13	16	312	DD6	C15-C14-C13	-5.09	115.22	125.99
8	19	304	CLA	C2B-C1B-NB	5.09	115.61	110.33
8	18	302	CLA	O2D-CGD-CBD	5.09	120.13	111.23
8	13	311	CLA	C3B-C2B-C1B	-5.09	101.17	107.17
8	19	307	CLA	C2C-C1C-NC	5.09	115.33	109.98
10	11	314	A86	C12-C11-C13	5.09	124.25	116.00
8	17	310	CLA	C2B-C1B-NB	5.09	115.60	110.33
8	20	309	CLA	C3B-C2B-C1B	-5.09	101.17	107.17
10	21	211	A86	C41-C32-C31	-5.08	105.92	110.47
9	17	303	KC1	CHC-C1C-C2C	-5.08	117.01	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	19	312	DD6	C21-C20-C15	-5.08	113.94	122.30
8	12	307	CLA	O2D-CGD-CBD	5.08	120.11	111.23
10	21	211	A86	C3-C2-C1	-5.08	120.16	127.28
8	16	303	CLA	CAA-C2A-C3A	-5.08	99.28	113.00
9	16	305	KC1	CHD-C4C-C3C	-5.07	115.87	125.23
8	21	209	CLA	C2B-C1B-NB	5.06	115.58	110.33
9	12	308	KC1	C3C-C4C-NC	5.06	115.33	109.90
10	13	314	A86	C25-C26-C27	-5.06	120.18	127.28
8	19	310	CLA	C2B-C1B-NB	5.06	115.58	110.33
8	13	304	CLA	C2C-C1C-NC	5.06	115.30	109.98
8	17	310	CLA	C4A-NA-C1A	-5.06	104.37	106.68
10	14	313	A86	C41-C32-C31	-5.06	105.94	110.47
8	20	302	CLA	O2D-CGD-CBD	5.06	120.08	111.23
9	11	302	KC1	CMA-C3A-C2A	-5.06	116.19	128.43
8	17	302	CLA	C2B-C1B-NB	5.06	115.57	110.33
8	17	308	CLA	C2B-C1B-NB	5.06	115.57	110.33
9	12	308	KC1	CHD-C4C-C3C	-5.06	115.91	125.23
10	12	302	A86	C33-C32-C31	5.05	114.12	109.21
10	11	312	A86	C36-C31-C32	-5.05	114.68	119.70
9	19	308	KC1	CHD-C4C-C3C	-5.05	115.91	125.23
9	14	304	KC1	O2D-CGD-CBD	5.05	120.06	111.23
8	11	301	CLA	C3B-C2B-C1B	-5.05	101.22	107.17
8	14	301	CLA	C3B-C2B-C1B	-5.05	101.22	107.17
8	18	310	CLA	C3B-C2B-C1B	-5.05	101.22	107.17
10	12	313	A86	O4-C38-C39	5.05	120.09	111.09
13	16	312	DD6	C7-C6-C8	-5.05	110.38	118.09
10	21	214	A86	O4-C38-C39	5.04	120.08	111.09
9	12	308	KC1	C2B-C1B-NB	5.04	115.12	110.13
9	17	305	KC1	O2D-CGD-CBD	5.04	120.04	111.23
8	13	304	CLA	C4A-NA-C1A	-5.04	104.38	106.68
8	20	308	CLA	C2B-C1B-NB	5.04	115.55	110.33
8	14	302	CLA	C3B-C2B-C1B	-5.03	101.24	107.17
8	21	205	CLA	C3D-C2D-C1D	-5.03	98.96	105.83
9	14	306	KC1	C3C-C4C-NC	5.03	115.29	109.90
9	15	306	KC1	CHD-C4C-C3C	-5.03	115.96	125.23
8	11	303	CLA	C2C-C1C-NC	5.03	115.26	109.98
8	13	306	CLA	C3B-C2B-C1B	-5.02	101.25	107.17
8	12	307	CLA	C3B-C2B-C1B	-5.02	101.25	107.17
8	15	307	CLA	C3B-C2B-C1B	-5.02	101.25	107.17
9	16	305	KC1	CMA-C3A-C2A	-5.02	116.28	128.43
9	17	306	KC1	C2D-C1D-ND	5.02	115.53	110.33
8	15	310	CLA	C3B-C2B-C1B	-5.01	101.26	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	11	308	KC1	C2D-C1D-ND	5.01	115.53	110.33
10	14	314	A86	O4-C38-C39	5.01	120.03	111.09
10	20	311	A86	O4-C38-C39	5.01	120.02	111.09
9	11	304	KC1	C2D-C1D-ND	5.01	115.52	110.33
13	19	312	DD6	C-C1-C24	-5.01	110.44	118.09
8	21	202	CLA	C2B-C1B-NB	5.01	115.52	110.33
9	15	302	KC1	O2D-CGD-CBD	5.01	119.98	111.23
8	15	301	CLA	C3B-C2B-C1B	-5.00	101.27	107.17
8	13	311	CLA	C2C-C1C-NC	5.00	115.24	109.98
8	18	301	CLA	C3D-C2D-C1D	-5.00	99.00	105.83
8	18	308	CLA	C2C-C1C-NC	5.00	115.24	109.98
10	15	314	A86	O4-C38-C39	5.00	120.00	111.09
9	14	306	KC1	CHD-C4C-C3C	-5.00	116.02	125.23
8	20	302	CLA	C2B-C1B-NB	4.99	115.50	110.33
9	13	303	KC1	C2D-C1D-ND	4.99	115.50	110.33
10	16	313	A86	C25-C26-C27	-4.99	120.28	127.28
8	14	301	CLA	C2B-C1B-NB	4.99	115.50	110.33
8	21	205	CLA	C2B-C1B-NB	4.99	115.50	110.33
9	15	304	KC1	C2D-C1D-ND	4.99	115.50	110.33
8	21	206	CLA	C3B-C2B-C1B	-4.99	101.29	107.17
8	12	305	CLA	C2B-C1B-NB	4.99	115.50	110.33
9	13	305	KC1	CHD-C4C-C3C	-4.99	116.03	125.23
9	13	305	KC1	O2D-CGD-CBD	4.99	119.95	111.23
10	21	215	A86	C36-C31-C32	-4.98	114.75	119.70
13	21	216	DD6	C24-C1-C2	-4.98	111.17	119.01
8	11	305	CLA	C3B-C2B-C1B	-4.98	101.30	107.17
8	18	303	CLA	CAA-C2A-C3A	-4.98	99.55	113.00
9	15	304	KC1	O2D-CGD-CBD	4.98	119.93	111.23
9	17	305	KC1	C2D-C1D-ND	4.97	115.48	110.33
8	21	205	CLA	C3B-C2B-C1B	-4.97	101.31	107.17
10	21	213	A86	O4-C38-C39	4.97	119.95	111.09
8	21	208	CLA	C3B-C2B-C1B	-4.97	101.31	107.17
9	17	305	KC1	CMA-C3A-C2A	-4.97	116.41	128.43
10	13	312	A86	O4-C38-C39	4.97	119.94	111.09
8	12	311	CLA	C3B-C2B-C1B	-4.96	101.32	107.17
9	11	306	KC1	C3C-C4C-NC	4.96	115.22	109.90
8	11	307	CLA	C2C-C1C-NC	4.96	115.19	109.98
8	21	206	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
10	12	315	A86	C40-C32-C31	-4.96	106.03	110.47
8	20	310	CLA	C2B-C1B-NB	4.96	115.47	110.33
10	12	314	A86	O4-C38-C39	4.96	119.93	111.09
8	14	302	CLA	O2D-CGD-CBD	4.96	119.90	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	19	309	CLA	O2D-CGD-CBD	4.95	119.88	111.23
9	21	203	KC1	C1A-NA-C4A	-4.95	104.42	106.68
9	17	303	KC1	CBC-CAC-C3C	-4.94	99.02	112.42
13	19	312	DD6	C7-C6-C8	-4.94	110.53	118.09
8	15	305	CLA	C3B-C2B-C1B	-4.94	101.34	107.17
8	19	301	CLA	C2B-C1B-NB	4.94	115.45	110.33
8	16	301	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
9	20	306	KC1	C2C-C1C-NC	4.94	116.56	110.45
10	20	311	A86	C25-C26-C27	-4.94	120.36	127.28
9	11	308	KC1	CHC-C1C-C2C	-4.94	117.24	125.03
9	20	305	KC1	C2D-C1D-ND	4.93	115.44	110.33
8	20	304	CLA	C4A-NA-C1A	-4.93	104.43	106.68
8	19	304	CLA	CAC-C3C-C4C	4.93	131.21	124.79
8	14	305	CLA	C2C-C1C-NC	4.93	115.16	109.98
9	13	305	KC1	C3C-C4C-NC	4.93	115.18	109.90
9	18	306	KC1	CHD-C4C-C3C	-4.93	116.14	125.23
10	20	313	A86	O4-C38-C39	4.93	119.88	111.09
10	18	311	A86	O4-C38-C39	4.93	119.87	111.09
8	13	308	CLA	C2C-C1C-NC	4.93	115.16	109.98
8	18	302	CLA	C3B-C2B-C1B	-4.92	101.37	107.17
8	16	303	CLA	C2B-C1B-NB	4.92	115.43	110.33
9	21	207	KC1	CHD-C4C-C3C	-4.92	116.15	125.23
8	19	309	CLA	C3B-C2B-C1B	-4.92	101.37	107.17
8	18	301	CLA	C3B-C2B-C1B	-4.92	101.37	107.17
10	20	301	A86	C10-C9-C8	-4.92	108.95	123.20
10	15	319	A86	C3-C2-C1	-4.92	120.38	127.28
10	13	316	A86	C3-C2-C1	-4.92	120.38	127.28
8	15	308	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
13	21	212	DD6	C-C1-C24	-4.91	110.58	118.09
10	18	312	A86	C3-C2-C1	-4.91	120.39	127.28
9	11	308	KC1	C1A-C2A-C3A	-4.91	102.77	107.28
8	18	302	CLA	C2C-C1C-NC	4.91	115.14	109.98
8	15	307	CLA	C4A-NA-C1A	-4.91	104.44	106.68
9	17	306	KC1	C3B-C2B-C1B	-4.91	102.40	107.05
8	19	301	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
8	19	306	CLA	C2B-C1B-NB	4.91	115.42	110.33
8	14	310	CLA	C2C-C1C-NC	4.91	115.14	109.98
8	21	205	CLA	C2C-C1C-NC	4.91	115.14	109.98
9	18	309	KC1	CMA-C3A-C2A	-4.90	116.56	128.43
8	21	210	CLA	C4A-NA-C1A	-4.90	104.44	106.68
8	16	303	CLA	C2C-C1C-NC	4.90	115.13	109.98
8	18	307	CLA	O2D-CGD-CBD	4.90	119.80	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	15	309	KC1	CHD-C4C-C3C	-4.90	116.19	125.23
13	19	312	DD6	C12-C11-C13	-4.90	110.60	118.09
8	14	301	CLA	C3D-C2D-C1D	-4.90	99.15	105.83
9	15	309	KC1	C3C-C4C-NC	4.90	115.14	109.90
10	13	314	A86	C41-C32-C31	-4.89	106.09	110.47
8	16	303	CLA	C3B-C2B-C1B	-4.89	101.41	107.17
8	18	307	CLA	C3B-C2B-C1B	-4.89	101.41	107.17
8	18	307	CLA	C2C-C1C-NC	4.88	115.11	109.98
8	18	307	CLA	C2B-C1B-NB	4.88	115.39	110.33
8	13	304	CLA	CAA-C2A-C3A	-4.88	99.82	113.00
8	20	309	CLA	C2B-C1B-NB	4.88	115.38	110.33
10	15	319	A86	C4-C5-C6	-4.87	120.44	127.28
9	13	310	KC1	C2D-C1D-ND	4.87	115.38	110.33
10	16	310	A86	O4-C38-C39	4.87	119.78	111.09
10	17	315	A86	O4-C38-C39	4.87	119.78	111.09
9	21	207	KC1	C3D-C4D-ND	4.87	116.99	110.20
8	14	303	CLA	C2C-C1C-NC	4.87	115.10	109.98
8	19	305	CLA	C2C-C1C-NC	4.87	115.10	109.98
8	19	305	CLA	C3D-C2D-C1D	-4.87	99.19	105.83
8	15	301	CLA	C3D-C2D-C1D	-4.87	99.19	105.83
8	13	311	CLA	C4A-NA-C1A	-4.86	104.46	106.68
8	18	305	CLA	C2C-C1C-NC	4.86	115.09	109.98
8	14	305	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
8	20	310	CLA	C2C-C1C-NC	4.86	115.09	109.98
9	20	305	KC1	CHC-C1C-C2C	-4.86	117.36	125.03
8	17	310	CLA	C3B-C2B-C1B	-4.86	101.45	107.17
8	12	304	CLA	C2B-C1B-NB	4.85	115.36	110.33
9	14	304	KC1	C1A-NA-C4A	-4.85	104.47	106.68
8	18	308	CLA	C2B-C1B-NB	4.85	115.36	110.33
8	11	305	CLA	C2C-C1C-NC	4.85	115.08	109.98
9	15	306	KC1	C3C-C4C-NC	4.85	115.10	109.90
9	12	310	KC1	CHD-C4C-C3C	-4.85	116.28	125.23
8	17	304	CLA	C2C-C1C-NC	4.85	115.08	109.98
8	11	309	CLA	C3B-C2B-C1B	-4.85	101.46	107.17
8	14	310	CLA	C3B-C2B-C1B	-4.84	101.46	107.17
10	16	313	A86	C33-C32-C31	4.84	113.92	109.21
8	12	309	CLA	C4A-NA-C1A	-4.84	104.47	106.68
10	15	313	A86	O4-C38-C39	4.84	119.72	111.09
9	20	303	KC1	CHD-C4C-C3C	-4.84	116.30	125.23
8	20	310	CLA	O2D-CGD-CBD	4.84	119.69	111.23
10	13	312	A86	C41-C32-C31	-4.84	106.14	110.47
8	16	309	CLA	C3B-C2B-C1B	-4.84	101.47	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	18	303	CLA	C3B-C2B-C1B	-4.83	101.47	107.17
8	18	305	CLA	C3B-C2B-C1B	-4.83	101.47	107.17
9	21	203	KC1	C2D-C1D-ND	4.83	115.34	110.33
8	20	309	CLA	O2D-CGD-CBD	4.83	119.67	111.23
9	11	304	KC1	CHC-C1C-C2C	-4.83	117.41	125.03
10	17	313	A86	C3-C2-C1	-4.83	120.51	127.28
8	16	306	CLA	O2D-CGD-CBD	4.82	119.65	111.23
8	20	308	CLA	C3B-C2B-C1B	-4.81	101.49	107.17
8	20	304	CLA	C3B-C2B-C1B	-4.81	101.50	107.17
9	16	304	KC1	C3C-C4C-NC	4.81	115.05	109.90
9	16	304	KC1	CHD-C4C-C3C	-4.81	116.36	125.23
8	19	305	CLA	C3B-C2B-C1B	-4.81	101.50	107.17
9	13	307	KC1	CHD-C4C-C3C	-4.81	116.37	125.23
8	15	310	CLA	C2C-C1C-NC	4.80	115.03	109.98
8	14	302	CLA	C2C-C1C-NC	4.80	115.03	109.98
8	18	307	CLA	C4A-NA-C1A	-4.80	104.49	106.68
8	14	310	CLA	O2D-CGD-CBD	4.80	119.62	111.23
8	12	301	CLA	C2C-C1C-NC	4.80	115.02	109.98
10	14	314	A86	C25-C26-C27	-4.80	120.55	127.28
8	16	307	CLA	C2B-C1B-NB	4.79	115.30	110.33
9	14	309	KC1	C3C-C4C-NC	4.79	115.03	109.90
8	12	305	CLA	C4A-NA-C1A	-4.79	104.49	106.68
8	21	204	CLA	C4A-NA-C1A	-4.79	104.49	106.68
8	20	308	CLA	O2D-CGD-CBD	4.78	119.59	111.23
9	20	303	KC1	O2D-CGD-CBD	4.78	119.59	111.23
8	19	306	CLA	C3B-C2B-C1B	-4.78	101.53	107.17
9	16	308	KC1	CHC-C1C-C2C	-4.78	117.48	125.03
13	20	312	DD6	C21-C20-C19	-4.78	108.87	114.24
9	19	308	KC1	C3C-C4C-NC	4.78	115.02	109.90
10	15	313	A86	C3-C2-C1	-4.78	120.58	127.28
9	11	302	KC1	CHD-C4C-C3C	-4.77	116.42	125.23
8	15	303	CLA	CAA-C2A-C3A	-4.77	100.10	113.00
8	19	304	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
8	21	204	CLA	C2C-C1C-NC	4.77	114.99	109.98
9	17	309	KC1	CHD-C4C-C3C	-4.77	116.44	125.23
9	17	306	KC1	C4B-C3B-C2B	-4.77	102.68	106.81
9	16	302	KC1	C3B-C2B-C1B	-4.77	102.53	107.05
9	18	309	KC1	CHC-C1C-C2C	-4.77	117.50	125.03
13	20	312	DD6	C25-C24-C1	-4.76	113.31	126.36
8	12	305	CLA	CAA-C2A-C3A	-4.76	100.14	113.00
8	19	307	CLA	C3D-C2D-C1D	-4.76	99.34	105.83
8	15	305	CLA	C2C-C1C-NC	4.76	114.98	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	12	310	KC1	C3C-C4C-NC	4.75	114.99	109.90
8	15	303	CLA	C2C-C1C-NC	4.75	114.97	109.98
8	11	309	CLA	C2C-C1C-NC	4.75	114.97	109.98
8	16	301	CLA	C2B-C1B-NB	4.75	115.25	110.33
9	14	304	KC1	CHD-C4C-C3C	-4.75	116.47	125.23
9	17	306	KC1	C2C-C1C-NC	4.75	116.33	110.45
8	20	310	CLA	C4A-NA-C1A	-4.75	104.51	106.68
9	19	308	KC1	C3D-C4D-ND	4.75	116.82	110.20
13	21	216	DD6	C21-C20-C19	-4.74	108.91	114.24
10	12	312	A86	O4-C38-C39	4.74	119.55	111.09
8	11	303	CLA	C4A-NA-C1A	-4.74	104.52	106.68
10	13	312	A86	C25-C26-C27	-4.74	120.63	127.28
8	16	306	CLA	C2B-C1B-NB	4.73	115.23	110.33
8	11	301	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
8	17	308	CLA	C3B-C2B-C1B	-4.73	101.60	107.17
8	20	308	CLA	C2C-C1C-NC	4.73	114.95	109.98
8	13	301	CLA	C2B-C1B-NB	4.73	115.23	110.33
8	20	310	CLA	C3B-C2B-C1B	-4.73	101.60	107.17
8	21	209	CLA	C2C-C1C-NC	4.73	114.94	109.98
9	21	207	KC1	C3C-C4C-NC	4.72	114.96	109.90
8	19	309	CLA	C2C-C1C-NC	4.72	114.94	109.98
8	17	308	CLA	C2C-C1C-NC	4.72	114.94	109.98
8	21	208	CLA	C2C-C1C-NC	4.72	114.94	109.98
10	18	312	A86	O4-C38-C39	4.72	119.51	111.09
8	11	301	CLA	O2D-CGD-CBD	4.72	119.47	111.23
8	19	302	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
8	14	302	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
9	13	310	KC1	CHC-C1C-C2C	-4.71	117.59	125.03
8	11	303	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
8	15	307	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
8	13	302	CLA	C3D-C2D-C1D	-4.70	99.41	105.83
8	20	307	CLA	C4A-NA-C1A	-4.70	104.53	106.68
8	21	209	CLA	C3B-C2B-C1B	-4.70	101.63	107.17
9	18	309	KC1	CHD-C4C-C3C	-4.70	116.56	125.23
10	11	312	A86	C4-C5-C6	-4.70	120.69	127.28
10	12	314	A86	C4-C5-C6	-4.70	120.69	127.28
9	17	305	KC1	C3D-C4D-ND	4.70	116.75	110.20
9	21	203	KC1	C3C-C4C-NC	4.70	114.93	109.90
8	21	202	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
9	14	304	KC1	C3D-C4D-ND	4.70	116.75	110.20
8	19	301	CLA	C3B-C2B-C1B	-4.70	101.63	107.17
9	13	303	KC1	CHC-C1C-C2C	-4.69	117.62	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	18	304	KC1	C3D-C4D-ND	4.69	116.74	110.20
10	20	301	A86	C28-C27-C26	-4.68	115.23	122.82
9	21	207	KC1	C1A-NA-C4A	-4.68	104.54	106.68
8	12	304	CLA	C3D-C2D-C1D	-4.68	99.45	105.83
8	16	303	CLA	C4A-NA-C1A	-4.68	104.55	106.68
8	19	307	CLA	C3B-C2B-C1B	-4.67	101.66	107.17
8	11	307	CLA	C3D-C2D-C1D	-4.67	99.45	105.83
8	20	302	CLA	C3D-C4D-ND	4.67	117.58	109.99
8	13	306	CLA	C2C-C1C-NC	4.67	114.89	109.98
8	16	309	CLA	C2C-C1C-NC	4.67	114.89	109.98
8	15	301	CLA	C3D-C4D-ND	4.67	117.58	109.99
8	20	302	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
9	16	308	KC1	C3C-C4C-NC	4.67	114.90	109.90
10	21	214	A86	C3-C2-C1	-4.67	120.73	127.28
8	16	309	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
8	21	202	CLA	C3B-C2B-C1B	-4.66	101.67	107.17
9	18	309	KC1	C3C-C4C-NC	4.66	114.90	109.90
9	15	304	KC1	CHC-C1C-C2C	-4.66	117.67	125.03
8	15	310	CLA	C4A-NA-C1A	-4.66	104.55	106.68
8	20	302	CLA	CHD-C1D-ND	-4.66	118.25	124.80
10	17	311	A86	C25-C26-C27	-4.66	120.74	127.28
8	13	309	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
9	11	302	KC1	CHC-C1C-C2C	-4.66	117.68	125.03
8	13	301	CLA	C3B-C2B-C1B	-4.66	101.68	107.17
9	12	306	KC1	CAC-C3C-C2C	4.65	136.11	127.56
8	15	301	CLA	CHD-C1D-ND	-4.65	118.26	124.80
10	18	312	A86	C40-C32-C31	-4.65	106.31	110.47
9	16	308	KC1	CHD-C4C-C3C	-4.65	116.65	125.23
9	17	309	KC1	C1A-C2A-C3A	-4.65	103.01	107.28
13	21	216	DD6	O1-C20-C21	-4.65	109.85	115.05
9	20	306	KC1	C2D-C1D-ND	4.65	115.15	110.33
8	12	303	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
8	17	310	CLA	C2C-C1C-NC	4.65	114.86	109.98
8	12	301	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
9	15	302	KC1	CHD-C4C-C3C	-4.64	116.66	125.23
13	21	212	DD6	C12-C11-C13	-4.64	111.00	118.09
8	16	301	CLA	O2D-CGD-CBD	4.64	119.34	111.23
8	12	305	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
8	21	210	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
9	21	203	KC1	CHD-C4C-C3C	-4.64	116.68	125.23
9	13	303	KC1	O2D-CGD-CBD	4.63	119.33	111.23
9	13	310	KC1	CMA-C3A-C2A	-4.63	117.22	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	20	302	CLA	C4A-NA-C1A	-4.63	104.57	106.68
9	16	302	KC1	C4B-C3B-C2B	-4.63	102.80	106.81
8	11	303	CLA	CAA-C2A-C3A	-4.63	100.50	113.00
8	19	303	CLA	C4A-NA-C1A	-4.63	104.57	106.68
9	13	307	KC1	C3D-C4D-ND	4.62	116.65	110.20
8	19	303	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
8	19	302	CLA	C2B-C1B-NB	4.62	115.12	110.33
8	12	307	CLA	C2C-C1C-NC	4.62	114.84	109.98
8	20	309	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
8	19	309	CLA	C4A-NA-C1A	-4.62	104.57	106.68
10	17	312	A86	O4-C38-C39	4.62	119.33	111.09
9	11	304	KC1	CHD-C4C-C3C	-4.62	116.71	125.23
8	20	308	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
8	13	308	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
8	18	302	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
8	20	304	CLA	C2C-C1C-NC	4.62	114.83	109.98
8	18	308	CLA	C3B-C2B-C1B	-4.61	101.73	107.17
10	16	313	A86	C12-C11-C13	4.61	123.48	116.00
9	14	304	KC1	C3C-C4C-NC	4.61	114.84	109.90
8	13	306	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
8	11	305	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
10	12	314	A86	C25-C26-C27	-4.61	120.82	127.28
9	15	304	KC1	C3D-C4D-ND	4.61	116.62	110.20
13	21	212	DD6	C24-C1-C2	-4.61	111.76	119.01
8	19	302	CLA	O2D-CGD-O1D	-4.61	114.88	123.85
8	18	305	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
8	21	202	CLA	C3B-C4B-NB	4.60	114.64	110.53
9	15	302	KC1	C3D-C4D-ND	4.60	116.61	110.20
9	17	303	KC1	CHD-C4C-C3C	-4.59	116.76	125.23
8	12	307	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
10	15	311	A86	C3-C2-C1	-4.59	120.84	127.28
8	19	306	CLA	O2D-CGD-CBD	4.59	119.25	111.23
8	12	305	CLA	C2C-C1C-NC	4.58	114.79	109.98
8	12	311	CLA	C2C-C1C-NC	4.58	114.79	109.98
8	19	305	CLA	C2B-C1B-NB	4.58	115.08	110.33
8	11	309	CLA	C3D-C2D-C1D	-4.58	99.59	105.83
8	15	303	CLA	C3B-C2B-C1B	-4.58	101.78	107.17
8	15	308	CLA	C3B-C2B-C1B	-4.57	101.78	107.17
8	15	301	CLA	C2B-C1B-NB	4.57	115.07	110.33
10	21	213	A86	C41-C32-C31	-4.57	106.38	110.47
8	12	311	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
8	21	209	CLA	C3D-C2D-C1D	-4.57	99.60	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	21	208	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
8	14	310	CLA	C4A-NA-C1A	-4.57	104.60	106.68
9	15	302	KC1	CHC-C1C-C2C	-4.56	117.82	125.03
9	16	302	KC1	O2D-CGD-CBD	4.56	119.21	111.23
10	14	312	A86	C3-C2-C1	-4.56	120.88	127.28
8	15	305	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
8	21	210	CLA	C3D-C4D-ND	4.56	117.40	109.99
9	11	304	KC1	C3C-C4C-NC	4.56	114.78	109.90
8	19	302	CLA	C2C-C1C-NC	4.56	114.77	109.98
8	18	307	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
8	17	308	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
8	14	305	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
9	18	304	KC1	C3C-C4C-NC	4.56	114.78	109.90
9	13	303	KC1	C3D-C4D-ND	4.55	116.55	110.20
8	15	308	CLA	C2B-C1B-NB	4.55	115.05	110.33
8	13	302	CLA	O2D-CGD-CBD	4.55	119.18	111.23
8	18	308	CLA	C3D-C2D-C1D	-4.55	99.63	105.83
8	19	302	CLA	C3B-C2B-C1B	-4.55	101.81	107.17
8	14	301	CLA	O2D-CGD-CBD	4.55	119.18	111.23
10	15	315	A86	C25-C26-C27	-4.55	120.90	127.28
10	18	313	A86	C25-C26-C27	-4.54	120.91	127.28
9	17	306	KC1	C2B-C1B-NB	4.54	114.61	110.13
8	12	309	CLA	C3D-C2D-C1D	-4.53	99.64	105.83
8	19	310	CLA	O2D-CGD-CBD	4.53	119.16	111.23
8	20	307	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
9	20	305	KC1	C3D-C4D-ND	4.53	116.52	110.20
8	17	307	CLA	C2C-C1C-NC	4.53	114.74	109.98
8	17	307	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
8	13	311	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
8	14	308	CLA	C2B-C1B-NB	4.52	115.01	110.33
8	19	303	CLA	C3D-C4D-ND	4.52	117.33	109.99
9	19	308	KC1	C1A-NA-C4A	-4.52	104.62	106.68
8	12	307	CLA	C3D-C4D-ND	4.52	117.33	109.99
9	15	304	KC1	CHD-C4C-C3C	-4.52	116.90	125.23
9	18	309	KC1	C1A-C2A-C3A	-4.51	103.13	107.28
8	12	311	CLA	C4A-NA-C1A	-4.51	104.62	106.68
8	19	301	CLA	O2D-CGD-CBD	4.51	119.12	111.23
9	11	302	KC1	C3C-C4C-NC	4.51	114.73	109.90
10	21	211	A86	C25-C26-C27	-4.51	120.95	127.28
9	18	304	KC1	CHD-C4C-C3C	-4.51	116.91	125.23
9	17	305	KC1	CHC-C1C-C2C	-4.51	117.91	125.03
8	19	303	CLA	C3B-C2B-C1B	-4.51	101.86	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	15	319	A86	C33-C32-C31	4.51	113.59	109.21
10	20	313	A86	C3-C2-C1	-4.51	120.96	127.28
8	16	307	CLA	C2C-C1C-NC	4.51	114.71	109.98
8	21	210	CLA	C2C-C1C-NC	4.50	114.71	109.98
8	17	304	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
10	17	314	A86	C40-C32-C31	-4.50	106.44	110.47
8	14	303	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
8	15	301	CLA	O2D-CGD-CBD	4.50	119.09	111.23
8	21	209	CLA	C4A-NA-C1A	-4.50	104.63	106.68
8	13	309	CLA	C2B-C1B-NB	4.49	114.99	110.33
9	19	308	KC1	C2A-C1A-NA	4.49	116.54	109.34
9	17	306	KC1	CHD-C4C-C3C	-4.49	116.94	125.23
8	21	204	CLA	C3D-C4D-ND	4.49	117.29	109.99
8	13	309	CLA	C3B-C2B-C1B	-4.49	101.87	107.17
9	13	303	KC1	C4B-C3B-C2B	-4.49	102.92	106.81
9	21	203	KC1	C4B-C3B-C2B	-4.49	102.92	106.81
8	15	303	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
9	16	304	KC1	C3D-C4D-ND	4.49	116.46	110.20
10	11	312	A86	C41-C32-C31	-4.49	106.45	110.47
8	19	306	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
8	17	302	CLA	C3D-C4D-ND	4.49	117.28	109.99
8	13	301	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
8	19	306	CLA	C3D-C4D-ND	4.49	117.28	109.99
9	13	307	KC1	C3C-C4C-NC	4.48	114.70	109.90
10	21	215	A86	C4-C5-C6	-4.48	120.99	127.28
8	21	204	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
9	16	302	KC1	CHD-C4C-C3C	-4.48	116.96	125.23
8	20	304	CLA	C2B-C1B-NB	4.48	114.97	110.33
8	19	304	CLA	C4A-NA-C1A	-4.47	104.64	106.68
8	15	305	CLA	C4A-NA-C1A	-4.47	104.64	106.68
8	20	302	CLA	C2C-C1C-NC	4.47	114.67	109.98
9	15	306	KC1	C3D-C4D-ND	4.47	116.43	110.20
8	12	303	CLA	O2D-CGD-CBD	4.46	119.03	111.23
9	17	309	KC1	C3D-C4D-ND	4.46	116.42	110.20
8	14	310	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
9	13	305	KC1	CHC-C1C-C2C	-4.46	117.98	125.03
9	11	308	KC1	CHD-C4C-C3C	-4.46	117.00	125.23
10	14	313	A86	C3-C2-C1	-4.46	121.02	127.28
8	20	308	CLA	C4A-NA-C1A	-4.46	104.64	106.68
9	20	303	KC1	C3D-C4D-ND	4.46	116.42	110.20
8	17	302	CLA	C2C-C1C-NC	4.46	114.66	109.98
8	17	310	CLA	C3D-C2D-C1D	-4.46	99.75	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	13	305	KC1	C3D-C4D-ND	4.45	116.41	110.20
10	13	313	A86	C36-C31-C32	-4.45	115.28	119.70
9	16	305	KC1	CHC-C1C-C2C	-4.45	118.00	125.03
8	21	208	CLA	O2D-CGD-CBD	4.45	119.01	111.23
8	21	204	CLA	CHD-C1D-ND	-4.45	118.54	124.80
9	17	303	KC1	C1C-C2C-C3C	-4.45	102.30	106.98
9	13	310	KC1	CHD-C4C-C3C	-4.45	117.03	125.23
8	19	303	CLA	C2B-C1B-NB	4.45	114.94	110.33
10	18	312	A86	C23-C16-C22	-4.45	100.91	107.37
9	13	303	KC1	C1A-NA-C4A	-4.45	104.65	106.68
8	17	302	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
9	16	304	KC1	CHC-C1C-C2C	-4.44	118.02	125.03
9	12	306	KC1	C3D-C4D-ND	4.44	116.39	110.20
8	15	310	CLA	C3D-C2D-C1D	-4.44	99.78	105.83
8	13	304	CLA	C3D-C2D-C1D	-4.44	99.78	105.83
9	17	309	KC1	CHC-C1C-C2C	-4.43	118.03	125.03
9	15	302	KC1	C3C-C4C-NC	4.43	114.65	109.90
15	17	317	LHG	O4-P-O5	4.43	133.06	112.44
8	19	310	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
9	20	305	KC1	CBA-CAA-C2A	-4.43	107.68	125.45
8	18	310	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
10	17	314	A86	C41-C32-C31	-4.42	106.51	110.47
8	16	303	CLA	C3D-C4D-ND	4.42	117.18	109.99
9	11	308	KC1	C3C-C4C-NC	4.42	114.64	109.90
8	16	303	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
10	15	315	A86	C3-C2-C1	-4.42	121.08	127.28
10	19	313	A86	C36-C31-C32	-4.42	115.31	119.70
10	14	316	A86	C25-C26-C27	-4.42	121.09	127.28
8	14	308	CLA	C3B-C2B-C1B	-4.42	101.97	107.17
8	19	304	CLA	CHD-C4C-C3C	-4.41	118.34	124.77
9	18	306	KC1	CHC-C1C-C2C	-4.41	118.06	125.03
15	21	217	LHG	O4-P-O5	4.41	132.97	112.44
9	18	304	KC1	CHC-C1C-C2C	-4.41	118.06	125.03
8	17	302	CLA	CHD-C1D-ND	-4.41	118.59	124.80
10	12	302	A86	O4-C38-C39	4.41	118.95	111.09
9	20	303	KC1	CHC-C1C-C2C	-4.41	118.07	125.03
8	19	304	CLA	C2C-C1C-NC	4.41	114.61	109.98
8	16	301	CLA	C3D-C4D-ND	4.41	117.15	109.99
9	13	303	KC1	CHD-C4C-C3C	-4.40	117.11	125.23
10	21	214	A86	C4-C5-C6	-4.40	121.11	127.28
8	12	301	CLA	C3B-C2B-C1B	-4.40	101.99	107.17
9	18	309	KC1	C3D-C4D-ND	4.40	116.33	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	17	309	KC1	C3C-C4C-NC	4.40	114.61	109.90
8	19	304	CLA	C3D-C4D-ND	4.39	117.13	109.99
10	18	312	A86	C36-C31-C32	-4.39	115.34	119.70
13	21	216	DD6	C15-C14-C13	4.39	135.27	125.99
8	13	311	CLA	C3D-C4D-ND	4.39	117.12	109.99
9	14	304	KC1	CHC-C1C-C2C	-4.38	118.11	125.03
9	20	305	KC1	CHD-C4C-C3C	-4.38	117.15	125.23
8	16	307	CLA	C3D-C4D-ND	4.38	117.11	109.99
8	15	301	CLA	C2C-C1C-NC	4.38	114.58	109.98
9	15	304	KC1	C1A-NA-C4A	-4.38	104.68	106.68
8	12	304	CLA	C3B-C2B-C1B	-4.38	102.01	107.17
8	17	302	CLA	O2D-CGD-CBD	4.38	118.88	111.23
8	12	307	CLA	CHD-C1D-ND	-4.38	118.64	124.80
9	16	302	KC1	C2C-C1C-NC	4.38	115.87	110.45
9	11	302	KC1	C3D-C4D-ND	4.38	116.30	110.20
8	21	206	CLA	CHD-C1D-ND	-4.38	118.64	124.80
8	12	307	CLA	C4A-NA-C1A	-4.38	104.68	106.68
9	12	308	KC1	C3D-C4D-ND	4.37	116.30	110.20
8	15	303	CLA	C3D-C4D-ND	4.37	117.09	109.99
9	13	310	KC1	C3D-C4D-ND	4.37	116.29	110.20
9	13	307	KC1	CHC-C1C-C2C	-4.37	118.13	125.03
8	18	310	CLA	C3D-C4D-ND	4.37	117.08	109.99
15	21	201	LHG	O4-P-O5	4.37	132.76	112.44
8	17	304	CLA	CHD-C1D-ND	-4.37	118.66	124.80
10	11	314	A86	C4-C5-C6	-4.36	121.16	127.28
9	15	309	KC1	CHC-C1C-C2C	-4.36	118.15	125.03
8	19	309	CLA	C3D-C4D-ND	4.35	117.06	109.99
8	14	308	CLA	C3D-C2D-C1D	-4.34	99.90	105.83
8	19	305	CLA	C3D-C4D-ND	4.34	117.05	109.99
8	12	309	CLA	C2C-C1C-NC	4.34	114.54	109.98
8	11	309	CLA	C3D-C4D-ND	4.34	117.04	109.99
8	16	307	CLA	C3B-C2B-C1B	-4.33	102.06	107.17
10	16	311	A86	O4-C38-C39	4.33	118.81	111.09
8	21	206	CLA	C2C-C1C-NC	4.33	114.53	109.98
9	12	310	KC1	C3D-C4D-ND	4.33	116.23	110.20
8	20	310	CLA	C3D-C2D-C1D	-4.33	99.93	105.83
9	18	304	KC1	C1A-NA-C4A	-4.32	104.71	106.68
9	12	308	KC1	CHC-C1C-C2C	-4.32	118.20	125.03
9	14	309	KC1	C3D-C4D-ND	4.32	116.22	110.20
9	16	302	KC1	C1C-C2C-C3C	-4.32	102.44	106.98
8	14	307	CLA	C2C-C1C-NC	4.32	114.52	109.98
10	19	311	A86	C3-C4-C5	-4.31	114.69	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	21	210	CLA	CHD-C1D-ND	-4.31	118.73	124.80
8	18	303	CLA	C3D-C4D-ND	4.31	117.00	109.99
9	21	203	KC1	C3D-C4D-ND	4.31	116.21	110.20
8	18	310	CLA	C4A-NA-C1A	-4.31	104.71	106.68
10	17	315	A86	C4-C3-C2	-4.31	114.70	123.52
9	20	303	KC1	C3C-C4C-NC	4.31	114.52	109.90
9	18	306	KC1	C2C-C1C-NC	4.30	115.78	110.45
8	19	306	CLA	C1D-CHD-C4C	-4.30	116.88	126.02
8	14	307	CLA	C4A-NA-C1A	-4.30	104.72	106.68
13	21	212	DD6	O1-C20-C21	-4.30	110.24	115.05
8	13	309	CLA	C3D-C4D-ND	4.30	116.97	109.99
9	17	303	KC1	CMA-C3A-C2A	-4.30	118.03	128.43
9	13	310	KC1	C3C-C4C-NC	4.30	114.50	109.90
8	14	301	CLA	C3D-C4D-ND	4.30	116.97	109.99
9	17	303	KC1	C4B-C3B-C2B	-4.29	103.09	106.81
8	21	209	CLA	C3D-C4D-ND	4.29	116.97	109.99
9	14	309	KC1	C1A-C2A-C3A	-4.29	103.33	107.28
8	19	306	CLA	C4A-NA-C1A	-4.29	104.72	106.68
8	13	301	CLA	C3D-C4D-ND	4.29	116.96	109.99
9	15	304	KC1	C3C-C4C-NC	4.29	114.50	109.90
9	20	306	KC1	CHD-C4C-C3C	-4.28	117.33	125.23
8	16	307	CLA	C3D-C2D-C1D	-4.28	99.99	105.83
9	13	305	KC1	CBA-CAA-C2A	-4.28	108.28	125.45
8	15	305	CLA	C3D-C4D-ND	4.28	116.94	109.99
10	17	321	A86	C25-C26-C27	-4.27	121.29	127.28
8	13	309	CLA	C4A-NA-C1A	-4.27	104.73	106.68
8	17	310	CLA	C3D-C4D-ND	4.27	116.92	109.99
9	11	308	KC1	C3D-C4D-ND	4.27	116.15	110.20
8	14	305	CLA	C3D-C4D-ND	4.26	116.92	109.99
8	21	205	CLA	O2D-CGD-CBD	4.26	118.69	111.23
9	13	310	KC1	CBA-CAA-C2A	-4.26	108.34	125.45
8	13	304	CLA	C3D-C4D-ND	4.26	116.92	109.99
8	17	304	CLA	C3D-C4D-ND	4.26	116.92	109.99
8	15	310	CLA	C3D-C4D-ND	4.26	116.91	109.99
8	14	310	CLA	C3D-C4D-ND	4.26	116.91	109.99
8	14	303	CLA	C3D-C4D-ND	4.26	116.91	109.99
8	14	307	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
9	17	306	KC1	C1C-C2C-C3C	-4.26	102.50	106.98
8	18	305	CLA	C3D-C4D-ND	4.26	116.90	109.99
9	20	306	KC1	C1C-C2C-C3C	-4.25	102.51	106.98
15	19	314	LHG	O4-P-O5	4.25	132.23	112.44
8	20	308	CLA	C3D-C4D-ND	4.25	116.90	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	13	306	CLA	C3D-C4D-ND	4.25	116.89	109.99
10	12	312	A86	C25-C26-C27	-4.25	121.32	127.28
8	20	304	CLA	CBA-CAA-C2A	4.25	126.43	113.79
8	13	302	CLA	C3D-C4D-ND	4.25	116.89	109.99
9	15	309	KC1	C3D-C4D-ND	4.24	116.12	110.20
10	17	316	A86	C25-C26-C27	-4.24	121.33	127.28
9	13	303	KC1	C2A-C1A-NA	4.24	116.14	109.34
8	17	308	CLA	C3D-C4D-ND	4.24	116.89	109.99
9	15	306	KC1	CHC-C1C-C2C	-4.24	118.33	125.03
14	16	314	SQD	O7-S-C6	4.24	113.09	106.76
9	14	306	KC1	C3D-C4D-ND	4.24	116.11	110.20
9	17	305	KC1	C2A-C1A-NA	4.24	116.13	109.34
8	12	301	CLA	C3D-C4D-ND	4.24	116.88	109.99
9	13	303	KC1	C3C-C4C-NC	4.24	114.44	109.90
8	18	303	CLA	C3D-C2D-C1D	-4.24	100.05	105.83
8	19	301	CLA	C3D-C4D-ND	4.24	116.87	109.99
8	16	309	CLA	C3D-C4D-ND	4.23	116.87	109.99
9	11	306	KC1	CHC-C1C-C2C	-4.23	118.34	125.03
8	20	304	CLA	C1D-CHD-C4C	-4.23	117.03	126.02
8	17	310	CLA	CHD-C1D-ND	-4.23	118.85	124.80
8	20	310	CLA	C3D-C4D-ND	4.23	116.86	109.99
8	12	305	CLA	C3D-C4D-ND	4.23	116.86	109.99
10	17	311	A86	C3-C2-C1	-4.22	121.35	127.28
8	18	301	CLA	C3D-C4D-ND	4.22	116.85	109.99
8	21	208	CLA	C3D-C4D-ND	4.22	116.85	109.99
10	17	315	A86	C9-C10-C11	-4.22	114.70	126.64
8	16	306	CLA	C3D-C4D-ND	4.22	116.85	109.99
9	16	302	KC1	C3D-C4D-ND	4.22	116.09	110.20
8	13	302	CLA	CHD-C1D-ND	-4.22	118.86	124.80
9	14	304	KC1	C2A-C1A-NA	4.22	116.10	109.34
8	11	307	CLA	C1C-C2C-C3C	-4.22	102.54	106.98
9	17	303	KC1	C2C-C1C-NC	4.22	115.67	110.45
9	11	304	KC1	C3D-C4D-ND	4.22	116.08	110.20
10	21	214	A86	C36-C31-C32	-4.22	115.51	119.70
10	20	311	A86	C41-C32-C31	-4.22	106.70	110.47
8	19	307	CLA	O2D-CGD-CBD	4.22	118.60	111.23
8	14	308	CLA	C1D-CHD-C4C	-4.21	117.07	126.02
8	13	302	CLA	C2C-C1C-NC	4.21	114.40	109.98
9	20	305	KC1	C2C-C1C-NC	4.21	115.66	110.45
8	16	303	CLA	CHD-C1D-ND	-4.21	118.88	124.80
9	15	302	KC1	C2A-C1A-NA	4.21	116.08	109.34
9	20	305	KC1	C3C-C4C-NC	4.21	114.41	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	13	301	CLA	C4A-NA-C1A	-4.21	104.76	106.68
10	18	313	A86	C41-C32-C31	-4.21	106.71	110.47
9	14	306	KC1	CHC-C1C-C2C	-4.21	118.39	125.03
9	21	207	KC1	C2A-C1A-NA	4.21	116.08	109.34
8	19	305	CLA	CHD-C1D-ND	-4.20	118.89	124.80
10	18	312	A86	C25-C26-C27	-4.20	121.39	127.28
8	11	301	CLA	C3D-C4D-ND	4.20	116.81	109.99
10	17	312	A86	C36-C31-C32	-4.20	115.53	119.70
8	18	308	CLA	C1D-CHD-C4C	-4.20	117.10	126.02
8	20	302	CLA	C1D-CHD-C4C	-4.19	117.10	126.02
8	11	305	CLA	C3D-C4D-ND	4.19	116.80	109.99
8	21	202	CLA	CHD-C1D-ND	-4.19	118.91	124.80
9	21	203	KC1	C2A-C1A-NA	4.19	116.05	109.34
9	16	302	KC1	C3C-C4C-NC	4.19	114.39	109.90
8	13	311	CLA	CHD-C1D-ND	-4.19	118.91	124.80
10	20	301	A86	C40-C32-C31	-4.19	106.73	110.47
9	11	302	KC1	C4B-C3B-C2B	-4.19	103.19	106.81
8	13	306	CLA	CHD-C1D-ND	-4.18	118.92	124.80
10	14	316	A86	C4-C3-C2	-4.18	114.96	123.52
9	11	306	KC1	C1C-C2C-C3C	-4.18	102.58	106.98
10	17	311	A86	C41-C32-C31	-4.18	106.73	110.47
10	20	313	A86	C40-C32-C31	-4.18	106.73	110.47
9	18	304	KC1	C2A-C1A-NA	4.18	116.04	109.34
9	16	305	KC1	C3D-C4D-ND	4.18	116.03	110.20
10	18	311	A86	C4-C5-C6	-4.18	121.42	127.28
8	18	310	CLA	CHD-C1D-ND	-4.18	118.92	124.80
8	20	307	CLA	C3D-C4D-ND	4.18	116.78	109.99
8	14	310	CLA	CHD-C1D-ND	-4.18	118.92	124.80
13	20	312	DD6	O1-C20-C21	-4.18	110.38	115.05
8	12	303	CLA	C1D-CHD-C4C	-4.17	117.15	126.02
10	14	316	A86	C35-C34-C33	4.17	117.38	109.89
8	15	308	CLA	CHD-C1D-ND	-4.17	118.93	124.80
8	19	301	CLA	C4A-NA-C1A	-4.17	104.78	106.68
8	19	302	CLA	C3D-C4D-ND	4.17	116.77	109.99
8	16	306	CLA	C3D-C2D-C1D	-4.17	100.14	105.83
9	15	304	KC1	C2A-C1A-NA	4.17	116.02	109.34
8	18	302	CLA	C4A-NA-C1A	-4.17	104.78	106.68
8	20	310	CLA	C1D-CHD-C4C	-4.17	117.16	126.02
10	12	319	A86	C10-C9-C8	-4.17	111.13	123.20
8	19	307	CLA	C1D-CHD-C4C	-4.17	117.17	126.02
8	15	308	CLA	C3D-C4D-ND	4.16	116.76	109.99
9	17	303	KC1	C3D-C4D-ND	4.16	116.00	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	19	303	CLA	CHD-C1D-ND	-4.16	118.95	124.80
9	21	203	KC1	CHC-C1C-C2C	-4.16	118.46	125.03
13	21	212	DD6	C35-C36-C31	-4.16	111.84	120.50
8	14	301	CLA	CHD-C1D-ND	-4.16	118.95	124.80
10	16	311	A86	C12-C11-C13	4.16	122.74	116.00
9	17	305	KC1	CHD-C4C-C3C	-4.16	117.56	125.23
9	20	303	KC1	C4B-C3B-C2B	-4.16	103.21	106.81
8	19	310	CLA	C3D-C4D-ND	4.16	116.74	109.99
9	20	303	KC1	C1C-C2C-C3C	-4.15	102.61	106.98
8	18	307	CLA	C3D-C4D-ND	4.15	116.73	109.99
8	21	202	CLA	C3D-C4D-ND	4.15	116.73	109.99
8	11	309	CLA	CHD-C1D-ND	-4.15	118.96	124.80
8	18	301	CLA	CHD-C1D-ND	-4.15	118.96	124.80
8	14	308	CLA	C3D-C4D-ND	4.15	116.73	109.99
8	21	206	CLA	C3D-C4D-ND	4.15	116.73	109.99
8	15	305	CLA	CHD-C1D-ND	-4.15	118.97	124.80
8	19	307	CLA	C3D-C4D-ND	4.15	116.73	109.99
9	20	303	KC1	C1A-NA-C4A	-4.14	104.79	106.68
8	20	307	CLA	C2C-C1C-NC	4.14	114.33	109.98
8	17	308	CLA	O2D-CGD-CBD	4.14	118.47	111.23
8	19	304	CLA	CHD-C1D-ND	-4.14	118.98	124.80
10	12	316	A86	C12-C11-C13	4.14	122.71	116.00
13	19	312	DD6	C21-C20-C19	-4.14	109.59	114.24
8	20	308	CLA	C1D-CHD-C4C	-4.14	117.23	126.02
10	11	311	A86	C26-C25-C24	-4.14	111.22	123.20
9	15	309	KC1	C1A-C2A-C3A	-4.14	103.48	107.28
9	14	309	KC1	CHC-C1C-C2C	-4.13	118.50	125.03
8	21	205	CLA	CHD-C1D-ND	-4.13	118.98	124.80
10	21	215	A86	C3-C2-C1	-4.13	121.48	127.28
9	18	304	KC1	CBA-CAA-C2A	-4.13	108.86	125.45
8	19	303	CLA	CBA-CAA-C2A	4.13	126.08	113.79
8	16	309	CLA	CHD-C1D-ND	-4.13	118.99	124.80
9	11	306	KC1	C3D-C4D-ND	4.13	115.96	110.20
8	21	208	CLA	CHD-C1D-ND	-4.13	118.99	124.80
8	14	305	CLA	CHD-C1D-ND	-4.13	118.99	124.80
8	18	303	CLA	C1D-CHD-C4C	-4.13	117.25	126.02
8	12	305	CLA	CHD-C1D-ND	-4.13	119.00	124.80
8	15	310	CLA	CHD-C1D-ND	-4.12	119.00	124.80
8	16	307	CLA	O2D-CGD-CBD	4.12	118.44	111.23
10	17	313	A86	C12-C11-C13	4.12	122.68	116.00
9	11	304	KC1	C2A-C1A-NA	4.12	115.94	109.34
9	12	308	KC1	C2A-C1A-NA	4.12	115.94	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	17	303	KC1	C3C-C4C-NC	4.12	114.31	109.90
9	11	304	KC1	C2C-C1C-NC	4.11	115.54	110.45
9	16	308	KC1	C3D-C4D-ND	4.11	115.94	110.20
9	16	308	KC1	C4B-C3B-C2B	-4.11	103.25	106.81
8	16	301	CLA	CHD-C1D-ND	-4.11	119.02	124.80
8	11	301	CLA	C1D-CHD-C4C	-4.11	117.29	126.02
9	13	307	KC1	C2A-C1A-NA	4.11	115.92	109.34
8	18	301	CLA	C1D-CHD-C4C	-4.10	117.30	126.02
13	20	314	DD6	O1-C20-C21	-4.10	110.46	115.05
9	18	306	KC1	C4B-C3B-C2B	-4.10	103.25	106.81
8	19	309	CLA	C3D-C2D-C1D	-4.10	100.23	105.83
8	21	209	CLA	CHD-C1D-ND	-4.10	119.03	124.80
8	11	303	CLA	C3D-C4D-ND	4.10	116.65	109.99
8	13	309	CLA	CHD-C1D-ND	-4.10	119.03	124.80
8	12	301	CLA	O2D-CGD-CBD	4.10	118.39	111.23
8	14	301	CLA	C1D-CHD-C4C	-4.10	117.31	126.02
8	11	305	CLA	CHD-C1D-ND	-4.10	119.04	124.80
9	17	305	KC1	C3C-C4C-NC	4.09	114.29	109.90
8	18	301	CLA	O2D-CGD-CBD	4.09	118.38	111.23
9	15	306	KC1	C2A-C1A-NA	4.09	115.90	109.34
8	18	308	CLA	C3D-C4D-ND	4.09	116.64	109.99
8	17	308	CLA	CHD-C1D-ND	-4.09	119.05	124.80
8	21	205	CLA	C3D-C4D-ND	4.09	116.64	109.99
9	19	308	KC1	CHC-C1C-C2C	-4.09	118.58	125.03
13	20	314	DD6	C15-C14-C13	4.09	134.63	125.99
8	18	305	CLA	C4A-NA-C1A	-4.09	104.81	106.68
9	20	305	KC1	C1C-C2C-C3C	-4.08	102.69	106.98
10	20	311	A86	C3-C2-C1	-4.08	121.56	127.28
8	11	307	CLA	C3D-C4D-ND	4.08	116.62	109.99
9	13	310	KC1	C1C-C2C-C3C	-4.08	102.69	106.98
8	11	303	CLA	CHD-C1D-ND	-4.07	119.07	124.80
13	19	312	DD6	C19-C18-C17	4.07	118.41	110.79
9	11	302	KC1	C1C-C2C-C3C	-4.07	102.70	106.98
10	15	316	A86	C25-C26-C27	-4.07	121.57	127.28
8	21	209	CLA	C1D-CHD-C4C	-4.07	117.37	126.02
9	12	306	KC1	CHC-C1C-C2C	-4.07	118.60	125.03
9	18	306	KC1	C3D-C4D-ND	4.07	115.87	110.20
8	13	309	CLA	O2D-CGD-CBD	4.06	118.33	111.23
8	15	303	CLA	CHD-C1D-ND	-4.06	119.09	124.80
8	12	301	CLA	CHD-C1D-ND	-4.06	119.09	124.80
10	13	315	A86	C36-C31-C32	-4.06	115.67	119.70
8	14	303	CLA	CHD-C1D-ND	-4.06	119.09	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	15	308	CLA	C1C-C2C-C3C	-4.06	102.71	106.98
9	14	306	KC1	C4B-C3B-C2B	-4.06	103.30	106.81
8	19	303	CLA	C2C-C1C-NC	4.06	114.24	109.98
14	16	314	SQD	O6-C1-C2	4.06	114.43	108.27
8	13	304	CLA	CHD-C1D-ND	-4.05	119.10	124.80
8	11	301	CLA	CHD-C1D-ND	-4.05	119.10	124.80
8	19	301	CLA	CHD-C1D-ND	-4.05	119.10	124.80
8	19	302	CLA	C1D-CHD-C4C	-4.05	117.41	126.02
9	16	304	KC1	C2A-C1A-NA	4.05	115.83	109.34
9	16	305	KC1	C2A-C1A-NA	4.05	115.83	109.34
9	14	306	KC1	CBA-CAA-C2A	-4.05	109.19	125.45
8	13	301	CLA	C1D-CHD-C4C	-4.05	117.41	126.02
8	17	308	CLA	C4A-NA-C1A	-4.05	104.83	106.68
10	14	315	A86	C25-C24-C1	-4.05	115.26	126.36
9	11	304	KC1	C1C-C2C-C3C	-4.05	102.72	106.98
8	15	307	CLA	C2C-C1C-NC	4.05	114.23	109.98
9	12	306	KC1	C4B-C3B-C2B	-4.04	103.31	106.81
8	11	307	CLA	C1D-CHD-C4C	-4.04	117.43	126.02
8	18	308	CLA	O2D-CGD-CBD	4.04	118.29	111.23
13	19	312	DD6	C15-C14-C13	4.04	134.53	125.99
10	12	316	A86	C35-C34-C33	4.03	117.13	109.89
10	14	315	A86	O4-C38-C39	4.03	118.28	111.09
8	11	307	CLA	C4A-NA-C1A	-4.03	104.84	106.68
8	12	301	CLA	C4A-NA-C1A	-4.03	104.84	106.68
9	13	307	KC1	C4B-C3B-C2B	-4.03	103.32	106.81
8	12	303	CLA	C4A-NA-C1A	-4.03	104.84	106.68
9	13	310	KC1	C2C-C1C-NC	4.03	115.44	110.45
8	20	309	CLA	C1D-CHD-C4C	-4.03	117.46	126.02
8	18	303	CLA	C2C-C1C-NC	4.03	114.21	109.98
9	13	307	KC1	C1C-C2C-C3C	-4.02	102.75	106.98
13	21	212	DD6	C37-C36-C35	-4.02	107.03	114.42
9	18	309	KC1	C4B-C3B-C2B	-4.02	103.33	106.81
10	14	312	A86	C4-C5-C6	-4.02	121.64	127.28
9	12	306	KC1	CBA-CAA-C2A	-4.02	109.31	125.45
9	16	308	KC1	C2C-C1C-NC	4.02	115.43	110.45
8	14	308	CLA	C1C-C2C-C3C	-4.02	102.75	106.98
8	20	309	CLA	C3D-C4D-ND	4.02	116.52	109.99
8	19	303	CLA	O2D-CGD-CBD	4.02	118.25	111.23
9	20	306	KC1	C3D-C4D-ND	4.01	115.80	110.20
9	15	302	KC1	C1A-NA-C4A	-4.01	104.85	106.68
14	16	314	SQD	O9-S-O7	-4.01	100.78	113.82
8	17	307	CLA	C4A-NA-C1A	-4.01	104.85	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	15	307	CLA	C1D-CHD-C4C	-4.01	117.50	126.02
9	20	306	KC1	C2A-C1A-NA	4.01	115.76	109.34
8	16	306	CLA	C2C-C1C-NC	4.01	114.19	109.98
9	13	310	KC1	C4B-C3B-C2B	-4.01	103.34	106.81
8	11	301	CLA	CAA-CBA-CGA	-4.01	101.83	113.21
8	12	309	CLA	C3D-C4D-ND	4.00	116.48	109.99
8	19	305	CLA	O2D-CGD-CBD	4.00	118.22	111.23
8	15	301	CLA	C1D-CHD-C4C	-4.00	117.52	126.02
9	20	305	KC1	C2A-C1A-NA	4.00	115.74	109.34
9	13	303	KC1	C2C-C1C-NC	3.99	115.39	110.45
8	20	308	CLA	CHD-C1D-ND	-3.99	119.19	124.80
8	18	305	CLA	CHD-C1D-ND	-3.99	119.19	124.80
10	11	318	A86	C12-C11-C13	3.99	122.47	116.00
9	15	304	KC1	C1C-C2C-C3C	-3.99	102.78	106.98
8	12	303	CLA	C2C-C1C-NC	3.98	114.17	109.98
8	14	307	CLA	C1D-CHD-C4C	-3.98	117.55	126.02
10	15	319	A86	C12-C11-C13	3.98	122.46	116.00
8	18	307	CLA	C1D-CHD-C4C	-3.98	117.56	126.02
8	14	302	CLA	C1D-CHD-C4C	-3.98	117.56	126.02
9	16	305	KC1	C1A-NA-C4A	-3.98	104.86	106.68
10	12	302	A86	C25-C26-C27	-3.98	121.70	127.28
10	14	315	A86	C3-C4-C5	-3.97	115.39	123.52
8	21	206	CLA	C1D-CHD-C4C	-3.97	117.57	126.02
8	12	311	CLA	C3D-C4D-ND	3.97	116.44	109.99
8	12	303	CLA	C3D-C4D-ND	3.97	116.44	109.99
9	14	306	KC1	C1C-C2C-C3C	-3.97	102.81	106.98
9	12	310	KC1	CHC-C1C-C2C	-3.97	118.76	125.03
13	20	312	DD6	C24-C1-C2	-3.97	112.77	119.01
8	13	308	CLA	O2D-CGD-CBD	3.97	118.16	111.23
9	15	304	KC1	C2C-C1C-NC	3.97	115.36	110.45
9	11	308	KC1	C2C-C1C-NC	3.96	115.36	110.45
10	11	310	A86	C41-C32-C31	-3.96	106.92	110.47
9	20	306	KC1	C4B-C3B-C2B	-3.96	103.38	106.81
8	11	307	CLA	C3C-C4C-NC	3.96	115.50	110.43
9	11	302	KC1	C2C-C1C-NC	3.96	115.35	110.45
8	21	202	CLA	C1D-CHD-C4C	-3.96	117.61	126.02
8	11	303	CLA	CBA-CAA-C2A	3.96	125.57	113.79
13	20	314	DD6	C33-C32-C31	3.96	117.29	109.49
9	11	304	KC1	C1A-NA-C4A	-3.96	104.87	106.68
8	20	307	CLA	C1D-CHD-C4C	-3.96	117.61	126.02
9	12	306	KC1	C2A-C1A-NA	3.95	115.68	109.34
8	11	309	CLA	C4A-NA-C1A	-3.95	104.88	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	16	310	A86	C12-C11-C13	3.95	122.41	116.00
9	20	303	KC1	CBC-CAC-C3C	-3.95	101.71	112.42
8	19	310	CLA	CHD-C1D-ND	-3.95	119.25	124.80
8	19	306	CLA	C3C-C4C-NC	3.95	115.48	110.43
10	14	315	A86	C4-C5-C6	-3.94	121.75	127.28
10	14	314	A86	C41-C32-C31	-3.94	106.94	110.47
8	16	301	CLA	C1D-CHD-C4C	-3.94	117.64	126.02
8	12	304	CLA	C3D-C4D-ND	3.94	116.39	109.99
9	18	306	KC1	C1C-C2C-C3C	-3.94	102.84	106.98
9	18	306	KC1	O2D-CGD-O1D	-3.94	116.18	123.85
10	11	313	A86	C3-C4-C5	-3.94	115.46	123.52
8	14	302	CLA	C4A-NA-C1A	-3.94	104.88	106.68
9	15	306	KC1	C1C-C2C-C3C	-3.94	102.84	106.98
8	13	301	CLA	CHD-C1D-ND	-3.94	119.26	124.80
9	15	302	KC1	C4B-C3B-C2B	-3.94	103.40	106.81
8	12	303	CLA	CHD-C1D-ND	-3.94	119.26	124.80
8	18	302	CLA	CHD-C1D-ND	-3.94	119.26	124.80
9	14	306	KC1	C2C-C1C-NC	3.93	115.32	110.45
9	13	310	KC1	C1A-NA-C4A	-3.93	104.89	106.68
8	19	303	CLA	C1D-CHD-C4C	-3.93	117.67	126.02
10	15	314	A86	C36-C31-C32	-3.93	115.80	119.70
8	19	305	CLA	C1D-CHD-C4C	-3.92	117.68	126.02
8	13	308	CLA	C1D-CHD-C4C	-3.92	117.68	126.02
8	15	310	CLA	C1D-CHD-C4C	-3.92	117.68	126.02
10	16	313	A86	C9-C8-C6	-3.92	115.61	126.36
10	18	314	A86	C41-C32-C31	-3.92	106.96	110.47
8	16	307	CLA	CHD-C1D-ND	-3.92	119.29	124.80
8	14	310	CLA	C1C-C2C-C3C	-3.92	102.86	106.98
8	15	301	CLA	C1C-C2C-C3C	-3.92	102.86	106.98
9	13	303	KC1	C1C-C2C-C3C	-3.92	102.86	106.98
9	15	302	KC1	C1C-C2C-C3C	-3.92	102.86	106.98
8	17	310	CLA	O2D-CGD-O1D	-3.92	116.23	123.85
8	19	301	CLA	C1-C2-C3	-3.91	119.78	126.20
9	12	308	KC1	C2C-C1C-NC	3.91	115.29	110.45
8	19	310	CLA	C1C-C2C-C3C	-3.91	102.86	106.98
8	13	308	CLA	C1C-C2C-C3C	-3.91	102.86	106.98
10	20	301	A86	C24-C1-C2	3.91	125.16	119.01
8	19	310	CLA	C1D-CHD-C4C	-3.91	117.71	126.02
8	20	304	CLA	C3C-C4C-NC	3.91	115.44	110.43
8	19	302	CLA	CHD-C1D-ND	-3.91	119.30	124.80
9	13	305	KC1	C2C-C1C-NC	3.91	115.29	110.45
8	12	304	CLA	C1D-CHD-C4C	-3.91	117.71	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	21	210	CLA	C1D-CHD-C4C	-3.91	117.71	126.02
8	17	302	CLA	C4A-NA-C1A	-3.91	104.90	106.68
13	21	216	DD6	C35-C36-C31	-3.91	112.37	120.50
9	16	302	KC1	CBA-CAA-C2A	-3.91	109.78	125.45
14	17	301	SQD	O9-S-O7	-3.91	101.12	113.82
8	15	305	CLA	C1D-CHD-C4C	-3.90	117.72	126.02
8	21	205	CLA	C4A-NA-C1A	-3.90	104.90	106.68
8	13	302	CLA	C1D-CHD-C4C	-3.90	117.72	126.02
8	16	303	CLA	C3B-C4B-NB	3.90	114.01	110.53
9	18	306	KC1	CBA-CAA-C2A	-3.90	109.80	125.45
8	14	305	CLA	C1C-C2C-C3C	-3.90	102.88	106.98
9	12	310	KC1	C2A-C1A-NA	3.90	115.59	109.34
8	18	305	CLA	C1D-CHD-C4C	-3.90	117.73	126.02
8	16	307	CLA	C4A-NA-C1A	-3.90	104.90	106.68
10	11	310	A86	C36-C31-C32	-3.89	115.83	119.70
9	15	306	KC1	C2C-C1C-NC	3.89	115.27	110.45
13	21	212	DD6	O1-C15-C14	-3.89	105.73	116.88
10	11	312	A86	C12-C11-C13	3.89	122.31	116.00
8	14	308	CLA	O2D-CGD-CBD	3.89	118.03	111.23
8	19	309	CLA	CHD-C1D-ND	-3.89	119.33	124.80
10	17	321	A86	C41-C32-C31	-3.89	106.99	110.47
9	20	303	KC1	C1D-CHD-C4C	-3.89	117.11	126.25
8	15	307	CLA	C3D-C4D-ND	3.89	116.31	109.99
9	16	304	KC1	C1A-NA-C4A	-3.89	104.91	106.68
8	13	309	CLA	C1D-CHD-C4C	-3.89	117.76	126.02
8	18	302	CLA	C1D-CHD-C4C	-3.89	117.76	126.02
8	12	311	CLA	CHD-C1D-ND	-3.88	119.34	124.80
8	20	304	CLA	CHD-C1D-ND	-3.88	119.34	124.80
9	16	305	KC1	C2C-C1C-NC	3.88	115.25	110.45
8	14	302	CLA	C3D-C4D-ND	3.88	116.29	109.99
8	19	307	CLA	CHD-C1D-ND	-3.88	119.34	124.80
9	18	304	KC1	C2C-C1C-NC	3.88	115.25	110.45
8	12	305	CLA	CBA-CAA-C2A	3.88	125.32	113.79
13	16	312	DD6	C37-C36-C35	-3.87	107.30	114.42
10	11	311	A86	C3-C4-C5	-3.87	115.59	123.52
10	21	213	A86	C4-C5-C6	-3.87	121.84	127.28
9	11	302	KC1	C2A-C1A-NA	3.87	115.55	109.34
8	21	205	CLA	CAC-C3C-C4C	3.87	129.83	124.79
8	15	310	CLA	CAA-C2A-C3A	-3.87	102.54	113.00
8	11	305	CLA	C1D-CHD-C4C	-3.87	117.79	126.02
8	16	307	CLA	C1D-CHD-C4C	-3.87	117.79	126.02
9	15	309	KC1	C1D-CHD-C4C	-3.87	117.15	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	16	309	CLA	C1D-CHD-C4C	-3.87	117.80	126.02
10	14	311	A86	C4-C5-C6	-3.87	121.85	127.28
8	13	311	CLA	C1C-C2C-C3C	-3.87	102.91	106.98
9	18	306	KC1	C1D-CHD-C4C	-3.87	117.15	126.25
10	11	313	A86	C25-C26-C27	-3.87	121.85	127.28
8	15	308	CLA	C1D-CHD-C4C	-3.87	117.80	126.02
10	15	313	A86	C25-C26-C27	-3.87	121.86	127.28
8	17	307	CLA	C1D-CHD-C4C	-3.87	117.80	126.02
9	11	306	KC1	O2D-CGD-O1D	-3.87	116.32	123.85
8	12	301	CLA	CAC-C3C-C4C	3.87	129.82	124.79
9	12	308	KC1	C1C-C2C-C3C	-3.86	102.92	106.98
9	11	304	KC1	C4B-C3B-C2B	-3.86	103.46	106.81
9	12	306	KC1	C2C-C1C-NC	3.86	115.23	110.45
8	17	307	CLA	C3D-C4D-ND	3.86	116.27	109.99
8	16	306	CLA	C1D-CHD-C4C	-3.86	117.81	126.02
8	18	308	CLA	C1C-C2C-C3C	-3.86	102.92	106.98
10	13	315	A86	C4-C5-C6	-3.86	121.87	127.28
8	14	307	CLA	C3D-C4D-ND	3.86	116.26	109.99
9	12	306	KC1	C1C-C2C-C3C	-3.86	102.92	106.98
10	18	314	A86	C25-C26-C27	-3.86	121.87	127.28
9	17	309	KC1	C4B-C3B-C2B	-3.85	103.47	106.81
9	13	305	KC1	C1C-C2C-C3C	-3.85	102.93	106.98
8	18	310	CLA	C1C-C2C-C3C	-3.85	102.93	106.98
8	11	305	CLA	C1C-C2C-C3C	-3.85	102.93	106.98
9	18	309	KC1	C2C-C1C-NC	3.85	115.21	110.45
8	11	303	CLA	C1C-C2C-C3C	-3.84	102.94	106.98
10	17	321	A86	C12-C11-C13	3.84	122.23	116.00
8	21	206	CLA	C4A-NA-C1A	-3.84	104.93	106.68
8	14	310	CLA	C1D-CHD-C4C	-3.84	117.85	126.02
9	20	303	KC1	C2A-C1A-NA	3.84	115.50	109.34
8	14	303	CLA	C1D-CHD-C4C	-3.84	117.86	126.02
8	13	302	CLA	C4A-NA-C1A	-3.84	104.93	106.68
10	15	316	A86	C35-C34-C33	3.84	116.78	109.89
10	11	313	A86	C10-C9-C8	-3.84	112.08	123.20
8	14	308	CLA	CHD-C1D-ND	-3.84	119.40	124.80
9	17	305	KC1	C1A-NA-C4A	-3.84	104.93	106.68
8	13	301	CLA	C1C-C2C-C3C	-3.83	102.95	106.98
8	21	204	CLA	C1C-C2C-C3C	-3.83	102.95	106.98
8	19	307	CLA	C4A-NA-C1A	-3.83	104.93	106.68
9	18	304	KC1	C1C-C2C-C3C	-3.83	102.95	106.98
9	12	306	KC1	C1D-CHD-C4C	-3.83	117.23	126.25
10	12	319	A86	C25-C26-C27	-3.83	121.91	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	15	309	KC1	C1C-C2C-C3C	-3.83	102.95	106.98
8	12	307	CLA	C1C-C2C-C3C	-3.83	102.95	106.98
8	12	303	CLA	CMC-C2C-C1C	3.83	131.01	125.03
8	20	310	CLA	CHD-C1D-ND	-3.83	119.42	124.80
8	15	308	CLA	CAC-C3C-C4C	3.83	129.77	124.79
8	12	301	CLA	C1D-CHD-C4C	-3.83	117.89	126.02
8	16	306	CLA	C3B-C2B-C1B	-3.83	102.66	107.17
9	13	305	KC1	C2A-C1A-NA	3.83	115.47	109.34
9	13	307	KC1	C2C-C1C-NC	3.83	115.19	110.45
8	12	304	CLA	C1C-C2C-C3C	-3.82	102.96	106.98
9	21	203	KC1	C2C-C1C-NC	3.82	115.18	110.45
8	11	309	CLA	O2D-CGD-CBD	3.82	117.91	111.23
8	14	305	CLA	C4A-NA-C1A	-3.82	104.94	106.68
9	12	308	KC1	C1D-CHD-C4C	-3.82	117.26	126.25
9	12	306	KC1	C1A-NA-C4A	-3.82	104.94	106.68
10	14	312	A86	C36-C31-C32	-3.82	115.91	119.70
9	14	309	KC1	C1D-CHD-C4C	-3.82	117.28	126.25
8	18	302	CLA	C3D-C4D-ND	3.81	116.19	109.99
8	17	304	CLA	C1C-C2C-C3C	-3.81	102.97	106.98
8	18	305	CLA	C1C-C2C-C3C	-3.81	102.97	106.98
13	19	312	DD6	C35-C36-C31	-3.81	112.57	120.50
9	20	305	KC1	C4B-C3B-C2B	-3.81	103.51	106.81
10	14	314	A86	C3-C4-C5	-3.81	115.73	123.52
8	12	309	CLA	CHD-C1D-ND	-3.81	119.45	124.80
9	15	302	KC1	C2C-C1C-NC	3.81	115.16	110.45
13	20	314	DD6	C21-C20-C15	-3.81	116.04	122.30
8	17	304	CLA	C3B-C4B-NB	3.80	113.93	110.53
8	13	311	CLA	C1D-CHD-C4C	-3.80	117.94	126.02
10	16	310	A86	C34-O4-C38	-3.80	111.14	117.85
9	18	309	KC1	C1D-CHD-C4C	-3.80	117.31	126.25
9	17	303	KC1	C2A-C1A-NA	3.80	115.43	109.34
8	13	306	CLA	C4A-NA-C1A	-3.80	104.95	106.68
8	13	306	CLA	C1C-C2C-C3C	-3.80	102.98	106.98
13	20	314	DD6	C23-C16-C15	3.80	120.30	110.05
10	13	312	A86	C12-C11-C13	3.80	122.16	116.00
13	19	312	DD6	C23-C16-C22	-3.80	101.85	107.37
9	15	306	KC1	CBA-CAA-C2A	-3.80	110.22	125.45
8	14	301	CLA	C2C-C1C-NC	3.79	113.97	109.98
9	17	305	KC1	CAC-C3C-C4C	3.79	129.72	124.79
9	20	303	KC1	C2C-C1C-NC	3.79	115.14	110.45
9	17	306	KC1	C3D-C4D-ND	3.79	115.48	110.20
10	20	301	A86	C8-C6-C5	3.79	124.97	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	12	316	A86	C25-C26-C27	-3.79	121.96	127.28
8	12	311	CLA	C1D-CHD-C4C	-3.79	117.97	126.02
9	17	306	KC1	O2D-CGD-O1D	-3.79	116.48	123.85
8	19	310	CLA	C4A-NA-C1A	-3.79	104.95	106.68
13	21	212	DD6	C25-C26-C27	3.78	137.20	126.61
8	16	306	CLA	C3C-C4C-NC	3.78	115.28	110.43
9	15	304	KC1	CBA-CAA-C2A	-3.78	110.27	125.45
8	16	303	CLA	C1C-C2C-C3C	-3.78	103.00	106.98
9	13	310	KC1	C2A-C1A-NA	3.78	115.40	109.34
10	17	312	A86	C3-C4-C5	-3.78	115.78	123.52
8	13	306	CLA	C1D-CHD-C4C	-3.78	117.98	126.02
8	13	304	CLA	C1C-C2C-C3C	-3.78	103.00	106.98
8	14	302	CLA	CHD-C1D-ND	-3.78	119.48	124.80
8	16	301	CLA	C4A-NA-C1A	-3.78	104.95	106.68
8	12	304	CLA	CHD-C1D-ND	-3.78	119.48	124.80
8	19	305	CLA	CMB-C2B-C1B	3.78	131.17	125.42
8	18	307	CLA	C3C-C4C-NC	3.78	115.27	110.43
9	16	302	KC1	C1D-CHD-C4C	-3.78	117.37	126.25
8	18	301	CLA	C2C-C1C-NC	3.78	113.95	109.98
9	15	309	KC1	C2C-C1C-NC	3.77	115.12	110.45
8	19	301	CLA	C2C-C1C-NC	3.77	113.94	109.98
8	17	302	CLA	C1D-CHD-C4C	-3.77	118.01	126.02
10	16	311	A86	C35-C34-C33	3.77	116.66	109.89
8	16	301	CLA	C2C-C1C-NC	3.77	113.94	109.98
9	11	306	KC1	CBA-CAA-C2A	-3.77	110.33	125.45
9	17	305	KC1	C1C-C2C-C3C	-3.77	103.02	106.98
9	21	203	KC1	CBA-CAA-C2A	-3.77	110.33	125.45
10	16	310	A86	C26-C25-C24	-3.77	112.29	123.20
9	11	308	KC1	C4B-C3B-C2B	-3.77	103.55	106.81
9	14	304	KC1	C1C-C2C-C3C	-3.77	103.02	106.98
8	20	309	CLA	C1C-C2C-C3C	-3.76	103.02	106.98
9	19	308	KC1	C1D-CHD-C4C	-3.76	117.40	126.25
9	14	306	KC1	C1D-CHD-C4C	-3.76	117.41	126.25
8	14	303	CLA	C1C-C2C-C3C	-3.76	103.03	106.98
10	15	316	A86	C4-C3-C2	-3.76	115.83	123.52
9	13	307	KC1	CBA-CAA-C2A	-3.76	110.37	125.45
8	18	310	CLA	C1D-CHD-C4C	-3.76	118.03	126.02
9	17	305	KC1	C2C-C1C-NC	3.76	115.10	110.45
9	17	309	KC1	C1D-CHD-C4C	-3.75	117.42	126.25
10	17	316	A86	C35-C34-C33	3.75	116.63	109.89
8	14	305	CLA	C1D-CHD-C4C	-3.75	118.04	126.02
8	18	308	CLA	C3C-C4C-NC	3.75	115.24	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	11	311	A86	C25-C26-C27	-3.75	122.01	127.28
8	12	304	CLA	C4A-NA-C1A	-3.75	104.97	106.68
9	12	310	KC1	CBA-CAA-C2A	-3.75	110.39	125.45
8	13	308	CLA	C3D-C4D-ND	3.75	116.09	109.99
9	11	306	KC1	C2C-C1C-NC	3.75	115.09	110.45
9	14	304	KC1	CBA-CAA-C2A	-3.75	110.39	125.45
8	17	304	CLA	CBA-CAA-C2A	3.75	124.95	113.79
8	18	301	CLA	C4A-NA-C1A	-3.75	104.97	106.68
10	17	314	A86	C3-C4-C5	-3.75	115.85	123.52
8	15	305	CLA	C1C-C2C-C3C	-3.75	103.04	106.98
13	20	312	DD6	C35-C36-C31	-3.75	112.70	120.50
8	11	309	CLA	C1C-C2C-C3C	-3.74	103.04	106.98
10	19	311	A86	C25-C24-C1	-3.74	116.10	126.36
8	17	310	CLA	C1C-C2C-C3C	-3.74	103.04	106.98
8	11	309	CLA	C3C-C4C-NC	3.74	115.22	110.43
8	15	303	CLA	C1C-C2C-C3C	-3.74	103.05	106.98
9	13	305	KC1	C1D-CHD-C4C	-3.74	117.45	126.25
8	18	307	CLA	C1C-C2C-C3C	-3.74	103.05	106.98
8	19	306	CLA	C1-C2-C3	-3.74	120.08	126.20
8	11	303	CLA	C1D-CHD-C4C	-3.74	118.08	126.02
8	15	308	CLA	C4A-NA-C1A	-3.73	104.97	106.68
8	19	310	CLA	C3C-C4C-NC	3.73	115.21	110.43
8	17	310	CLA	C1D-CHD-C4C	-3.73	118.08	126.02
8	19	305	CLA	C3C-C4C-NC	3.73	115.21	110.43
8	15	310	CLA	C1C-C2C-C3C	-3.73	103.06	106.98
9	16	308	KC1	C1C-C2C-C3C	-3.73	103.06	106.98
10	15	313	A86	C41-C32-C31	-3.73	107.13	110.47
8	19	301	CLA	C3C-C4C-NC	3.73	115.20	110.43
9	11	306	KC1	C2A-C1A-NA	3.73	115.31	109.34
8	13	304	CLA	C1D-CHD-C4C	-3.72	118.10	126.02
8	20	310	CLA	C1C-C2C-C3C	-3.72	103.06	106.98
8	16	301	CLA	C3C-C4C-NC	3.72	115.20	110.43
8	16	306	CLA	CHD-C1D-ND	-3.72	119.57	124.80
10	11	312	A86	C4-C3-C2	-3.72	115.91	123.52
10	12	313	A86	C12-C11-C13	3.72	122.03	116.00
10	13	316	A86	C25-C26-C27	-3.72	122.06	127.28
8	21	206	CLA	O2D-CGD-CBD	3.72	117.73	111.23
9	19	308	KC1	C1C-C2C-C3C	-3.72	103.07	106.98
9	18	306	KC1	C2A-C1A-NA	3.71	115.29	109.34
8	13	301	CLA	O2D-CGD-CBD	3.71	117.72	111.23
8	15	303	CLA	C1D-CHD-C4C	-3.71	118.13	126.02
8	16	301	CLA	CAC-C3C-C4C	3.71	129.62	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	13	301	CLA	CAC-C3C-C4C	3.71	129.62	124.79
9	12	308	KC1	C1A-NA-C4A	-3.71	104.99	106.68
9	15	306	KC1	C1D-CHD-C4C	-3.71	117.53	126.25
8	17	307	CLA	C3C-C4C-NC	3.71	115.18	110.43
8	12	301	CLA	C1C-C2C-C3C	-3.71	103.08	106.98
8	21	204	CLA	C1D-CHD-C4C	-3.70	118.14	126.02
9	17	306	KC1	C2A-C1A-NA	3.70	115.28	109.34
9	11	308	KC1	C1C-C2C-C3C	-3.70	103.08	106.98
8	12	309	CLA	C1D-CHD-C4C	-3.70	118.15	126.02
9	16	304	KC1	C4B-C3B-C2B	-3.70	103.60	106.81
8	19	307	CLA	C3C-C4C-NC	3.70	115.17	110.43
8	18	301	CLA	C3C-C4C-NC	3.70	115.17	110.43
10	17	321	A86	C3-C2-C1	-3.70	122.09	127.28
8	19	301	CLA	C1D-CHD-C4C	-3.70	118.15	126.02
10	13	312	A86	C4-C5-C6	-3.70	122.09	127.28
10	20	301	A86	C25-C26-C27	3.70	132.47	127.28
8	21	208	CLA	C1C-C2C-C3C	-3.70	103.09	106.98
9	14	304	KC1	C2C-C1C-NC	3.70	115.02	110.45
9	16	305	KC1	C1D-CHD-C4C	-3.69	117.56	126.25
9	11	306	KC1	C1D-CHD-C4C	-3.69	117.56	126.25
8	12	307	CLA	CAA-C2A-C3A	-3.69	103.02	113.00
9	11	302	KC1	CBC-CAC-C3C	-3.69	102.41	112.42
9	20	305	KC1	CAC-C3C-C4C	3.69	129.59	124.79
8	13	309	CLA	C1C-C2C-C3C	-3.69	103.10	106.98
9	13	303	KC1	C1D-CHD-C4C	-3.69	117.57	126.25
8	18	303	CLA	CBA-CAA-C2A	3.69	124.77	113.79
9	16	304	KC1	C1D-CHD-C4C	-3.69	117.58	126.25
8	17	302	CLA	C1C-C2C-C3C	-3.69	103.10	106.98
10	12	316	A86	C4-C3-C2	-3.69	115.98	123.52
9	21	203	KC1	C1C-C2C-C3C	-3.68	103.11	106.98
8	11	301	CLA	C3C-C4C-NC	3.68	115.15	110.43
9	20	305	KC1	C1D-CHD-C4C	-3.68	117.59	126.25
8	16	307	CLA	C1C-C2C-C3C	-3.68	103.11	106.98
10	16	311	A86	C4-C5-C6	-3.68	122.12	127.28
8	15	307	CLA	CHD-C1D-ND	-3.68	119.62	124.80
9	16	308	KC1	C2A-C1A-NA	3.68	115.23	109.34
10	12	315	A86	C12-C11-C13	3.67	121.95	116.00
10	17	321	A86	C10-C9-C8	-3.67	112.57	123.20
9	15	304	KC1	C4B-C3B-C2B	-3.67	103.63	106.81
13	20	312	DD6	O1-C15-C14	-3.67	106.37	116.88
8	21	202	CLA	CAC-C3C-C4C	3.67	129.56	124.79
8	20	309	CLA	CHD-C1D-ND	-3.67	119.64	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	17	303	KC1	C1D-CHD-C4C	-3.67	117.62	126.25
9	21	207	KC1	CHC-C1C-C2C	-3.67	119.24	125.03
10	11	311	A86	C4-C5-C6	-3.67	122.14	127.28
9	16	305	KC1	C4B-C3B-C2B	-3.66	103.64	106.81
8	19	309	CLA	CAA-C2A-C3A	-3.66	103.10	113.00
8	11	303	CLA	C3B-C4B-NB	3.66	113.80	110.53
8	17	308	CLA	C1D-CHD-C4C	-3.66	118.23	126.02
8	20	307	CLA	CHD-C1D-ND	-3.66	119.65	124.80
9	11	308	KC1	C1D-CHD-C4C	-3.66	117.63	126.25
9	14	304	KC1	C4B-C3B-C2B	-3.66	103.64	106.81
8	19	305	CLA	C1C-C2C-C3C	-3.66	103.13	106.98
9	18	304	KC1	C4B-C3B-C2B	-3.66	103.64	106.81
9	16	304	KC1	C2C-C1C-NC	3.66	114.98	110.45
10	15	316	A86	C33-C32-C31	3.66	112.77	109.21
8	14	308	CLA	C3C-C4C-NC	3.66	115.12	110.43
8	19	309	CLA	C1D-CHD-C4C	-3.66	118.25	126.02
8	18	302	CLA	C1C-C2C-C3C	-3.66	103.13	106.98
10	19	313	A86	C26-C25-C24	-3.66	112.61	123.20
9	12	310	KC1	C1A-NA-C4A	-3.66	105.01	106.68
8	18	310	CLA	C3B-C4B-NB	3.65	113.79	110.53
8	21	206	CLA	C1C-C2C-C3C	-3.65	103.14	106.98
9	13	310	KC1	C1D-CHD-C4C	-3.65	117.66	126.25
13	16	312	DD6	C19-C18-C17	3.65	117.62	110.79
8	19	302	CLA	C1C-C2C-C3C	-3.65	103.14	106.98
10	11	311	A86	C36-C31-C32	-3.65	116.08	119.70
9	11	302	KC1	C1D-CHD-C4C	-3.65	117.67	126.25
9	19	308	KC1	C4B-C3B-C2B	-3.65	103.65	106.81
8	12	307	CLA	C1D-CHD-C4C	-3.65	118.27	126.02
8	12	305	CLA	C1D-CHD-C4C	-3.64	118.27	126.02
8	15	308	CLA	C3B-C4B-NB	3.64	113.78	110.53
9	15	309	KC1	C4B-C3B-C2B	-3.64	103.66	106.81
10	12	314	A86	C41-C32-C31	-3.64	107.21	110.47
10	15	315	A86	C12-C11-C13	3.64	121.90	116.00
9	16	304	KC1	CBA-CAA-C2A	-3.64	110.86	125.45
8	19	309	CLA	C1C-C2C-C3C	-3.64	103.16	106.98
8	15	303	CLA	CBA-CAA-C2A	3.64	124.61	113.79
8	12	311	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
10	12	313	A86	C41-C32-C31	-3.63	107.22	110.47
8	21	208	CLA	C1D-CHD-C4C	-3.63	118.30	126.02
8	20	304	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
9	21	203	KC1	C1D-CHD-C4C	-3.63	117.71	126.25
9	15	304	KC1	C1D-CHD-C4C	-3.63	117.71	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	16	311	A86	C34-O4-C38	-3.63	111.44	117.85
8	16	309	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
8	16	301	CLA	CMC-C2C-C1C	3.63	130.70	125.03
8	20	308	CLA	C1C-C2C-C3C	-3.63	103.17	106.98
10	13	314	A86	C36-C31-C32	-3.63	116.10	119.70
9	12	310	KC1	C1D-CHD-C4C	-3.63	117.72	126.25
8	14	302	CLA	C3C-C4C-NC	3.62	115.07	110.43
9	12	306	KC1	C4C-C3C-C2C	-3.62	101.62	106.89
13	21	212	DD6	C21-C20-C15	-3.62	116.34	122.30
10	15	314	A86	C41-C32-C31	-3.62	107.23	110.47
9	13	307	KC1	C1A-NA-C4A	-3.62	105.03	106.68
8	16	303	CLA	C1D-CHD-C4C	-3.61	118.34	126.02
9	15	302	KC1	C1D-CHD-C4C	-3.61	117.75	126.25
8	11	307	CLA	CHD-C1D-ND	-3.61	119.72	124.80
8	19	303	CLA	C3C-C4C-NC	3.61	115.06	110.43
8	17	308	CLA	C1C-C2C-C3C	-3.61	103.18	106.98
8	21	209	CLA	C1C-C2C-C3C	-3.61	103.18	106.98
8	21	202	CLA	C1C-C2C-C3C	-3.61	103.18	106.98
10	19	313	A86	C40-C32-C31	-3.61	107.24	110.47
9	14	304	KC1	C1D-CHD-C4C	-3.61	117.76	126.25
9	16	308	KC1	C1D-CHD-C4C	-3.61	117.76	126.25
9	18	309	KC1	C1C-C2C-C3C	-3.61	103.19	106.98
8	19	302	CLA	CAA-C2A-C3A	-3.61	103.25	113.00
9	20	306	KC1	O2D-CGD-O1D	-3.61	116.83	123.85
8	14	301	CLA	C3C-C4C-NC	3.60	115.05	110.43
10	21	211	A86	C4-C5-C6	-3.60	122.23	127.28
9	12	310	KC1	C4B-C3B-C2B	-3.60	103.69	106.81
10	17	316	A86	C9-C8-C6	-3.60	116.50	126.36
10	16	310	A86	C3-C4-C5	-3.59	116.17	123.52
9	20	306	KC1	C1A-NA-C4A	-3.59	105.04	106.68
9	17	305	KC1	C4B-C3B-C2B	-3.59	103.70	106.81
8	21	205	CLA	C1C-C2C-C3C	-3.59	103.20	106.98
10	14	311	A86	C12-C11-C13	3.59	121.82	116.00
8	21	205	CLA	C1D-CHD-C4C	-3.59	118.40	126.02
9	17	306	KC1	C1D-CHD-C4C	-3.59	117.82	126.25
8	13	304	CLA	C3B-C4B-NB	3.58	113.73	110.53
10	18	311	A86	C3-C2-C1	-3.58	122.25	127.28
8	13	304	CLA	CAC-C3C-C4C	3.58	129.45	124.79
10	12	312	A86	C12-C11-C13	3.58	121.81	116.00
8	13	308	CLA	C4A-NA-C1A	-3.58	105.05	106.68
10	16	310	A86	C4-C5-C6	-3.58	122.26	127.28
10	15	316	A86	C41-C32-C31	-3.58	107.27	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	13	305	KC1	C1A-NA-C4A	-3.58	105.05	106.68
9	11	304	KC1	C1D-CHD-C4C	-3.58	117.84	126.25
8	12	305	CLA	C3C-C4C-NC	3.58	115.01	110.43
8	12	305	CLA	C1C-C2C-C3C	-3.57	103.22	106.98
10	14	315	A86	C41-C32-C31	-3.57	107.28	110.47
13	21	216	DD6	C37-C36-C35	-3.57	107.86	114.42
13	19	312	DD6	C37-C36-C35	-3.57	107.86	114.42
8	17	307	CLA	C1C-C2C-C3C	-3.56	103.23	106.98
8	19	307	CLA	C1C-C2C-C3C	-3.56	103.23	106.98
8	12	304	CLA	C3C-C4C-NC	3.56	115.00	110.43
8	11	309	CLA	C1D-CHD-C4C	-3.56	118.45	126.02
8	18	307	CLA	CHD-C1D-ND	-3.56	119.79	124.80
8	14	302	CLA	C1C-C2C-C3C	-3.56	103.24	106.98
8	14	307	CLA	C3C-C4C-NC	3.56	114.99	110.43
8	11	301	CLA	C4A-NA-C1A	-3.56	105.06	106.68
8	11	305	CLA	CAA-C2A-C3A	-3.55	103.39	113.00
10	13	316	A86	C41-C32-C31	-3.55	107.29	110.47
8	18	305	CLA	C3B-C4B-NB	3.55	113.70	110.53
10	12	302	A86	C41-C32-C31	-3.55	107.29	110.47
8	11	301	CLA	C2C-C1C-NC	3.55	113.71	109.98
8	21	210	CLA	C1C-C2C-C3C	-3.55	103.25	106.98
9	21	207	KC1	CAA-CBA-CGA	-3.55	109.01	127.05
10	15	312	A86	C3-C4-C5	-3.55	116.26	123.52
10	14	311	A86	C3-C2-C1	-3.55	122.31	127.28
10	21	215	A86	C25-C26-C27	-3.54	122.31	127.28
9	13	307	KC1	C1D-CHD-C4C	-3.54	117.91	126.25
8	15	301	CLA	C3C-C4C-NC	3.54	114.97	110.43
10	11	313	A86	C12-C11-C13	3.54	121.74	116.00
8	19	306	CLA	C2C-C1C-NC	3.54	113.70	109.98
8	13	308	CLA	C3C-C4C-NC	3.54	114.97	110.43
9	17	303	KC1	CBA-CAA-C2A	-3.54	111.24	125.45
8	20	309	CLA	C3C-C4C-NC	3.54	114.97	110.43
8	18	308	CLA	CHD-C1D-ND	-3.54	119.82	124.80
8	14	308	CLA	C3B-C4B-NB	3.54	113.69	110.53
9	11	304	KC1	CBA-CAA-C2A	-3.54	111.26	125.45
9	12	308	KC1	C4B-C3B-C2B	-3.53	103.75	106.81
8	17	308	CLA	CAC-C3C-C4C	3.53	129.39	124.79
10	14	315	A86	C33-C32-C31	3.53	112.64	109.21
8	20	304	CLA	C3D-C4D-ND	3.53	115.73	109.99
10	15	319	A86	C10-C9-C8	-3.53	112.98	123.20
9	13	303	KC1	CAA-CBA-CGA	-3.53	109.12	127.05
8	21	204	CLA	CBA-CAA-C2A	3.53	124.28	113.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	21	206	CLA	CAA-C2A-C3A	-3.53	103.47	113.00
8	16	303	CLA	CBA-CAA-C2A	3.52	124.28	113.79
8	17	310	CLA	C1-C2-C3	-3.52	120.42	126.20
10	13	313	A86	C12-C11-C13	3.52	121.72	116.00
8	18	302	CLA	C3C-C4C-NC	3.52	114.94	110.43
9	14	306	KC1	C2A-C1A-NA	3.52	114.99	109.34
8	21	208	CLA	CAC-C3C-C4C	3.52	129.37	124.79
8	18	303	CLA	C3C-C4C-NC	3.52	114.94	110.43
8	12	303	CLA	CAC-C3C-C4C	3.52	129.37	124.79
8	21	208	CLA	C4A-NA-C1A	-3.52	105.07	106.68
10	14	312	A86	C12-C11-C13	3.52	121.71	116.00
10	12	319	A86	C4-C3-C2	-3.52	116.32	123.52
13	19	312	DD6	C14-C13-C11	-3.52	120.07	125.53
8	13	301	CLA	C3C-C4C-NC	3.52	114.94	110.43
9	14	309	KC1	C4B-C3B-C2B	-3.52	103.77	106.81
9	13	305	KC1	C4B-C3B-C2B	-3.52	103.77	106.81
10	11	314	A86	C10-C9-C8	-3.51	113.02	123.20
10	12	313	A86	C36-C31-C32	-3.51	116.21	119.70
9	15	306	KC1	C1A-NA-C4A	-3.51	105.08	106.68
8	14	310	CLA	CAA-C2A-C3A	-3.51	103.51	113.00
8	14	303	CLA	C3B-C4B-NB	3.51	113.66	110.53
9	19	308	KC1	C2C-C1C-NC	3.51	114.80	110.45
10	18	314	A86	C3-C2-C1	-3.51	122.36	127.28
8	20	307	CLA	C3C-C4C-NC	3.51	114.92	110.43
10	12	319	A86	C7-C6-C8	3.50	123.44	118.09
8	12	309	CLA	C3C-C4C-NC	3.50	114.91	110.43
8	13	304	CLA	CBA-CAA-C2A	3.50	124.20	113.79
8	21	210	CLA	C3C-C4C-NC	3.50	114.91	110.43
8	21	202	CLA	C4B-C3B-C2B	-3.50	102.95	107.30
9	13	307	KC1	CBC-CAC-C3C	-3.49	102.95	112.42
10	19	313	A86	C19-C18-C17	3.49	117.32	110.79
8	12	311	CLA	O2D-CGD-O1D	-3.49	117.05	123.85
10	18	314	A86	C4-C3-C2	-3.49	116.37	123.52
10	12	312	A86	C25-C24-C1	-3.49	116.79	126.36
9	20	305	KC1	C1A-NA-C4A	-3.49	105.09	106.68
8	13	301	CLA	C3B-C4B-NB	3.49	113.64	110.53
8	17	307	CLA	CHD-C1D-ND	-3.48	119.90	124.80
8	13	309	CLA	CAC-C3C-C4C	3.48	129.32	124.79
10	13	312	A86	C10-C9-C8	-3.48	113.11	123.20
13	16	312	DD6	C21-C20-C19	-3.48	110.34	114.24
9	16	304	KC1	C1C-C2C-C3C	-3.48	103.32	106.98
8	16	306	CLA	C4B-C3B-C2B	-3.48	102.98	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	13	309	CLA	C3C-C4C-NC	3.48	114.88	110.43
8	17	304	CLA	C1D-CHD-C4C	-3.47	118.63	126.02
8	11	305	CLA	C3B-C4B-NB	3.47	113.63	110.53
8	15	307	CLA	C3C-C4C-NC	3.47	114.88	110.43
10	11	318	A86	C10-C9-C8	-3.47	113.14	123.20
9	15	304	KC1	CAA-CBA-CGA	-3.47	109.41	127.05
9	13	303	KC1	CBA-CAA-C2A	-3.47	111.53	125.45
9	17	305	KC1	CBA-CAA-C2A	-3.46	111.55	125.45
14	16	314	SQD	O47-C7-C8	3.46	118.97	111.48
9	20	303	KC1	CBA-CAA-C2A	-3.46	111.56	125.45
10	12	319	A86	C33-C32-C31	3.46	112.57	109.21
10	11	314	A86	C3-C4-C5	-3.46	116.44	123.52
8	14	307	CLA	CHD-C1D-ND	-3.46	119.93	124.80
9	16	305	KC1	C1C-C2C-C3C	-3.46	103.34	106.98
8	15	308	CLA	C1-C2-C3	-3.46	120.53	126.20
10	18	312	A86	C3-C4-C5	-3.46	116.44	123.52
9	21	207	KC1	C1D-CHD-C4C	-3.46	118.12	126.25
8	18	303	CLA	CHD-C1D-ND	-3.46	119.94	124.80
8	20	309	CLA	C4A-NA-C1A	-3.45	105.10	106.68
8	19	309	CLA	CAC-C3C-C4C	3.45	129.28	124.79
8	20	310	CLA	C3C-C4C-NC	3.45	114.85	110.43
8	14	301	CLA	CHD-C4C-NC	3.45	129.58	124.23
8	21	206	CLA	C3C-C4C-NC	3.45	114.85	110.43
10	17	314	A86	C10-C9-C8	-3.45	113.21	123.20
10	11	312	A86	C9-C8-C6	-3.45	116.91	126.36
10	14	314	A86	C12-C11-C13	3.44	121.59	116.00
10	12	315	A86	C4-C5-C6	-3.44	122.45	127.28
10	14	315	A86	C10-C9-C8	-3.44	113.22	123.20
9	17	305	KC1	C1D-CHD-C4C	-3.44	118.15	126.25
10	12	319	A86	C26-C25-C24	-3.44	113.23	123.20
8	17	302	CLA	C3C-C4C-NC	3.44	114.84	110.43
10	18	313	A86	C9-C8-C6	-3.44	116.93	126.36
9	11	306	KC1	C4B-C3B-C2B	-3.44	103.83	106.81
8	18	310	CLA	C3C-C4C-NC	3.43	114.83	110.43
8	14	310	CLA	C3B-C4B-NB	3.43	113.59	110.53
8	21	204	CLA	C3B-C4B-NB	3.43	113.59	110.53
8	12	311	CLA	C3C-C4C-NC	3.43	114.83	110.43
10	18	311	A86	C7-C6-C8	3.43	123.33	118.09
8	12	309	CLA	C1C-C2C-C3C	-3.43	103.37	106.98
8	19	306	CLA	C4C-C3C-C2C	-3.43	101.90	106.89
9	16	302	KC1	CBC-CAC-C3C	-3.43	103.13	112.42
8	15	308	CLA	C3C-C4C-NC	3.43	114.82	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	14	309	KC1	C1C-C2C-C3C	-3.42	103.38	106.98
11	16	315	LMG	O6-C1-O1	-3.42	101.95	110.04
8	13	308	CLA	C3B-C4B-NB	3.42	113.58	110.53
8	19	306	CLA	CHD-C1D-ND	-3.42	119.99	124.80
9	20	306	KC1	C4C-C3C-C2C	-3.42	101.91	106.89
8	16	307	CLA	C3C-C4C-NC	3.41	114.80	110.43
8	14	301	CLA	C4A-NA-C1A	-3.41	105.12	106.68
9	18	304	KC1	C1D-CHD-C4C	-3.41	118.22	126.25
9	14	309	KC1	CMA-C3A-C2A	-3.41	120.18	128.43
10	11	310	A86	C35-C34-C33	3.41	116.01	109.89
8	18	305	CLA	C3C-C4C-NC	3.41	114.80	110.43
10	14	311	A86	C3-C4-C5	-3.41	116.55	123.52
8	20	304	CLA	CMC-C2C-C1C	3.40	130.35	125.03
8	15	303	CLA	C3C-C4C-NC	3.40	114.79	110.43
9	12	310	KC1	CMA-C3A-C2A	-3.40	120.19	128.43
8	13	302	CLA	C3C-C4C-NC	3.40	114.78	110.43
8	14	308	CLA	CHC-C1C-C2C	-3.40	117.29	126.95
8	21	205	CLA	C3C-C4C-NC	3.40	114.78	110.43
9	17	309	KC1	C2C-C1C-NC	3.39	114.65	110.45
8	20	302	CLA	C1C-C2C-C3C	-3.39	103.41	106.98
10	17	314	A86	C25-C26-C27	-3.39	122.52	127.28
10	14	314	A86	C10-C9-C8	-3.39	113.37	123.20
9	17	309	KC1	C1C-C2C-C3C	-3.39	103.41	106.98
8	20	302	CLA	C3C-C4C-NC	3.39	114.77	110.43
10	12	316	A86	C3-C2-C1	-3.39	122.52	127.28
10	15	319	A86	C25-C24-C1	-3.39	117.08	126.36
9	21	207	KC1	CHD-C1D-ND	-3.38	118.97	124.05
8	20	304	CLA	C1-O2A-CGA	3.38	124.84	116.65
8	11	303	CLA	CAC-C3C-C4C	3.38	129.19	124.79
8	15	301	CLA	C4A-NA-C1A	-3.38	105.14	106.68
10	12	315	A86	C36-C31-C32	-3.38	116.34	119.70
8	12	301	CLA	C4B-C3B-C2B	-3.38	103.10	107.30
10	21	213	A86	C35-C34-C33	3.38	115.95	109.89
8	12	303	CLA	C3C-C4C-NC	3.38	114.75	110.43
8	11	305	CLA	C4A-NA-C1A	-3.38	105.14	106.68
9	14	309	KC1	C2C-C1C-NC	3.38	114.63	110.45
8	15	305	CLA	C3C-C4C-NC	3.37	114.75	110.43
10	11	310	A86	C12-C11-C13	3.37	121.47	116.00
8	19	305	CLA	CAA-C2A-C3A	-3.37	103.89	113.00
10	18	313	A86	C3-C4-C5	-3.37	116.62	123.52
8	17	308	CLA	C3C-C4C-NC	3.37	114.75	110.43
10	17	313	A86	C4-C3-C2	-3.37	116.62	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	13	309	CLA	C3B-C4B-NB	3.37	113.54	110.53
10	17	314	A86	C12-C11-C13	3.37	121.46	116.00
10	13	315	A86	C41-C32-C31	-3.36	107.46	110.47
9	12	310	KC1	C2C-C1C-NC	3.36	114.61	110.45
9	13	310	KC1	CBC-CAC-C3C	-3.36	103.31	112.42
9	14	306	KC1	O2D-CGD-O1D	-3.36	117.31	123.85
9	11	302	KC1	CAA-CBA-CGA	-3.36	109.96	127.05
8	18	308	CLA	C3B-C4B-NB	3.36	113.53	110.53
8	19	307	CLA	C3B-C4B-NB	3.36	113.53	110.53
9	15	309	KC1	CMA-C3A-C2A	-3.36	120.30	128.43
9	12	310	KC1	C1C-C2C-C3C	-3.36	103.45	106.98
8	13	308	CLA	CHD-C1D-ND	-3.36	120.08	124.80
10	21	215	A86	C34-O4-C38	-3.36	111.92	117.85
8	21	206	CLA	CHD-C4C-NC	3.35	129.43	124.23
8	21	208	CLA	C3B-C4B-NB	3.35	113.52	110.53
8	12	311	CLA	CAA-C2A-C3A	-3.35	103.95	113.00
10	13	312	A86	C3-C2-C1	-3.35	122.58	127.28
10	12	316	A86	C33-C32-C31	3.35	112.47	109.21
8	19	306	CLA	CAC-C3C-C4C	3.35	129.15	124.79
9	17	309	KC1	CAC-C3C-C4C	3.35	129.14	124.79
9	16	305	KC1	C4C-C3C-C2C	-3.35	102.02	106.89
10	14	312	A86	C40-C32-C31	-3.35	107.48	110.47
10	11	310	A86	C3-C2-C1	-3.34	122.59	127.28
10	14	311	A86	C10-C9-C8	-3.34	113.52	123.20
8	14	301	CLA	CMC-C2C-C1C	3.34	130.25	125.03
9	16	308	KC1	CAC-C3C-C4C	3.34	129.14	124.79
10	12	302	A86	C12-C11-C13	3.34	121.42	116.00
8	19	303	CLA	C1-C2-C3	-3.34	120.72	126.20
8	15	307	CLA	C1C-C2C-C3C	-3.34	103.47	106.98
8	14	307	CLA	CAC-C3C-C4C	3.34	129.13	124.79
8	20	309	CLA	C3B-C4B-NB	3.34	113.51	110.53
9	17	305	KC1	CHD-C1D-ND	-3.33	119.05	124.05
8	20	307	CLA	CAA-C2A-C3A	-3.33	104.00	113.00
8	20	308	CLA	C3C-C4C-NC	3.33	114.70	110.43
8	18	301	CLA	C1-C2-C3	-3.33	120.74	126.20
9	16	302	KC1	C2A-C1A-NA	3.33	114.68	109.34
10	16	311	A86	C41-C32-C31	-3.33	107.49	110.47
8	15	310	CLA	C3C-C4C-NC	3.33	114.69	110.43
10	11	318	A86	C3-C4-C5	-3.33	116.71	123.52
9	16	304	KC1	CAA-CBA-CGA	-3.32	110.14	127.05
10	17	314	A86	C4-C5-C6	-3.32	122.62	127.28
9	16	308	KC1	CBA-CAA-C2A	-3.32	112.12	125.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	19	311	A86	C4-C5-C6	-3.32	122.62	127.28
8	16	309	CLA	C3C-C4C-NC	3.32	114.68	110.43
8	14	305	CLA	CAA-C2A-C3A	-3.32	104.03	113.00
10	12	312	A86	C41-C32-C31	-3.32	107.50	110.47
8	13	311	CLA	C3B-C4B-NB	3.31	113.49	110.53
8	11	301	CLA	CHD-C4C-NC	3.31	129.37	124.23
10	21	214	A86	C25-C26-C27	-3.31	122.63	127.28
8	14	308	CLA	CAC-C3C-C4C	3.31	129.10	124.79
10	16	313	A86	C26-C25-C24	-3.31	113.61	123.20
9	11	306	KC1	CHD-C4C-NC	3.30	129.29	124.31
8	19	309	CLA	C3C-C4C-NC	3.30	114.66	110.43
9	18	304	KC1	CAC-C3C-C4C	3.30	129.09	124.79
8	18	302	CLA	C1-C2-C3	-3.30	120.78	126.20
8	13	311	CLA	C3C-C4C-NC	3.30	114.66	110.43
8	19	305	CLA	C1-O2A-CGA	3.30	124.64	116.65
8	18	307	CLA	C3B-C4B-NB	3.30	113.48	110.53
8	16	306	CLA	C1C-C2C-C3C	-3.30	103.51	106.98
9	11	302	KC1	CBA-CAA-C2A	-3.30	112.21	125.45
8	14	308	CLA	C4B-C3B-C2B	-3.30	103.20	107.30
8	21	202	CLA	CHC-C1C-C2C	-3.30	117.58	126.95
9	13	303	KC1	CAC-C3C-C4C	3.29	129.08	124.79
10	17	316	A86	C33-C32-C31	3.29	112.41	109.21
9	20	303	KC1	CAA-CBA-CGA	-3.29	110.31	127.05
9	12	306	KC1	CHD-C4C-NC	3.29	129.27	124.31
8	15	303	CLA	CAC-C3C-C4C	3.29	129.07	124.79
10	19	311	A86	C41-C32-C31	-3.29	107.53	110.47
10	12	315	A86	C10-C9-C8	-3.29	113.67	123.20
10	13	315	A86	C12-C11-C13	3.29	121.33	116.00
9	11	308	KC1	CAC-C3C-C4C	3.28	129.06	124.79
8	19	302	CLA	C3C-C4C-NC	3.28	114.64	110.43
8	14	303	CLA	C3C-C4C-NC	3.28	114.63	110.43
8	11	301	CLA	C4C-C3C-C2C	-3.28	102.11	106.89
10	15	315	A86	C41-C32-C31	-3.28	107.54	110.47
8	20	309	CLA	CAC-C3C-C4C	3.28	129.05	124.79
10	11	318	A86	C28-C27-C26	3.28	128.12	122.82
8	21	205	CLA	C3B-C4B-NB	3.28	113.45	110.53
13	20	314	DD6	C21-C20-C19	-3.27	110.56	114.24
8	13	302	CLA	C1C-C2C-C3C	-3.27	103.54	106.98
10	11	314	A86	C25-C24-C1	-3.27	117.39	126.36
8	12	304	CLA	CHC-C1C-C2C	-3.27	117.66	126.95
8	12	305	CLA	C3B-C4B-NB	3.27	113.45	110.53
9	20	306	KC1	C1D-CHD-C4C	-3.26	118.57	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	12	315	A86	C3-C4-C5	-3.26	116.84	123.52
10	12	313	A86	C10-C9-C8	-3.26	113.75	123.20
9	18	306	KC1	CAC-C3C-C4C	3.26	129.03	124.79
10	12	312	A86	C4-C5-C6	-3.26	122.70	127.28
8	12	307	CLA	C3C-C4C-NC	3.26	114.61	110.43
9	14	309	KC1	CAC-C3C-C4C	3.26	129.03	124.79
8	16	307	CLA	C4B-C3B-C2B	-3.26	103.25	107.30
9	15	302	KC1	CAA-CBA-CGA	-3.26	110.48	127.05
9	18	304	KC1	CHD-C1D-ND	-3.26	119.16	124.05
8	19	304	CLA	C4C-C3C-C2C	-3.26	102.15	106.89
8	19	307	CLA	CHC-C1C-C2C	-3.26	117.70	126.95
8	14	305	CLA	C3C-C4C-NC	3.25	114.60	110.43
8	12	301	CLA	C3B-C4B-NB	3.25	113.44	110.53
9	12	308	KC1	CBA-CAA-C2A	-3.25	112.40	125.45
8	15	308	CLA	CED-O2D-CGD	3.25	123.29	115.92
8	14	305	CLA	C3B-C4B-NB	3.25	113.43	110.53
8	19	304	CLA	C1D-CHD-C4C	-3.25	119.11	126.02
9	15	304	KC1	CHD-C1D-ND	-3.25	119.17	124.05
8	19	310	CLA	CHC-C1C-C2C	-3.25	117.72	126.95
8	19	301	CLA	CHD-C4C-NC	3.25	129.27	124.23
8	16	301	CLA	C4C-C3C-C2C	-3.25	102.17	106.89
9	13	303	KC1	CAB-C3B-C4B	3.25	132.57	124.82
13	20	312	DD6	C37-C36-C35	-3.25	108.45	114.42
10	14	315	A86	C12-C11-C13	3.25	121.26	116.00
8	13	306	CLA	C3C-C4C-NC	3.24	114.59	110.43
9	12	310	KC1	CAC-C3C-C4C	3.24	129.01	124.79
8	15	308	CLA	CHC-C1C-C2C	-3.24	117.73	126.95
9	20	305	KC1	CAA-CBA-CGA	-3.24	110.56	127.05
8	18	302	CLA	CHC-C1C-C2C	-3.24	117.73	126.95
9	16	302	KC1	CMB-C2B-C1B	3.24	130.44	124.73
8	20	307	CLA	CAC-C3C-C4C	3.24	129.01	124.79
9	17	303	KC1	CAA-CBA-CGA	-3.24	110.57	127.05
8	21	204	CLA	C4-C3-C5	3.24	120.85	115.23
8	20	302	CLA	CAC-C3C-C4C	3.24	129.00	124.79
8	20	302	CLA	C4-C3-C5	3.24	120.85	115.23
10	14	316	A86	C12-C11-C13	3.24	121.25	116.00
8	16	303	CLA	CAC-C3C-C4C	3.24	129.00	124.79
10	18	311	A86	C34-O4-C38	-3.24	112.13	117.85
8	15	303	CLA	C4B-C3B-C2B	-3.24	103.28	107.30
9	11	308	KC1	CHD-C1D-ND	-3.24	119.20	124.05
8	19	307	CLA	C4B-C3B-C2B	-3.23	103.28	107.30
10	12	313	A86	C3-C4-C5	-3.23	116.90	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	19	306	CLA	CHD-C4C-NC	3.23	129.25	124.23
9	18	309	KC1	CAC-C3C-C4C	3.23	129.00	124.79
9	21	207	KC1	C1C-C2C-C3C	-3.23	103.58	106.98
8	12	309	CLA	C4-C3-C5	3.23	120.84	115.23
10	14	314	A86	C36-C31-C32	-3.23	116.49	119.70
9	20	303	KC1	CHD-C4C-NC	3.23	129.17	124.31
10	12	302	A86	C35-C34-C33	3.22	115.68	109.89
8	21	209	CLA	C3C-C4C-NC	3.22	114.56	110.43
8	14	301	CLA	CAC-C3C-C4C	3.22	128.98	124.79
8	17	310	CLA	C3C-C4C-NC	3.22	114.56	110.43
9	15	302	KC1	CBA-CAA-C2A	-3.22	112.53	125.45
8	12	303	CLA	C1C-C2C-C3C	-3.22	103.59	106.98
10	13	315	A86	C3-C4-C5	-3.22	116.94	123.52
8	13	304	CLA	C3C-C4C-NC	3.22	114.55	110.43
8	15	308	CLA	C4B-C3B-C2B	-3.21	103.31	107.30
8	12	309	CLA	O2D-CGD-O1D	-3.21	117.59	123.85
8	11	303	CLA	C3C-C4C-NC	3.21	114.55	110.43
8	21	202	CLA	C4A-NA-C1A	-3.21	105.21	106.68
8	12	301	CLA	C3C-C4C-NC	3.21	114.55	110.43
9	21	203	KC1	CAC-C3C-C4C	3.21	128.97	124.79
8	16	307	CLA	C1-C2-C3	-3.21	120.94	126.20
8	13	309	CLA	CHC-C1C-C2C	-3.21	117.83	126.95
13	20	312	DD6	C12-C11-C13	-3.21	113.19	118.09
9	19	308	KC1	CBA-CAA-C2A	-3.20	112.61	125.45
10	21	213	A86	C36-C31-C32	-3.20	116.52	119.70
9	14	309	KC1	CHD-C4C-NC	3.20	129.13	124.31
8	11	305	CLA	C3C-C4C-NC	3.20	114.53	110.43
8	12	304	CLA	CAA-C2A-C1A	3.20	122.46	111.97
8	15	307	CLA	CHD-C4C-NC	3.20	129.19	124.23
8	19	305	CLA	C4-C3-C5	3.20	119.89	116.13
10	15	312	A86	C36-C31-C32	-3.20	116.52	119.70
8	14	307	CLA	C1C-C2C-C3C	-3.20	103.62	106.98
10	11	318	A86	C25-C24-C1	-3.20	117.60	126.36
10	19	311	A86	C12-C11-C13	3.20	121.18	116.00
8	19	304	CLA	C3C-C4C-NC	3.19	114.52	110.43
8	19	303	CLA	C1C-C2C-C3C	-3.19	103.62	106.98
10	15	315	A86	C21-C20-C15	-3.19	113.05	123.35
9	15	306	KC1	C4B-C3B-C2B	-3.19	104.05	106.81
9	18	309	KC1	C2A-C1A-NA	3.19	114.45	109.34
10	15	313	A86	C12-C11-C13	3.19	121.17	116.00
8	12	303	CLA	CHD-C4C-NC	3.19	129.17	124.23
8	15	310	CLA	C3B-C4B-NB	3.18	113.37	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	11	318	A86	C25-C26-C27	3.18	131.74	127.28
13	16	312	DD6	C3-C4-C5	-3.18	117.00	123.52
8	18	302	CLA	CAA-C2A-C1A	3.18	122.41	111.97
9	11	304	KC1	CHD-C1D-ND	-3.18	119.28	124.05
10	14	312	A86	C10-C9-C8	-3.18	113.98	123.20
8	21	205	CLA	CAA-C2A-C3A	-3.18	104.41	113.00
10	11	313	A86	C8-C6-C5	-3.18	114.01	119.01
8	13	301	CLA	CHC-C1C-C2C	-3.18	117.92	126.95
10	11	311	A86	C41-C32-C31	-3.18	107.63	110.47
9	20	306	KC1	CHD-C1D-ND	-3.18	119.28	124.05
8	20	302	CLA	C1-C2-C3	-3.17	121.00	126.20
10	17	315	A86	C25-C24-C1	-3.17	117.66	126.36
10	18	313	A86	C36-C31-C32	-3.17	116.55	119.70
8	16	301	CLA	CHD-C4C-NC	3.17	129.15	124.23
8	18	310	CLA	CHC-C1C-C2C	-3.17	117.93	126.95
8	19	307	CLA	C4C-C3C-C2C	-3.17	102.28	106.89
8	20	308	CLA	C3B-C4B-NB	3.17	113.36	110.53
10	17	312	A86	C12-C11-C13	3.17	121.14	116.00
8	14	310	CLA	CHC-C1C-C2C	-3.17	117.94	126.95
9	20	305	KC1	CHD-C1D-ND	-3.17	119.30	124.05
9	14	304	KC1	CHD-C1D-ND	-3.17	119.30	124.05
8	13	306	CLA	C3B-C4B-NB	3.17	113.36	110.53
10	15	312	A86	C34-O4-C38	-3.17	112.25	117.85
8	19	307	CLA	CAA-C2A-C3A	-3.17	104.44	113.00
8	21	208	CLA	CHC-C1C-C2C	-3.17	117.95	126.95
8	20	309	CLA	CHC-C1C-C2C	-3.17	117.95	126.95
8	11	301	CLA	CAC-C3C-C4C	3.17	128.91	124.79
8	17	304	CLA	CHC-C1C-C2C	-3.16	117.96	126.95
10	18	311	A86	C41-C32-C31	-3.16	107.64	110.47
8	15	307	CLA	CMC-C2C-C1C	3.16	129.98	125.03
8	21	202	CLA	C3C-C4C-NC	3.16	114.48	110.43
10	16	311	A86	C4-C3-C2	-3.16	117.05	123.52
9	19	308	KC1	CHD-C4C-NC	3.16	129.07	124.31
9	12	310	KC1	O2D-CGD-O1D	-3.16	117.70	123.85
10	19	313	A86	C21-C20-C15	-3.16	113.15	123.35
8	14	308	CLA	C4A-NA-C1A	-3.16	105.24	106.68
8	15	305	CLA	C3B-C4B-NB	3.16	113.35	110.53
8	21	209	CLA	CAC-C3C-C4C	3.16	128.90	124.79
10	15	319	A86	C41-C32-C31	-3.16	107.65	110.47
8	19	303	CLA	CAC-C3C-C4C	3.15	128.89	124.79
8	20	310	CLA	CHC-C1C-C2C	-3.15	117.99	126.95
10	15	316	A86	C3-C2-C1	-3.15	122.86	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	13	307	KC1	CHD-C1D-ND	-3.15	119.32	124.05
8	21	205	CLA	CHC-C1C-C2C	-3.15	118.00	126.95
14	17	301	SQD	O9-S-C6	3.15	111.46	106.76
14	16	314	SQD	O48-C23-C24	3.15	121.44	111.83
8	17	307	CLA	CAA-C2A-C1A	3.15	122.29	111.97
8	16	306	CLA	CMC-C2C-C1C	3.15	129.95	125.03
8	20	307	CLA	C4C-C3C-C2C	-3.15	102.31	106.89
8	18	301	CLA	CHD-C4C-NC	3.15	129.11	124.23
8	19	301	CLA	C4C-C3C-C2C	-3.15	102.31	106.89
8	19	303	CLA	CHD-C4C-NC	3.15	129.11	124.23
8	14	305	CLA	CHC-C1C-C2C	-3.14	118.02	126.95
9	15	306	KC1	CAA-CBA-CGA	-3.14	111.07	127.05
9	11	308	KC1	C2A-C1A-NA	3.14	114.38	109.34
8	11	303	CLA	CHC-C1C-C2C	-3.14	118.02	126.95
8	14	302	CLA	CHC-C1C-C2C	-3.14	118.03	126.95
14	16	314	SQD	O5-C5-C4	3.14	115.36	109.70
8	18	308	CLA	C4B-C3B-C2B	-3.14	103.40	107.30
10	13	313	A86	C3-C4-C5	-3.14	117.10	123.52
10	16	313	A86	C4-C3-C2	-3.14	117.10	123.52
8	14	303	CLA	CAC-C3C-C4C	3.14	128.87	124.79
10	13	312	A86	C7-C6-C8	3.13	122.88	118.09
8	14	310	CLA	C3C-C4C-NC	3.13	114.45	110.43
8	18	301	CLA	C4C-C3C-C2C	-3.13	102.33	106.89
9	16	302	KC1	CAA-CBA-CGA	-3.13	111.12	127.05
10	11	314	A86	C36-C31-C32	-3.13	116.59	119.70
9	16	302	KC1	CMA-C3A-C2A	-3.13	120.85	128.43
9	16	304	KC1	C4C-C3C-C2C	-3.13	102.33	106.89
10	15	313	A86	C21-C20-C15	-3.13	113.24	123.35
8	21	208	CLA	C3C-C4C-NC	3.13	114.44	110.43
9	18	309	KC1	C1A-NA-C4A	-3.13	105.25	106.68
13	20	314	DD6	C24-C1-C2	-3.13	114.09	119.01
8	16	303	CLA	C3C-C4C-NC	3.13	114.44	110.43
8	17	304	CLA	C3C-C4C-NC	3.13	114.44	110.43
8	11	301	CLA	C1-C2-C3	-3.13	121.07	126.20
9	12	310	KC1	CHD-C1D-ND	-3.13	119.36	124.05
8	16	303	CLA	CHC-C1C-C2C	-3.13	118.06	126.95
8	18	303	CLA	C4B-C3B-C2B	-3.13	103.41	107.30
8	12	304	CLA	C4B-C3B-C2B	-3.13	103.42	107.30
11	17	318	LMG	C1-C2-C3	-3.12	103.44	110.01
9	16	305	KC1	CBA-CAA-C2A	-3.12	112.92	125.45
9	13	305	KC1	CHD-C1D-ND	-3.12	119.36	124.05
9	16	305	KC1	CAA-CBA-CGA	-3.12	111.17	127.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	13	309	CLA	CMB-C2B-C1B	3.12	130.17	125.42
9	17	306	KC1	C4C-C3C-C2C	-3.12	102.35	106.89
10	15	311	A86	C12-C11-C13	3.12	121.06	116.00
8	21	209	CLA	CHC-C1C-C2C	-3.12	118.09	126.95
10	13	313	A86	C34-O4-C38	-3.12	112.34	117.85
10	21	214	A86	C41-C32-C31	-3.12	107.68	110.47
9	16	308	KC1	C1A-NA-C4A	-3.11	105.26	106.68
8	17	304	CLA	CAC-C3C-C4C	3.11	128.84	124.79
8	11	309	CLA	C3B-C4B-NB	3.11	113.31	110.53
8	13	301	CLA	C4B-C3B-C2B	-3.11	103.43	107.30
8	12	304	CLA	O2A-CGA-CBA	3.11	121.33	111.83
8	14	303	CLA	O2A-CGA-CBA	3.11	121.32	111.83
10	17	313	A86	C21-C20-C15	-3.11	113.31	123.35
10	14	312	A86	C26-C25-C24	-3.11	114.19	123.20
8	19	306	CLA	CMB-C2B-C1B	3.11	130.15	125.42
9	21	207	KC1	CAC-C3C-C4C	3.11	128.83	124.79
9	15	306	KC1	CHD-C1D-ND	-3.11	119.39	124.05
8	13	309	CLA	C4B-C3B-C2B	-3.10	103.44	107.30
8	18	303	CLA	C4C-C3C-C2C	-3.10	102.37	106.89
8	11	307	CLA	CHD-C4C-NC	3.10	129.04	124.23
8	11	305	CLA	CHC-C1C-C2C	-3.10	118.13	126.95
9	20	303	KC1	CHD-C1D-ND	-3.10	119.40	124.05
9	14	304	KC1	CAA-CBA-CGA	-3.10	111.28	127.05
8	20	304	CLA	CAC-C3C-C4C	3.10	128.82	124.79
9	13	310	KC1	CHD-C1D-ND	-3.10	119.40	124.05
8	18	303	CLA	C1C-C2C-C3C	-3.10	103.72	106.98
8	20	304	CLA	C3B-C4B-NB	3.10	113.29	110.53
10	13	316	A86	C35-C34-C33	3.10	115.45	109.89
9	15	302	KC1	CHD-C1D-ND	-3.09	119.41	124.05
10	21	215	A86	C12-C11-C13	3.09	121.01	116.00
8	20	308	CLA	CAC-C3C-C4C	3.09	128.81	124.79
10	14	312	A86	C3-C4-C5	-3.09	117.19	123.52
8	13	311	CLA	CAA-C2A-C3A	-3.09	104.65	113.00
9	17	309	KC1	C2A-C1A-NA	3.09	114.29	109.34
10	18	311	A86	C10-C9-C8	-3.09	114.25	123.20
10	18	312	A86	C26-C25-C24	-3.09	114.26	123.20
10	12	302	A86	C3-C4-C5	-3.09	117.20	123.52
9	12	308	KC1	CAA-CBA-CGA	-3.09	111.36	127.05
9	17	309	KC1	CHD-C1D-ND	-3.08	119.42	124.05
9	13	310	KC1	CAC-C3C-C4C	3.08	128.80	124.79
10	19	311	A86	C28-C27-C26	3.08	127.81	122.82
8	19	305	CLA	CHC-C1C-C2C	-3.08	118.19	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	18	305	CLA	C4B-C3B-C2B	-3.08	103.47	107.30
9	21	207	KC1	C2C-C1C-NC	3.08	114.26	110.45
8	16	307	CLA	CHD-C4C-NC	3.08	129.01	124.23
10	14	312	A86	C41-C32-C31	-3.08	107.72	110.47
8	18	310	CLA	C4C-C3C-C2C	-3.08	102.41	106.89
9	17	309	KC1	CHD-C4C-NC	3.08	128.95	124.31
8	12	301	CLA	CHC-C1C-C2C	-3.08	118.19	126.95
9	15	304	KC1	CAC-C3C-C4C	3.08	128.80	124.79
8	14	302	CLA	CMB-C2B-C1B	3.08	130.11	125.42
8	21	210	CLA	C3B-C4B-NB	3.08	113.28	110.53
8	17	304	CLA	C4B-C3B-C2B	-3.08	103.47	107.30
10	18	312	A86	C21-C20-C15	-3.08	113.41	123.35
8	11	303	CLA	C1-O2A-CGA	3.08	124.10	116.65
9	11	302	KC1	C1A-NA-C4A	-3.08	105.28	106.68
8	15	310	CLA	CHC-C1C-C2C	-3.07	118.21	126.95
10	12	314	A86	C36-C31-C32	-3.07	116.64	119.70
8	18	301	CLA	CAC-C3C-C4C	3.07	128.79	124.79
9	15	306	KC1	CHD-C4C-NC	3.07	128.94	124.31
8	14	307	CLA	C4C-C3C-C2C	-3.07	102.42	106.89
8	19	301	CLA	C1C-C2C-C3C	-3.07	103.75	106.98
9	16	308	KC1	O2D-CGD-O1D	-3.07	117.86	123.85
8	21	204	CLA	CHC-C1C-C2C	-3.07	118.22	126.95
9	18	306	KC1	C4C-C3C-C2C	-3.07	102.42	106.89
8	17	307	CLA	C3B-C4B-NB	3.07	113.27	110.53
9	13	303	KC1	CHD-C1D-ND	-3.07	119.44	124.05
10	13	315	A86	C25-C24-C1	-3.07	117.95	126.36
8	12	307	CLA	C3B-C4B-NB	3.07	113.27	110.53
13	21	216	DD6	C23-C16-C15	3.07	118.33	110.05
8	19	309	CLA	CHC-C1C-C2C	-3.07	118.23	126.95
8	13	302	CLA	CHD-C4C-NC	3.07	128.99	124.23
8	14	310	CLA	C4B-C3B-C2B	-3.07	103.49	107.30
9	13	307	KC1	CHD-C4C-NC	3.07	128.93	124.31
10	11	318	A86	C4-C5-C6	-3.07	122.98	127.28
10	14	316	A86	C41-C32-C31	-3.07	107.73	110.47
8	12	304	CLA	CMB-C2B-C1B	3.07	130.09	125.42
9	17	303	KC1	CHD-C4C-NC	3.07	128.93	124.31
9	13	307	KC1	CAA-CBA-CGA	-3.07	111.46	127.05
9	19	308	KC1	CAA-CBA-CGA	-3.06	111.47	127.05
8	19	302	CLA	C4B-C3B-C2B	-3.06	103.49	107.30
9	16	302	KC1	CAB-C3B-C4B	3.06	132.13	124.82
8	15	307	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
8	18	303	CLA	CHD-C4C-NC	3.06	128.98	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	14	301	CLA	C4C-C3C-C2C	-3.06	102.44	106.89
8	15	301	CLA	CHD-C4C-NC	3.06	128.98	124.23
9	17	309	KC1	CBC-CAC-C3C	-3.06	104.12	112.42
8	21	206	CLA	C3B-C4B-NB	3.06	113.26	110.53
10	17	312	A86	C34-O4-C38	-3.06	112.45	117.85
8	11	309	CLA	C4C-C3C-C2C	-3.06	102.44	106.89
9	14	309	KC1	CHD-C1D-ND	-3.06	119.47	124.05
10	16	310	A86	C35-C34-C33	3.05	115.37	109.89
9	21	203	KC1	CAA-CBA-CGA	-3.05	111.52	127.05
10	12	319	A86	C-C1-C24	3.05	122.75	118.09
10	14	313	A86	C21-C20-C15	-3.05	113.50	123.35
8	11	303	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
13	19	312	DD6	C25-C24-C1	-3.05	118.00	126.36
8	19	303	CLA	C4C-C3C-C2C	-3.05	102.45	106.89
9	13	305	KC1	CAA-CBA-CGA	-3.05	111.54	127.05
8	19	304	CLA	C1C-C2C-C3C	-3.05	103.77	106.98
10	12	312	A86	C10-C9-C8	-3.05	114.37	123.20
8	19	306	CLA	CMC-C2C-C1C	3.05	129.80	125.03
8	18	308	CLA	CHC-C1C-C2C	-3.04	118.30	126.95
8	18	308	CLA	C4A-NA-C1A	-3.04	105.29	106.68
9	18	306	KC1	C1A-NA-C4A	-3.04	105.29	106.68
9	16	304	KC1	CHD-C1D-ND	-3.04	119.49	124.05
9	16	305	KC1	CHD-C1D-ND	-3.04	119.49	124.05
9	11	302	KC1	CHD-C1D-ND	-3.04	119.49	124.05
8	19	304	CLA	CHC-C1C-C2C	-3.04	118.31	126.95
10	16	311	A86	C40-C32-C31	-3.04	107.75	110.47
8	21	205	CLA	C4C-C3C-C2C	-3.04	102.47	106.89
10	12	302	A86	C26-C25-C24	-3.04	114.40	123.20
8	16	306	CLA	CHD-C4C-NC	3.04	128.94	124.23
9	21	207	KC1	CHD-C4C-NC	3.04	128.88	124.31
10	19	313	A86	C9-C8-C6	-3.04	118.04	126.36
8	13	309	CLA	C4C-C3C-C2C	-3.04	102.47	106.89
10	17	311	A86	C23-C16-C22	-3.03	102.96	107.37
10	14	311	A86	C4-C3-C2	-3.03	117.31	123.52
9	18	309	KC1	O2D-CGD-O1D	-3.03	117.94	123.85
8	20	308	CLA	CHC-C1C-C2C	-3.03	118.33	126.95
8	21	204	CLA	CAC-C3C-C4C	3.03	128.74	124.79
8	11	301	CLA	CMC-C2C-C1C	3.03	129.77	125.03
8	14	307	CLA	CAA-C2A-C1A	3.03	121.91	111.97
10	16	311	A86	C26-C25-C24	-3.03	114.42	123.20
9	21	207	KC1	C4C-C3C-C2C	-3.03	102.48	106.89
10	12	316	A86	C21-C20-C15	-3.03	113.57	123.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	11	307	CLA	O2A-CGA-CBA	3.03	121.06	111.83
8	21	204	CLA	C3C-C4C-NC	3.02	114.31	110.43
8	20	310	CLA	CHD-C4C-NC	3.02	128.92	124.23
8	11	307	CLA	C4C-C3C-C2C	-3.02	102.49	106.89
8	18	303	CLA	C3B-C4B-NB	3.02	113.23	110.53
8	13	308	CLA	CHC-C1C-C2C	-3.02	118.36	126.95
8	14	307	CLA	CHC-C1C-C2C	-3.02	118.36	126.95
8	16	301	CLA	C1-C2-C3	-3.02	121.25	126.20
8	17	307	CLA	CMC-C2C-C1C	3.02	129.75	125.03
8	15	301	CLA	CMB-C2B-C1B	3.02	130.02	125.42
8	17	310	CLA	CED-O2D-CGD	3.02	122.76	115.92
8	13	304	CLA	CHC-C1C-C2C	-3.02	118.38	126.95
8	18	303	CLA	CAC-C3C-C4C	3.02	128.71	124.79
8	12	309	CLA	CAC-C3C-C4C	3.01	128.71	124.79
8	13	306	CLA	CHC-C1C-C2C	-3.01	118.38	126.95
8	11	309	CLA	CAA-C2A-C3A	-3.01	104.86	113.00
9	16	308	KC1	CHD-C1D-ND	-3.01	119.53	124.05
8	13	309	CLA	O2A-CGA-CBA	3.01	121.02	111.83
8	17	302	CLA	C4C-C3C-C2C	-3.01	102.51	106.89
8	12	303	CLA	C3B-C4B-NB	3.01	113.22	110.53
8	16	303	CLA	C4B-C3B-C2B	-3.01	103.56	107.30
9	18	309	KC1	C4C-C3C-C2C	-3.01	102.51	106.89
10	19	313	A86	C25-C26-C27	-3.01	123.06	127.28
8	21	209	CLA	C4B-C3B-C2B	-3.01	103.56	107.30
9	11	302	KC1	CHD-C4C-NC	3.01	128.84	124.31
8	17	308	CLA	CHC-C1C-C2C	-3.01	118.41	126.95
8	17	310	CLA	CHC-C1C-C2C	-3.01	118.41	126.95
8	16	306	CLA	C4C-C3C-C2C	-3.00	102.52	106.89
8	20	307	CLA	C1C-C2C-C3C	-3.00	103.82	106.98
10	21	211	A86	C9-C8-C6	-3.00	118.13	126.36
8	12	311	CLA	C3B-C4B-NB	3.00	113.21	110.53
13	21	216	DD6	C21-C20-C15	-3.00	117.36	122.30
8	18	307	CLA	C4B-C3B-C2B	-3.00	103.57	107.30
8	18	305	CLA	CHC-C1C-C2C	-3.00	118.42	126.95
8	19	302	CLA	CHD-C4C-NC	3.00	128.88	124.23
10	11	313	A86	C7-C6-C8	3.00	122.67	118.09
8	17	310	CLA	CAA-C2A-C1A	-3.00	102.15	111.97
8	20	310	CLA	C4B-C3B-C2B	-3.00	103.57	107.30
9	16	308	KC1	C4C-C3C-C2C	-3.00	102.53	106.89
8	19	302	CLA	CAC-C3C-C4C	3.00	128.69	124.79
8	18	307	CLA	CAC-C3C-C4C	3.00	128.69	124.79
8	19	302	CLA	CHC-C1C-C2C	-3.00	118.44	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	14	311	A86	C7-C6-C8	2.99	122.66	118.09
8	12	304	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
10	20	301	A86	C12-C11-C10	-2.99	116.40	123.67
8	20	307	CLA	C1-C2-C3	-2.99	121.92	126.76
8	13	302	CLA	C4C-C3C-C2C	-2.99	102.54	106.89
8	17	310	CLA	C3B-C4B-NB	2.99	113.20	110.53
8	19	305	CLA	C4C-C3C-C2C	-2.99	102.54	106.89
8	18	308	CLA	C4C-C3C-C2C	-2.99	102.54	106.89
8	21	209	CLA	C3B-C4B-NB	2.99	113.20	110.53
9	12	308	KC1	C4C-C3C-C2C	-2.98	102.55	106.89
8	12	307	CLA	CHC-C1C-C2C	-2.98	118.47	126.95
8	14	301	CLA	CMB-C2B-C1B	2.98	129.96	125.42
8	19	310	CLA	C4C-C3C-C2C	-2.98	102.55	106.89
8	19	303	CLA	CMC-C2C-C1C	2.98	129.69	125.03
8	20	304	CLA	CHD-C4C-NC	2.98	128.85	124.23
8	19	309	CLA	C3B-C4B-NB	2.98	113.19	110.53
8	16	307	CLA	CHC-C1C-C2C	-2.98	118.48	126.95
9	11	306	KC1	CHD-C1D-ND	-2.98	119.58	124.05
10	17	311	A86	C4-C3-C2	-2.98	117.43	123.52
10	14	312	A86	C7-C6-C8	2.98	122.64	118.09
8	20	304	CLA	CAA-C2A-C1A	2.98	121.73	111.97
8	13	308	CLA	CED-O2D-CGD	2.97	122.66	115.92
10	16	313	A86	C21-C20-C15	-2.97	113.75	123.35
9	21	207	KC1	C4B-C3B-C2B	-2.97	104.23	106.81
8	11	309	CLA	C4B-C3B-C2B	-2.97	103.60	107.30
8	14	302	CLA	C4C-C3C-C2C	-2.97	102.56	106.89
9	21	203	KC1	O2D-CGD-O1D	-2.97	118.06	123.85
9	13	305	KC1	CHD-C4C-NC	2.97	128.79	124.31
10	16	311	A86	C10-C9-C8	-2.97	114.59	123.20
15	21	201	LHG	O8-C23-C24	2.97	120.90	111.83
9	18	304	KC1	CAA-CBA-CGA	-2.97	111.94	127.05
8	12	309	CLA	C4C-C3C-C2C	-2.97	102.57	106.89
14	16	314	SQD	O9-S-C6	2.97	111.19	106.76
10	17	311	A86	C25-C24-C1	-2.97	118.22	126.36
8	20	304	CLA	C4C-C3C-C2C	-2.97	102.57	106.89
10	16	311	A86	C36-C31-C32	-2.97	116.75	119.70
8	20	304	CLA	C4-C3-C5	2.97	120.38	115.23
8	12	311	CLA	CHC-C1C-C2C	-2.97	118.51	126.95
8	13	308	CLA	CBC-CAC-C3C	-2.97	104.38	112.42
10	19	311	A86	C7-C6-C8	2.97	122.62	118.09
8	14	303	CLA	CBA-CAA-C2A	2.97	122.62	113.79
10	15	319	A86	C-C1-C24	2.96	122.62	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	15	307	CLA	C4B-C3B-C2B	-2.96	103.62	107.30
14	17	301	SQD	C4-C3-C2	2.96	116.03	110.83
8	12	311	CLA	CHD-C4C-NC	2.96	128.82	124.23
9	12	308	KC1	CHD-C4C-NC	2.96	128.77	124.31
8	20	307	CLA	C3B-C4B-NB	2.96	113.17	110.53
8	17	304	CLA	C1-O2A-CGA	2.96	123.81	116.65
9	11	308	KC1	CMB-C2B-C1B	2.96	129.94	124.73
9	11	306	KC1	CMB-C2B-C1B	2.96	129.94	124.73
8	16	307	CLA	CAA-C2A-C3A	-2.96	105.00	113.00
10	19	313	A86	C7-C6-C5	-2.96	118.03	122.82
8	13	311	CLA	CHC-C1C-C2C	-2.96	118.55	126.95
8	14	301	CLA	C1C-C2C-C3C	-2.96	103.87	106.98
8	11	307	CLA	CAC-C3C-C2C	2.96	132.99	127.56
8	15	303	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
8	12	307	CLA	CHD-C4C-NC	2.96	128.81	124.23
8	20	308	CLA	C4B-C3B-C2B	-2.96	103.63	107.30
8	17	307	CLA	C4C-C3C-C2C	-2.96	102.59	106.89
9	17	303	KC1	CHD-C1D-ND	-2.96	119.62	124.05
8	13	311	CLA	C4B-C3B-C2B	-2.95	103.63	107.30
8	18	302	CLA	C4C-C3C-C2C	-2.95	102.59	106.89
10	17	314	A86	C7-C6-C8	2.95	122.60	118.09
8	18	310	CLA	C4B-C3B-C2B	-2.95	103.63	107.30
8	19	301	CLA	CMC-C2C-C1C	2.95	129.65	125.03
8	21	202	CLA	C4C-C3C-C2C	-2.95	102.60	106.89
8	17	307	CLA	CAC-C3C-C4C	2.95	128.63	124.79
9	12	310	KC1	CAA-CBA-CGA	-2.95	112.05	127.05
10	15	319	A86	C7-C6-C8	2.95	122.59	118.09
8	18	307	CLA	C4C-C3C-C2C	-2.95	102.60	106.89
8	17	302	CLA	C3B-C4B-NB	2.95	113.16	110.53
10	19	313	A86	C4-C3-C2	-2.95	117.48	123.52
8	15	305	CLA	CHC-C1C-C2C	-2.95	118.57	126.95
9	11	304	KC1	CAA-CBA-CGA	-2.95	112.05	127.05
8	15	307	CLA	CAC-C3C-C4C	2.95	128.63	124.79
8	12	307	CLA	C1-C2-C3	-2.95	121.99	126.76
9	19	308	KC1	C4C-C3C-C2C	-2.95	102.60	106.89
8	14	303	CLA	CHC-C1C-C2C	-2.95	118.58	126.95
8	12	305	CLA	C1-O2A-CGA	2.94	123.78	116.65
9	14	309	KC1	C4C-C3C-C2C	-2.94	102.61	106.89
9	15	309	KC1	CAC-C3C-C4C	2.94	128.62	124.79
8	14	305	CLA	C4B-C3B-C2B	-2.94	103.64	107.30
8	21	208	CLA	C4B-C3B-C2B	-2.94	103.64	107.30
8	12	305	CLA	CAC-C3C-C4C	2.94	128.62	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	16	307	CLA	C3B-C4B-NB	2.94	113.16	110.53
9	12	310	KC1	C4C-C3C-C2C	-2.94	102.61	106.89
8	11	305	CLA	C4B-C3B-C2B	-2.94	103.64	107.30
10	11	312	A86	C21-C20-C15	-2.94	113.85	123.35
8	17	307	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
9	16	302	KC1	CAC-C3C-C4C	2.94	128.62	124.79
8	19	310	CLA	C3B-C4B-NB	2.94	113.16	110.53
9	18	306	KC1	CMB-C2B-C1B	2.94	129.91	124.73
8	20	302	CLA	CHD-C4C-NC	2.94	128.79	124.23
10	12	319	A86	C3-C4-C5	-2.94	117.51	123.52
10	19	311	A86	C21-C20-C15	-2.93	113.88	123.35
8	20	310	CLA	C4C-C3C-C2C	-2.93	102.62	106.89
9	15	302	KC1	CAC-C3C-C4C	2.93	128.61	124.79
10	11	312	A86	C40-C32-C31	-2.93	107.85	110.47
8	11	305	CLA	CHB-C4A-NA	2.93	128.63	124.40
8	20	302	CLA	C4C-C3C-C2C	-2.93	102.63	106.89
9	17	309	KC1	CMA-C3A-C2A	-2.93	121.34	128.43
8	19	302	CLA	C3B-C4B-NB	2.93	113.14	110.53
10	14	313	A86	C25-C24-C1	-2.93	118.33	126.36
8	11	305	CLA	CHD-C4C-NC	2.93	128.77	124.23
8	16	307	CLA	CAC-C3C-C4C	2.93	128.60	124.79
8	12	305	CLA	C4C-C3C-C2C	-2.93	102.63	106.89
9	20	306	KC1	CBA-CAA-C2A	-2.93	113.70	125.45
8	16	309	CLA	C4C-C3C-C2C	-2.93	102.63	106.89
8	17	308	CLA	C4B-C3B-C2B	-2.93	103.66	107.30
8	13	306	CLA	CHD-C4C-NC	2.93	128.77	124.23
10	12	316	A86	C41-C32-C31	-2.93	107.85	110.47
9	12	310	KC1	CHD-C4C-NC	2.93	128.72	124.31
10	11	310	A86	C10-C9-C8	-2.93	114.72	123.20
8	21	210	CLA	C4C-C3C-C2C	-2.92	102.63	106.89
8	12	303	CLA	C4-C3-C5	2.92	120.30	115.23
8	18	302	CLA	C3B-C4B-NB	2.92	113.14	110.53
8	12	301	CLA	C1-C2-C3	-2.92	121.41	126.20
8	19	310	CLA	CAC-C3C-C4C	2.92	128.59	124.79
8	21	202	CLA	O2A-CGA-CBA	2.92	120.74	111.83
9	11	308	KC1	C4C-C3C-C2C	-2.92	102.64	106.89
8	20	308	CLA	C4C-C3C-C2C	-2.92	102.64	106.89
8	20	309	CLA	C4C-C3C-C2C	-2.92	102.64	106.89
8	21	206	CLA	O2A-CGA-CBA	2.92	120.74	111.83
8	14	307	CLA	CHD-C4C-NC	2.92	128.76	124.23
8	18	305	CLA	CHD-C4C-NC	2.92	128.76	124.23
8	15	310	CLA	C4B-C3B-C2B	-2.92	103.67	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	14	315	A86	C7-C6-C8	2.92	122.55	118.09
8	14	302	CLA	CHD-C4C-NC	2.92	128.76	124.23
8	18	301	CLA	C1C-C2C-C3C	-2.92	103.91	106.98
8	16	309	CLA	CHC-C1C-C2C	-2.92	118.66	126.95
8	12	304	CLA	C4C-C3C-C2C	-2.92	102.65	106.89
9	14	306	KC1	C4C-C3C-C2C	-2.92	102.65	106.89
13	16	312	DD6	C35-C36-C31	-2.92	114.43	120.50
9	19	308	KC1	CHD-C1D-ND	-2.92	119.67	124.05
10	14	315	A86	C36-C31-C32	-2.91	116.80	119.70
10	14	316	A86	C21-C20-C15	-2.91	113.94	123.35
8	11	305	CLA	CMB-C2B-C1B	2.91	129.86	125.42
9	11	308	KC1	CAA-CBA-CGA	-2.91	112.24	127.05
8	17	307	CLA	C4B-C3B-C2B	-2.91	103.68	107.30
8	16	301	CLA	CMB-C2B-C1B	2.91	129.85	125.42
8	20	310	CLA	C3B-C4B-NB	2.91	113.13	110.53
9	21	203	KC1	C4C-C3C-C2C	-2.91	102.65	106.89
8	19	309	CLA	C4C-C3C-C2C	-2.91	102.65	106.89
9	15	306	KC1	CMB-C2B-C1B	2.91	129.85	124.73
9	14	304	KC1	CHD-C4C-NC	2.91	128.69	124.31
9	14	306	KC1	CHD-C4C-NC	2.91	128.69	124.31
13	21	212	DD6	C4-C3-C2	-2.91	117.57	123.52
10	17	321	A86	C4-C3-C2	-2.91	117.57	123.52
10	14	312	A86	C4-C3-C2	-2.91	117.57	123.52
8	13	301	CLA	C1-C2-C3	-2.91	121.44	126.20
10	15	319	A86	C36-C31-C32	-2.91	116.81	119.70
9	15	302	KC1	CHD-C4C-NC	2.91	128.69	124.31
9	14	304	KC1	C4C-C3C-C2C	-2.90	102.66	106.89
10	17	312	A86	C8-C6-C5	-2.90	114.44	119.01
9	14	309	KC1	C2A-C1A-NA	2.90	113.99	109.34
10	11	313	A86	C34-O4-C38	-2.90	112.72	117.85
8	17	302	CLA	CHC-C1C-C2C	-2.90	118.70	126.95
9	12	306	KC1	CAA-CBA-CGA	-2.90	112.30	127.05
8	17	310	CLA	C4B-C3B-C2B	-2.90	103.70	107.30
8	19	305	CLA	CBC-CAC-C3C	-2.90	104.56	112.42
10	14	316	A86	C33-C32-C31	2.90	112.03	109.21
8	17	308	CLA	C3B-C4B-NB	2.90	113.12	110.53
10	13	312	A86	C34-O4-C38	-2.90	112.73	117.85
8	15	303	CLA	C4C-C3C-C2C	-2.90	102.68	106.89
8	12	311	CLA	C4C-C3C-C2C	-2.90	102.68	106.89
10	17	321	A86	C36-C31-C32	-2.90	116.82	119.70
9	21	207	KC1	CMB-C2B-C1B	2.89	129.83	124.73
8	13	308	CLA	CAC-C3C-C4C	2.89	128.56	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	13	311	CLA	C4C-C3C-C2C	-2.89	102.68	106.89
9	17	309	KC1	O2D-CGD-O1D	-2.89	118.22	123.85
8	14	305	CLA	CAC-C3C-C4C	2.89	128.55	124.79
9	11	302	KC1	O2D-CGD-O1D	-2.89	118.22	123.85
8	13	301	CLA	C4C-C3C-C2C	-2.89	102.68	106.89
9	13	305	KC1	C4C-C3C-C2C	-2.89	102.68	106.89
10	15	315	A86	C4-C3-C2	-2.89	117.61	123.52
8	15	303	CLA	C3B-C4B-NB	2.89	113.11	110.53
10	19	313	A86	C3-C2-C1	-2.89	123.23	127.28
8	17	308	CLA	C4C-C3C-C2C	-2.89	102.69	106.89
9	15	309	KC1	C4C-C3C-C2C	-2.89	102.69	106.89
8	20	308	CLA	CHD-C4C-NC	2.89	128.71	124.23
10	12	313	A86	C21-C20-C15	-2.89	114.03	123.35
8	17	310	CLA	C4C-C3C-C2C	-2.89	102.69	106.89
8	11	307	CLA	C1-C2-C3	-2.89	121.47	126.20
8	15	303	CLA	CHC-C1C-C2C	-2.89	118.74	126.95
8	16	307	CLA	C4C-C3C-C2C	-2.89	102.69	106.89
10	17	316	A86	C41-C32-C31	-2.89	107.89	110.47
9	11	304	KC1	CAC-C3C-C4C	2.89	128.54	124.79
10	15	316	A86	C21-C20-C15	-2.88	114.04	123.35
9	21	203	KC1	CHD-C1D-ND	-2.88	119.72	124.05
14	17	301	SQD	O7-S-C6	2.88	111.06	106.76
8	21	202	CLA	CMB-C2B-C1B	2.88	129.81	125.42
8	16	309	CLA	C4B-C3B-C2B	-2.88	103.72	107.30
8	12	305	CLA	CHD-C4C-NC	2.88	128.70	124.23
9	15	309	KC1	CHD-C4C-NC	2.88	128.65	124.31
10	12	312	A86	C34-O4-C38	-2.88	112.76	117.85
8	15	310	CLA	C4C-C3C-C2C	-2.88	102.70	106.89
9	12	306	KC1	CHD-C1D-ND	-2.88	119.73	124.05
9	18	309	KC1	CHD-C1D-ND	-2.88	119.73	124.05
8	21	209	CLA	C4C-C3C-C2C	-2.87	102.71	106.89
9	12	310	KC1	CMC-C2C-C1C	2.87	129.52	125.03
10	11	311	A86	C23-C16-C22	-2.87	103.20	107.37
8	14	310	CLA	CHD-C4C-NC	2.87	128.69	124.23
8	19	303	CLA	C4B-C3B-C2B	-2.87	103.73	107.30
9	14	306	KC1	CMB-C2B-C1B	2.87	129.79	124.73
8	21	210	CLA	CAA-C2A-C3A	-2.87	105.24	113.00
10	14	316	A86	C3-C2-C1	-2.87	123.25	127.28
8	17	307	CLA	CHD-C4C-NC	2.87	128.68	124.23
9	16	302	KC1	CHD-C4C-NC	2.87	128.63	124.31
8	21	202	CLA	CHB-C4A-NA	2.87	128.54	124.40
8	11	309	CLA	CHC-C1C-C2C	-2.87	118.80	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	16	310	A86	C21-C20-C15	-2.87	114.09	123.35
10	11	314	A86	C41-C32-C31	-2.87	107.91	110.47
8	19	301	CLA	CAC-C3C-C4C	2.87	128.52	124.79
10	14	313	A86	C12-C11-C13	2.87	120.65	116.00
8	13	306	CLA	C4B-C3B-C2B	-2.87	103.74	107.30
9	14	309	KC1	CMC-C2C-C1C	2.86	129.51	125.03
8	15	305	CLA	C4B-C3B-C2B	-2.86	103.74	107.30
9	16	305	KC1	CMB-C2B-C1B	2.86	129.77	124.73
8	17	310	CLA	O2A-CGA-CBA	2.86	120.57	111.83
8	19	303	CLA	C3B-C4B-NB	2.86	113.09	110.53
10	15	314	A86	C3-C4-C5	-2.86	117.66	123.52
9	17	303	KC1	C1A-NA-C4A	-2.86	105.37	106.68
10	13	313	A86	C4-C5-C6	-2.86	123.27	127.28
10	14	314	A86	C21-C20-C15	-2.86	114.12	123.35
8	21	204	CLA	CHD-C4C-NC	2.86	128.66	124.23
8	18	302	CLA	C4B-C3B-C2B	-2.86	103.75	107.30
8	14	303	CLA	C4C-C3C-C2C	-2.86	102.73	106.89
8	21	206	CLA	CHC-C1C-C2C	-2.86	118.83	126.95
8	18	302	CLA	CHD-C4C-NC	2.86	128.66	124.23
9	17	309	KC1	C4C-C3C-C2C	-2.86	102.73	106.89
9	18	304	KC1	C4C-C3C-C2C	-2.86	102.73	106.89
9	12	308	KC1	CMB-C2B-C1B	2.86	129.76	124.73
8	12	305	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
10	13	312	A86	C25-C24-C1	-2.85	118.53	126.36
10	13	316	A86	C21-C20-C15	-2.85	114.14	123.35
8	13	302	CLA	CHB-C4A-NA	2.85	128.52	124.40
9	18	309	KC1	CBC-CAC-C3C	-2.85	104.69	112.42
10	15	319	A86	C4-C3-C2	-2.85	117.68	123.52
10	14	311	A86	C25-C24-C1	-2.85	118.54	126.36
9	17	305	KC1	CAA-CBA-CGA	-2.85	112.55	127.05
8	11	307	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
9	15	304	KC1	CHD-C4C-NC	2.85	128.60	124.31
8	19	302	CLA	C4C-C3C-C2C	-2.85	102.74	106.89
8	20	304	CLA	C4B-C3B-C2B	-2.85	103.76	107.30
10	12	319	A86	C34-O4-C38	-2.85	112.82	117.85
8	12	307	CLA	O2A-CGA-CBA	2.85	120.51	111.83
8	19	301	CLA	CMB-C2B-C1B	2.85	129.75	125.42
10	21	214	A86	C4-C3-C2	-2.85	117.70	123.52
8	17	307	CLA	CHC-C1C-C2C	-2.84	118.86	126.95
8	19	304	CLA	C3B-C4B-NB	2.84	113.07	110.53
8	13	302	CLA	CMB-C2B-C1B	2.84	129.75	125.42
10	13	312	A86	C4-C3-C2	-2.84	117.70	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	16	311	A86	C7-C6-C8	2.84	122.43	118.09
8	16	309	CLA	CHD-C4C-NC	2.84	128.64	124.23
8	16	303	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
8	21	208	CLA	CAA-C2A-C3A	-2.84	105.32	113.00
10	12	302	A86	C21-C20-C15	-2.84	114.18	123.35
8	18	307	CLA	CHD-C4C-NC	2.84	128.64	124.23
10	14	313	A86	C35-C34-C33	2.84	114.99	109.89
8	12	309	CLA	CHC-C1C-C2C	-2.84	118.87	126.95
8	19	307	CLA	CAC-C3C-C4C	2.84	128.49	124.79
9	16	308	KC1	CAA-CBA-CGA	-2.84	112.60	127.05
8	21	210	CLA	CHD-C4C-NC	2.84	128.63	124.23
8	12	311	CLA	C4B-C3B-C2B	-2.84	103.77	107.30
10	18	312	A86	C7-C6-C8	2.84	122.42	118.09
9	16	304	KC1	CHD-C4C-NC	2.84	128.59	124.31
8	12	309	CLA	CHD-C4C-NC	2.84	128.63	124.23
10	17	321	A86	C26-C25-C24	-2.83	114.99	123.20
8	20	307	CLA	CHC-C1C-C2C	-2.83	118.90	126.95
8	15	305	CLA	CHD-C4C-NC	2.83	128.62	124.23
8	17	304	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
8	16	301	CLA	C1C-C2C-C3C	-2.83	104.00	106.98
8	19	305	CLA	CAC-C3C-C4C	2.83	128.47	124.79
10	15	316	A86	C36-C31-C32	-2.83	116.89	119.70
10	12	314	A86	C21-C20-C15	-2.83	114.22	123.35
9	15	309	KC1	CHD-C1D-ND	-2.83	119.81	124.05
8	18	305	CLA	CAC-C3C-C4C	2.83	128.47	124.79
8	15	307	CLA	C4C-C3C-C2C	-2.83	102.78	106.89
8	15	305	CLA	CAC-C3C-C4C	2.83	128.47	124.79
8	16	306	CLA	CAC-C3C-C4C	2.83	128.47	124.79
9	11	306	KC1	CAA-CBA-CGA	-2.83	112.67	127.05
8	14	305	CLA	CHD-C4C-NC	2.83	128.61	124.23
8	15	307	CLA	C4-C3-C5	2.83	120.13	115.23
9	17	306	KC1	C1A-NA-C4A	-2.83	105.39	106.68
8	21	205	CLA	C4B-C3B-C2B	-2.82	103.79	107.30
10	13	315	A86	C40-C32-C31	-2.82	107.95	110.47
8	18	305	CLA	C4C-C3C-C2C	-2.82	102.78	106.89
8	12	304	CLA	C3B-C4B-NB	2.82	113.05	110.53
8	21	209	CLA	CHD-C4C-NC	2.82	128.60	124.23
8	13	304	CLA	C4-C3-C5	2.82	120.12	115.23
8	13	302	CLA	CHC-C1C-C2C	-2.82	118.94	126.95
9	18	309	KC1	O1D-CGD-CBD	-2.82	118.96	124.52
10	15	314	A86	C4-C5-C6	-2.82	123.33	127.28
8	19	309	CLA	C4B-C3B-C2B	-2.82	103.80	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	16	304	KC1	CAC-C3C-C4C	2.82	128.45	124.79
10	18	311	A86	C25-C26-C27	-2.82	123.33	127.28
8	17	310	CLA	CHD-C4C-NC	2.82	128.60	124.23
8	13	306	CLA	CAC-C3C-C4C	2.82	128.45	124.79
9	14	309	KC1	C1A-NA-C4A	-2.81	105.39	106.68
8	16	303	CLA	C1-C2-C3	-2.81	121.59	126.20
10	18	312	A86	C35-C34-C33	2.81	114.94	109.89
8	15	305	CLA	C4C-C3C-C2C	-2.81	102.80	106.89
10	11	311	A86	C34-O4-C38	-2.81	112.88	117.85
10	15	311	A86	C10-C9-C8	-2.81	115.05	123.20
8	16	303	CLA	CBC-CAC-C3C	-2.81	104.80	112.42
8	13	308	CLA	C4C-C3C-C2C	-2.81	102.80	106.89
8	19	307	CLA	C1-C2-C3	-2.81	121.59	126.20
10	18	311	A86	C23-C16-C22	-2.81	103.29	107.37
8	15	310	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
8	20	307	CLA	CHD-C4C-NC	2.81	128.59	124.23
8	14	308	CLA	C4C-C3C-C2C	-2.81	102.80	106.89
8	18	303	CLA	C1-O2A-CGA	2.81	123.45	116.65
8	20	302	CLA	CAA-C2A-C3A	-2.81	105.41	113.00
8	19	305	CLA	C4A-NA-C1A	-2.81	105.40	106.68
9	14	309	KC1	CBC-CAC-C3C	-2.80	104.82	112.42
10	21	214	A86	C12-C11-C13	2.80	120.55	116.00
9	18	309	KC1	CHD-C4C-NC	2.80	128.53	124.31
8	12	309	CLA	C3B-C4B-NB	2.80	113.03	110.53
8	21	206	CLA	C4B-C3B-C2B	-2.80	103.82	107.30
9	14	306	KC1	CAA-CBA-CGA	-2.80	112.81	127.05
8	13	304	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
8	20	310	CLA	CAA-C2A-C3A	-2.80	105.44	113.00
8	17	307	CLA	C4-C3-C5	2.80	120.08	115.23
10	17	313	A86	C40-C32-C31	-2.80	107.97	110.47
9	15	302	KC1	CBC-CAC-C3C	-2.80	104.84	112.42
9	15	309	KC1	CBC-CAC-C3C	-2.80	104.84	112.42
13	21	212	DD6	C33-C32-C31	2.80	115.00	109.49
8	15	301	CLA	C1-C2-C3	-2.80	121.62	126.20
8	19	302	CLA	CGD-CBD-CAD	-2.80	101.80	110.85
8	12	301	CLA	C4C-C3C-C2C	-2.80	102.82	106.89
10	18	313	A86	C21-C20-C15	-2.79	114.33	123.35
10	14	311	A86	C23-C16-C22	-2.79	103.31	107.37
8	18	307	CLA	CHC-C1C-C2C	-2.79	119.01	126.95
8	12	307	CLA	C4B-C3B-C2B	-2.79	103.83	107.30
8	21	202	CLA	C1-C2-C3	-2.79	121.62	126.20
9	15	306	KC1	C4C-C3C-C2C	-2.79	102.83	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	15	315	A86	C36-C31-C32	-2.79	116.93	119.70
9	16	302	KC1	CHD-C1D-ND	-2.79	119.86	124.05
9	20	305	KC1	O2D-CGD-O1D	-2.79	118.42	123.85
10	13	313	A86	C21-C20-C15	-2.79	114.35	123.35
8	21	205	CLA	CMB-C2B-C1B	2.79	129.66	125.42
8	13	304	CLA	C4C-C3C-C2C	-2.79	102.84	106.89
8	11	309	CLA	C4-C3-C5	2.79	119.41	116.13
9	15	309	KC1	CMB-C2B-C1B	2.79	129.63	124.73
9	17	303	KC1	O2D-CGD-O1D	-2.78	118.43	123.85
8	13	302	CLA	CAC-C3C-C4C	2.78	128.41	124.79
8	11	301	CLA	CMB-C2B-C1B	2.78	129.66	125.42
8	19	301	CLA	C4B-C3B-C2B	-2.78	103.84	107.30
9	11	304	KC1	CHD-C4C-NC	2.78	128.50	124.31
10	14	314	A86	C25-C24-C1	-2.78	118.74	126.36
8	18	301	CLA	CMC-C2C-C1C	2.78	129.38	125.03
8	18	303	CLA	CMC-C2C-C1C	2.78	129.38	125.03
13	20	312	DD6	C21-C20-C15	-2.78	117.72	122.30
8	16	309	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
8	12	307	CLA	C4C-C3C-C2C	-2.78	102.85	106.89
9	21	207	KC1	CMC-C2C-C1C	2.78	129.38	125.03
9	20	305	KC1	CMB-C2B-C1B	2.78	129.62	124.73
9	16	305	KC1	CHD-C4C-NC	2.78	128.50	124.31
8	18	308	CLA	CHD-C4C-NC	2.78	128.54	124.23
8	11	303	CLA	C4C-C3C-C2C	-2.78	102.85	106.89
8	19	305	CLA	C3B-C4B-NB	2.78	113.01	110.53
10	11	313	A86	C21-C20-C15	-2.78	114.39	123.35
8	20	307	CLA	O2A-CGA-CBA	2.77	120.30	111.83
9	13	307	KC1	CAC-C3C-C4C	2.77	128.40	124.79
8	12	305	CLA	C4-C3-C5	2.77	120.04	115.23
11	11	315	LMG	C1-O6-C5	-2.77	108.30	113.72
10	15	313	A86	C36-C31-C32	-2.77	116.94	119.70
10	12	316	A86	C8-C6-C5	2.77	123.37	119.01
8	15	301	CLA	C4C-C3C-C2C	-2.77	102.85	106.89
9	19	308	KC1	CAA-C2A-C1A	-2.77	112.50	124.64
15	17	317	LHG	O8-C23-C24	2.77	120.28	111.83
10	11	313	A86	C36-C31-C32	-2.77	116.95	119.70
10	19	311	A86	C35-C34-C33	2.77	114.86	109.89
8	11	305	CLA	CBC-CAC-C3C	-2.77	104.91	112.42
8	12	305	CLA	CAA-C2A-C1A	2.77	121.05	111.97
10	11	318	A86	O4-C38-O5	-2.77	117.64	122.99
8	19	303	CLA	CMB-C2B-C1B	2.77	129.64	125.42
8	21	210	CLA	CMB-C2B-C1B	2.77	129.64	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	11	311	A86	C10-C9-C8	-2.77	115.18	123.20
10	18	314	A86	C21-C20-C15	-2.77	114.42	123.35
10	17	312	A86	C28-C27-C26	2.77	127.30	122.82
10	17	313	A86	C36-C31-C32	-2.77	116.95	119.70
10	20	301	A86	C21-C20-C15	-2.76	114.43	123.35
8	16	303	CLA	C4C-C3C-C2C	-2.76	102.87	106.89
9	17	306	KC1	CBA-CAA-C2A	-2.76	114.36	125.45
9	11	308	KC1	O2D-CGD-O1D	-2.76	118.47	123.85
10	12	302	A86	C9-C8-C6	-2.76	118.79	126.36
8	13	302	CLA	C4-C3-C5	2.76	120.02	115.23
8	12	305	CLA	CHC-C1C-C2C	-2.76	119.10	126.95
8	12	304	CLA	CHD-C4C-NC	2.76	128.51	124.23
10	15	316	A86	C40-C32-C31	2.76	112.94	110.47
10	18	312	A86	C41-C32-C31	-2.76	108.00	110.47
8	12	305	CLA	C4B-C3B-C2B	-2.76	103.87	107.30
10	12	312	A86	C3-C2-C1	-2.76	123.41	127.28
8	12	303	CLA	C4C-C3C-C2C	-2.76	102.88	106.89
8	20	302	CLA	CHC-C1C-C2C	-2.76	119.11	126.95
8	14	303	CLA	CHD-C4C-NC	2.76	128.51	124.23
9	13	310	KC1	CHD-C4C-NC	2.76	128.46	124.31
8	21	206	CLA	C4C-C3C-C2C	-2.76	102.88	106.89
8	13	308	CLA	C4-C3-C5	2.76	120.01	115.23
10	12	312	A86	C3-C4-C5	-2.76	117.88	123.52
10	12	315	A86	C7-C6-C8	2.76	122.30	118.09
10	15	312	A86	C10-C9-C8	-2.76	115.21	123.20
8	21	208	CLA	C4C-C3C-C2C	-2.75	102.88	106.89
10	17	315	A86	C33-C32-C31	2.75	111.89	109.21
10	21	215	A86	C40-C32-C31	2.75	112.94	110.47
8	12	304	CLA	CAC-C3C-C4C	2.75	128.37	124.79
8	11	305	CLA	C4C-C3C-C2C	-2.75	102.88	106.89
10	15	314	A86	C34-O4-C38	-2.75	112.98	117.85
10	15	315	A86	C26-C25-C24	-2.75	115.23	123.20
10	15	314	A86	C21-C20-C15	-2.75	114.47	123.35
8	11	309	CLA	CHD-C4C-NC	2.75	128.50	124.23
8	21	206	CLA	CBC-CAC-C3C	-2.75	104.96	112.42
8	20	304	CLA	C1-C2-C3	-2.75	121.69	126.20
8	13	306	CLA	C4C-C3C-C2C	-2.75	102.89	106.89
8	14	301	CLA	C1-C2-C3	-2.75	121.69	126.20
10	16	310	A86	C25-C26-C27	-2.75	123.42	127.28
10	17	314	A86	C25-C24-C1	-2.75	118.83	126.36
8	19	304	CLA	CAA-C2A-C3A	-2.75	105.57	113.00
8	15	310	CLA	CHD-C4C-NC	2.75	128.49	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	20	302	CLA	C3B-C4B-NB	2.75	112.98	110.53
8	17	304	CLA	C4C-C3C-C2C	-2.75	102.89	106.89
9	13	303	KC1	CHD-C4C-NC	2.75	128.45	124.31
8	15	308	CLA	C4C-C3C-C2C	-2.74	102.90	106.89
9	20	305	KC1	CHD-C4C-NC	2.74	128.44	124.31
9	15	309	KC1	C2A-C1A-NA	2.74	113.74	109.34
8	11	307	CLA	CHC-C1C-C2C	-2.74	119.15	126.95
9	16	308	KC1	CHD-C4C-NC	2.74	128.44	124.31
10	14	312	A86	C-C1-C24	2.74	122.28	118.09
8	15	303	CLA	CHD-C4C-NC	2.74	128.48	124.23
10	16	310	A86	C10-C9-C8	-2.74	115.27	123.20
8	18	302	CLA	CAC-C3C-C4C	2.74	128.35	124.79
9	13	310	KC1	O2D-CGD-O1D	-2.74	118.52	123.85
10	17	314	A86	C21-C20-C15	-2.74	114.51	123.35
8	19	307	CLA	CHD-C4C-NC	2.74	128.47	124.23
9	11	306	KC1	C4C-C3C-C2C	-2.74	102.91	106.89
10	17	312	A86	C21-C20-C15	-2.74	114.52	123.35
8	13	308	CLA	CHD-C4C-NC	2.74	128.47	124.23
8	17	304	CLA	C4-C3-C5	2.74	119.98	115.23
10	12	315	A86	C21-C20-C15	-2.74	114.52	123.35
8	14	307	CLA	C4-C3-C5	2.73	119.97	115.23
8	14	305	CLA	C4C-C3C-C2C	-2.73	102.91	106.89
8	12	305	CLA	CMC-C2C-C1C	2.73	129.30	125.03
10	20	311	A86	C4-C3-C2	-2.73	117.93	123.52
8	11	309	CLA	O2A-CGA-CBA	2.73	120.16	111.83
8	16	303	CLA	CHD-C4C-NC	2.73	128.46	124.23
9	16	308	KC1	CMA-C3A-C2A	-2.73	121.83	128.43
8	21	204	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
10	18	313	A86	C4-C5-C6	-2.73	123.45	127.28
13	20	314	DD6	C19-C18-C17	2.73	115.89	110.79
8	21	209	CLA	CAA-C2A-C3A	-2.73	105.64	113.00
9	15	309	KC1	CAA-CBA-CGA	-2.72	113.19	127.05
8	14	302	CLA	CAC-C3C-C4C	2.72	128.34	124.79
9	13	303	KC1	C4C-C3C-C2C	-2.72	102.93	106.89
8	12	309	CLA	C4B-C3B-C2B	-2.72	103.92	107.30
14	17	301	SQD	O47-C7-C8	2.72	117.37	111.48
10	15	316	A86	C12-C11-C13	2.72	120.41	116.00
8	21	210	CLA	CHC-C1C-C2C	-2.72	119.22	126.95
8	21	208	CLA	C4-C3-C5	2.72	119.95	115.23
10	12	312	A86	C7-C6-C8	2.72	122.24	118.09
9	21	207	KC1	CBA-CAA-C2A	-2.72	114.55	125.45
8	18	302	CLA	C4-C3-C5	2.72	119.94	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	20	309	CLA	CHD-C4C-NC	2.72	128.44	124.23
8	12	301	CLA	O2A-CGA-CBA	2.72	120.12	111.83
8	15	307	CLA	CHC-C1C-C2C	-2.72	119.23	126.95
10	17	312	A86	C25-C24-C1	-2.72	118.92	126.36
8	20	310	CLA	CAC-C3C-C4C	2.72	128.32	124.79
8	14	310	CLA	C4C-C3C-C2C	-2.72	102.94	106.89
9	13	310	KC1	CAA-CBA-CGA	-2.72	113.24	127.05
8	12	311	CLA	CAC-C3C-C4C	2.71	128.32	124.79
10	17	312	A86	C41-C32-C31	-2.71	108.04	110.47
10	17	312	A86	C7-C6-C8	2.71	122.23	118.09
8	21	208	CLA	O2A-CGA-CBA	2.71	120.11	111.83
9	13	307	KC1	CMB-C2B-C1B	2.71	129.50	124.73
8	16	309	CLA	CAA-CBA-CGA	-2.71	105.26	112.49
9	19	308	KC1	O2D-CGD-O1D	-2.71	118.57	123.85
8	17	302	CLA	CHB-C4A-NA	2.71	128.31	124.40
8	13	308	CLA	CHB-C4A-NA	2.71	128.31	124.40
9	11	304	KC1	C4C-C3C-C2C	-2.71	102.95	106.89
8	18	307	CLA	CMC-C2C-C1C	2.71	129.27	125.03
10	17	316	A86	C21-C20-C15	-2.71	114.61	123.35
8	18	302	CLA	CBA-CAA-C2A	-2.71	105.73	113.79
10	18	313	A86	C40-C32-C31	-2.71	108.05	110.47
8	11	307	CLA	C3B-C4B-NB	2.70	112.94	110.53
10	15	312	A86	C7-C6-C8	2.70	122.22	118.09
8	19	305	CLA	CHD-C4C-NC	2.70	128.42	124.23
8	19	305	CLA	CHB-C4A-NA	2.70	128.30	124.40
9	21	203	KC1	CHD-C4C-NC	2.70	128.38	124.31
10	13	316	A86	C12-C11-C13	2.70	120.38	116.00
10	20	311	A86	C25-C24-C1	-2.70	118.96	126.36
13	19	312	DD6	C4-C3-C2	-2.70	117.99	123.52
13	21	212	DD6	C19-C18-C17	2.70	115.84	110.79
10	14	314	A86	C34-O4-C38	-2.70	113.08	117.85
8	11	305	CLA	CAC-C3C-C4C	2.70	128.30	124.79
10	17	316	A86	C22-C16-C17	-2.70	104.23	108.97
10	11	311	A86	C7-C6-C8	2.70	122.20	118.09
10	16	310	A86	C23-C16-C22	-2.69	103.46	107.37
8	13	311	CLA	CAC-C3C-C4C	2.69	128.29	124.79
9	17	306	KC1	CHC-C4B-C3B	-2.69	120.67	125.21
14	17	301	SQD	O6-C1-C2	2.69	112.36	108.27
8	14	302	CLA	CAA-C2A-C1A	2.69	120.80	111.97
8	18	308	CLA	O2A-CGA-CBA	2.69	120.04	111.83
10	15	312	A86	C12-C11-C13	2.69	120.36	116.00
9	14	309	KC1	O2D-CGD-O1D	-2.69	118.61	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	15	309	KC1	O2D-CGD-O1D	-2.69	118.61	123.85
8	12	309	CLA	CMC-C2C-C1C	2.69	129.24	125.03
13	20	314	DD6	C14-C13-C11	-2.69	121.36	125.53
9	15	302	KC1	C4C-C3C-C2C	-2.69	102.98	106.89
9	17	305	KC1	O2D-CGD-O1D	-2.69	118.62	123.85
10	20	313	A86	C9-C8-C6	-2.69	119.00	126.36
10	11	311	A86	C12-C11-C13	2.69	120.36	116.00
9	17	305	KC1	C4C-C3C-C2C	-2.69	102.98	106.89
8	19	306	CLA	C4-C3-C5	2.69	119.89	115.23
10	15	312	A86	C21-C20-C15	-2.69	114.68	123.35
9	11	306	KC1	C1A-NA-C4A	-2.69	105.45	106.68
9	11	308	KC1	CHD-C4C-NC	2.68	128.35	124.31
8	14	308	CLA	CHD-C4C-NC	2.68	128.39	124.23
9	17	303	KC1	CAC-C3C-C4C	2.68	128.28	124.79
9	16	305	KC1	O2D-CGD-O1D	-2.68	118.63	123.85
10	18	313	A86	C7-C6-C8	2.68	122.19	118.09
8	19	306	CLA	O2A-CGA-CBA	2.68	120.01	111.83
10	12	312	A86	C21-C20-C15	-2.68	114.69	123.35
10	15	315	A86	C7-C6-C8	2.68	122.18	118.09
9	11	308	KC1	CMA-C3A-C2A	-2.68	121.94	128.43
10	12	319	A86	C21-C20-C15	-2.68	114.70	123.35
8	17	310	CLA	CAA-CBA-CGA	-2.68	105.60	113.21
10	15	316	A86	C8-C6-C5	2.68	123.22	119.01
8	20	309	CLA	C4B-C3B-C2B	-2.68	103.97	107.30
8	13	306	CLA	CHB-C4A-NA	2.68	128.26	124.40
8	19	302	CLA	O2A-CGA-CBA	2.68	119.99	111.83
8	21	204	CLA	CBC-CAC-C3C	-2.68	105.17	112.42
8	17	302	CLA	CHD-C4C-NC	2.67	128.38	124.23
8	20	304	CLA	CHC-C1C-C2C	-2.67	119.35	126.95
8	15	310	CLA	CAC-C3C-C4C	2.67	128.27	124.79
10	12	316	A86	C7-C6-C5	-2.67	118.49	122.82
9	18	306	KC1	CAA-CBA-CGA	-2.67	113.46	127.05
8	19	309	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
15	19	314	LHG	O8-C23-C24	2.67	119.98	111.83
10	21	214	A86	C21-C20-C15	-2.67	114.73	123.35
8	15	301	CLA	CHC-C1C-C2C	-2.67	119.36	126.95
13	21	216	DD6	C19-C18-C17	2.67	115.78	110.79
8	13	308	CLA	C4B-C3B-C2B	-2.67	103.98	107.30
10	17	311	A86	C9-C10-C11	-2.67	119.10	126.64
9	13	305	KC1	CAC-C3C-C4C	2.67	128.26	124.79
10	16	311	A86	C21-C20-C15	-2.67	114.74	123.35
10	11	313	A86	C25-C24-C1	-2.67	119.06	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	20	314	DD6	C37-C36-C35	-2.66	109.52	114.42
8	14	302	CLA	C3B-C4B-NB	2.66	112.91	110.53
9	15	304	KC1	C4C-C3C-C2C	-2.66	103.02	106.89
8	19	303	CLA	C1-O2A-CGA	2.66	123.09	116.65
10	17	312	A86	C10-C9-C8	-2.66	115.49	123.20
10	19	311	A86	C10-C9-C8	-2.66	115.49	123.20
9	12	308	KC1	CHD-C1D-ND	-2.66	120.06	124.05
9	21	207	KC1	CAA-C2A-C1A	-2.66	112.99	124.64
8	14	307	CLA	C3B-C4B-NB	2.66	112.90	110.53
8	17	302	CLA	CMB-C2B-C1B	2.66	129.47	125.42
8	19	304	CLA	C4B-C3B-C2B	-2.66	104.00	107.30
10	18	314	A86	C35-C34-C33	2.66	114.66	109.89
9	14	309	KC1	CMB-C2B-C1B	2.66	129.41	124.73
8	19	307	CLA	O2A-CGA-CBA	2.66	119.93	111.83
8	14	303	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
10	13	312	A86	C21-C20-C15	-2.66	114.78	123.35
8	15	308	CLA	CMB-C2B-C1B	2.66	129.46	125.42
9	18	304	KC1	CHD-C4C-NC	2.66	128.31	124.31
10	17	315	A86	C3-C2-C1	-2.65	123.56	127.28
9	11	308	KC1	CHB-C4A-NA	2.65	128.35	124.23
10	18	311	A86	C21-C20-C15	-2.65	114.78	123.35
8	20	307	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
10	17	316	A86	C12-C11-C13	2.65	120.30	116.00
10	12	312	A86	C23-C16-C22	-2.65	103.52	107.37
8	19	304	CLA	CHB-C4A-NA	2.65	128.23	124.40
8	13	311	CLA	CHD-C4C-NC	2.65	128.34	124.23
8	19	310	CLA	C4B-C3B-C2B	-2.65	104.01	107.30
10	11	318	A86	C21-C20-C15	-2.65	114.80	123.35
10	16	311	A86	C23-C16-C22	-2.65	103.52	107.37
8	14	307	CLA	O2A-CGA-CBA	2.65	119.91	111.83
14	17	301	SQD	O48-C23-C24	2.65	119.91	111.83
8	15	307	CLA	C3B-C4B-NB	2.65	112.89	110.53
13	16	312	DD6	C25-C24-C1	-2.65	119.11	126.36
8	13	302	CLA	C3B-C4B-NB	2.65	112.89	110.53
10	11	314	A86	C21-C20-C15	-2.65	114.81	123.35
13	21	216	DD6	C14-C13-C11	-2.64	121.43	125.53
9	17	309	KC1	CHB-C4A-NA	2.64	128.33	124.23
9	14	304	KC1	CAC-C3C-C4C	2.64	128.23	124.79
8	19	309	CLA	CHD-C4C-NC	2.64	128.33	124.23
9	20	306	KC1	CMB-C2B-C1B	2.64	129.38	124.73
9	15	309	KC1	CHB-C4A-NA	2.64	128.33	124.23
9	20	305	KC1	C4C-C3C-C2C	-2.64	103.05	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	14	308	CLA	C1-C2-C3	-2.64	121.87	126.20
10	12	314	A86	C12-C11-C13	2.64	120.28	116.00
8	19	310	CLA	CAA-C2A-C3A	-2.64	105.87	113.00
8	11	303	CLA	C4B-C3B-C2B	-2.64	104.02	107.30
8	15	308	CLA	CMC-C2C-C1C	2.64	129.16	125.03
9	14	309	KC1	CAA-CBA-CGA	-2.64	113.64	127.05
9	18	309	KC1	CAA-CBA-CGA	-2.64	113.64	127.05
8	18	305	CLA	CBC-CAC-C3C	-2.64	105.27	112.42
10	21	213	A86	C21-C20-C15	-2.64	114.84	123.35
8	19	310	CLA	O2A-CGA-CBA	2.64	119.87	111.83
8	21	204	CLA	C4C-C3C-C2C	-2.63	103.06	106.89
8	21	210	CLA	CAC-C3C-C4C	2.63	128.22	124.79
8	15	303	CLA	C1-C2-C3	-2.63	121.88	126.20
8	11	303	CLA	CHD-C4C-NC	2.63	128.31	124.23
10	17	311	A86	C21-C20-C15	-2.63	114.85	123.35
8	18	308	CLA	CMB-C2B-C1B	2.63	129.43	125.42
10	14	316	A86	C7-C6-C5	-2.63	118.55	122.82
9	17	306	KC1	CHD-C1D-ND	-2.63	120.10	124.05
8	13	304	CLA	CMB-C2B-C1B	2.63	129.42	125.42
8	17	304	CLA	CHD-C4C-NC	2.63	128.31	124.23
8	18	301	CLA	CHC-C1C-C2C	-2.63	119.47	126.95
10	15	311	A86	C8-C6-C5	-2.63	114.87	119.01
10	17	321	A86	C7-C6-C8	2.63	122.10	118.09
8	18	301	CLA	C4B-C3B-C2B	-2.63	104.03	107.30
8	21	210	CLA	C4B-C3B-C2B	-2.63	104.04	107.30
9	17	309	KC1	CMB-C2B-C1B	2.63	129.35	124.73
8	20	304	CLA	O2D-CGD-O1D	-2.63	118.74	123.85
9	17	305	KC1	CMB-C2B-C1B	2.63	129.35	124.73
8	15	303	CLA	CMC-C2C-C1C	2.62	129.14	125.03
9	15	306	KC1	CAC-C3C-C4C	2.62	128.21	124.79
9	20	303	KC1	O2D-CGD-O1D	-2.62	118.74	123.85
8	12	301	CLA	CHD-C4C-NC	2.62	128.30	124.23
8	13	308	CLA	CMC-C2C-C1C	2.62	129.13	125.03
10	15	314	A86	C7-C6-C8	2.62	122.10	118.09
8	15	308	CLA	CBC-CAC-C3C	-2.62	105.31	112.42
8	14	308	CLA	O2A-CGA-CBA	2.62	119.82	111.83
8	16	307	CLA	O2A-CGA-CBA	2.62	119.82	111.83
8	19	301	CLA	C3B-C4B-NB	2.62	112.87	110.53
8	19	307	CLA	CHB-C4A-NA	2.62	128.18	124.40
8	18	303	CLA	CHC-C1C-C2C	-2.62	119.51	126.95
9	15	302	KC1	CMB-C2B-C1B	2.62	129.33	124.73
9	12	306	KC1	O2D-CGD-O1D	-2.62	118.76	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	20	302	CLA	CMB-C2B-C1B	2.62	129.40	125.42
10	15	314	A86	C25-C24-C1	-2.61	119.19	126.36
8	13	308	CLA	CAA-C2A-C3A	-2.61	105.94	113.00
10	12	319	A86	C40-C32-C31	-2.61	108.13	110.47
10	14	313	A86	C36-C31-C32	-2.61	117.10	119.70
8	14	305	CLA	CBC-CAC-C3C	-2.61	105.34	112.42
10	11	314	A86	C19-C18-C17	-2.61	105.91	110.79
9	11	302	KC1	C4C-C3C-C2C	-2.61	103.09	106.89
8	13	301	CLA	CED-O2D-CGD	2.61	121.84	115.92
8	21	202	CLA	CHD-C4C-NC	2.61	128.28	124.23
8	21	204	CLA	C4B-C3B-C2B	-2.61	104.06	107.30
10	13	312	A86	C3-C4-C5	-2.61	118.18	123.52
8	11	301	CLA	C1C-C2C-C3C	-2.61	104.24	106.98
10	18	314	A86	C7-C6-C5	-2.61	118.59	122.82
8	16	306	CLA	CHB-C1B-C2B	-2.60	119.86	127.43
8	20	307	CLA	C4B-C3B-C2B	-2.60	104.06	107.30
8	13	309	CLA	C1-C2-C3	-2.60	121.93	126.20
9	18	306	KC1	CHD-C4C-NC	2.60	128.23	124.31
10	12	315	A86	C25-C24-C1	-2.60	119.23	126.36
8	17	304	CLA	CBC-CAC-C3C	-2.60	105.37	112.42
8	14	307	CLA	CHA-C1A-NA	-2.60	120.50	126.39
9	14	306	KC1	CHD-C1D-ND	-2.60	120.15	124.05
8	13	311	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
8	20	308	CLA	CMB-C2B-C1B	2.60	129.38	125.42
9	11	302	KC1	CAC-C3C-C4C	2.60	128.17	124.79
9	13	307	KC1	C4C-C3C-C2C	-2.60	103.11	106.89
8	19	303	CLA	CHC-C1C-C2C	-2.60	119.57	126.95
8	15	301	CLA	C3B-C4B-NB	2.60	112.85	110.53
8	21	208	CLA	CHB-C4A-NA	2.60	128.15	124.40
8	16	309	CLA	C3B-C4B-NB	2.60	112.85	110.53
8	13	301	CLA	O2A-CGA-CBA	2.60	119.75	111.83
10	12	315	A86	C34-O4-C38	-2.59	113.27	117.85
8	19	309	CLA	CMB-C2B-C1B	2.59	129.37	125.42
8	12	303	CLA	C4B-C3B-C2B	-2.59	104.08	107.30
9	16	308	KC1	CMB-C2B-C1B	2.59	129.29	124.73
8	19	301	CLA	CHC-C1C-C2C	-2.59	119.58	126.95
8	19	310	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
9	21	203	KC1	CBC-CAC-C3C	-2.59	105.40	112.42
8	18	310	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
9	19	308	KC1	CMB-C2B-C1B	2.59	129.29	124.73
10	12	312	A86	C4-C3-C2	-2.59	118.22	123.52
8	18	303	CLA	C4-C3-C5	2.59	119.72	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	13	315	A86	C21-C20-C15	-2.59	115.00	123.35
8	16	306	CLA	CHC-C1C-C2C	-2.59	119.60	126.95
8	19	304	CLA	CMB-C2B-C1B	2.59	129.36	125.42
9	17	309	KC1	CAA-CBA-CGA	-2.59	113.90	127.05
8	14	303	CLA	C1-O2A-CGA	2.58	122.91	116.65
8	12	311	CLA	CMB-C2B-C1B	2.58	129.35	125.42
10	17	312	A86	C40-C32-C31	-2.58	108.16	110.47
9	12	308	KC1	O2D-CGD-O1D	-2.58	118.82	123.85
9	21	203	KC1	CHB-C1B-C2B	-2.58	120.12	125.49
8	20	308	CLA	CAA-C2A-C3A	-2.58	106.02	113.00
8	17	308	CLA	CMC-C2C-C1C	2.58	129.07	125.03
8	17	308	CLA	CHD-C4C-NC	2.58	128.23	124.23
8	12	303	CLA	CHB-C4A-NA	2.58	128.12	124.40
8	19	306	CLA	C1C-C2C-C3C	-2.58	104.27	106.98
8	17	307	CLA	O2A-CGA-CBA	2.58	119.70	111.83
8	17	304	CLA	CMB-C2B-C3B	2.58	132.62	126.55
8	13	304	CLA	CHD-C4C-NC	2.58	128.23	124.23
8	21	208	CLA	CHD-C4C-NC	2.58	128.23	124.23
8	11	301	CLA	CHC-C1C-C2C	-2.58	119.62	126.95
10	15	315	A86	C10-C9-C8	-2.58	115.73	123.20
13	20	312	DD6	C3-C4-C5	-2.58	118.24	123.52
10	13	313	A86	C7-C6-C8	2.58	122.03	118.09
8	21	210	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
10	13	314	A86	C35-C34-C33	2.58	114.51	109.89
8	11	301	CLA	CHB-C4A-NA	2.58	128.12	124.40
8	21	204	CLA	O2A-CGA-CBA	2.58	119.69	111.83
8	14	301	CLA	CHC-C1C-C2C	-2.58	119.63	126.95
8	17	308	CLA	CAA-C2A-C3A	-2.58	106.04	113.00
10	21	215	A86	C25-C24-C1	-2.58	119.30	126.36
8	19	305	CLA	C4B-C3B-C2B	-2.58	104.10	107.30
9	12	308	KC1	CAC-C3C-C4C	2.58	128.14	124.79
10	17	321	A86	C40-C32-C31	-2.58	108.17	110.47
9	13	310	KC1	C4C-C3C-C2C	-2.57	103.14	106.89
10	13	316	A86	C36-C31-C32	-2.57	117.14	119.70
8	12	303	CLA	CHC-C1C-C2C	-2.57	119.63	126.95
10	18	311	A86	C12-C11-C13	2.57	120.17	116.00
10	18	312	A86	C12-C11-C13	2.57	120.17	116.00
8	15	308	CLA	CHD-C4C-NC	2.57	128.22	124.23
10	14	316	A86	C40-C32-C31	2.57	112.77	110.47
8	16	301	CLA	CBA-CAA-C2A	2.57	121.44	113.79
9	16	308	KC1	O1D-CGD-CBD	-2.57	119.45	124.52
8	20	310	CLA	O2D-CGD-O1D	-2.57	118.84	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	19	310	CLA	CHD-C4C-NC	2.57	128.22	124.23
11	11	316	LMG	O6-C1-O1	-2.57	103.97	110.04
8	11	303	CLA	C4-C3-C5	2.57	119.69	115.23
10	11	318	A86	C7-C6-C8	2.57	122.01	118.09
9	14	309	KC1	CHB-C4A-NA	2.57	128.22	124.23
9	18	309	KC1	CMB-C2B-C1B	2.57	129.25	124.73
8	20	302	CLA	CBC-CAC-C3C	-2.57	105.46	112.42
8	12	311	CLA	CHB-C4A-NA	2.57	128.11	124.40
8	12	303	CLA	C1-C2-C3	-2.57	121.99	126.20
10	17	316	A86	C7-C6-C5	-2.57	118.66	122.82
10	17	316	A86	C36-C31-C32	-2.57	117.15	119.70
9	11	308	KC1	C1A-NA-C4A	-2.57	105.51	106.68
8	19	301	CLA	CHB-C4A-NA	2.57	128.10	124.40
10	14	315	A86	C21-C20-C15	-2.57	115.07	123.35
8	12	309	CLA	O2A-CGA-CBA	2.57	119.66	111.83
8	14	302	CLA	O2A-CGA-CBA	2.57	119.66	111.83
8	15	308	CLA	CAA-C2A-C3A	-2.56	106.07	113.00
9	13	305	KC1	CMB-C2B-C1B	2.56	129.24	124.73
8	12	301	CLA	CAA-CBA-CGA	-2.56	105.93	113.21
8	18	301	CLA	O2A-CGA-CBA	2.56	119.65	111.83
8	14	308	CLA	CAA-C2A-C3A	-2.56	106.08	113.00
8	18	301	CLA	CMB-C2B-C1B	2.56	129.32	125.42
10	12	319	A86	C8-C6-C5	-2.56	114.98	119.01
8	15	307	CLA	CHB-C1B-C2B	-2.56	120.00	127.43
8	13	301	CLA	CMB-C2B-C1B	2.56	129.32	125.42
10	11	310	A86	C21-C20-C15	-2.56	115.09	123.35
8	21	206	CLA	CMB-C2B-C1B	2.56	129.31	125.42
10	13	312	A86	C8-C6-C5	-2.55	114.99	119.01
8	17	302	CLA	C4-C3-C5	2.55	119.66	115.23
8	13	308	CLA	CMB-C2B-C1B	2.55	129.30	125.42
9	17	305	KC1	CHD-C4C-NC	2.55	128.15	124.31
9	15	306	KC1	CMC-C2C-C1C	2.55	129.02	125.03
8	15	307	CLA	CHA-C1A-NA	-2.55	120.62	126.39
8	11	301	CLA	C4-C3-C5	2.55	119.65	115.23
8	14	310	CLA	CAC-C3C-C4C	2.55	128.10	124.79
10	14	313	A86	C9-C8-C6	-2.55	119.38	126.36
8	18	310	CLA	CAC-C3C-C4C	2.54	128.10	124.79
8	21	206	CLA	CMC-C2C-C1C	2.54	129.01	125.03
8	21	208	CLA	CMB-C2B-C1B	2.54	129.29	125.42
8	14	301	CLA	C3B-C4B-NB	2.54	112.80	110.53
8	18	301	CLA	CHB-C4A-NA	2.54	128.06	124.40
10	15	311	A86	C21-C20-C15	-2.54	115.16	123.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	18	302	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
13	21	212	DD6	C23-C16-C17	-2.54	104.51	108.97
9	15	306	KC1	O2D-CGD-O1D	-2.54	118.91	123.85
8	21	209	CLA	CMB-C2B-C1B	2.54	129.28	125.42
8	19	301	CLA	CMA-C3A-C2A	-2.54	104.18	113.98
8	18	308	CLA	C1-C2-C3	-2.53	122.05	126.20
9	13	307	KC1	O2D-CGD-O1D	-2.53	118.92	123.85
8	11	307	CLA	CHB-C4A-NA	2.53	128.05	124.40
9	20	303	KC1	C4C-C3C-C2C	-2.53	103.21	106.89
10	12	302	A86	C34-O4-C38	-2.53	113.38	117.85
9	20	306	KC1	O1D-CGD-CBD	-2.53	119.53	124.52
8	20	309	CLA	O2A-CGA-CBA	2.53	119.54	111.83
10	18	311	A86	C4-C3-C2	-2.53	118.35	123.52
8	13	306	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
8	16	309	CLA	CAC-C3C-C4C	2.53	128.08	124.79
9	13	303	KC1	CBC-CAC-C3C	-2.52	105.58	112.42
8	13	306	CLA	CAA-C2A-C3A	-2.52	106.18	113.00
8	16	307	CLA	CHB-C4A-NA	2.52	128.04	124.40
8	18	308	CLA	CAA-C2A-C3A	-2.52	106.18	113.00
8	19	306	CLA	CAA-C2A-C3A	-2.52	106.18	113.00
9	15	304	KC1	CAA-C2A-C1A	-2.52	113.60	124.64
8	12	309	CLA	CHB-C4A-NA	2.52	128.04	124.40
10	14	311	A86	C34-O4-C38	-2.52	113.39	117.85
8	14	305	CLA	CHB-C4A-NA	2.52	128.04	124.40
9	16	304	KC1	O2D-CGD-O1D	-2.52	118.94	123.85
8	12	309	CLA	C1-C2-C3	-2.52	122.07	126.20
8	17	307	CLA	CHB-C4A-NA	2.52	128.03	124.40
8	18	303	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
8	14	302	CLA	C4B-C3B-C2B	-2.52	104.17	107.30
10	21	215	A86	C10-C9-C8	-2.52	115.91	123.20
10	11	311	A86	C40-C32-C31	-2.52	108.22	110.47
8	13	309	CLA	CBC-CAC-C3C	-2.51	105.61	112.42
8	20	302	CLA	O2A-CGA-CBA	2.51	119.50	111.83
8	18	305	CLA	CAA-C2A-C3A	-2.51	106.21	113.00
8	21	209	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
10	13	314	A86	C9-C10-C11	-2.51	119.54	126.64
10	13	313	A86	C41-C32-C31	-2.51	108.22	110.47
8	14	305	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
10	13	313	A86	C25-C24-C1	-2.51	119.48	126.36
10	14	314	A86	C7-C6-C8	2.51	121.92	118.09
9	21	207	KC1	O1D-CGD-CBD	-2.51	119.57	124.52
10	11	312	A86	C25-C26-C27	-2.51	123.76	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	18	305	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
8	21	208	CLA	C1-C2-C3	-2.51	122.09	126.20
8	17	307	CLA	CHA-C1A-NA	-2.51	120.72	126.39
9	20	303	KC1	CAC-C3C-C4C	2.50	128.05	124.79
8	15	308	CLA	O2D-CGD-CBD	2.50	115.61	111.23
8	13	302	CLA	CAA-CBA-CGA	-2.50	106.10	113.21
9	13	307	KC1	CMC-C2C-C1C	2.50	128.94	125.03
10	13	315	A86	C7-C6-C8	2.50	121.91	118.09
8	13	301	CLA	CAA-C2A-C3A	-2.50	106.24	113.00
8	21	206	CLA	C1-C2-C3	-2.50	122.10	126.20
10	11	312	A86	C-C1-C24	2.50	121.91	118.09
8	17	302	CLA	C4B-C3B-C2B	-2.50	104.19	107.30
8	14	303	CLA	C4B-C3B-C2B	-2.50	104.19	107.30
10	12	312	A86	C8-C6-C5	-2.50	115.08	119.01
9	11	306	KC1	CHB-C4A-NA	2.50	128.10	124.23
8	16	301	CLA	CHC-C1C-C2C	-2.50	119.85	126.95
9	17	309	KC1	C1A-NA-C4A	-2.49	105.54	106.68
8	11	303	CLA	O1D-CGD-CBD	-2.49	119.60	124.52
10	14	316	A86	C8-C6-C5	2.49	122.93	119.01
10	12	314	A86	C23-C16-C22	-2.49	103.75	107.37
8	11	303	CLA	O2A-CGA-CBA	2.49	119.43	111.83
8	11	305	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
10	17	321	A86	C21-C20-C15	-2.49	115.31	123.35
8	11	301	CLA	C4B-C3B-C2B	-2.49	104.20	107.30
15	21	201	LHG	C11-C10-C9	-2.49	101.80	114.37
8	19	302	CLA	C4-C3-C5	2.49	119.54	115.23
10	21	211	A86	C21-C20-C15	-2.49	115.32	123.35
10	15	312	A86	C25-C24-C1	-2.49	119.55	126.36
10	18	313	A86	C12-C11-C13	2.49	120.03	116.00
8	12	307	CLA	CAC-C3C-C4C	2.48	128.02	124.79
8	15	305	CLA	CHB-C4A-NA	2.48	127.98	124.40
8	14	307	CLA	CHB-C4A-NA	2.48	127.98	124.40
9	16	302	KC1	C4C-C3C-C2C	-2.48	103.28	106.89
8	21	205	CLA	CHB-C4A-NA	2.48	127.98	124.40
8	16	301	CLA	C3B-C4B-NB	2.48	112.74	110.53
8	18	307	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
8	12	305	CLA	CBC-CAC-C3C	-2.48	105.70	112.42
9	14	306	KC1	CHB-C4A-NA	2.48	128.07	124.23
8	17	310	CLA	CAC-C3C-C4C	2.48	128.01	124.79
10	21	215	A86	C33-C32-C31	2.48	111.62	109.21
8	17	310	CLA	CMB-C2B-C1B	2.47	129.19	125.42
10	18	311	A86	C25-C24-C1	-2.47	119.58	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	20	308	CLA	O2D-CGD-O1D	-2.47	119.03	123.85
8	14	308	CLA	CMB-C2B-C1B	2.47	129.18	125.42
8	21	205	CLA	CHD-C4C-NC	2.47	128.06	124.23
10	18	314	A86	C36-C31-C32	-2.47	117.25	119.70
9	17	309	KC1	CMC-C2C-C1C	2.47	128.89	125.03
8	15	305	CLA	CAA-C2A-C3A	-2.47	106.33	113.00
8	18	307	CLA	O2A-CGA-CBA	2.47	119.36	111.83
8	15	301	CLA	C4B-C3B-C2B	-2.47	104.23	107.30
9	18	309	KC1	CHB-C4A-NA	2.47	128.06	124.23
8	17	308	CLA	C1-C2-C3	-2.47	122.15	126.20
8	19	304	CLA	O2D-CGD-O1D	-2.47	119.05	123.85
10	11	318	A86	C8-C6-C5	-2.47	115.13	119.01
16	19	315	LMU	C1B-O1B-C4'	-2.47	112.13	117.98
10	21	214	A86	C10-C9-C8	-2.46	116.06	123.20
8	17	302	CLA	C1-O2A-CGA	2.46	122.61	116.65
10	12	302	A86	C7-C6-C5	-2.46	118.83	122.82
9	12	310	KC1	CBC-CAC-C3C	-2.46	105.75	112.42
8	19	306	CLA	C4B-C3B-C2B	-2.46	104.24	107.30
8	13	311	CLA	O1D-CGD-CBD	-2.46	119.67	124.52
8	17	304	CLA	CHB-C4A-NA	2.46	127.95	124.40
8	18	310	CLA	CMB-C2B-C1B	2.46	129.16	125.42
10	13	315	A86	C34-O4-C38	-2.46	113.50	117.85
10	14	314	A86	C8-C6-C5	-2.46	115.14	119.01
8	12	307	CLA	CBC-CAC-C3C	-2.46	105.76	112.42
8	12	301	CLA	CMB-C2B-C1B	2.46	129.16	125.42
8	12	303	CLA	CMB-C2B-C1B	2.45	129.16	125.42
9	14	306	KC1	CHB-C1B-NB	-2.45	121.35	124.80
8	14	310	CLA	CBC-CAC-C3C	-2.45	105.77	112.42
8	20	307	CLA	CHB-C4A-NA	2.45	127.94	124.40
8	17	308	CLA	CMB-C2B-C1B	2.45	129.15	125.42
8	11	307	CLA	CHA-C1A-NA	-2.45	120.84	126.39
8	12	301	CLA	CBC-CAC-C3C	-2.45	105.78	112.42
10	20	313	A86	C41-C32-C31	-2.45	108.28	110.47
8	13	308	CLA	O2A-CGA-CBA	2.45	119.30	111.83
8	18	308	CLA	CBC-CAC-C3C	-2.45	105.78	112.42
8	18	301	CLA	C4-C3-C5	2.45	119.48	115.23
8	15	305	CLA	CBC-CAC-C3C	-2.45	105.78	112.42
9	14	306	KC1	CAC-C3C-C4C	2.45	127.97	124.79
9	20	303	KC1	CAB-C3B-C4B	2.45	130.66	124.82
8	20	309	CLA	CMB-C2B-C1B	2.45	129.14	125.42
8	20	304	CLA	CHA-C1A-NA	-2.45	120.85	126.39
11	17	318	LMG	O6-C1-O1	-2.44	104.27	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	19	310	CLA	CHB-C4A-NA	2.44	127.93	124.40
8	14	303	CLA	CHB-C4A-NA	2.44	127.92	124.40
10	20	313	A86	C9-C10-C11	-2.44	119.74	126.64
8	12	307	CLA	CAA-C2A-C1A	-2.44	103.97	111.97
10	14	311	A86	C8-C6-C5	-2.44	115.17	119.01
10	20	313	A86	C34-O4-C38	-2.44	113.54	117.85
8	15	305	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
8	12	301	CLA	CMC-C2C-C1C	2.44	128.85	125.03
10	12	315	A86	C8-C6-C5	-2.44	115.17	119.01
8	15	307	CLA	O2A-CGA-CBA	2.44	119.27	111.83
10	17	314	A86	C8-C6-C5	-2.44	115.17	119.01
8	15	310	CLA	CHB-C4A-NA	2.44	127.92	124.40
8	12	309	CLA	CHA-C1A-NA	-2.44	120.87	126.39
9	12	310	KC1	CHB-C1B-C2B	-2.44	120.42	125.49
10	17	313	A86	C25-C24-C1	-2.44	119.68	126.36
8	12	307	CLA	CMB-C2B-C1B	2.44	129.13	125.42
13	19	312	DD6	C33-C32-C31	2.44	114.29	109.49
10	16	311	A86	C3-C4-C5	-2.44	118.54	123.52
11	16	315	LMG	O1-C1-C2	-2.43	104.58	108.27
9	16	305	KC1	CAC-C3C-C4C	2.43	127.95	124.79
8	14	303	CLA	CMB-C2B-C1B	2.43	129.12	125.42
14	17	301	SQD	C1-O5-C5	2.43	118.47	113.72
9	19	308	KC1	CAB-C3B-C4B	2.43	130.63	124.82
8	20	302	CLA	CMC-C2C-C1C	2.43	128.83	125.03
9	12	310	KC1	CHB-C4A-NA	2.43	128.00	124.23
10	11	313	A86	C41-C32-C31	-2.43	108.30	110.47
10	14	314	A86	C40-C32-C31	-2.43	108.30	110.47
8	18	310	CLA	CHB-C4A-NA	2.43	127.91	124.40
8	12	301	CLA	C4-C3-C5	2.43	119.44	115.23
9	20	303	KC1	CMB-C2B-C1B	2.43	129.01	124.73
9	16	302	KC1	C1A-NA-C4A	-2.43	105.57	106.68
8	15	305	CLA	CMB-C2B-C1B	2.43	129.12	125.42
8	12	303	CLA	O2A-CGA-CBA	2.43	119.24	111.83
8	14	310	CLA	CHB-C4A-NA	2.43	127.90	124.40
8	11	307	CLA	C4B-C3B-C2B	-2.42	104.29	107.30
8	15	307	CLA	CAA-C2A-C1A	2.42	119.92	111.97
9	14	306	KC1	CMC-C2C-C1C	2.42	128.82	125.03
9	18	306	KC1	CMC-C2C-C1C	2.42	128.82	125.03
8	18	302	CLA	CHB-C4A-NA	2.42	127.90	124.40
8	11	303	CLA	CAA-C2A-C1A	2.42	119.91	111.97
8	11	309	CLA	CAC-C3C-C4C	2.42	127.94	124.79
9	15	309	KC1	CMC-C2C-C1C	2.42	128.82	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	16	302	KC1	CHB-C4A-NA	2.42	127.98	124.23
8	18	308	CLA	CAC-C3C-C4C	2.42	127.94	124.79
8	18	307	CLA	CAA-C2A-C3A	-2.42	106.46	113.00
8	21	202	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
8	15	307	CLA	CHB-C4A-NA	2.42	127.89	124.40
8	18	308	CLA	C4-C3-C5	2.42	119.42	115.23
8	12	309	CLA	O1D-CGD-CBD	-2.42	119.75	124.52
10	13	312	A86	C23-C16-C22	-2.42	103.86	107.37
8	15	305	CLA	CMC-C2C-C1C	2.42	128.81	125.03
8	20	304	CLA	O2A-CGA-CBA	2.42	119.20	111.83
8	13	301	CLA	CHD-C4C-NC	2.42	127.98	124.23
8	17	310	CLA	C4-C3-C5	2.42	119.42	115.23
8	19	306	CLA	CHC-C1C-C2C	-2.42	120.08	126.95
8	11	301	CLA	C3B-C4B-NB	2.42	112.69	110.53
8	18	301	CLA	C3B-C4B-NB	2.42	112.69	110.53
9	15	302	KC1	CGD-CBD-CAD	-2.41	103.03	110.85
9	21	207	KC1	CHB-C4A-NA	2.41	127.97	124.23
8	14	301	CLA	C4B-C3B-C2B	-2.41	104.30	107.30
8	12	309	CLA	CMB-C2B-C3B	2.41	132.23	126.55
8	11	303	CLA	CHB-C4A-NA	2.41	127.88	124.40
10	14	311	A86	C21-C20-C15	-2.41	115.56	123.35
9	19	308	KC1	CMC-C2C-C1C	2.41	128.80	125.03
10	15	315	A86	C40-C32-C31	-2.41	108.31	110.47
10	18	314	A86	C8-C6-C5	2.41	122.80	119.01
8	14	307	CLA	C4B-C3B-C2B	-2.41	104.31	107.30
8	21	206	CLA	CAC-C3C-C4C	2.41	127.92	124.79
10	14	313	A86	C4-C3-C2	-2.41	118.59	123.52
10	14	316	A86	C36-C31-C32	-2.41	117.31	119.70
8	16	306	CLA	C1-C2-C3	-2.41	122.25	126.20
9	11	308	KC1	O1D-CGD-CBD	-2.41	119.77	124.52
8	18	305	CLA	CHB-C4A-NA	2.41	127.88	124.40
10	16	310	A86	C36-C31-C32	-2.41	117.31	119.70
9	14	306	KC1	O1D-CGD-CBD	-2.41	119.77	124.52
8	13	304	CLA	CMC-C2C-C1C	2.41	128.79	125.03
10	14	315	A86	C35-C34-C33	2.41	114.21	109.89
9	11	304	KC1	O2D-CGD-O1D	-2.41	119.17	123.85
10	17	315	A86	C23-C16-C22	-2.41	103.88	107.37
8	21	204	CLA	CHB-C4A-NA	2.40	127.87	124.40
9	15	306	KC1	CBC-CAC-C3C	-2.40	105.91	112.42
8	15	307	CLA	O1D-CGD-CBD	-2.40	119.78	124.52
8	14	302	CLA	CHB-C4A-NA	2.40	127.86	124.40
10	17	313	A86	C-C1-C24	2.40	121.75	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	21	217	LHG	C11-C10-C9	-2.40	102.24	114.37
8	18	308	CLA	CHB-C4A-NA	2.40	127.86	124.40
8	12	309	CLA	CHB-C1B-C2B	-2.40	120.46	127.43
8	14	307	CLA	C1-C2-C3	-2.40	122.27	126.20
8	17	308	CLA	CHB-C4A-NA	2.40	127.86	124.40
10	21	211	A86	C25-C24-C1	-2.40	119.79	126.36
8	16	306	CLA	CBC-CAC-C3C	-2.40	105.92	112.42
8	18	307	CLA	C4-C3-C5	2.40	119.39	115.23
8	12	309	CLA	CAA-C2A-C3A	-2.40	106.52	113.00
13	21	212	DD6	C22-C16-C15	2.40	116.52	110.05
9	13	310	KC1	CHB-C4A-NA	2.40	127.95	124.23
10	16	311	A86	C8-C6-C5	-2.40	115.24	119.01
8	15	308	CLA	O2A-CGA-CBA	2.39	119.14	111.83
8	19	303	CLA	O2A-CGA-CBA	2.39	119.13	111.83
9	15	306	KC1	CAA-C2A-C1A	-2.39	114.16	124.64
8	19	301	CLA	CBC-CAC-C3C	-2.39	105.93	112.42
8	11	309	CLA	C1-C2-C3	-2.39	122.28	126.20
8	12	307	CLA	CHB-C4A-NA	2.39	127.85	124.40
8	12	309	CLA	CAA-C2A-C1A	2.39	119.81	111.97
9	17	306	KC1	CAC-C3C-C4C	2.39	127.90	124.79
8	13	304	CLA	CBC-CAC-C3C	-2.39	105.94	112.42
8	16	309	CLA	CAA-C2A-C1A	-2.39	104.15	111.97
10	19	313	A86	C-C1-C24	2.39	121.74	118.09
9	16	305	KC1	CHB-C4A-NA	2.39	127.93	124.23
8	20	304	CLA	CMB-C2B-C1B	2.39	129.06	125.42
10	17	313	A86	C41-C32-C31	-2.39	108.33	110.47
15	21	217	LHG	O8-C23-C24	2.39	119.11	111.83
10	17	315	A86	C36-C31-C32	-2.39	117.33	119.70
10	14	316	A86	C26-C25-C24	-2.39	116.28	123.20
10	15	316	A86	C7-C6-C5	-2.39	118.95	122.82
8	18	307	CLA	CHB-C4A-NA	2.39	127.84	124.40
8	17	304	CLA	O2A-CGA-CBA	2.39	119.11	111.83
9	18	304	KC1	O2D-CGD-O1D	-2.39	119.20	123.85
8	14	302	CLA	CHA-C1A-NA	-2.39	120.99	126.39
8	16	303	CLA	CMB-C2B-C1B	2.38	129.05	125.42
8	18	308	CLA	C1-O2A-CGA	2.38	122.42	116.65
8	19	301	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
10	17	313	A86	O4-C34-C33	2.38	113.73	107.64
10	14	312	A86	C8-C6-C5	-2.38	115.26	119.01
9	20	303	KC1	CMC-C2C-C1C	2.38	128.75	125.03
8	13	306	CLA	CBC-CAC-C3C	-2.38	105.97	112.42
10	13	316	A86	C7-C6-C5	-2.38	118.96	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	21	215	A86	C21-C20-C15	-2.38	115.67	123.35
8	15	307	CLA	C1-O2A-CGA	2.38	122.41	116.65
8	17	308	CLA	O2A-CGA-CBA	2.38	119.08	111.83
9	11	308	KC1	CGD-CBD-CAD	-2.38	103.15	110.85
9	21	207	KC1	O2D-CGD-O1D	-2.38	119.22	123.85
10	13	314	A86	C21-C20-C15	-2.38	115.68	123.35
8	12	305	CLA	O2A-CGA-CBA	2.37	119.08	111.83
10	12	316	A86	C36-C31-C32	-2.37	117.34	119.70
8	12	304	CLA	CHA-C1A-NA	-2.37	121.02	126.39
10	11	311	A86	C21-C20-C15	-2.37	115.69	123.35
8	16	306	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
10	13	314	A86	C10-C9-C8	-2.37	116.33	123.20
8	14	303	CLA	CBC-CAC-C3C	-2.37	105.99	112.42
8	15	310	CLA	O1D-CGD-CBD	-2.37	119.84	124.52
8	12	305	CLA	CHB-C4A-NA	2.37	127.82	124.40
8	13	308	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
8	13	304	CLA	C4B-C3B-C2B	-2.37	104.36	107.30
15	21	201	LHG	O3-C3-C2	-2.37	99.87	109.63
10	14	312	A86	C34-O4-C38	-2.37	113.66	117.85
10	20	311	A86	C21-C20-C15	-2.37	115.70	123.35
8	18	302	CLA	CHA-C1A-NA	-2.37	121.03	126.39
8	19	306	CLA	CHB-C4A-NA	2.37	127.82	124.40
8	13	309	CLA	CHD-C4C-NC	2.37	127.90	124.23
10	21	213	A86	C10-C9-C8	-2.37	116.34	123.20
8	11	309	CLA	CHB-C4A-NA	2.37	127.81	124.40
8	11	303	CLA	CBC-CAC-C3C	-2.36	106.01	112.42
8	13	302	CLA	CMC-C2C-C1C	2.36	128.73	125.03
8	14	308	CLA	CED-O2D-CGD	2.36	121.28	115.92
8	13	304	CLA	CHB-C4A-NA	2.36	127.81	124.40
9	15	304	KC1	CMB-C2B-C1B	2.36	128.89	124.73
8	14	308	CLA	CMC-C2C-C1C	2.36	128.73	125.03
9	17	306	KC1	CAA-CBA-CGA	-2.36	115.04	127.05
8	13	304	CLA	CAA-C2A-C1A	2.36	119.71	111.97
10	13	316	A86	C26-C25-C24	-2.36	116.37	123.20
8	18	305	CLA	CMB-C2B-C1B	2.36	129.01	125.42
8	17	304	CLA	CHB-C1B-C2B	-2.36	120.58	127.43
10	11	314	A86	C8-C6-C5	-2.36	115.30	119.01
8	18	303	CLA	CBC-CAC-C3C	-2.36	106.03	112.42
8	14	307	CLA	CMC-C2C-C1C	2.36	128.72	125.03
8	19	305	CLA	CMC-C2C-C1C	2.35	128.71	125.03
10	13	314	A86	C7-C6-C5	-2.35	119.00	122.82
8	21	204	CLA	O1D-CGD-CBD	-2.35	119.88	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	20	304	CLA	OBD-CAD-C3D	-2.35	122.92	128.42
8	20	302	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
10	11	318	A86	C33-C32-C31	2.35	111.50	109.21
8	13	308	CLA	CGD-CBD-CAD	-2.35	103.23	110.85
8	15	303	CLA	O2A-CGA-CBA	2.35	119.01	111.83
15	19	314	LHG	C27-C26-C25	-2.35	102.48	114.37
13	20	314	DD6	C25-C24-C1	-2.35	119.91	126.36
8	17	310	CLA	CHB-C4A-NA	2.35	127.79	124.40
9	15	306	KC1	CHB-C4A-NA	2.35	127.88	124.23
8	17	308	CLA	C1-O2A-CGA	2.35	122.34	116.65
9	20	305	KC1	CMC-C2C-C1C	2.35	128.71	125.03
8	12	307	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
10	12	315	A86	C41-C32-C31	-2.35	108.37	110.47
8	12	311	CLA	CMC-C2C-C1C	2.35	128.70	125.03
8	13	302	CLA	C4B-C3B-C2B	-2.35	104.38	107.30
10	19	313	A86	C24-C1-C2	-2.35	115.32	119.01
9	18	306	KC1	CHD-C1D-ND	-2.35	120.53	124.05
8	14	310	CLA	CMB-C2B-C1B	2.34	128.99	125.42
8	17	310	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
8	13	311	CLA	CHB-C4A-NA	2.34	127.78	124.40
10	14	312	A86	C21-C20-C15	-2.34	115.79	123.35
8	21	209	CLA	CBC-CAC-C3C	-2.34	106.07	112.42
10	17	314	A86	C-C1-C24	2.34	121.67	118.09
8	19	301	CLA	CBA-CAA-C2A	2.34	120.76	113.79
8	18	310	CLA	CHD-C4C-NC	2.34	127.86	124.23
9	11	302	KC1	CHB-C4A-NA	2.34	127.86	124.23
9	18	306	KC1	CHB-C4A-NA	2.34	127.86	124.23
8	16	307	CLA	CMC-C2C-C1C	2.34	128.69	125.03
8	15	301	CLA	CMC-C2C-C1C	2.34	128.69	125.03
8	19	301	CLA	O2A-CGA-CBA	2.34	118.97	111.83
8	16	303	CLA	CHB-C4A-NA	2.34	127.78	124.40
9	17	303	KC1	CHC-C4B-C3B	-2.34	121.27	125.21
14	17	301	SQD	C44-O6-C1	2.34	118.81	113.80
8	13	302	CLA	C1-O2A-CGA	2.34	122.31	116.65
15	17	317	LHG	C20-C19-C18	-2.34	102.56	114.37
8	14	307	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
8	14	302	CLA	C4-C3-C5	2.33	119.28	115.23
8	16	303	CLA	C1-O2A-CGA	2.33	122.30	116.65
8	14	301	CLA	CHB-C4A-NA	2.33	127.76	124.40
8	19	310	CLA	C4-C3-C5	2.33	119.27	115.23
8	18	305	CLA	CMC-C2C-C1C	2.33	128.68	125.03
8	15	307	CLA	CMB-C2B-C3B	2.33	132.03	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	15	308	CLA	C1-O2A-CGA	2.33	122.28	116.65
9	17	305	KC1	CHB-C4A-NA	2.33	127.84	124.23
9	14	304	KC1	O2D-CGD-O1D	-2.33	119.32	123.85
8	20	302	CLA	C4B-C3B-C2B	-2.33	104.41	107.30
9	13	307	KC1	C3D-C2D-C1D	-2.33	98.97	106.40
8	15	301	CLA	O2A-CGA-CBA	2.32	118.92	111.83
9	15	302	KC1	CHB-C4A-NA	2.32	127.83	124.23
8	17	307	CLA	C1-C2-C3	-2.32	122.39	126.20
11	16	315	LMG	O3-C3-C2	-2.32	104.91	110.38
9	17	303	KC1	CHB-C4A-NA	2.32	127.83	124.23
9	11	308	KC1	CBC-CAC-C3C	-2.32	106.13	112.42
8	18	301	CLA	CAA-CBA-CGA	-2.32	106.62	113.21
8	18	310	CLA	CAA-C2A-C3A	-2.32	106.74	113.00
8	15	303	CLA	CAA-C2A-C1A	2.32	119.56	111.97
10	15	312	A86	C41-C32-C31	-2.31	108.40	110.47
8	12	304	CLA	CHB-C4A-NA	2.31	127.74	124.40
9	18	304	KC1	CHB-C4A-NA	2.31	127.82	124.23
8	20	309	CLA	CHB-C4A-NA	2.31	127.74	124.40
8	13	306	CLA	CMB-C2B-C1B	2.31	128.94	125.42
8	21	206	CLA	CHB-C4A-NA	2.31	127.74	124.40
10	11	313	A86	C35-C34-C33	2.31	114.04	109.89
8	12	311	CLA	O1D-CGD-CBD	-2.31	119.96	124.52
8	14	303	CLA	C4-C3-C5	2.31	119.24	115.23
9	20	306	KC1	CHB-C4A-NA	2.31	127.81	124.23
8	16	306	CLA	C2A-C3A-C4A	-2.31	98.14	101.87
8	12	301	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
8	12	303	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
8	16	303	CLA	O2A-CGA-CBA	2.31	118.87	111.83
9	13	310	KC1	CMB-C2B-C1B	2.31	128.79	124.73
8	14	308	CLA	CBC-CAC-C3C	-2.31	106.17	112.42
8	11	305	CLA	CMA-C3A-C4A	-2.31	105.57	111.77
10	15	312	A86	C8-C6-C5	-2.31	115.38	119.01
8	18	302	CLA	O2A-CGA-CBA	2.31	118.86	111.83
8	14	305	CLA	CMB-C2B-C1B	2.31	128.93	125.42
9	13	303	KC1	CMB-C2B-C1B	2.30	128.78	124.73
9	20	303	KC1	CHB-C4A-NA	2.30	127.80	124.23
8	11	301	CLA	O2D-CGD-O1D	-2.30	119.37	123.85
10	11	318	A86	C19-C18-C17	-2.30	106.49	110.79
8	18	303	CLA	O2A-CGA-CBA	2.30	118.85	111.83
9	11	306	KC1	C3D-C2D-C1D	-2.30	99.06	106.40
8	20	309	CLA	CAA-C2A-C1A	2.30	119.51	111.97
8	20	304	CLA	CBC-CAC-C3C	-2.30	106.20	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	12	312	A86	C36-C31-C32	-2.30	117.42	119.70
13	21	216	DD6	C9-C8-C6	-2.30	120.07	126.36
9	18	304	KC1	CMC-C2C-C1C	2.29	128.62	125.03
10	11	310	A86	C23-C16-C22	-2.29	104.04	107.37
8	13	306	CLA	CMC-C2C-C1C	2.29	128.62	125.03
10	11	313	A86	C-C1-C24	2.29	121.59	118.09
8	14	305	CLA	O1D-CGD-CBD	-2.29	120.00	124.52
15	21	217	LHG	C27-C26-C25	-2.29	102.78	114.37
8	11	305	CLA	CMC-C2C-C1C	2.29	128.61	125.03
10	18	313	A86	C8-C6-C5	-2.29	115.41	119.01
8	16	301	CLA	C4B-C3B-C2B	-2.29	104.46	107.30
8	21	210	CLA	O1D-CGD-CBD	-2.29	120.00	124.52
8	19	305	CLA	O2A-CGA-CBA	2.29	118.81	111.83
8	13	309	CLA	CAA-C2A-C3A	-2.29	106.82	113.00
8	20	309	CLA	CHA-C1A-NA	-2.29	121.21	126.39
8	12	301	CLA	CAA-C2A-C3A	-2.29	106.82	113.00
9	17	306	KC1	CHB-C4A-NA	2.29	127.78	124.23
8	15	310	CLA	CBC-CAC-C3C	-2.29	106.22	112.42
9	16	302	KC1	O2D-CGD-O1D	-2.29	119.40	123.85
10	21	214	A86	C25-C24-C1	-2.28	120.10	126.36
8	18	308	CLA	CED-O2D-CGD	2.28	121.10	115.92
13	20	314	DD6	C3-C4-C5	-2.28	118.85	123.52
8	20	310	CLA	CHB-C4A-NA	2.28	127.69	124.40
8	21	206	CLA	C4-C3-C5	2.28	119.19	115.23
10	11	312	A86	C19-C18-C17	-2.28	106.52	110.79
10	21	213	A86	C12-C11-C13	2.28	119.70	116.00
10	15	316	A86	C9-C10-C11	-2.28	120.19	126.64
8	16	307	CLA	C1-O2A-CGA	2.28	122.17	116.65
9	15	304	KC1	O2D-CGD-O1D	-2.28	119.41	123.85
9	15	306	KC1	CGD-CBD-CAD	-2.28	103.47	110.85
8	13	301	CLA	CBC-CAC-C3C	-2.28	106.25	112.42
8	13	304	CLA	C1-C2-C3	-2.27	122.47	126.20
8	14	307	CLA	CHB-C1B-C2B	-2.27	120.83	127.43
8	15	310	CLA	CMB-C2B-C1B	2.27	128.88	125.42
8	18	303	CLA	CAA-C2A-C1A	2.27	119.42	111.97
9	18	306	KC1	CHB-C1B-NB	-2.27	121.61	124.80
9	13	310	KC1	CHB-C1B-C2B	-2.27	120.77	125.49
9	15	304	KC1	CHB-C4A-NA	2.27	127.75	124.23
10	11	311	A86	C19-C18-C17	2.27	115.03	110.79
8	16	306	CLA	C1-O2A-CGA	2.27	122.14	116.65
8	19	303	CLA	O2D-CGD-O1D	-2.27	119.43	123.85
8	20	309	CLA	O2D-CGD-O1D	-2.27	119.44	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	20	305	KC1	CHB-C4A-NA	2.27	127.75	124.23
8	13	304	CLA	C1-O2A-CGA	2.27	122.14	116.65
9	13	303	KC1	CHC-C4B-NB	-2.27	121.61	124.80
8	16	301	CLA	CBC-CAC-C3C	-2.27	106.28	112.42
8	11	303	CLA	CMB-C2B-C1B	2.27	128.87	125.42
13	21	212	DD6	C9-C8-C6	-2.27	120.15	126.36
10	15	319	A86	C34-O4-C38	-2.27	113.84	117.85
8	19	309	CLA	CHB-C4A-NA	2.26	127.67	124.40
8	12	304	CLA	C4-C3-C5	2.26	119.16	115.23
9	21	203	KC1	CMC-C2C-C1C	2.26	128.57	125.03
9	17	303	KC1	CMC-C2C-C1C	2.26	128.57	125.03
9	17	303	KC1	C4C-C3C-C2C	-2.26	103.60	106.89
10	17	314	A86	C36-C31-C32	-2.26	117.45	119.70
8	21	210	CLA	CMC-C2C-C1C	2.26	128.57	125.03
10	13	316	A86	C4-C3-C2	-2.26	118.89	123.52
15	19	314	LHG	C11-C10-C9	-2.26	102.95	114.37
9	14	304	KC1	CHB-C4A-NA	2.26	127.73	124.23
10	19	313	A86	C22-C16-C17	-2.26	105.00	108.97
9	20	306	KC1	O2A-CGA-O1A	-2.26	118.10	122.70
8	11	307	CLA	CAA-C2A-C1A	2.26	119.37	111.97
9	12	306	KC1	C3D-C2D-C1D	-2.25	99.20	106.40
8	19	309	CLA	CMC-C2C-C1C	2.25	128.55	125.03
8	19	307	CLA	CMB-C2B-C1B	2.25	128.85	125.42
9	18	306	KC1	CAB-C3B-C4B	2.25	130.19	124.82
8	16	309	CLA	CHB-C1B-C2B	-2.25	120.89	127.43
8	16	306	CLA	C4-C3-C5	2.25	119.13	115.23
9	13	305	KC1	O2D-CGD-O1D	-2.25	119.47	123.85
9	13	303	KC1	CHB-C4A-NA	2.25	127.72	124.23
9	16	308	KC1	CHB-C4A-NA	2.25	127.72	124.23
8	17	304	CLA	O1D-CGD-CBD	-2.25	120.08	124.52
13	21	216	DD6	C3-C4-C5	-2.25	118.92	123.52
9	20	306	KC1	CMC-C2C-C3C	2.25	132.22	126.15
10	20	301	A86	C34-O4-C38	-2.25	113.88	117.85
8	12	304	CLA	C1-C2-C3	-2.25	122.52	126.20
9	17	306	KC1	O1D-CGD-CBD	-2.25	120.09	124.52
10	15	313	A86	C9-C8-C6	-2.24	120.21	126.36
8	12	301	CLA	CHB-C4A-NA	2.24	127.64	124.40
8	14	310	CLA	O2D-CGD-O1D	-2.24	119.48	123.85
9	14	306	KC1	C3D-C2D-C1D	-2.24	99.24	106.40
9	12	310	KC1	CMB-C2B-C1B	2.24	128.68	124.73
8	20	302	CLA	CHB-C4A-NA	2.24	127.64	124.40
8	14	303	CLA	CHB-C1B-C2B	-2.24	120.92	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	14	301	CLA	C4-C3-C5	2.24	119.12	115.23
10	19	313	A86	C41-C32-C31	-2.24	108.47	110.47
8	17	307	CLA	CBC-CAC-C3C	-2.24	106.35	112.42
8	19	306	CLA	O2D-CGD-O1D	-2.24	119.49	123.85
9	15	302	KC1	CMC-C2C-C1C	2.24	128.53	125.03
8	16	307	CLA	CBC-CAC-C3C	-2.24	106.36	112.42
8	15	303	CLA	CHB-C4A-NA	2.24	127.63	124.40
10	11	314	A86	C7-C6-C8	2.24	121.50	118.09
9	13	305	KC1	C3D-C2D-C1D	-2.24	99.26	106.40
9	13	305	KC1	CHB-C4A-NA	2.24	127.70	124.23
8	17	302	CLA	CAA-CBA-CGA	-2.24	106.86	113.21
9	16	304	KC1	CMB-C2B-C1B	2.24	128.66	124.73
8	19	310	CLA	C1-C2-C3	-2.23	122.54	126.20
8	14	302	CLA	O2D-CGD-O1D	-2.23	119.50	123.85
8	20	304	CLA	CHB-C4A-NA	2.23	127.62	124.40
11	11	315	LMG	O1-C7-C8	-2.23	105.39	110.82
9	13	310	KC1	CMC-C2C-C1C	2.23	128.52	125.03
10	14	313	A86	C19-C18-C17	-2.23	106.62	110.79
9	17	306	KC1	CHD-C4C-NC	2.23	127.67	124.31
9	15	306	KC1	C3D-C2D-C1D	-2.23	99.28	106.40
10	12	313	A86	C34-O4-C38	-2.23	113.91	117.85
10	20	311	A86	C34-O4-C38	-2.23	113.91	117.85
8	12	304	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
8	20	307	CLA	CMC-C2C-C1C	2.23	128.52	125.03
10	14	313	A86	C23-C16-C22	-2.23	104.13	107.37
10	12	319	A86	C41-C32-C31	-2.23	108.48	110.47
10	13	314	A86	C25-C24-C1	-2.23	120.26	126.36
10	19	311	A86	C8-C6-C5	-2.23	115.51	119.01
8	14	303	CLA	O1D-CGD-CBD	-2.23	120.13	124.52
9	17	305	KC1	CMC-C2C-C1C	2.23	128.51	125.03
10	15	319	A86	C8-C6-C5	-2.22	115.51	119.01
9	16	305	KC1	C3D-C2D-C1D	-2.22	99.30	106.40
10	17	314	A86	C34-O4-C38	-2.22	113.92	117.85
10	14	316	A86	C9-C10-C11	-2.22	120.36	126.64
8	20	308	CLA	CBC-CAC-C3C	-2.22	106.40	112.42
10	18	313	A86	C34-O4-C38	-2.22	113.92	117.85
9	16	304	KC1	CHB-C4A-NA	2.22	127.68	124.23
8	18	303	CLA	CHB-C4A-NA	2.22	127.60	124.40
10	17	313	A86	C19-C18-C17	-2.22	106.64	110.79
9	20	303	KC1	C3D-C2D-C1D	-2.22	99.32	106.40
8	20	308	CLA	CMC-C2C-C1C	2.22	128.50	125.03
10	21	213	A86	C25-C24-C1	-2.22	120.29	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	15	311	A86	C7-C6-C8	2.22	121.47	118.09
8	19	302	CLA	CMC-C2C-C1C	2.21	128.49	125.03
9	17	306	KC1	CMB-C2B-C1B	2.21	128.62	124.73
9	16	304	KC1	C3D-C2D-C1D	-2.21	99.33	106.40
8	15	303	CLA	CBC-CAC-C3C	-2.21	106.43	112.42
10	15	319	A86	C3-C4-C5	-2.21	119.00	123.52
8	13	301	CLA	CMC-C2C-C1C	2.21	128.48	125.03
9	12	308	KC1	CAA-C2A-C1A	-2.21	114.97	124.64
8	11	301	CLA	CBC-CAC-C3C	-2.21	106.44	112.42
10	12	316	A86	C26-C25-C24	-2.20	116.81	123.20
15	17	317	LHG	C18-C17-C16	-2.20	103.22	114.37
10	17	316	A86	C3-C4-C5	-2.20	119.01	123.52
9	19	308	KC1	CHB-C4A-NA	2.20	127.65	124.23
8	19	302	CLA	CBC-CAC-C3C	-2.20	106.44	112.42
9	12	308	KC1	CMC-C2C-C1C	2.20	128.48	125.03
8	18	303	CLA	CHB-C1B-C2B	-2.20	121.03	127.43
10	14	311	A86	C36-C31-C32	-2.20	117.51	119.70
10	18	314	A86	C12-C11-C13	2.20	119.57	116.00
9	18	304	KC1	CMB-C2B-C1B	2.20	128.61	124.73
8	16	303	CLA	O1D-CGD-CBD	-2.20	120.17	124.52
10	15	313	A86	C4-C3-C2	-2.20	119.01	123.52
10	12	313	A86	C7-C6-C8	2.20	121.45	118.09
10	17	315	A86	C34-O4-C38	-2.20	113.96	117.85
8	18	307	CLA	CHA-C1A-NA	-2.20	121.41	126.39
13	19	312	DD6	C10-C9-C8	-2.20	116.83	123.20
10	19	311	A86	C25-C26-C27	2.20	130.36	127.28
9	11	308	KC1	C3D-C2D-C1D	-2.20	99.38	106.40
8	14	307	CLA	CBC-CAC-C3C	-2.20	106.46	112.42
8	11	301	CLA	O2A-CGA-CBA	2.20	118.54	111.83
13	19	312	DD6	C23-C16-C15	2.20	115.98	110.05
8	17	307	CLA	CMB-C2B-C3B	2.20	131.72	126.55
8	15	308	CLA	CHB-C4A-NA	2.20	127.57	124.40
8	13	301	CLA	CHB-C4A-NA	2.19	127.57	124.40
8	18	302	CLA	CMB-C2B-C1B	2.19	128.76	125.42
8	15	303	CLA	CHB-C1B-C2B	-2.19	121.06	127.43
10	12	312	A86	C35-C34-C33	2.19	113.83	109.89
8	12	303	CLA	CHA-C1A-NA	-2.19	121.42	126.39
9	13	305	KC1	CMC-C2C-C1C	2.19	128.46	125.03
8	19	310	CLA	CBC-CAC-C3C	-2.19	106.48	112.42
8	21	204	CLA	CMC-C2C-C1C	2.19	128.46	125.03
8	11	309	CLA	CMB-C2B-C1B	2.19	128.75	125.42
8	16	306	CLA	CMB-C2B-C3B	2.19	131.70	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	13	302	CLA	CBC-CAC-C3C	-2.19	106.49	112.42
9	16	308	KC1	C3D-C2D-C1D	-2.19	99.41	106.40
8	21	205	CLA	O2A-CGA-CBA	2.19	120.91	114.00
10	12	316	A86	C9-C8-C6	-2.19	120.36	126.36
8	11	301	CLA	CHA-C1A-NA	-2.19	121.44	126.39
9	14	309	KC1	CHB-C1B-C2B	-2.19	120.94	125.49
8	11	303	CLA	CMC-C2C-C1C	2.19	128.45	125.03
10	12	302	A86	C22-C16-C17	-2.19	105.13	108.97
14	17	301	SQD	O8-S-C6	2.19	110.19	105.97
8	11	309	CLA	CMC-C2C-C1C	2.18	128.45	125.03
9	12	310	KC1	O2A-CGA-O1A	-2.18	118.25	122.70
8	17	308	CLA	CBC-CAC-C3C	-2.18	106.50	112.42
9	17	309	KC1	C3D-C2D-C1D	-2.18	99.43	106.40
9	15	302	KC1	O2D-CGD-O1D	-2.18	119.60	123.85
8	14	305	CLA	CMC-C2C-C1C	2.18	128.44	125.03
8	12	305	CLA	CMB-C2B-C1B	2.18	128.74	125.42
8	17	308	CLA	C4-C3-C5	2.18	119.01	115.23
8	15	303	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
9	18	304	KC1	C3D-C2D-C1D	-2.18	99.44	106.40
9	11	304	KC1	C3D-C2D-C1D	-2.18	99.45	106.40
9	14	304	KC1	CMB-C2B-C1B	2.17	128.56	124.73
13	19	312	DD6	C3-C4-C5	-2.17	119.07	123.52
11	17	318	LMG	O7-C10-O9	-2.17	118.62	123.70
8	20	308	CLA	CHB-C4A-NA	2.17	127.54	124.40
8	19	307	CLA	CBC-CAC-C3C	-2.17	106.53	112.42
8	14	303	CLA	C1-C2-C3	-2.17	122.64	126.20
8	18	301	CLA	CHA-C1A-NA	-2.17	121.48	126.39
10	14	316	A86	O4-C38-O5	-2.17	118.80	122.99
8	18	302	CLA	CHB-C1B-C2B	-2.17	121.13	127.43
10	16	313	A86	C3-C4-C5	-2.17	119.08	123.52
8	14	307	CLA	O1D-CGD-CBD	-2.17	120.24	124.52
8	11	303	CLA	CHA-C1A-NA	-2.17	121.48	126.39
9	17	303	KC1	CGD-CBD-CAD	-2.17	103.83	110.85
10	18	313	A86	C25-C24-C1	-2.17	120.42	126.36
8	18	303	CLA	O1D-CGD-CBD	-2.17	120.24	124.52
8	17	302	CLA	CED-O2D-CGD	2.17	120.83	115.92
9	15	309	KC1	C1A-NA-C4A	-2.17	105.69	106.68
9	14	309	KC1	C3D-C2D-C1D	-2.17	99.48	106.40
8	21	205	CLA	CHA-C1A-NA	-2.17	121.48	126.39
14	17	301	SQD	O47-C7-O49	-2.17	118.64	123.70
10	12	316	A86	O4-C38-O5	-2.17	118.81	122.99
9	17	303	KC1	C3D-C2D-C1D	-2.17	99.48	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	19	302	CLA	CMB-C2B-C1B	2.17	128.72	125.42
8	21	210	CLA	CHB-C4A-NA	2.16	127.52	124.40
9	17	306	KC1	C3D-C2D-C1D	-2.16	99.49	106.40
8	15	303	CLA	C1-O2A-CGA	2.16	121.89	116.65
10	17	313	A86	C10-C9-C8	-2.16	116.93	123.20
8	20	309	CLA	CMC-C2C-C1C	2.16	128.41	125.03
8	19	303	CLA	C4-C3-C5	2.16	118.98	115.23
9	17	309	KC1	CHB-C1B-C2B	-2.16	120.99	125.49
9	16	305	KC1	CAA-C2A-C1A	-2.16	115.17	124.64
8	19	310	CLA	CMB-C2B-C1B	2.16	128.71	125.42
10	18	314	A86	C29-C30-C31	-2.16	175.11	177.66
9	21	207	KC1	C3D-C2D-C1D	-2.16	99.50	106.40
10	11	314	A86	C22-C16-C17	-2.16	105.17	108.97
8	14	308	CLA	CMA-C3A-C2A	-2.16	105.63	113.98
9	15	309	KC1	C3D-C2D-C1D	-2.16	99.50	106.40
8	21	208	CLA	CMC-C2C-C1C	2.16	128.41	125.03
8	21	209	CLA	CMC-C2C-C1C	2.16	128.41	125.03
9	20	303	KC1	CHC-C4B-NB	-2.16	121.77	124.80
8	16	301	CLA	CHB-C4A-NA	2.16	127.51	124.40
9	11	304	KC1	O1D-CGD-CBD	-2.16	120.27	124.52
9	19	308	KC1	CBC-CAC-C3C	-2.16	106.58	112.42
8	14	308	CLA	CHB-C4A-NA	2.16	127.51	124.40
10	12	319	A86	C25-C24-C1	-2.16	120.45	126.36
10	13	316	A86	C19-C18-C17	-2.15	106.76	110.79
9	18	306	KC1	O2A-CGA-O1A	-2.15	118.31	122.70
9	16	302	KC1	C3D-C2D-C1D	-2.15	99.52	106.40
8	18	301	CLA	CBC-CAC-C3C	-2.15	106.58	112.42
10	11	313	A86	C23-C16-C22	-2.15	104.24	107.37
10	12	313	A86	C9-C10-C11	-2.15	120.55	126.64
9	12	308	KC1	C3D-C2D-C1D	-2.15	99.53	106.40
8	15	301	CLA	CHB-C4A-NA	2.15	127.51	124.40
13	21	212	DD6	C22-C16-C17	2.15	112.75	108.97
8	16	309	CLA	CHB-C4A-NA	2.15	127.50	124.40
8	19	301	CLA	CMA-C3A-C4A	-2.15	105.99	111.77
10	15	319	A86	C21-C20-C15	-2.15	116.41	123.35
9	13	307	KC1	CHB-C4A-NA	2.15	127.57	124.23
8	15	305	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
8	13	308	CLA	CMA-C3A-C4A	-2.15	106.00	111.77
8	18	305	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
8	21	204	CLA	C1-O2A-CGA	2.15	121.85	116.65
8	18	307	CLA	CAA-C2A-C1A	2.15	119.02	111.97
10	11	311	A86	C8-C6-C5	-2.15	115.63	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	19	307	CLA	C4-C3-C5	2.15	118.96	115.23
10	20	301	A86	C-C1-C24	-2.15	114.81	118.09
15	19	314	LHG	C20-C19-C18	-2.15	103.52	114.37
9	12	308	KC1	CHB-C4A-NA	2.15	127.56	124.23
8	16	309	CLA	O2A-CGA-CBA	2.15	120.78	114.00
8	16	307	CLA	O2D-CGD-O1D	-2.15	119.67	123.85
9	14	304	KC1	C3D-C2D-C1D	-2.15	99.55	106.40
10	13	312	A86	C35-C34-C33	2.15	113.74	109.89
10	21	214	A86	C9-C10-C11	-2.14	120.58	126.64
15	17	317	LHG	C27-C26-C25	-2.14	103.53	114.37
10	21	214	A86	C-C1-C24	2.14	121.36	118.09
8	14	302	CLA	CAA-C2A-C3A	-2.14	107.21	113.00
9	11	304	KC1	CMC-C2C-C1C	2.14	128.38	125.03
8	20	307	CLA	CMB-C2B-C1B	2.14	128.68	125.42
8	21	202	CLA	CBC-CAC-C3C	-2.14	106.62	112.42
10	13	314	A86	C4-C3-C2	-2.14	119.14	123.52
9	15	304	KC1	C3D-C2D-C1D	-2.14	99.57	106.40
8	18	308	CLA	CMC-C2C-C1C	2.14	128.37	125.03
8	20	307	CLA	CHB-C1B-C2B	-2.14	121.23	127.43
10	15	314	A86	C40-C32-C31	-2.14	108.56	110.47
8	15	303	CLA	C4-C3-C5	2.14	118.93	115.23
11	16	315	LMG	O7-C10-O9	-2.13	118.71	123.70
8	14	301	CLA	O2D-CGD-O1D	-2.13	119.69	123.85
9	11	302	KC1	C3D-C2D-C1D	-2.13	99.58	106.40
8	16	309	CLA	CBC-CAC-C3C	-2.13	106.64	112.42
9	17	303	KC1	CHB-C1B-NB	-2.13	121.80	124.80
10	15	314	A86	C9-C8-C6	-2.13	120.51	126.36
9	17	306	KC1	CHC-C1C-NC	2.13	127.54	124.23
8	21	204	CLA	C1-C2-C3	-2.13	122.70	126.20
9	20	306	KC1	CAA-CBA-CGA	-2.13	116.20	127.05
8	13	311	CLA	CMB-C2B-C1B	2.13	128.66	125.42
9	18	306	KC1	C3D-C2D-C1D	-2.13	99.59	106.40
8	17	307	CLA	CHB-C1B-C2B	-2.13	121.24	127.43
10	20	301	A86	C36-C31-C32	-2.13	117.58	119.70
10	21	213	A86	C-C1-C2	-2.13	119.36	122.82
10	14	314	A86	C23-C16-C22	-2.13	104.28	107.37
8	14	302	CLA	CMC-C2C-C1C	2.13	128.36	125.03
8	19	303	CLA	C2A-C1A-CHA	-2.13	120.17	123.87
10	14	314	A86	C4-C5-C6	-2.13	124.29	127.28
9	15	302	KC1	C3D-C2D-C1D	-2.13	99.60	106.40
10	11	313	A86	C4-C5-C6	-2.13	124.29	127.28
8	19	309	CLA	CBC-CAC-C3C	-2.13	106.65	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	20	313	A86	C25-C24-C1	-2.13	120.53	126.36
8	17	310	CLA	C2A-C3A-C4A	-2.13	98.43	101.87
9	14	304	KC1	CAA-C2A-C1A	-2.13	115.33	124.64
8	21	205	CLA	O2D-CGD-O1D	-2.13	119.71	123.85
8	12	311	CLA	CHB-C1B-C2B	-2.13	121.26	127.43
8	12	307	CLA	CMC-C2C-C1C	2.12	128.35	125.03
9	18	306	KC1	CBC-CAC-C3C	-2.12	106.67	112.42
8	19	305	CLA	CMA-C3A-C4A	-2.12	106.07	111.77
9	12	310	KC1	O1D-CGD-CBD	-2.12	120.33	124.52
9	11	302	KC1	CMC-C2C-C1C	2.12	128.34	125.03
8	16	306	CLA	CBA-CAA-C2A	2.12	120.10	113.79
8	13	301	CLA	C4-C3-C5	2.12	118.91	115.23
11	17	318	LMG	O3-C3-C2	-2.12	105.38	110.38
9	12	310	KC1	C3D-C2D-C1D	-2.12	99.64	106.40
13	16	312	DD6	O1-C20-C21	-2.12	112.68	115.05
8	14	301	CLA	O2A-CGA-CBA	2.12	118.29	111.83
8	17	304	CLA	CHA-C1A-NA	-2.12	121.60	126.39
8	12	305	CLA	CHA-C1A-NA	-2.12	121.60	126.39
8	13	301	CLA	O2D-CGD-O1D	-2.12	119.73	123.85
8	13	309	CLA	CHB-C4A-NA	2.11	127.45	124.40
9	17	303	KC1	CMB-C2B-C1B	2.11	128.45	124.73
8	19	303	CLA	CGD-CBD-CAD	-2.11	104.01	110.85
9	13	303	KC1	C3D-C2D-C1D	-2.11	99.65	106.40
10	11	310	A86	C9-C10-C11	-2.11	120.67	126.64
8	12	305	CLA	O1D-CGD-CBD	-2.11	120.35	124.52
10	20	301	A86	C7-C6-C5	-2.11	119.40	122.82
14	16	314	SQD	C1-O5-C5	2.11	117.84	113.72
8	16	306	CLA	C3B-C4B-NB	2.11	112.41	110.53
10	17	315	A86	C21-C20-C15	-2.11	116.54	123.35
10	11	314	A86	C34-O4-C38	-2.11	114.12	117.85
8	17	310	CLA	CBC-CAC-C3C	-2.11	106.70	112.42
8	21	209	CLA	CHB-C4A-NA	2.11	127.44	124.40
9	18	306	KC1	O1D-CGD-CBD	-2.11	120.36	124.52
8	20	302	CLA	CHA-C1A-NA	-2.11	121.62	126.39
11	17	318	LMG	C6-C5-C4	-2.11	107.84	113.02
9	20	305	KC1	C3D-C2D-C1D	-2.11	99.67	106.40
9	18	309	KC1	C3D-C2D-C1D	-2.11	99.68	106.40
10	11	311	A86	C9-C10-C11	-2.10	120.69	126.64
10	14	315	A86	C8-C6-C5	-2.10	115.70	119.01
9	19	308	KC1	O2A-CGA-O1A	-2.10	118.42	122.70
8	19	307	CLA	CHA-C1A-NA	-2.10	121.63	126.39
9	19	308	KC1	CAC-C3C-C4C	2.10	127.53	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	21	203	KC1	CMB-C2B-C3B	2.10	133.51	128.43
11	11	316	LMG	O3-C3-C2	-2.10	105.42	110.38
8	19	306	CLA	CBC-CAC-C3C	-2.10	106.72	112.42
8	13	308	CLA	CHA-C1A-NA	-2.10	121.64	126.39
8	14	303	CLA	CMC-C2C-C1C	2.10	128.31	125.03
8	21	202	CLA	CMA-C3A-C4A	-2.10	106.13	111.77
9	13	305	KC1	CBC-CAC-C3C	-2.10	106.73	112.42
8	20	308	CLA	O2A-CGA-CBA	2.10	120.63	114.00
9	21	203	KC1	C3D-C2D-C1D	-2.10	99.70	106.40
10	17	312	A86	C25-C26-C27	2.10	130.22	127.28
8	18	307	CLA	C1-C2-C3	-2.10	122.76	126.20
9	19	308	KC1	C3D-C2D-C1D	-2.10	99.70	106.40
9	15	304	KC1	CMC-C2C-C1C	2.10	128.31	125.03
8	18	310	CLA	O1D-CGD-CBD	-2.10	120.38	124.52
8	19	307	CLA	CED-O2D-CGD	2.10	120.67	115.92
9	20	303	KC1	CHB-C1B-C2B	-2.10	121.13	125.49
8	21	206	CLA	CHB-C1B-C2B	-2.09	121.35	127.43
8	14	302	CLA	C1-O2A-CGA	2.09	121.72	116.65
9	17	305	KC1	C3D-C2D-C1D	-2.09	99.72	106.40
9	12	308	KC1	CBC-CAC-C3C	-2.09	106.75	112.42
8	13	311	CLA	CHB-C1B-C2B	-2.09	121.36	127.43
13	19	312	DD6	C41-C32-C31	-2.09	106.78	110.52
10	17	315	A86	C23-C16-C17	-2.09	105.30	108.97
8	21	204	CLA	CGD-CBD-CAD	-2.09	104.09	110.85
9	15	302	KC1	O1D-CGD-CBD	-2.09	120.40	124.52
9	11	304	KC1	CHB-C4A-NA	2.09	127.47	124.23
8	21	208	CLA	O2D-CGD-O1D	-2.09	119.79	123.85
8	20	307	CLA	CHA-C1A-NA	-2.08	121.67	126.39
13	21	212	DD6	C15-C14-C13	-2.08	121.59	125.99
8	20	309	CLA	CBC-CAC-C3C	-2.08	106.77	112.42
8	21	204	CLA	CHA-C1A-NA	-2.08	121.67	126.39
9	15	304	KC1	CBC-CAC-C3C	-2.08	106.78	112.42
9	16	304	KC1	CAA-C2A-C1A	-2.08	115.52	124.64
8	20	310	CLA	CBC-CAC-C3C	-2.08	106.78	112.42
8	18	302	CLA	CGD-CBD-CAD	-2.08	104.11	110.85
8	13	309	CLA	CED-O2D-CGD	2.08	120.64	115.92
8	14	302	CLA	CBC-CAC-C3C	-2.08	106.78	112.42
8	17	310	CLA	OBD-CAD-C3D	-2.08	123.56	128.42
10	12	313	A86	C4-C3-C2	-2.08	119.27	123.52
9	12	306	KC1	CAB-C3B-C4B	2.08	129.78	124.82
10	19	311	A86	O4-C38-O5	-2.08	118.98	122.99
11	11	316	LMG	O2-C2-C1	-2.08	105.13	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	18	307	CLA	CBC-CAC-C3C	-2.08	106.79	112.42
9	15	306	KC1	O1D-CGD-CBD	-2.08	120.42	124.52
8	14	308	CLA	C1-O2A-CGA	2.08	121.68	116.65
8	17	304	CLA	CAA-C2A-C1A	2.08	118.78	111.97
8	21	202	CLA	C4-C3-C5	2.08	118.83	115.23
8	18	303	CLA	CHA-C1A-NA	-2.08	121.69	126.39
8	19	307	CLA	CHB-C1B-C2B	-2.07	121.40	127.43
10	13	313	A86	C8-C6-C5	-2.07	115.75	119.01
9	14	309	KC1	O1D-CGD-CBD	-2.07	120.43	124.52
9	11	304	KC1	CMB-C2B-C1B	2.07	128.38	124.73
9	14	306	KC1	C1A-NA-C4A	-2.07	105.73	106.68
9	18	304	KC1	O1D-CGD-CBD	-2.07	120.43	124.52
8	15	301	CLA	O2D-CGD-O1D	-2.07	119.81	123.85
8	20	302	CLA	CMA-C3A-C4A	-2.07	106.20	111.77
9	21	207	KC1	CHB-C1B-C2B	-2.07	121.18	125.49
8	11	307	CLA	O1D-CGD-CBD	-2.07	120.43	124.52
10	14	312	A86	C19-C18-C17	2.07	114.66	110.79
8	14	308	CLA	C4-C3-C5	2.07	118.82	115.23
10	12	302	A86	C19-C18-C17	-2.07	106.92	110.79
10	17	316	A86	C25-C24-C1	-2.07	120.69	126.36
8	18	303	CLA	CMB-C2B-C3B	2.07	131.42	126.55
9	13	303	KC1	CMC-C2C-C1C	2.07	128.27	125.03
8	14	308	CLA	O2D-CGD-O1D	-2.07	119.82	123.85
10	18	312	A86	C4-C3-C2	-2.07	119.29	123.52
8	11	307	CLA	CHB-C1B-C2B	-2.07	121.43	127.43
10	17	321	A86	O4-C38-O5	-2.07	119.00	122.99
8	13	309	CLA	O2D-CGD-O1D	-2.07	119.83	123.85
10	11	318	A86	C40-C32-C31	-2.06	108.63	110.47
8	11	307	CLA	CMB-C2B-C1B	2.06	128.56	125.42
9	21	207	KC1	CBC-CAC-C3C	-2.06	106.83	112.42
15	19	314	LHG	C18-C17-C16	-2.06	103.95	114.37
8	13	302	CLA	O2D-CGD-O1D	-2.06	119.84	123.85
9	11	306	KC1	O2A-CGA-O1A	-2.06	118.50	122.70
10	13	313	A86	C10-C9-C8	-2.06	117.23	123.20
10	12	316	A86	C22-C16-C17	-2.06	105.35	108.97
8	17	307	CLA	O1D-CGD-CBD	-2.06	120.46	124.52
10	18	311	A86	C3-C4-C5	-2.06	119.31	123.52
13	20	312	DD6	C9-C8-C6	-2.06	120.72	126.36
9	13	307	KC1	CHB-C1B-NB	-2.06	121.91	124.80
9	13	303	KC1	CHB-C1B-C2B	-2.06	121.21	125.49
9	20	306	KC1	C3D-C2D-C1D	-2.05	99.84	106.40
9	13	310	KC1	C3D-C2D-C1D	-2.05	99.85	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	16	305	KC1	CAB-C3B-C4B	2.05	129.72	124.82
8	14	301	CLA	CBC-CAC-C3C	-2.05	106.86	112.42
8	13	302	CLA	CHA-C1A-NA	-2.05	121.75	126.39
8	15	310	CLA	CHB-C1B-C2B	-2.05	121.48	127.43
10	17	321	A86	C-C1-C24	2.05	121.22	118.09
9	21	203	KC1	O1D-CGD-CBD	-2.05	120.48	124.52
9	16	302	KC1	CHC-C1C-NC	2.05	127.41	124.23
10	15	319	A86	C24-C1-C2	-2.05	115.79	119.01
14	16	314	SQD	O8-S-C6	2.05	109.92	105.97
8	16	303	CLA	CMC-C2C-C1C	2.05	128.23	125.03
16	19	315	LMU	O3'-C3'-C2'	-2.05	105.56	110.38
9	14	306	KC1	O2A-CGA-O1A	-2.04	118.54	122.70
10	21	215	A86	C-C1-C24	2.04	121.21	118.09
9	11	308	KC1	CHC-C1C-NC	2.04	127.40	124.23
8	12	307	CLA	CHB-C1B-C2B	-2.04	121.50	127.43
10	15	312	A86	C4-C5-C6	-2.04	124.41	127.28
9	13	310	KC1	O1D-CGD-CBD	-2.04	120.49	124.52
10	15	319	A86	C40-C32-C31	-2.04	108.64	110.47
8	18	301	CLA	CHB-C1B-C2B	-2.04	121.50	127.43
9	13	303	KC1	O2D-CGD-O1D	-2.04	119.87	123.85
15	17	317	LHG	C11-C10-C9	-2.04	104.05	114.37
10	15	316	A86	C26-C25-C24	-2.04	117.28	123.20
8	12	301	CLA	CED-O2D-CGD	2.04	120.54	115.92
9	12	310	KC1	CGD-CBD-CAD	-2.04	104.24	110.85
10	21	214	A86	C34-O4-C38	-2.04	114.25	117.85
14	16	314	SQD	O48-C23-O10	-2.04	118.53	123.63
8	21	208	CLA	CED-O2D-CGD	2.04	120.53	115.92
9	15	309	KC1	O1D-CGD-CBD	-2.03	120.50	124.52
10	15	315	A86	C25-C24-C1	-2.03	120.78	126.36
8	12	311	CLA	CBC-CAC-C3C	-2.03	106.91	112.42
8	13	304	CLA	CHA-C1A-NA	-2.03	121.79	126.39
8	17	304	CLA	CMC-C2C-C1C	2.03	128.21	125.03
10	13	314	A86	O4-C34-C33	2.03	112.84	107.64
8	21	202	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
8	13	304	CLA	O2A-CGA-CBA	2.03	118.03	111.83
9	16	308	KC1	CMC-C2C-C1C	2.03	128.21	125.03
8	19	306	CLA	C7-C6-C5	-2.03	107.85	113.26
8	21	206	CLA	CED-O2D-CGD	2.03	120.52	115.92
10	15	311	A86	C9-C10-C11	-2.03	120.90	126.64
8	19	309	CLA	CHB-C1B-C2B	-2.03	121.53	127.43
8	19	305	CLA	O2D-CGD-O1D	-2.03	119.90	123.85
8	21	205	CLA	CMC-C2C-C1C	2.03	128.21	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	21	208	CLA	CBC-CAC-C3C	-2.03	106.92	112.42
9	17	309	KC1	CAB-C3B-C4B	2.03	129.67	124.82
11	11	315	LMG	O7-C10-O9	-2.03	118.96	123.70
9	20	306	KC1	CHB-C1B-NB	-2.03	121.95	124.80
8	21	202	CLA	O1D-CGD-CBD	-2.03	120.52	124.52
10	16	311	A86	C23-C16-C17	-2.03	105.41	108.97
9	17	306	KC1	CMC-C2C-C3C	2.03	131.63	126.15
10	21	215	A86	C23-C16-C22	-2.03	104.42	107.37
8	15	308	CLA	CHA-C1A-NA	-2.03	121.80	126.39
8	21	204	CLA	CAA-C2A-C1A	2.03	118.61	111.97
8	17	308	CLA	O2D-CGD-O1D	-2.02	119.91	123.85
8	19	304	CLA	O2A-CGA-CBA	2.02	120.40	114.00
10	17	313	A86	C9-C8-C6	-2.02	120.82	126.36
14	16	314	SQD	O47-C7-O49	-2.02	118.98	123.70
9	18	309	KC1	CAB-C3B-C4B	2.02	129.65	124.82
10	15	316	A86	O4-C38-O5	-2.02	119.09	122.99
10	11	310	A86	C28-C27-C26	2.02	126.09	122.82
15	21	201	LHG	C27-C26-C25	-2.02	104.16	114.37
8	19	306	CLA	CHA-C1A-NA	-2.02	121.82	126.39
8	19	302	CLA	C1-C2-C3	-2.02	122.89	126.20
11	16	315	LMG	O1-C7-C8	-2.02	105.91	110.82
8	14	303	CLA	CHA-C1A-NA	-2.02	121.82	126.39
8	15	303	CLA	CHA-C1A-NA	-2.02	121.82	126.39
8	20	310	CLA	O2A-CGA-CBA	2.02	120.38	114.00
8	13	311	CLA	CMC-C2C-C1C	2.02	128.19	125.03
9	11	306	KC1	CMC-C2C-C1C	2.02	128.19	125.03
11	16	315	LMG	O8-C28-O10	-2.02	118.58	123.63
8	16	303	CLA	CHA-C1A-NA	-2.02	121.83	126.39
8	20	307	CLA	O2A-CGA-O1A	-2.02	118.59	123.63
8	15	307	CLA	CBC-CAC-C3C	-2.02	106.96	112.42
8	20	304	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
8	13	311	CLA	CHA-C1A-NA	-2.01	121.83	126.39
8	11	309	CLA	CBC-CAC-C3C	-2.01	106.96	112.42
8	12	304	CLA	CBC-CAC-C3C	-2.01	106.96	112.42
8	11	301	CLA	CHB-C1B-C2B	-2.01	121.59	127.43
8	12	309	CLA	C2A-C3A-C4A	-2.01	98.62	101.87
8	20	309	CLA	CMA-C3A-C4A	2.01	117.18	111.77
8	12	307	CLA	C5-C3-C4	2.01	119.22	114.59
8	19	303	CLA	CHB-C4A-NA	2.01	127.30	124.40
9	12	306	KC1	O1D-CGD-CBD	-2.01	120.56	124.52
8	19	310	CLA	CMC-C2C-C1C	2.01	128.17	125.03
10	11	314	A86	C40-C32-C31	-2.01	108.67	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	17	316	A86	C4-C3-C2	-2.01	119.41	123.52
10	12	319	A86	O4-C38-O5	-2.01	119.12	122.99
8	11	307	CLA	C4-C3-C5	2.01	118.71	115.23
10	15	314	A86	C12-C11-C13	2.01	119.25	116.00
8	19	310	CLA	CHB-C1B-C2B	-2.01	121.61	127.43
8	18	310	CLA	CHA-C1A-NA	-2.01	121.85	126.39
8	16	303	CLA	C4-C3-C5	2.00	118.71	115.23
10	20	311	A86	C7-C6-C8	2.00	121.15	118.09
10	12	302	A86	C4-C3-C2	-2.00	119.42	123.52
10	11	318	A86	C41-C32-C31	-2.00	108.68	110.47
8	18	310	CLA	O2A-CGA-CBA	2.00	120.33	114.00
10	12	314	A86	C3-C4-C5	-2.00	119.42	123.52
8	17	310	CLA	CHB-C1B-C2B	-2.00	121.61	127.43
8	13	302	CLA	CHB-C1B-C2B	-2.00	121.62	127.43
9	13	305	KC1	O1D-CGD-CBD	-2.00	120.57	124.52
8	20	302	CLA	CMA-C3A-C2A	-2.00	106.25	113.98
9	18	304	KC1	CAA-C2A-C1A	-2.00	115.87	124.64
8	13	308	CLA	C1-O2A-CGA	2.00	121.49	116.65
8	14	303	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
10	18	314	A86	C25-C24-C1	-2.00	120.88	126.36
9	15	309	KC1	CHB-C1B-C2B	-2.00	121.33	125.49

All (55) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	11	303	CLA	ND
8	11	305	CLA	ND
8	11	309	CLA	ND
8	12	301	CLA	ND
8	12	303	CLA	ND
8	12	304	CLA	ND
8	12	305	CLA	ND
8	12	309	CLA	ND
8	12	311	CLA	ND
8	13	304	CLA	ND
8	13	306	CLA	ND
8	13	308	CLA	ND
8	14	302	CLA	ND
8	14	305	CLA	ND
8	14	307	CLA	ND
8	14	308	CLA	ND
8	14	310	CLA	ND

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Mol	Chain	Res	Type	Atom
8	15	303	CLA	ND
8	15	305	CLA	ND
8	15	307	CLA	ND
8	15	308	CLA	ND
8	15	310	CLA	ND
8	16	303	CLA	ND
8	16	306	CLA	ND
8	16	307	CLA	ND
8	16	309	CLA	ND
8	17	304	CLA	ND
8	17	307	CLA	ND
8	17	308	CLA	ND
8	17	310	CLA	ND
8	18	302	CLA	ND
8	18	303	CLA	ND
8	18	305	CLA	ND
8	18	307	CLA	ND
8	18	308	CLA	ND
8	19	301	CLA	ND
8	19	302	CLA	ND
8	19	303	CLA	ND
8	19	304	CLA	ND
8	19	305	CLA	ND
8	19	306	CLA	ND
8	19	307	CLA	ND
8	19	309	CLA	ND
8	19	310	CLA	ND
8	20	304	CLA	ND
8	20	307	CLA	ND
8	20	308	CLA	ND
8	20	309	CLA	ND
8	20	310	CLA	ND
8	21	202	CLA	ND
8	21	204	CLA	ND
8	21	205	CLA	ND
8	21	206	CLA	ND
8	21	208	CLA	ND
8	21	209	CLA	ND

All (1610) torsion outliers are listed below:

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Mol	Chain	Res	Type	Atoms
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Mol	Chain	Res	Type	Atoms
8	11	301	CLA	C1A-C2A-CAA-CBA
8	11	301	CLA	C3A-C2A-CAA-CBA
8	11	301	CLA	C2B-C3B-CAB-CBB
8	11	301	CLA	C4B-C3B-CAB-CBB
8	11	303	CLA	C1A-C2A-CAA-CBA
8	11	309	CLA	CBD-CGD-O2D-CED
8	12	303	CLA	C3A-C2A-CAA-CBA
8	12	304	CLA	C1A-C2A-CAA-CBA
8	12	304	CLA	CAD-CBD-CGD-O2D
8	12	305	CLA	C1A-C2A-CAA-CBA
8	12	311	CLA	CHA-CBD-CGD-O1D
8	12	311	CLA	CHA-CBD-CGD-O2D
8	13	302	CLA	C2B-C3B-CAB-CBB
8	13	302	CLA	C4B-C3B-CAB-CBB
8	13	304	CLA	C1A-C2A-CAA-CBA
8	13	308	CLA	CHA-CBD-CGD-O1D
8	13	308	CLA	CHA-CBD-CGD-O2D
8	14	301	CLA	C1A-C2A-CAA-CBA
8	14	301	CLA	C3A-C2A-CAA-CBA
8	14	302	CLA	C6-C7-C8-C9
8	14	303	CLA	C2B-C3B-CAB-CBB
8	14	303	CLA	C4B-C3B-CAB-CBB
8	14	307	CLA	C2B-C3B-CAB-CBB
8	14	307	CLA	C4B-C3B-CAB-CBB
8	15	301	CLA	C1A-C2A-CAA-CBA
8	15	301	CLA	C3A-C2A-CAA-CBA
8	15	301	CLA	C2B-C3B-CAB-CBB
8	15	301	CLA	C4B-C3B-CAB-CBB
8	15	303	CLA	C1A-C2A-CAA-CBA
8	15	310	CLA	CHA-CBD-CGD-O1D
8	15	310	CLA	CHA-CBD-CGD-O2D
8	16	301	CLA	C1A-C2A-CAA-CBA
8	16	301	CLA	C3A-C2A-CAA-CBA
8	16	301	CLA	C2B-C3B-CAB-CBB
8	16	301	CLA	C4B-C3B-CAB-CBB
8	16	303	CLA	C1A-C2A-CAA-CBA
8	16	306	CLA	C1A-C2A-CAA-CBA
8	16	306	CLA	C2B-C3B-CAB-CBB
8	16	306	CLA	C4B-C3B-CAB-CBB
8	17	302	CLA	C2B-C3B-CAB-CBB
8	17	302	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
8	17	304	CLA	C1A-C2A-CAA-CBA
8	17	310	CLA	CHA-CBD-CGD-O1D
8	17	310	CLA	CHA-CBD-CGD-O2D
8	17	310	CLA	CBD-CGD-O2D-CED
8	18	301	CLA	C1A-C2A-CAA-CBA
8	18	301	CLA	C3A-C2A-CAA-CBA
8	18	301	CLA	CBD-CGD-O2D-CED
8	18	303	CLA	C1A-C2A-CAA-CBA
8	19	301	CLA	C3A-C2A-CAA-CBA
8	19	301	CLA	C4B-C3B-CAB-CBB
8	19	305	CLA	C2-C3-C5-C6
8	19	310	CLA	C2-C3-C5-C6
8	19	310	CLA	C4-C3-C5-C6
8	20	302	CLA	C1A-C2A-CAA-CBA
8	20	302	CLA	C2B-C3B-CAB-CBB
8	20	302	CLA	C4B-C3B-CAB-CBB
8	20	308	CLA	CHA-CBD-CGD-O1D
8	20	308	CLA	CHA-CBD-CGD-O2D
8	21	202	CLA	C1A-C2A-CAA-CBA
8	21	204	CLA	C1A-C2A-CAA-CBA
8	21	209	CLA	CHA-CBD-CGD-O1D
8	21	209	CLA	CHA-CBD-CGD-O2D
8	21	210	CLA	CHA-CBD-CGD-O1D
8	21	210	CLA	CHA-CBD-CGD-O2D
9	11	302	KC1	C3A-C2A-CAA-CBA
9	11	302	KC1	C2A-CAA-CBA-CGA
9	11	304	KC1	C2B-C3B-CAB-CBB
9	11	304	KC1	C2A-CAA-CBA-CGA
9	11	306	KC1	C3A-C2A-CAA-CBA
9	11	306	KC1	C2B-C3B-CAB-CBB
9	11	306	KC1	C2A-CAA-CBA-CGA
9	11	308	KC1	C3A-C2A-CAA-CBA
9	11	308	KC1	C2A-CAA-CBA-CGA
9	11	308	KC1	CHA-CBD-CGD-O1D
9	11	308	KC1	CHA-CBD-CGD-O2D
9	12	306	KC1	C3A-C2A-CAA-CBA
9	12	306	KC1	C2A-CAA-CBA-CGA
9	12	308	KC1	C3A-C2A-CAA-CBA
9	12	308	KC1	C2A-CAA-CBA-CGA
9	12	310	KC1	C3A-C2A-CAA-CBA
9	12	310	KC1	C2A-CAA-CBA-CGA
9	13	303	KC1	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
9	13	303	KC1	C2A-CAA-CBA-CGA
9	13	305	KC1	C3A-C2A-CAA-CBA
9	13	305	KC1	C2B-C3B-CAB-CBB
9	13	305	KC1	C2A-CAA-CBA-CGA
9	13	307	KC1	C3A-C2A-CAA-CBA
9	13	307	KC1	C2A-CAA-CBA-CGA
9	13	310	KC1	C3A-C2A-CAA-CBA
9	13	310	KC1	C2A-CAA-CBA-CGA
9	14	304	KC1	C2A-CAA-CBA-CGA
9	14	306	KC1	C3A-C2A-CAA-CBA
9	14	306	KC1	C2A-CAA-CBA-CGA
9	14	309	KC1	C3A-C2A-CAA-CBA
9	15	302	KC1	C3A-C2A-CAA-CBA
9	15	302	KC1	C2A-CAA-CBA-CGA
9	15	304	KC1	C3A-C2A-CAA-CBA
9	15	304	KC1	C2B-C3B-CAB-CBB
9	15	304	KC1	C2A-CAA-CBA-CGA
9	15	306	KC1	C3A-C2A-CAA-CBA
9	15	306	KC1	C2B-C3B-CAB-CBB
9	15	306	KC1	C2A-CAA-CBA-CGA
9	15	309	KC1	C3A-C2A-CAA-CBA
9	15	309	KC1	C2A-CAA-CBA-CGA
9	15	309	KC1	CHA-CBD-CGD-O2D
9	16	302	KC1	C3A-C2A-CAA-CBA
9	16	302	KC1	C2A-CAA-CBA-CGA
9	16	304	KC1	C3A-C2A-CAA-CBA
9	16	304	KC1	C2A-CAA-CBA-CGA
9	16	305	KC1	C2A-CAA-CBA-CGA
9	16	308	KC1	C3A-C2A-CAA-CBA
9	17	303	KC1	C3A-C2A-CAA-CBA
9	17	303	KC1	C2A-CAA-CBA-CGA
9	17	305	KC1	C2A-CAA-CBA-CGA
9	17	306	KC1	C3A-C2A-CAA-CBA
9	17	306	KC1	C2A-CAA-CBA-CGA
9	17	309	KC1	C3A-C2A-CAA-CBA
9	17	309	KC1	C2A-CAA-CBA-CGA
9	18	304	KC1	C3A-C2A-CAA-CBA
9	18	304	KC1	C2A-CAA-CBA-CGA
9	18	306	KC1	C3A-C2A-CAA-CBA
9	18	306	KC1	C2A-CAA-CBA-CGA
9	18	306	KC1	CHA-CBD-CGD-O1D
9	18	306	KC1	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
9	18	309	KC1	C3A-C2A-CAA-CBA
9	19	308	KC1	C2A-CAA-CBA-CGA
9	20	303	KC1	C3A-C2A-CAA-CBA
9	20	303	KC1	C2A-CAA-CBA-CGA
9	20	303	KC1	CBD-CGD-O2D-CED
9	20	305	KC1	C3A-C2A-CAA-CBA
9	20	305	KC1	C2A-CAA-CBA-CGA
9	20	306	KC1	C2A-CAA-CBA-CGA
9	21	203	KC1	C3A-C2A-CAA-CBA
9	21	203	KC1	C2A-CAA-CBA-CGA
9	21	207	KC1	C3A-C2A-CAA-CBA
9	21	207	KC1	C2B-C3B-CAB-CBB
10	11	310	A86	C24-C25-C26-C27
10	11	312	A86	C24-C25-C26-C27
10	11	312	A86	C39-C38-O4-C34
10	11	312	A86	O5-C38-O4-C34
10	11	313	A86	C-C1-C24-C25
10	11	313	A86	C2-C1-C24-C25
10	11	313	A86	C10-C11-C13-O
10	11	313	A86	C12-C11-C13-O
10	11	314	A86	C39-C38-O4-C34
10	11	314	A86	O5-C38-O4-C34
10	11	318	A86	C24-C25-C26-C27
10	12	302	A86	C11-C10-C9-C8
10	12	302	A86	C10-C11-C13-O
10	12	302	A86	C12-C11-C13-O
10	12	302	A86	C13-C14-C15-C16
10	12	302	A86	C39-C38-O4-C34
10	12	302	A86	C5-C6-C8-C9
10	12	312	A86	C-C1-C24-C25
10	12	312	A86	C2-C1-C24-C25
10	12	314	A86	C26-C27-C29-C30
10	12	314	A86	C28-C27-C29-C30
10	12	314	A86	C35-C34-O4-C38
10	12	315	A86	C-C1-C24-C25
10	12	315	A86	C2-C1-C24-C25
10	12	315	A86	C39-C38-O4-C34
10	12	315	A86	C5-C6-C8-C9
10	12	316	A86	O-C13-C14-C15
10	12	316	A86	C11-C13-C14-C15
10	12	316	A86	C13-C14-C15-C16
10	12	316	A86	O5-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
10	12	319	A86	C-C1-C24-C25
10	12	319	A86	C2-C1-C24-C25
10	12	319	A86	C11-C10-C9-C8
10	12	319	A86	O5-C38-O4-C34
10	12	319	A86	C3-C4-C5-C6
10	13	312	A86	C-C1-C24-C25
10	13	312	A86	C2-C1-C24-C25
10	13	313	A86	C39-C38-O4-C34
10	13	313	A86	C5-C6-C8-C9
10	13	313	A86	C7-C6-C8-C9
10	13	314	A86	C10-C11-C13-C14
10	13	314	A86	C12-C11-C13-C14
10	13	314	A86	O-C13-C14-C15
10	13	314	A86	C11-C13-C14-C15
10	13	314	A86	C33-C34-O4-C38
10	13	314	A86	C39-C38-O4-C34
10	13	315	A86	C11-C10-C9-C8
10	13	315	A86	C13-C14-C15-C16
10	13	315	A86	C39-C38-O4-C34
10	13	316	A86	C13-C14-C15-C16
10	13	316	A86	O5-C38-O4-C34
10	14	311	A86	O-C13-C14-C15
10	14	311	A86	C39-C38-O4-C34
10	14	313	A86	C-C1-C24-C25
10	14	313	A86	C2-C1-C24-C25
10	14	313	A86	O-C13-C14-C15
10	14	313	A86	C24-C25-C26-C27
10	14	313	A86	C26-C27-C29-C30
10	14	313	A86	C33-C34-O4-C38
10	14	313	A86	C39-C38-O4-C34
10	14	313	A86	C5-C6-C8-C9
10	14	313	A86	C7-C6-C8-C9
10	14	314	A86	C-C1-C24-C25
10	14	314	A86	C2-C1-C24-C25
10	14	314	A86	C10-C11-C13-O
10	14	314	A86	C12-C11-C13-O
10	14	314	A86	C39-C38-O4-C34
10	14	314	A86	C5-C6-C8-C9
10	14	314	A86	C7-C6-C8-C9
10	14	316	A86	O-C13-C14-C15
10	14	316	A86	C11-C13-C14-C15
10	14	316	A86	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
10	15	311	A86	C24-C25-C26-C27
10	15	311	A86	O5-C38-O4-C34
10	15	312	A86	C39-C38-O4-C34
10	15	312	A86	C5-C6-C8-C9
10	15	314	A86	C-C1-C24-C25
10	15	314	A86	C2-C1-C24-C25
10	15	314	A86	C11-C10-C9-C8
10	15	314	A86	C39-C38-O4-C34
10	15	315	A86	C2-C1-C24-C25
10	15	315	A86	C39-C38-O4-C34
10	15	315	A86	O5-C38-O4-C34
10	15	315	A86	C5-C6-C8-C9
10	15	315	A86	C7-C6-C8-C9
10	15	316	A86	O-C13-C14-C15
10	15	316	A86	C11-C13-C14-C15
10	15	316	A86	C13-C14-C15-C16
10	15	316	A86	O5-C38-O4-C34
10	15	319	A86	C39-C38-O4-C34
10	15	319	A86	C5-C6-C8-C9
10	15	319	A86	C7-C6-C8-C9
10	16	311	A86	C24-C25-C26-C27
10	16	313	A86	C10-C11-C13-O
10	16	313	A86	C12-C11-C13-O
10	16	313	A86	C13-C14-C15-C16
10	16	313	A86	C39-C38-O4-C34
10	16	313	A86	O5-C38-O4-C34
10	17	311	A86	C24-C25-C26-C27
10	17	312	A86	C5-C6-C8-C9
10	17	312	A86	C7-C6-C8-C9
10	17	313	A86	C33-C34-O4-C38
10	17	313	A86	C39-C38-O4-C34
10	17	314	A86	C-C1-C24-C25
10	17	314	A86	C2-C1-C24-C25
10	17	315	A86	C-C1-C24-C25
10	17	315	A86	C2-C1-C24-C25
10	17	315	A86	C11-C13-C14-C15
10	17	315	A86	C5-C6-C8-C9
10	17	315	A86	C7-C6-C8-C9
10	17	316	A86	C11-C10-C9-C8
10	17	316	A86	C10-C11-C13-O
10	17	316	A86	C12-C11-C13-O
10	17	316	A86	C11-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
10	17	316	A86	C13-C14-C15-C16
10	17	321	A86	C2-C1-C24-C25
10	17	321	A86	C39-C38-O4-C34
10	18	311	A86	O-C13-C14-C15
10	18	311	A86	C24-C25-C26-C27
10	18	311	A86	C39-C38-O4-C34
10	18	312	A86	O-C13-C14-C15
10	18	312	A86	C5-C6-C8-C9
10	18	312	A86	C7-C6-C8-C9
10	18	313	A86	C-C1-C24-C25
10	18	313	A86	C2-C1-C24-C25
10	18	313	A86	C11-C10-C9-C8
10	18	314	A86	O-C13-C14-C15
10	18	314	A86	C11-C13-C14-C15
10	18	314	A86	C13-C14-C15-C16
10	18	314	A86	C39-C38-O4-C34
10	18	314	A86	O5-C38-O4-C34
10	19	313	A86	C2-C1-C24-C25
10	20	301	A86	C12-C11-C13-C14
10	20	311	A86	C11-C10-C9-C8
10	20	311	A86	O-C13-C14-C15
10	20	313	A86	C2-C1-C24-C25
10	20	313	A86	O-C13-C14-C15
10	20	313	A86	C11-C13-C14-C15
10	21	211	A86	C-C1-C24-C25
10	21	211	A86	C2-C1-C24-C25
10	21	211	A86	C11-C10-C9-C8
10	21	211	A86	O-C13-C14-C15
10	21	211	A86	O5-C38-O4-C34
10	21	211	A86	C5-C6-C8-C9
10	21	211	A86	C7-C6-C8-C9
10	21	213	A86	O-C13-C14-C15
10	21	214	A86	C-C1-C24-C25
10	21	214	A86	C2-C1-C24-C25
10	21	214	A86	O-C13-C14-C15
10	21	215	A86	C-C1-C24-C25
10	21	215	A86	C2-C1-C24-C25
11	11	315	LMG	O9-C10-O7-C8
11	11	315	LMG	C11-C10-O7-C8
11	17	318	LMG	O9-C10-O7-C8
11	17	318	LMG	C11-C10-O7-C8
13	16	312	DD6	C-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
13	16	312	DD6	C-C1-C24-C25
13	16	312	DD6	C2-C1-C24-C25
13	16	312	DD6	C9-C10-C11-C13
13	16	312	DD6	C10-C11-C13-C14
13	16	312	DD6	C4-C5-C6-C7
13	16	312	DD6	C7-C6-C8-C9
13	19	312	DD6	C-C1-C2-C3
13	19	312	DD6	C-C1-C24-C25
13	19	312	DD6	C9-C10-C11-C12
13	19	312	DD6	C4-C5-C6-C7
13	20	312	DD6	C-C1-C2-C3
13	20	312	DD6	C-C1-C24-C25
13	20	312	DD6	C2-C1-C24-C25
13	20	312	DD6	C9-C10-C11-C12
13	20	312	DD6	C9-C10-C11-C13
13	20	312	DD6	C10-C11-C13-C14
13	20	312	DD6	C3-C4-C5-C6
13	20	312	DD6	C4-C5-C6-C7
13	20	312	DD6	C4-C5-C6-C8
13	20	312	DD6	C5-C6-C8-C9
13	20	314	DD6	C-C1-C2-C3
13	20	314	DD6	C2-C1-C24-C25
13	20	314	DD6	C9-C10-C11-C12
13	20	314	DD6	C13-C14-C15-C16
13	20	314	DD6	C24-C25-C26-C27
13	20	314	DD6	C4-C5-C6-C7
13	20	314	DD6	C7-C6-C8-C9
13	21	212	DD6	C-C1-C2-C3
13	21	212	DD6	C9-C10-C11-C12
13	21	212	DD6	C12-C11-C13-C14
13	21	212	DD6	C3-C4-C5-C6
13	21	212	DD6	C4-C5-C6-C8
13	21	212	DD6	C7-C6-C8-C9
13	21	216	DD6	C-C1-C2-C3
13	21	216	DD6	C2-C1-C24-C25
13	21	216	DD6	C9-C10-C11-C12
13	21	216	DD6	C10-C11-C13-C14
13	21	216	DD6	C4-C5-C6-C7
13	21	216	DD6	C4-C5-C6-C8
13	21	216	DD6	C5-C6-C8-C9
14	16	314	SQD	O5-C5-C6-S
14	17	301	SQD	O5-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
14	17	301	SQD	C8-C7-O47-C45
14	17	301	SQD	C5-C6-S-O7
14	17	301	SQD	C5-C6-S-O8
14	17	301	SQD	C5-C6-S-O9
15	17	317	LHG	C4-O6-P-O5
15	19	314	LHG	O2-C2-C3-O3
15	19	314	LHG	C3-O3-P-O4
15	19	314	LHG	C3-O3-P-O6
15	21	201	LHG	C3-O3-P-O4
15	21	201	LHG	C3-O3-P-O6
15	21	201	LHG	C4-O6-P-O4
15	21	217	LHG	O1-C1-C2-C3
15	21	217	LHG	C3-O3-P-O5
15	21	217	LHG	C4-O6-P-O3
15	21	217	LHG	C4-O6-P-O4
15	21	217	LHG	C4-O6-P-O5
15	21	217	LHG	O7-C5-C6-O8
8	17	310	CLA	O1D-CGD-O2D-CED
10	11	313	A86	C39-C38-O4-C34
10	12	302	A86	O5-C38-O4-C34
10	12	314	A86	C39-C38-O4-C34
10	12	319	A86	C39-C38-O4-C34
10	13	313	A86	O5-C38-O4-C34
10	13	315	A86	O5-C38-O4-C34
10	14	314	A86	O5-C38-O4-C34
10	15	312	A86	O5-C38-O4-C34
10	15	313	A86	C39-C38-O4-C34
10	15	316	A86	C39-C38-O4-C34
10	16	310	A86	C39-C38-O4-C34
10	17	312	A86	C39-C38-O4-C34
10	17	316	A86	C39-C38-O4-C34
10	18	311	A86	O5-C38-O4-C34
10	18	313	A86	C39-C38-O4-C34
10	21	211	A86	C39-C38-O4-C34
10	21	213	A86	C39-C38-O4-C34
10	21	215	A86	C39-C38-O4-C34
10	11	310	A86	C39-C38-O4-C34
10	11	310	A86	O5-C38-O4-C34
10	11	311	A86	C39-C38-O4-C34
10	12	315	A86	O5-C38-O4-C34
10	13	314	A86	O5-C38-O4-C34
10	14	311	A86	O5-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
10	14	312	A86	C39-C38-O4-C34
10	14	313	A86	O5-C38-O4-C34
10	15	311	A86	C39-C38-O4-C34
10	15	314	A86	O5-C38-O4-C34
10	16	311	A86	C39-C38-O4-C34
10	17	313	A86	O5-C38-O4-C34
10	17	321	A86	O5-C38-O4-C34
8	14	301	CLA	CBD-CGD-O2D-CED
8	21	206	CLA	CBD-CGD-O2D-CED
9	12	306	KC1	C4C-C3C-CAC-CBC
10	12	316	A86	C39-C38-O4-C34
10	13	316	A86	C39-C38-O4-C34
10	15	313	A86	C35-C34-O4-C38
10	21	213	A86	C35-C34-O4-C38
8	21	206	CLA	O1D-CGD-O2D-CED
9	20	303	KC1	O1D-CGD-O2D-CED
11	17	318	LMG	C29-C28-O8-C9
10	15	319	A86	O5-C38-O4-C34
8	18	302	CLA	O1A-CGA-O2A-C1
11	17	318	LMG	O10-C28-O8-C9
8	11	309	CLA	O1D-CGD-O2D-CED
10	12	314	A86	O5-C38-O4-C34
8	18	301	CLA	O1D-CGD-O2D-CED
10	11	313	A86	O5-C38-O4-C34
10	15	313	A86	O5-C38-O4-C34
10	16	310	A86	O5-C38-O4-C34
10	17	316	A86	O5-C38-O4-C34
10	18	313	A86	O5-C38-O4-C34
10	21	213	A86	O5-C38-O4-C34
9	12	306	KC1	C2C-C3C-CAC-CBC
15	21	201	LHG	O9-C7-O7-C5
10	19	313	A86	C39-C38-O4-C34
8	11	301	CLA	C3-C5-C6-C7
8	13	302	CLA	C3-C5-C6-C7
8	15	308	CLA	C3-C5-C6-C7
8	21	202	CLA	C3-C5-C6-C7
8	21	206	CLA	C3-C5-C6-C7
8	13	309	CLA	CBA-CGA-O2A-C1
15	19	314	LHG	C24-C23-O8-C6
10	14	315	A86	C39-C38-O4-C34
10	17	314	A86	C39-C38-O4-C34
8	11	301	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
8	12	311	CLA	CBD-CGD-O2D-CED
8	16	307	CLA	CBD-CGD-O2D-CED
8	17	302	CLA	CBD-CGD-O2D-CED
8	17	308	CLA	CBD-CGD-O2D-CED
10	14	316	A86	O5-C38-O4-C34
10	19	313	A86	O5-C38-O4-C34
10	14	316	A86	C39-C38-O4-C34
10	17	312	A86	O5-C38-O4-C34
9	11	306	KC1	CAA-CBA-CGA-O1A
9	11	306	KC1	CAA-CBA-CGA-O2A
8	15	308	CLA	C4-C3-C5-C6
8	19	302	CLA	C4-C3-C5-C6
8	20	304	CLA	C4-C3-C5-C6
8	21	204	CLA	C4-C3-C5-C6
8	21	208	CLA	C4-C3-C5-C6
8	15	308	CLA	C2-C3-C5-C6
8	20	304	CLA	C2-C3-C5-C6
8	21	204	CLA	C2-C3-C5-C6
8	21	208	CLA	C2-C3-C5-C6
10	21	215	A86	O5-C38-O4-C34
8	11	307	CLA	C3-C5-C6-C7
8	12	304	CLA	C2A-CAA-CBA-CGA
8	12	309	CLA	C3-C5-C6-C7
8	13	308	CLA	C3-C5-C6-C7
8	14	307	CLA	C3-C5-C6-C7
8	15	307	CLA	C3-C5-C6-C7
8	17	307	CLA	C3-C5-C6-C7
8	12	304	CLA	C3-C5-C6-C7
8	19	310	CLA	C3-C5-C6-C7
8	18	302	CLA	CBA-CGA-O2A-C1
10	14	312	A86	O5-C38-O4-C34
11	11	315	LMG	O6-C5-C6-O5
11	17	318	LMG	O6-C5-C6-O5
10	11	318	A86	C39-C38-O4-C34
10	11	311	A86	C24-C25-C26-C27
10	11	314	A86	C24-C25-C26-C27
10	12	313	A86	C24-C25-C26-C27
10	12	316	A86	C11-C10-C9-C8
10	12	319	A86	C24-C25-C26-C27
10	13	313	A86	C24-C25-C26-C27
10	13	315	A86	C24-C25-C26-C27
10	13	316	A86	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
10	14	311	A86	C24-C25-C26-C27
10	14	315	A86	C24-C25-C26-C27
10	15	313	A86	C24-C25-C26-C27
10	17	311	A86	C11-C10-C9-C8
10	17	313	A86	C24-C25-C26-C27
10	17	314	A86	C24-C25-C26-C27
10	18	312	A86	C11-C10-C9-C8
10	18	314	A86	C11-C10-C9-C8
10	21	211	A86	C24-C25-C26-C27
10	21	214	A86	C24-C25-C26-C27
13	16	312	DD6	C24-C25-C26-C27
13	20	312	DD6	C1-C2-C3-C4
13	21	212	DD6	C24-C25-C26-C27
13	21	216	DD6	C1-C2-C3-C4
8	13	309	CLA	O1A-CGA-O2A-C1
15	19	314	LHG	O10-C23-O8-C6
11	16	315	LMG	O9-C10-O7-C8
8	14	301	CLA	O1D-CGD-O2D-CED
10	11	318	A86	O5-C38-O4-C34
10	19	311	A86	C39-C38-O4-C34
10	20	313	A86	C39-C38-O4-C34
8	17	302	CLA	C3-C5-C6-C7
8	18	307	CLA	C3-C5-C6-C7
8	19	307	CLA	C3-C5-C6-C7
8	13	308	CLA	CBD-CGD-O2D-CED
15	17	317	LHG	O2-C2-C3-O3
11	16	315	LMG	C29-C28-O8-C9
10	17	311	A86	C39-C38-O4-C34
10	17	311	A86	O5-C38-O4-C34
10	19	311	A86	O5-C38-O4-C34
8	18	302	CLA	CBD-CGD-O2D-CED
11	16	315	LMG	C11-C10-O7-C8
15	21	201	LHG	C8-C7-O7-C5
8	13	309	CLA	C3-C5-C6-C7
8	14	302	CLA	C3-C5-C6-C7
9	12	308	KC1	CAA-CBA-CGA-O2A
9	14	309	KC1	CAA-CBA-CGA-O2A
9	15	306	KC1	CAA-CBA-CGA-O2A
9	21	207	KC1	CAA-CBA-CGA-O2A
8	20	302	CLA	C4-C3-C5-C6
8	19	302	CLA	C2-C3-C5-C6
8	20	302	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	17	301	SQD	O10-C23-O48-C46
15	17	317	LHG	O9-C7-O7-C5
10	18	312	A86	C39-C38-O4-C34
8	16	306	CLA	CBD-CGD-O2D-CED
8	21	205	CLA	CBD-CGD-O2D-CED
11	11	315	LMG	C4-C5-C6-O5
11	17	318	LMG	C4-C5-C6-O5
14	16	314	SQD	O5-C1-O6-C44
8	19	307	CLA	CBA-CGA-O2A-C1
11	11	316	LMG	C29-C28-O8-C9
8	12	309	CLA	CBD-CGD-O2D-CED
8	16	309	CLA	CBD-CGD-O2D-CED
8	21	209	CLA	CBD-CGD-O2D-CED
11	11	316	LMG	O6-C5-C6-O5
9	11	308	KC1	CAA-CBA-CGA-O1A
9	11	308	KC1	CAA-CBA-CGA-O2A
9	12	308	KC1	CAA-CBA-CGA-O1A
9	15	302	KC1	CAA-CBA-CGA-O1A
9	15	306	KC1	CAA-CBA-CGA-O1A
15	21	217	LHG	C23-C24-C25-C26
10	11	313	A86	C24-C25-C26-C27
10	12	314	A86	C24-C25-C26-C27
10	14	314	A86	C24-C25-C26-C27
10	15	314	A86	C24-C25-C26-C27
10	15	316	A86	C11-C10-C9-C8
10	16	310	A86	C24-C25-C26-C27
10	20	313	A86	C11-C10-C9-C8
13	21	216	DD6	C24-C25-C26-C27
8	19	307	CLA	O1A-CGA-O2A-C1
15	19	314	LHG	C1-C2-C3-O3
8	12	301	CLA	CBA-CGA-O2A-C1
8	19	305	CLA	CBA-CGA-O2A-C1
14	17	301	SQD	C24-C23-O48-C46
8	13	301	CLA	CBD-CGD-O2D-CED
8	19	301	CLA	CBD-CGD-O2D-CED
11	11	316	LMG	C4-C5-C6-O5
10	16	311	A86	O5-C38-O4-C34
9	13	303	KC1	CAA-CBA-CGA-O2A
9	13	305	KC1	CAA-CBA-CGA-O1A
9	13	305	KC1	CAA-CBA-CGA-O2A
9	14	309	KC1	CAA-CBA-CGA-O1A
9	15	302	KC1	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
9	15	304	KC1	CAA-CBA-CGA-O1A
9	16	304	KC1	CAA-CBA-CGA-O1A
9	16	304	KC1	CAA-CBA-CGA-O2A
9	18	304	KC1	CAA-CBA-CGA-O2A
9	21	207	KC1	CAA-CBA-CGA-O1A
8	12	303	CLA	C3-C5-C6-C7
8	21	206	CLA	C11-C12-C13-C14
8	12	311	CLA	O1D-CGD-O2D-CED
10	11	311	A86	O5-C38-O4-C34
14	16	314	SQD	C2-C1-O6-C44
8	19	305	CLA	O1A-CGA-O2A-C1
10	11	311	A86	C-C1-C24-C25
10	11	312	A86	C7-C6-C8-C9
10	11	318	A86	C-C1-C24-C25
10	12	302	A86	C7-C6-C8-C9
10	12	314	A86	C-C1-C24-C25
10	12	315	A86	C7-C6-C8-C9
10	12	316	A86	C-C1-C24-C25
10	13	314	A86	C-C1-C24-C25
10	13	314	A86	C7-C6-C8-C9
10	13	315	A86	C-C1-C24-C25
10	13	316	A86	C7-C6-C8-C9
10	14	316	A86	C-C1-C24-C25
10	15	312	A86	C-C1-C24-C25
10	15	312	A86	C7-C6-C8-C9
10	15	314	A86	C7-C6-C8-C9
10	15	315	A86	C-C1-C24-C25
10	17	312	A86	C-C1-C24-C25
10	17	321	A86	C-C1-C24-C25
10	17	321	A86	C7-C6-C8-C9
10	19	313	A86	C-C1-C24-C25
10	20	301	A86	C-C1-C24-C25
10	20	301	A86	C7-C6-C8-C9
10	20	313	A86	C-C1-C24-C25
10	21	213	A86	C-C1-C24-C25
13	16	312	DD6	C12-C11-C13-C14
13	19	312	DD6	C12-C11-C13-C14
13	19	312	DD6	C7-C6-C8-C9
13	20	312	DD6	C7-C6-C8-C9
13	20	314	DD6	C12-C11-C13-C14
13	21	212	DD6	C-C1-C24-C25
13	21	216	DD6	C-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
13	21	216	DD6	C12-C11-C13-C14
13	21	216	DD6	C7-C6-C8-C9
10	11	311	A86	C2-C1-C24-C25
10	11	312	A86	C5-C6-C8-C9
10	11	318	A86	C2-C1-C24-C25
10	12	314	A86	C2-C1-C24-C25
10	12	319	A86	C5-C6-C8-C9
10	13	314	A86	C2-C1-C24-C25
10	13	314	A86	C5-C6-C8-C9
10	13	315	A86	C2-C1-C24-C25
10	13	316	A86	C5-C6-C8-C9
10	15	312	A86	C2-C1-C24-C25
10	17	312	A86	C2-C1-C24-C25
10	20	301	A86	C2-C1-C24-C25
10	20	301	A86	C5-C6-C8-C9
10	21	213	A86	C2-C1-C24-C25
8	19	309	CLA	C2A-CAA-CBA-CGA
9	15	304	KC1	CAA-CBA-CGA-O2A
9	20	303	KC1	CAA-CBA-CGA-O1A
8	19	306	CLA	CBA-CGA-O2A-C1
8	17	302	CLA	O1D-CGD-O2D-CED
11	11	316	LMG	C10-C11-C12-C13
8	13	308	CLA	O1D-CGD-O2D-CED
8	16	307	CLA	O1D-CGD-O2D-CED
9	18	304	KC1	CAA-CBA-CGA-O1A
9	20	303	KC1	CAA-CBA-CGA-O2A
8	13	309	CLA	C10-C11-C12-C13
10	12	315	A86	C24-C25-C26-C27
10	13	312	A86	C24-C25-C26-C27
10	13	314	A86	C11-C10-C9-C8
10	14	312	A86	C24-C25-C26-C27
10	14	316	A86	C11-C10-C9-C8
10	15	319	A86	C24-C25-C26-C27
10	16	313	A86	C11-C10-C9-C8
10	18	311	A86	C11-C10-C9-C8
10	18	313	A86	C24-C25-C26-C27
10	20	301	A86	C1-C2-C3-C4
10	21	215	A86	C24-C25-C26-C27
13	20	312	DD6	C24-C25-C26-C27
9	20	306	KC1	C2C-C3C-CAC-CBC
11	16	315	LMG	C10-C11-C12-C13
8	17	308	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
8	19	303	CLA	C8-C10-C11-C12
8	19	307	CLA	C10-C11-C12-C13
8	11	301	CLA	C2A-CAA-CBA-CGA
8	13	302	CLA	C2A-CAA-CBA-CGA
8	14	302	CLA	C2A-CAA-CBA-CGA
8	15	307	CLA	C2A-CAA-CBA-CGA
8	17	302	CLA	C2A-CAA-CBA-CGA
9	18	309	KC1	CAA-CBA-CGA-O2A
8	19	303	CLA	C13-C15-C16-C17
15	19	314	LHG	C23-C24-C25-C26
8	12	301	CLA	O1A-CGA-O2A-C1
8	12	303	CLA	C8-C10-C11-C12
8	12	303	CLA	C15-C16-C17-C18
8	13	301	CLA	C10-C11-C12-C13
8	18	308	CLA	C10-C11-C12-C13
8	15	307	CLA	CBD-CGD-O2D-CED
15	21	217	LHG	C7-C8-C9-C10
8	19	306	CLA	C10-C11-C12-C13
8	12	301	CLA	C10-C11-C12-C13
8	17	308	CLA	C10-C11-C12-C13
9	13	303	KC1	CAA-CBA-CGA-O1A
9	18	309	KC1	CAA-CBA-CGA-O1A
11	16	315	LMG	O10-C28-O8-C9
11	11	315	LMG	C28-C29-C30-C31
10	14	315	A86	O5-C38-O4-C34
8	19	307	CLA	C13-C15-C16-C17
8	14	308	CLA	CBA-CGA-O2A-C1
9	14	309	KC1	C2A-CAA-CBA-CGA
9	16	308	KC1	C2A-CAA-CBA-CGA
9	18	309	KC1	C2A-CAA-CBA-CGA
10	17	314	A86	O5-C38-O4-C34
10	12	312	A86	C24-C25-C26-C27
10	17	312	A86	C11-C10-C9-C8
10	17	315	A86	C11-C10-C9-C8
10	17	321	A86	C3-C4-C5-C6
10	20	301	A86	C3-C4-C5-C6
10	20	313	A86	C24-C25-C26-C27
10	21	213	A86	C3-C4-C5-C6
13	20	312	DD6	C11-C10-C9-C8
13	21	216	DD6	C3-C4-C5-C6
9	15	309	KC1	CAA-CBA-CGA-O2A
15	17	317	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
8	11	307	CLA	C2A-CAA-CBA-CGA
8	19	310	CLA	CBA-CGA-O2A-C1
8	21	208	CLA	CBA-CGA-O2A-C1
8	12	303	CLA	C13-C15-C16-C17
8	13	302	CLA	C15-C16-C17-C18
8	16	306	CLA	C8-C10-C11-C12
8	18	308	CLA	C13-C15-C16-C17
8	11	303	CLA	C3-C5-C6-C7
8	20	302	CLA	C3-C5-C6-C7
8	14	302	CLA	C8-C10-C11-C12
8	14	302	CLA	C10-C11-C12-C13
8	17	308	CLA	C13-C15-C16-C17
8	19	306	CLA	O1A-CGA-O2A-C1
8	20	304	CLA	CBD-CGD-O2D-CED
15	21	217	LHG	C8-C7-O7-C5
8	11	301	CLA	O1D-CGD-O2D-CED
14	17	301	SQD	O49-C7-O47-C45
14	17	301	SQD	C2-C1-O6-C44
8	13	304	CLA	C3-C5-C6-C7
10	11	314	A86	C-C1-C24-C25
10	12	319	A86	C7-C6-C8-C9
10	13	313	A86	C-C1-C24-C25
10	16	311	A86	C-C1-C24-C25
10	17	311	A86	C7-C6-C8-C9
10	19	311	A86	C-C1-C24-C25
13	20	314	DD6	C-C1-C24-C25
10	11	314	A86	C2-C1-C24-C25
10	13	313	A86	C2-C1-C24-C25
10	15	314	A86	C5-C6-C8-C9
10	16	310	A86	C2-C1-C24-C25
10	19	311	A86	C2-C1-C24-C25
8	18	301	CLA	C2A-CAA-CBA-CGA
8	18	307	CLA	C2A-CAA-CBA-CGA
8	19	306	CLA	C2A-CAA-CBA-CGA
8	21	208	CLA	C13-C15-C16-C17
8	12	301	CLA	C16-C17-C18-C20
8	19	310	CLA	O1A-CGA-O2A-C1
8	18	303	CLA	C3-C5-C6-C7
13	16	312	DD6	C24-C1-C2-C3
13	19	312	DD6	C4-C5-C6-C8
13	21	212	DD6	C24-C1-C2-C3
13	21	216	DD6	C24-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
9	15	309	KC1	CAA-CBA-CGA-O1A
8	19	301	CLA	C3-C5-C6-C7
8	19	303	CLA	C3-C5-C6-C7
8	12	301	CLA	C16-C17-C18-C19
8	14	308	CLA	O1A-CGA-O2A-C1
8	21	208	CLA	O1A-CGA-O2A-C1
11	16	315	LMG	O6-C5-C6-O5
8	11	307	CLA	C2C-C3C-CAC-CBC
15	17	317	LHG	C11-C10-C9-C8
15	19	314	LHG	C28-C29-C30-C31
14	16	314	SQD	C14-C15-C16-C17
14	17	301	SQD	C9-C10-C11-C12
8	18	302	CLA	O1D-CGD-O2D-CED
8	11	303	CLA	C4B-C3B-CAB-CBB
8	11	307	CLA	C4B-C3B-CAB-CBB
8	12	303	CLA	C4B-C3B-CAB-CBB
8	13	304	CLA	C4B-C3B-CAB-CBB
8	16	306	CLA	C16-C17-C18-C19
8	16	306	CLA	C16-C17-C18-C20
8	21	205	CLA	O1D-CGD-O2D-CED
8	16	301	CLA	C8-C10-C11-C12
8	19	306	CLA	C11-C12-C13-C15
10	20	313	A86	O5-C38-O4-C34
15	21	201	LHG	C10-C11-C12-C13
14	17	301	SQD	C27-C28-C29-C30
8	17	310	CLA	C3-C5-C6-C7
9	19	308	KC1	CAA-CBA-CGA-O1A
8	11	303	CLA	C3A-C2A-CAA-CBA
8	12	305	CLA	C3A-C2A-CAA-CBA
8	13	304	CLA	C3A-C2A-CAA-CBA
8	15	303	CLA	C3A-C2A-CAA-CBA
8	16	303	CLA	C3A-C2A-CAA-CBA
8	16	306	CLA	C3A-C2A-CAA-CBA
8	16	309	CLA	C3A-C2A-CAA-CBA
8	17	304	CLA	C3A-C2A-CAA-CBA
8	17	310	CLA	C3A-C2A-CAA-CBA
8	18	302	CLA	C3A-C2A-CAA-CBA
8	18	303	CLA	C3A-C2A-CAA-CBA
8	19	303	CLA	C3A-C2A-CAA-CBA
8	20	302	CLA	C3A-C2A-CAA-CBA
8	20	304	CLA	C3A-C2A-CAA-CBA
8	20	309	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
8	21	202	CLA	C3A-C2A-CAA-CBA
8	21	204	CLA	C3A-C2A-CAA-CBA
8	21	205	CLA	C3A-C2A-CAA-CBA
15	19	314	LHG	C26-C27-C28-C29
15	21	201	LHG	C11-C10-C9-C8
11	11	315	LMG	C13-C14-C15-C16
8	19	303	CLA	C10-C11-C12-C13
8	21	209	CLA	O1D-CGD-O2D-CED
10	11	312	A86	C11-C10-C9-C8
10	11	318	A86	C3-C4-C5-C6
10	13	314	A86	C24-C25-C26-C27
10	14	316	A86	C3-C4-C5-C6
10	15	316	A86	C3-C4-C5-C6
10	15	319	A86	C3-C4-C5-C6
14	17	301	SQD	C29-C30-C31-C32
8	13	301	CLA	CBA-CGA-O2A-C1
8	20	307	CLA	CBA-CGA-O2A-C1
14	16	314	SQD	C18-C19-C20-C21
15	21	217	LHG	C30-C31-C32-C33
15	19	314	LHG	C33-C34-C35-C36
9	16	305	KC1	CAA-CBA-CGA-O1A
9	17	306	KC1	CAA-CBA-CGA-O1A
8	16	306	CLA	O1D-CGD-O2D-CED
15	17	317	LHG	C16-C17-C18-C19
16	19	315	LMU	C1-C2-C3-C4
8	14	301	CLA	C2B-C3B-CAB-CBB
8	14	302	CLA	C2B-C3B-CAB-CBB
8	19	301	CLA	C2B-C3B-CAB-CBB
8	19	310	CLA	C2B-C3B-CAB-CBB
8	20	309	CLA	C2B-C3B-CAB-CBB
15	19	314	LHG	C11-C12-C13-C14
8	12	303	CLA	C10-C11-C12-C13
8	20	307	CLA	O1A-CGA-O2A-C1
15	21	201	LHG	C24-C25-C26-C27
10	18	312	A86	O5-C38-O4-C34
14	17	301	SQD	C11-C12-C13-C14
15	19	314	LHG	C30-C31-C32-C33
8	11	309	CLA	CBA-CGA-O2A-C1
8	21	206	CLA	CBA-CGA-O2A-C1
14	16	314	SQD	C24-C23-O48-C46
8	13	301	CLA	O1A-CGA-O2A-C1
11	16	315	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
11	11	315	LMG	C30-C31-C32-C33
11	11	316	LMG	O10-C28-O8-C9
9	19	308	KC1	CAA-CBA-CGA-O2A
15	17	317	LHG	C24-C23-O8-C6
10	14	314	A86	C3-C4-C5-C6
10	15	315	A86	C11-C10-C9-C8
10	15	315	A86	C24-C25-C26-C27
10	18	312	A86	C24-C25-C26-C27
8	16	303	CLA	CBD-CGD-O2D-CED
10	12	313	A86	C39-C38-O4-C34
10	16	310	A86	C-C1-C24-C25
10	12	316	A86	C2-C1-C24-C25
10	17	321	A86	C5-C6-C8-C9
8	12	309	CLA	C2A-CAA-CBA-CGA
8	12	311	CLA	C2A-CAA-CBA-CGA
9	17	306	KC1	CAA-CBA-CGA-O2A
8	15	307	CLA	C4-C3-C5-C6
8	17	304	CLA	C4-C3-C5-C6
8	17	307	CLA	C4-C3-C5-C6
9	11	308	KC1	C2B-C3B-CAB-CBB
9	12	310	KC1	C2B-C3B-CAB-CBB
9	13	307	KC1	C2B-C3B-CAB-CBB
9	14	304	KC1	C2B-C3B-CAB-CBB
9	14	306	KC1	C2B-C3B-CAB-CBB
9	15	302	KC1	C2B-C3B-CAB-CBB
9	15	309	KC1	C2B-C3B-CAB-CBB
9	16	304	KC1	C2B-C3B-CAB-CBB
9	16	305	KC1	C2B-C3B-CAB-CBB
9	17	305	KC1	C2B-C3B-CAB-CBB
9	18	304	KC1	C2B-C3B-CAB-CBB
9	20	305	KC1	C2B-C3B-CAB-CBB
9	20	306	KC1	C2B-C3B-CAB-CBB
15	19	314	LHG	C10-C11-C12-C13
15	21	217	LHG	C29-C30-C31-C32
11	17	318	LMG	C28-C29-C30-C31
8	19	310	CLA	C5-C6-C7-C8
11	11	315	LMG	C10-C11-C12-C13
8	21	206	CLA	C10-C11-C12-C13
8	12	309	CLA	O1D-CGD-O2D-CED
9	20	306	KC1	C4C-C3C-CAC-CBC
8	13	309	CLA	C5-C6-C7-C8
8	16	309	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	17	317	LHG	C27-C28-C29-C30
15	19	314	LHG	C32-C33-C34-C35
15	17	317	LHG	C13-C14-C15-C16
9	16	305	KC1	CAA-CBA-CGA-O2A
9	17	303	KC1	CAA-CBA-CGA-O2A
8	14	303	CLA	C2A-CAA-CBA-CGA
8	14	302	CLA	CBD-CGD-O2D-CED
8	19	302	CLA	CBD-CGD-O2D-CED
8	20	302	CLA	CBD-CGD-O2D-CED
14	16	314	SQD	C13-C14-C15-C16
15	21	217	LHG	O1-C1-C2-O2
8	16	306	CLA	C3-C5-C6-C7
9	12	310	KC1	CAA-CBA-CGA-O1A
9	17	303	KC1	CAA-CBA-CGA-O1A
9	20	306	KC1	CAA-CBA-CGA-O1A
8	11	305	CLA	C1A-C2A-CAA-CBA
8	11	309	CLA	C1A-C2A-CAA-CBA
8	12	303	CLA	C1A-C2A-CAA-CBA
8	13	301	CLA	C1A-C2A-CAA-CBA
8	13	309	CLA	C1A-C2A-CAA-CBA
8	14	303	CLA	C1A-C2A-CAA-CBA
8	14	305	CLA	C1A-C2A-CAA-CBA
8	16	307	CLA	C1A-C2A-CAA-CBA
8	16	309	CLA	C1A-C2A-CAA-CBA
8	17	308	CLA	C1A-C2A-CAA-CBA
8	17	310	CLA	C1A-C2A-CAA-CBA
8	18	302	CLA	C1A-C2A-CAA-CBA
8	19	301	CLA	C1A-C2A-CAA-CBA
8	19	303	CLA	C1A-C2A-CAA-CBA
8	19	305	CLA	C1A-C2A-CAA-CBA
8	19	306	CLA	C1A-C2A-CAA-CBA
8	19	307	CLA	C1A-C2A-CAA-CBA
8	19	310	CLA	C1A-C2A-CAA-CBA
8	20	304	CLA	C1A-C2A-CAA-CBA
8	20	309	CLA	C1A-C2A-CAA-CBA
8	21	205	CLA	C1A-C2A-CAA-CBA
8	21	206	CLA	C1A-C2A-CAA-CBA
8	21	208	CLA	C1A-C2A-CAA-CBA
16	19	315	LMU	C11-C10-C9-C8
8	11	309	CLA	O1A-CGA-O2A-C1
15	21	217	LHG	O9-C7-O7-C5
15	17	317	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
8	14	301	CLA	C6-C7-C8-C10
8	14	301	CLA	C12-C13-C15-C16
8	18	301	CLA	C12-C13-C15-C16
8	21	204	CLA	C6-C7-C8-C10
9	12	310	KC1	CAA-CBA-CGA-O2A
14	16	314	SQD	C23-C24-C25-C26
14	17	301	SQD	C7-C8-C9-C10
15	17	317	LHG	C7-C8-C9-C10
8	14	307	CLA	C2-C3-C5-C6
8	17	307	CLA	C2-C3-C5-C6
8	13	302	CLA	C5-C6-C7-C8
8	12	301	CLA	C14-C13-C15-C16
8	14	301	CLA	C6-C7-C8-C9
8	14	301	CLA	C14-C13-C15-C16
8	18	301	CLA	C11-C10-C8-C9
8	19	307	CLA	C14-C13-C15-C16
8	16	307	CLA	CBA-CGA-O2A-C1
8	15	308	CLA	C5-C6-C7-C8
15	19	314	LHG	C31-C32-C33-C34
8	11	307	CLA	C4C-C3C-CAC-CBC
8	12	305	CLA	C10-C11-C12-C13
8	13	301	CLA	O1D-CGD-O2D-CED
11	11	316	LMG	C7-C8-C9-O8
15	21	201	LHG	C4-C5-C6-O8
8	15	307	CLA	CBA-CGA-O2A-C1
8	21	206	CLA	O1A-CGA-O2A-C1
11	11	315	LMG	O10-C28-O8-C9
8	14	307	CLA	C4-C3-C5-C6
8	15	307	CLA	C2-C3-C5-C6
10	12	316	A86	C7-C6-C8-C9
10	15	316	A86	C7-C6-C8-C9
10	15	319	A86	C-C1-C24-C25
10	18	313	A86	C7-C6-C8-C9
10	18	314	A86	C7-C6-C8-C9
10	20	311	A86	C7-C6-C8-C9
10	14	315	A86	C2-C1-C24-C25
10	14	316	A86	C2-C1-C24-C25
10	14	316	A86	C5-C6-C8-C9
10	18	313	A86	C5-C6-C8-C9
10	18	314	A86	C5-C6-C8-C9
13	19	312	DD6	C5-C6-C8-C9
8	16	307	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
15	17	317	LHG	C12-C13-C14-C15
15	19	314	LHG	C7-C8-C9-C10
11	17	318	LMG	C15-C16-C17-C18
9	20	306	KC1	CAA-CBA-CGA-O2A
15	17	317	LHG	C4-C5-O7-C7
10	20	313	A86	C3-C4-C5-C6
13	19	312	DD6	C3-C4-C5-C6
11	17	318	LMG	C16-C17-C18-C19
15	21	217	LHG	C11-C10-C9-C8
13	20	314	DD6	C24-C1-C2-C3
13	20	314	DD6	C9-C10-C11-C13
14	16	314	SQD	C12-C13-C14-C15
8	13	304	CLA	C4-C3-C5-C6
16	19	315	LMU	C7-C8-C9-C10
15	19	314	LHG	C9-C10-C11-C12
15	21	217	LHG	C26-C27-C28-C29
11	11	316	LMG	O1-C7-C8-O7
11	11	316	LMG	C32-C33-C34-C35
8	18	307	CLA	CBA-CGA-O2A-C1
8	12	305	CLA	C3-C5-C6-C7
14	17	301	SQD	C12-C13-C14-C15
15	17	317	LHG	C9-C10-C11-C12
8	16	307	CLA	C10-C11-C12-C13
8	17	308	CLA	CBA-CGA-O2A-C1
11	16	315	LMG	C15-C16-C17-C18
11	17	318	LMG	C31-C32-C33-C34
14	17	301	SQD	C35-C36-C37-C38
8	15	308	CLA	C13-C15-C16-C17
10	17	312	A86	C24-C25-C26-C27
10	19	311	A86	C24-C25-C26-C27
10	19	313	A86	C11-C10-C9-C8
8	12	309	CLA	C4-C3-C5-C6
8	19	301	CLA	CBA-CGA-O2A-C1
8	16	306	CLA	C14-C13-C15-C16
8	21	204	CLA	C6-C7-C8-C9
8	12	305	CLA	C4B-C3B-CAB-CBB
8	13	308	CLA	C4B-C3B-CAB-CBB
8	14	301	CLA	C4B-C3B-CAB-CBB
8	14	302	CLA	C4B-C3B-CAB-CBB
8	17	307	CLA	C4B-C3B-CAB-CBB
8	18	307	CLA	C4B-C3B-CAB-CBB
8	19	310	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
8	20	304	CLA	C4B-C3B-CAB-CBB
8	20	307	CLA	C4B-C3B-CAB-CBB
8	20	309	CLA	C4B-C3B-CAB-CBB
8	21	205	CLA	C4B-C3B-CAB-CBB
8	21	202	CLA	CBA-CGA-O2A-C1
14	17	301	SQD	C14-C15-C16-C17
8	13	308	CLA	C2A-CAA-CBA-CGA
15	17	317	LHG	C29-C30-C31-C32
11	11	315	LMG	C2-C1-O1-C7
11	16	315	LMG	C2-C1-O1-C7
15	21	217	LHG	C32-C33-C34-C35
8	12	301	CLA	C12-C13-C15-C16
8	12	304	CLA	C6-C7-C8-C10
8	16	306	CLA	C12-C13-C15-C16
8	18	301	CLA	C11-C10-C8-C7
8	19	302	CLA	C6-C7-C8-C10
8	19	307	CLA	C12-C13-C15-C16
8	11	301	CLA	C8-C10-C11-C12
8	11	307	CLA	C4-C3-C5-C6
8	21	206	CLA	C4-C3-C5-C6
14	17	301	SQD	C30-C31-C32-C33
8	15	307	CLA	O1A-CGA-O2A-C1
10	13	312	A86	C11-C10-C9-C8
10	13	313	A86	C11-C10-C9-C8
10	15	312	A86	C24-C25-C26-C27
10	18	312	A86	C3-C4-C5-C6
10	18	313	A86	C3-C4-C5-C6
10	14	316	A86	C7-C6-C8-C9
14	16	314	SQD	C9-C10-C11-C12
8	19	305	CLA	C4-C3-C5-C6
15	21	201	LHG	C2-C3-O3-P
14	16	314	SQD	O10-C23-O48-C46
9	13	310	KC1	CAA-CBA-CGA-O1A
8	21	208	CLA	C10-C11-C12-C13
13	20	314	DD6	C10-C11-C13-C14
11	11	315	LMG	C29-C30-C31-C32
10	13	314	A86	C12-C11-C13-O
10	15	314	A86	C12-C11-C13-O
10	15	316	A86	C12-C11-C13-O
10	18	313	A86	C12-C11-C13-O
10	20	301	A86	C12-C11-C13-O
10	20	313	A86	C12-C11-C13-O

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Mol	Chain	Res	Type	Atoms
11	11	316	LMG	O1-C7-C8-C9
15	19	314	LHG	C4-C5-C6-O8
8	16	307	CLA	C3-C5-C6-C7
14	17	301	SQD	C26-C27-C28-C29
9	13	310	KC1	CAA-CBA-CGA-O2A
8	18	307	CLA	C4-C3-C5-C6
8	18	308	CLA	C4-C3-C5-C6
8	12	309	CLA	C2-C3-C5-C6
10	13	314	A86	C10-C11-C13-O
10	15	314	A86	C10-C11-C13-O
10	18	313	A86	C10-C11-C13-O
10	20	301	A86	C10-C11-C13-O
10	20	313	A86	C10-C11-C13-O
8	19	305	CLA	C2B-C3B-CAB-CBB
8	21	205	CLA	C2B-C3B-CAB-CBB
8	21	206	CLA	C2B-C3B-CAB-CBB
8	17	302	CLA	C8-C10-C11-C12
8	19	303	CLA	C5-C6-C7-C8
8	12	303	CLA	C5-C6-C7-C8
11	11	315	LMG	O7-C8-C9-O8
11	17	318	LMG	O1-C7-C8-O7
14	16	314	SQD	O47-C45-C46-O48
16	19	315	LMU	C3-C4-C5-C6
8	16	301	CLA	C3-C5-C6-C7
8	14	302	CLA	C5-C6-C7-C8
8	21	204	CLA	C5-C6-C7-C8
8	11	307	CLA	C2-C3-C5-C6
8	17	304	CLA	C2-C3-C5-C6
8	18	307	CLA	C2-C3-C5-C6
8	21	206	CLA	C2-C3-C5-C6
14	16	314	SQD	C19-C20-C21-C22
8	18	301	CLA	C14-C13-C15-C16
8	14	301	CLA	C8-C10-C11-C12
8	19	301	CLA	O1D-CGD-O2D-CED
15	21	201	LHG	C25-C26-C27-C28
8	13	308	CLA	CBA-CGA-O2A-C1
10	11	314	A86	C3-C4-C5-C6
10	15	314	A86	C3-C4-C5-C6
13	21	212	DD6	C11-C10-C9-C8
15	19	314	LHG	C15-C16-C17-C18
16	19	315	LMU	C4-C5-C6-C7
10	12	313	A86	O5-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
10	11	310	A86	C-C1-C24-C25
10	14	315	A86	C-C1-C24-C25
10	15	311	A86	C-C1-C24-C25
10	17	313	A86	C-C1-C24-C25
10	17	316	A86	C-C1-C24-C25
8	14	308	CLA	C12-C13-C15-C16
15	17	317	LHG	C30-C31-C32-C33
10	11	310	A86	C2-C1-C24-C25
10	12	316	A86	C5-C6-C8-C9
10	15	311	A86	C2-C1-C24-C25
10	15	316	A86	C5-C6-C8-C9
10	15	319	A86	C2-C1-C24-C25
10	17	311	A86	C5-C6-C8-C9
10	17	313	A86	C2-C1-C24-C25
10	20	311	A86	C5-C6-C8-C9
8	17	308	CLA	O1A-CGA-O2A-C1
8	18	307	CLA	O1A-CGA-O2A-C1
8	16	307	CLA	C14-C13-C15-C16
11	11	316	LMG	O9-C10-O7-C8
8	13	308	CLA	C4-C3-C5-C6
8	21	202	CLA	O1A-CGA-O2A-C1
9	12	308	KC1	C2B-C3B-CAB-CBB
9	13	310	KC1	C2B-C3B-CAB-CBB
9	14	309	KC1	C2B-C3B-CAB-CBB
9	16	308	KC1	C2B-C3B-CAB-CBB
9	17	306	KC1	C2B-C3B-CAB-CBB
9	17	309	KC1	C2B-C3B-CAB-CBB
8	18	308	CLA	CBA-CGA-O2A-C1
11	16	315	LMG	C9-C8-O7-C10
14	16	314	SQD	C11-C10-C9-C8
15	21	217	LHG	C31-C32-C33-C34
13	16	312	DD6	C4-C5-C6-C8
13	19	312	DD6	C24-C1-C2-C3
11	11	315	LMG	C7-C8-C9-O8
15	21	217	LHG	C4-C5-C6-O8
11	11	316	LMG	C28-C29-C30-C31
9	11	304	KC1	C4B-C3B-CAB-CBB
9	11	306	KC1	C4B-C3B-CAB-CBB
9	12	308	KC1	C4B-C3B-CAB-CBB
9	12	310	KC1	C4B-C3B-CAB-CBB
9	13	303	KC1	C4B-C3B-CAB-CBB
9	13	305	KC1	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
9	14	306	KC1	C4B-C3B-CAB-CBB
9	14	309	KC1	C4B-C3B-CAB-CBB
9	15	306	KC1	C4B-C3B-CAB-CBB
9	16	305	KC1	C4B-C3B-CAB-CBB
9	16	308	KC1	C4B-C3B-CAB-CBB
9	17	309	KC1	C4B-C3B-CAB-CBB
9	21	207	KC1	C4B-C3B-CAB-CBB
8	20	304	CLA	C3-C5-C6-C7
11	11	315	LMG	C20-C21-C22-C23
8	18	308	CLA	O1A-CGA-O2A-C1
10	15	313	A86	C28-C27-C29-C30
10	16	311	A86	C28-C27-C29-C30
15	21	201	LHG	O2-C2-C3-O3
11	16	315	LMG	C16-C17-C18-C19
11	11	316	LMG	O7-C8-C9-O8
14	17	301	SQD	O6-C44-C45-O47
8	14	308	CLA	C14-C13-C15-C16
8	20	302	CLA	CBA-CGA-O2A-C1
8	16	303	CLA	O1A-CGA-O2A-C1
8	19	301	CLA	O1A-CGA-O2A-C1
14	16	314	SQD	C17-C18-C19-C20
10	12	302	A86	C13-C14-C15-O1
10	12	316	A86	C13-C14-C15-O1
10	13	314	A86	C13-C14-C15-O1
10	13	315	A86	C13-C14-C15-O1
10	13	316	A86	C13-C14-C15-O1
10	14	316	A86	C13-C14-C15-O1
10	15	316	A86	C13-C14-C15-O1
10	16	313	A86	C13-C14-C15-O1
10	17	316	A86	C13-C14-C15-O1
10	18	314	A86	C13-C14-C15-O1
8	13	308	CLA	O1A-CGA-O2A-C1
15	17	317	LHG	C8-C7-O7-C5
10	11	310	A86	C1-C2-C3-C4
10	16	311	A86	C1-C2-C3-C4
8	16	303	CLA	CBA-CGA-O2A-C1
8	13	302	CLA	C10-C11-C12-C13
8	20	304	CLA	O1D-CGD-O2D-CED
15	21	217	LHG	C35-C36-C37-C38
10	15	313	A86	C-C1-C24-C25
8	11	305	CLA	C4B-C3B-CAB-CBB
8	12	307	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
8	13	306	CLA	C4B-C3B-CAB-CBB
8	14	305	CLA	C4B-C3B-CAB-CBB
8	14	310	CLA	C4B-C3B-CAB-CBB
8	15	305	CLA	C4B-C3B-CAB-CBB
8	15	307	CLA	C4B-C3B-CAB-CBB
8	15	308	CLA	C4B-C3B-CAB-CBB
8	18	302	CLA	C4B-C3B-CAB-CBB
8	18	305	CLA	C4B-C3B-CAB-CBB
8	18	310	CLA	C4B-C3B-CAB-CBB
8	19	303	CLA	C4B-C3B-CAB-CBB
8	19	304	CLA	C4B-C3B-CAB-CBB
8	19	305	CLA	C4B-C3B-CAB-CBB
8	19	309	CLA	C4B-C3B-CAB-CBB
8	21	202	CLA	C4B-C3B-CAB-CBB
8	21	206	CLA	C4B-C3B-CAB-CBB
8	21	208	CLA	C4B-C3B-CAB-CBB
8	21	210	CLA	C4B-C3B-CAB-CBB
10	11	312	A86	O-C13-C14-C15
10	12	312	A86	O-C13-C14-C15
10	12	314	A86	O-C13-C14-C15
10	13	312	A86	O-C13-C14-C15
10	14	314	A86	O-C13-C14-C15
10	15	311	A86	O-C13-C14-C15
10	15	313	A86	O-C13-C14-C15
10	15	314	A86	O-C13-C14-C15
10	17	311	A86	O-C13-C14-C15
10	17	314	A86	O-C13-C14-C15
10	17	315	A86	O-C13-C14-C15
10	17	316	A86	O-C13-C14-C15
10	19	311	A86	O-C13-C14-C15
10	20	301	A86	O-C13-C14-C15
8	18	301	CLA	C4-C3-C5-C6
15	21	217	LHG	O6-C4-C5-C6
9	17	305	KC1	CAA-CBA-CGA-O1A
15	19	314	LHG	O9-C7-O7-C5
8	14	308	CLA	C6-C7-C8-C10
8	15	308	CLA	C12-C13-C15-C16
8	21	206	CLA	C11-C12-C13-C15
15	17	317	LHG	C11-C12-C13-C14
8	20	302	CLA	O1A-CGA-O2A-C1
8	14	301	CLA	C4-C3-C5-C6
15	21	217	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
8	19	302	CLA	C6-C7-C8-C9
8	15	303	CLA	O1A-CGA-O2A-C1
10	13	316	A86	C3-C4-C5-C6
10	14	313	A86	C11-C10-C9-C8
10	21	214	A86	C3-C4-C5-C6
9	11	304	KC1	C3A-C2A-CAA-CBA
9	12	306	KC1	C1A-C2A-CAA-CBA
9	13	307	KC1	C1A-C2A-CAA-CBA
9	14	304	KC1	C3A-C2A-CAA-CBA
9	14	306	KC1	C1A-C2A-CAA-CBA
9	16	305	KC1	C3A-C2A-CAA-CBA
9	17	305	KC1	C3A-C2A-CAA-CBA
9	17	306	KC1	C1A-C2A-CAA-CBA
9	18	306	KC1	C1A-C2A-CAA-CBA
9	20	306	KC1	C1A-C2A-CAA-CBA
9	20	306	KC1	C3A-C2A-CAA-CBA
10	15	313	A86	C26-C27-C29-C30
10	16	311	A86	C26-C27-C29-C30
15	21	201	LHG	C15-C16-C17-C18
15	19	314	LHG	O7-C5-C6-O8
15	21	201	LHG	O7-C5-C6-O8
9	17	305	KC1	CAA-CBA-CGA-O2A
14	16	314	SQD	O6-C44-C45-C46
8	14	302	CLA	C4-C3-C5-C6
15	17	317	LHG	C10-C11-C12-C13
8	13	304	CLA	CAD-CBD-CGD-O2D
8	14	302	CLA	CAD-CBD-CGD-O2D
8	15	303	CLA	CAD-CBD-CGD-O2D
8	18	310	CLA	CAD-CBD-CGD-O2D
8	19	303	CLA	CAD-CBD-CGD-O2D
8	14	308	CLA	C13-C15-C16-C17
8	14	307	CLA	CBD-CGD-O2D-CED
8	15	305	CLA	C2A-CAA-CBA-CGA
14	16	314	SQD	C11-C12-C13-C14
8	11	305	CLA	CHA-CBD-CGD-O1D
8	11	305	CLA	CHA-CBD-CGD-O2D
8	11	307	CLA	CHA-CBD-CGD-O2D
8	12	304	CLA	CAD-CBD-CGD-O1D
8	13	304	CLA	CAD-CBD-CGD-O1D
8	14	302	CLA	CAD-CBD-CGD-O1D
8	14	307	CLA	CHA-CBD-CGD-O1D
8	14	307	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
8	15	303	CLA	CAD-CBD-CGD-O1D
8	15	307	CLA	CAD-CBD-CGD-O1D
8	17	307	CLA	CHA-CBD-CGD-O1D
8	17	307	CLA	CHA-CBD-CGD-O2D
8	18	305	CLA	CAD-CBD-CGD-O1D
8	18	307	CLA	CHA-CBD-CGD-O1D
8	18	307	CLA	CHA-CBD-CGD-O2D
8	18	310	CLA	CAD-CBD-CGD-O1D
8	19	303	CLA	CAD-CBD-CGD-O1D
9	12	310	KC1	CHA-CBD-CGD-O1D
9	15	309	KC1	CHA-CBD-CGD-O1D
9	17	306	KC1	CHA-CBD-CGD-O1D
9	18	309	KC1	CHA-CBD-CGD-O1D
9	18	309	KC1	CHA-CBD-CGD-O2D
9	20	306	KC1	CHA-CBD-CGD-O1D
9	20	306	KC1	CHA-CBD-CGD-O2D
9	21	207	KC1	CHA-CBD-CGD-O1D
9	21	207	KC1	CHA-CBD-CGD-O2D
10	11	313	A86	C10-C11-C13-C14
10	11	318	A86	C1-C2-C3-C4
10	14	312	A86	C11-C10-C9-C8
10	14	314	A86	C10-C11-C13-C14
10	15	314	A86	C10-C11-C13-C14
10	17	311	A86	C10-C11-C13-C14
10	20	313	A86	C10-C11-C13-C14
10	21	213	A86	C11-C10-C9-C8
13	21	216	DD6	C11-C10-C9-C8
15	17	317	LHG	C3-O3-P-O6
15	19	314	LHG	C3-O3-P-O5
15	21	201	LHG	C4-O6-P-O3
8	12	305	CLA	C4-C3-C5-C6
8	16	303	CLA	O1D-CGD-O2D-CED
8	11	303	CLA	C2B-C3B-CAB-CBB
8	11	305	CLA	C2B-C3B-CAB-CBB
8	11	307	CLA	C2B-C3B-CAB-CBB
8	12	303	CLA	C2B-C3B-CAB-CBB
8	12	307	CLA	C2B-C3B-CAB-CBB
8	13	304	CLA	C2B-C3B-CAB-CBB
8	15	305	CLA	C2B-C3B-CAB-CBB
8	18	307	CLA	C2B-C3B-CAB-CBB
8	18	310	CLA	C2B-C3B-CAB-CBB
8	19	303	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
8	19	304	CLA	C2B-C3B-CAB-CBB
8	20	308	CLA	C2B-C3B-CAB-CBB
8	20	310	CLA	C2B-C3B-CAB-CBB
8	21	210	CLA	C2B-C3B-CAB-CBB
8	13	308	CLA	C2-C3-C5-C6
10	12	302	A86	C-C1-C24-C25
10	14	312	A86	C7-C6-C8-C9
15	21	201	LHG	C5-C4-O6-P
15	19	314	LHG	C19-C20-C21-C22
10	11	313	A86	C12-C11-C13-C14
10	12	314	A86	C12-C11-C13-C14
10	14	314	A86	C12-C11-C13-C14
10	15	316	A86	C12-C11-C13-C14
10	17	311	A86	C12-C11-C13-C14
10	17	316	A86	C12-C11-C13-C14
10	20	313	A86	C12-C11-C13-C14
8	18	305	CLA	C2A-CAA-CBA-CGA
14	16	314	SQD	C10-C11-C12-C13
8	16	301	CLA	C15-C16-C17-C18
8	16	307	CLA	C12-C13-C15-C16
13	21	212	DD6	C1-C24-C25-C26
8	18	308	CLA	C2-C3-C5-C6
11	11	315	LMG	C12-C13-C14-C15
10	12	302	A86	C3-C4-C5-C6
8	15	301	CLA	C13-C15-C16-C17
11	16	315	LMG	C13-C14-C15-C16
8	15	308	CLA	C14-C13-C15-C16
8	19	302	CLA	O1D-CGD-O2D-CED
15	19	314	LHG	C34-C35-C36-C37
8	21	208	CLA	C12-C13-C15-C16
8	14	308	CLA	C5-C6-C7-C8
8	14	302	CLA	O1D-CGD-O2D-CED
8	19	303	CLA	O1A-CGA-O2A-C1
15	17	317	LHG	O7-C5-C6-O8
15	19	314	LHG	C11-C10-C9-C8
8	17	302	CLA	CAA-CBA-CGA-O2A
15	21	217	LHG	C25-C26-C27-C28
8	13	304	CLA	C2-C3-C5-C6
8	12	301	CLA	C8-C10-C11-C12
8	13	302	CLA	CAA-CBA-CGA-O2A
8	17	307	CLA	C2A-CAA-CBA-CGA
8	19	301	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
10	12	316	A86	C3-C4-C5-C6
8	13	302	CLA	CBD-CGD-O2D-CED
8	13	302	CLA	C4-C3-C5-C6
10	11	313	A86	C13-C14-C15-C16
10	12	312	A86	C13-C14-C15-C16
10	13	314	A86	C13-C14-C15-C16
10	14	314	A86	C13-C14-C15-C16
10	18	311	A86	C13-C14-C15-C16
10	18	312	A86	C13-C14-C15-C16
11	11	315	LMG	C29-C28-O8-C9
15	17	317	LHG	C2-C3-O3-P
8	12	309	CLA	C4B-C3B-CAB-CBB
8	15	310	CLA	C4B-C3B-CAB-CBB
8	18	301	CLA	C4B-C3B-CAB-CBB
8	20	308	CLA	C4B-C3B-CAB-CBB
8	20	310	CLA	C4B-C3B-CAB-CBB
15	21	217	LHG	C10-C11-C12-C13
8	15	303	CLA	CBA-CGA-O2A-C1
9	11	308	KC1	C4B-C3B-CAB-CBB
9	13	307	KC1	C4B-C3B-CAB-CBB
9	13	310	KC1	C4B-C3B-CAB-CBB
9	14	304	KC1	C4B-C3B-CAB-CBB
9	15	302	KC1	C4B-C3B-CAB-CBB
9	15	304	KC1	C4B-C3B-CAB-CBB
9	15	309	KC1	C4B-C3B-CAB-CBB
9	16	304	KC1	C4B-C3B-CAB-CBB
9	17	305	KC1	C4B-C3B-CAB-CBB
9	18	304	KC1	C4B-C3B-CAB-CBB
9	20	305	KC1	C4B-C3B-CAB-CBB
9	20	306	KC1	C4B-C3B-CAB-CBB
8	12	301	CLA	C11-C10-C8-C7
8	14	302	CLA	C6-C7-C8-C10
9	20	305	KC1	CAA-CBA-CGA-O1A
15	19	314	LHG	C17-C18-C19-C20
8	15	307	CLA	O1D-CGD-O2D-CED
8	19	303	CLA	CBA-CGA-O2A-C1
8	19	302	CLA	O1A-CGA-O2A-C1
8	12	303	CLA	C4-C3-C5-C6
8	12	304	CLA	C3A-C2A-CAA-CBA
11	16	315	LMG	C29-C30-C31-C32
8	14	302	CLA	C2-C3-C5-C6
8	18	301	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
8	12	301	CLA	C13-C15-C16-C17
10	20	301	A86	C25-C26-C27-C28
13	21	212	DD6	C4-C5-C6-C7
8	11	303	CLA	C10-C11-C12-C13
9	17	306	KC1	C2C-C3C-CAC-CBC
14	17	301	SQD	C11-C10-C9-C8
8	16	301	CLA	C2-C1-O2A-CGA
10	12	315	A86	C3-C4-C5-C6
10	17	315	A86	C24-C25-C26-C27
10	20	311	A86	C24-C25-C26-C27
8	11	309	CLA	C4-C3-C5-C6
10	17	316	A86	C2-C1-C24-C25
8	14	301	CLA	C2-C3-C5-C6
8	12	303	CLA	C2A-CAA-CBA-CGA
10	12	314	A86	C12-C11-C13-O
10	14	316	A86	C12-C11-C13-O
10	18	314	A86	C12-C11-C13-O
8	11	301	CLA	C6-C7-C8-C9
8	12	301	CLA	C11-C12-C13-C14
8	12	305	CLA	C6-C7-C8-C9
8	13	309	CLA	C6-C7-C8-C9
8	17	302	CLA	C11-C12-C13-C14
11	11	315	LMG	C31-C32-C33-C34
11	11	315	LMG	C14-C15-C16-C17
15	17	317	LHG	C26-C27-C28-C29
8	21	205	CLA	CAA-CBA-CGA-O1A
9	20	305	KC1	CAA-CBA-CGA-O2A
8	12	301	CLA	C1A-C2A-CAA-CBA
8	13	302	CLA	C1A-C2A-CAA-CBA
8	17	302	CLA	C1A-C2A-CAA-CBA
8	19	304	CLA	C1A-C2A-CAA-CBA
10	12	314	A86	C10-C11-C13-O
10	18	314	A86	C10-C11-C13-O
10	20	301	A86	C25-C26-C27-C29
8	16	301	CLA	C16-C17-C18-C19
14	16	314	SQD	C26-C27-C28-C29
8	11	309	CLA	C2B-C3B-CAB-CBB
8	12	305	CLA	C2B-C3B-CAB-CBB
8	12	309	CLA	C2B-C3B-CAB-CBB
8	13	301	CLA	C2B-C3B-CAB-CBB
8	13	306	CLA	C2B-C3B-CAB-CBB
8	13	308	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
8	13	311	CLA	C2B-C3B-CAB-CBB
8	14	305	CLA	C2B-C3B-CAB-CBB
8	14	310	CLA	C2B-C3B-CAB-CBB
8	15	307	CLA	C2B-C3B-CAB-CBB
8	15	308	CLA	C2B-C3B-CAB-CBB
8	15	310	CLA	C2B-C3B-CAB-CBB
8	16	303	CLA	C2B-C3B-CAB-CBB
8	18	301	CLA	C2B-C3B-CAB-CBB
8	18	302	CLA	C2B-C3B-CAB-CBB
8	18	305	CLA	C2B-C3B-CAB-CBB
8	19	302	CLA	C2B-C3B-CAB-CBB
8	19	309	CLA	C2B-C3B-CAB-CBB
8	20	307	CLA	C2B-C3B-CAB-CBB
8	21	202	CLA	C2B-C3B-CAB-CBB
8	21	208	CLA	C2B-C3B-CAB-CBB
8	17	310	CLA	CAA-CBA-CGA-O2A
8	19	302	CLA	CBA-CGA-O2A-C1
8	20	310	CLA	CAA-CBA-CGA-O2A
8	13	302	CLA	C2-C3-C5-C6
8	12	305	CLA	C6-C7-C8-C10
10	13	316	A86	C-C1-C24-C25
8	20	308	CLA	CAA-CBA-CGA-O2A
8	11	303	CLA	C4-C3-C5-C6
8	11	301	CLA	C5-C6-C7-C8
10	21	215	A86	C33-C34-O4-C38
8	14	307	CLA	CBA-CGA-O2A-C1
8	12	303	CLA	C2-C3-C5-C6
8	12	305	CLA	C2-C3-C5-C6
8	13	304	CLA	O1A-CGA-O2A-C1
8	20	308	CLA	CAA-CBA-CGA-O1A
8	20	310	CLA	CAA-CBA-CGA-O1A
8	21	205	CLA	CAA-CBA-CGA-O2A
8	20	302	CLA	O1D-CGD-O2D-CED
14	17	301	SQD	C44-C45-C46-O48
8	21	205	CLA	C2A-CAA-CBA-CGA
8	15	303	CLA	C5-C6-C7-C8
15	21	201	LHG	O6-C4-C5-O7
8	14	303	CLA	CAA-CBA-CGA-O2A
11	17	318	LMG	C11-C12-C13-C14
8	13	301	CLA	C4B-C3B-CAB-CBB
8	16	303	CLA	C4B-C3B-CAB-CBB
8	19	304	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
8	18	305	CLA	CAA-CBA-CGA-O2A
15	21	217	LHG	C12-C13-C14-C15
11	17	318	LMG	O7-C8-C9-O8
11	11	316	LMG	C31-C32-C33-C34
15	17	317	LHG	C19-C20-C21-C22
8	21	209	CLA	CAA-CBA-CGA-O2A
10	13	314	A86	C3-C4-C5-C6
8	21	210	CLA	CAA-CBA-CGA-O2A
8	14	302	CLA	C11-C12-C13-C14
8	17	304	CLA	C6-C7-C8-C9
14	17	301	SQD	C34-C35-C36-C37
8	13	306	CLA	CAA-CBA-CGA-O2A
8	16	309	CLA	CAA-CBA-CGA-O2A
8	14	307	CLA	C2A-CAA-CBA-CGA
8	14	308	CLA	C2-C1-O2A-CGA
8	18	308	CLA	C2-C1-O2A-CGA
15	21	201	LHG	C27-C28-C29-C30
8	13	302	CLA	C3A-C2A-CAA-CBA
8	18	305	CLA	CAA-CBA-CGA-O1A
8	19	304	CLA	CAA-CBA-CGA-O1A
9	12	306	KC1	C2B-C3B-CAB-CBB
9	17	303	KC1	C2B-C3B-CAB-CBB
8	15	305	CLA	CAA-CBA-CGA-O2A
8	12	309	CLA	CBA-CGA-O2A-C1
10	21	215	A86	C35-C34-O4-C38
8	18	303	CLA	C4-C3-C5-C6
8	15	305	CLA	CAA-CBA-CGA-O1A
8	21	209	CLA	CAA-CBA-CGA-O1A
13	19	312	DD6	C13-C14-C15-O1
8	13	306	CLA	CAA-CBA-CGA-O1A
14	16	314	SQD	C44-C45-C46-O48
9	17	303	KC1	C4B-C3B-CAB-CBB
9	17	306	KC1	C4B-C3B-CAB-CBB
14	16	314	SQD	C30-C31-C32-C33
8	16	309	CLA	CAA-CBA-CGA-O1A
10	14	315	A86	C3-C4-C5-C6
10	17	314	A86	C3-C4-C5-C6
10	11	311	A86	C28-C27-C29-C30
10	11	312	A86	C28-C27-C29-C30
10	14	313	A86	C28-C27-C29-C30
8	12	309	CLA	O1A-CGA-O2A-C1
8	14	308	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
8	18	303	CLA	C6-C7-C8-C9
8	21	208	CLA	C14-C13-C15-C16
8	14	307	CLA	CAA-CBA-CGA-O2A
8	15	307	CLA	CAA-CBA-CGA-O2A
8	18	307	CLA	CAA-CBA-CGA-O2A
8	21	210	CLA	CAA-CBA-CGA-O1A
10	20	301	A86	C13-C14-C15-O1
10	20	313	A86	C13-C14-C15-O1
9	17	306	KC1	C4C-C3C-CAC-CBC
8	14	302	CLA	C11-C12-C13-C15
8	16	307	CLA	C11-C10-C8-C7
8	17	302	CLA	C6-C7-C8-C10
8	17	304	CLA	C6-C7-C8-C10
8	17	307	CLA	C2B-C3B-CAB-CBB
8	20	304	CLA	C2B-C3B-CAB-CBB
8	12	303	CLA	C2-C1-O2A-CGA
8	15	308	CLA	C2-C1-O2A-CGA
8	17	310	CLA	C2-C1-O2A-CGA
13	19	312	DD6	C24-C25-C26-C27
10	18	314	A86	C33-C34-O4-C38
8	17	307	CLA	CAA-CBA-CGA-O2A
8	21	206	CLA	CAA-CBA-CGA-O2A
8	16	307	CLA	C8-C10-C11-C12
8	16	301	CLA	C4-C3-C5-C6
8	12	311	CLA	CAA-CBA-CGA-O2A
8	14	307	CLA	O1A-CGA-O2A-C1
8	12	309	CLA	CAA-CBA-CGA-O2A
11	11	315	LMG	C19-C20-C21-C22
11	16	315	LMG	C14-C15-C16-C17
8	21	202	CLA	CAA-CBA-CGA-O2A
8	14	310	CLA	CBD-CGD-O2D-CED
8	13	304	CLA	CBA-CGA-O2A-C1
8	14	308	CLA	C11-C10-C8-C9
8	18	301	CLA	CAA-CBA-CGA-O2A
8	20	302	CLA	CAA-CBA-CGA-O2A
8	17	302	CLA	C4C-C3C-CAC-CBC
8	11	309	CLA	C4B-C3B-CAB-CBB
8	12	309	CLA	C1A-C2A-CAA-CBA
8	12	311	CLA	C4B-C3B-CAB-CBB
8	13	309	CLA	C4B-C3B-CAB-CBB
8	13	311	CLA	C4B-C3B-CAB-CBB
8	14	302	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
8	14	307	CLA	C1A-C2A-CAA-CBA
8	14	308	CLA	C4B-C3B-CAB-CBB
8	16	307	CLA	C4B-C3B-CAB-CBB
8	17	307	CLA	C1A-C2A-CAA-CBA
8	17	308	CLA	C4B-C3B-CAB-CBB
8	18	303	CLA	C4B-C3B-CAB-CBB
8	18	308	CLA	C4B-C3B-CAB-CBB
8	19	302	CLA	C4B-C3B-CAB-CBB
8	19	306	CLA	C4B-C3B-CAB-CBB
8	20	308	CLA	C1A-C2A-CAA-CBA
10	12	302	A86	O-C13-C14-C15
10	12	315	A86	O-C13-C14-C15
10	13	315	A86	O-C13-C14-C15
10	13	316	A86	O-C13-C14-C15
10	16	313	A86	O-C13-C14-C15
10	18	313	A86	O-C13-C14-C15
10	19	313	A86	O-C13-C14-C15
10	17	315	A86	C39-C38-O4-C34
8	11	303	CLA	C2-C3-C5-C6
10	12	302	A86	C2-C1-C24-C25
10	14	312	A86	C5-C6-C8-C9
10	15	313	A86	C2-C1-C24-C25
13	21	212	DD6	C10-C11-C13-C14
10	15	312	A86	C11-C10-C9-C8
10	15	316	A86	C24-C25-C26-C27
10	17	316	A86	C24-C25-C26-C27
10	18	314	A86	C3-C4-C5-C6
10	20	313	A86	C1-C2-C3-C4
8	16	301	CLA	C16-C17-C18-C20
8	16	303	CLA	CAA-CBA-CGA-O2A
15	21	217	LHG	O7-C7-C8-C9
9	17	309	KC1	CAA-CBA-CGA-O1A
8	14	301	CLA	C13-C15-C16-C17
8	16	306	CLA	C10-C11-C12-C13
8	13	301	CLA	C2-C1-O2A-CGA
8	16	307	CLA	C2-C1-O2A-CGA
8	19	302	CLA	C12-C13-C15-C16
8	19	303	CLA	C12-C13-C15-C16
16	19	315	LMU	O1'-C1-C2-C3
9	17	309	KC1	CAA-CBA-CGA-O2A
8	13	308	CLA	CAA-CBA-CGA-O2A
14	17	301	SQD	O47-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
10	15	312	A86	C1-C2-C3-C4
8	17	304	CLA	O1A-CGA-O2A-C1
8	18	310	CLA	CAA-CBA-CGA-O2A
15	21	217	LHG	C28-C29-C30-C31
8	14	303	CLA	C3A-C2A-CAA-CBA
8	20	308	CLA	C3A-C2A-CAA-CBA
8	21	209	CLA	C3A-C2A-CAA-CBA
8	15	301	CLA	C8-C10-C11-C12
8	17	302	CLA	C15-C16-C17-C18
8	21	208	CLA	CAA-CBA-CGA-O2A
8	12	311	CLA	CAA-CBA-CGA-O1A
8	17	307	CLA	CAA-CBA-CGA-O1A
14	16	314	SQD	O47-C7-C8-C9
8	21	204	CLA	C3-C5-C6-C7
8	19	303	CLA	C14-C13-C15-C16
8	15	301	CLA	CAA-CBA-CGA-O2A
8	21	202	CLA	CAA-CBA-CGA-O1A
8	18	302	CLA	C5-C6-C7-C8
8	14	310	CLA	CAA-CBA-CGA-O2A
8	12	309	CLA	CAA-CBA-CGA-O1A
8	18	307	CLA	CAA-CBA-CGA-O1A
8	20	307	CLA	CAA-CBA-CGA-O2A
9	11	306	KC1	C1A-C2A-CAA-CBA
9	13	305	KC1	C1A-C2A-CAA-CBA
9	18	304	KC1	C1A-C2A-CAA-CBA
9	19	308	KC1	C3A-C2A-CAA-CBA
10	11	312	A86	C26-C27-C29-C30
10	13	314	A86	C26-C27-C29-C30
8	14	307	CLA	CAA-CBA-CGA-O1A
8	19	306	CLA	C8-C10-C11-C12
10	13	316	A86	C2-C1-C24-C25
8	15	307	CLA	CAA-CBA-CGA-O1A
8	20	302	CLA	CAA-CBA-CGA-O1A
15	21	217	LHG	O9-C7-C8-C9
15	17	317	LHG	O9-C7-C8-C9
10	12	316	A86	C12-C11-C13-O
10	19	313	A86	C12-C11-C13-O
8	18	301	CLA	CAA-CBA-CGA-O1A
8	21	206	CLA	CAA-CBA-CGA-O1A
8	19	309	CLA	CAA-CBA-CGA-O2A
9	12	310	KC1	CAD-CBD-CGD-O2D
9	14	306	KC1	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
9	15	306	KC1	CAD-CBD-CGD-O2D
9	16	308	KC1	CAD-CBD-CGD-O2D
8	13	301	CLA	C5-C6-C7-C8
15	17	317	LHG	O6-C4-C5-C6
8	12	301	CLA	C2-C1-O2A-CGA
8	16	301	CLA	C13-C15-C16-C17
8	12	305	CLA	CAA-CBA-CGA-O2A
8	13	304	CLA	CAA-CBA-CGA-O2A
8	16	307	CLA	CAA-CBA-CGA-O2A
8	20	304	CLA	CAA-CBA-CGA-O2A
8	20	307	CLA	CAA-CBA-CGA-O1A
8	11	303	CLA	CAA-CBA-CGA-O2A
8	17	304	CLA	CAA-CBA-CGA-O2A
8	18	303	CLA	CAA-CBA-CGA-O2A
8	14	302	CLA	O1A-CGA-O2A-C1

There are no ring outliers.

72 monomers are involved in 122 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	17	310	CLA	1	0
8	19	309	CLA	1	0
8	20	302	CLA	2	0
10	14	314	A86	1	0
8	13	309	CLA	4	0
8	12	309	CLA	1	0
8	12	301	CLA	3	0
8	17	307	CLA	1	0
8	13	308	CLA	1	0
15	19	314	LHG	2	0
8	15	308	CLA	5	0
10	13	312	A86	1	0
8	17	308	CLA	4	0
8	19	305	CLA	2	0
8	16	301	CLA	2	0
8	11	307	CLA	3	0
13	20	314	DD6	2	0
8	13	304	CLA	1	0
9	17	303	KC1	2	0
10	18	313	A86	1	0
8	11	303	CLA	1	0
8	12	305	CLA	2	0

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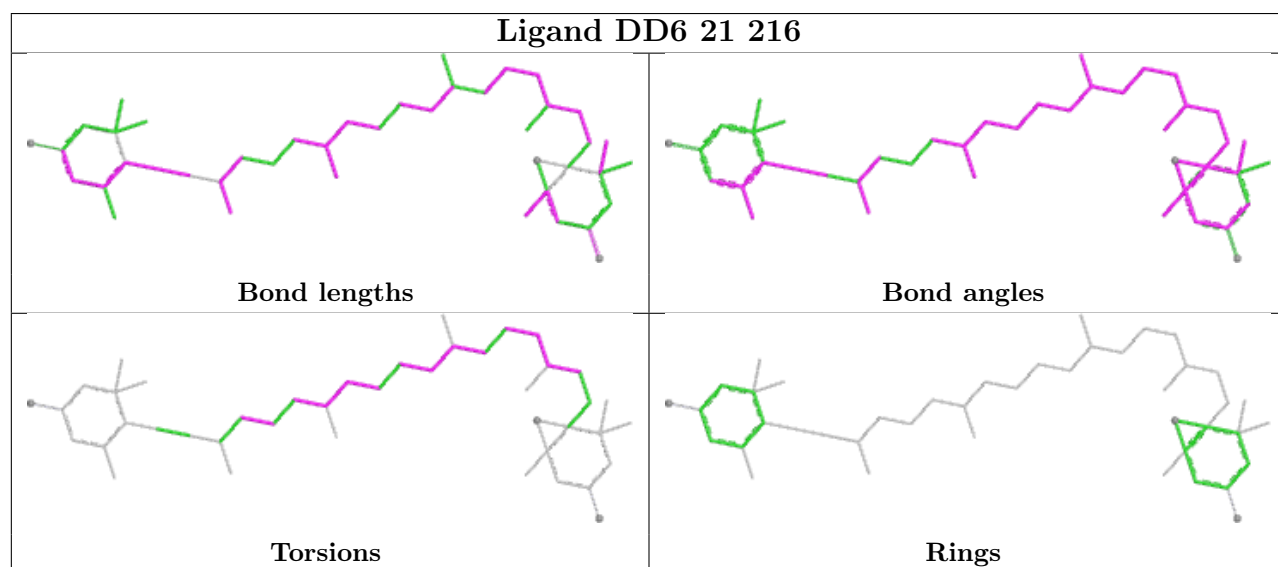
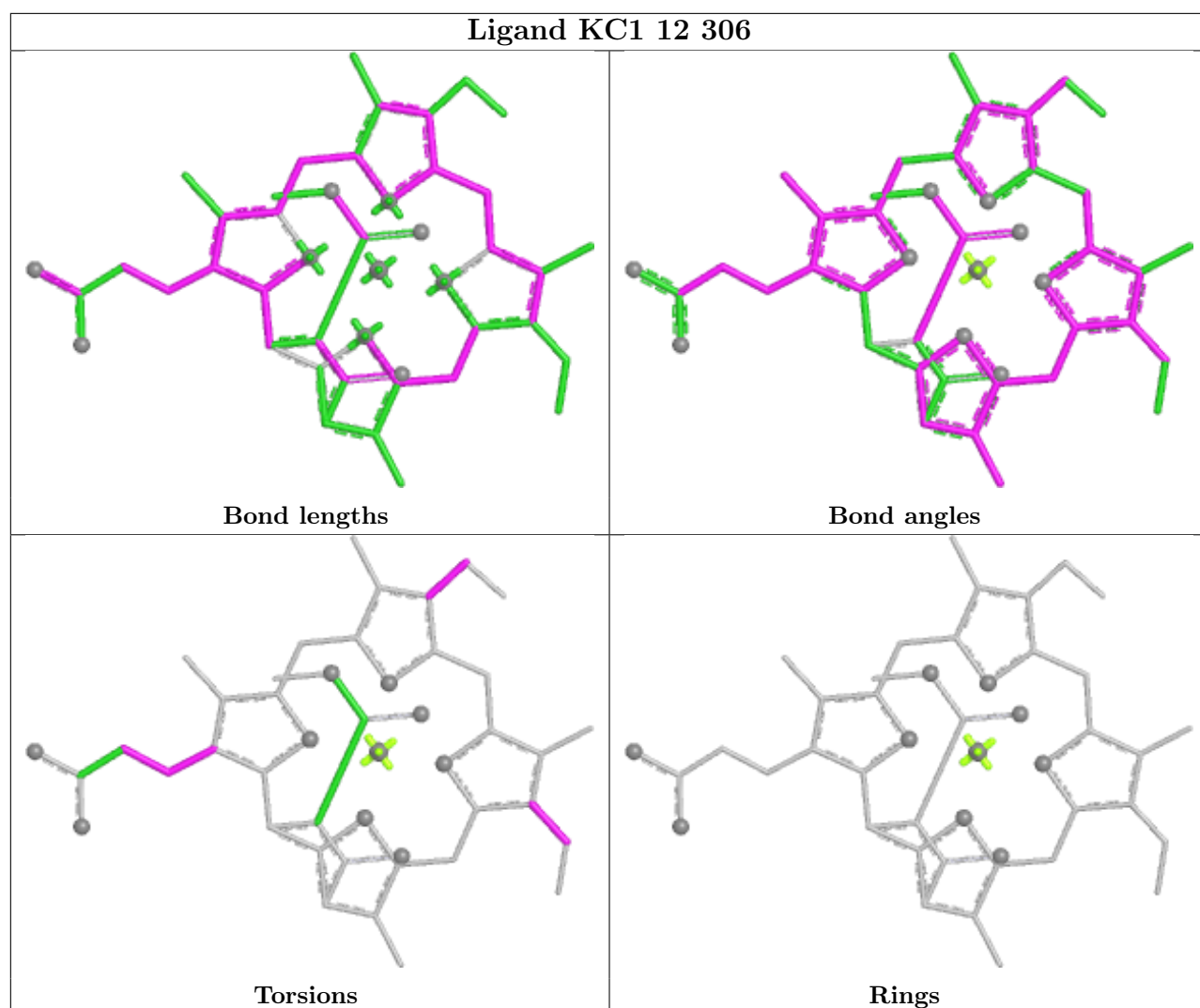
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	11	301	CLA	2	0
8	18	303	CLA	1	0
13	19	312	DD6	2	0
10	18	311	A86	1	0
8	19	310	CLA	1	0
8	19	304	CLA	1	0
10	11	318	A86	1	0
8	12	304	CLA	1	0
8	16	306	CLA	1	0
8	14	307	CLA	1	0
8	15	301	CLA	6	0
8	14	302	CLA	2	0
15	21	217	LHG	4	0
8	19	302	CLA	3	0
8	14	303	CLA	1	0
8	17	302	CLA	1	0
14	16	314	SQD	2	0
9	18	304	KC1	1	0
8	13	302	CLA	2	0
8	15	307	CLA	1	0
8	18	308	CLA	3	0
8	21	206	CLA	3	0
8	18	301	CLA	1	0
10	11	310	A86	1	0
8	19	301	CLA	2	0
8	21	202	CLA	2	0
8	18	307	CLA	2	0
16	19	315	LMU	1	0
8	15	310	CLA	1	0
8	20	307	CLA	1	0
8	15	303	CLA	1	0
8	18	310	CLA	1	0
8	19	307	CLA	1	0
8	12	311	CLA	1	0
8	18	302	CLA	4	0
8	16	307	CLA	3	0
10	15	311	A86	1	0
8	16	309	CLA	1	0
10	14	315	A86	1	0
8	14	301	CLA	2	0
8	21	208	CLA	1	0
8	19	306	CLA	1	0

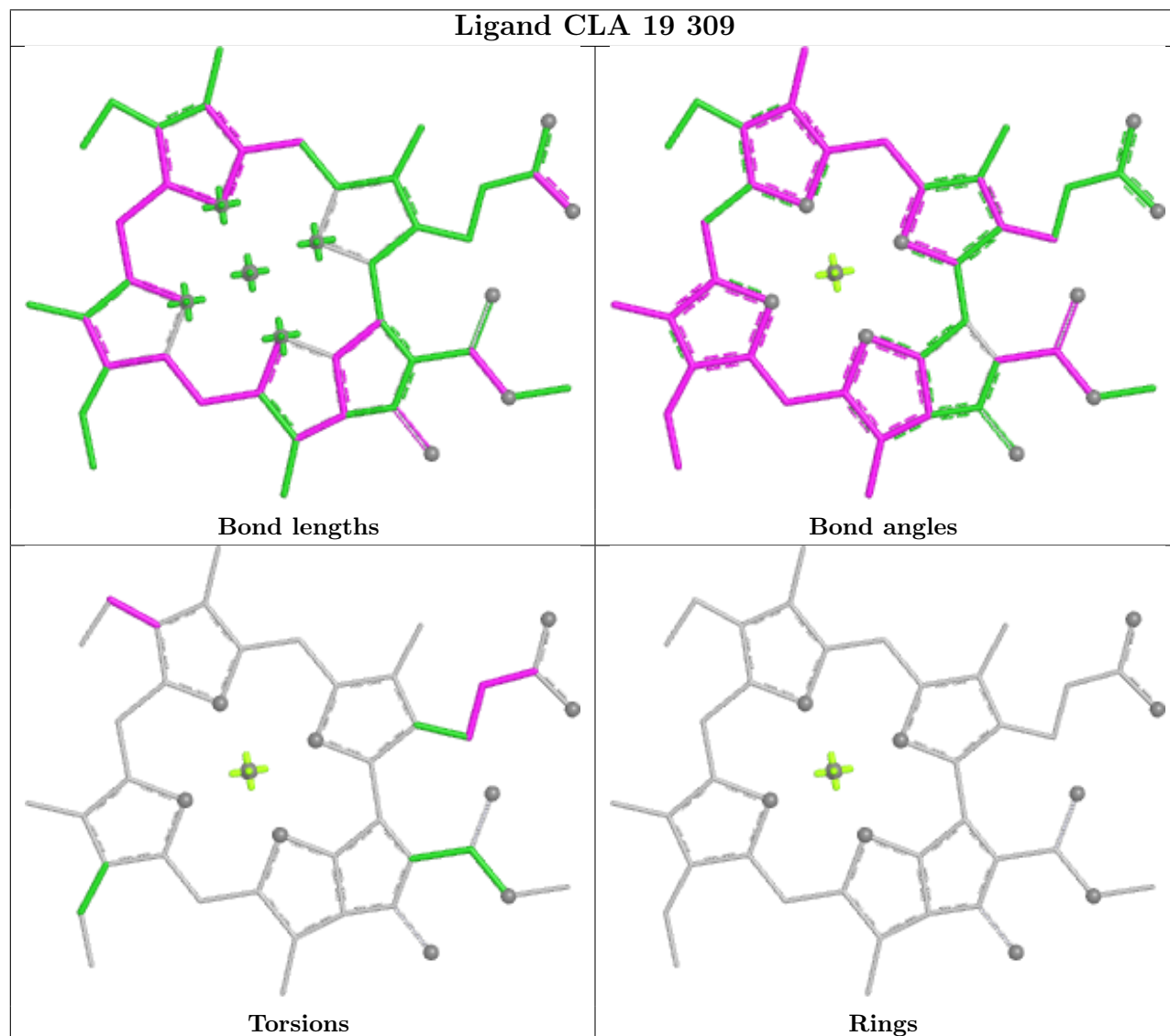
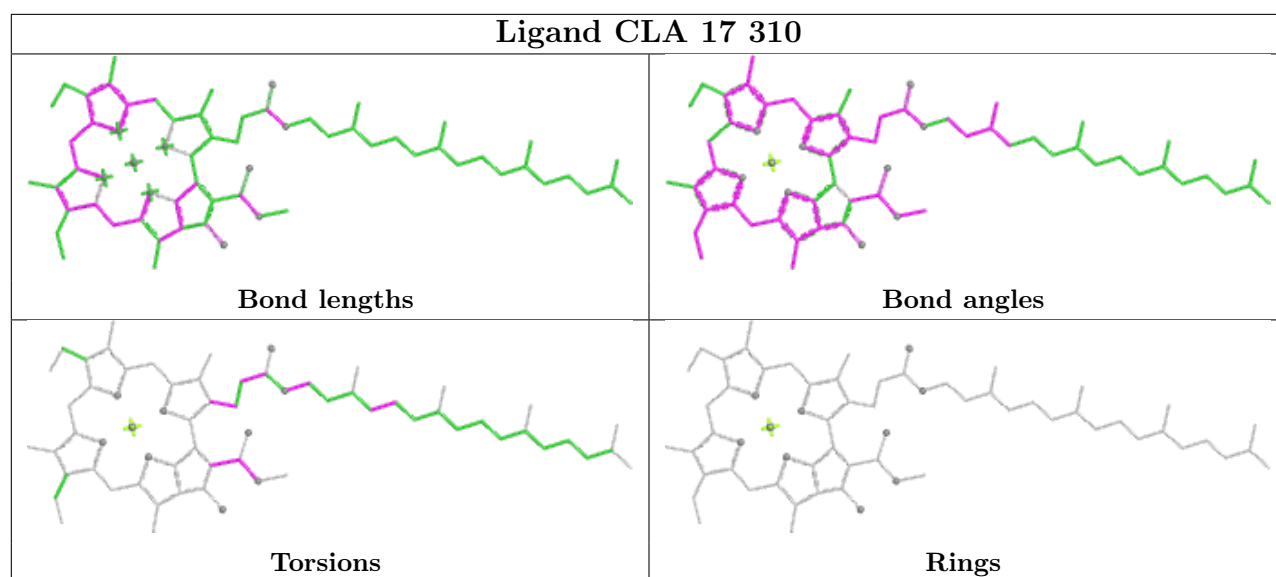
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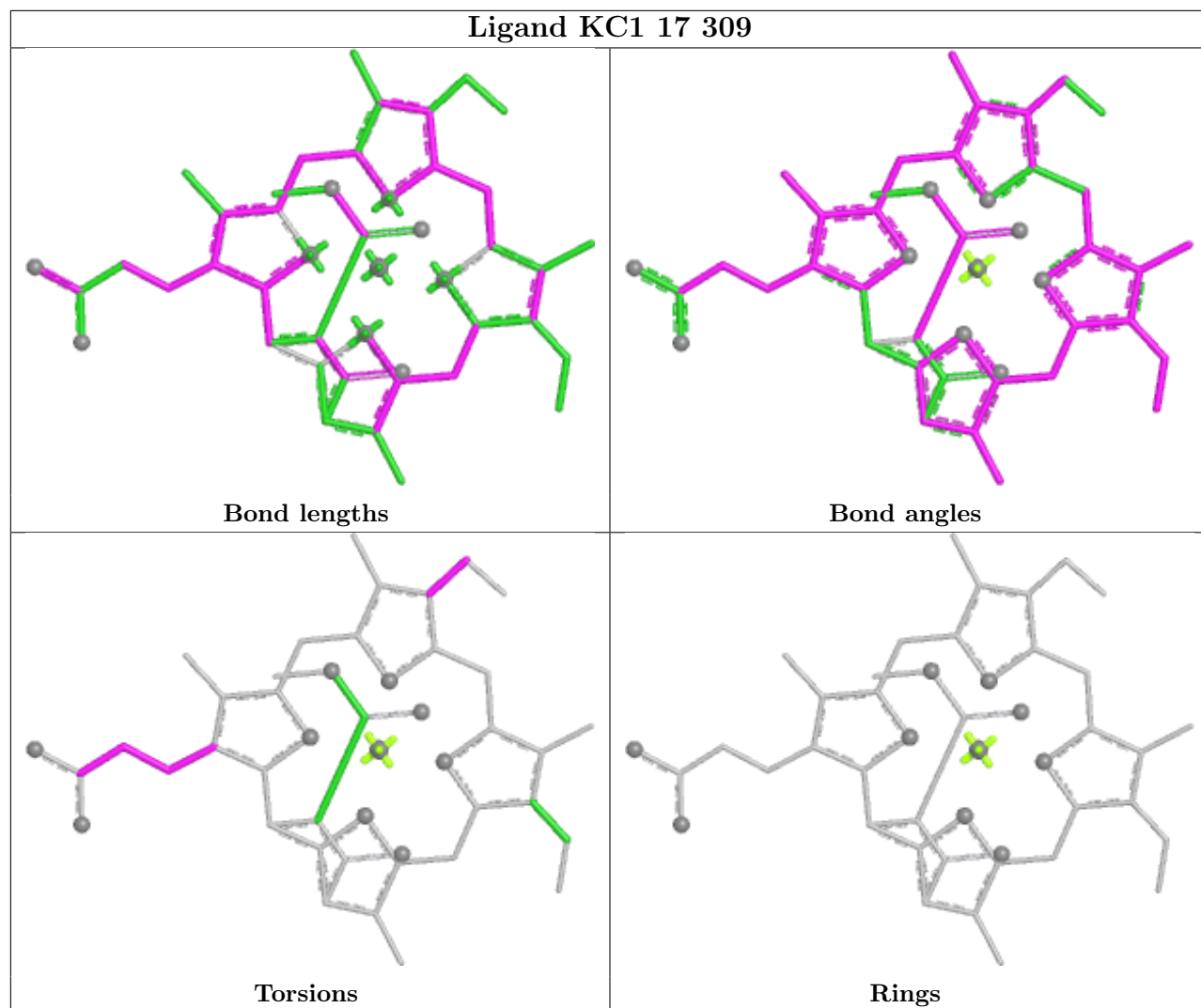
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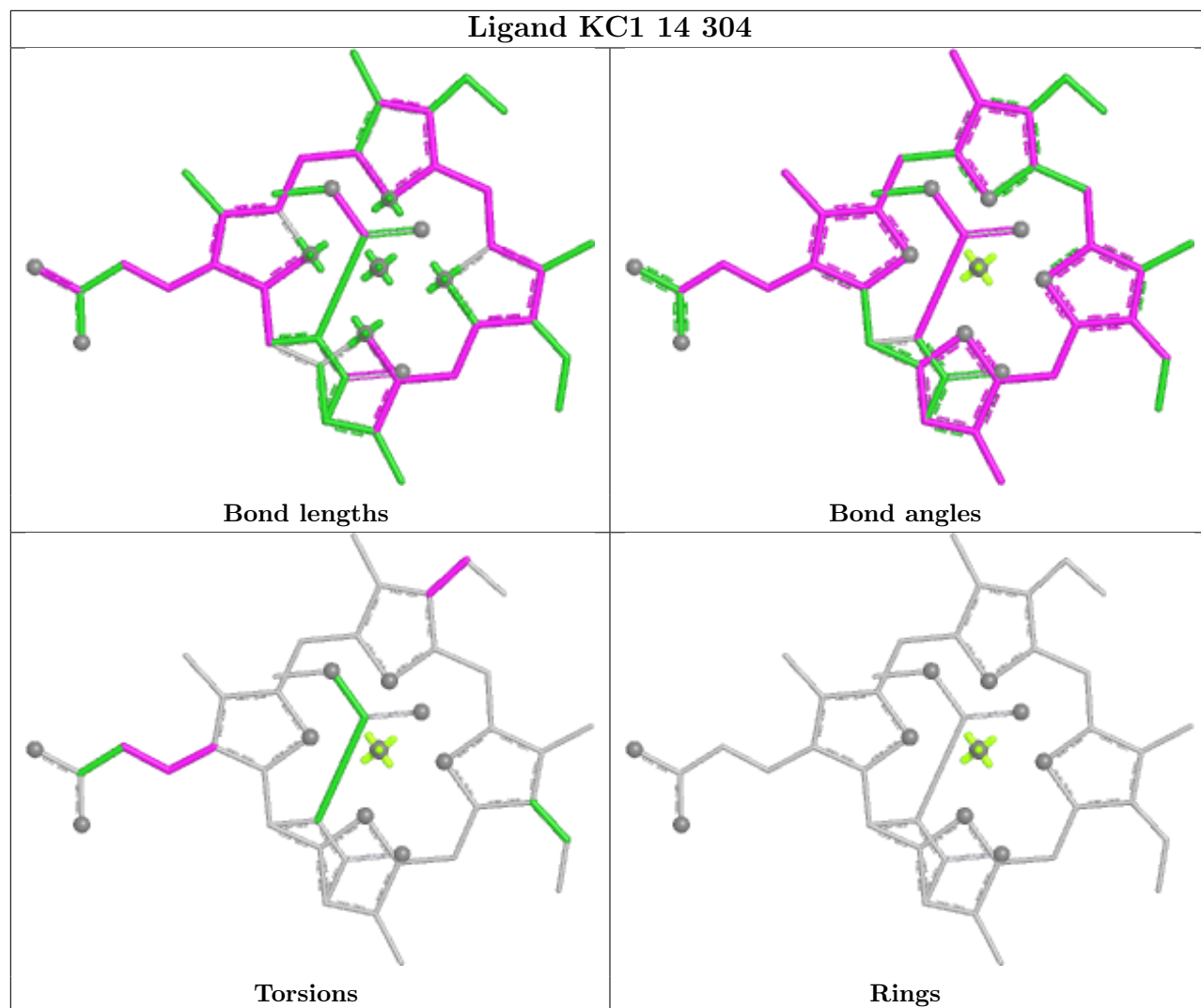
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	17	317	LHG	1	0
8	13	301	CLA	2	0
11	16	315	LMG	1	0
8	13	311	CLA	3	0
8	12	303	CLA	3	0
9	11	306	KC1	1	0
8	12	307	CLA	1	0
14	17	301	SQD	3	0

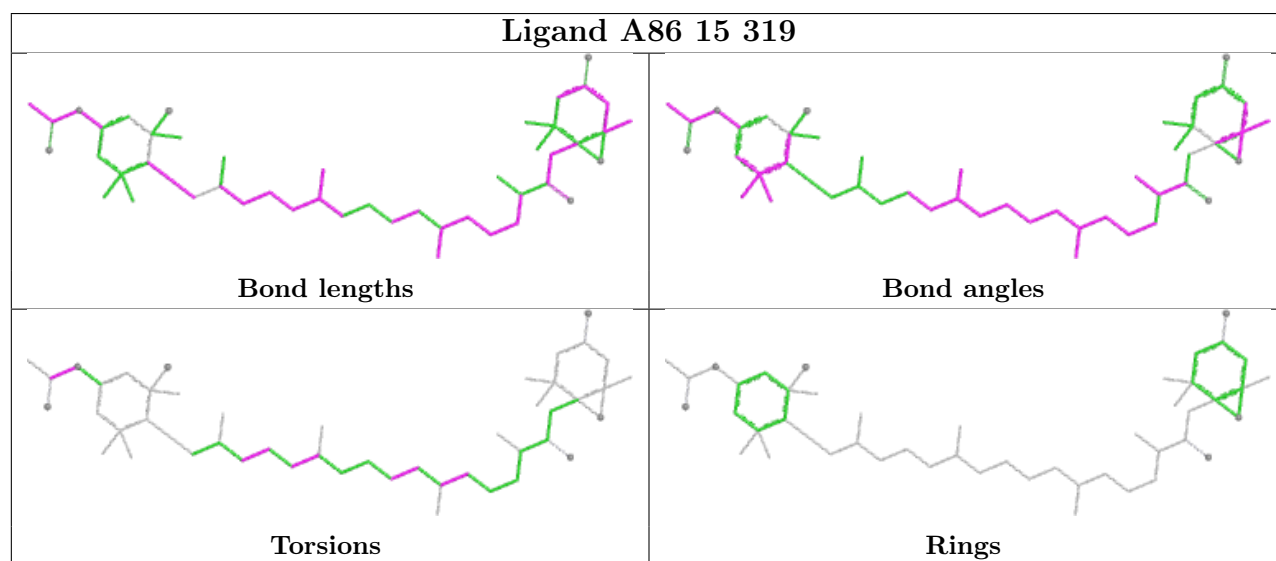
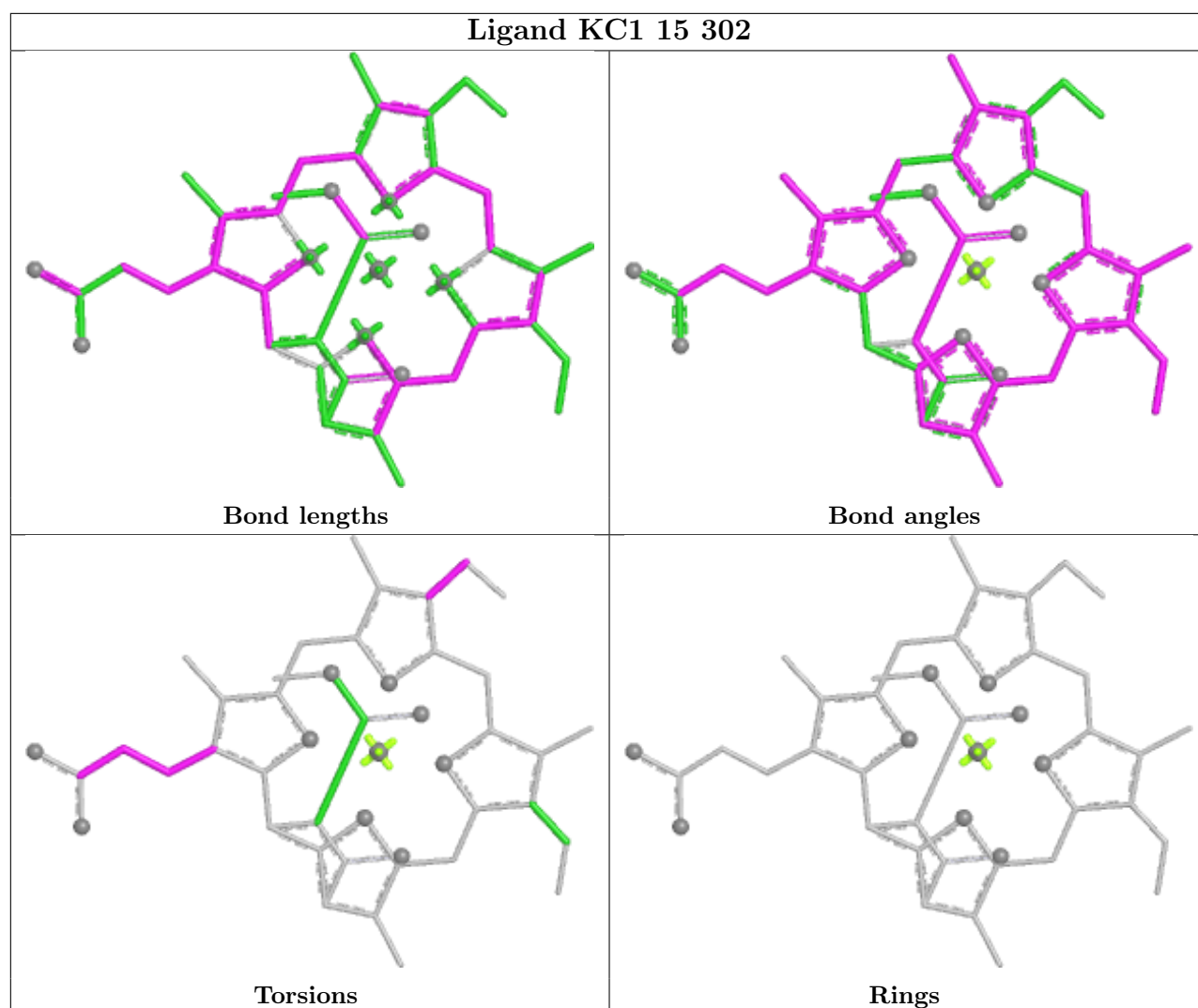
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

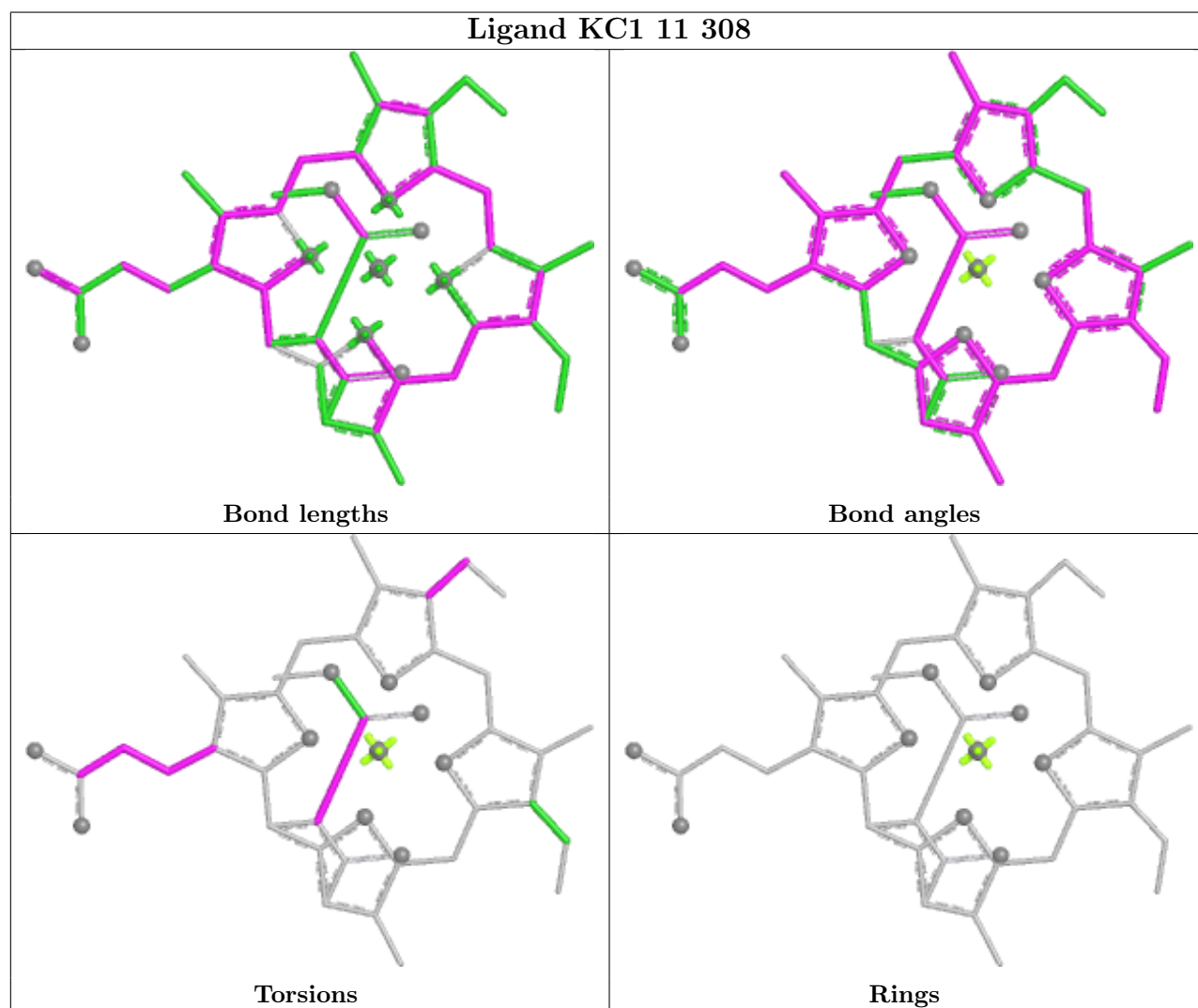
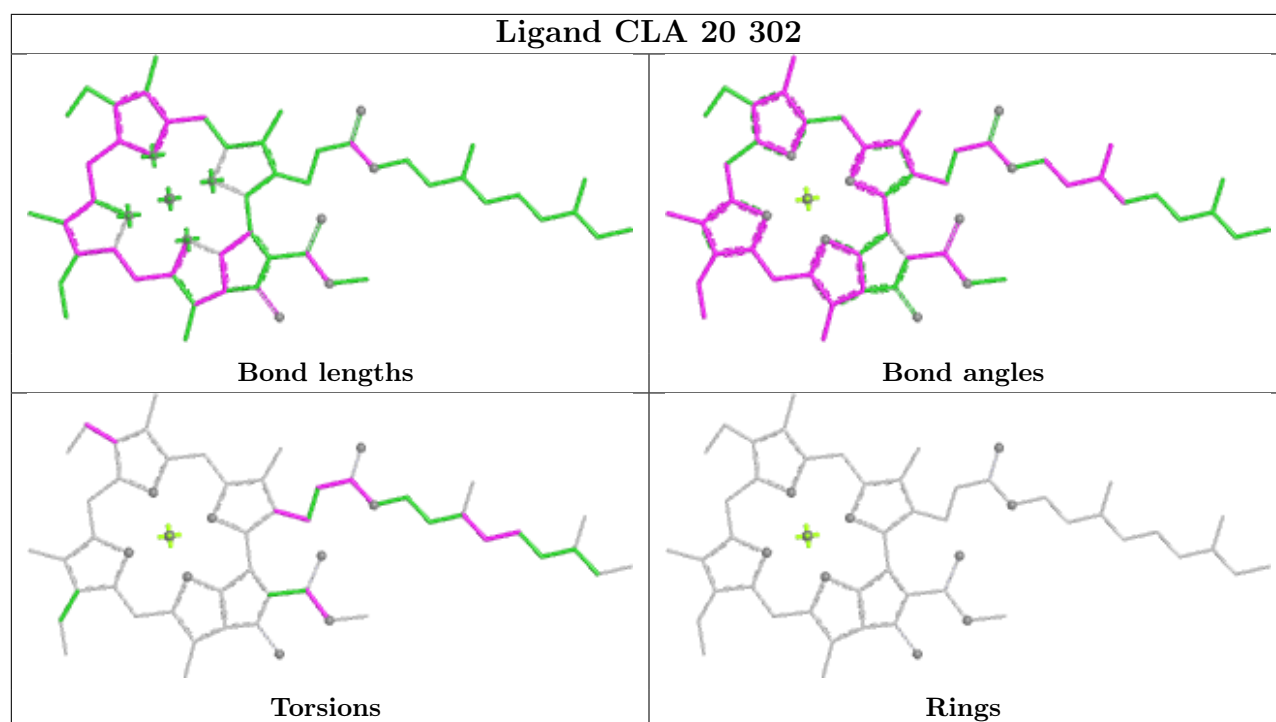


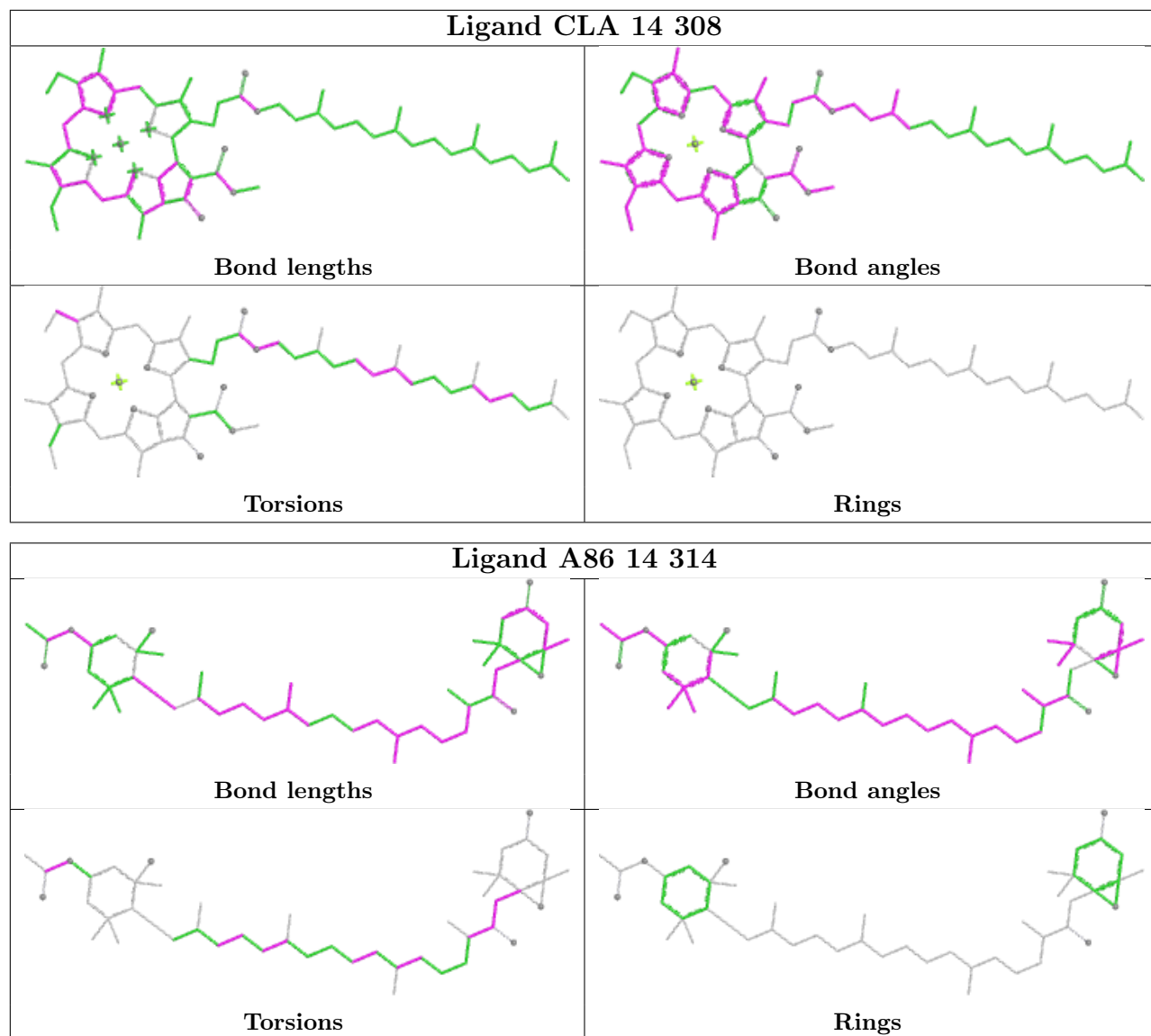


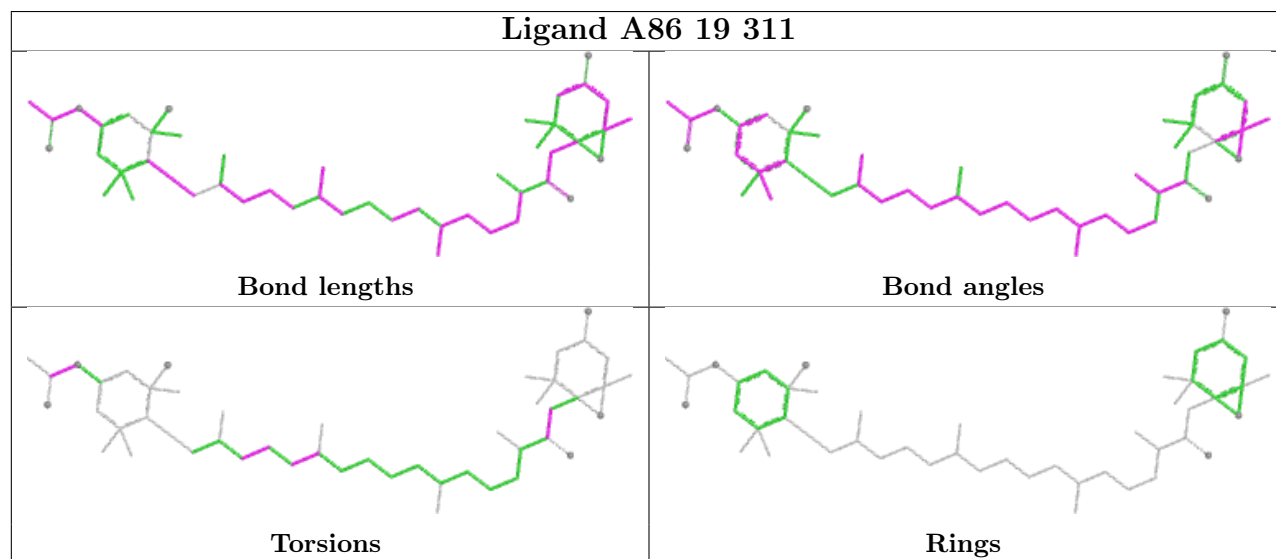
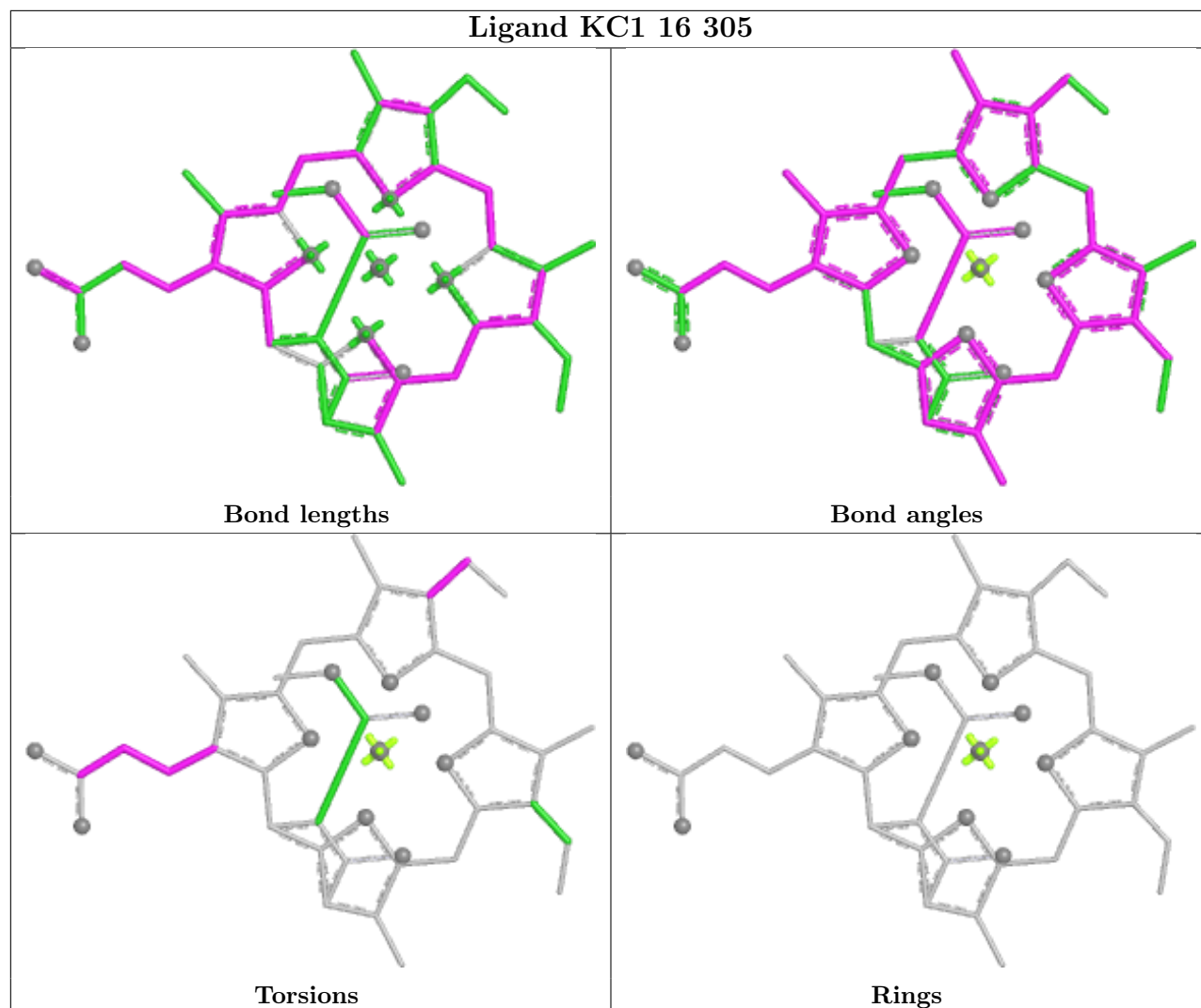


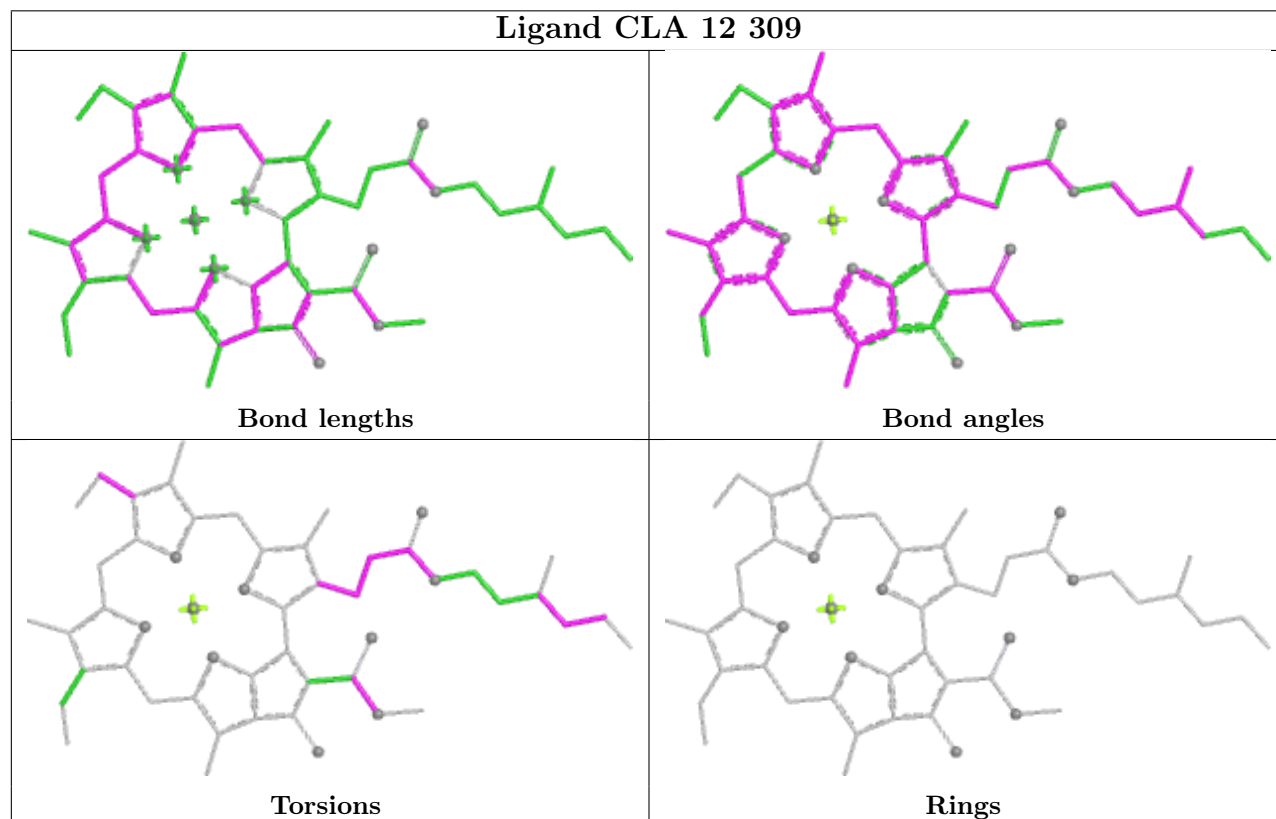
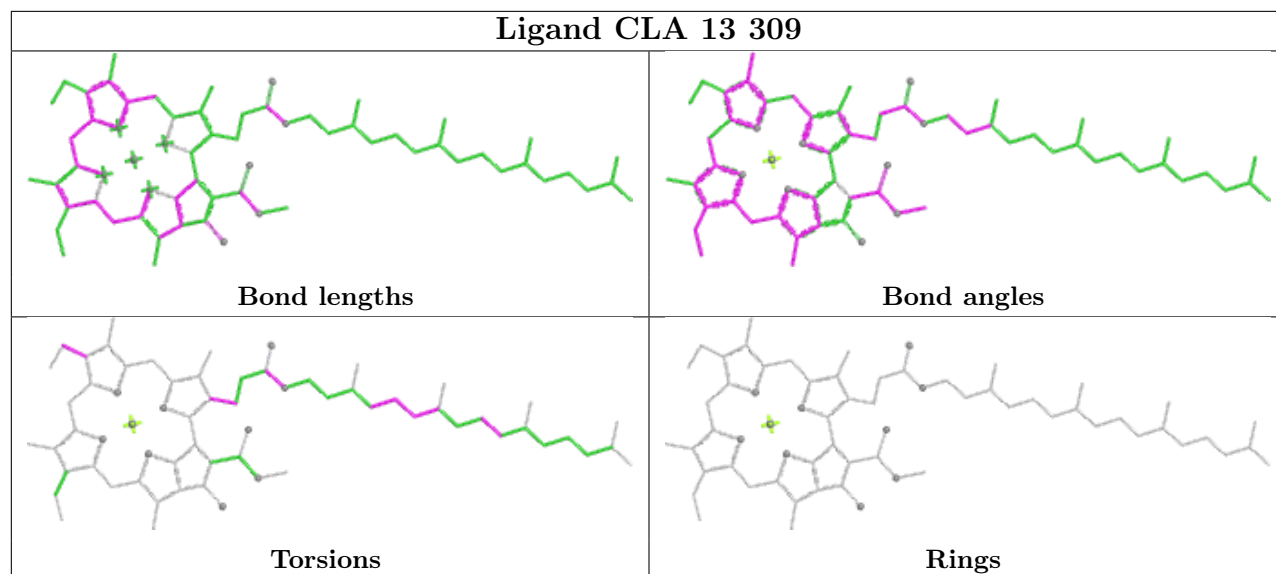


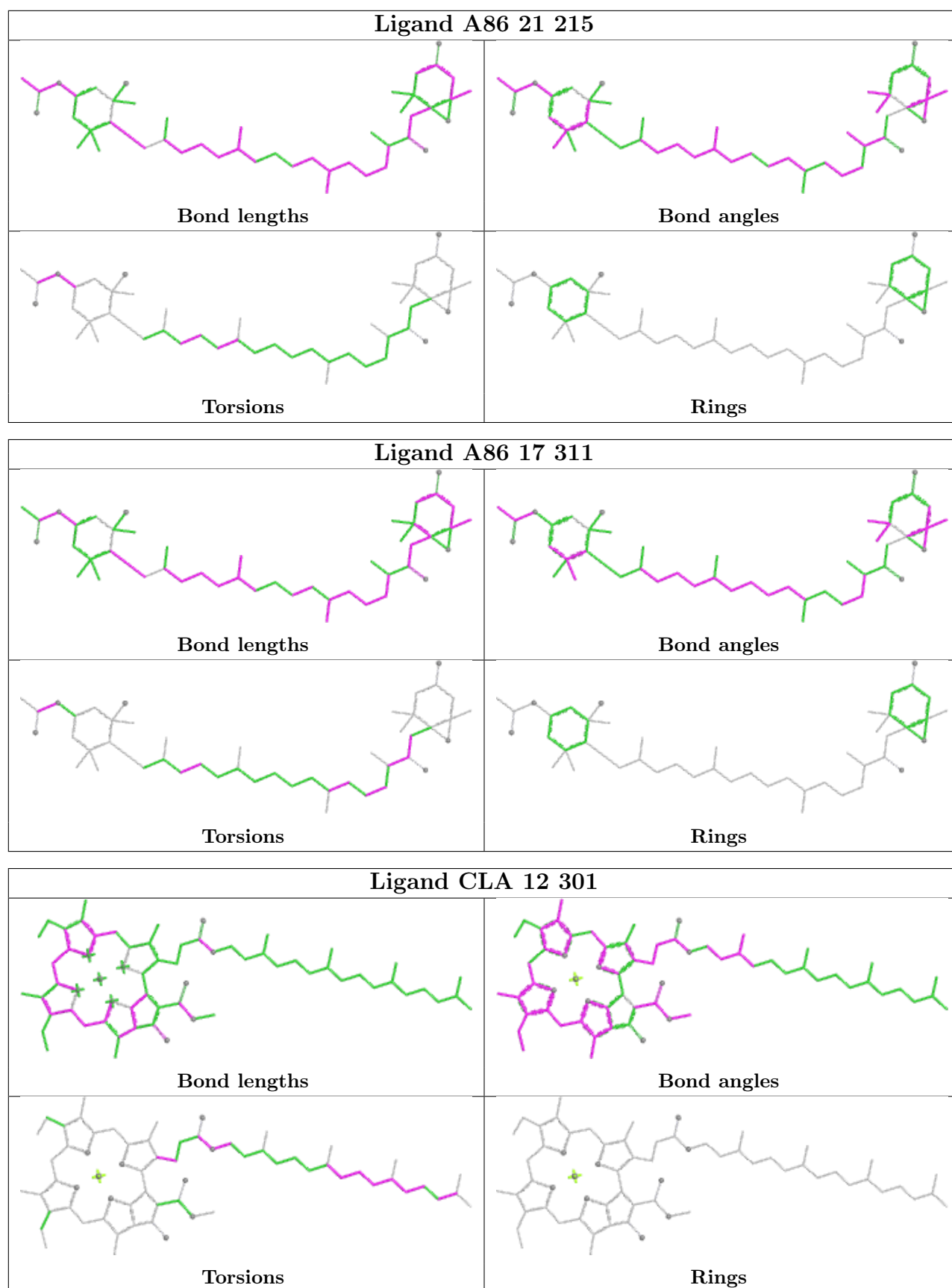


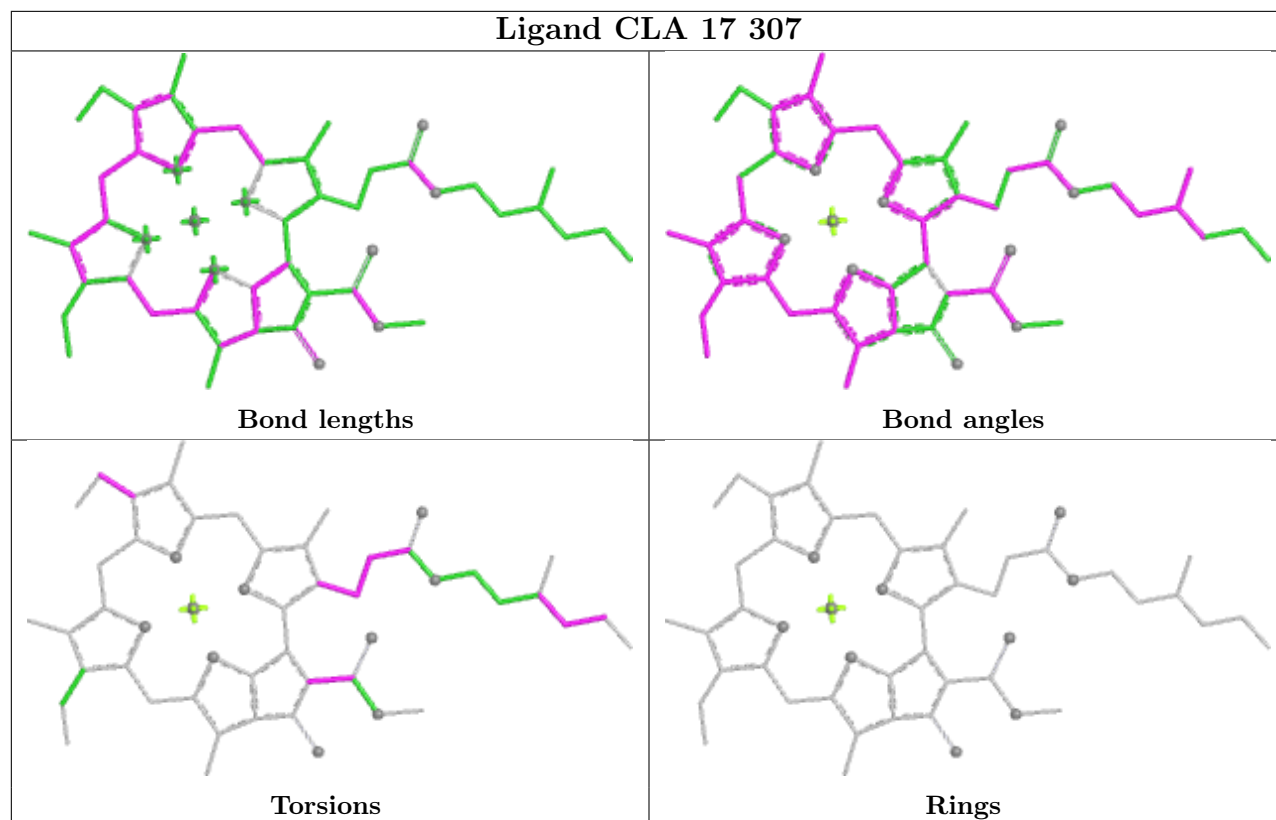


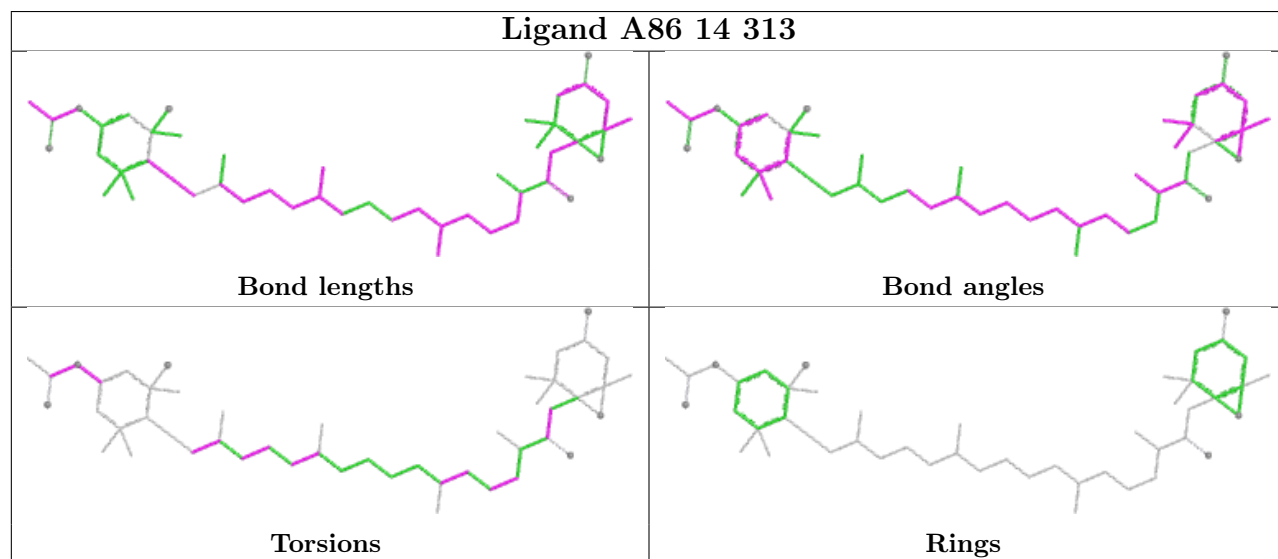
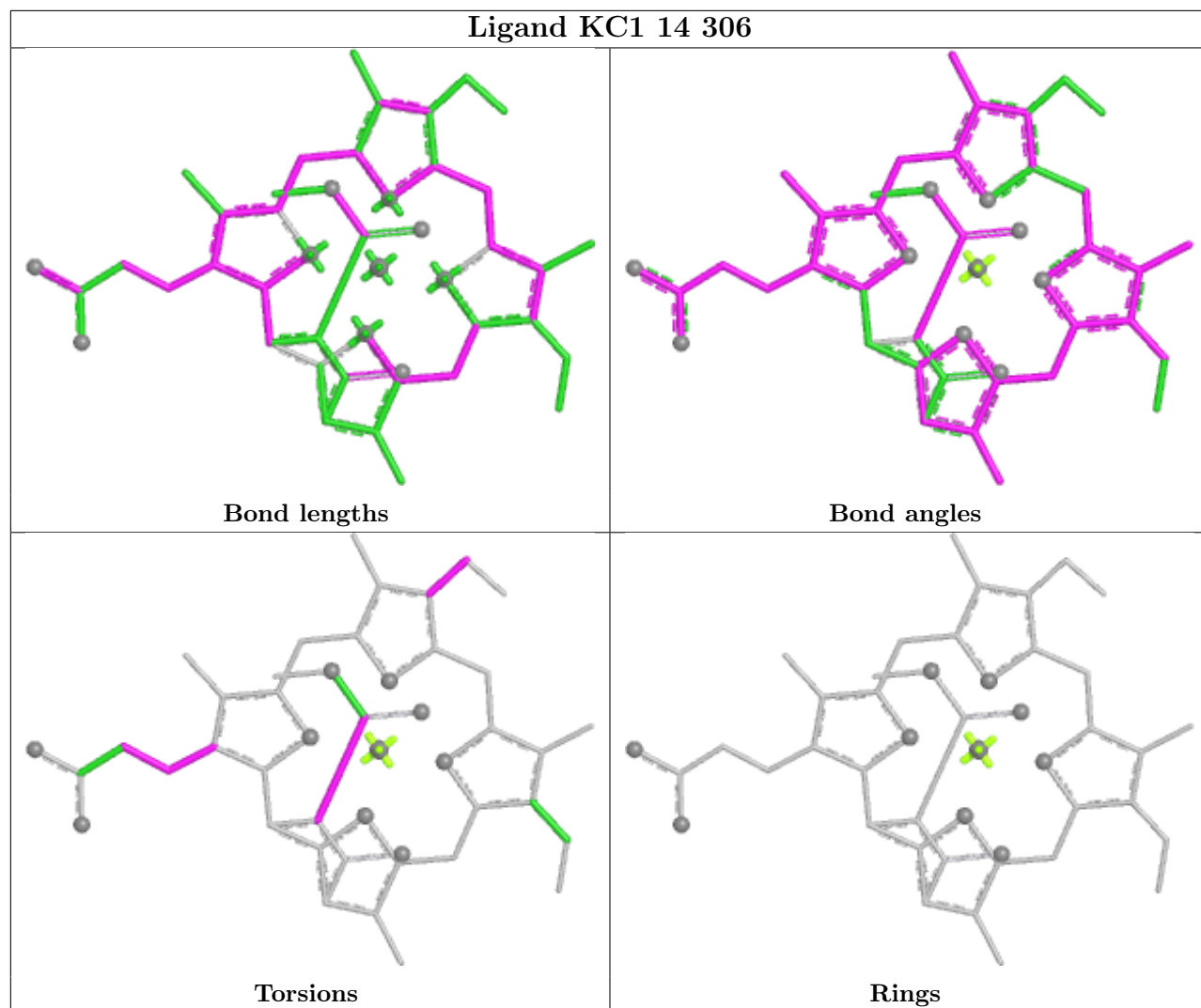


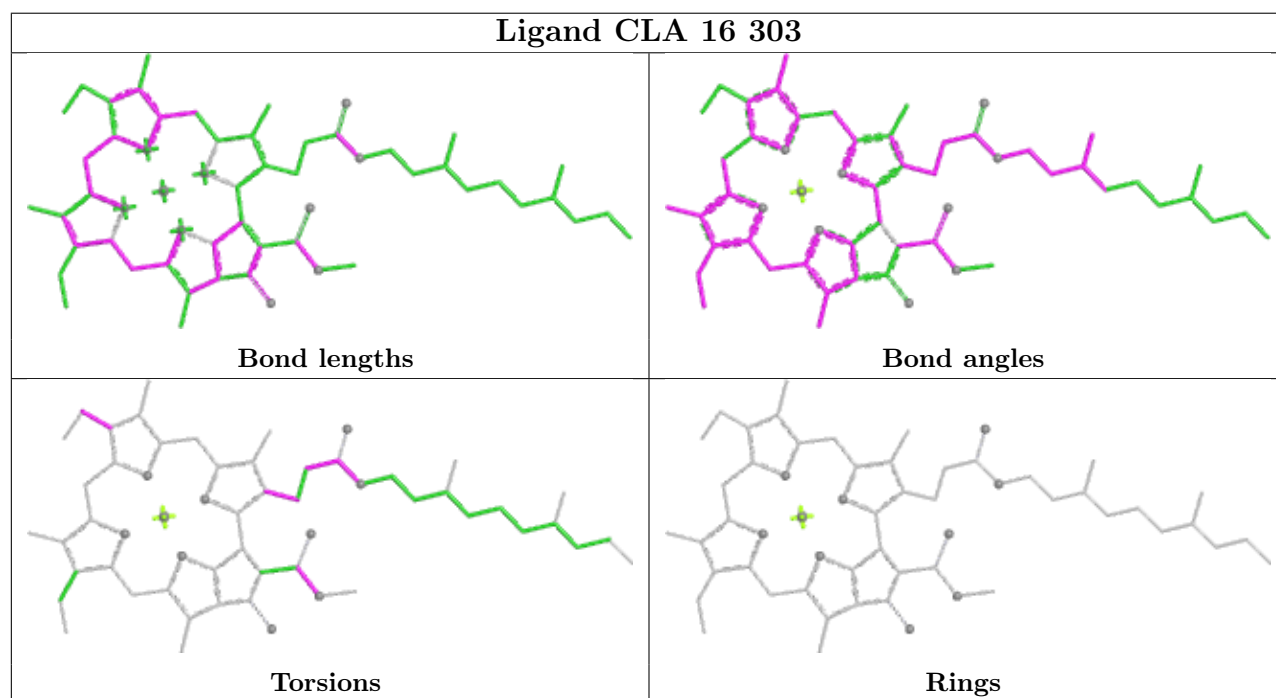
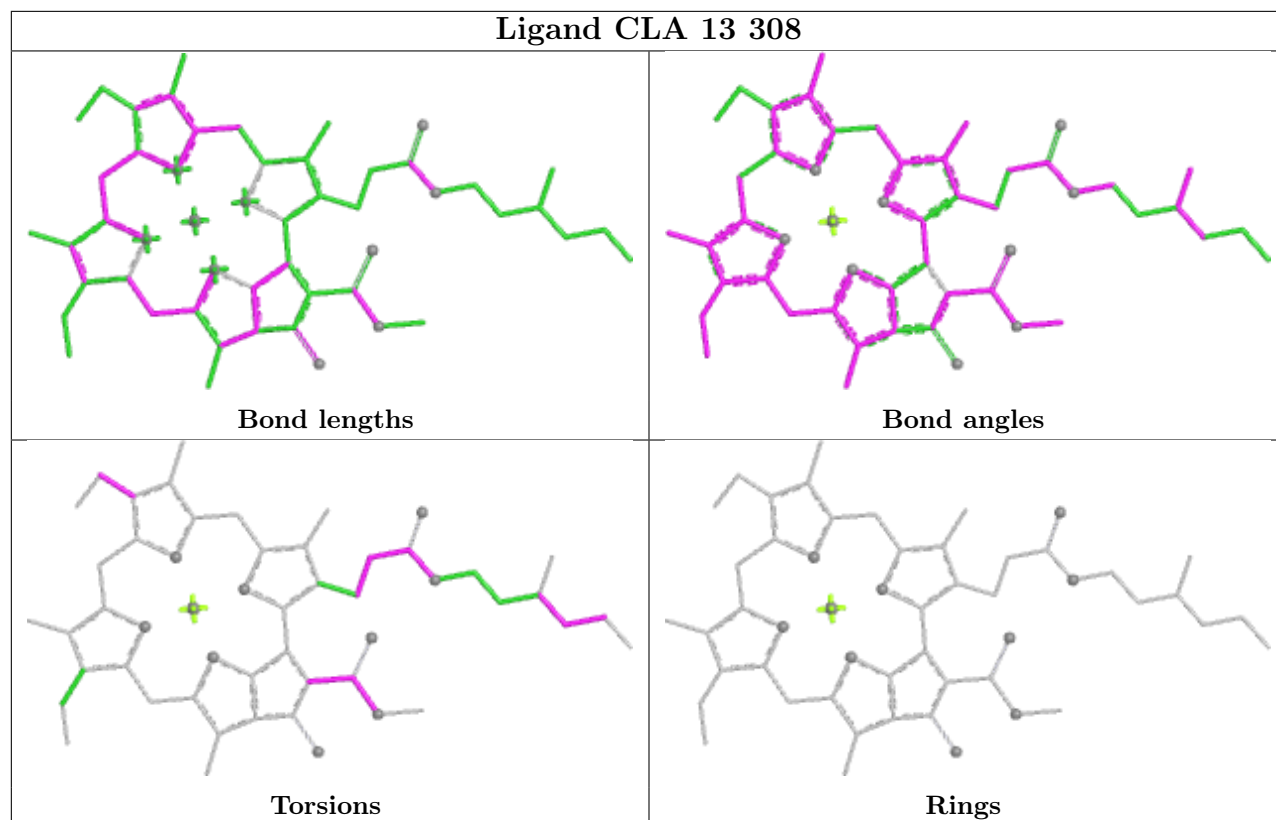


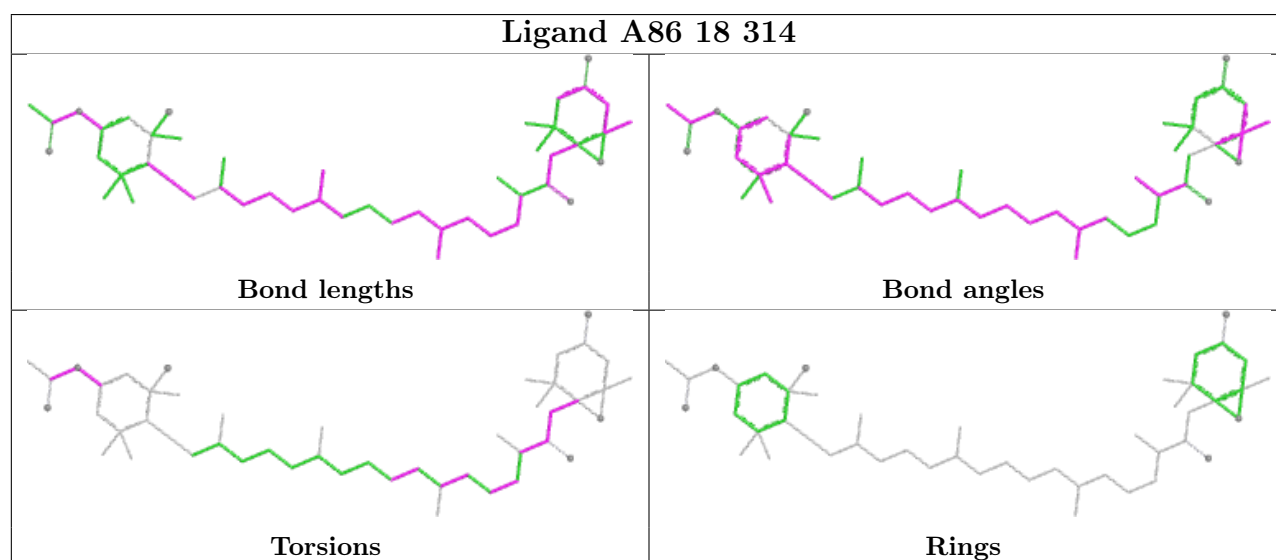
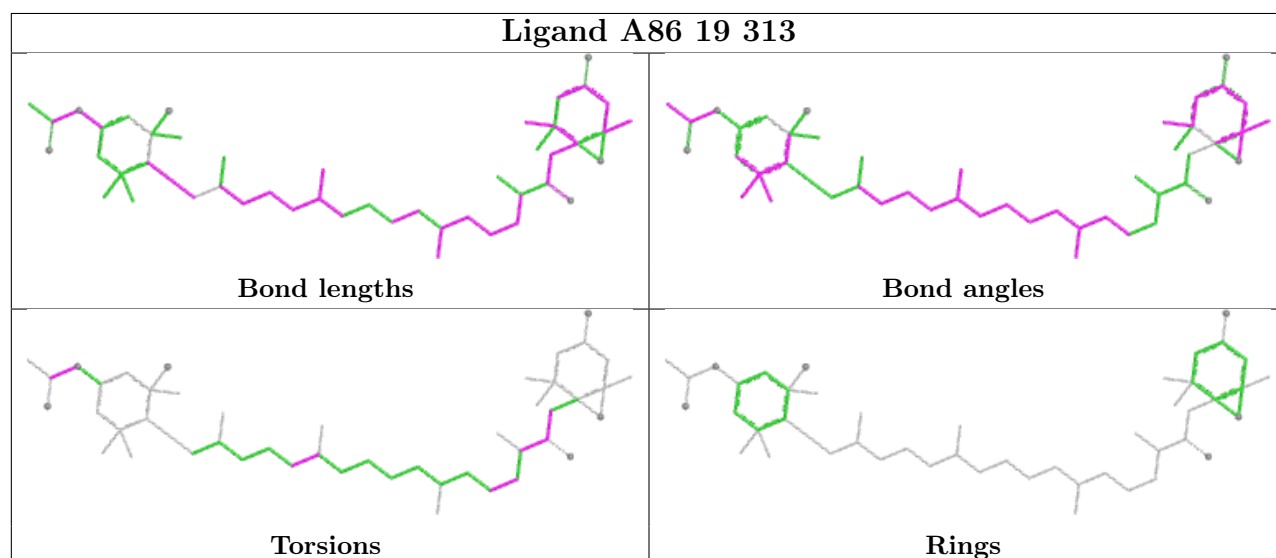
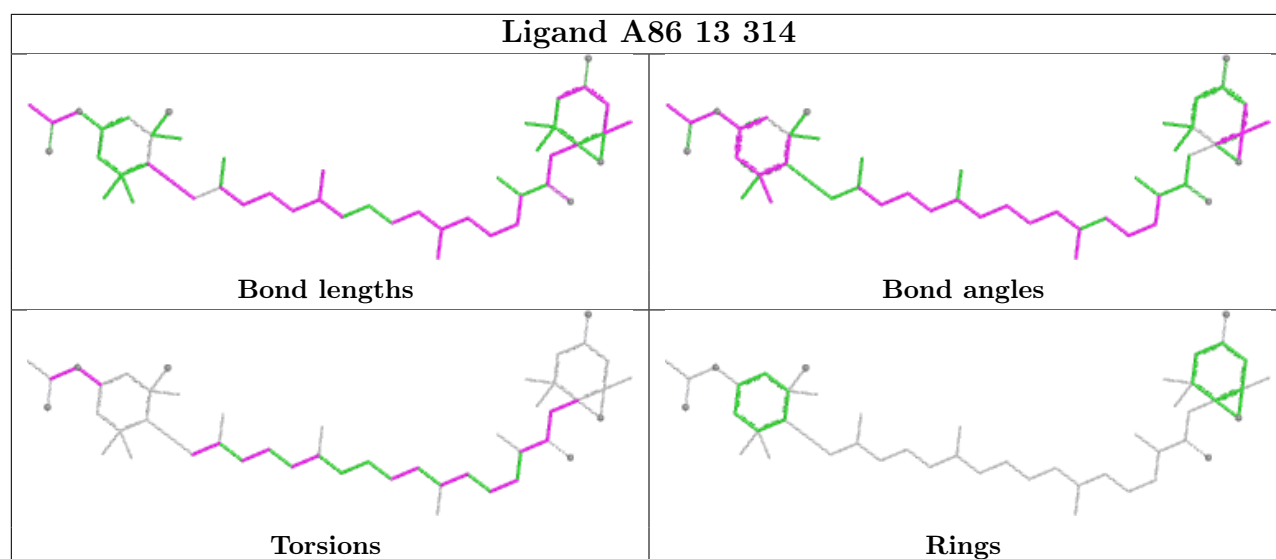


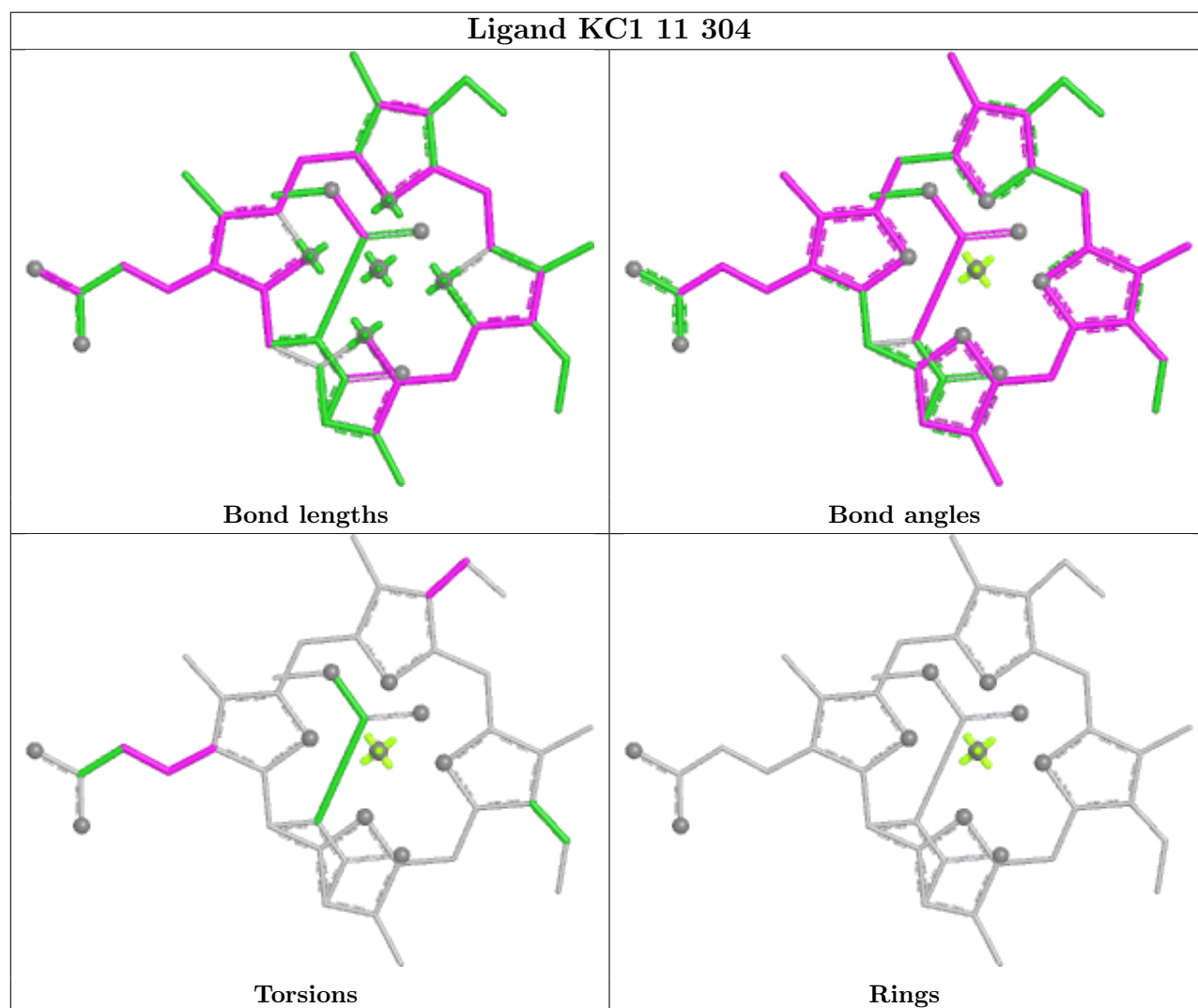
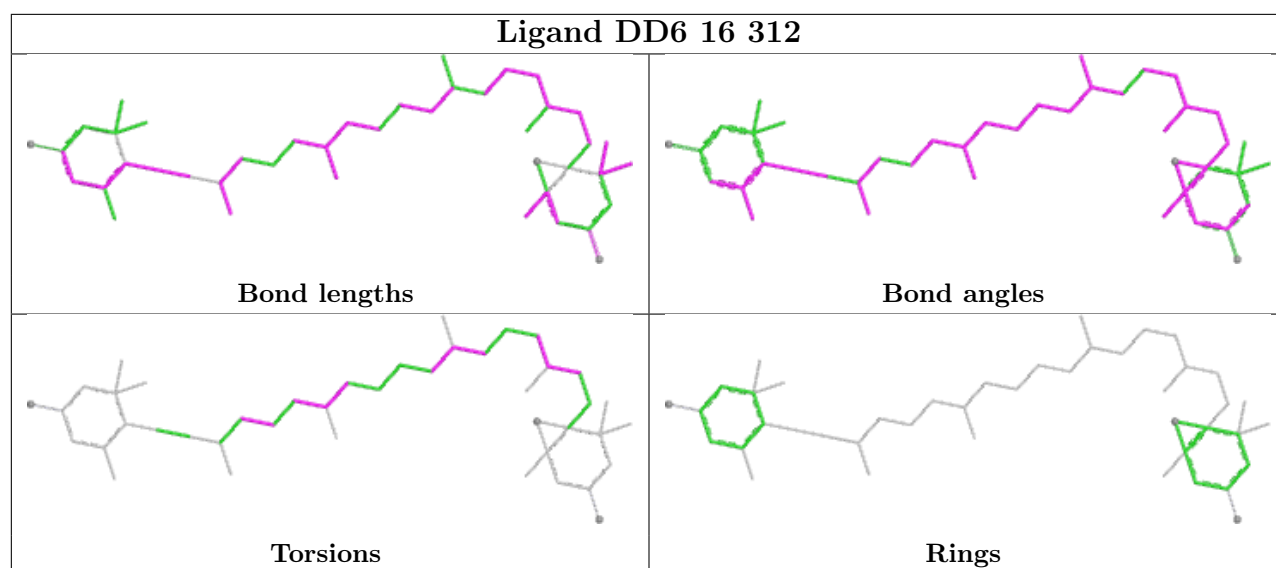


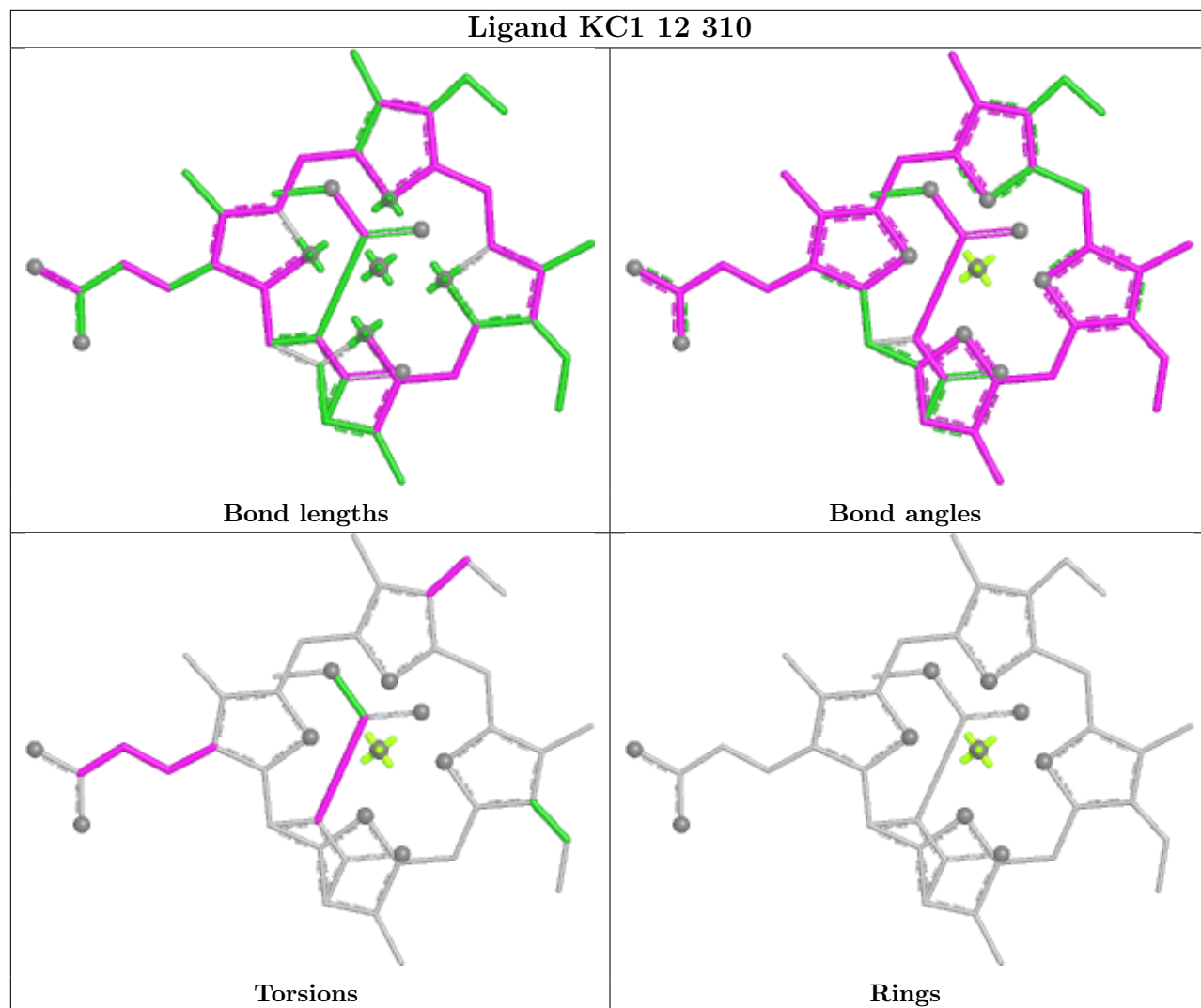


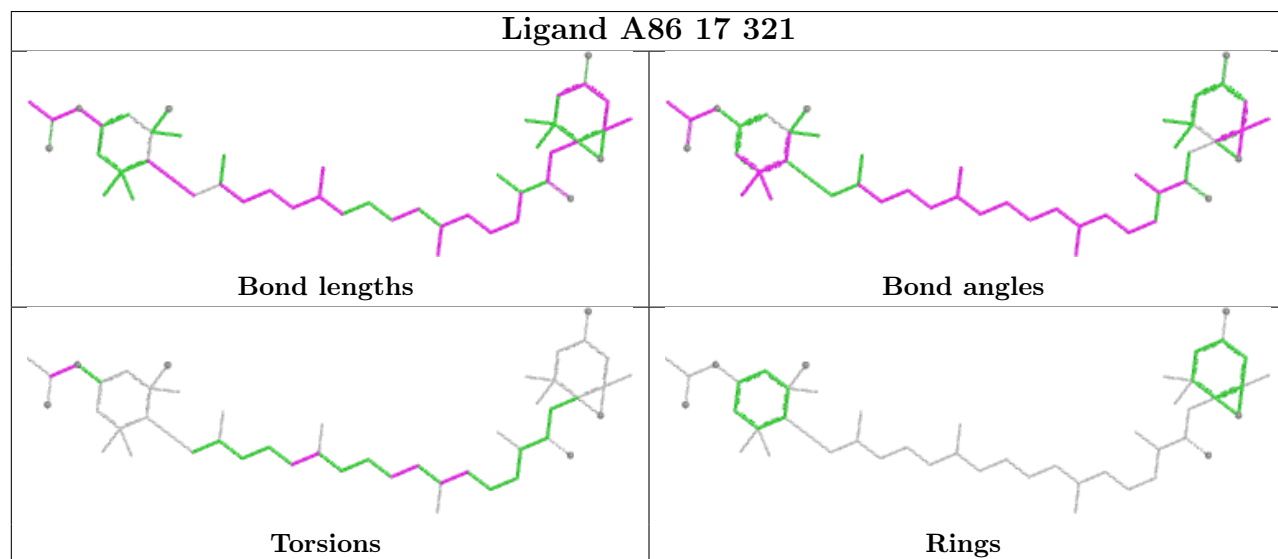
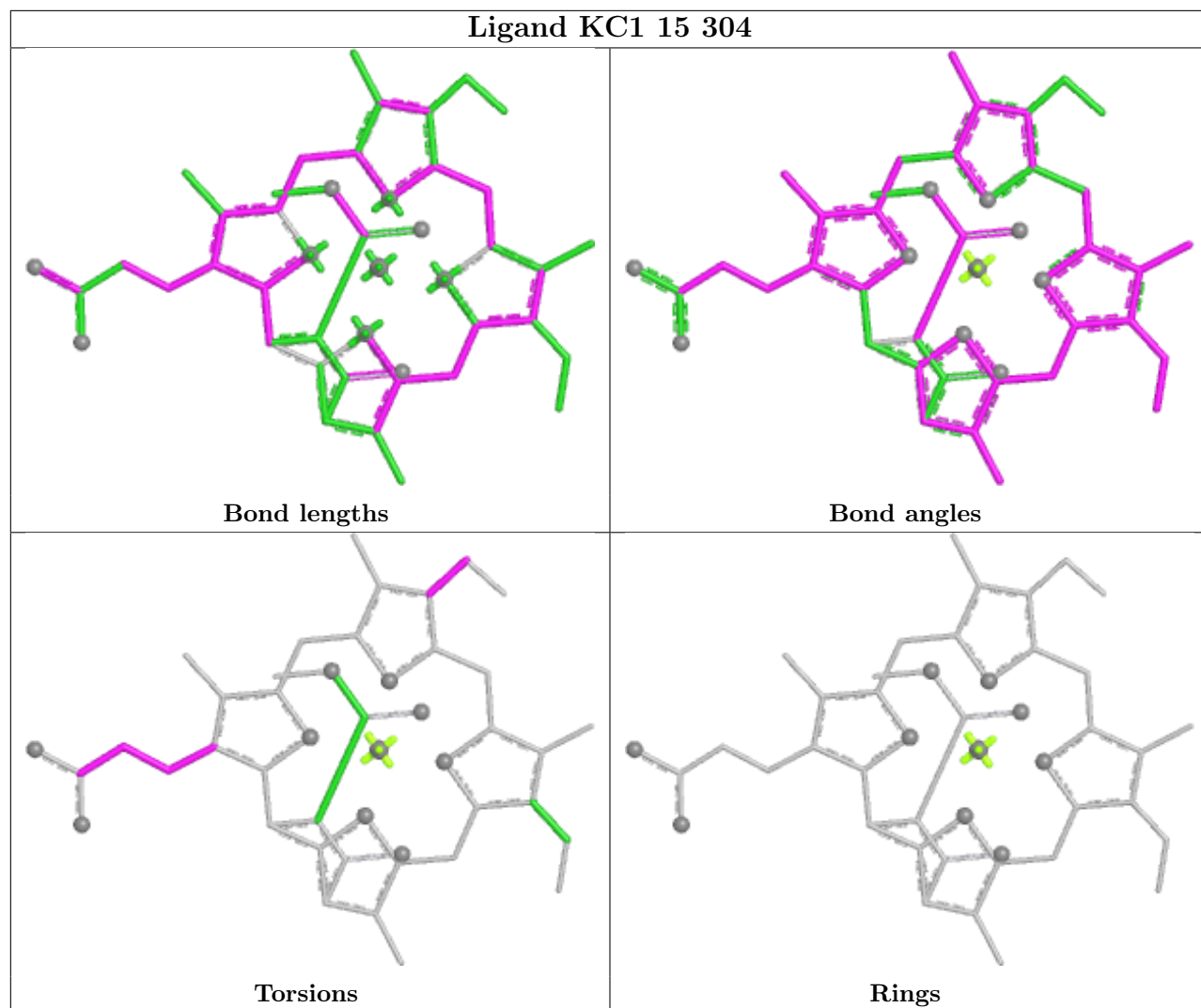


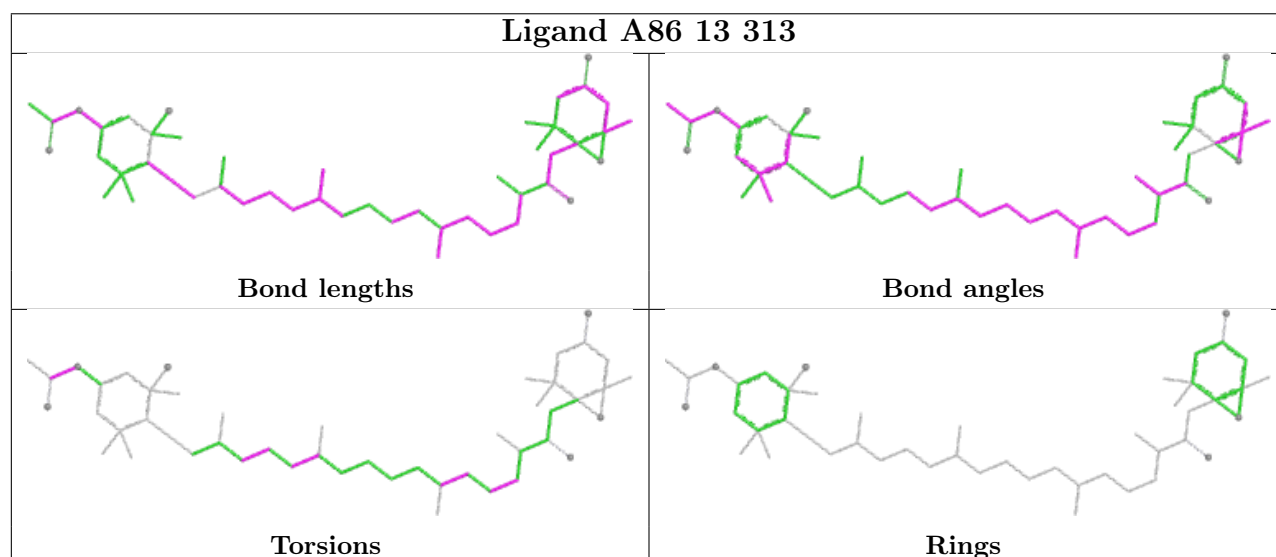
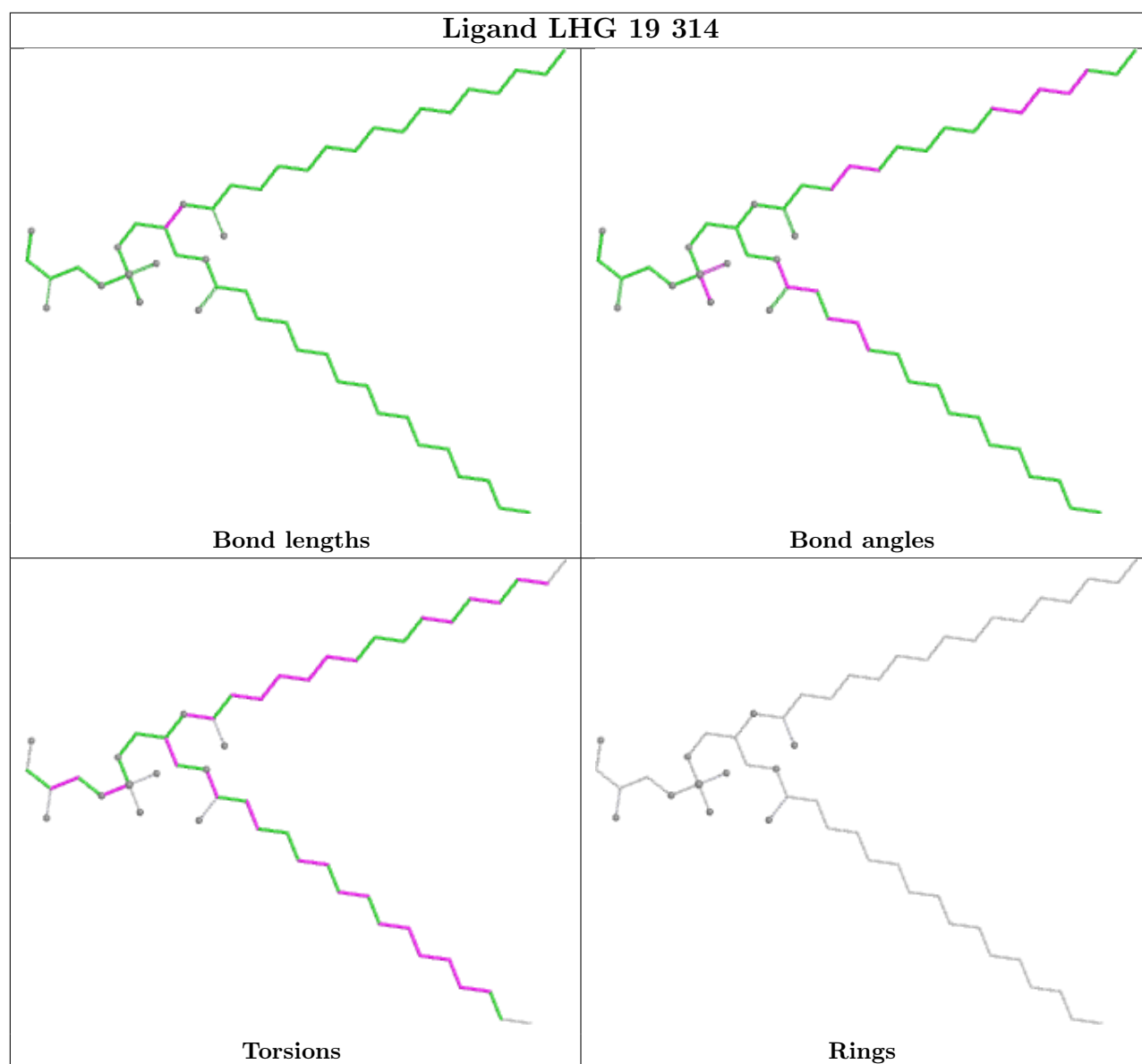


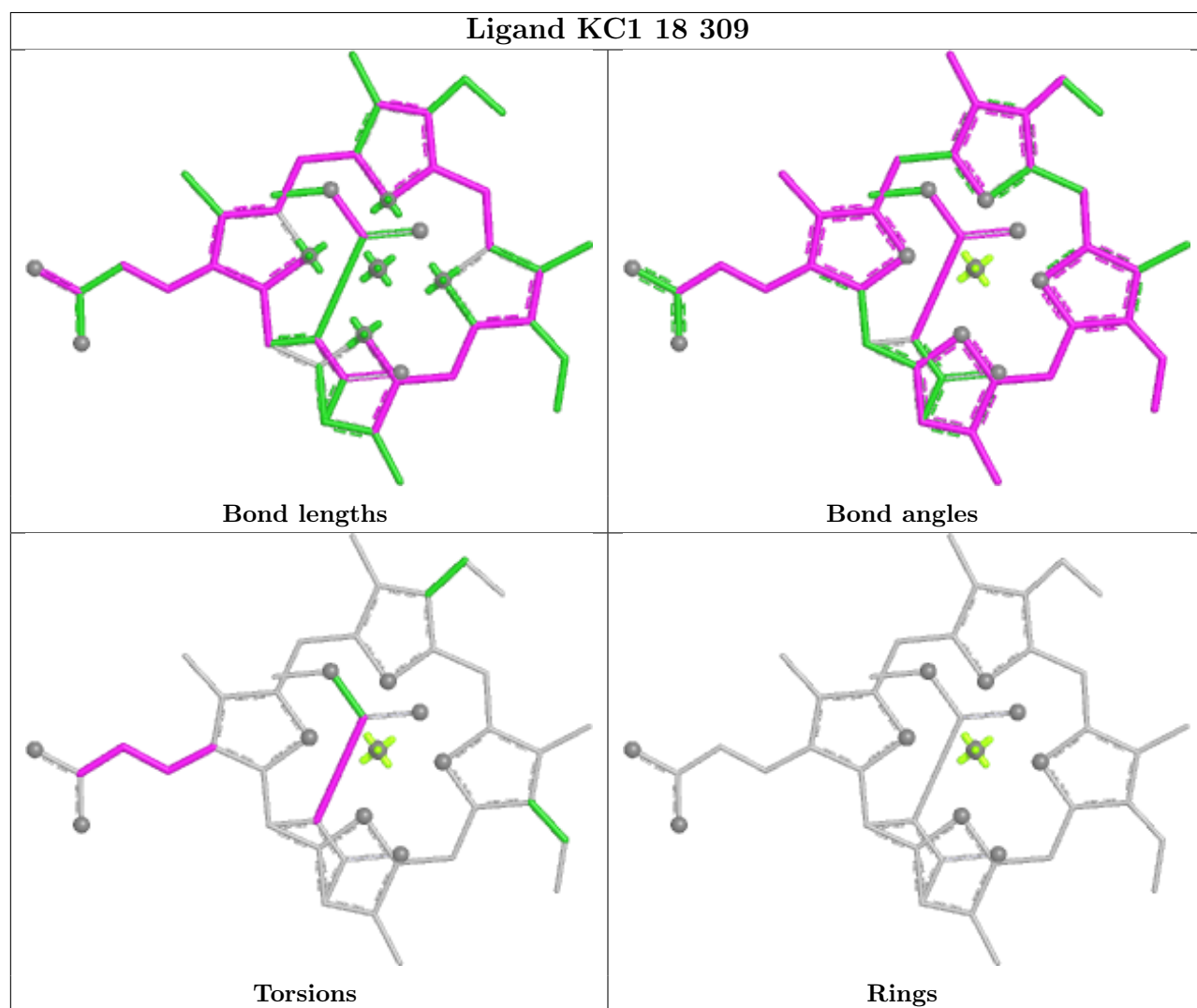
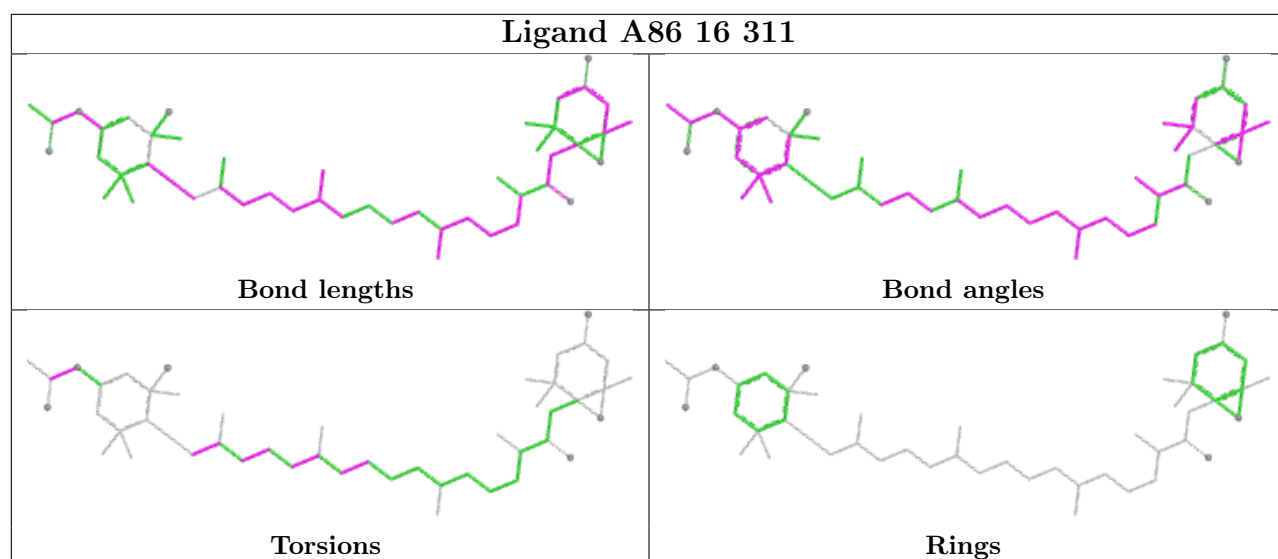


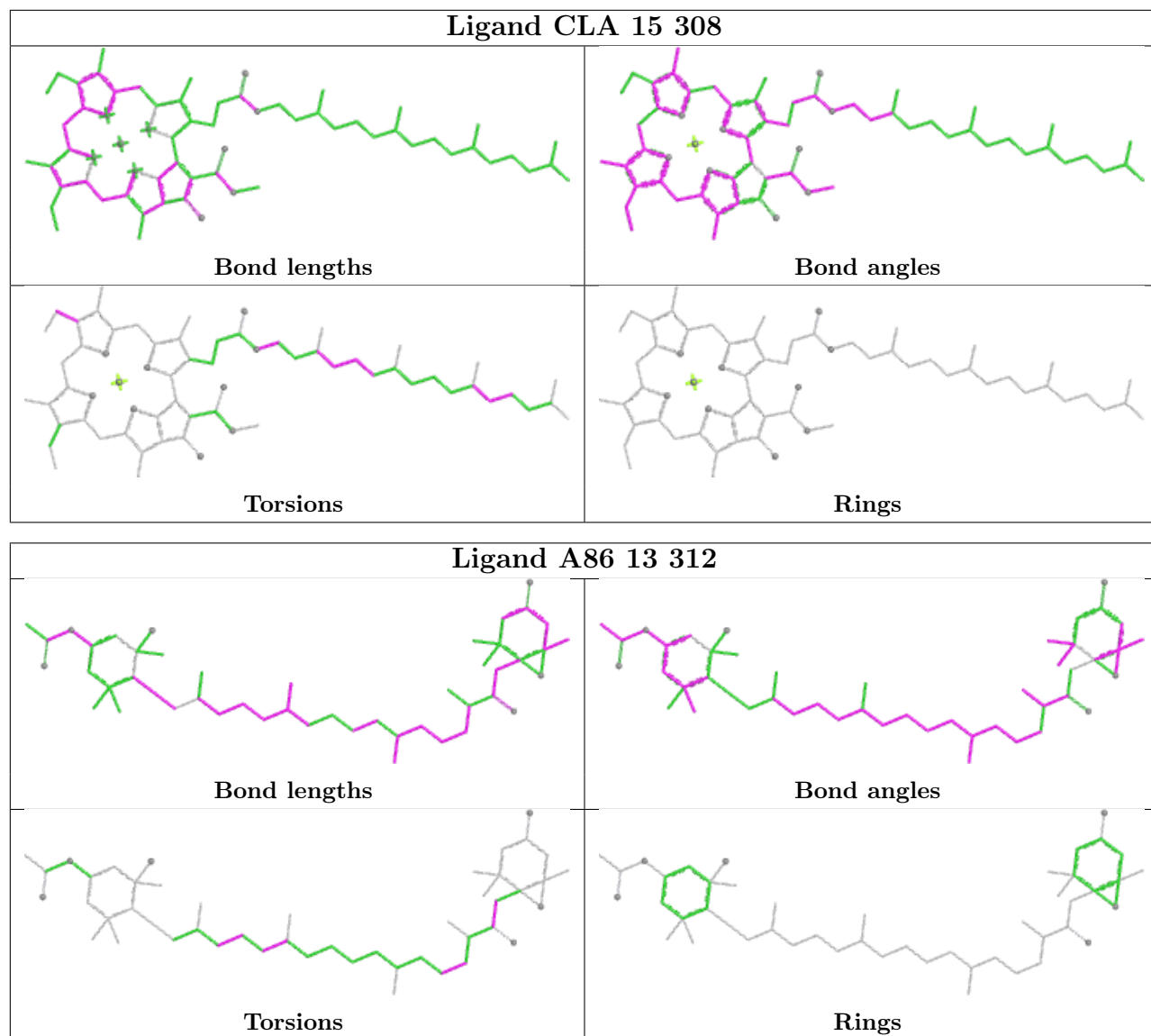


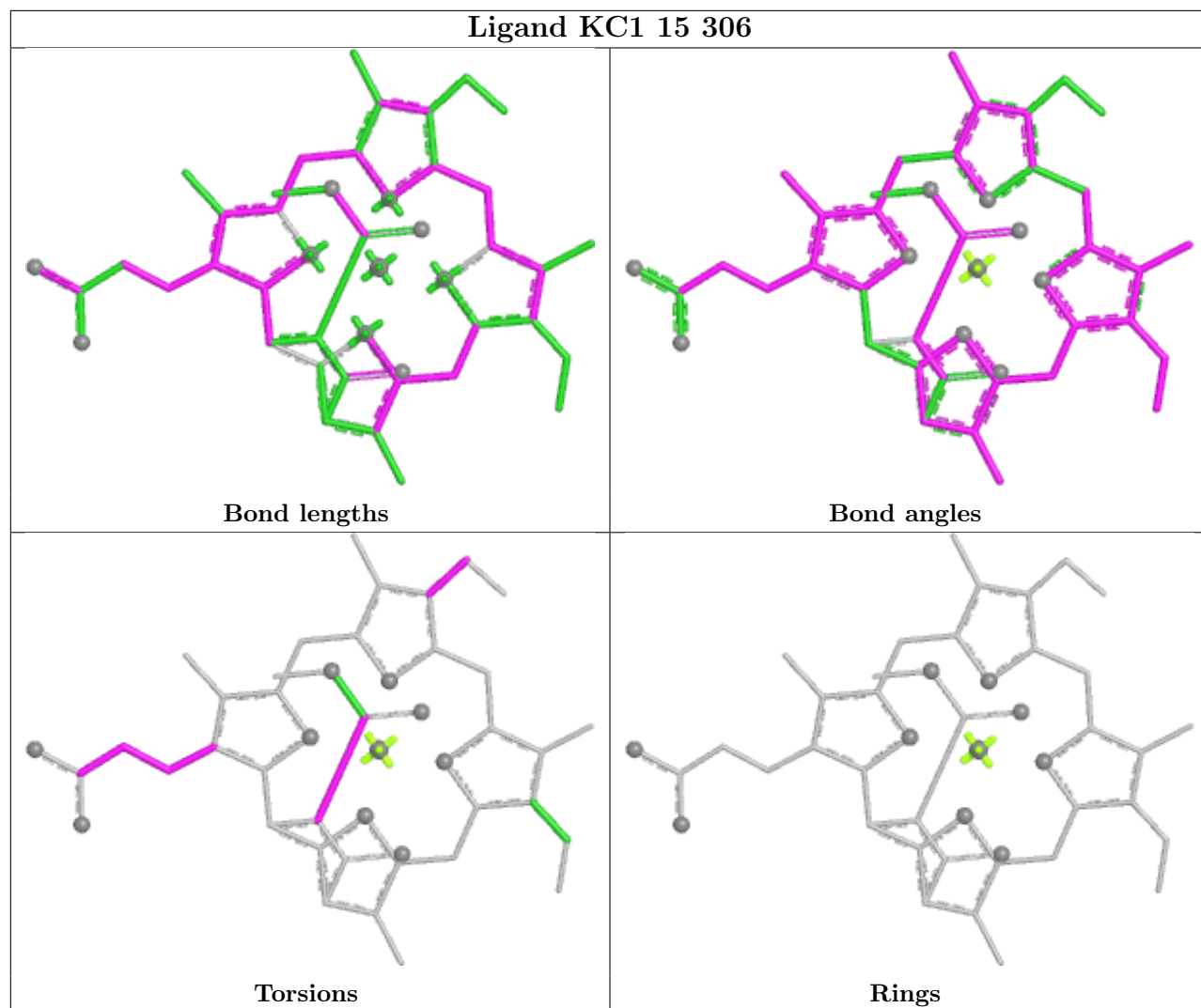


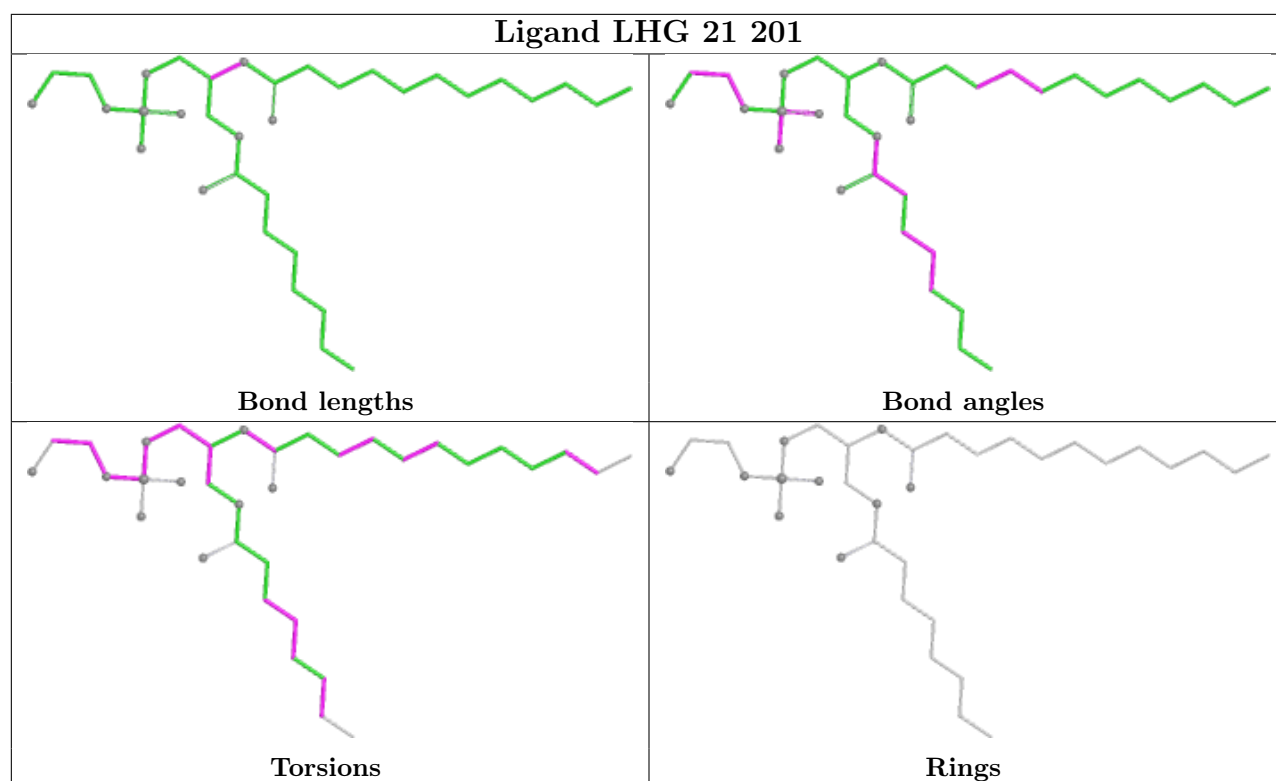


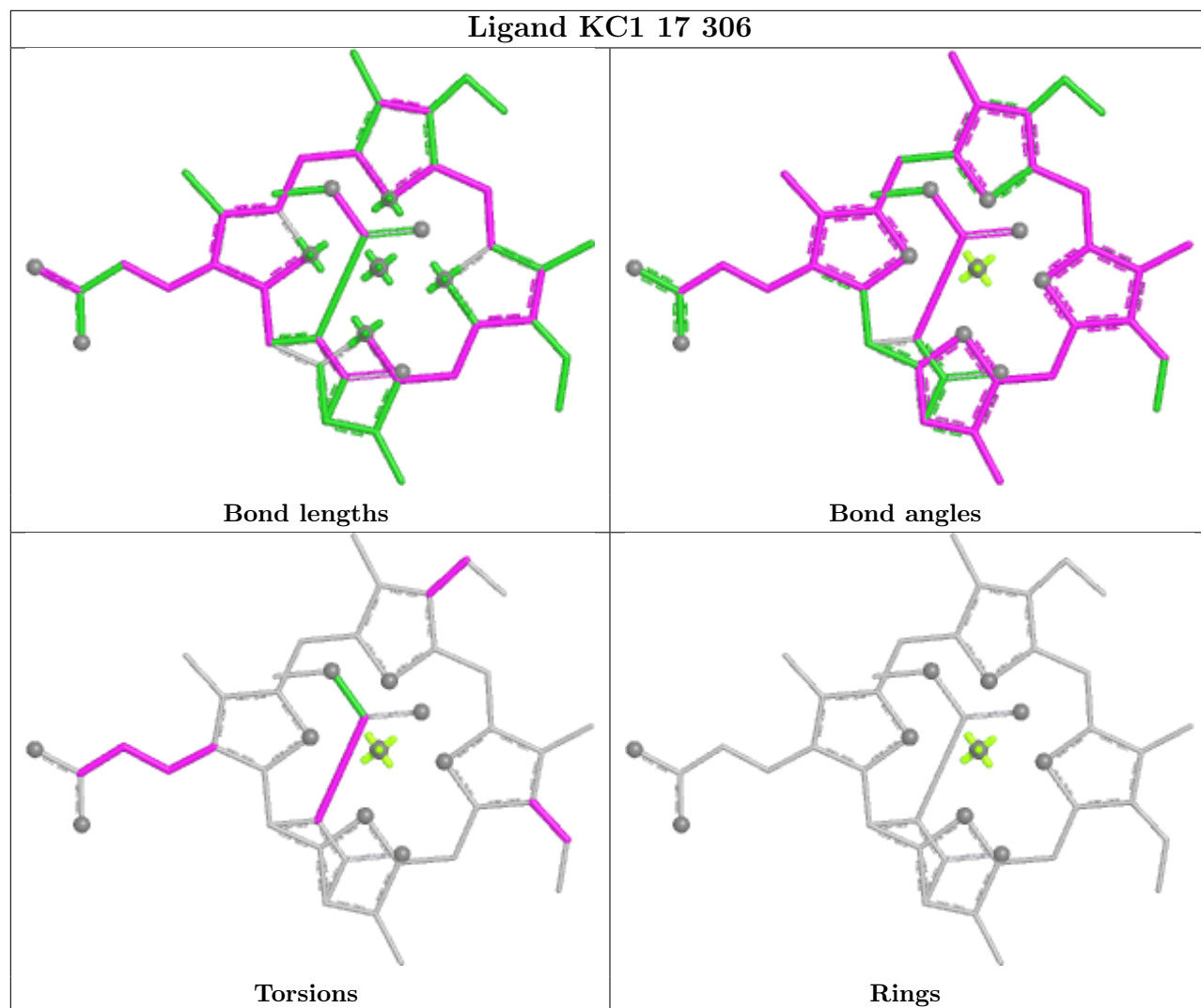


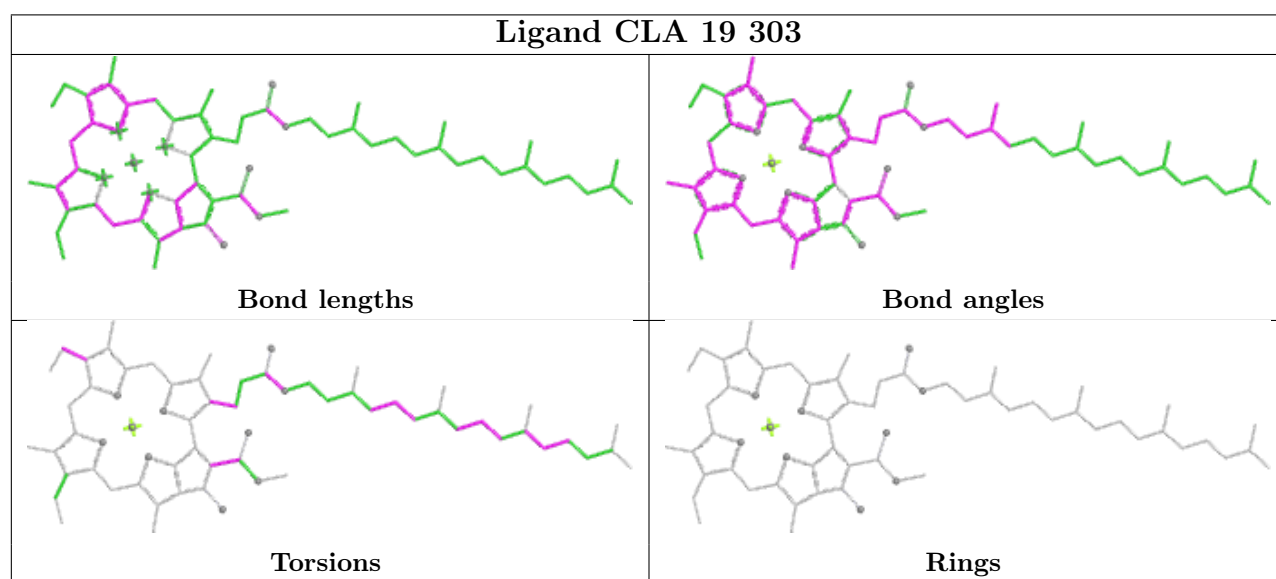
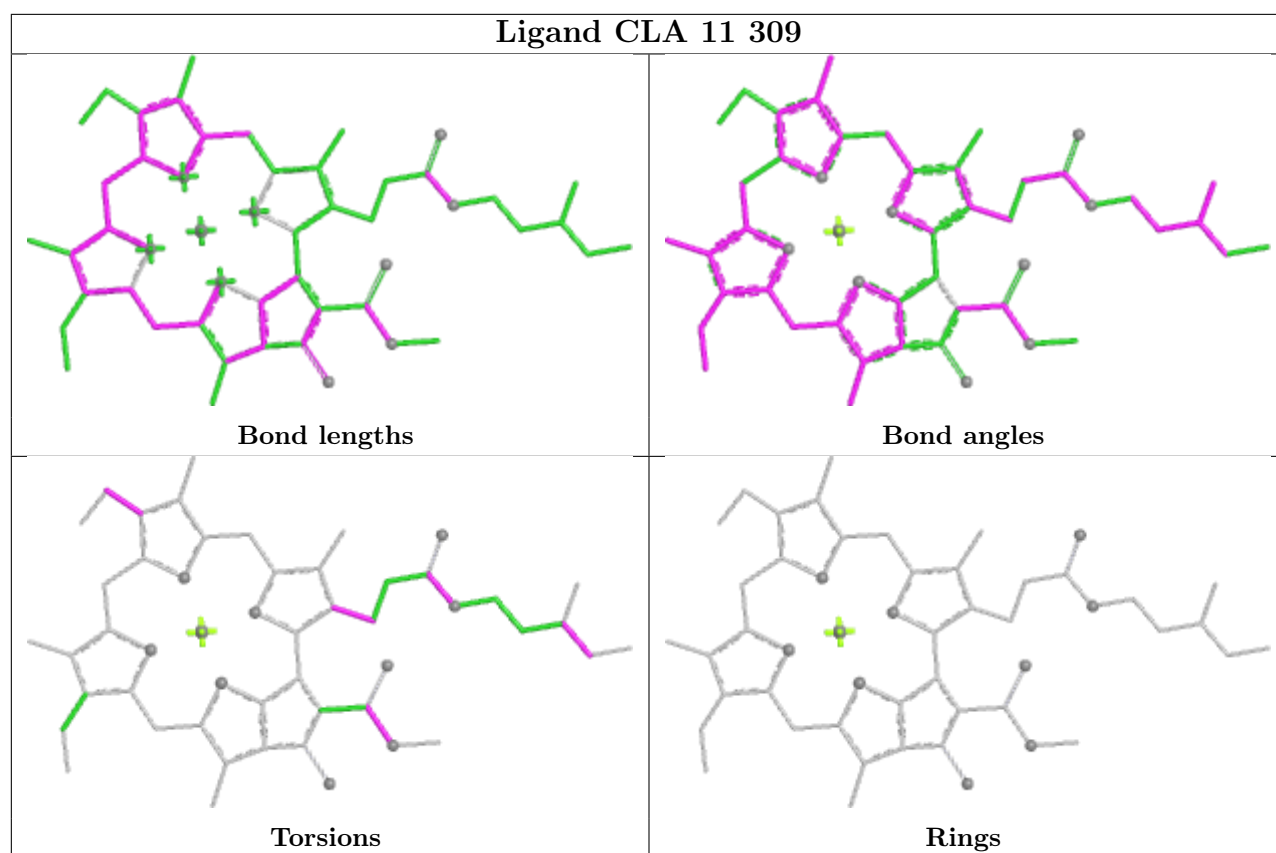


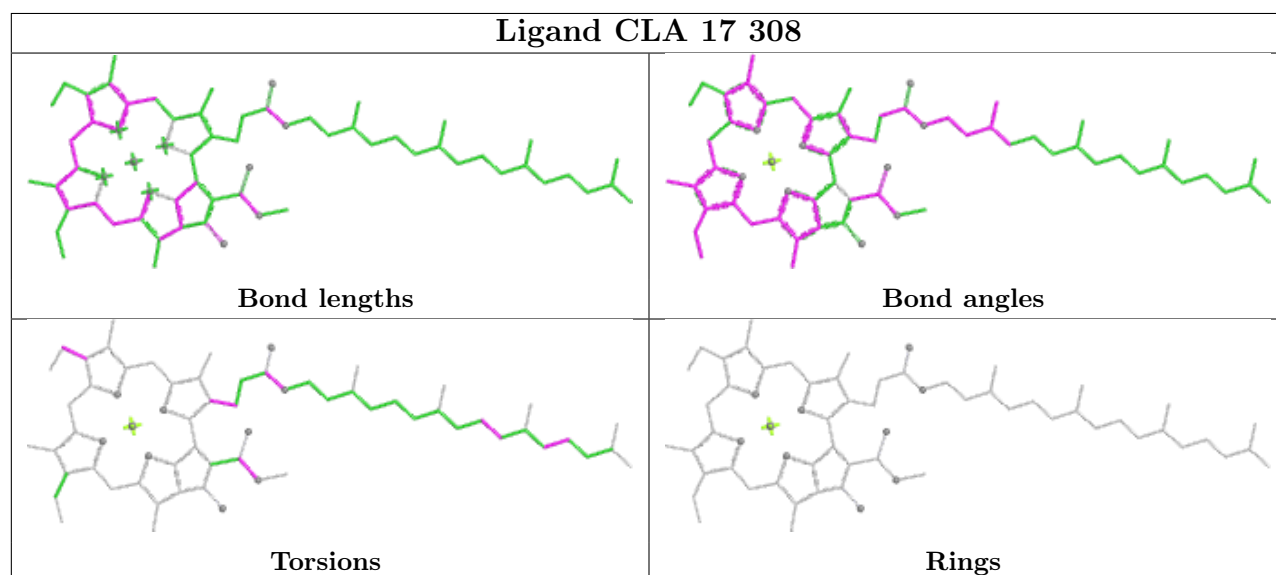
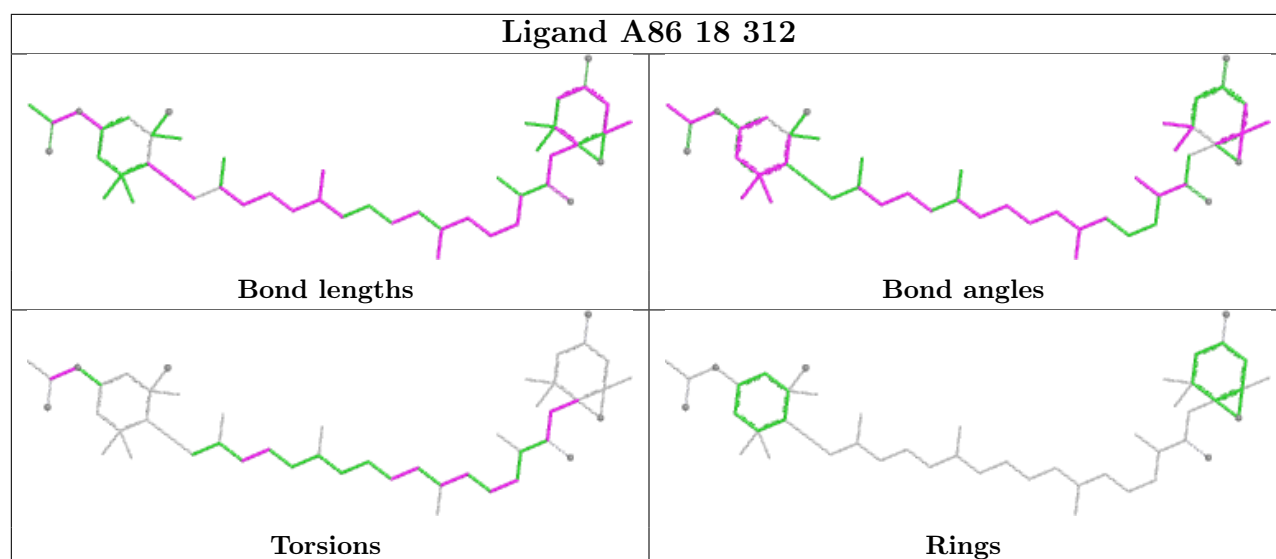


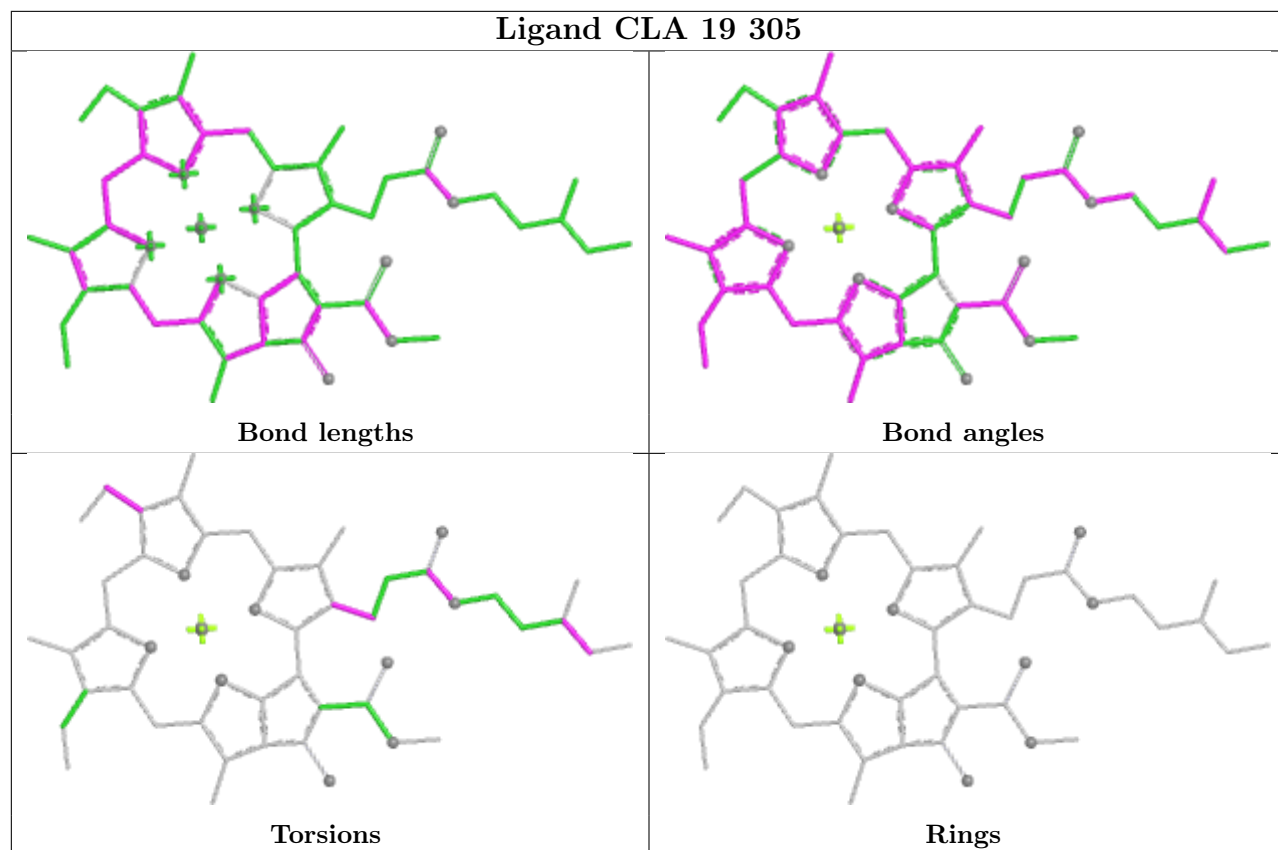


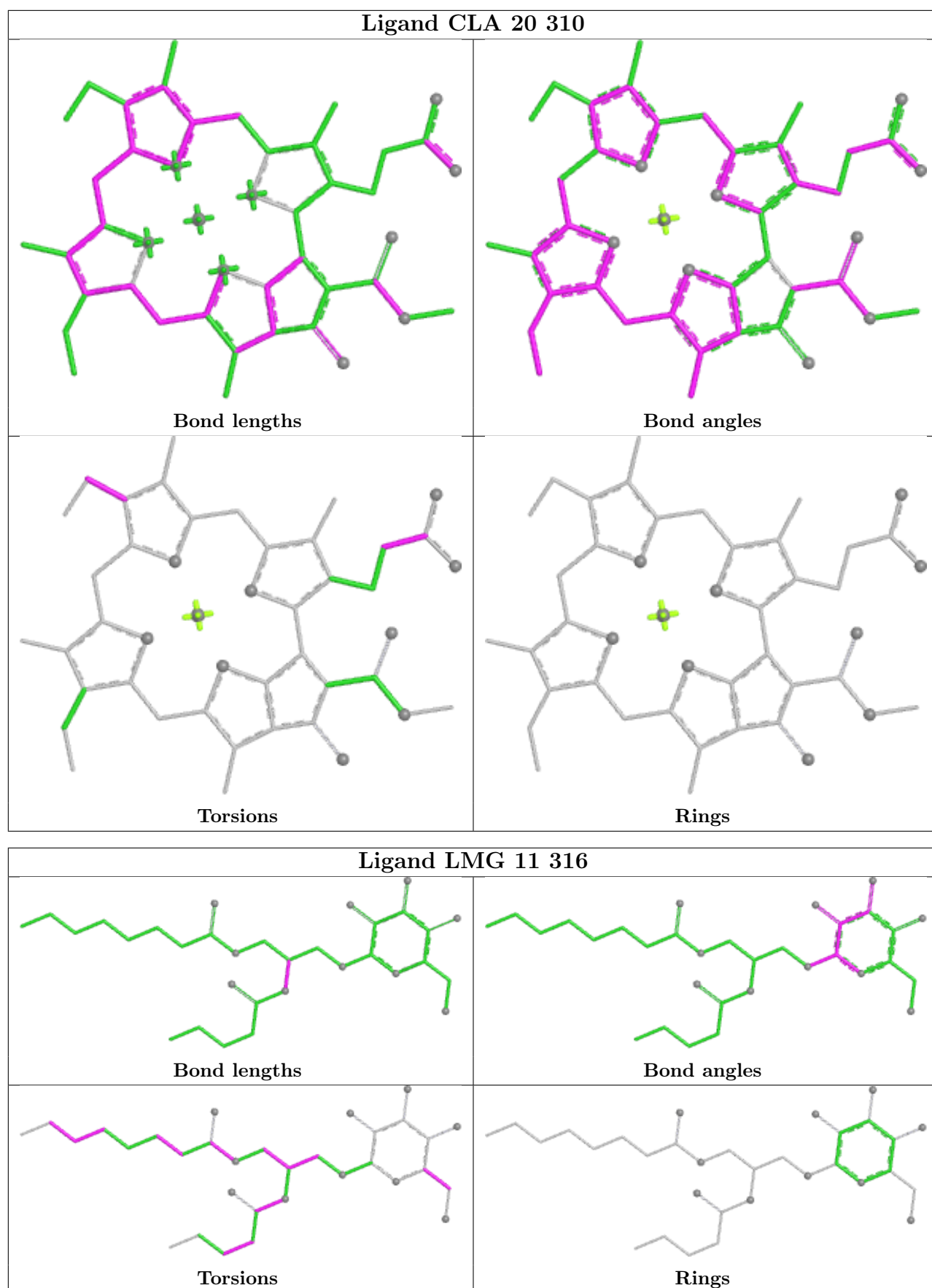


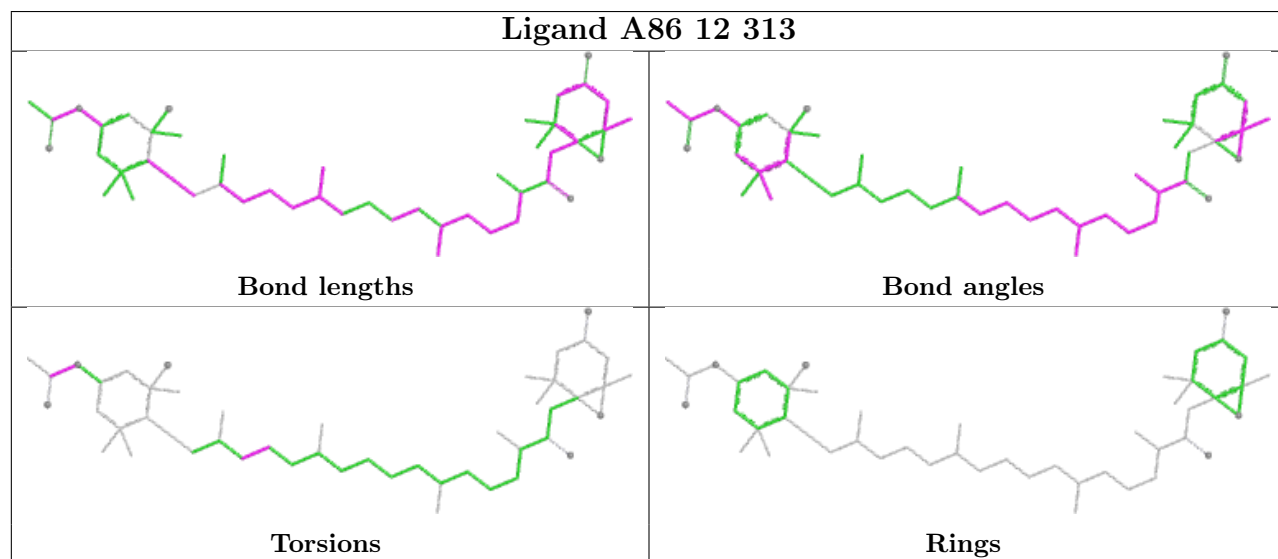
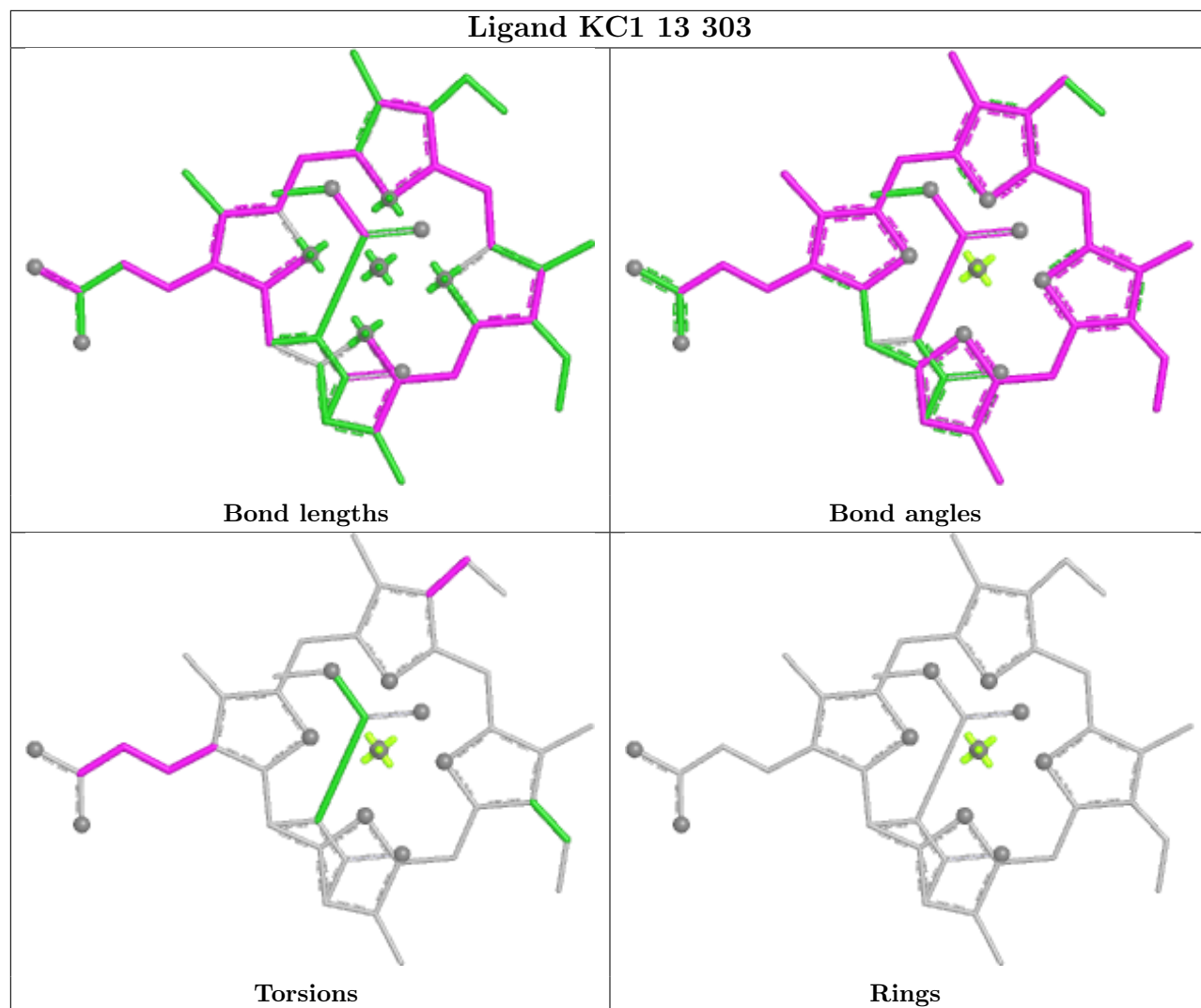


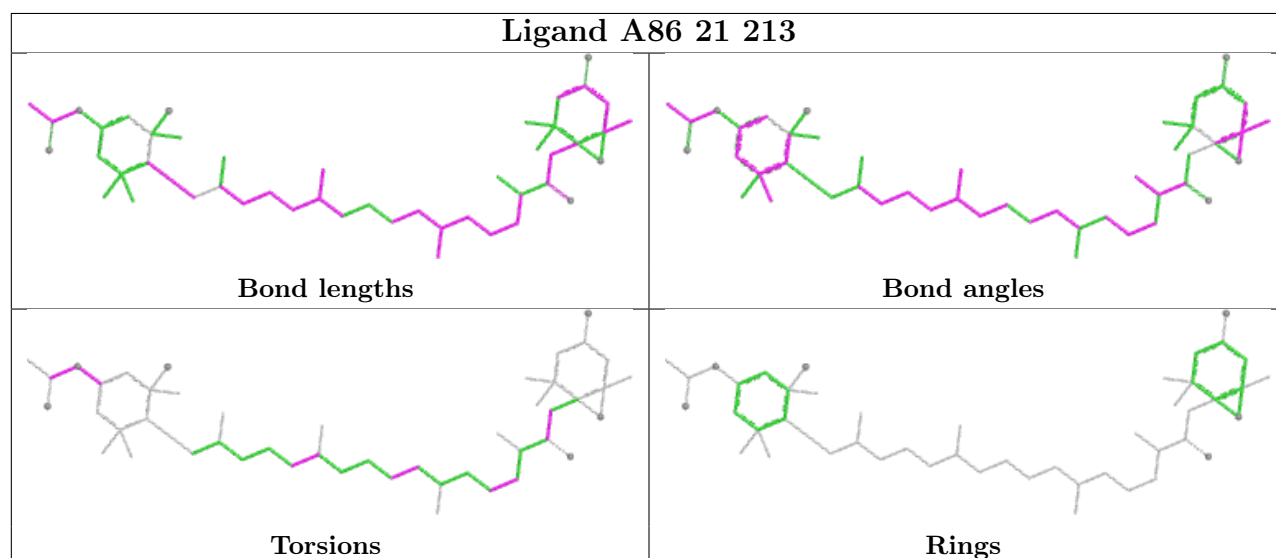
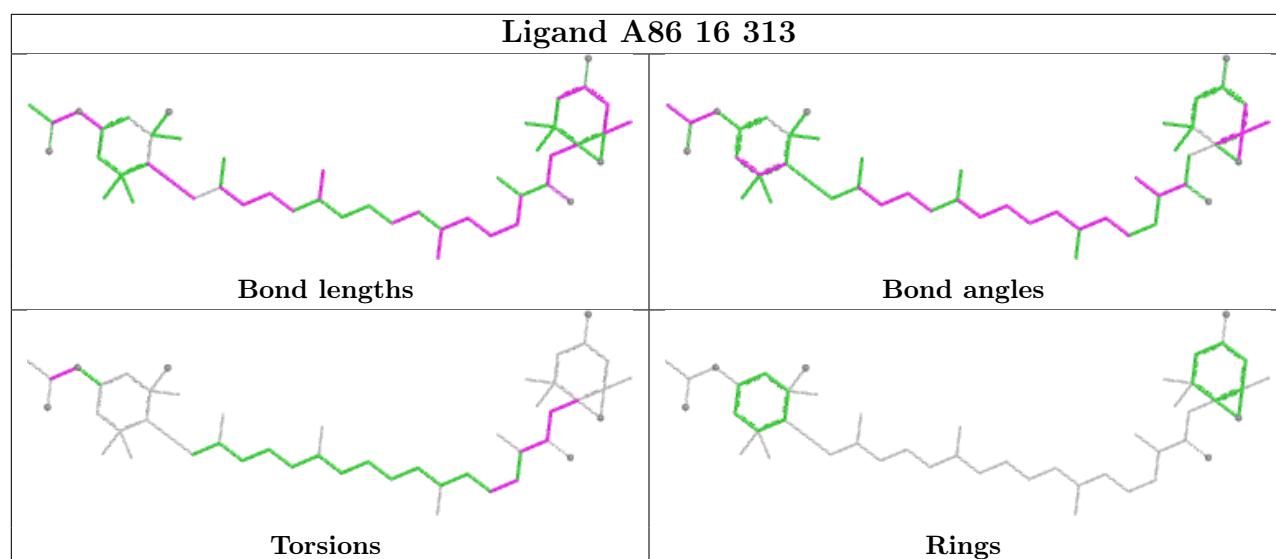


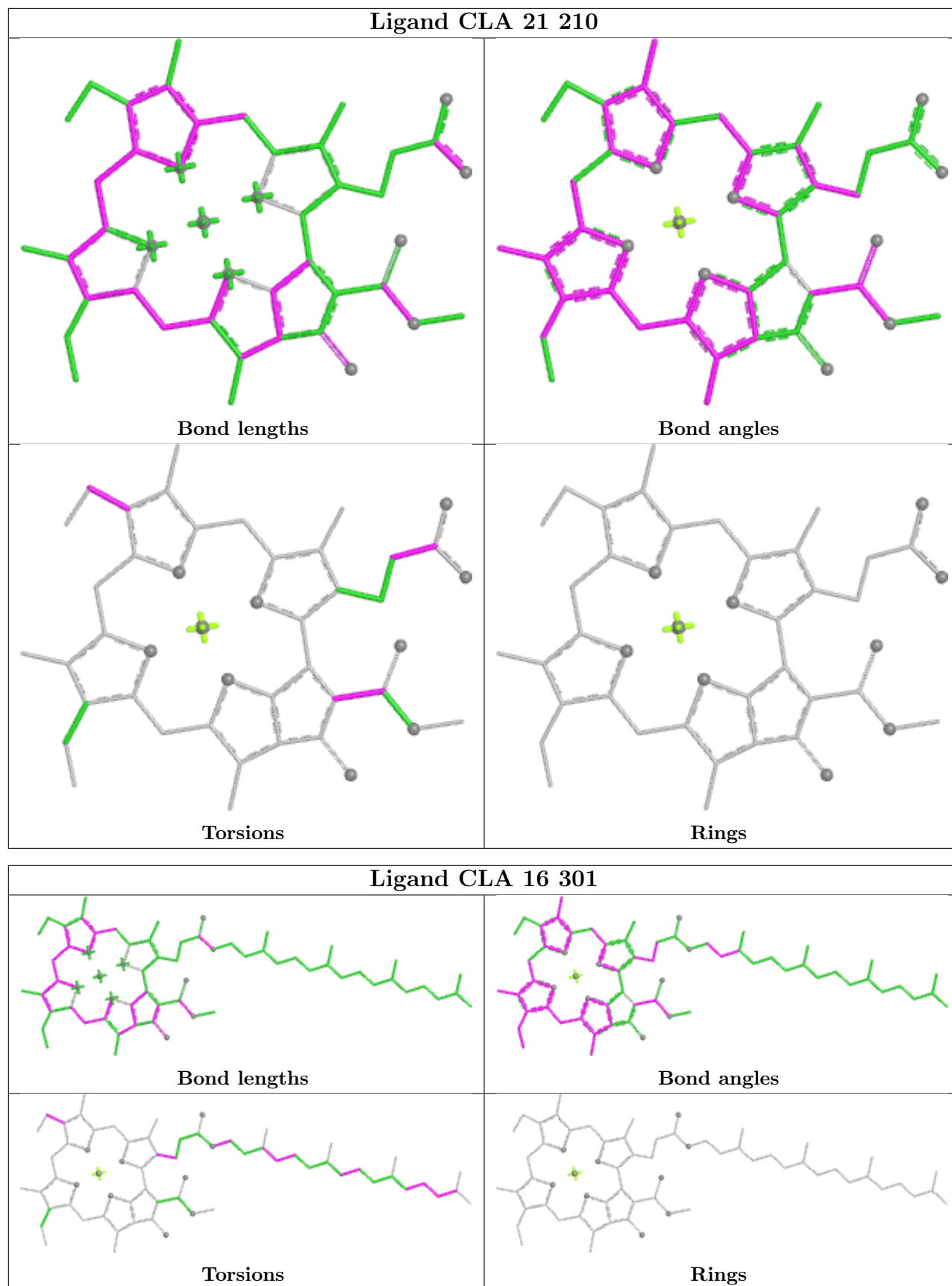


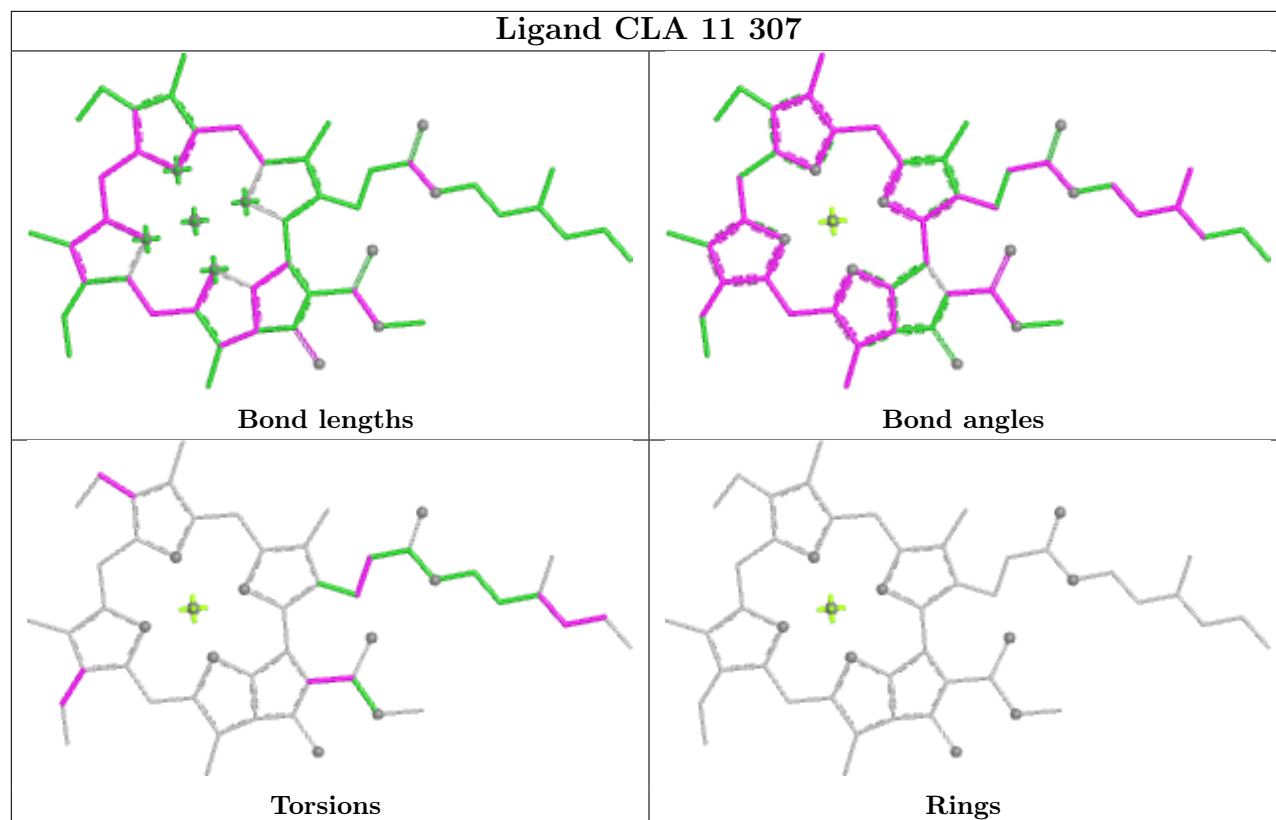


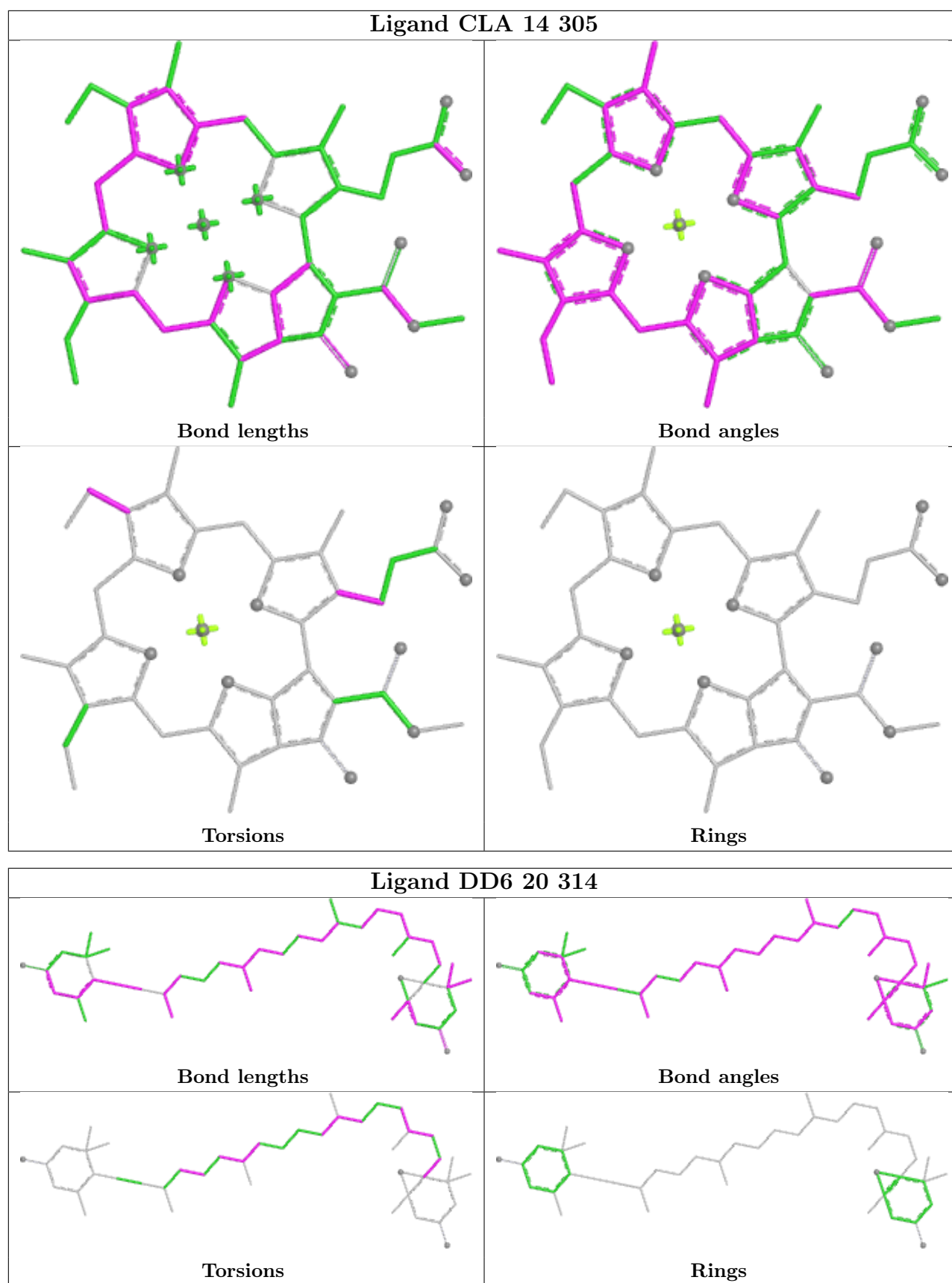


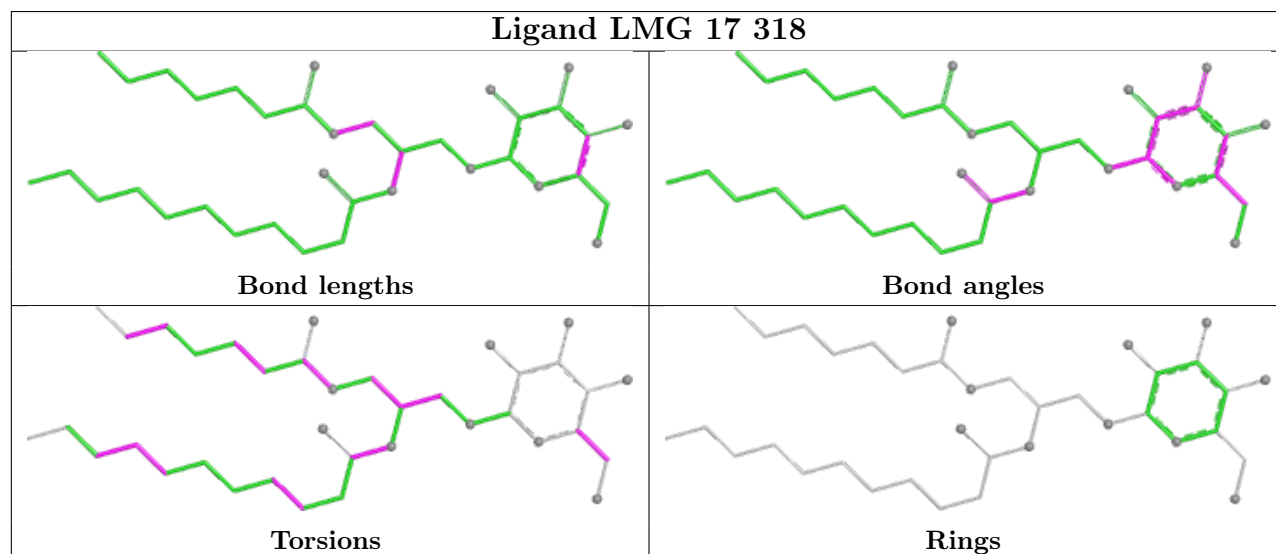
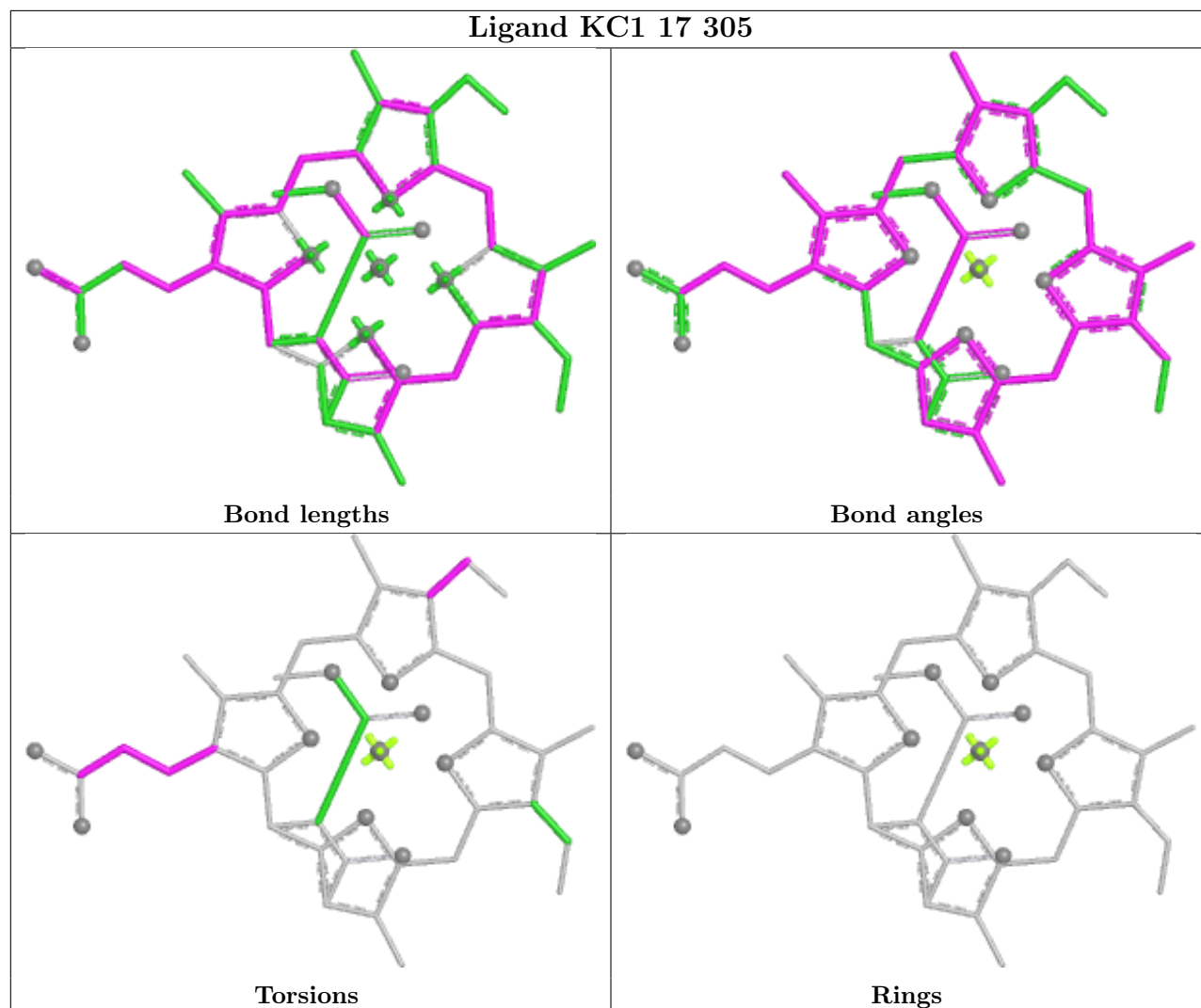


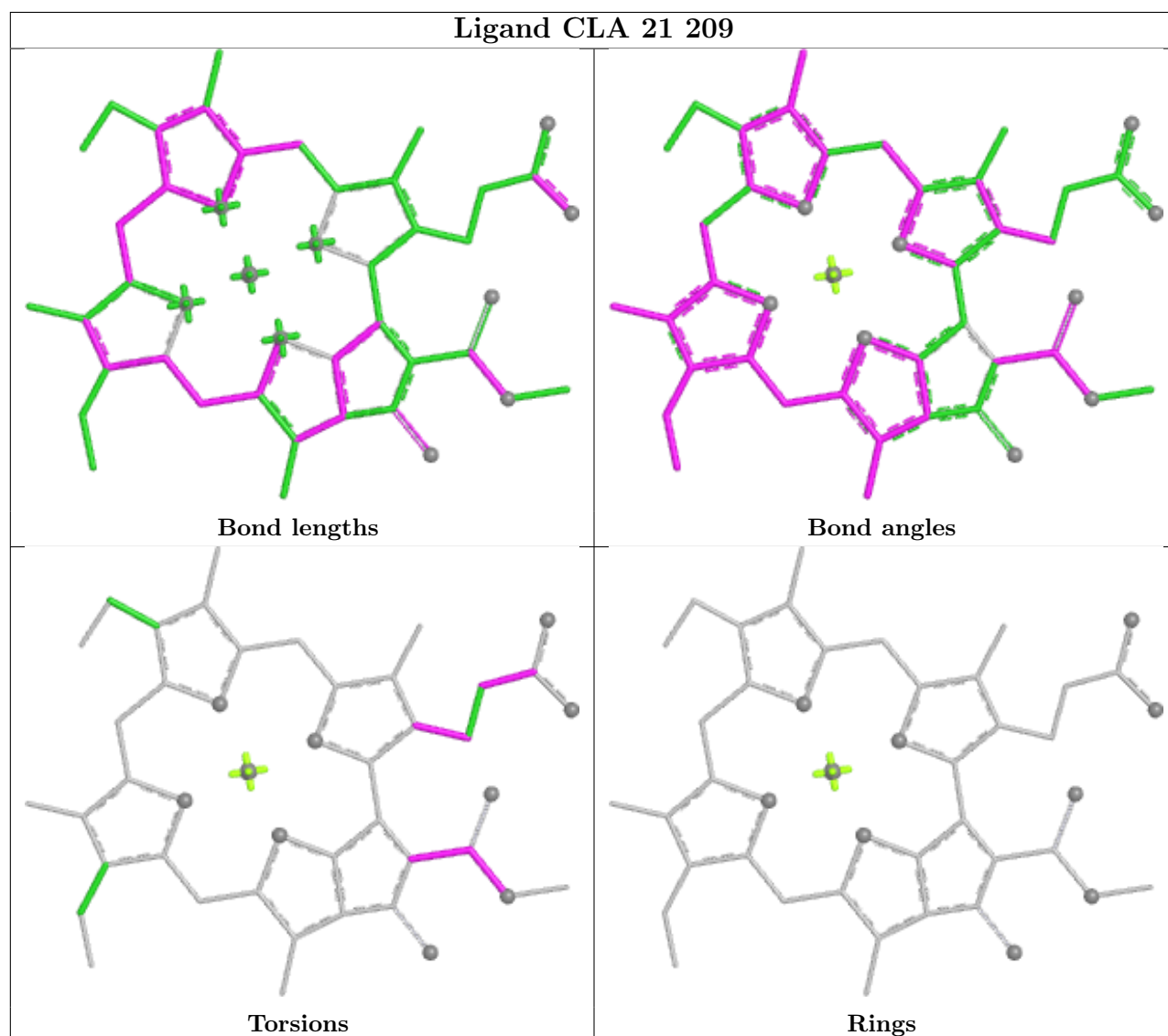
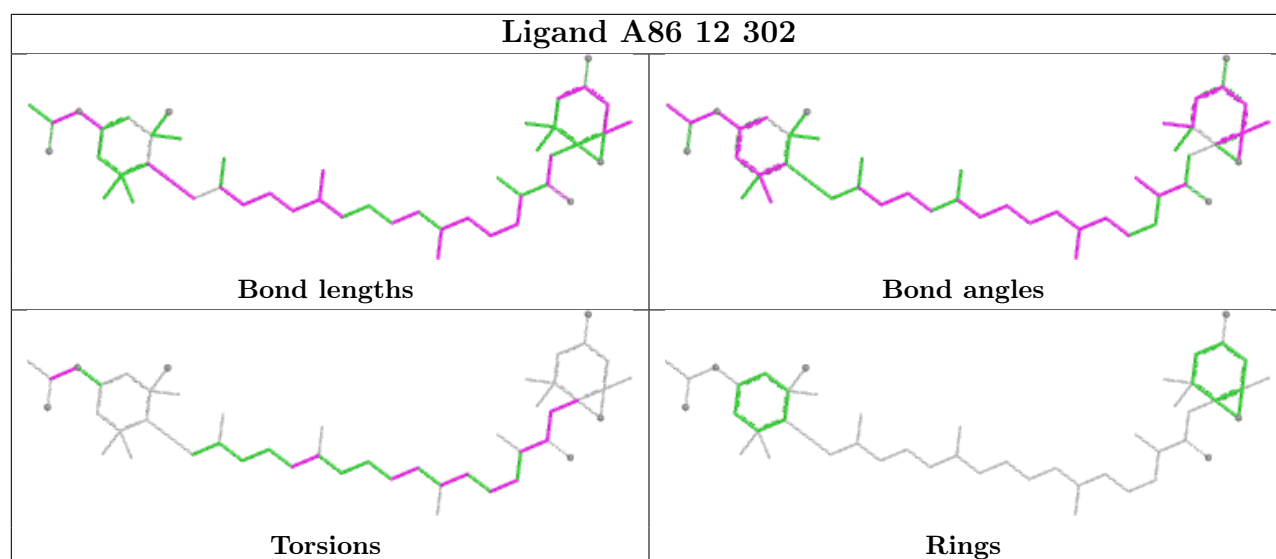


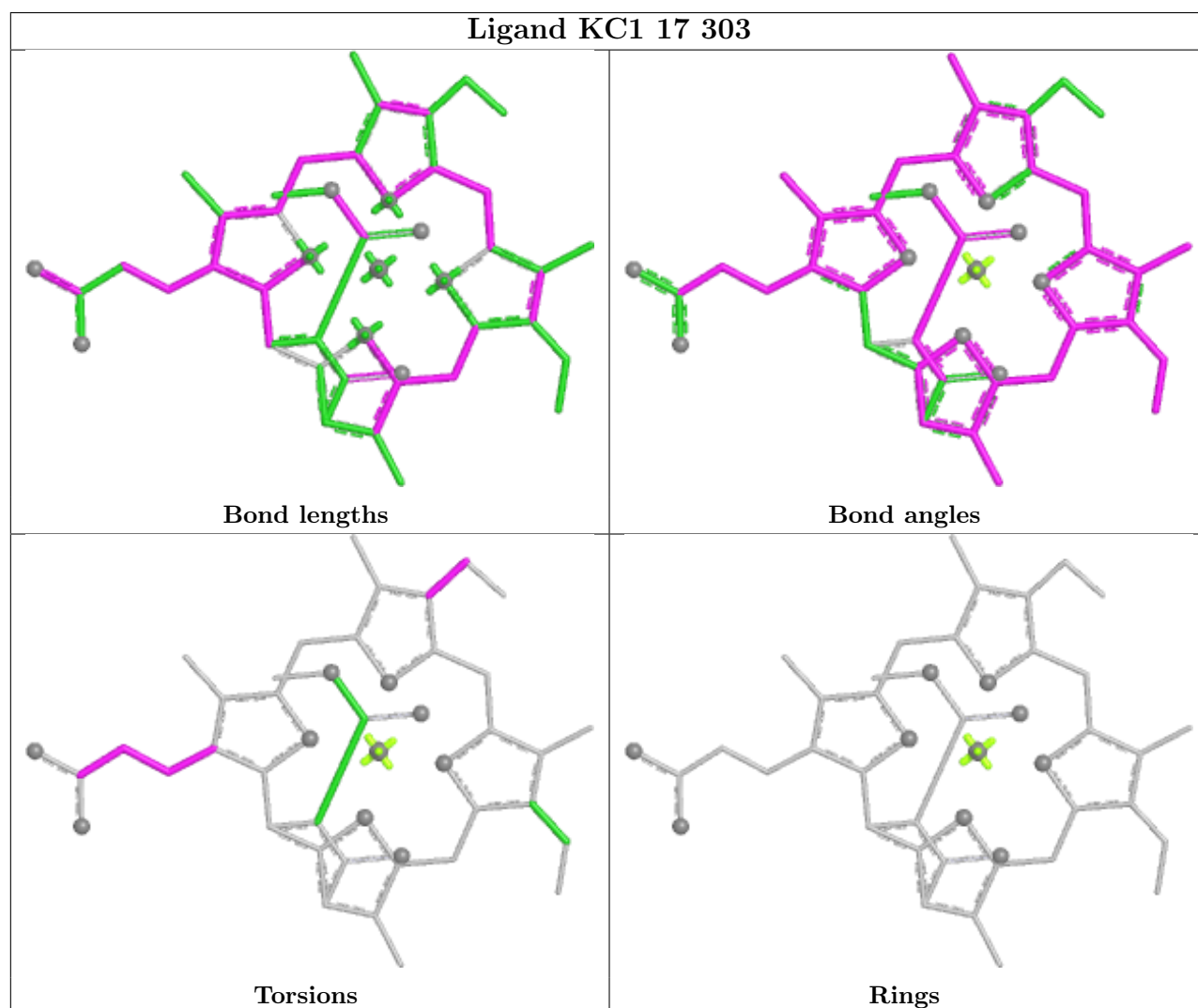
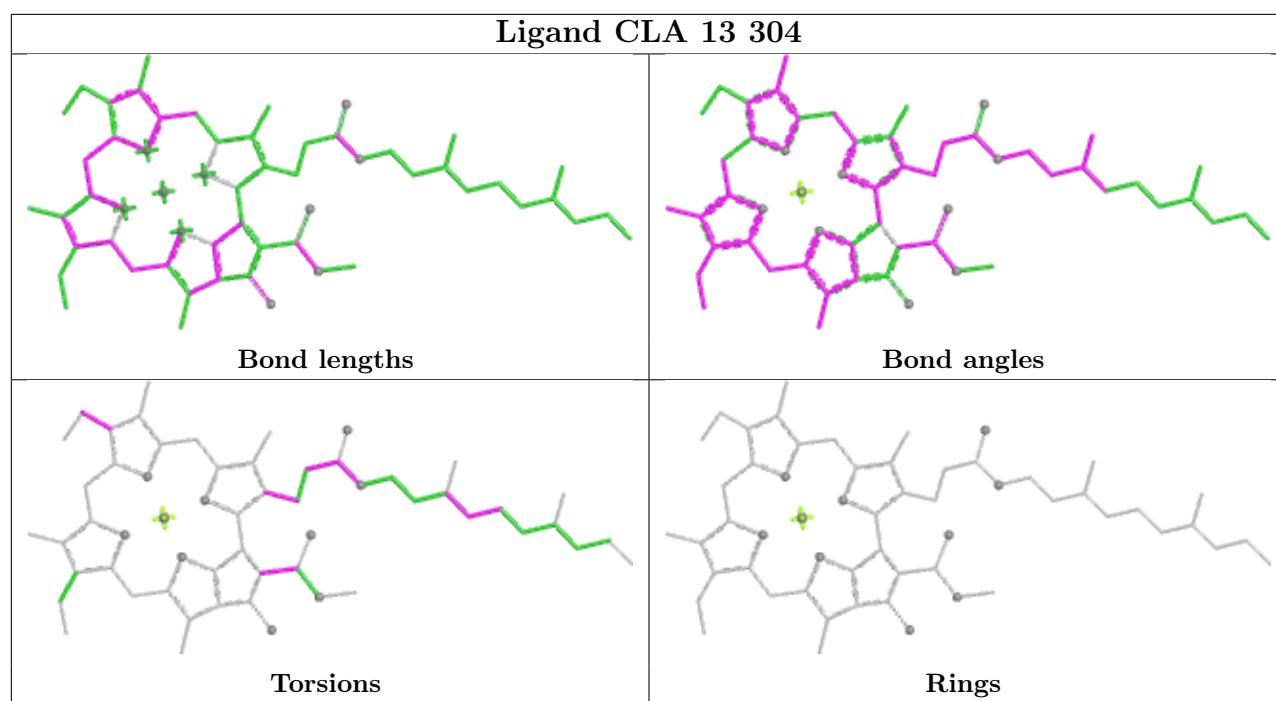


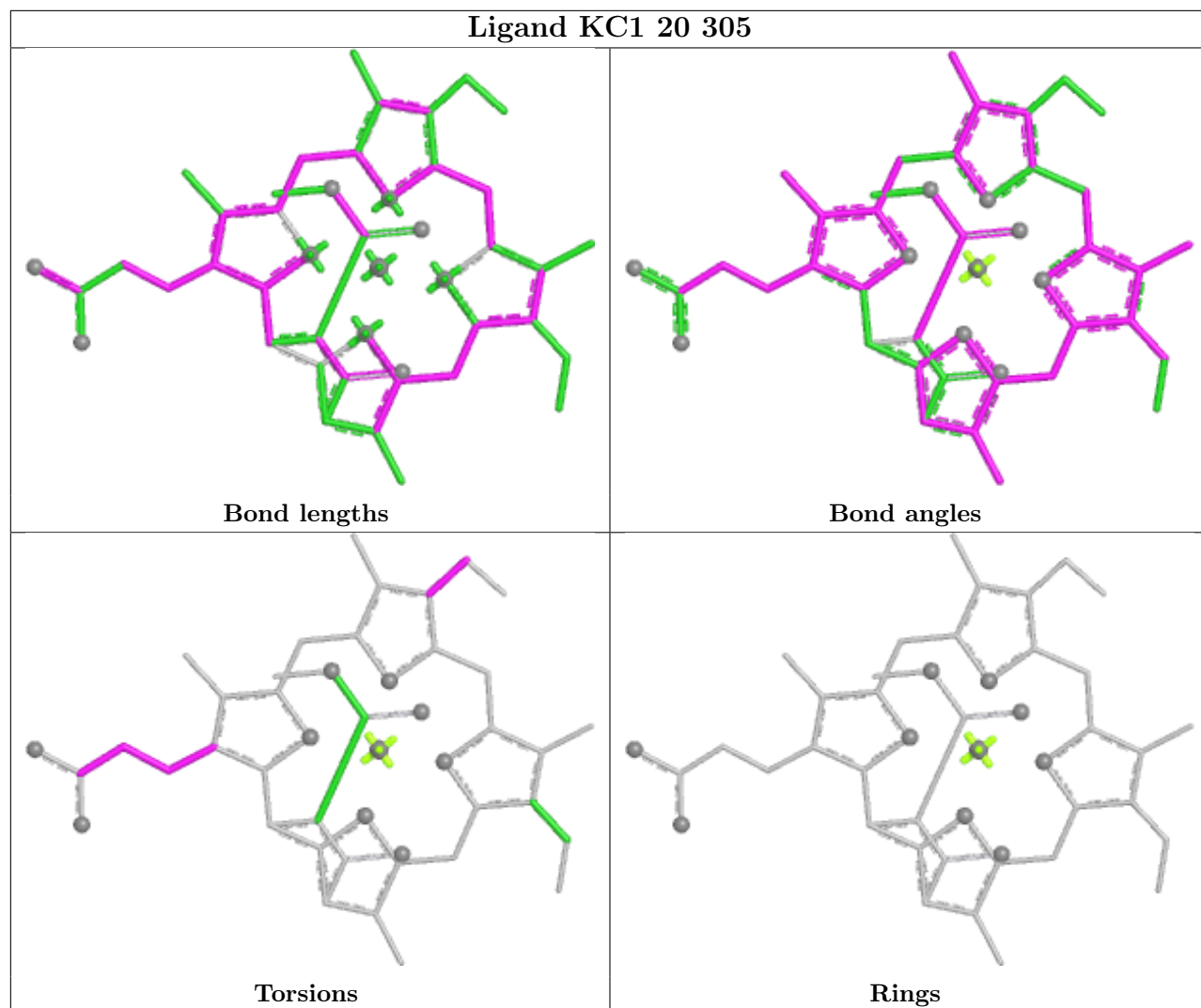


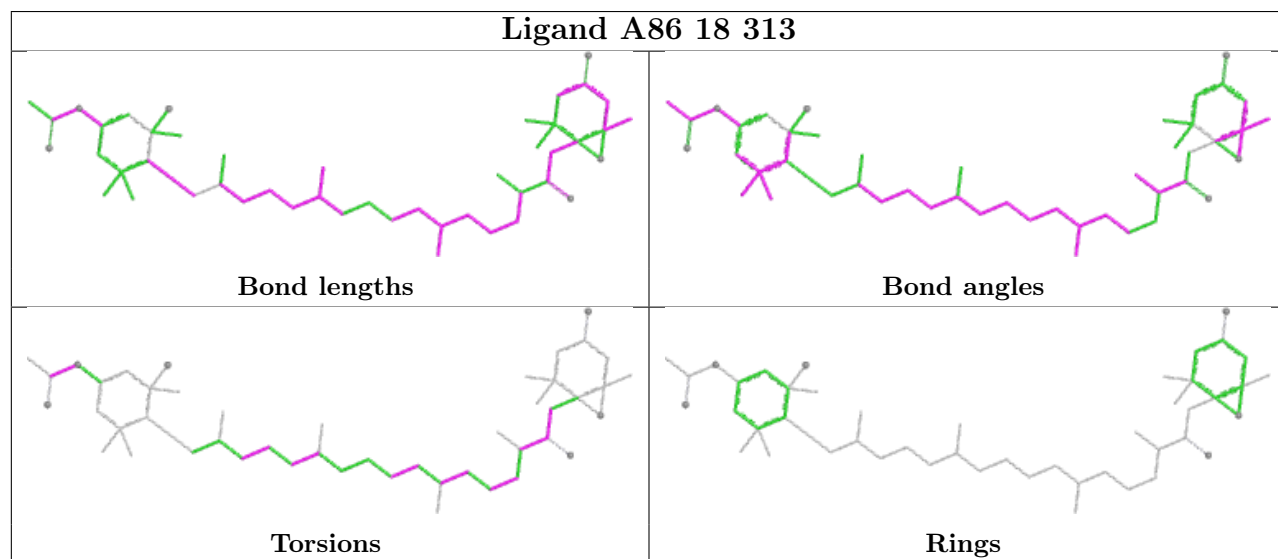
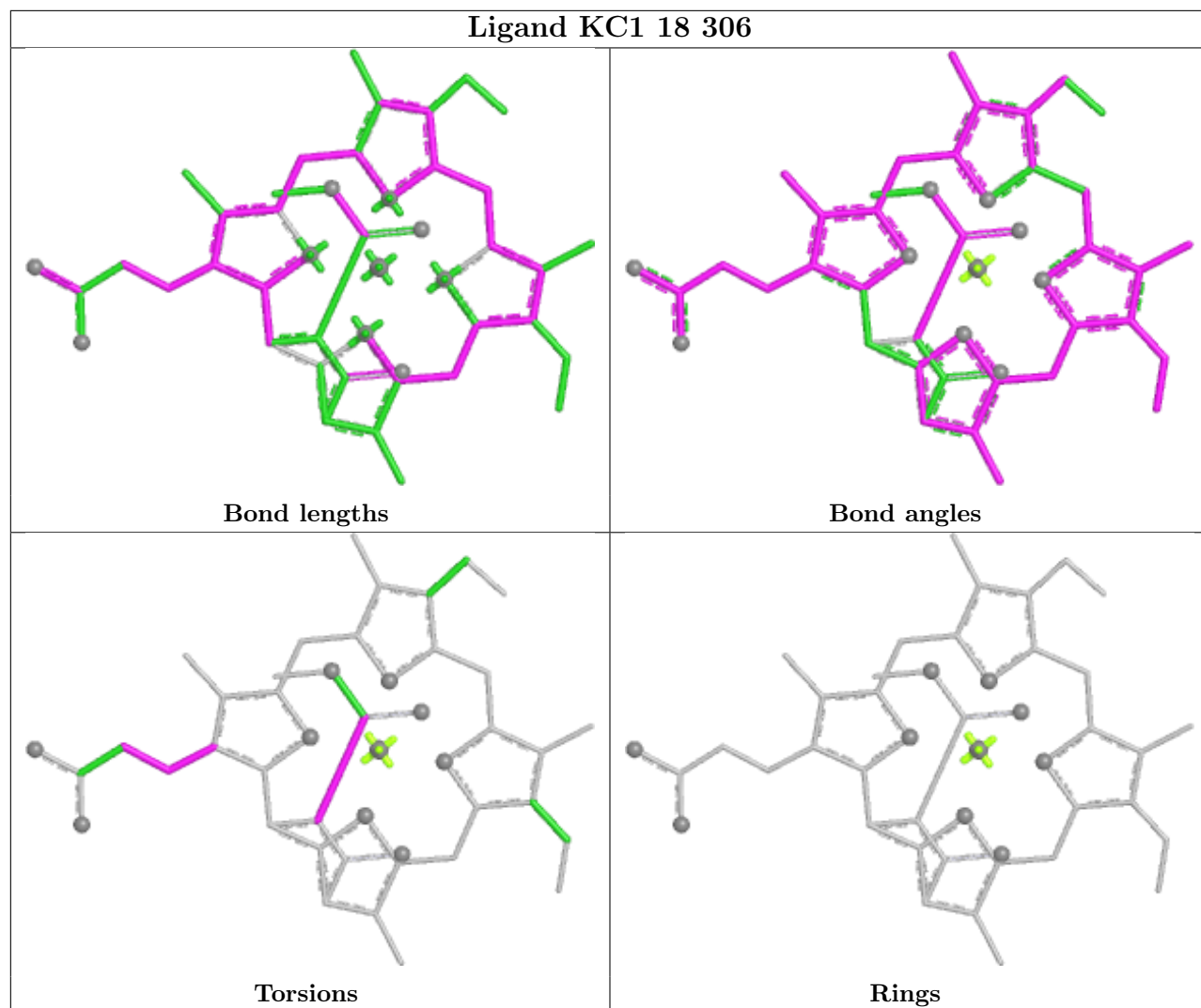


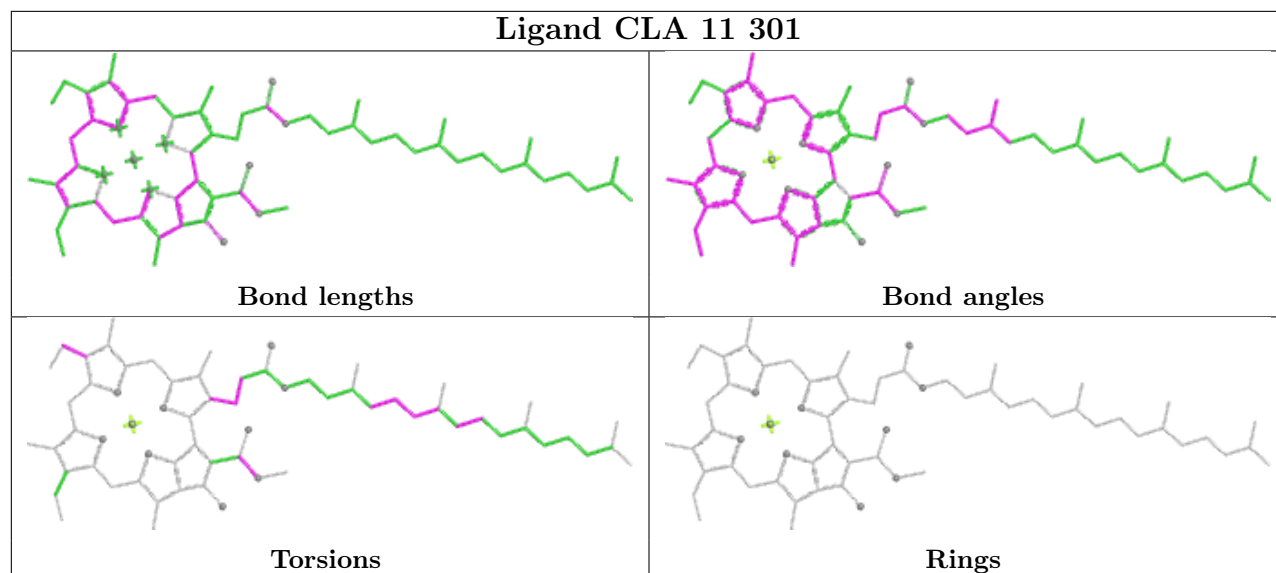
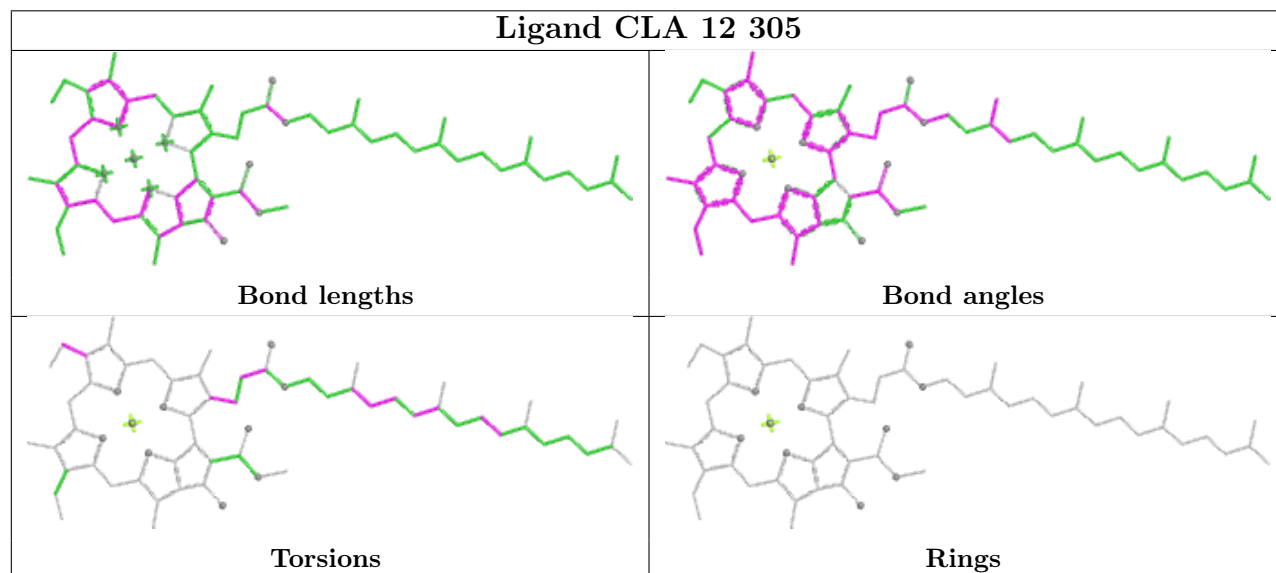
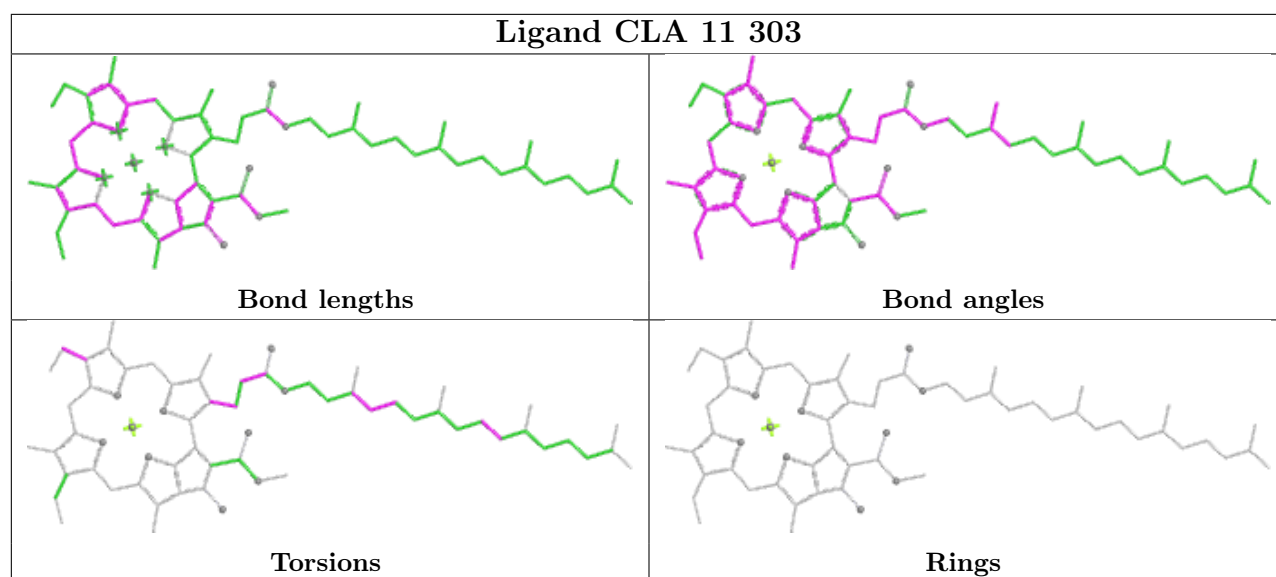


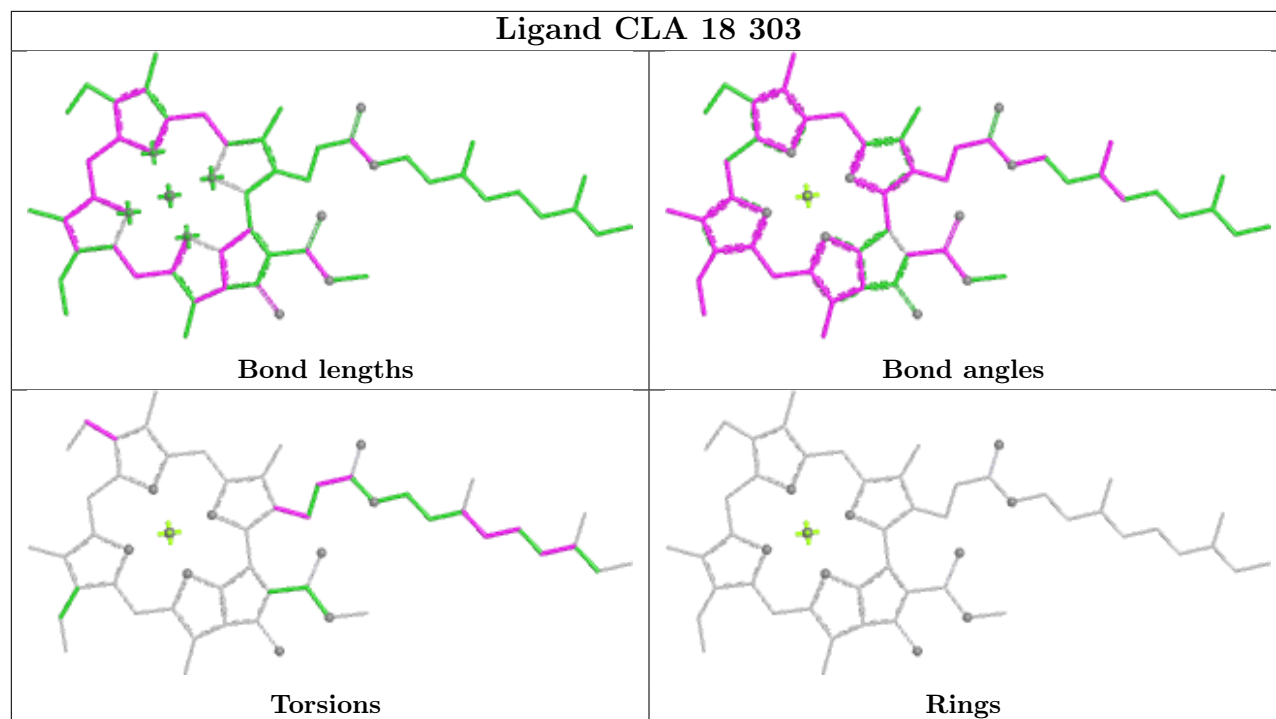


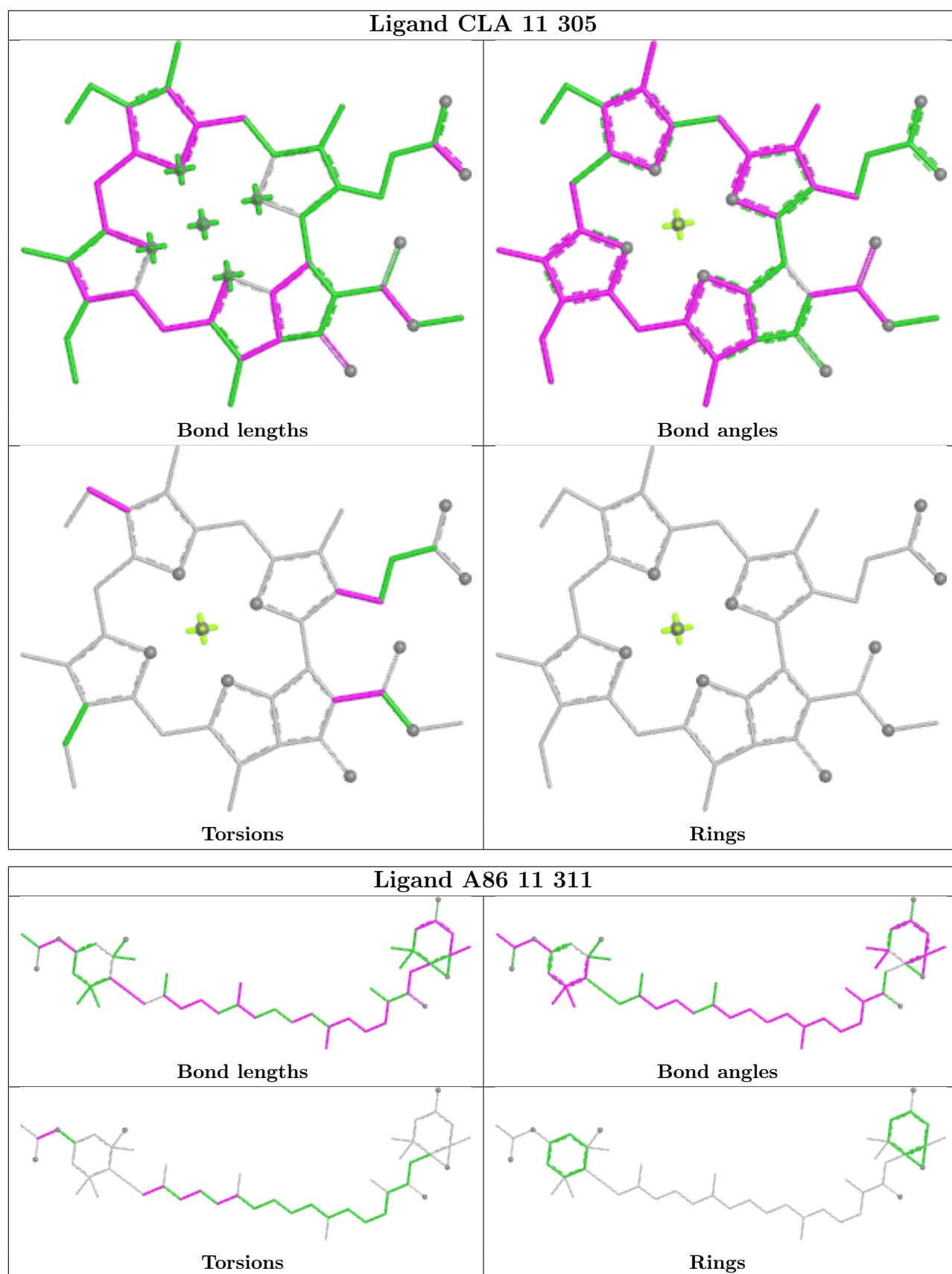


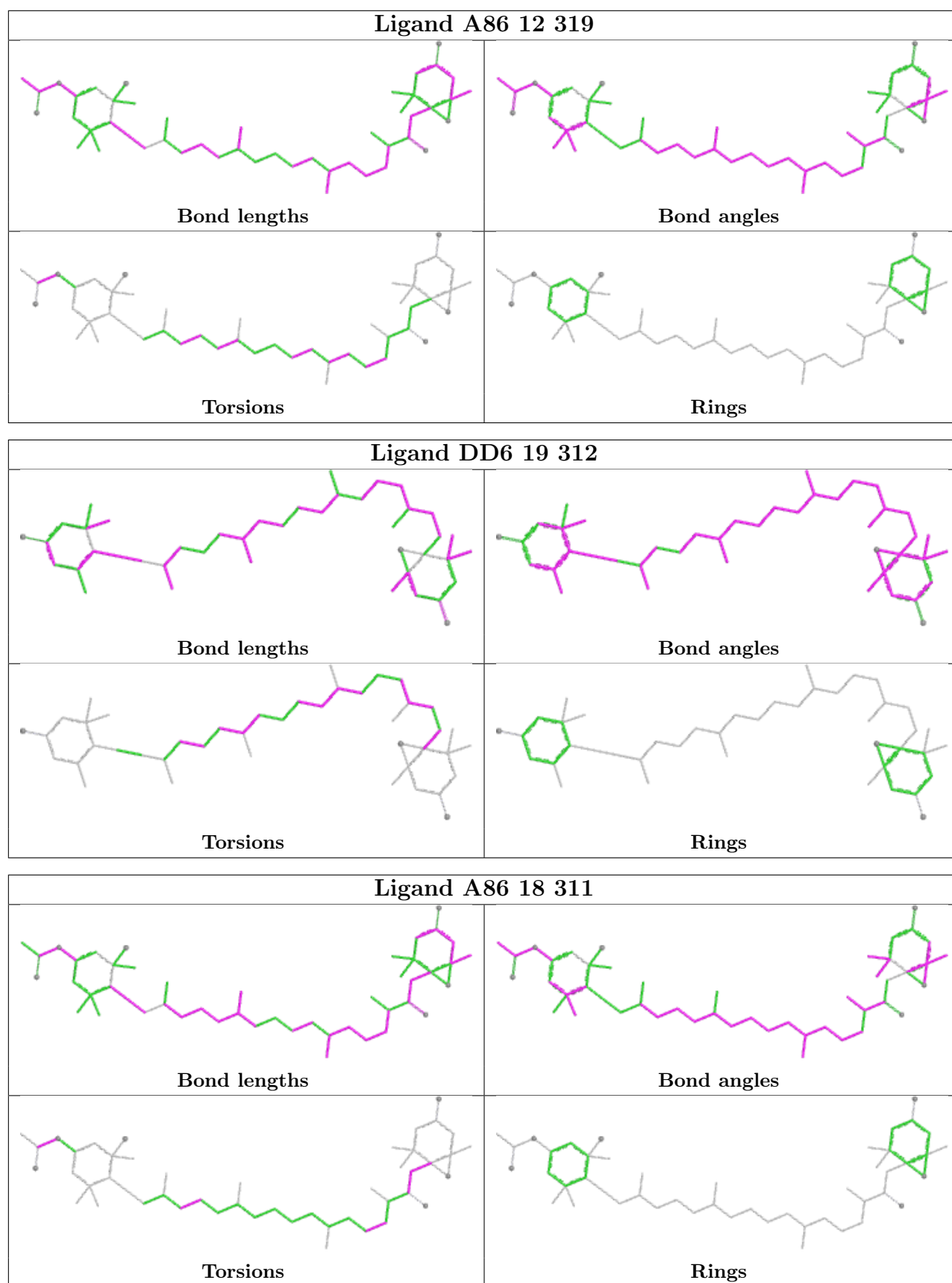


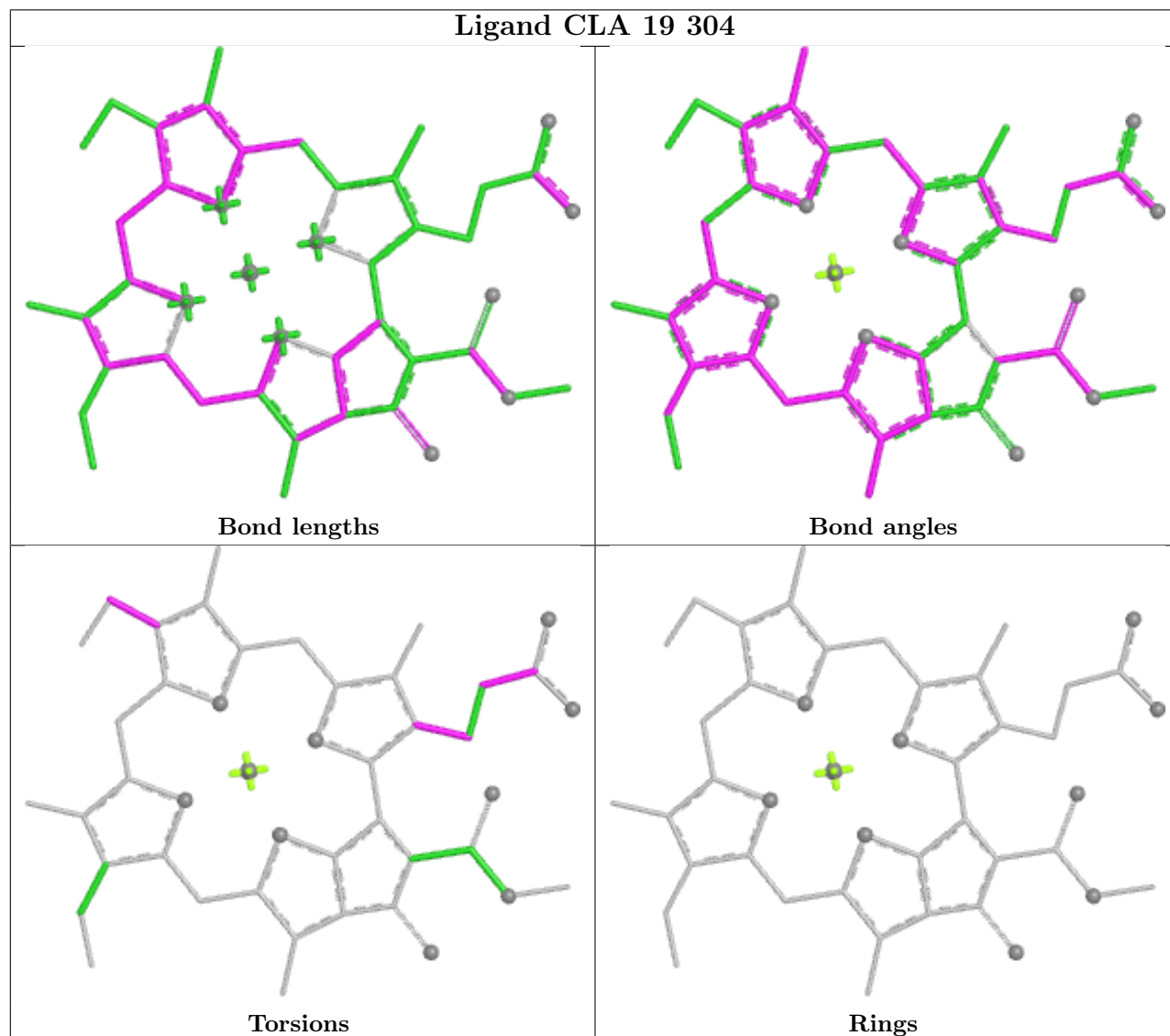
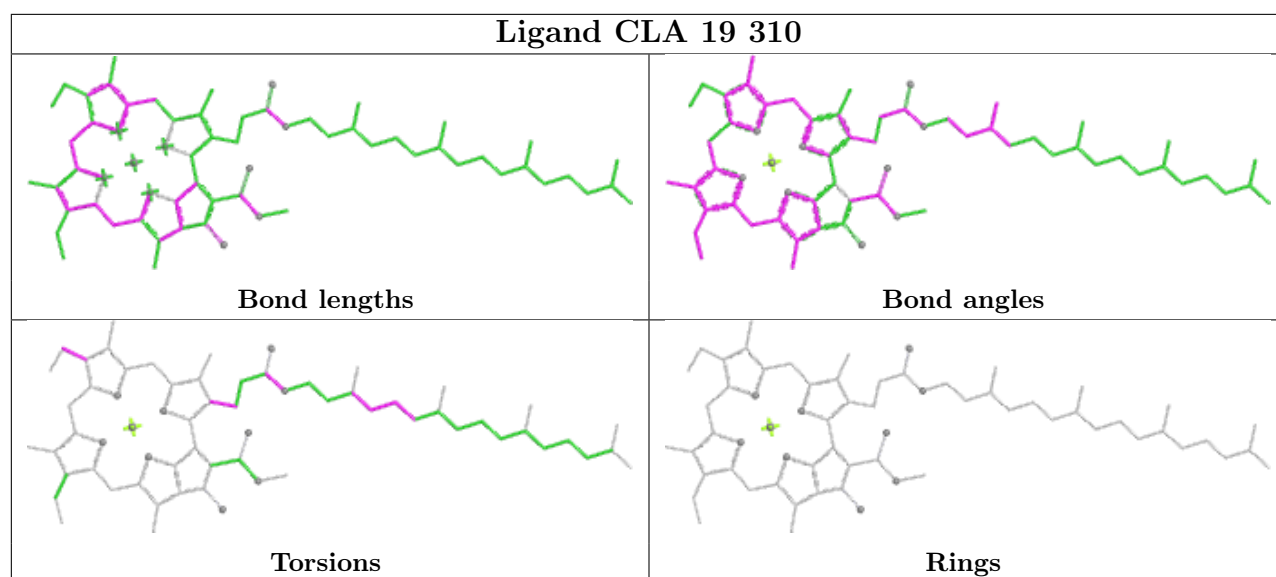


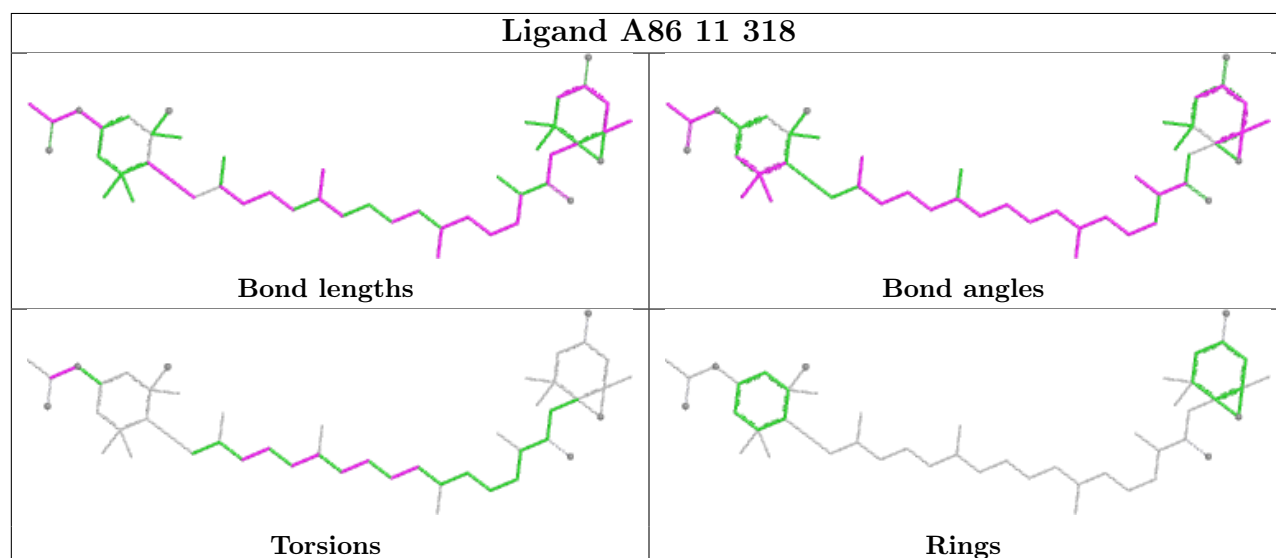
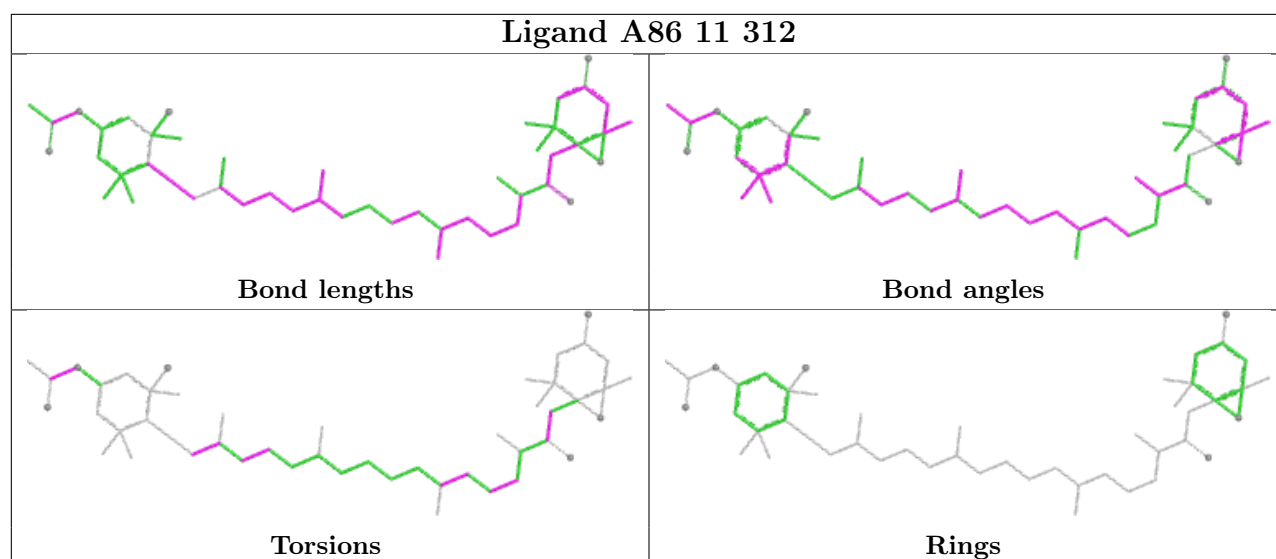


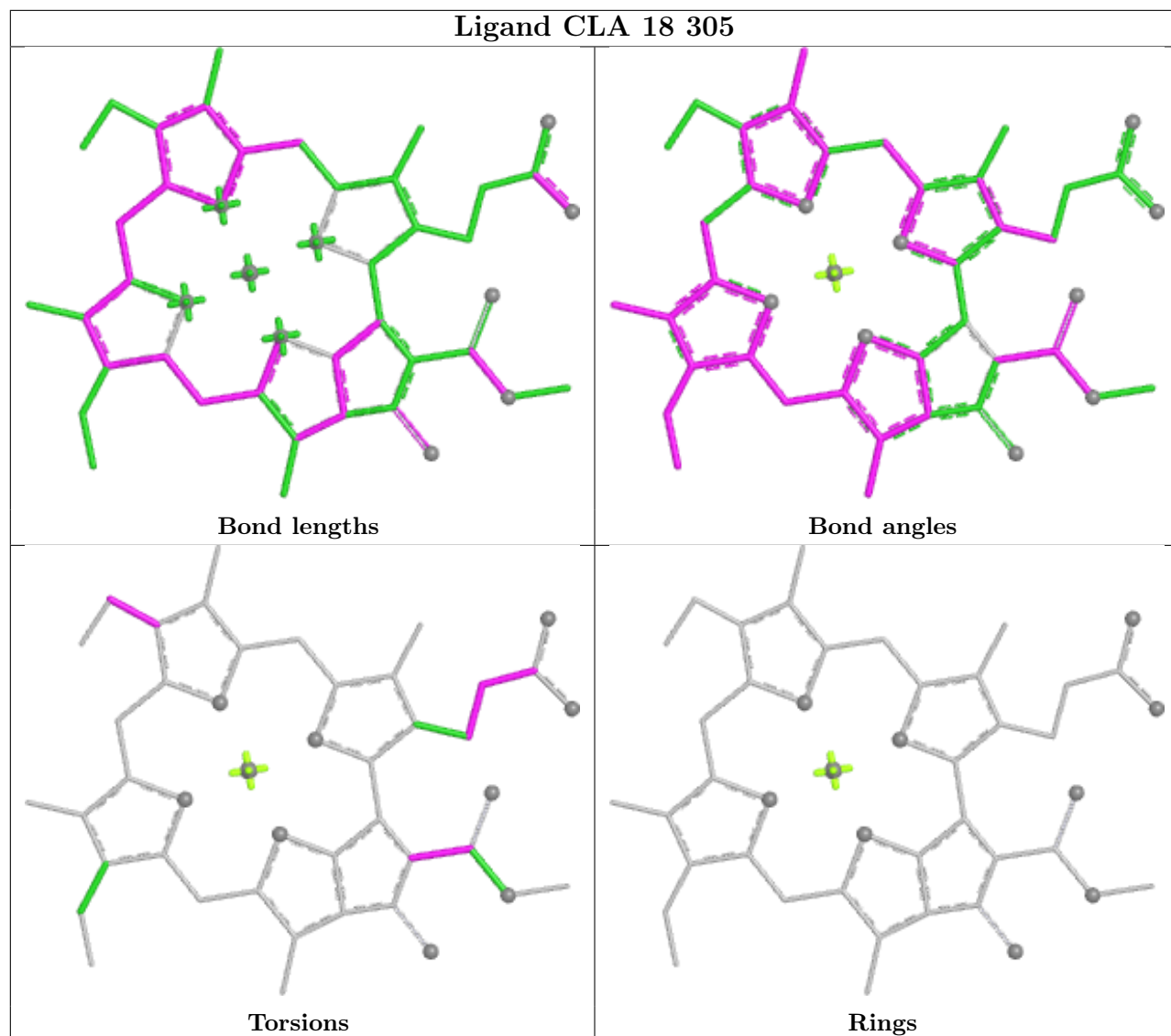


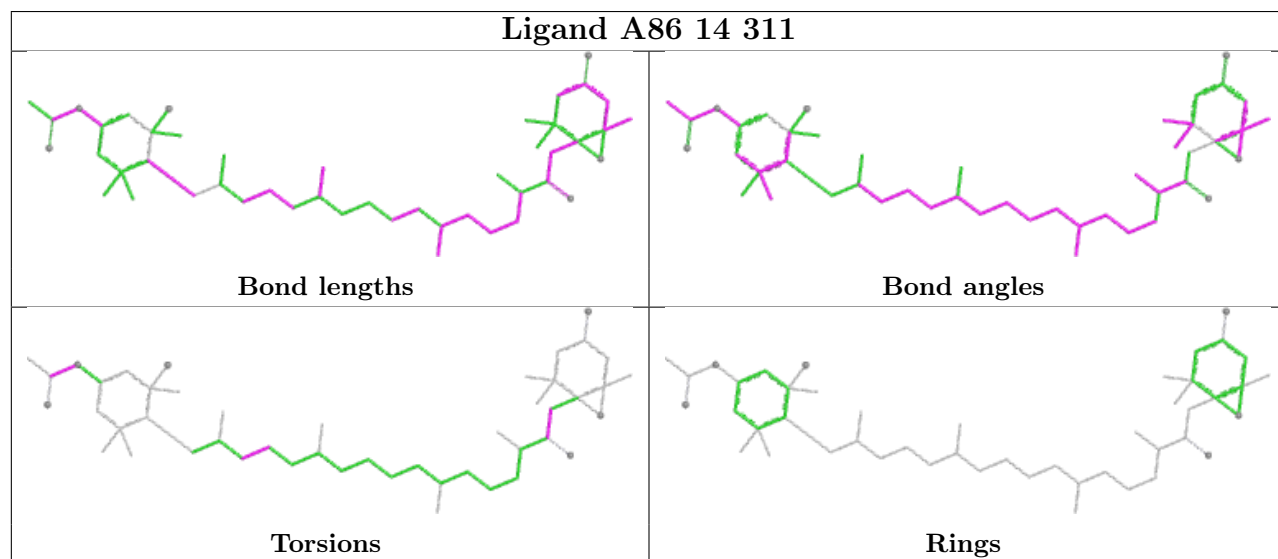
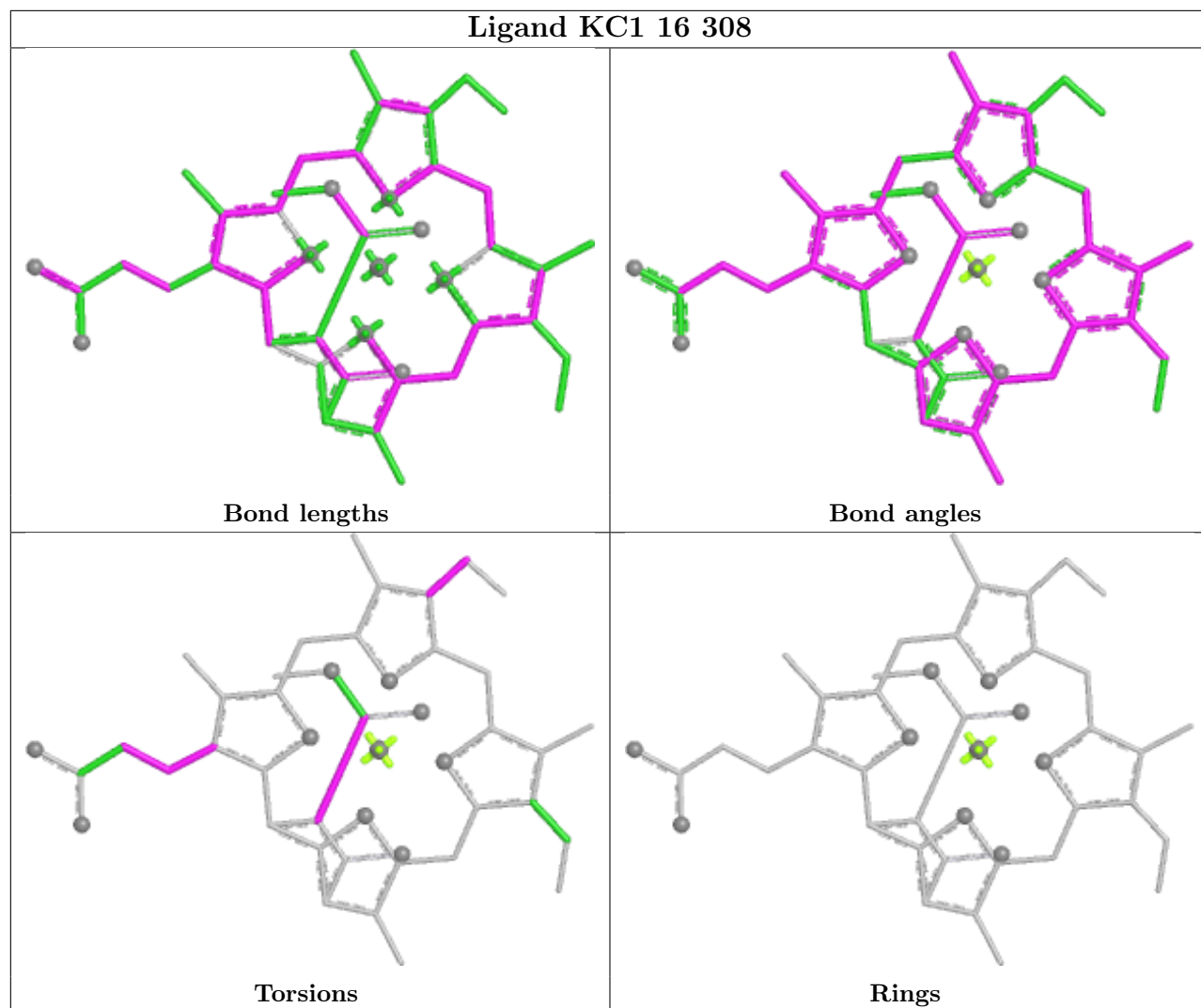


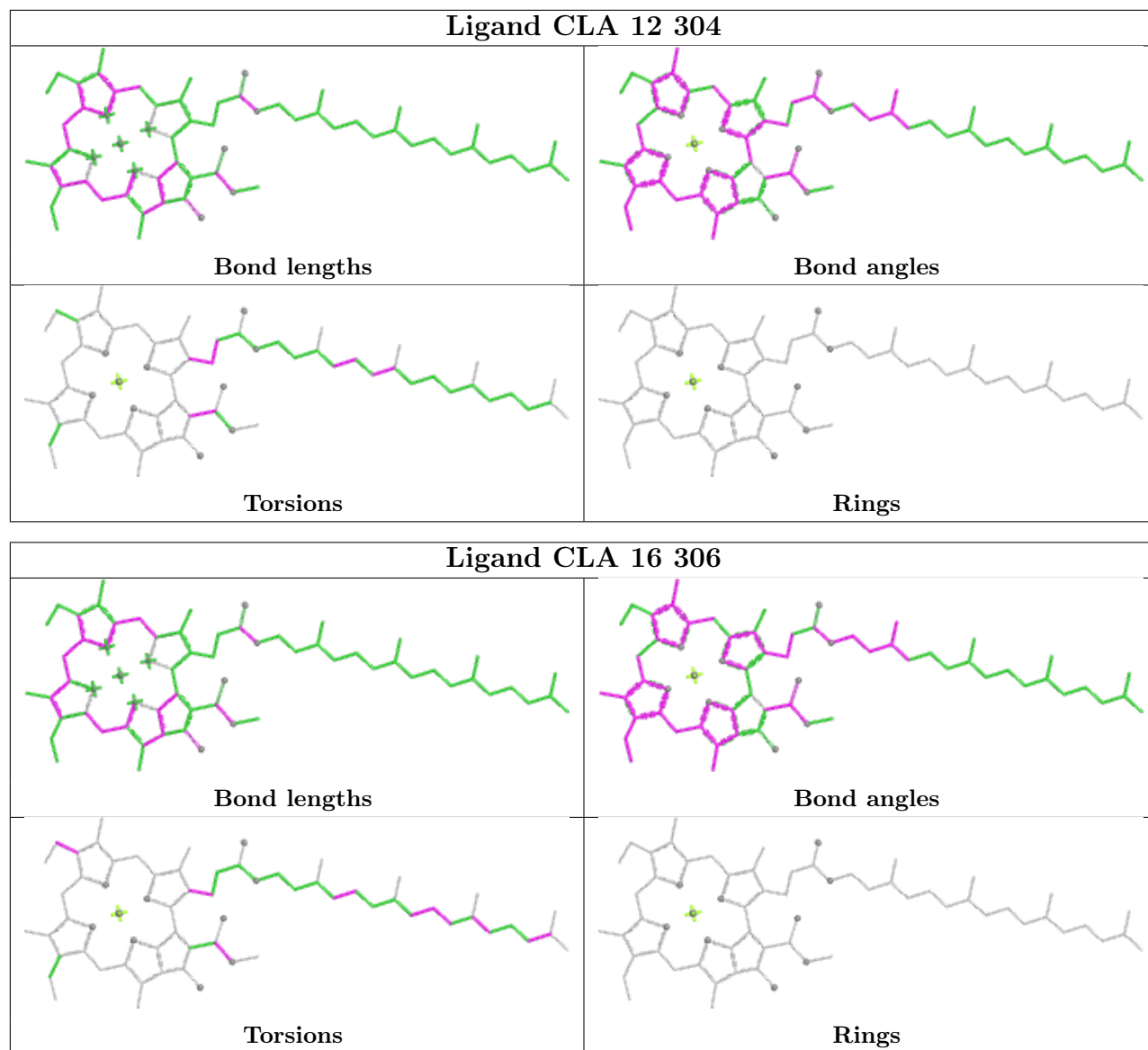


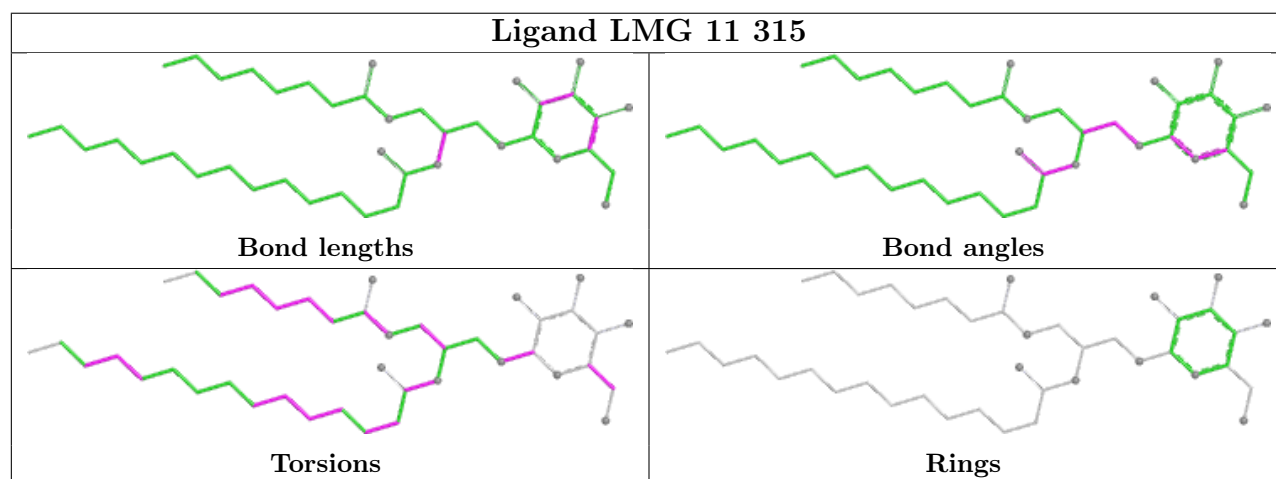
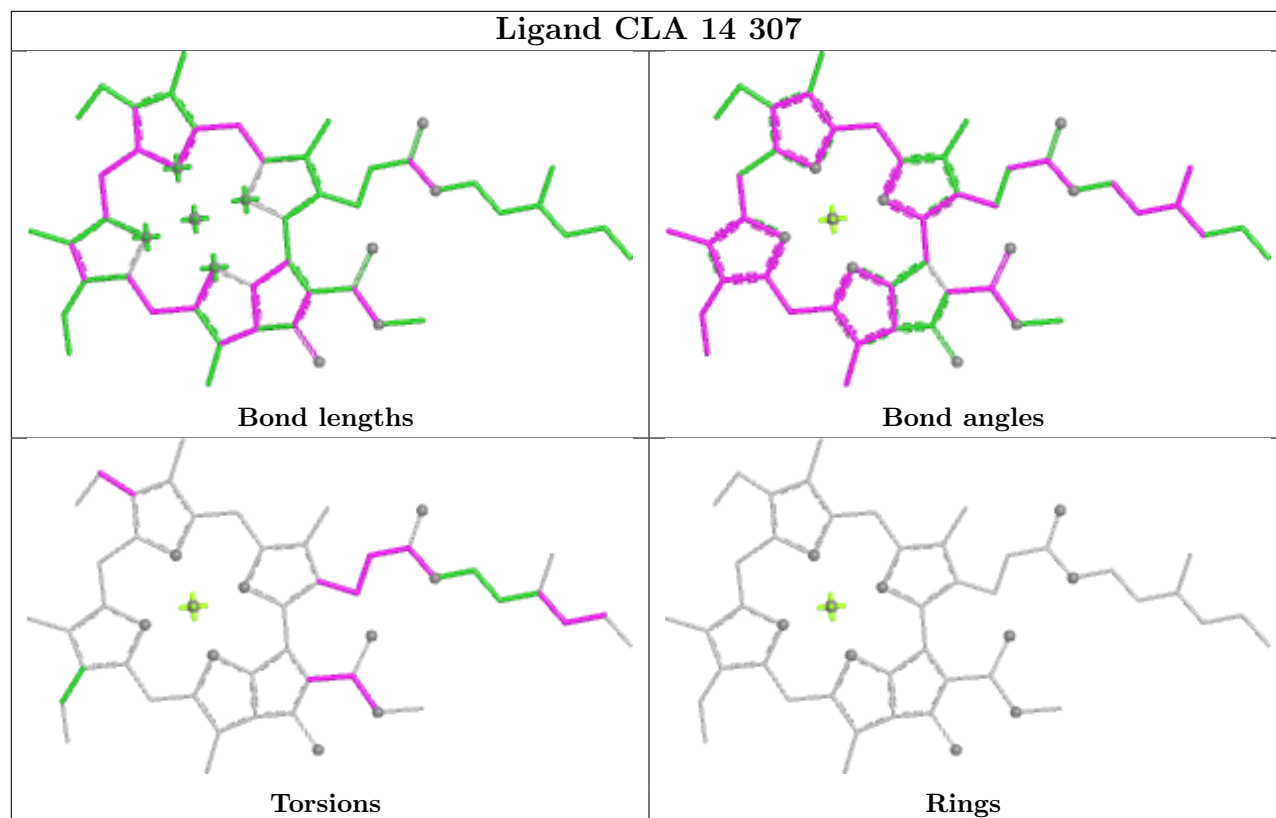


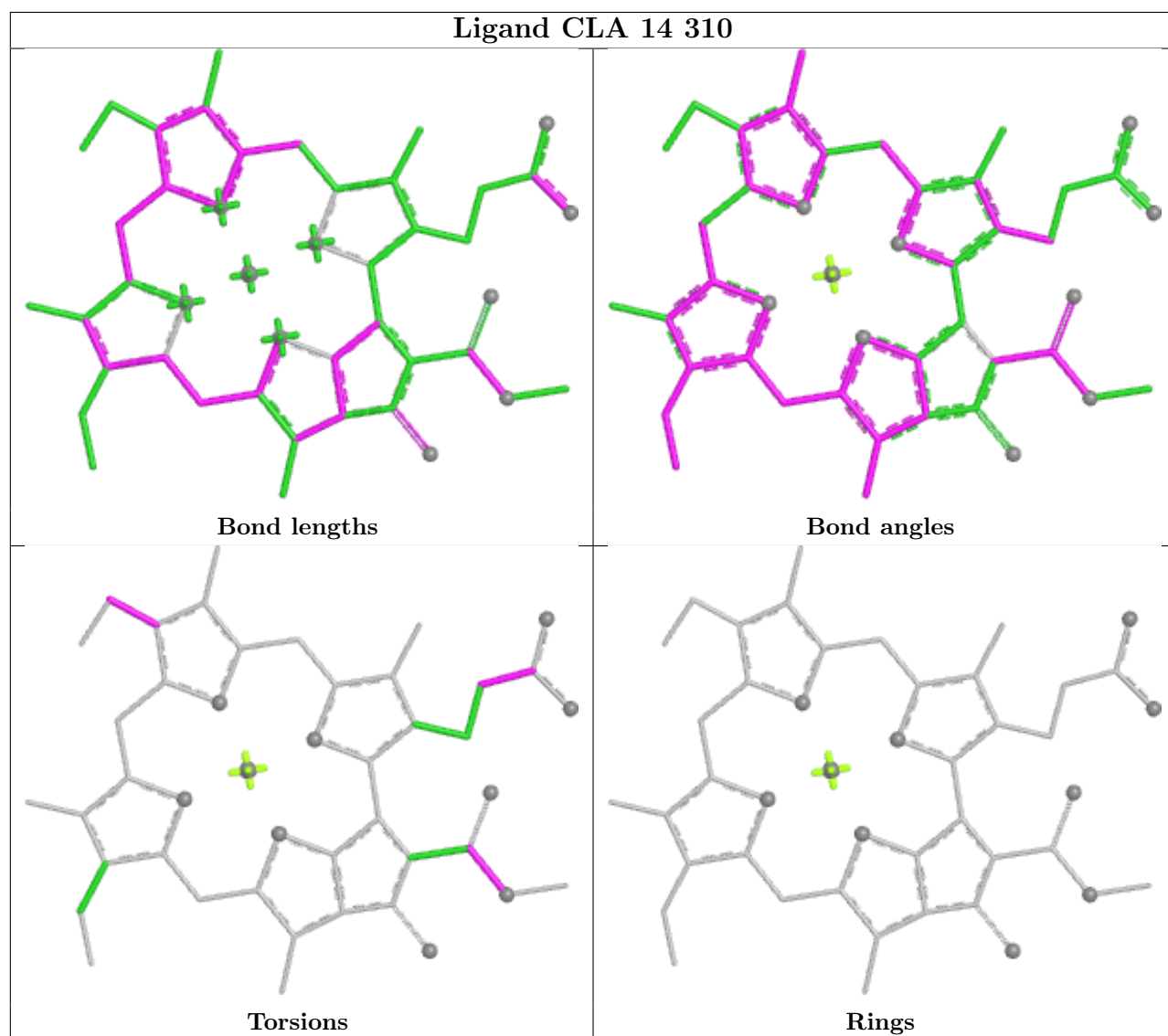
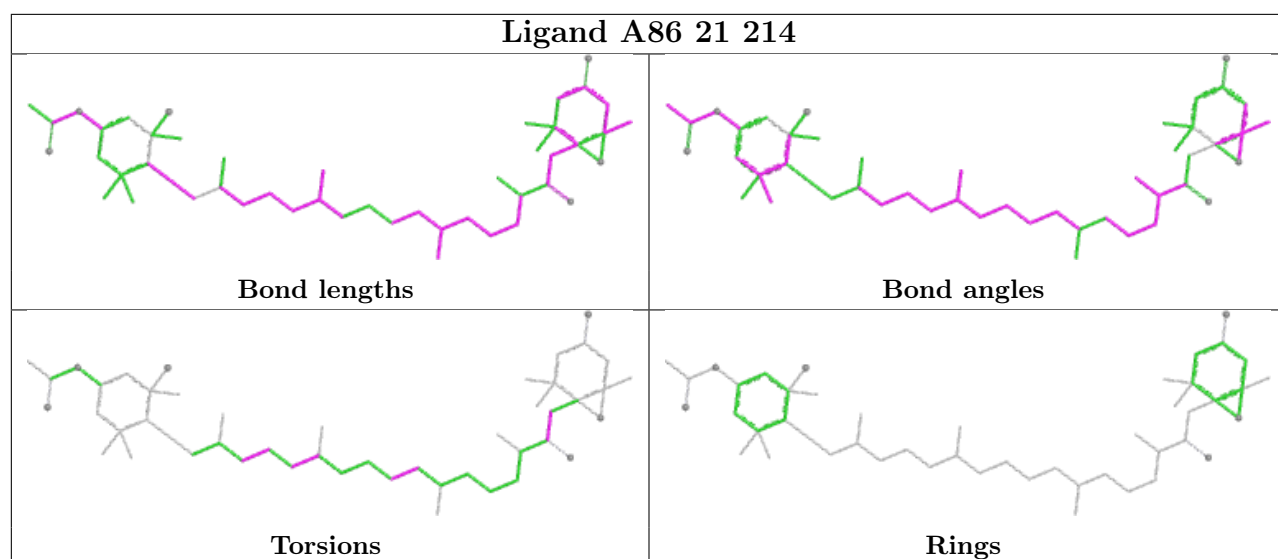


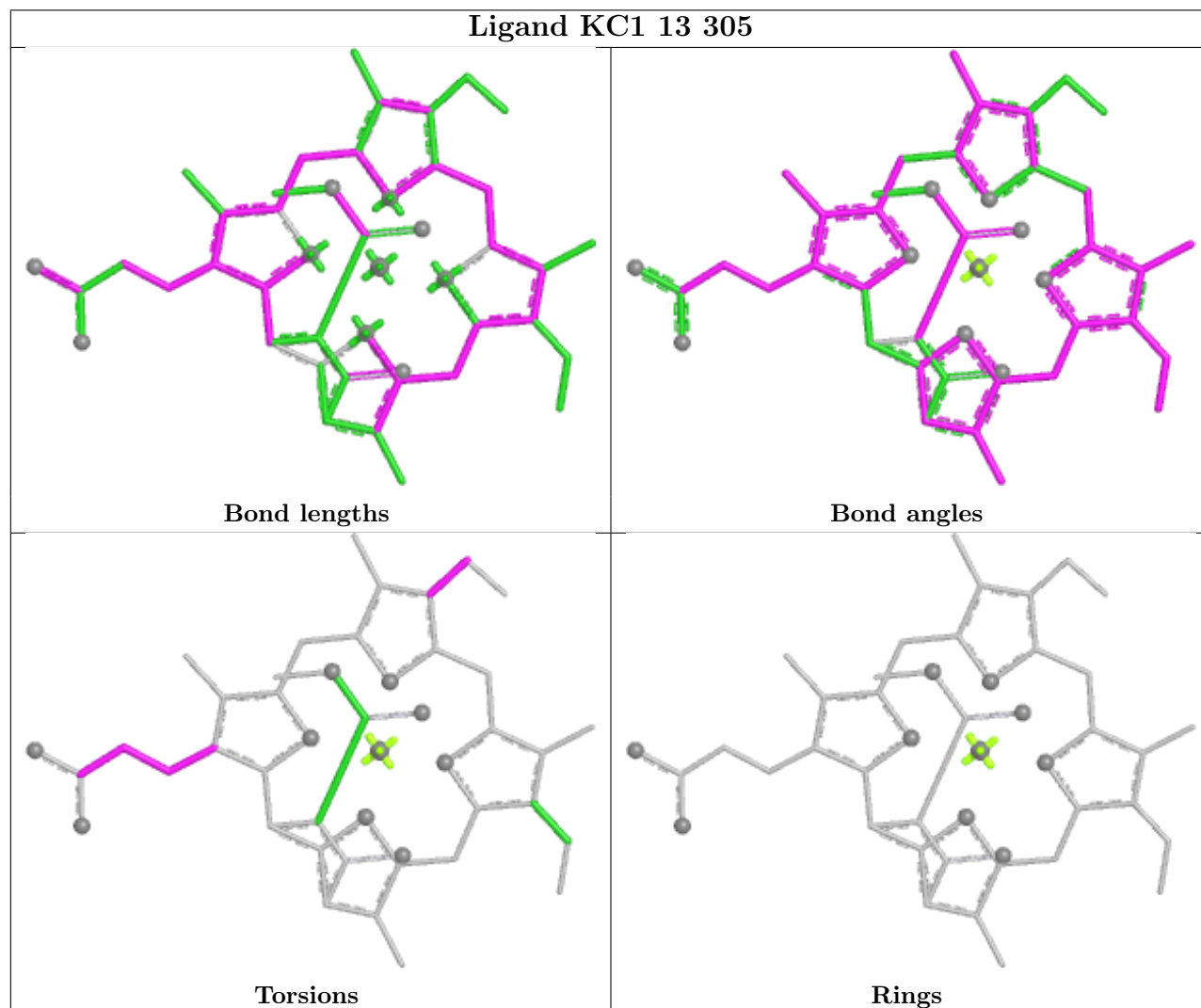
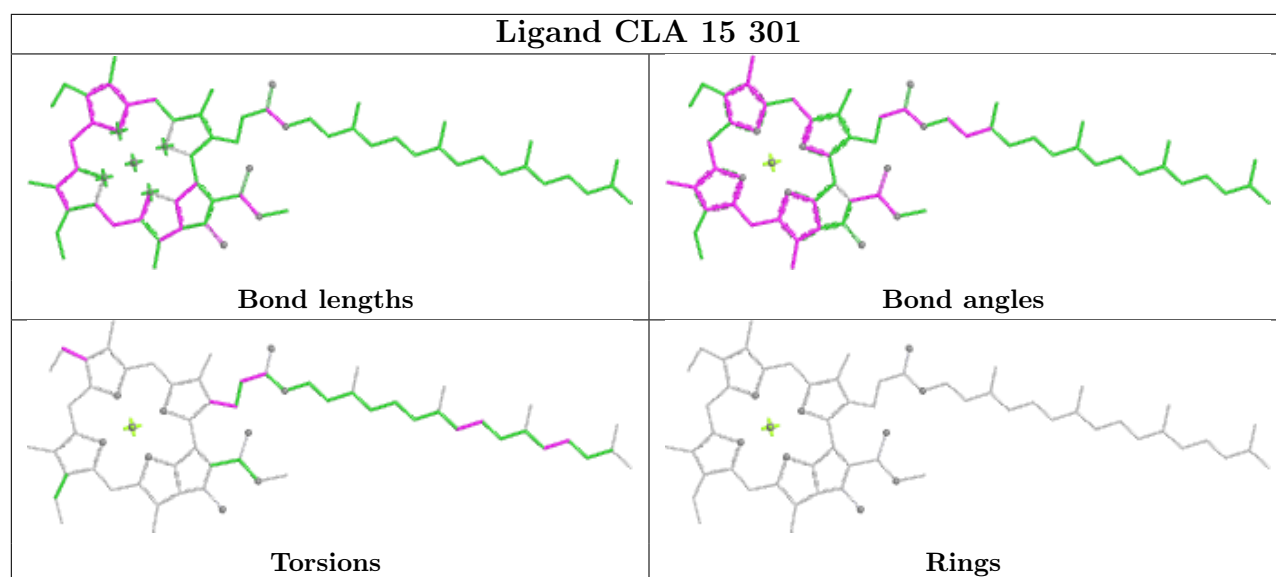


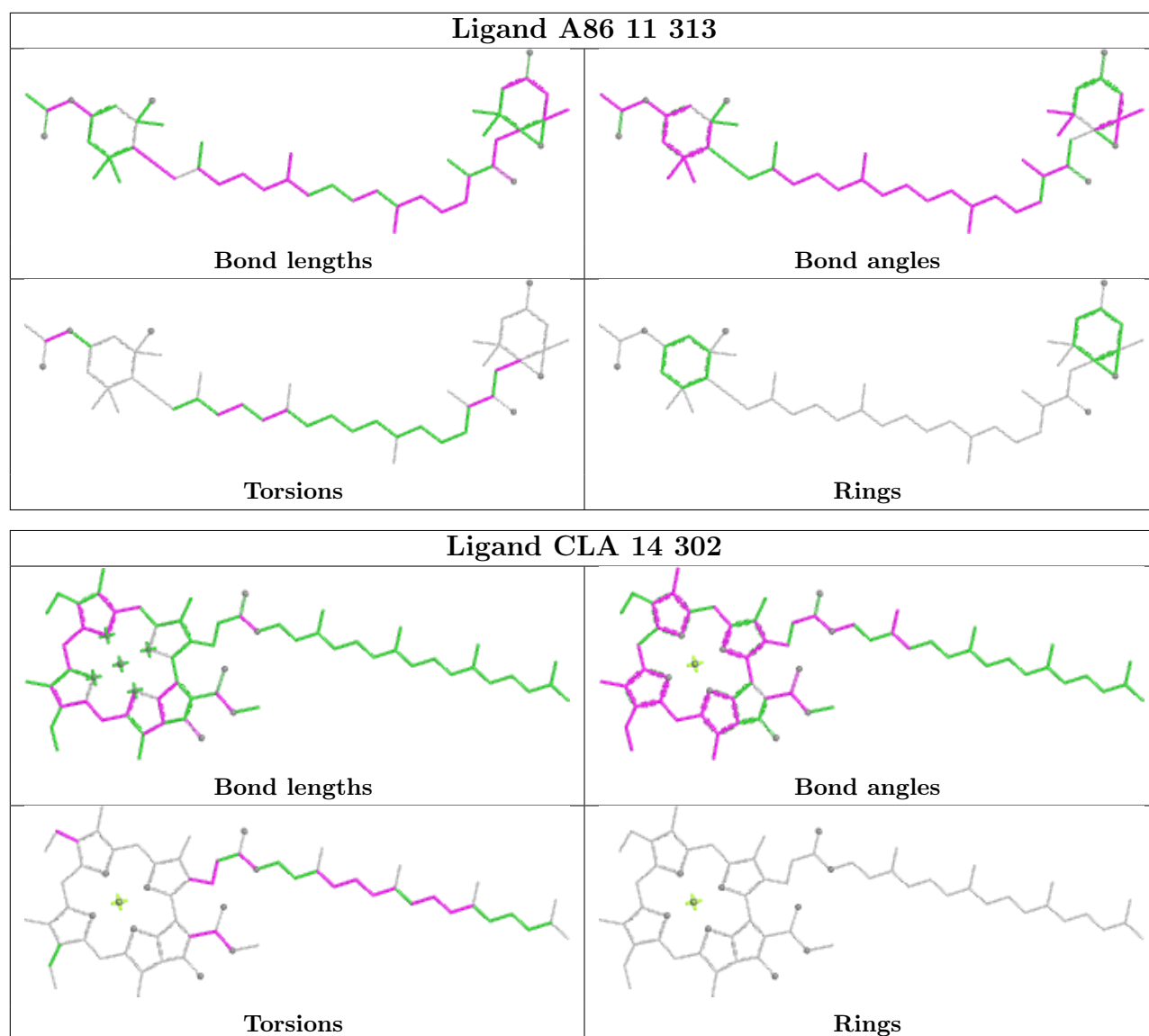


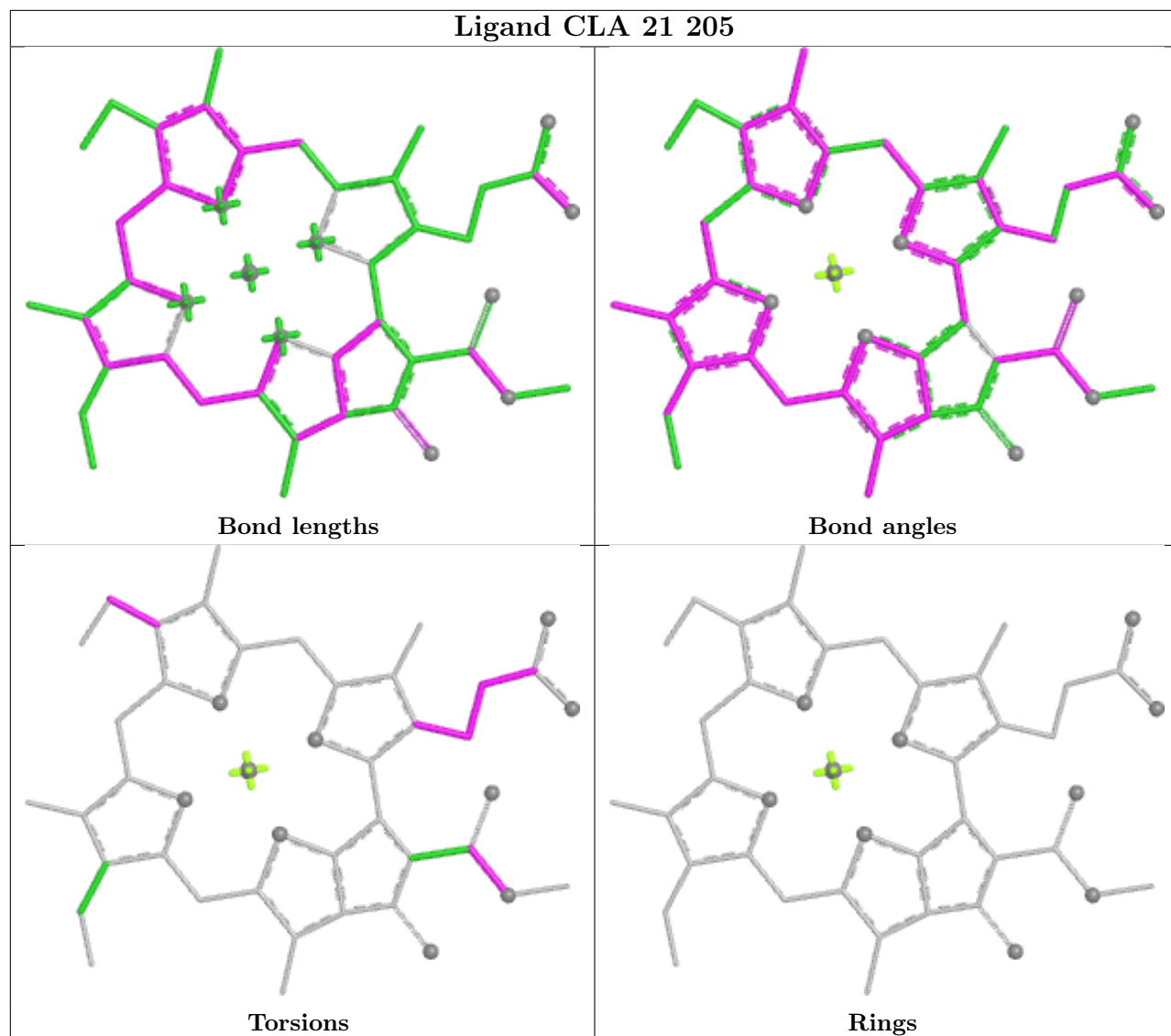


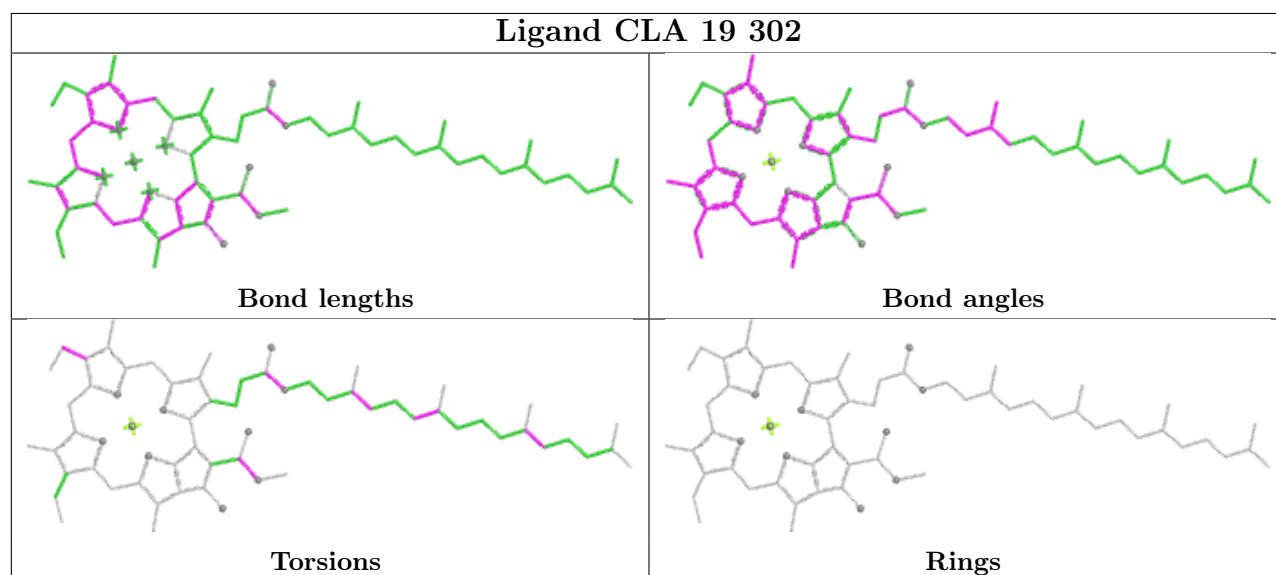
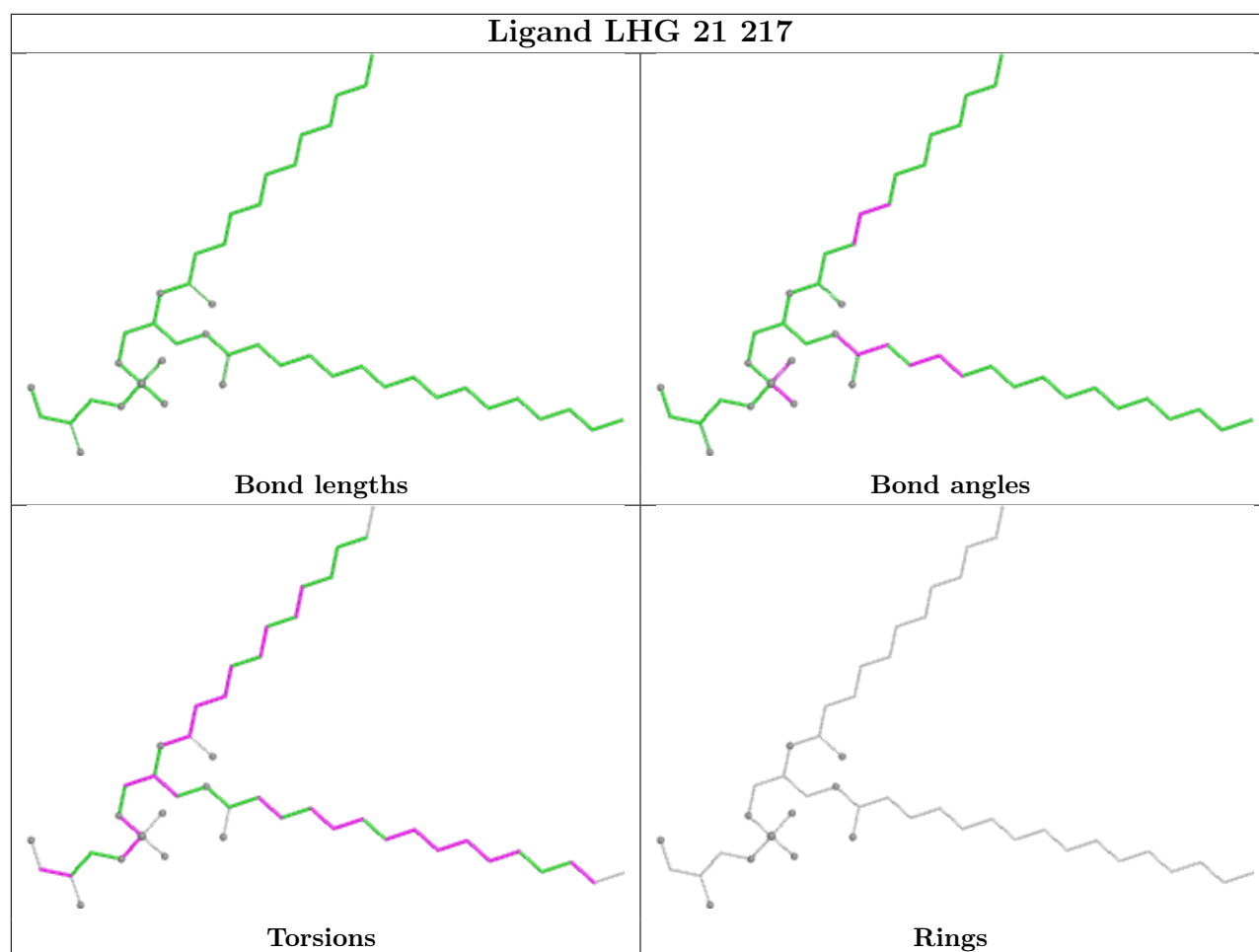


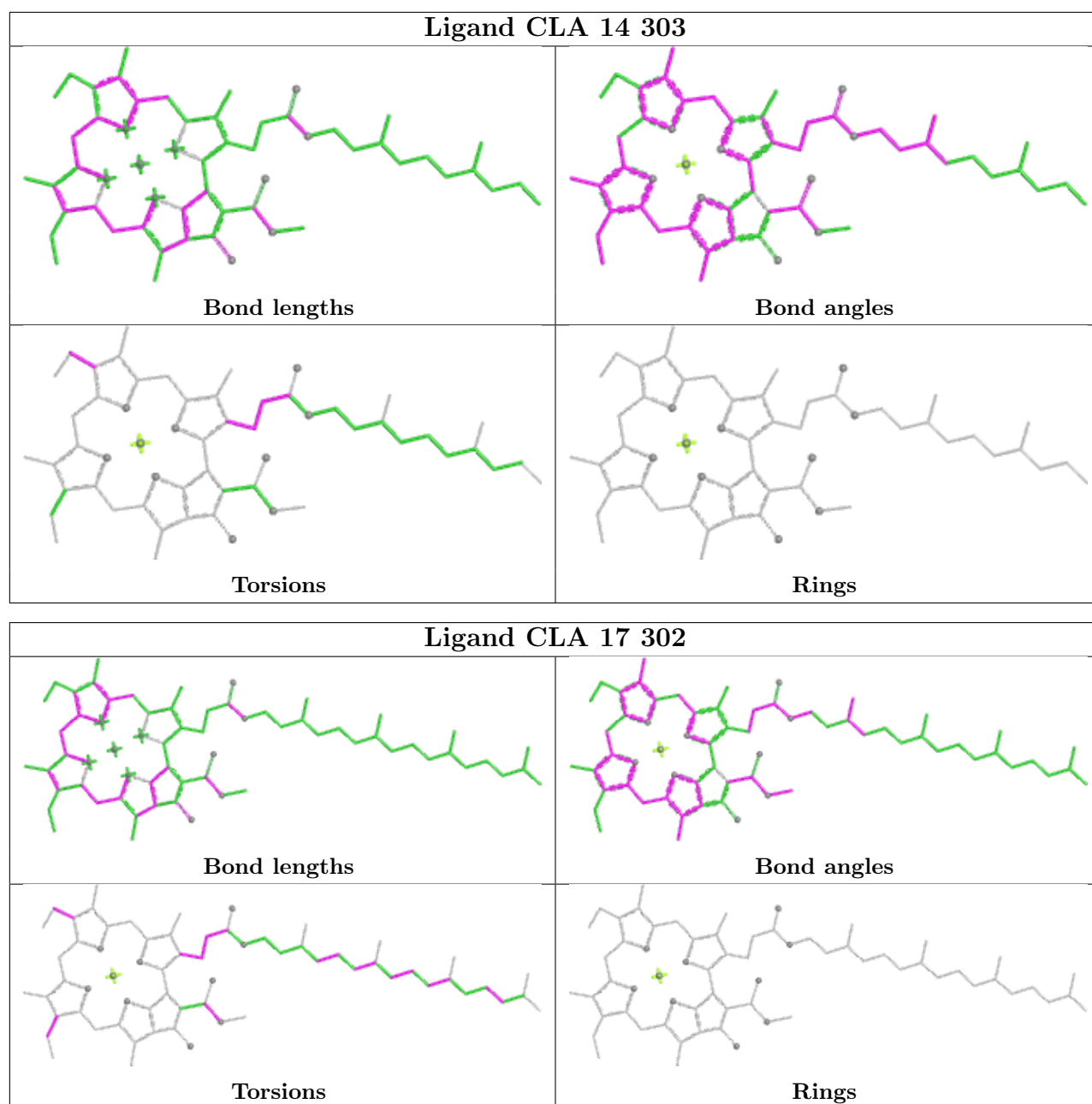


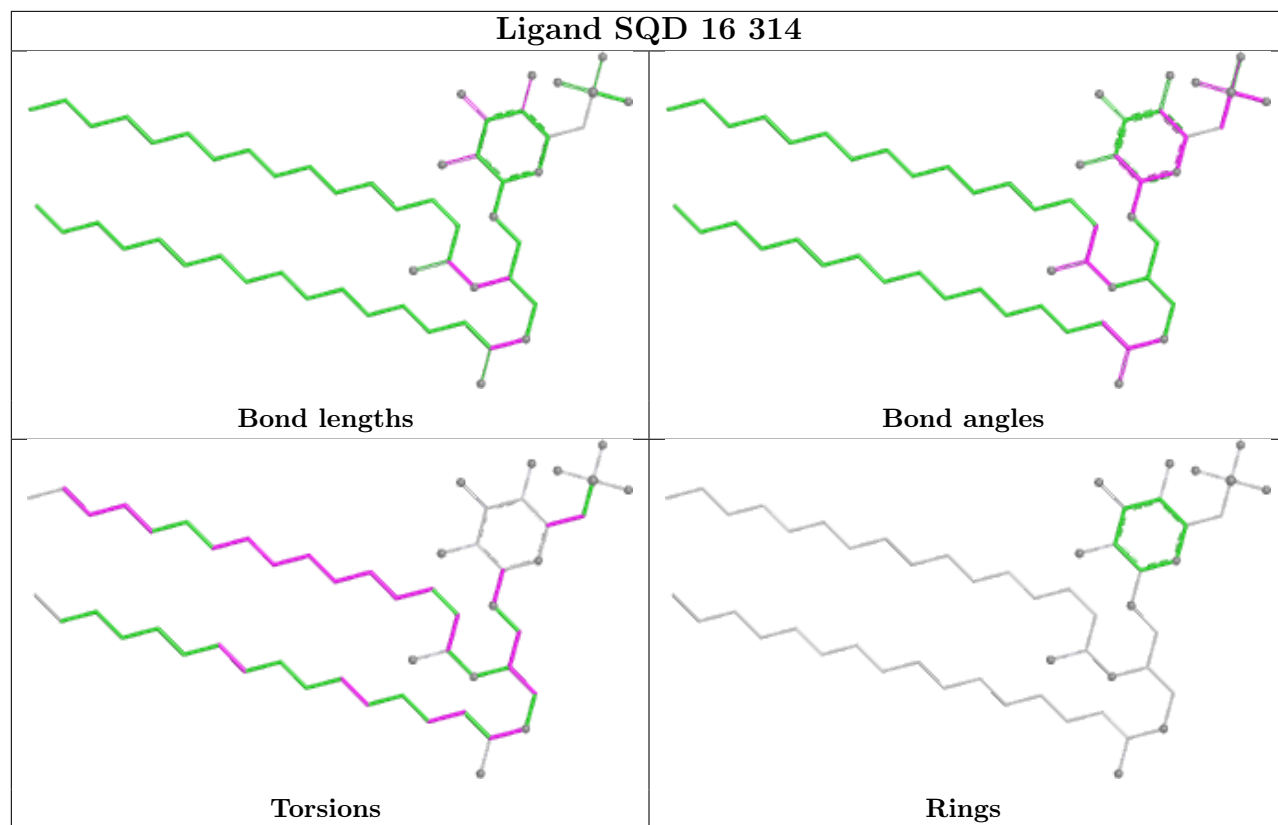


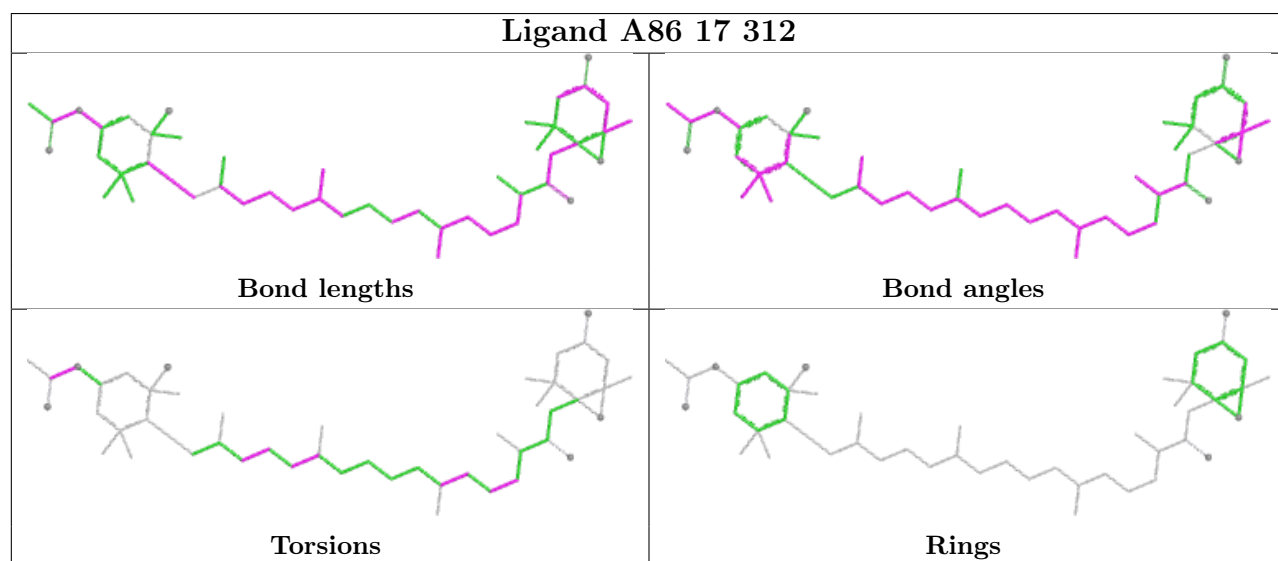
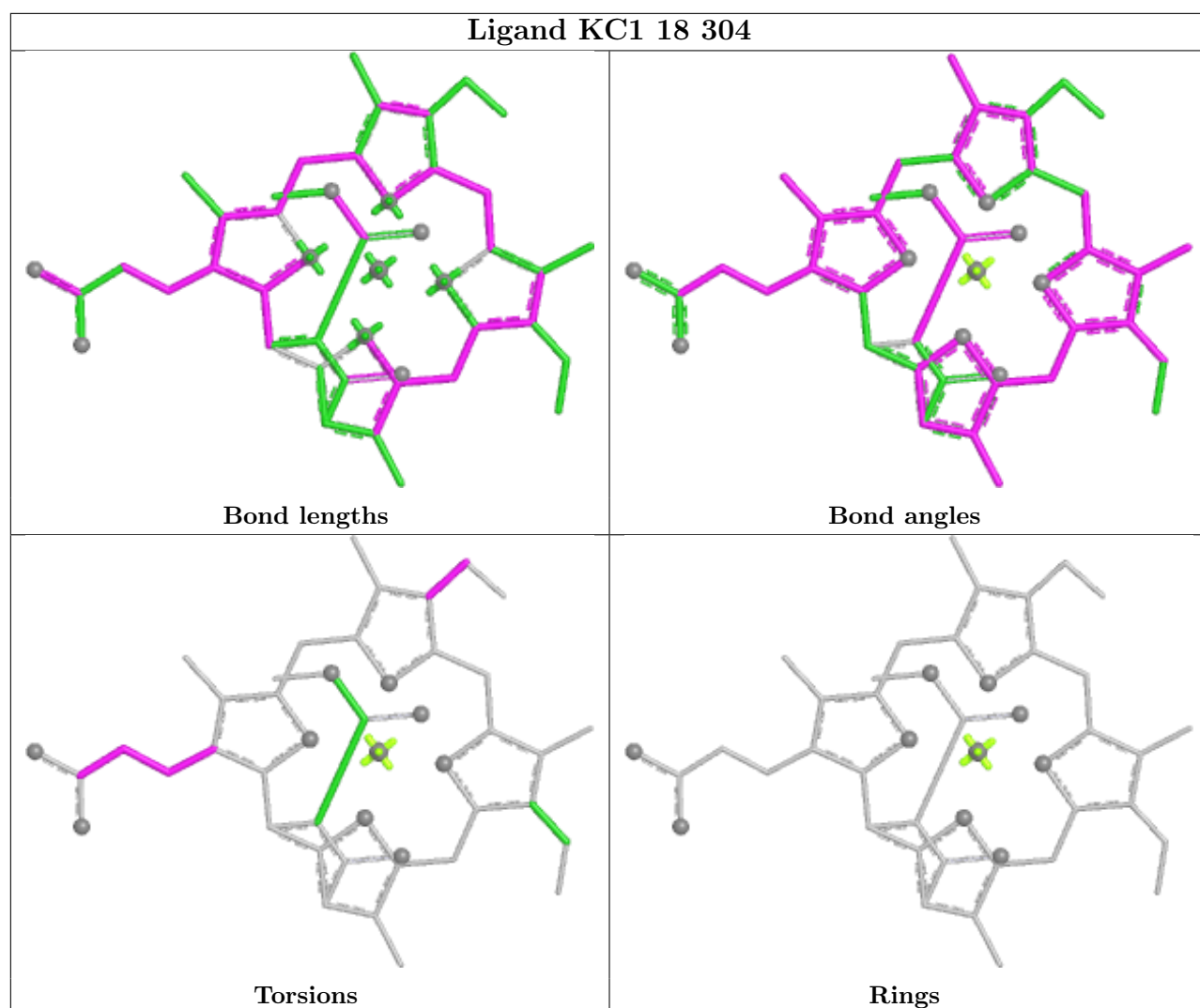


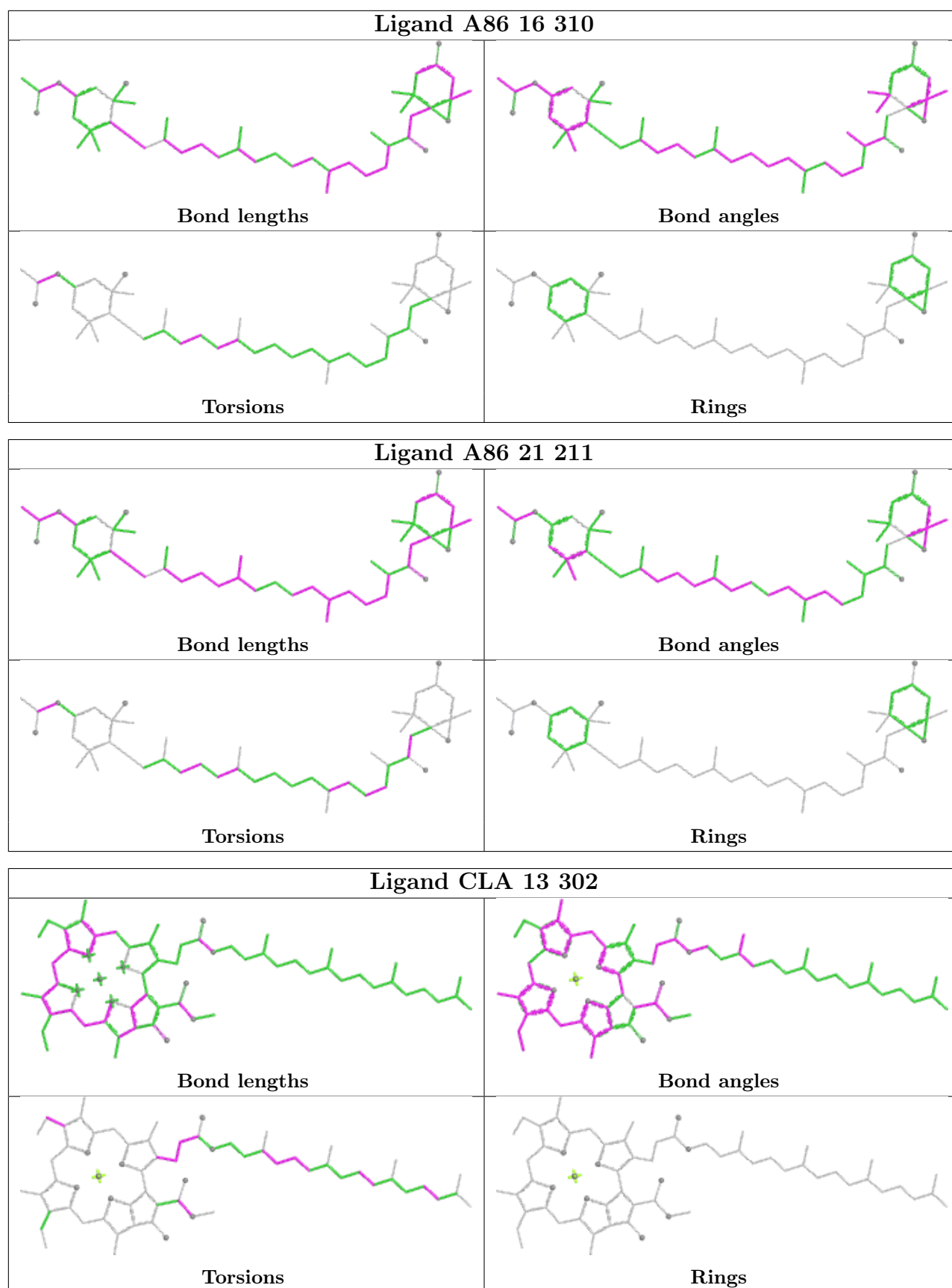


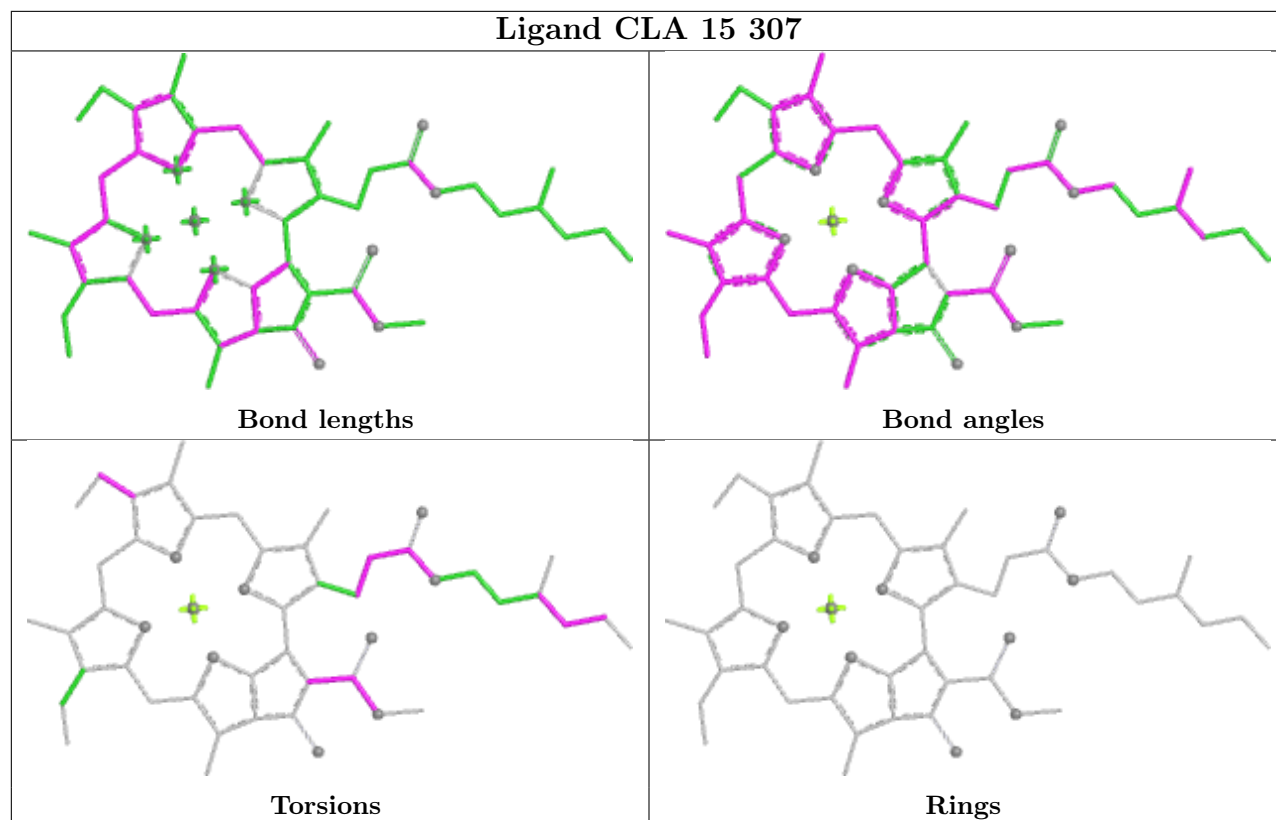


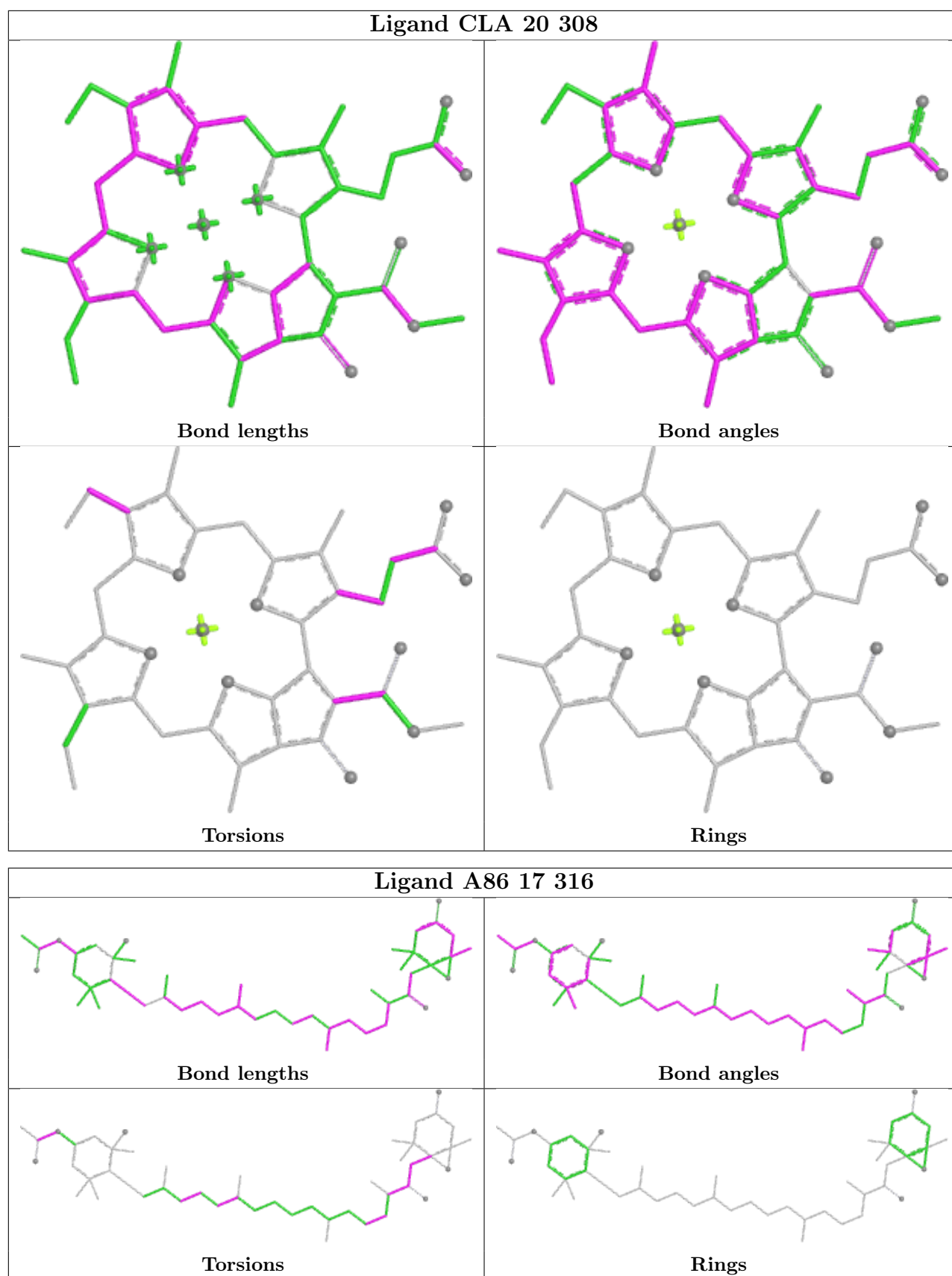


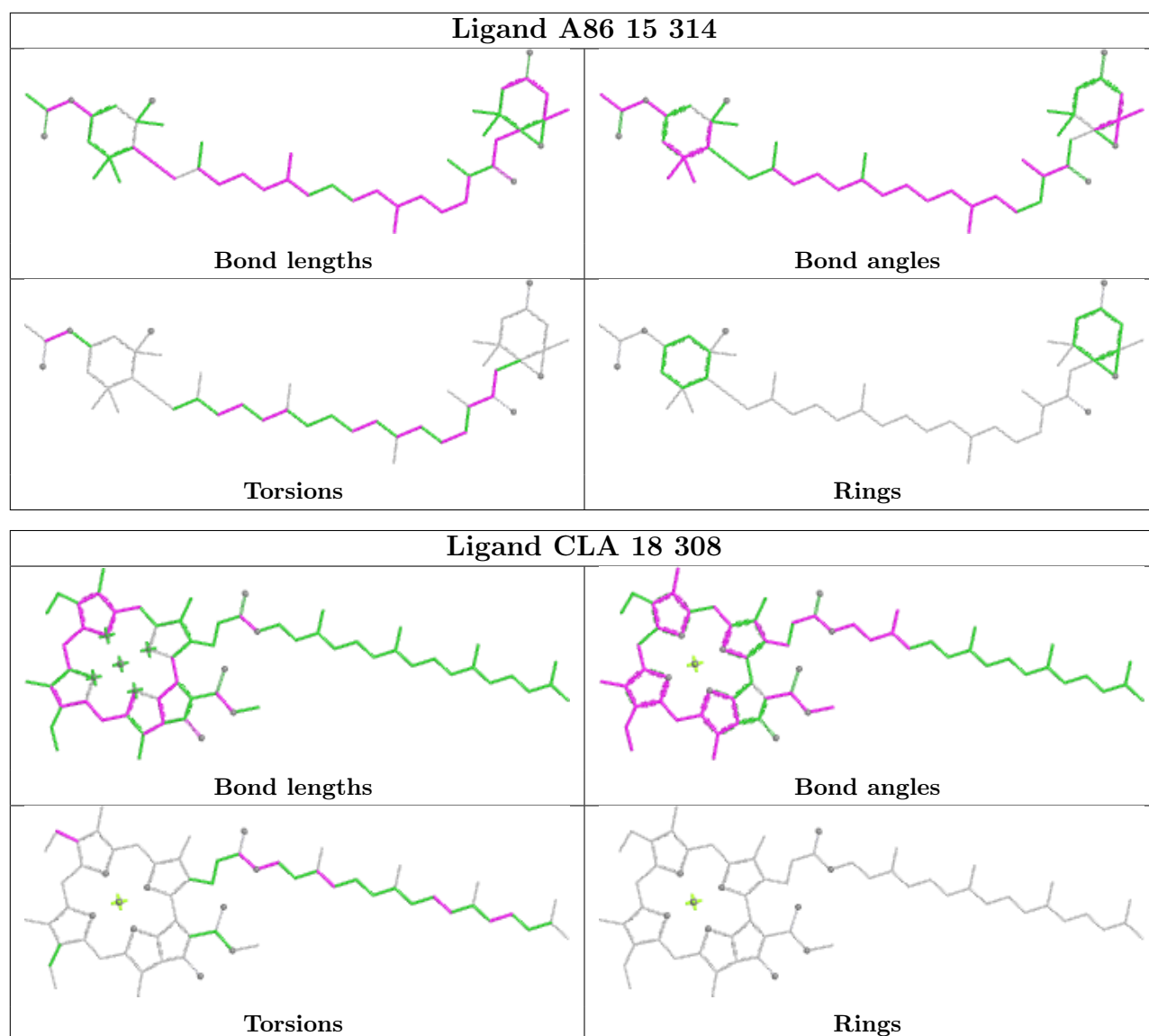


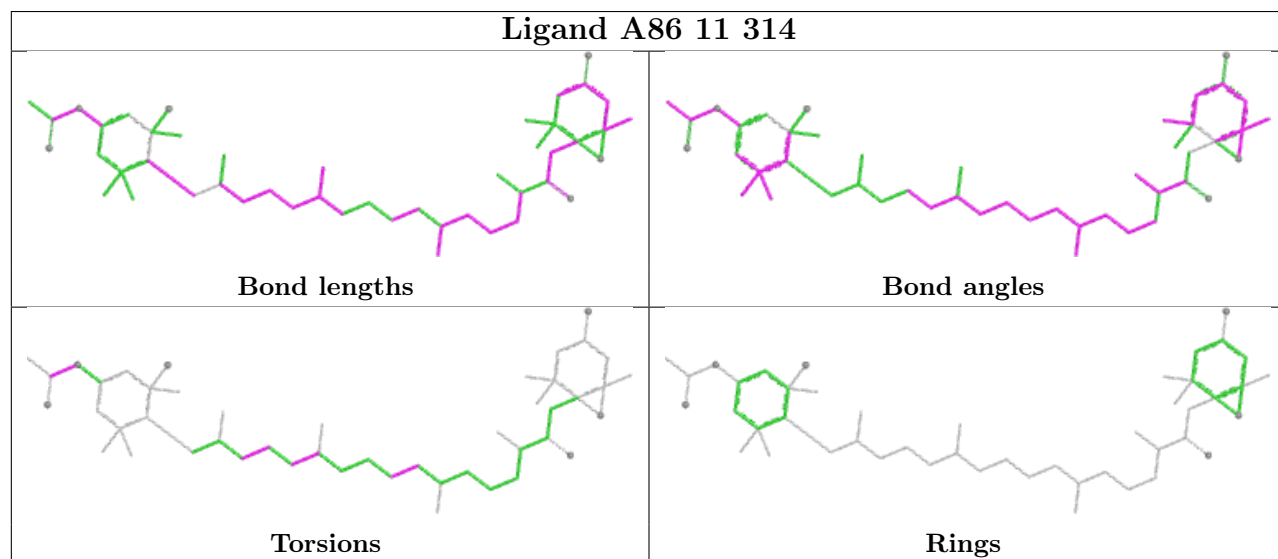
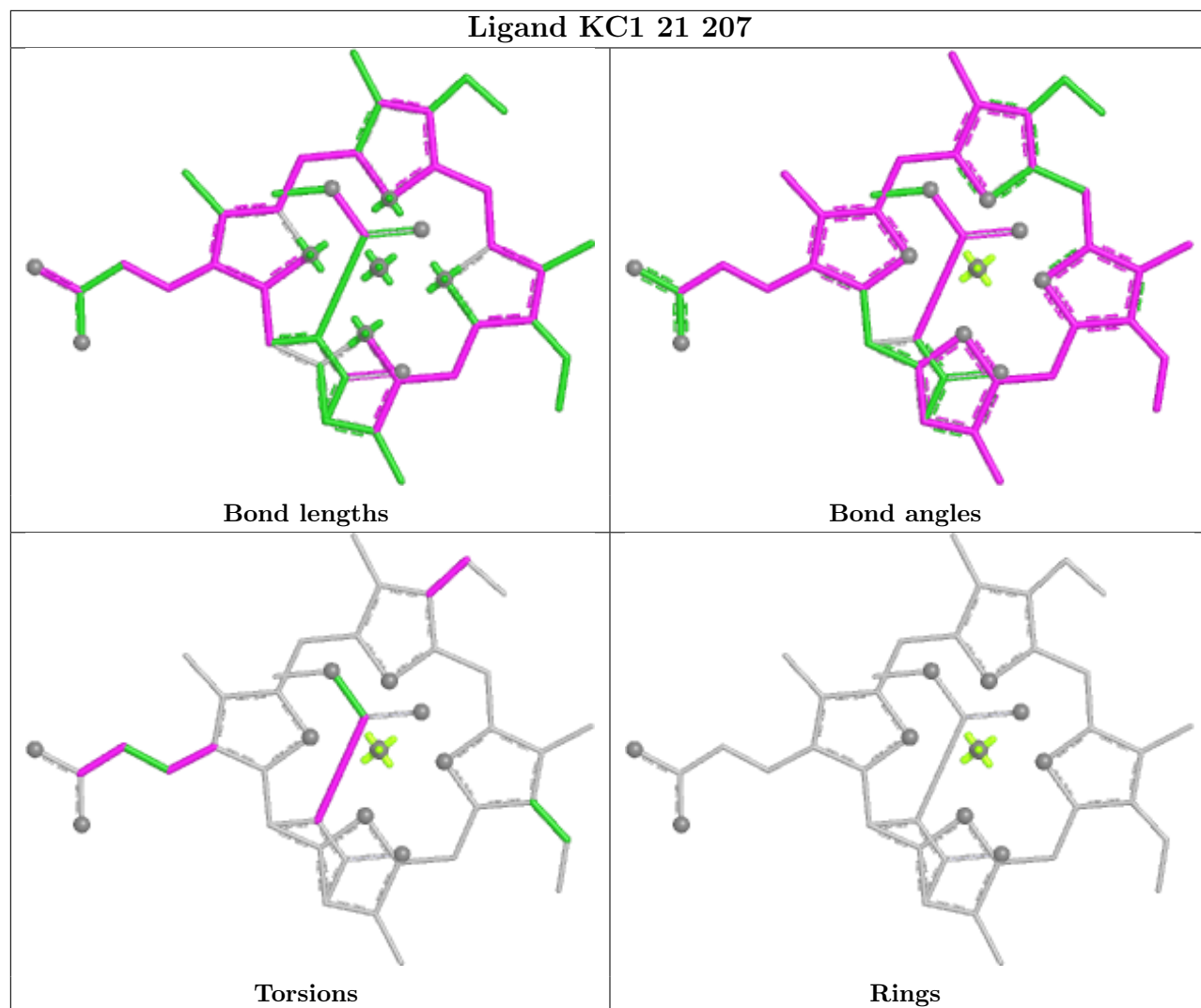


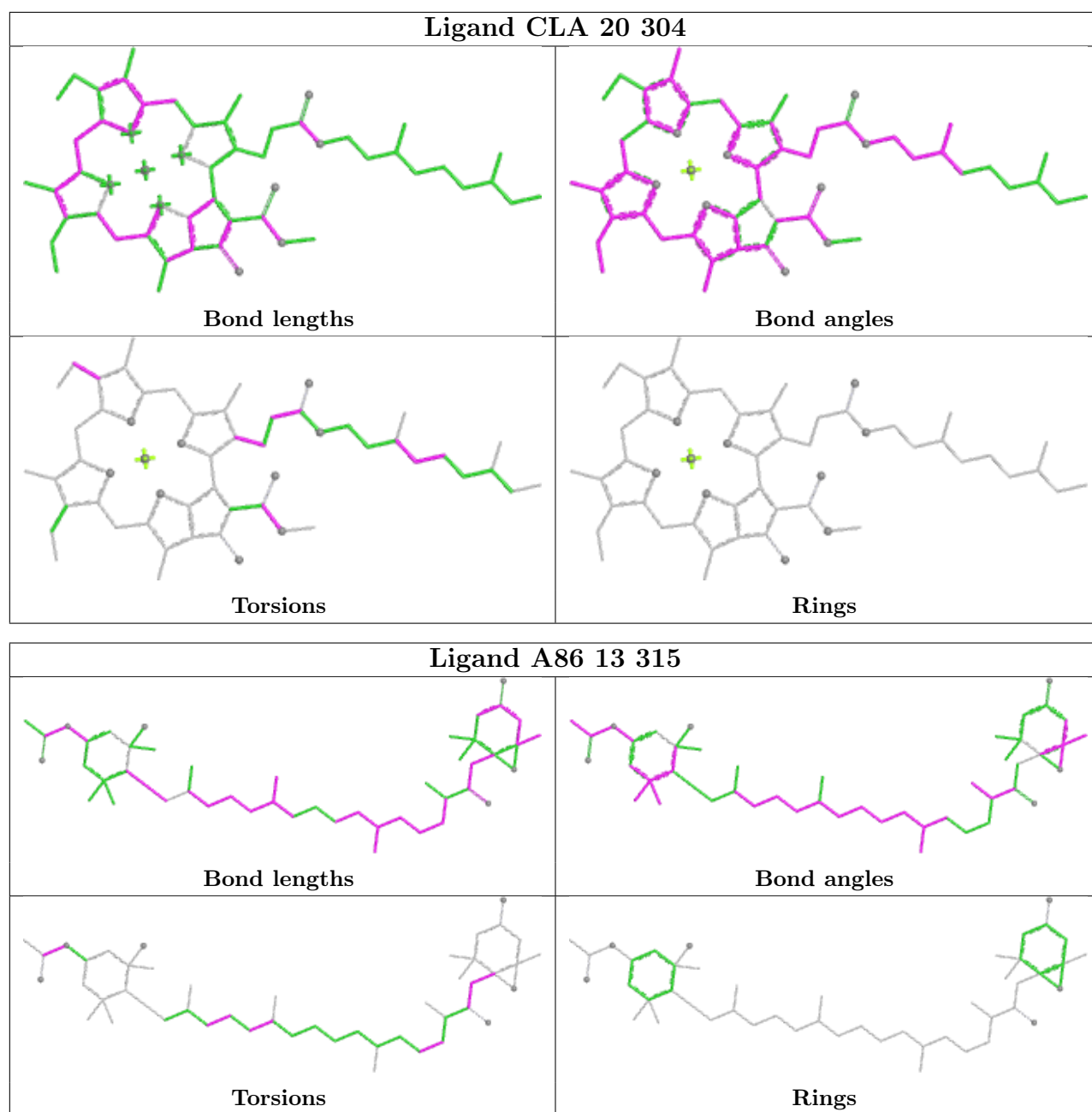


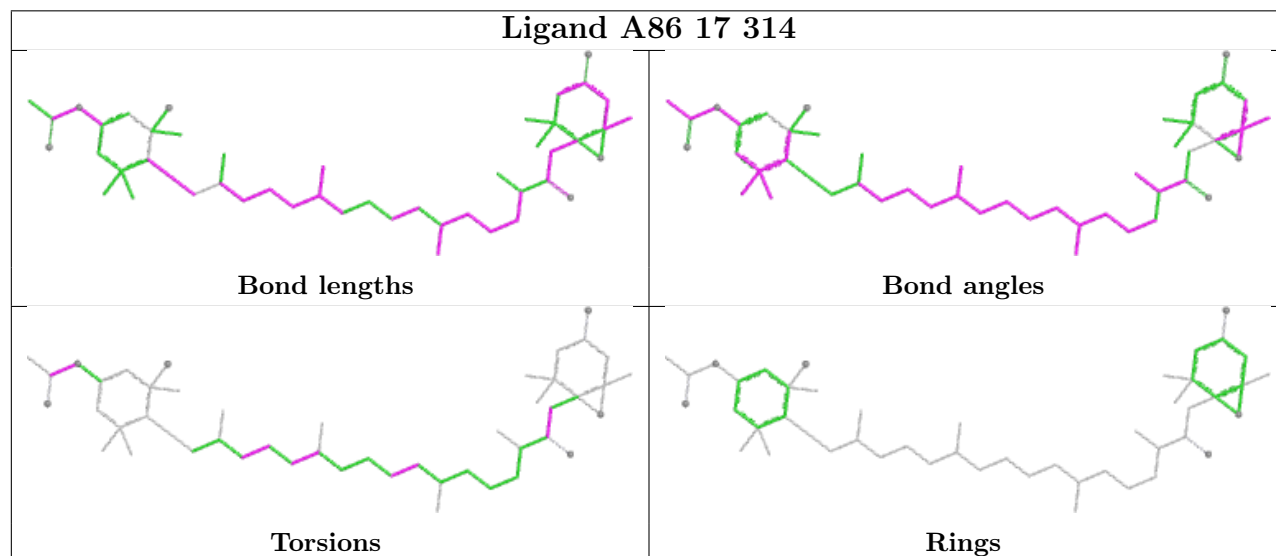
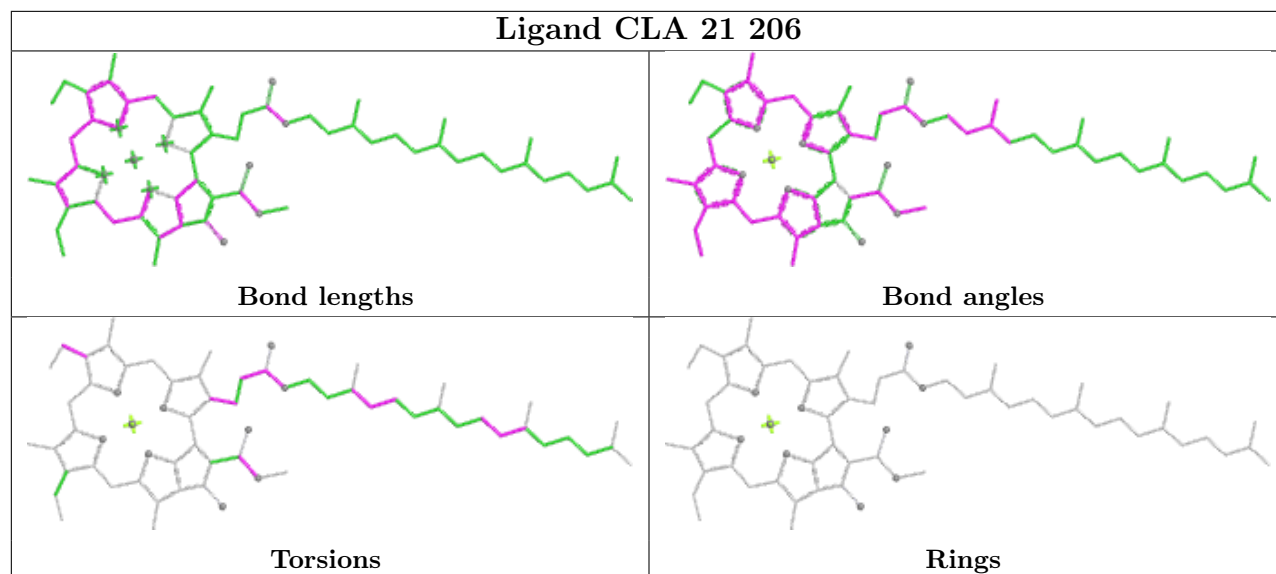


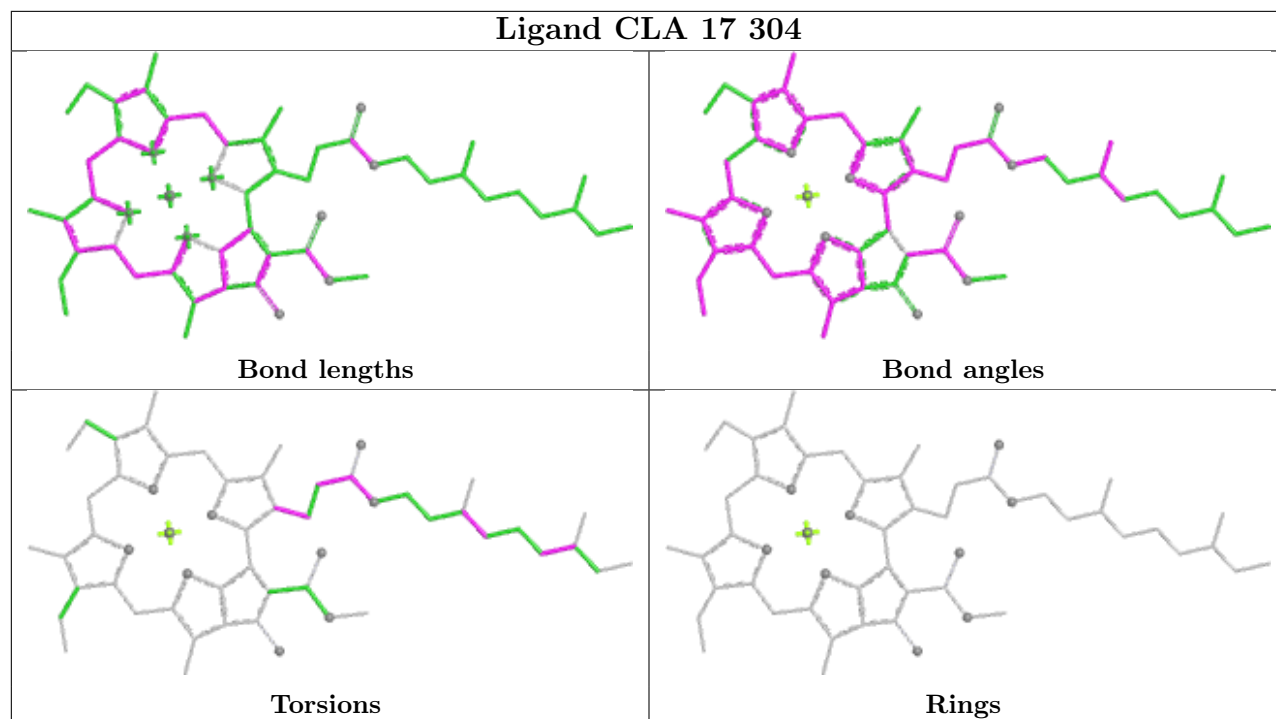


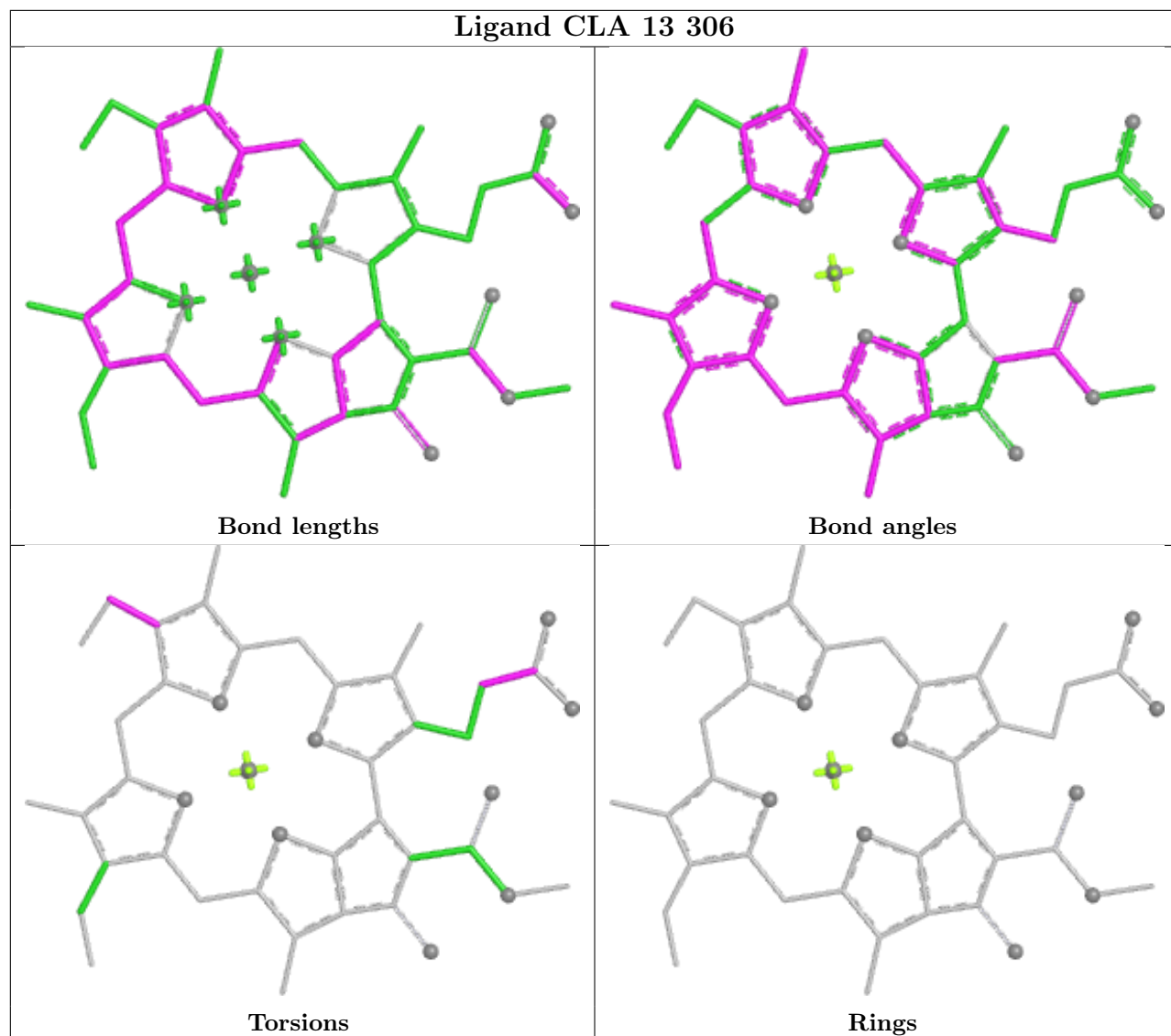


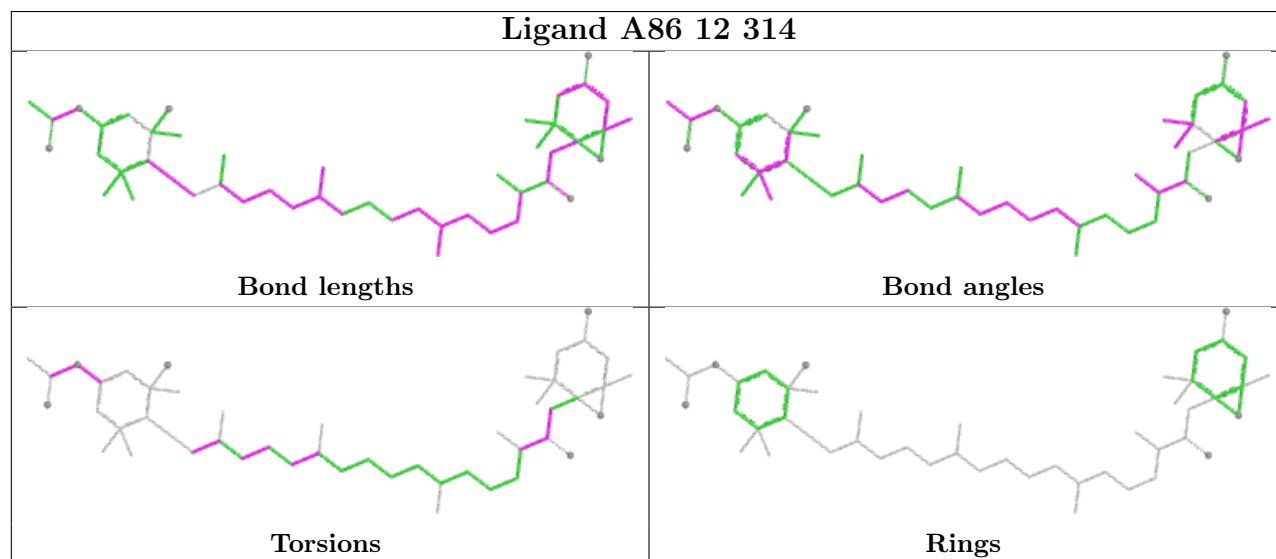
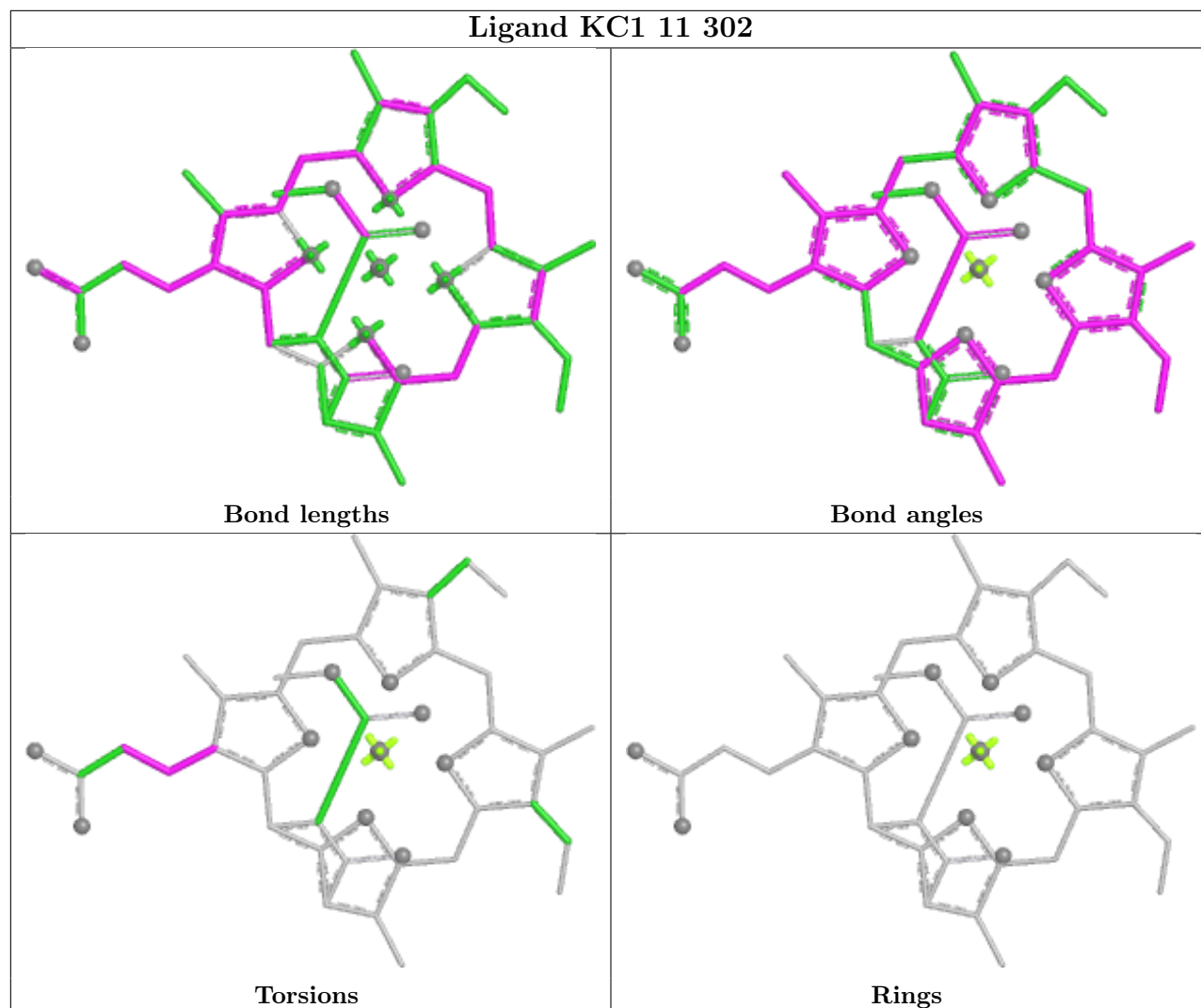


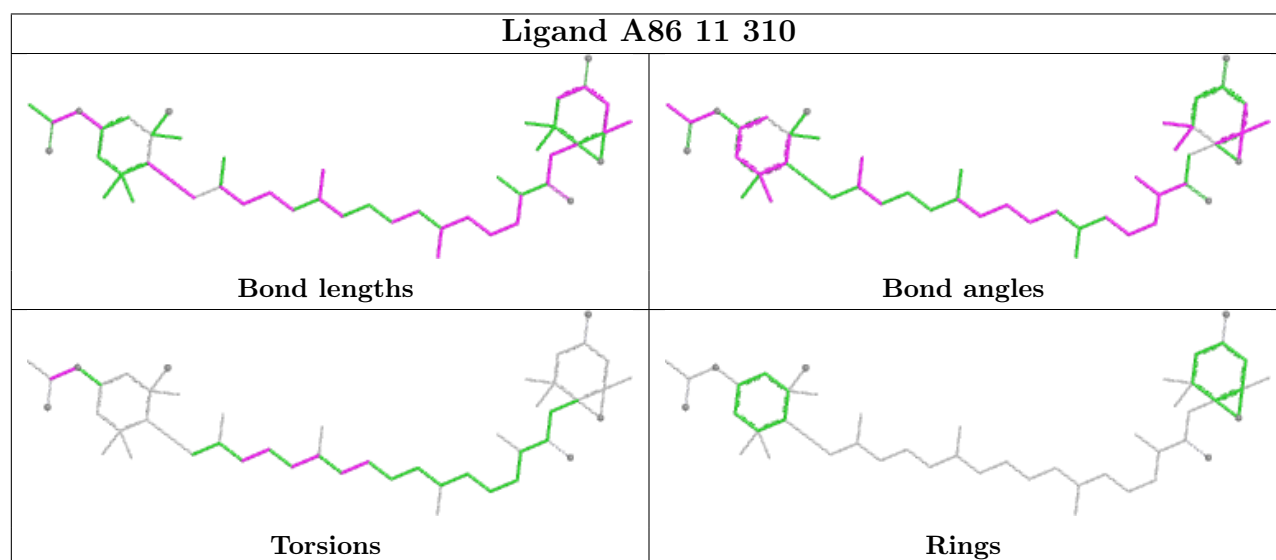
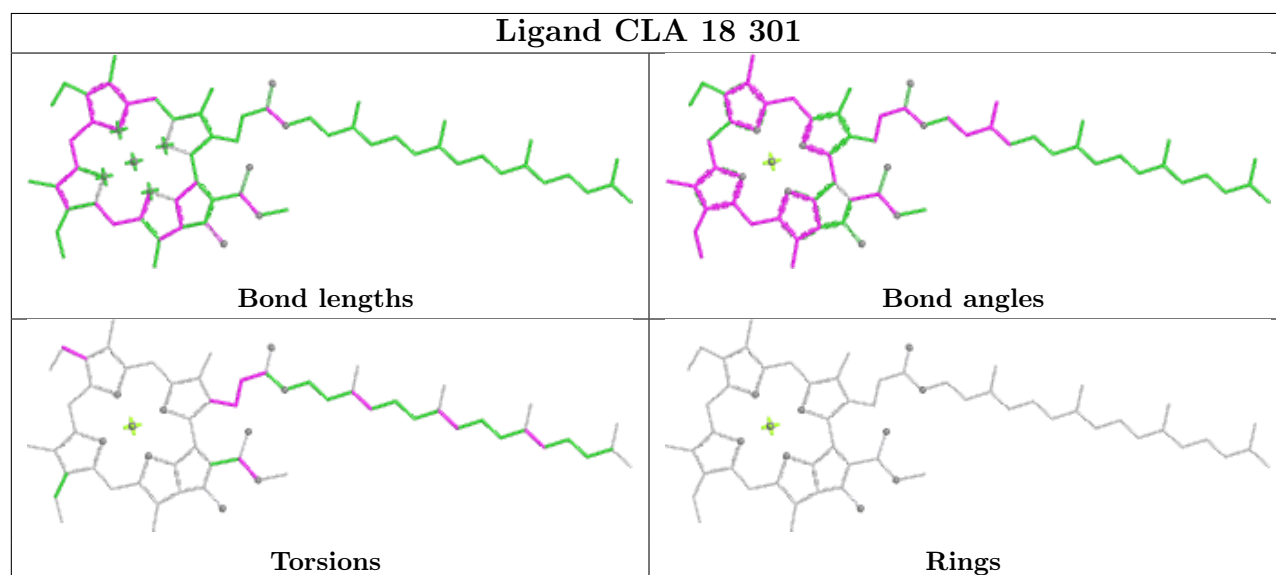
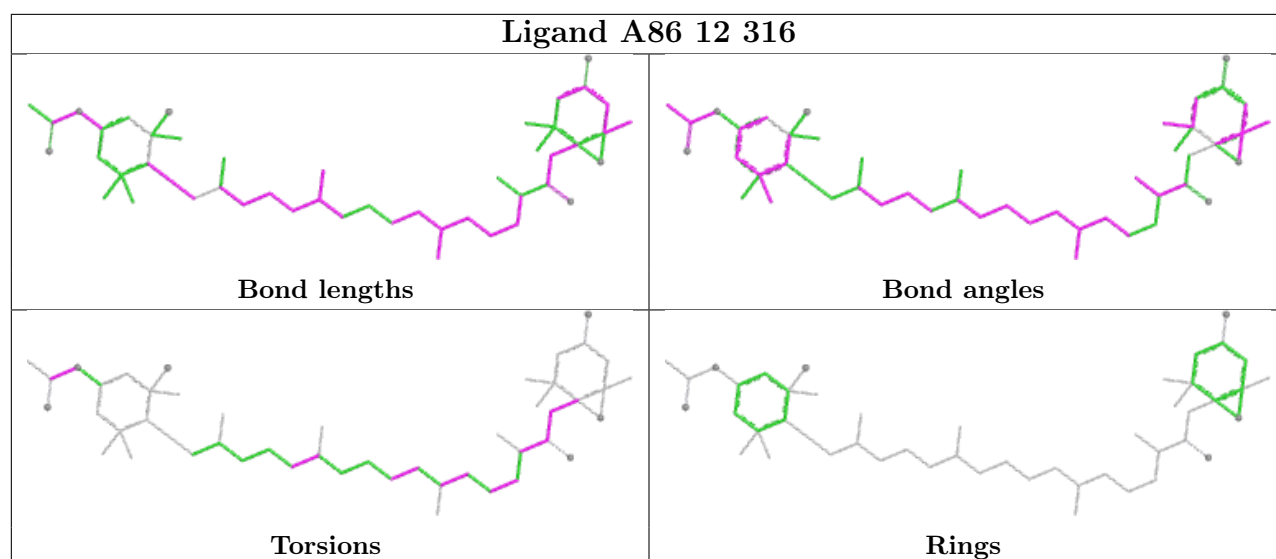


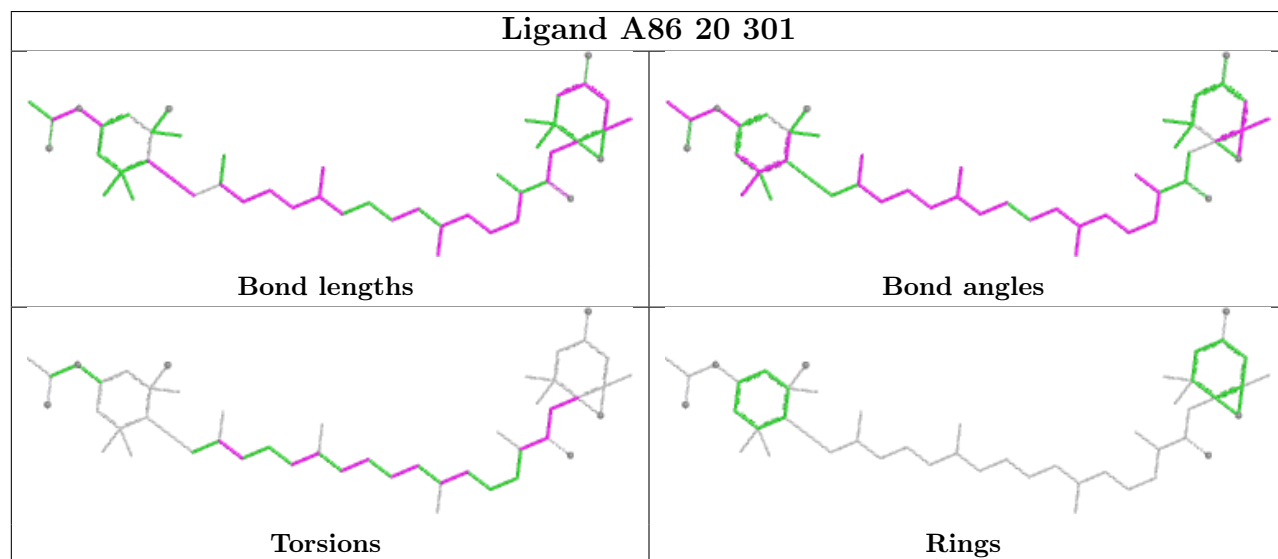
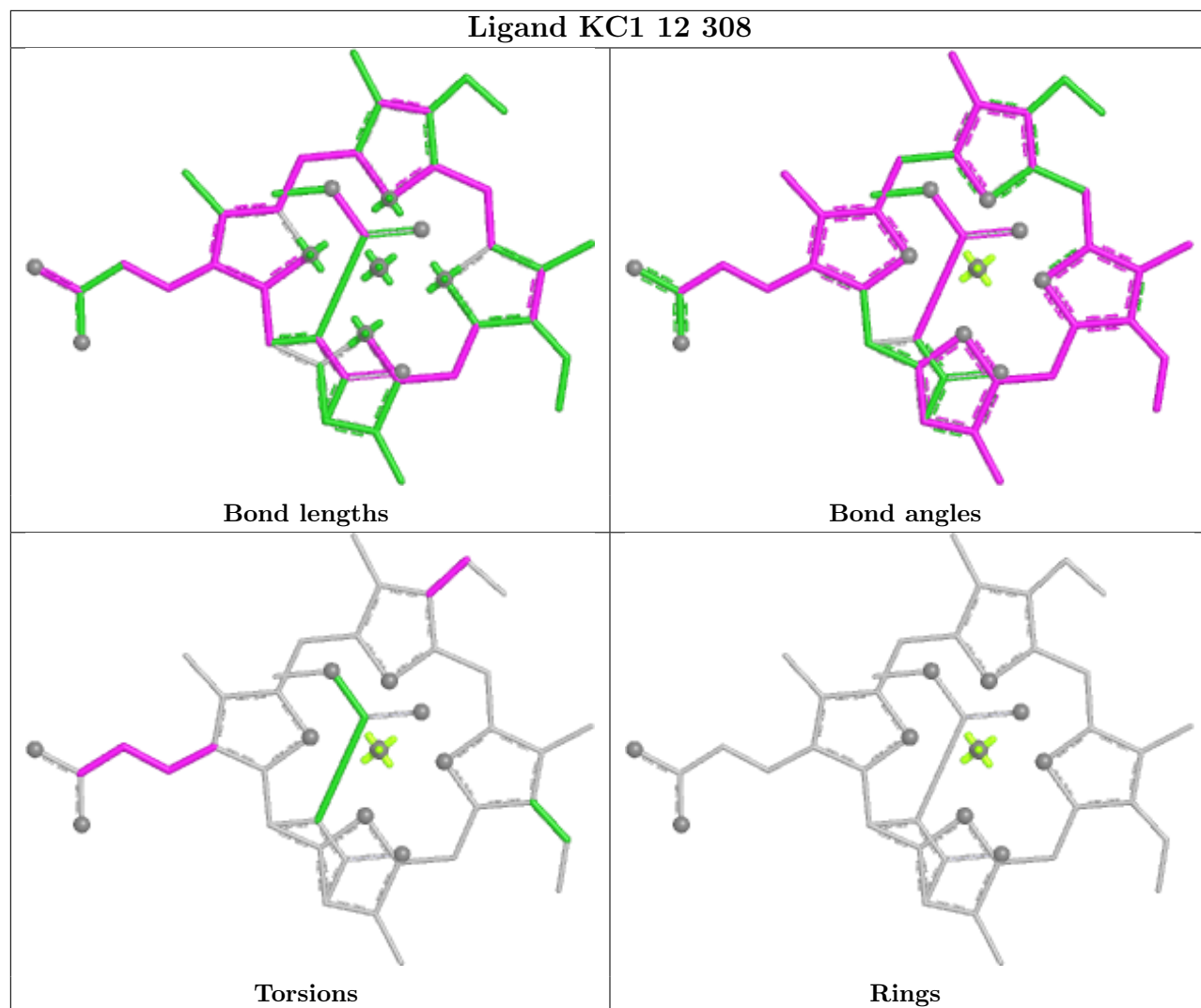


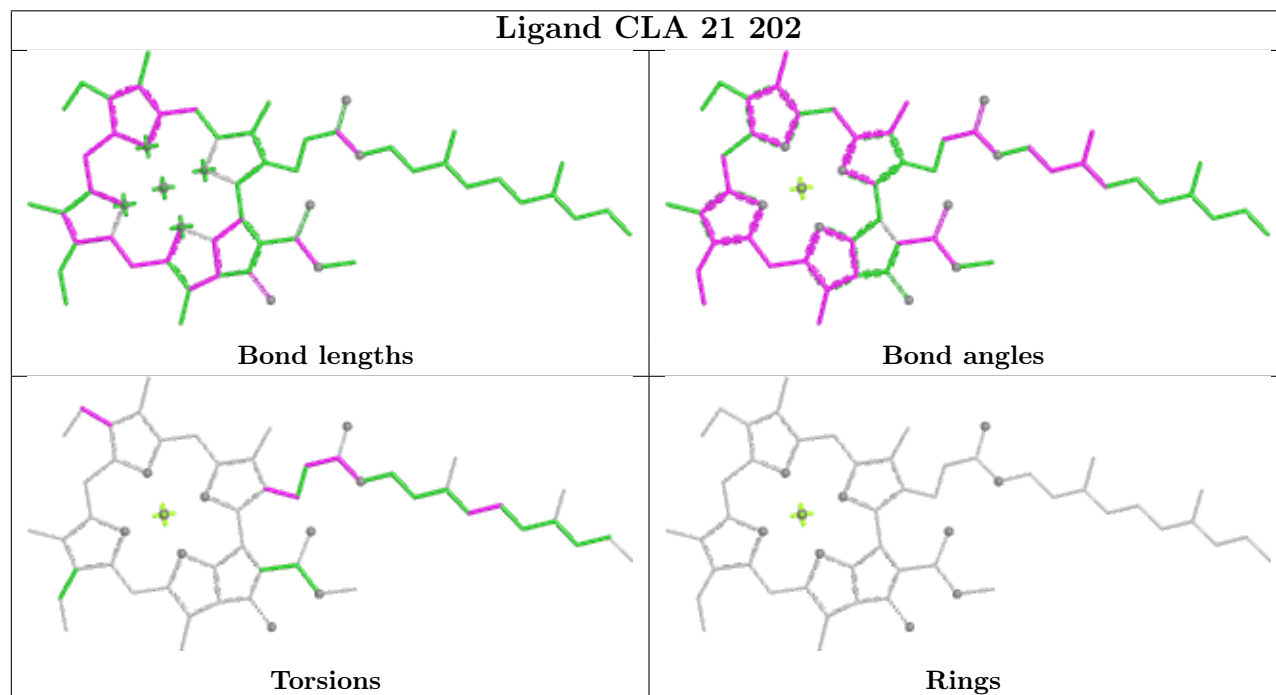
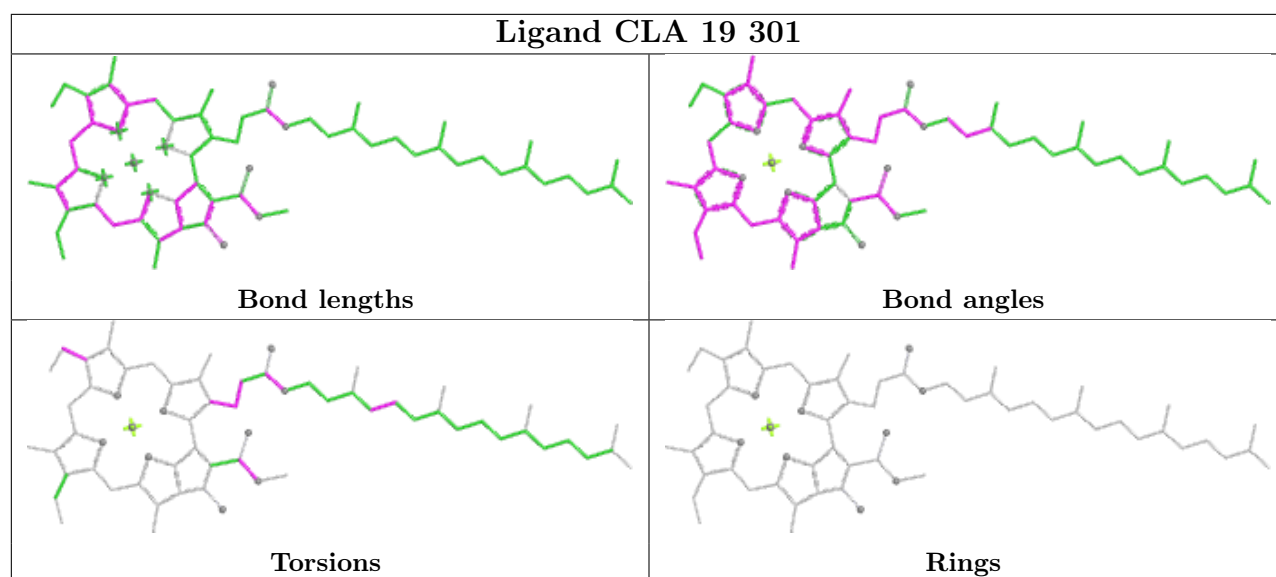


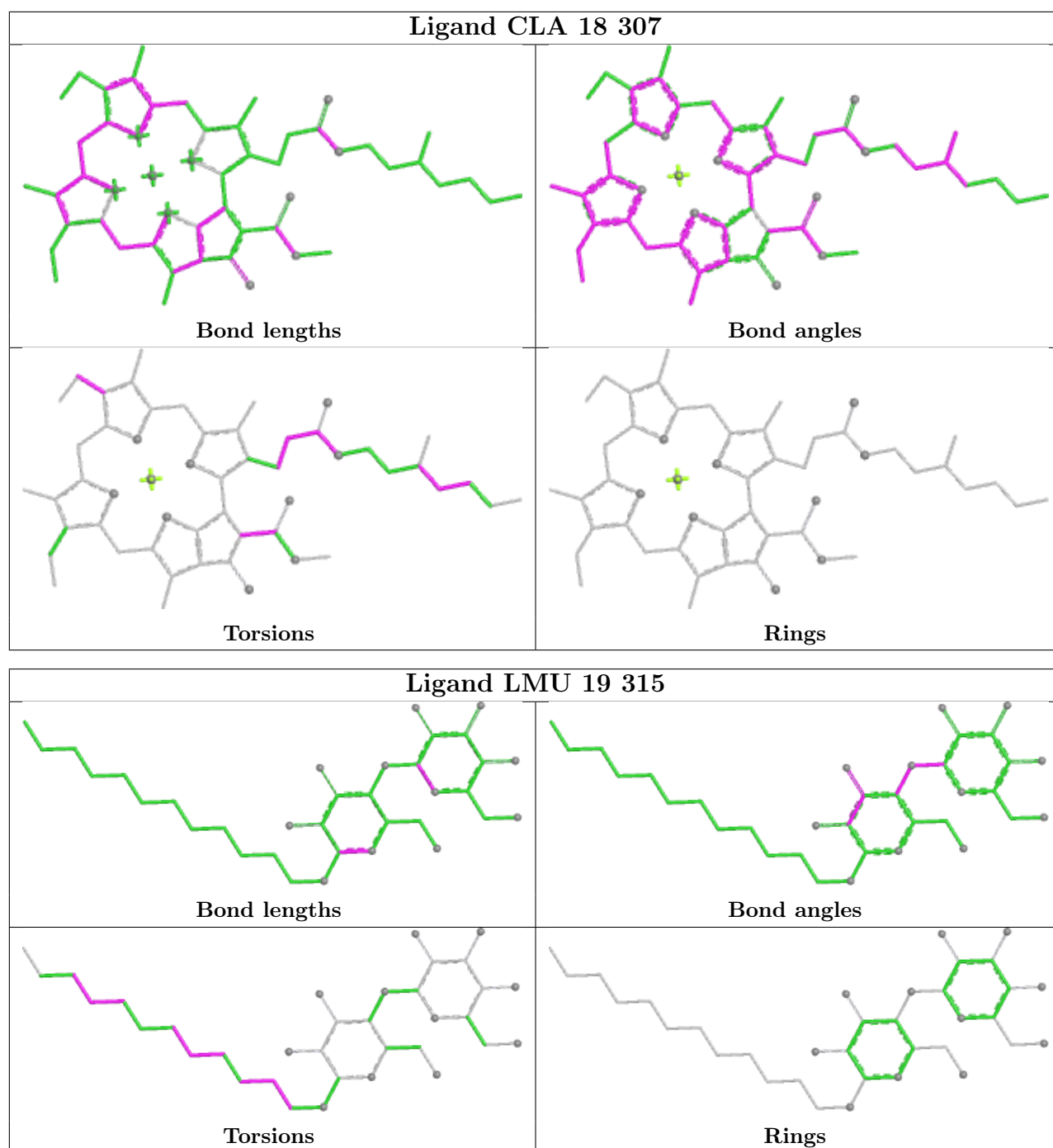


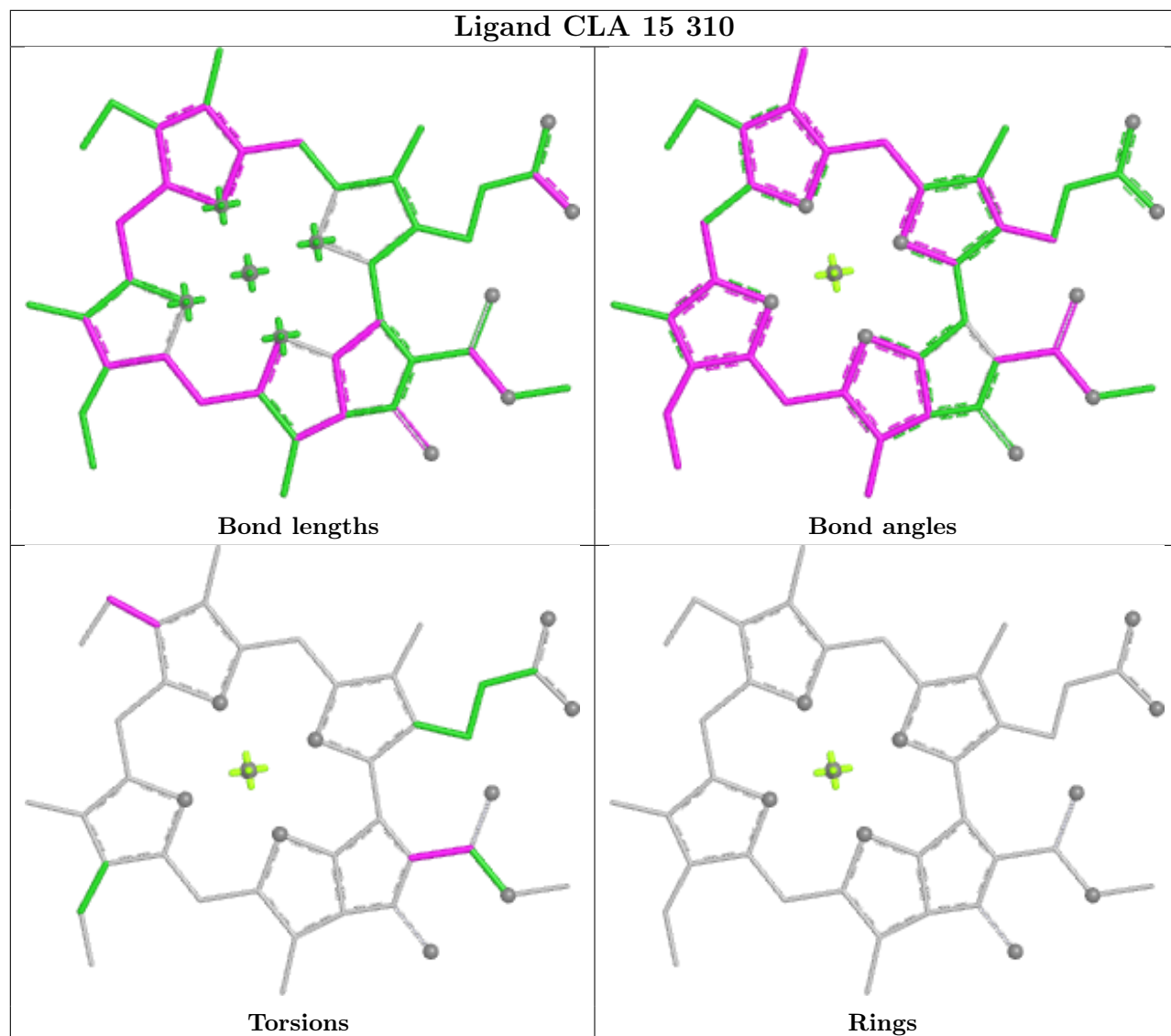


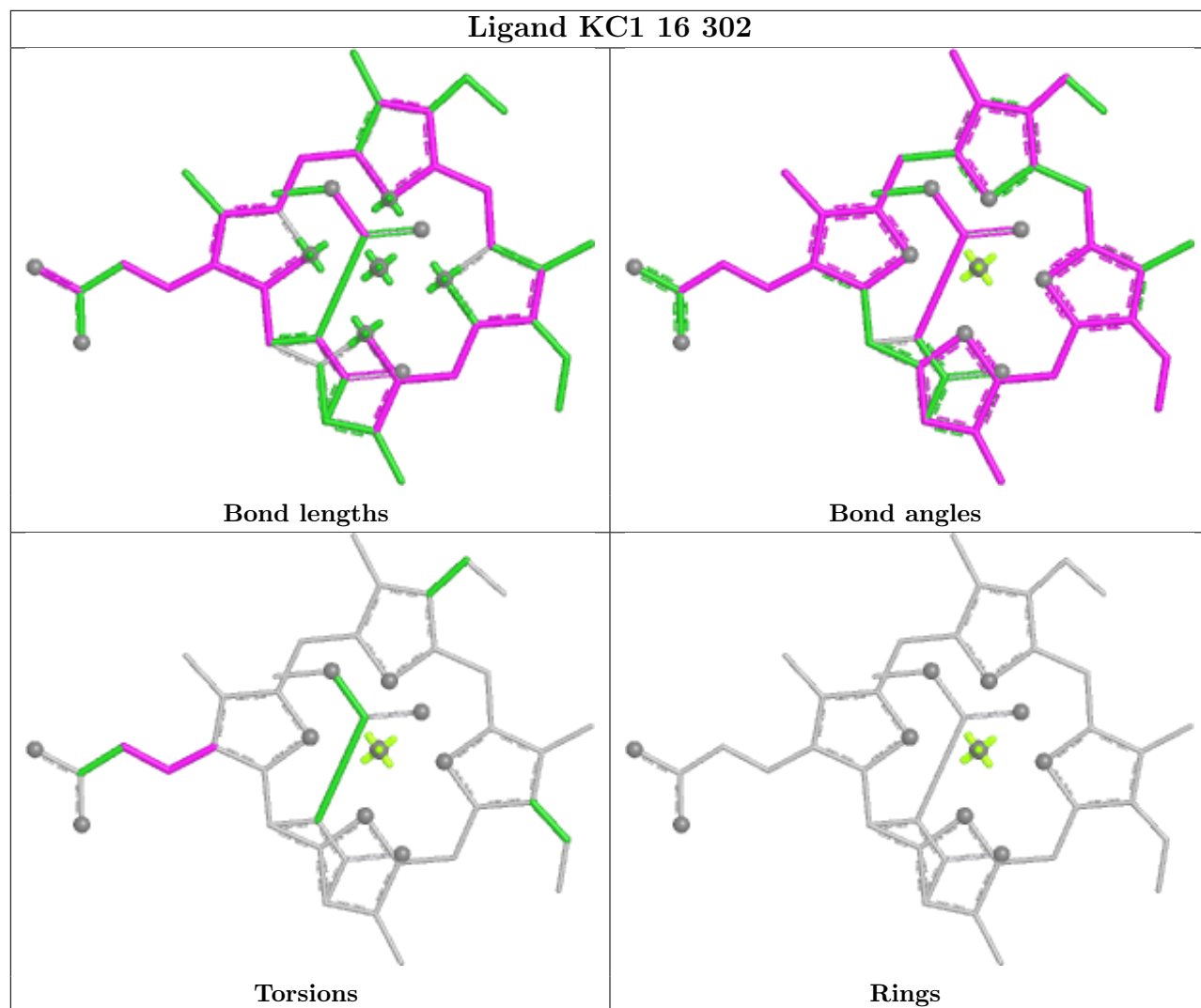


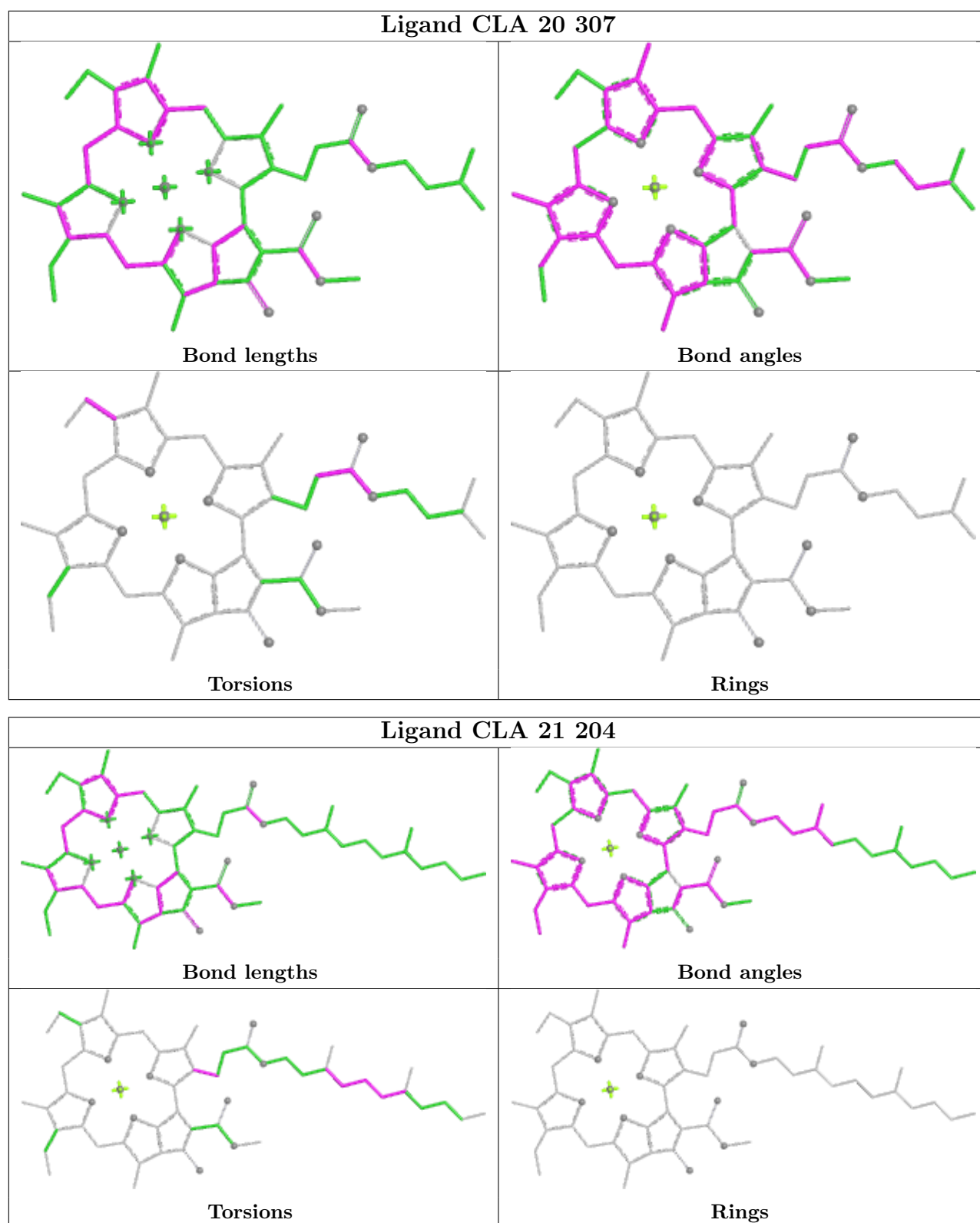


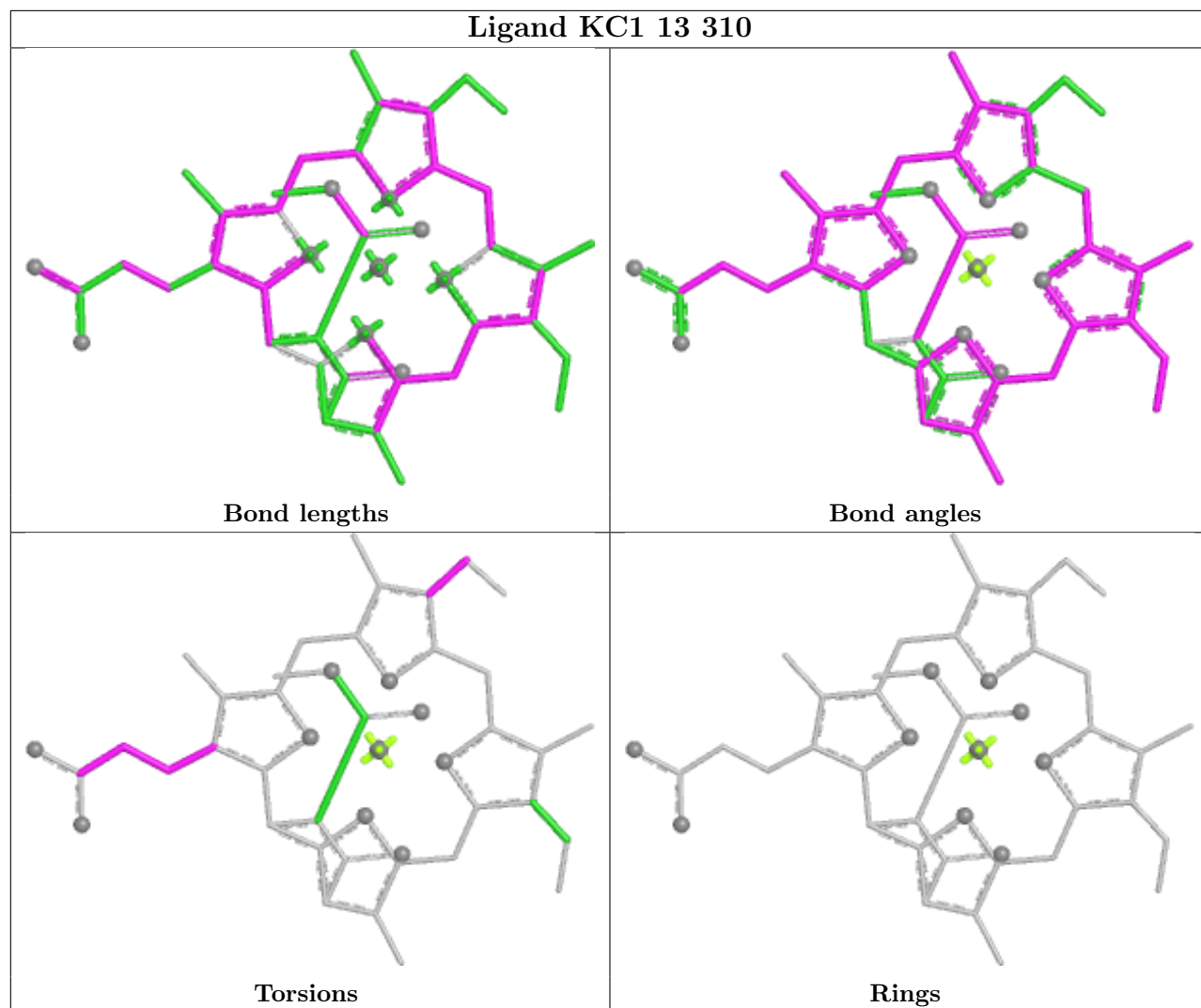


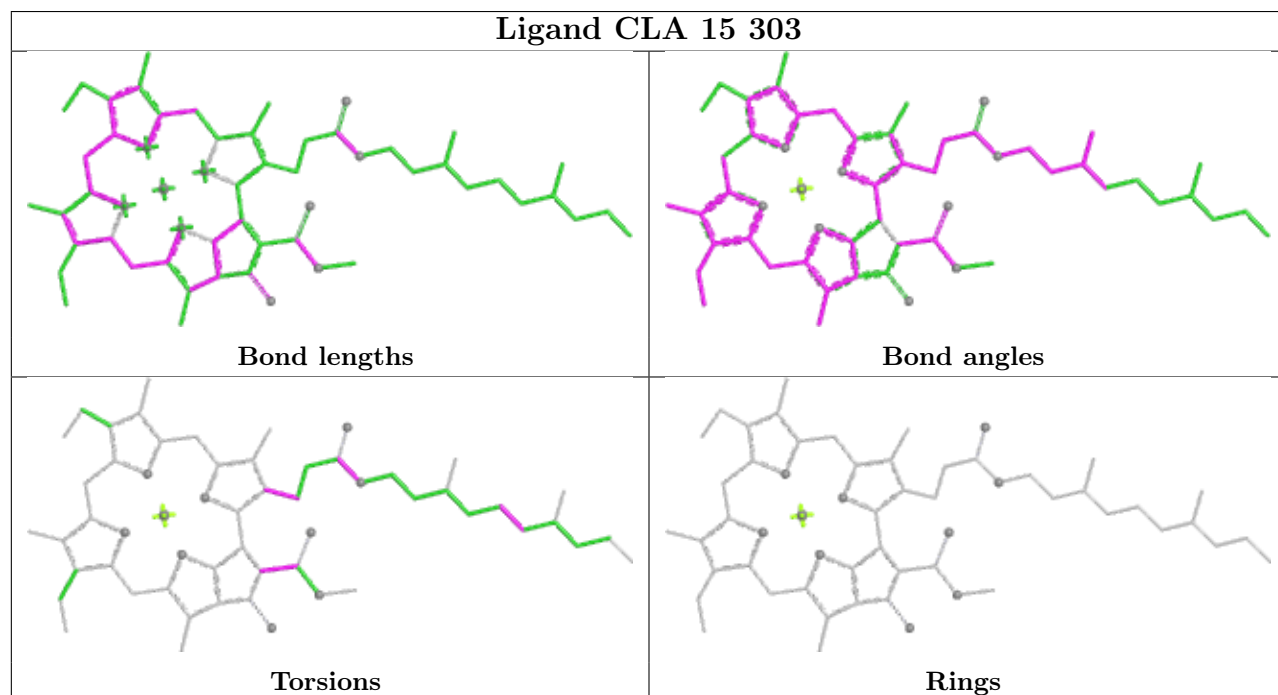
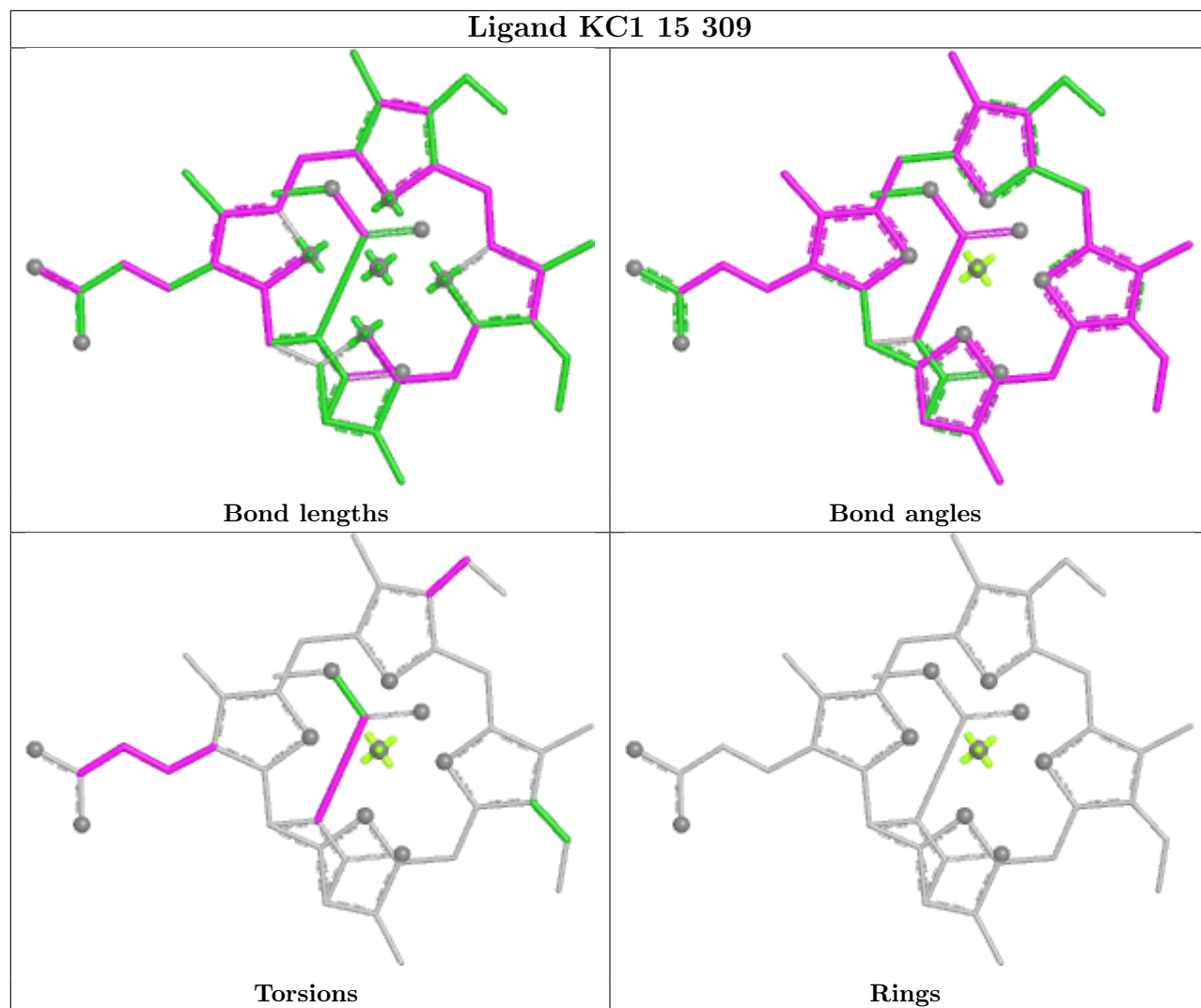


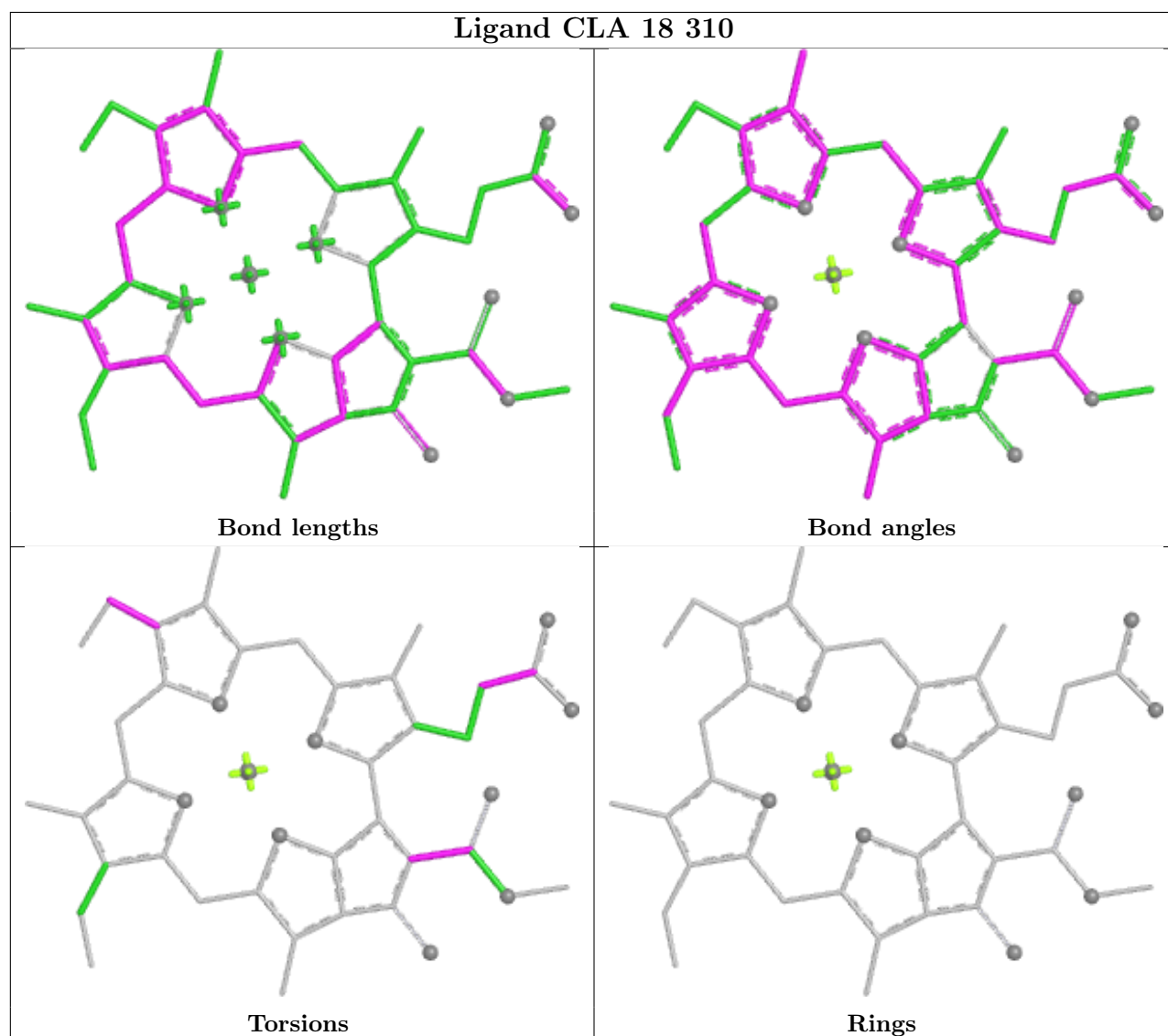
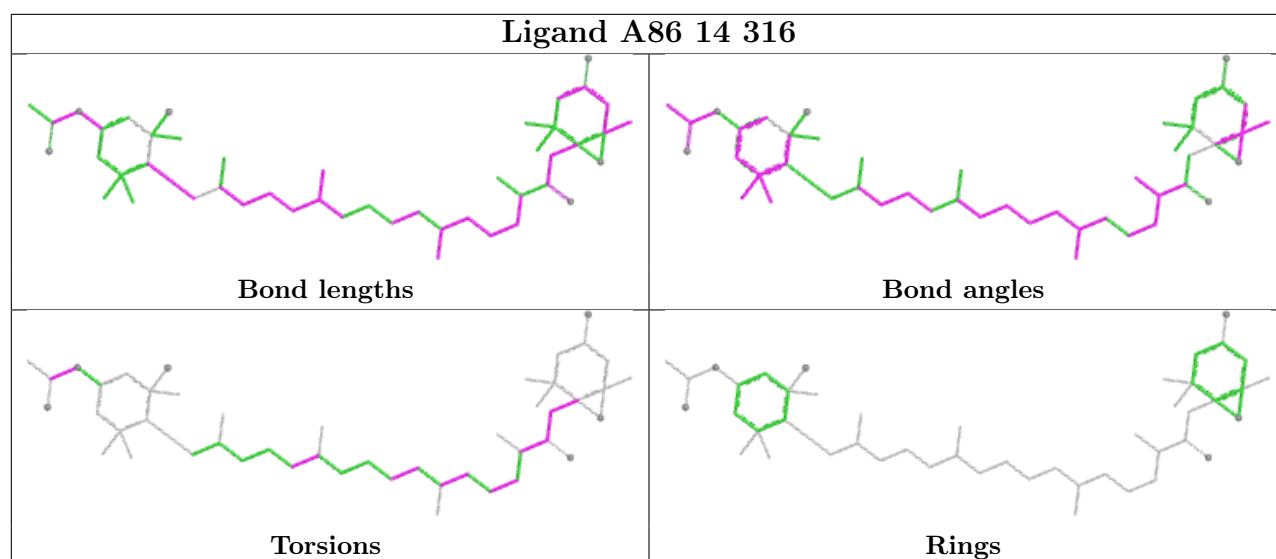


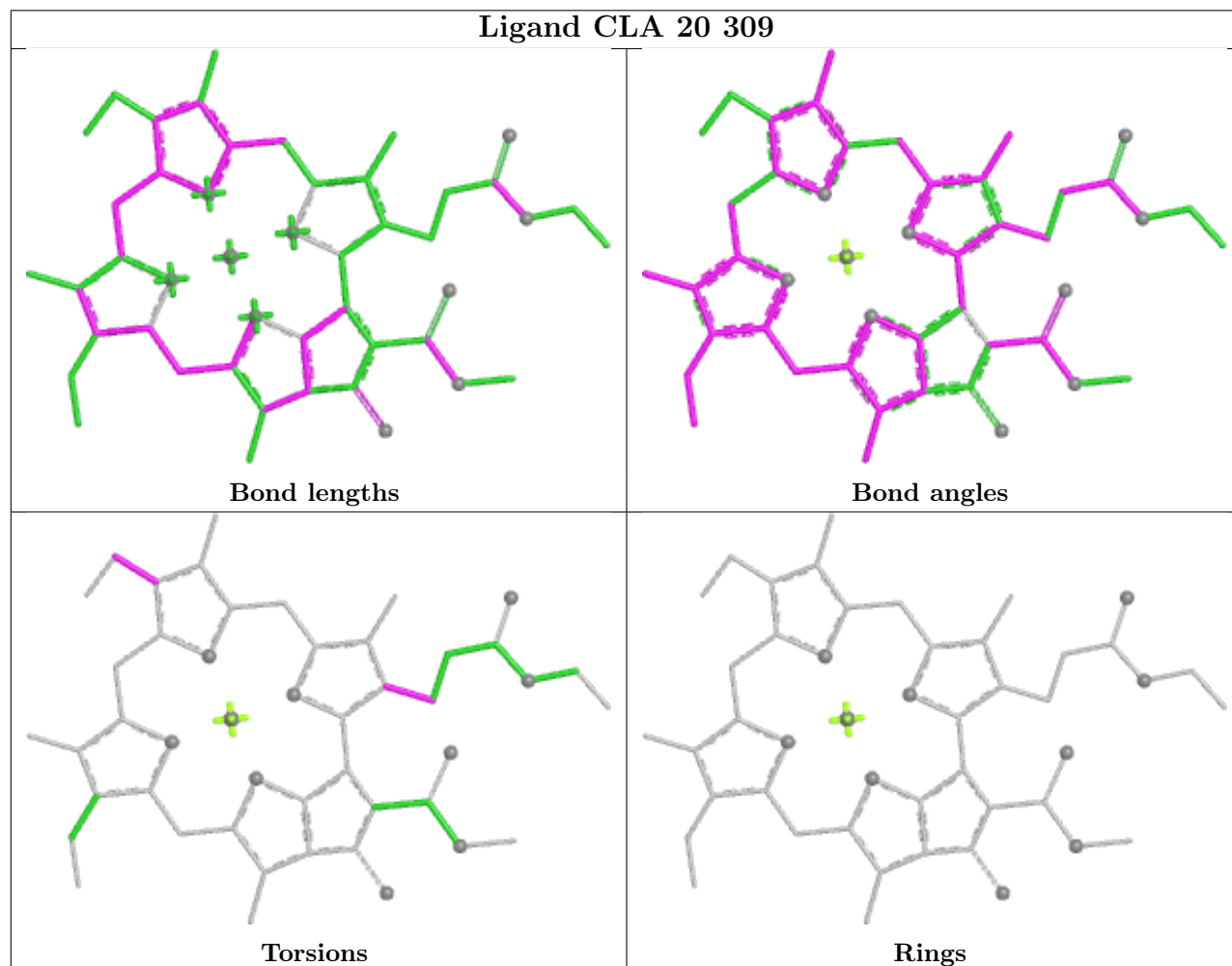
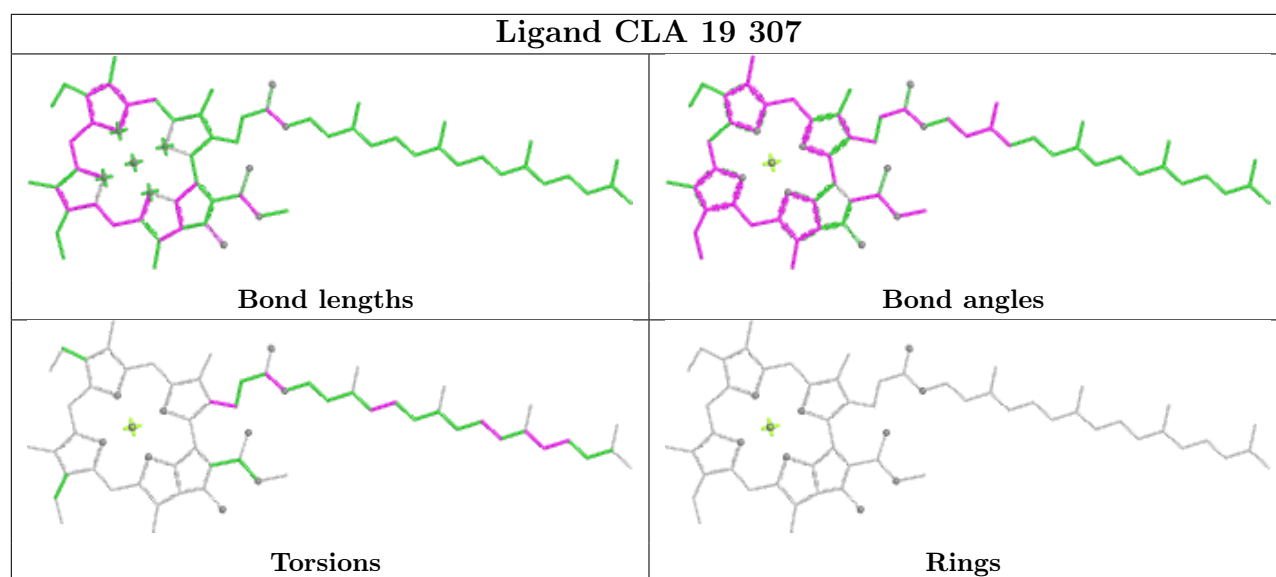


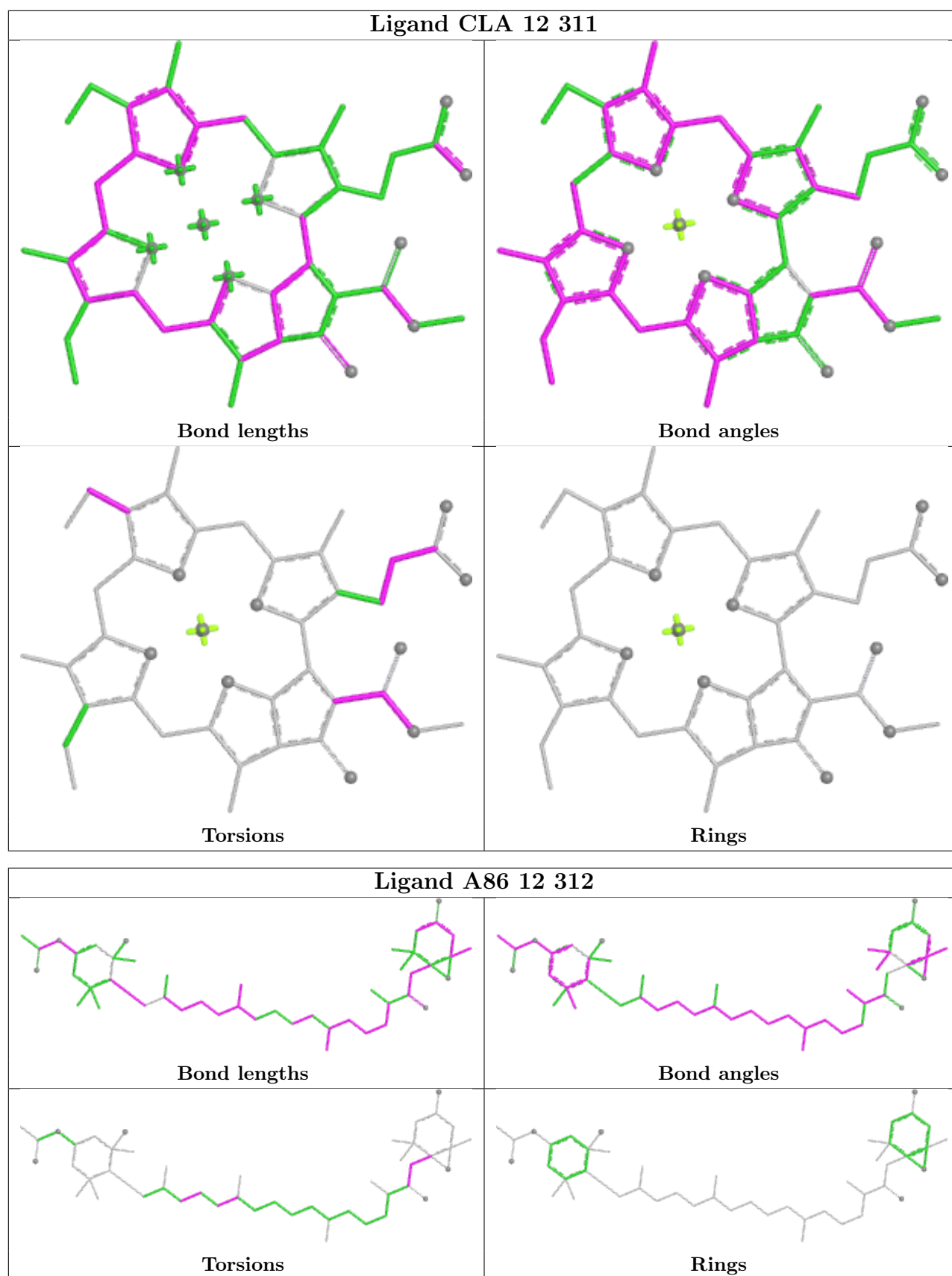


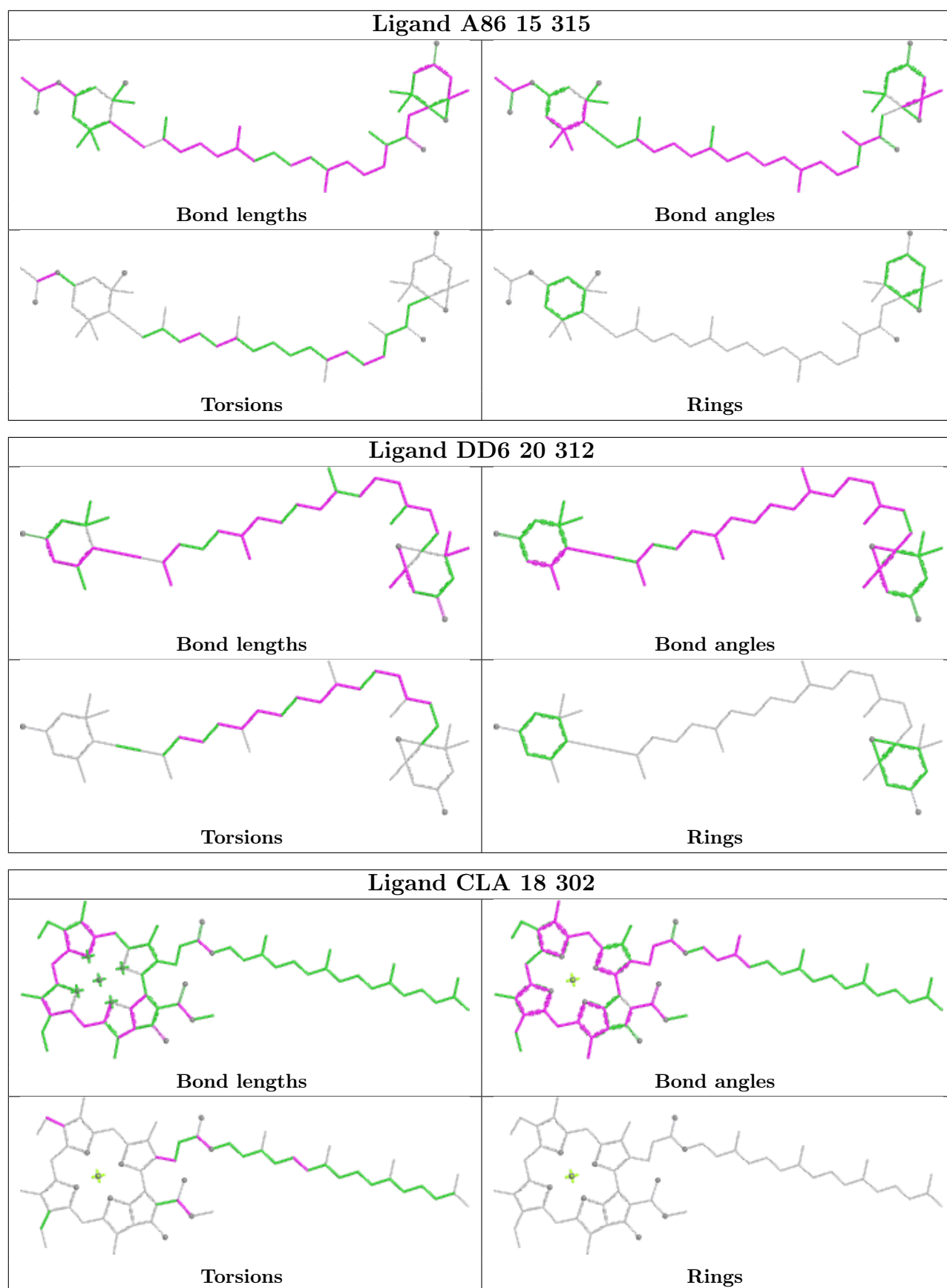


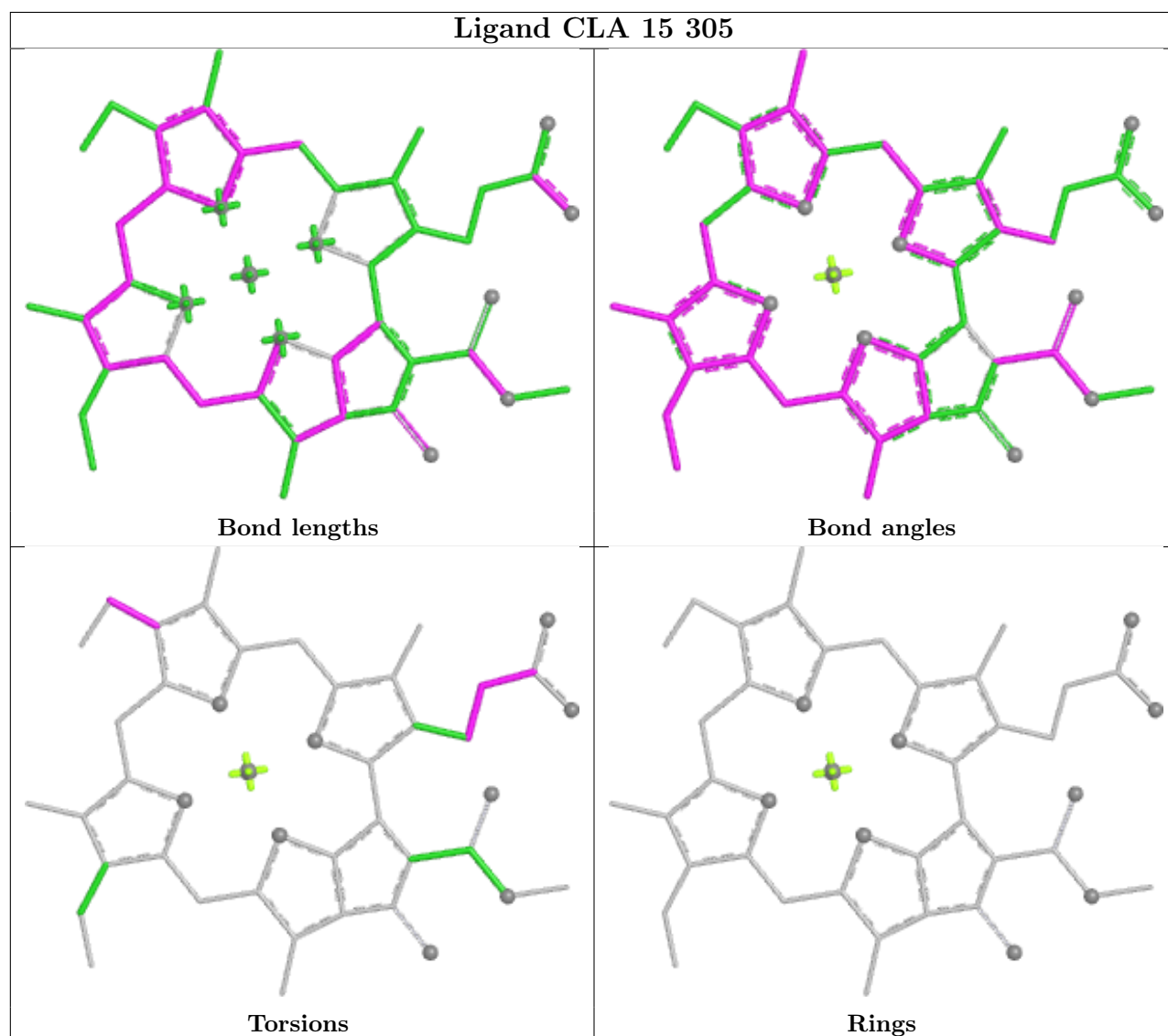
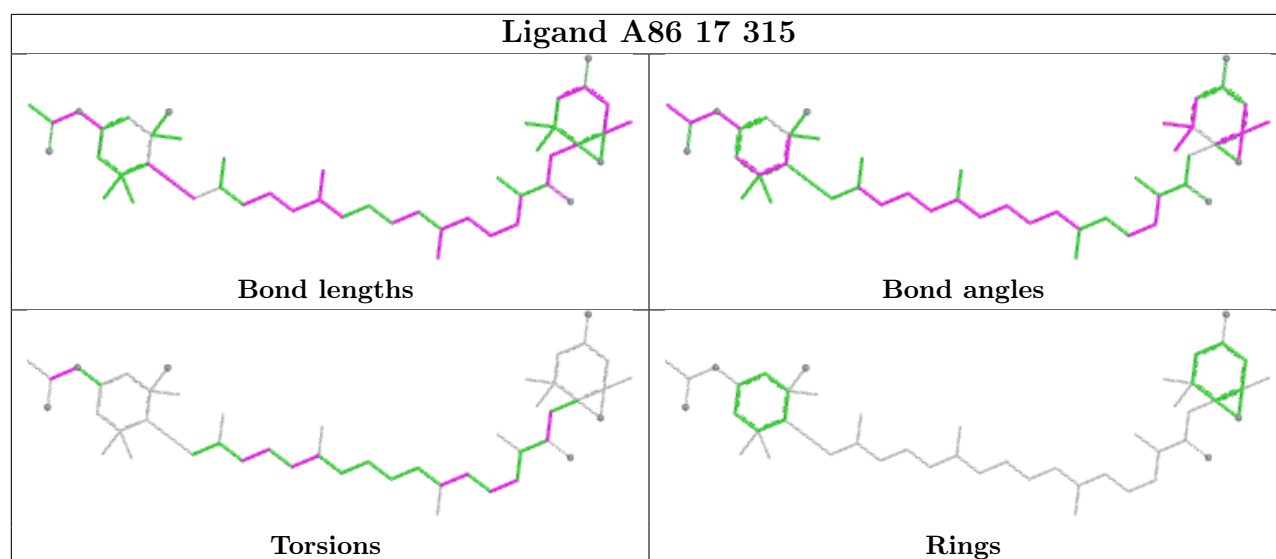




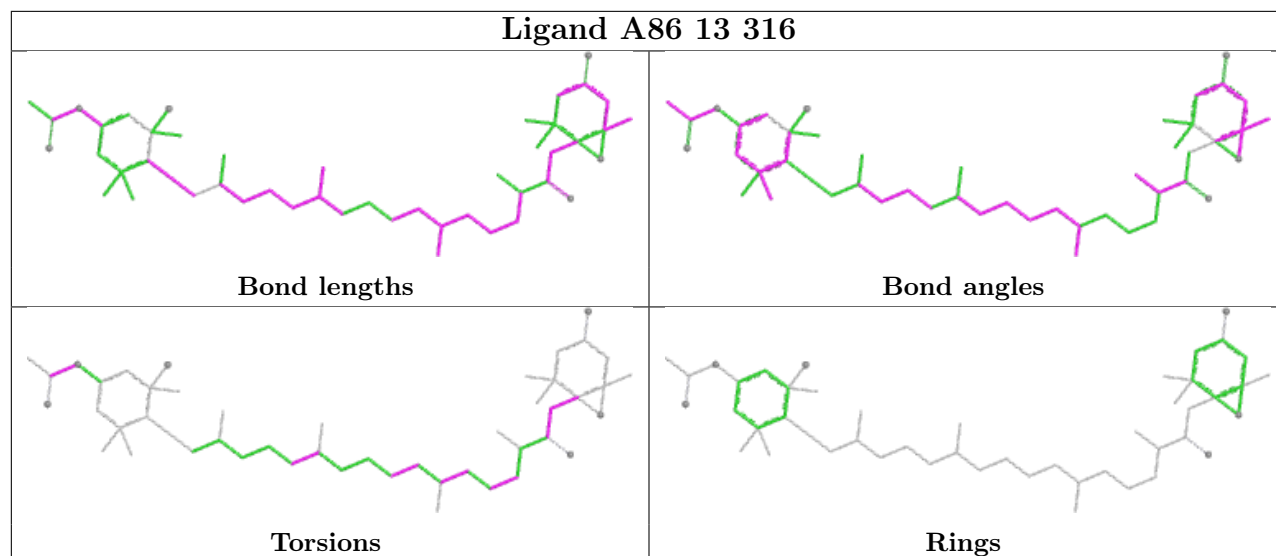




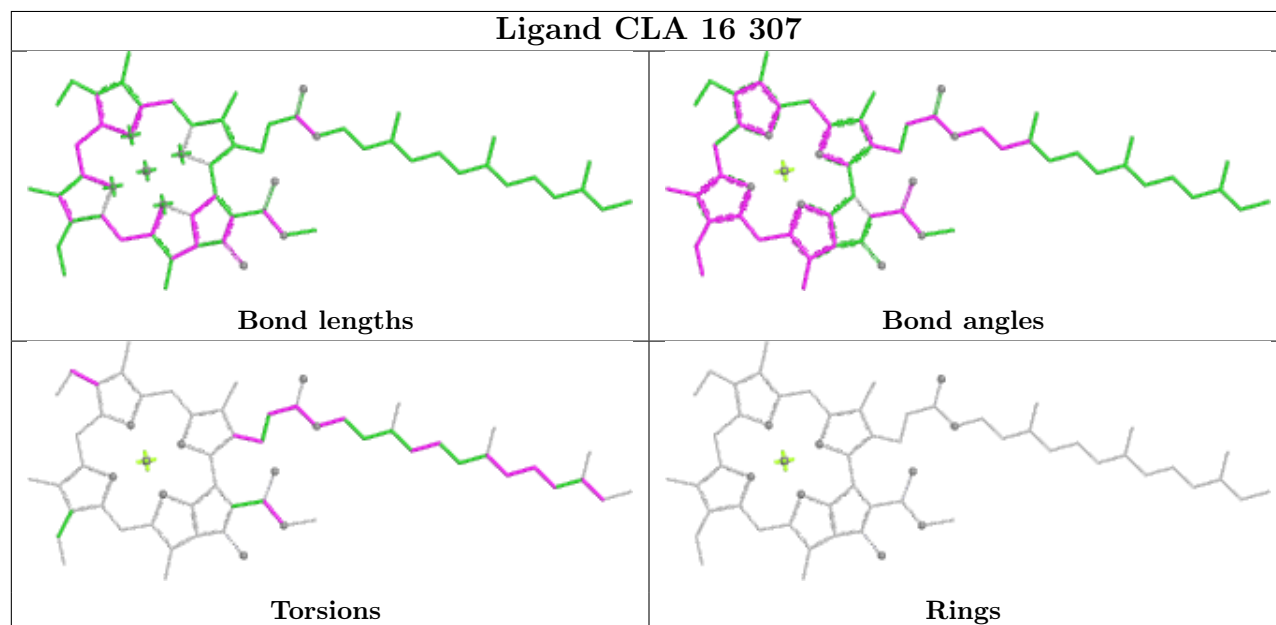




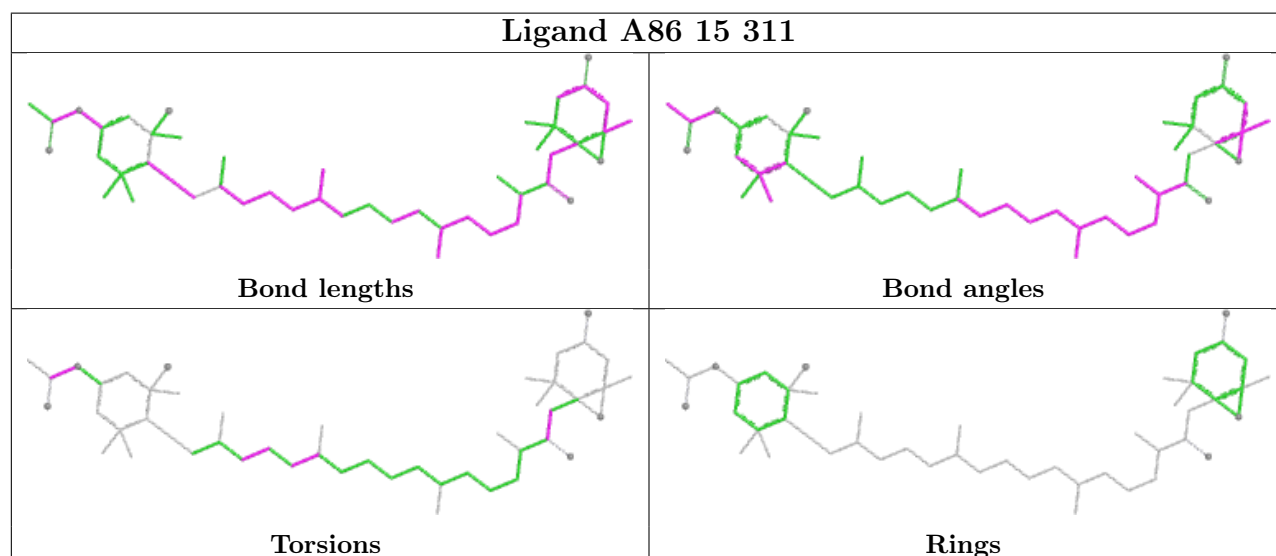
Ligand A86 13 316

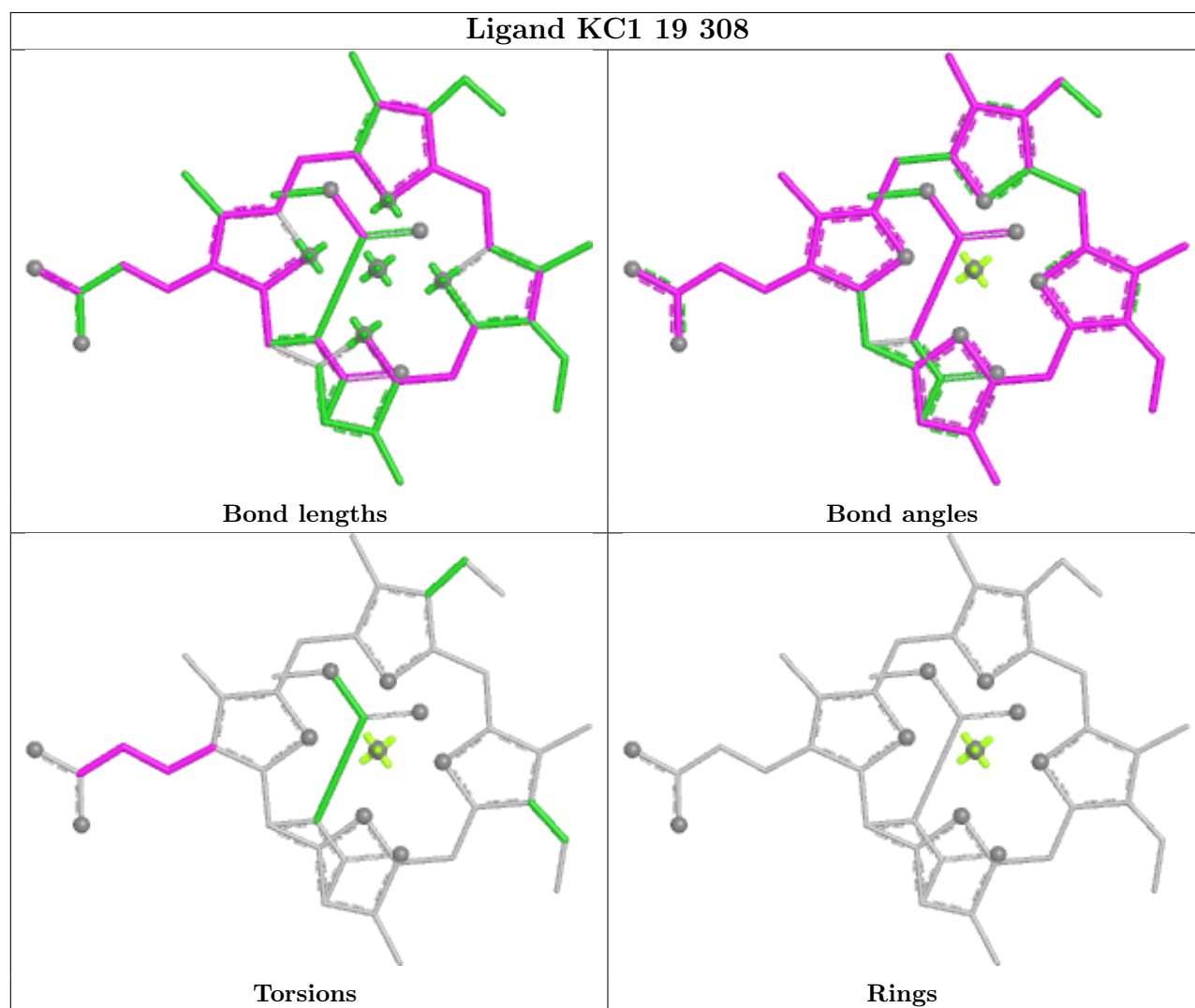
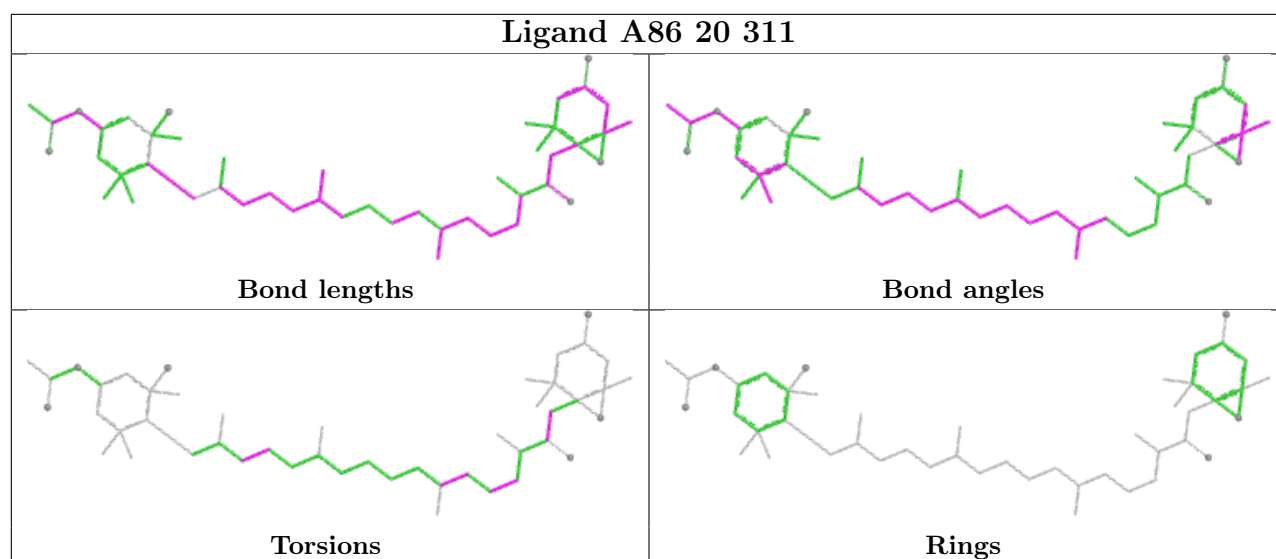


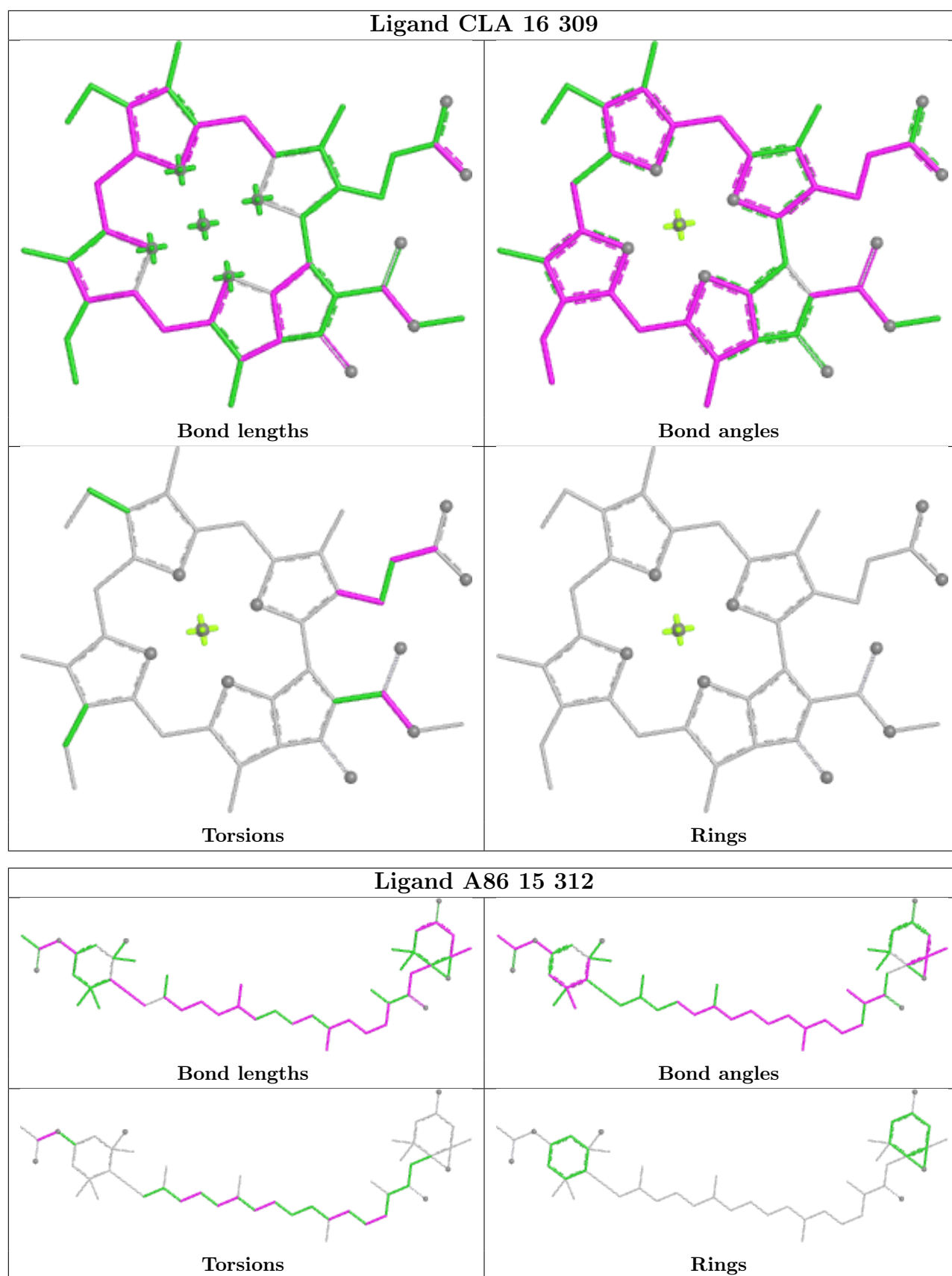
Ligand CLA 16 307

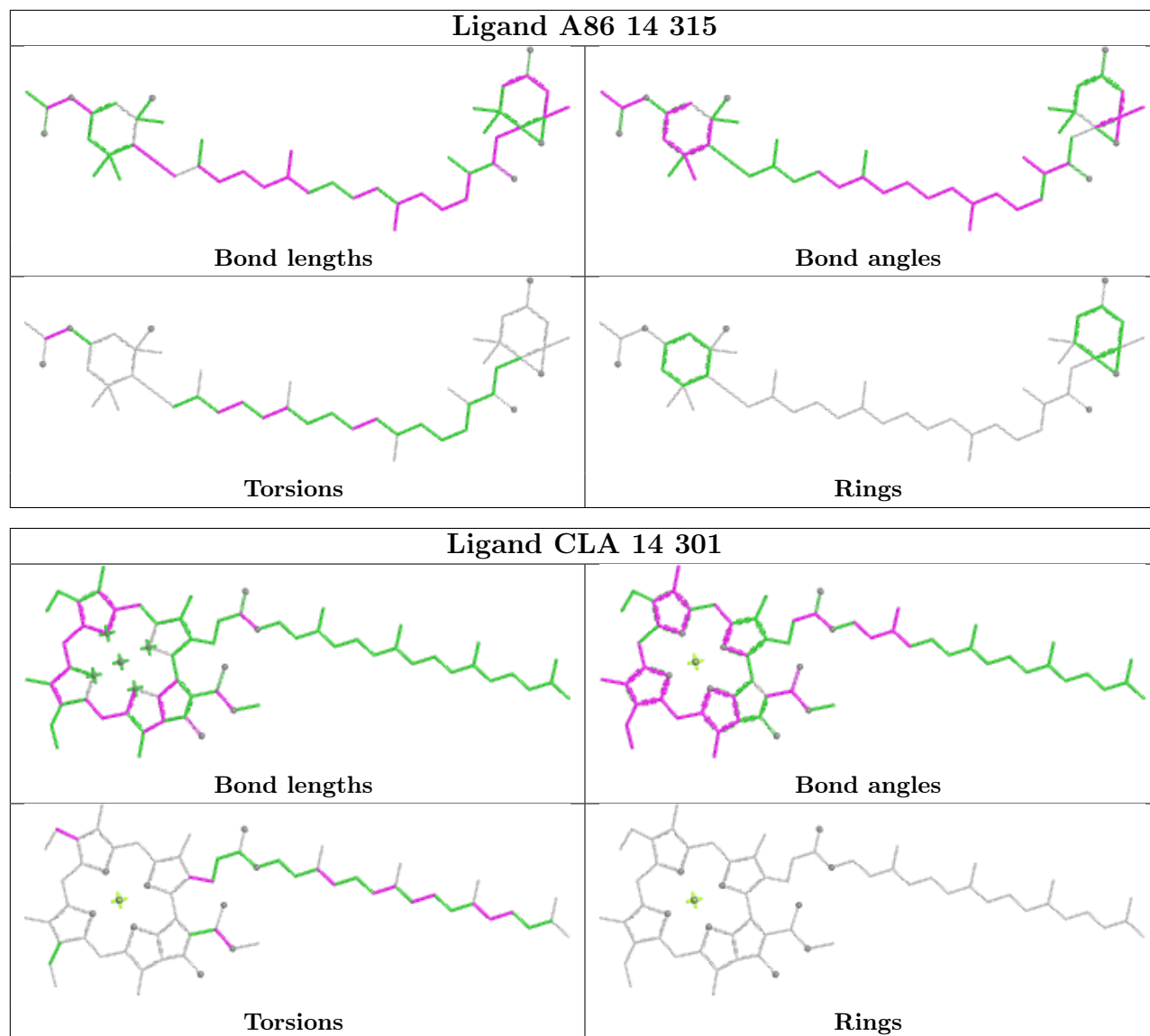


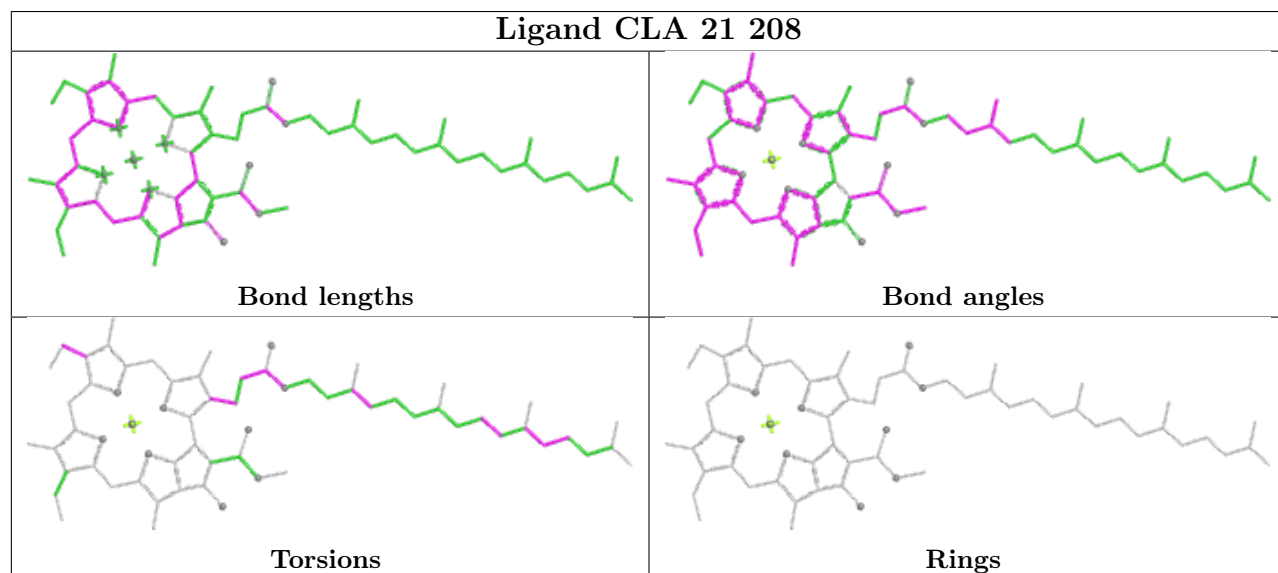
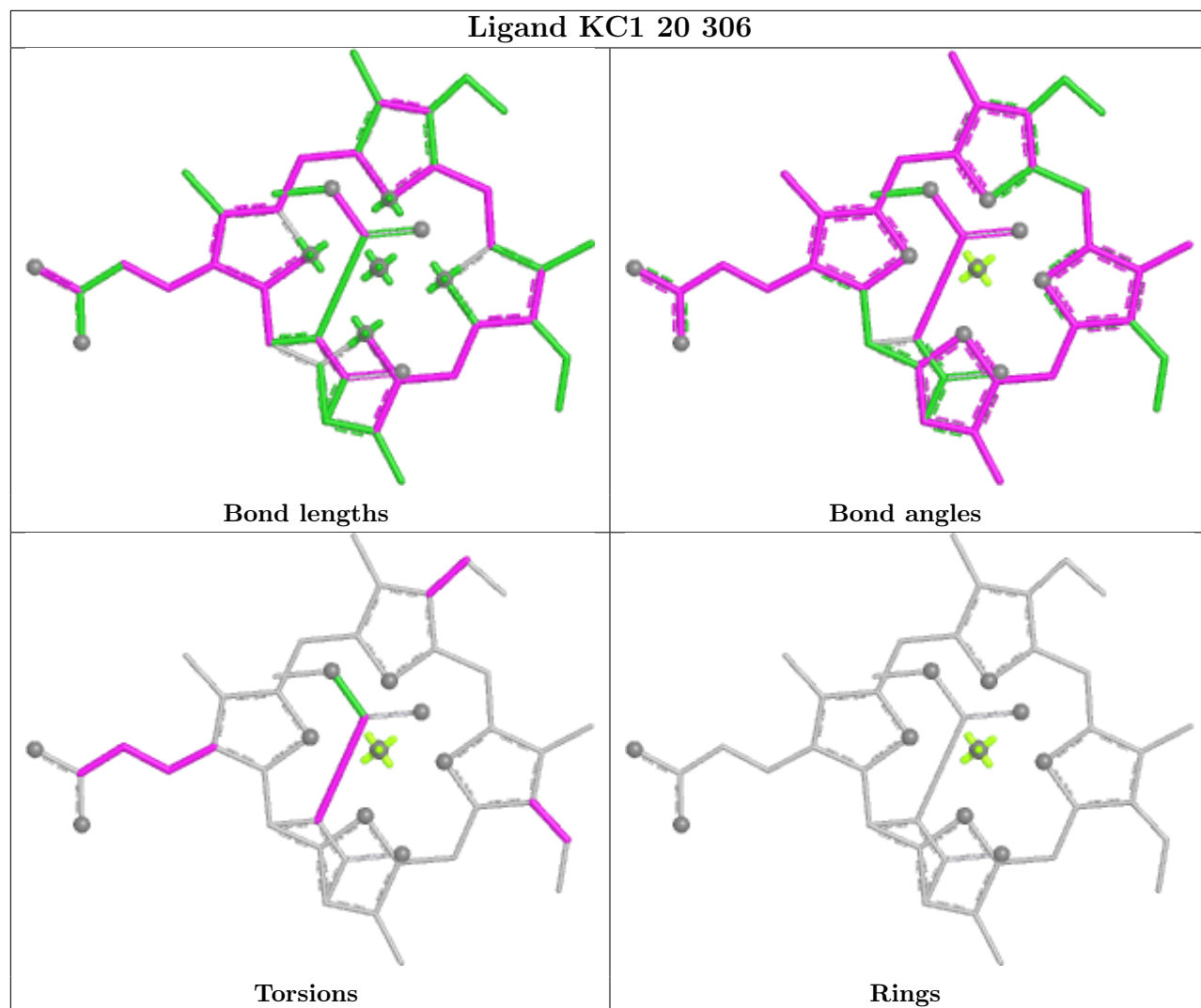
Ligand A86 15 311

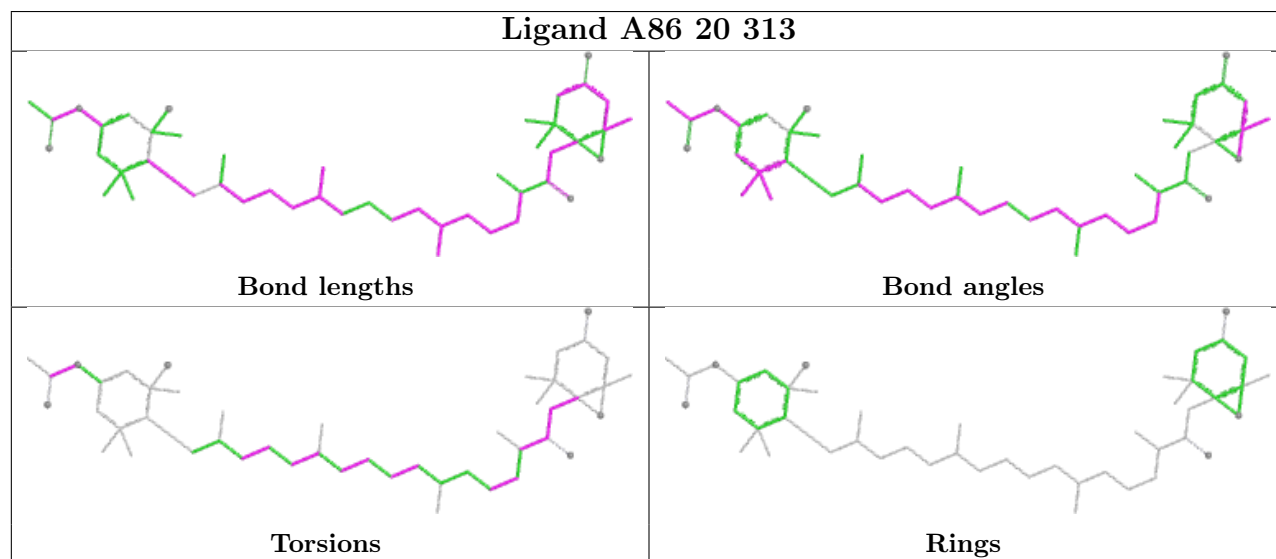
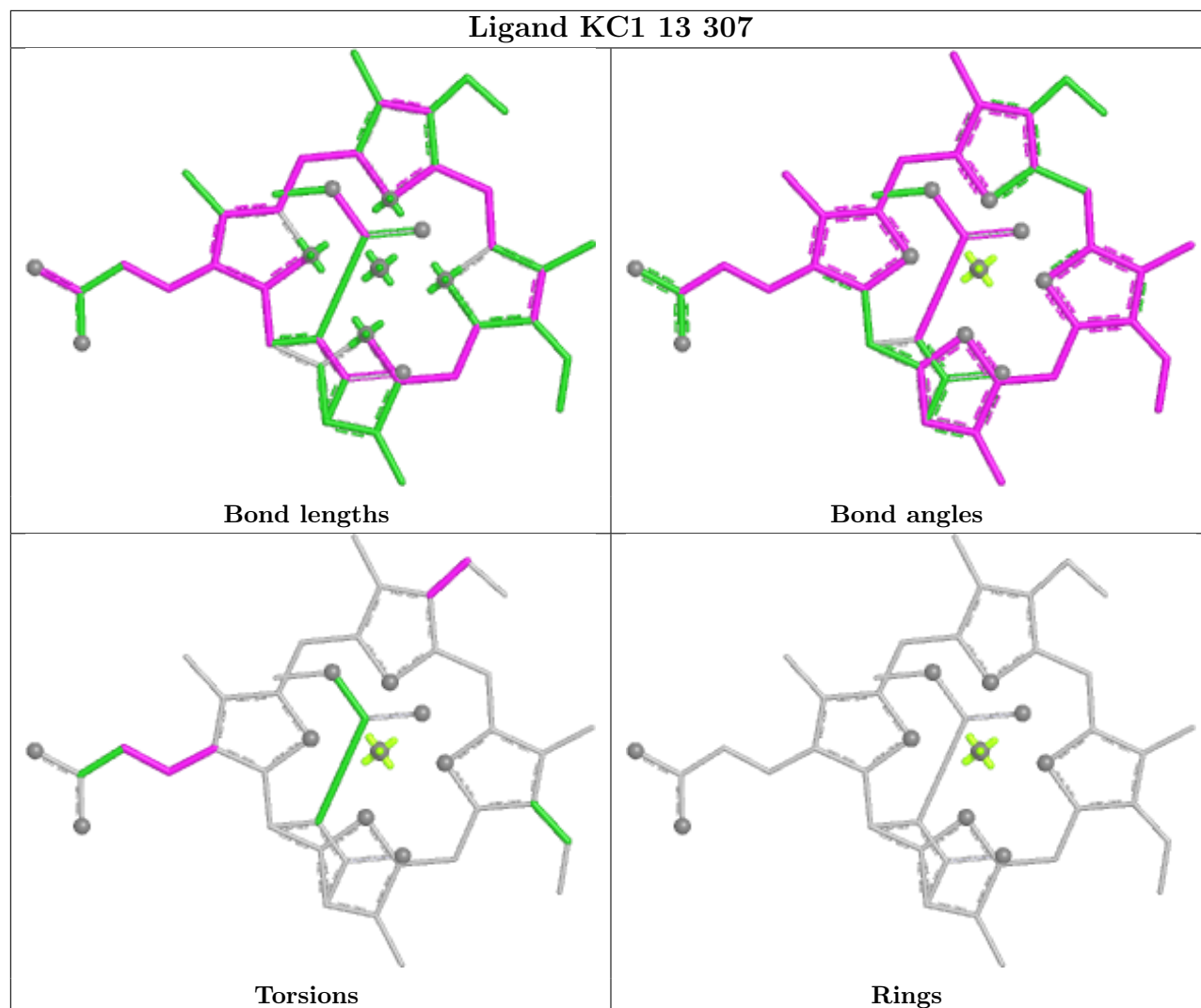


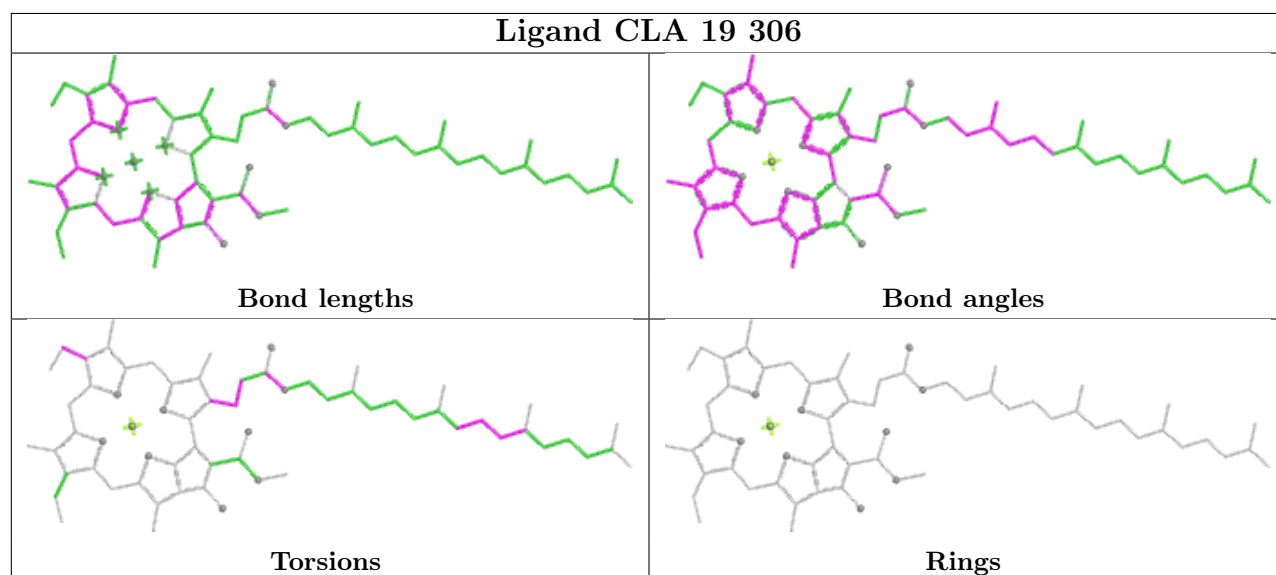
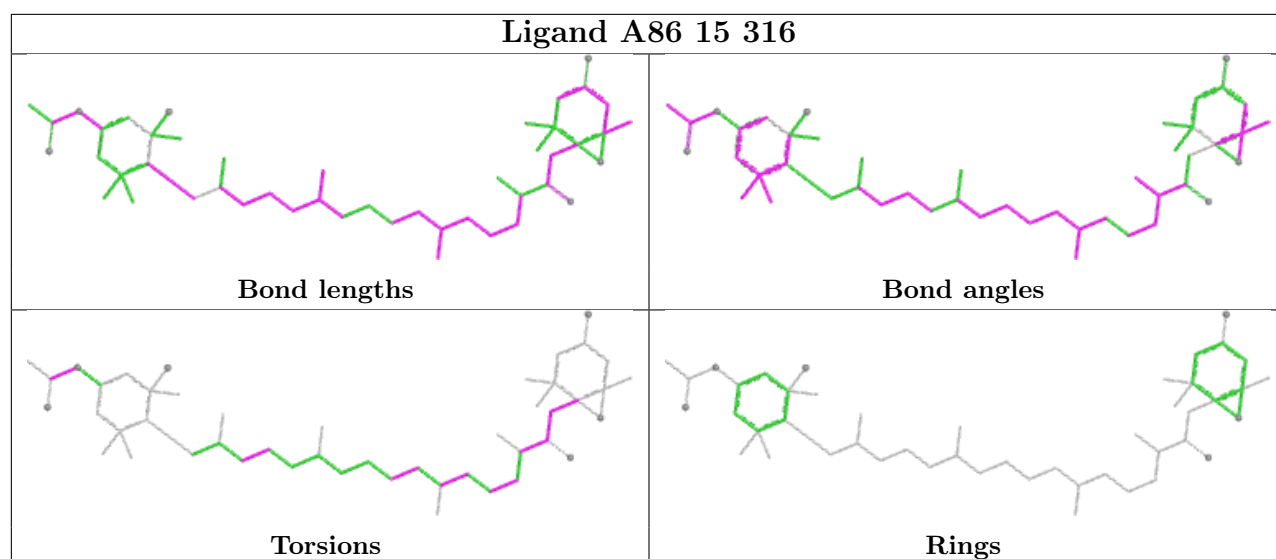


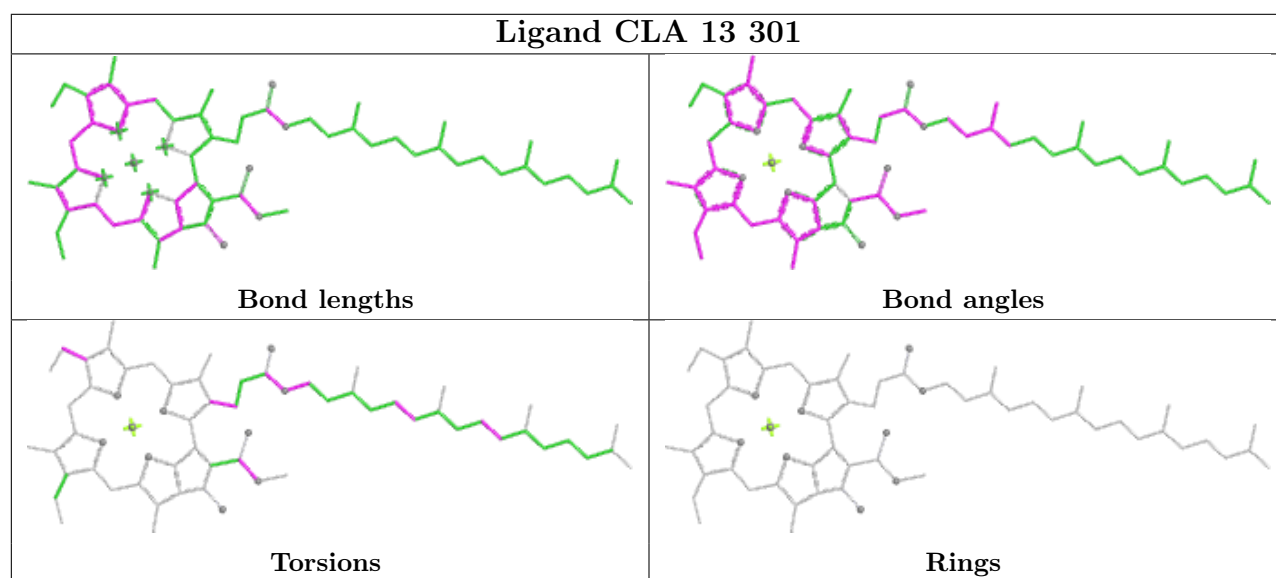
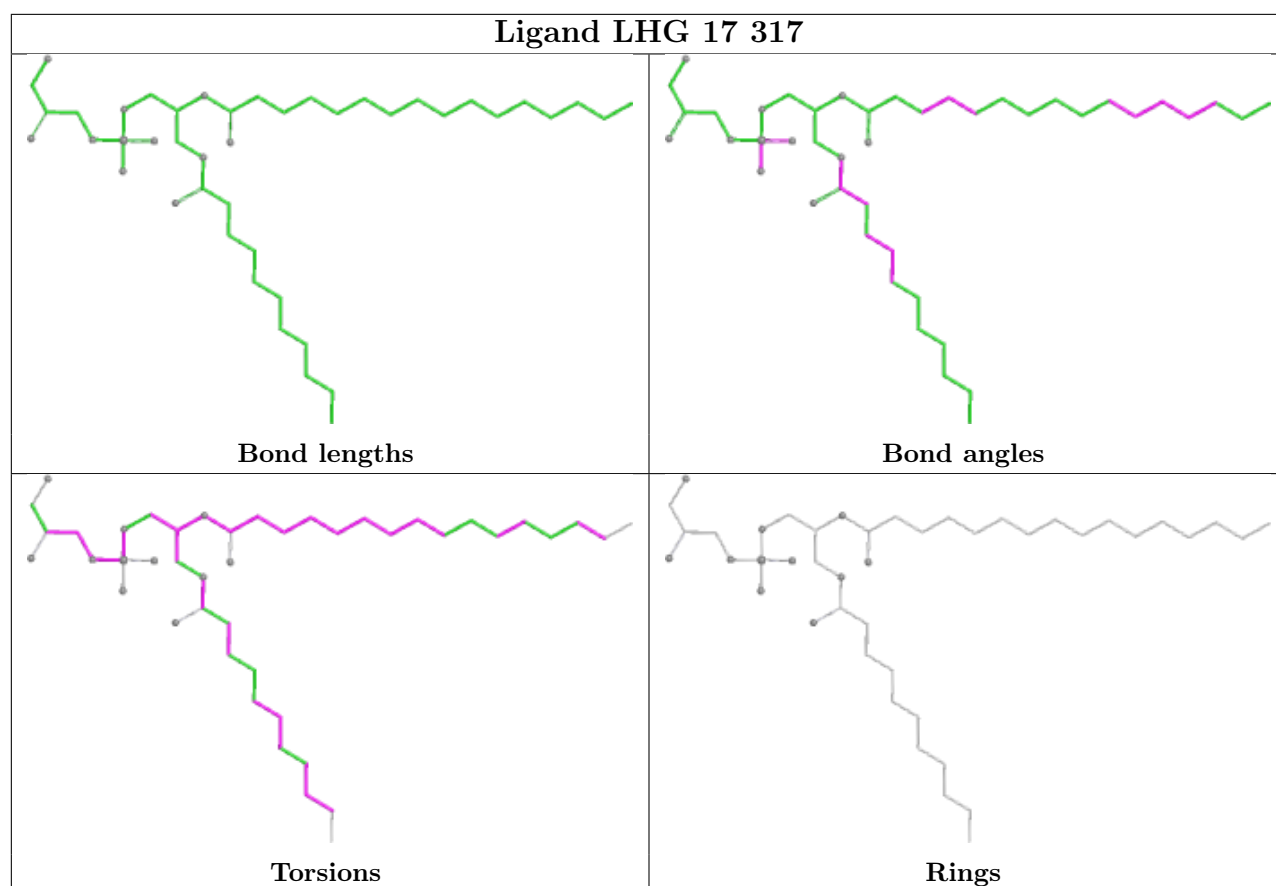


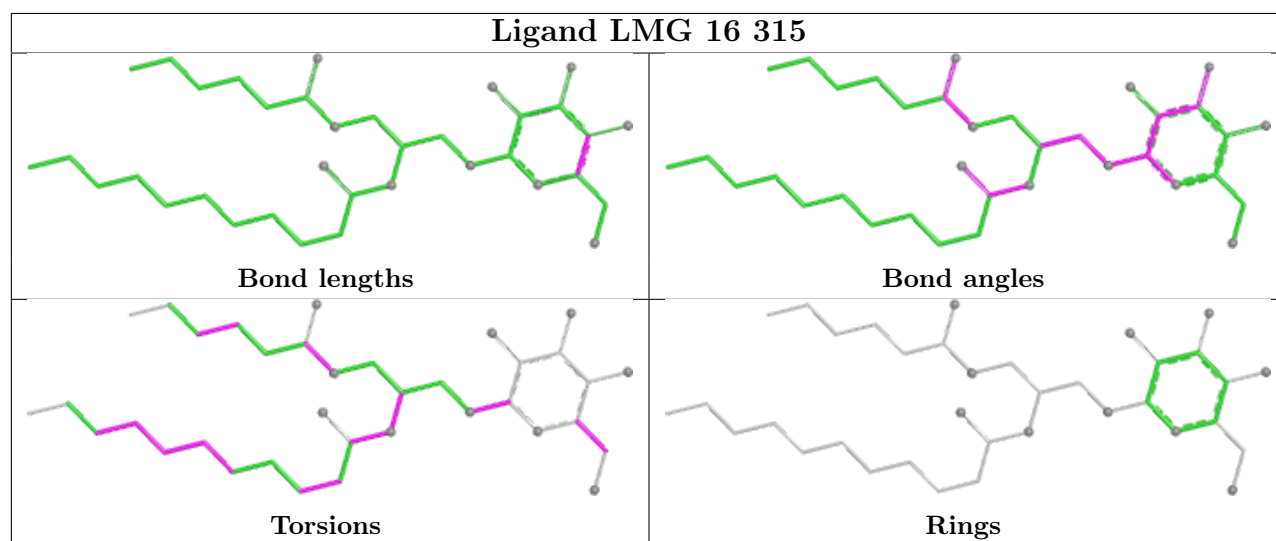
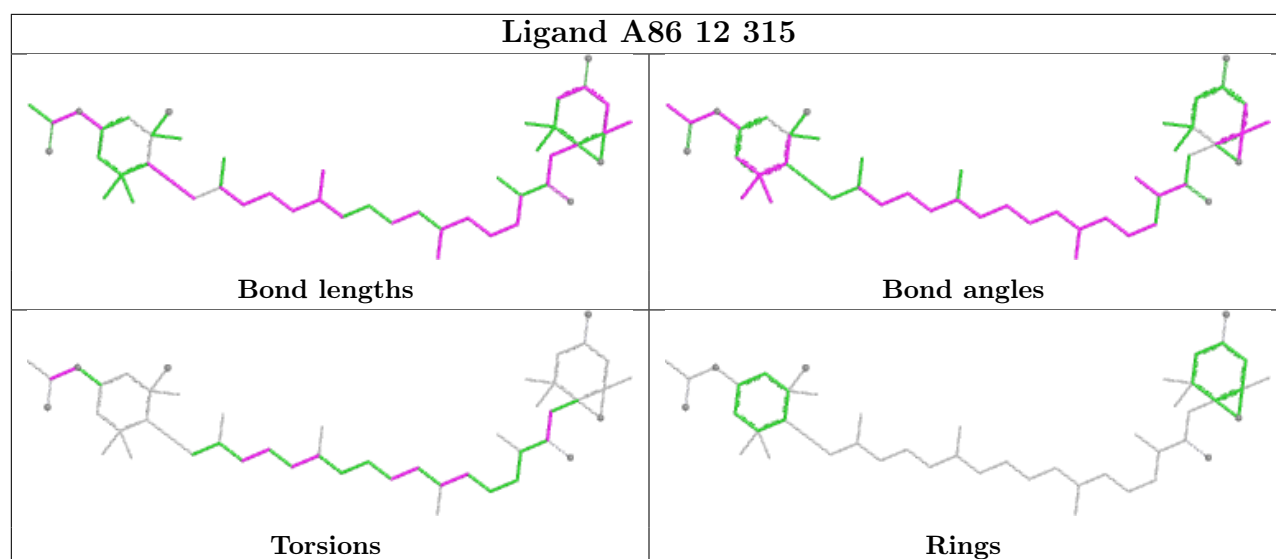


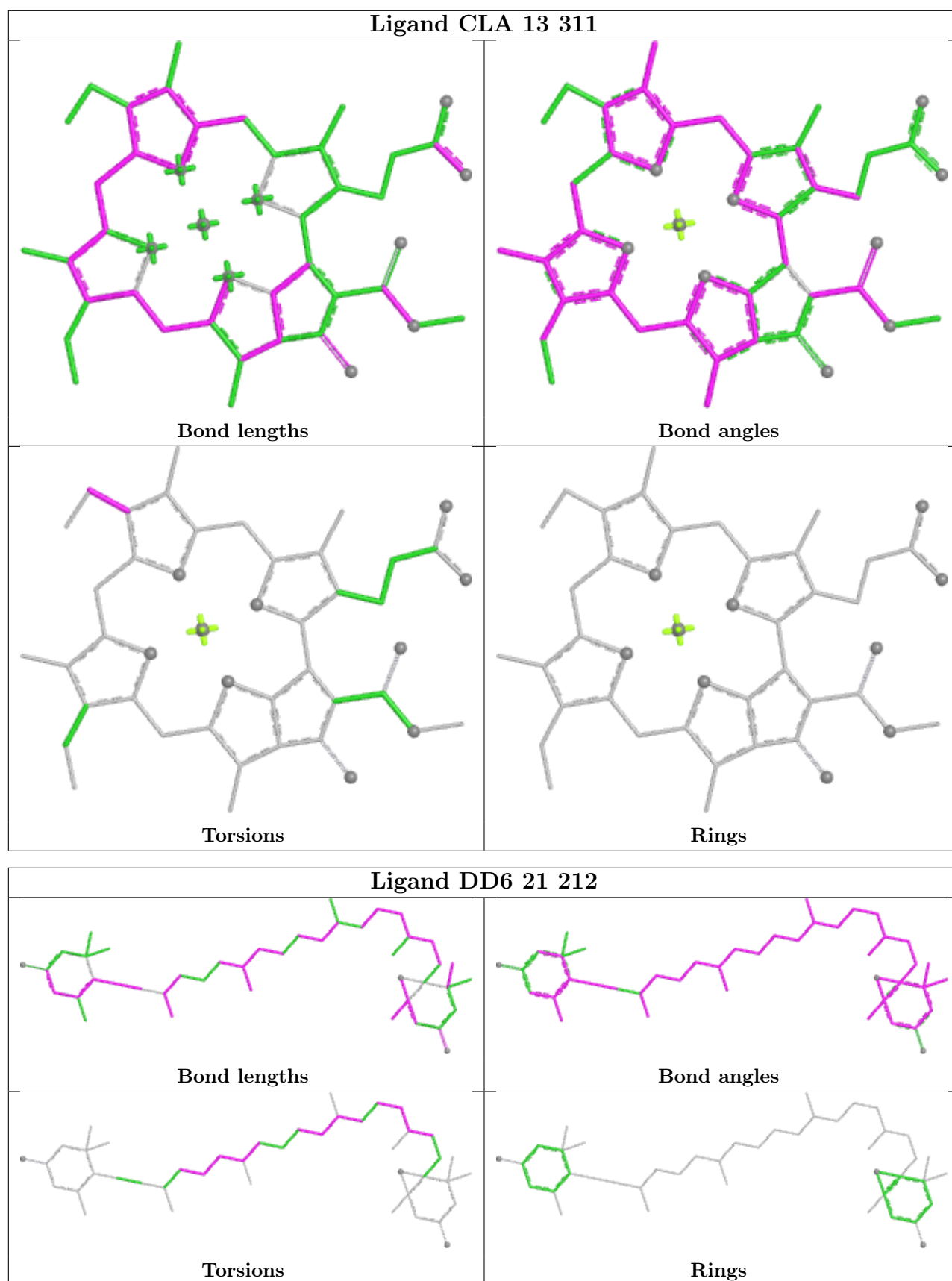


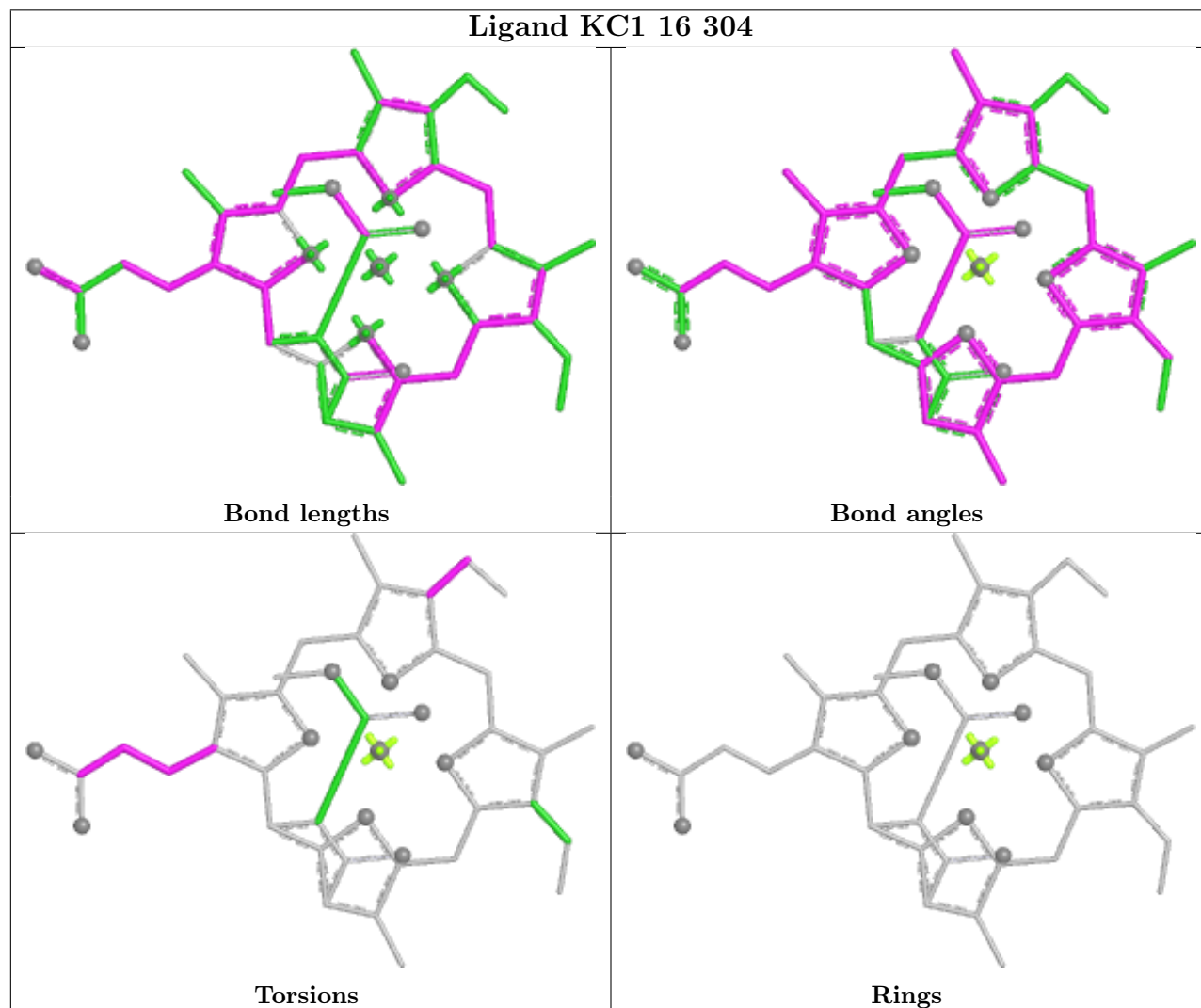
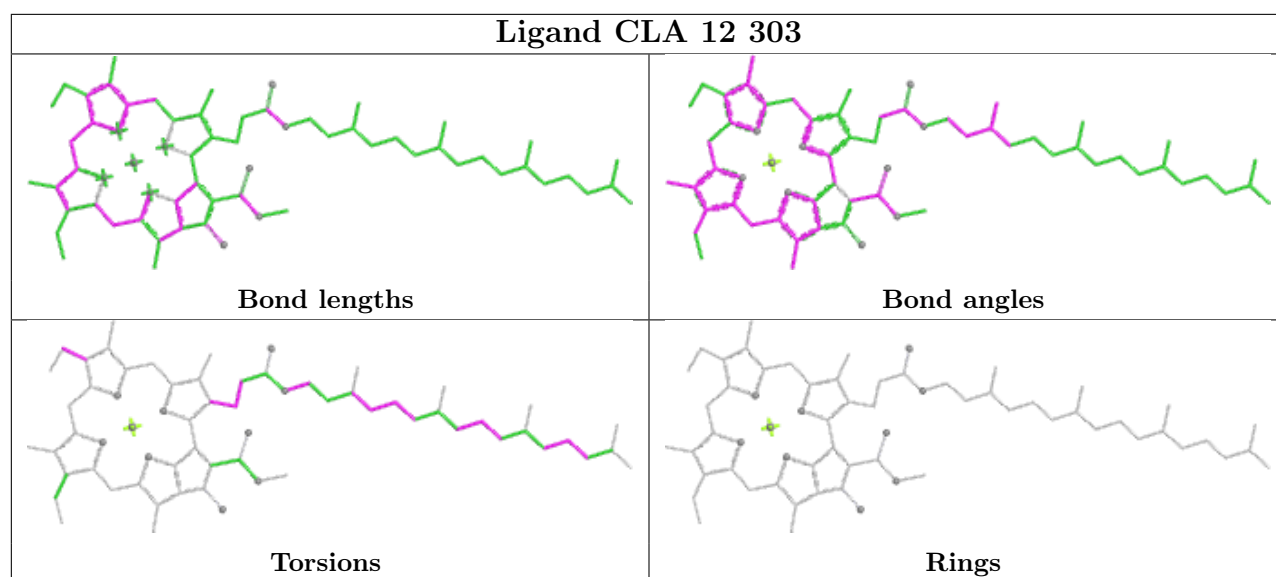


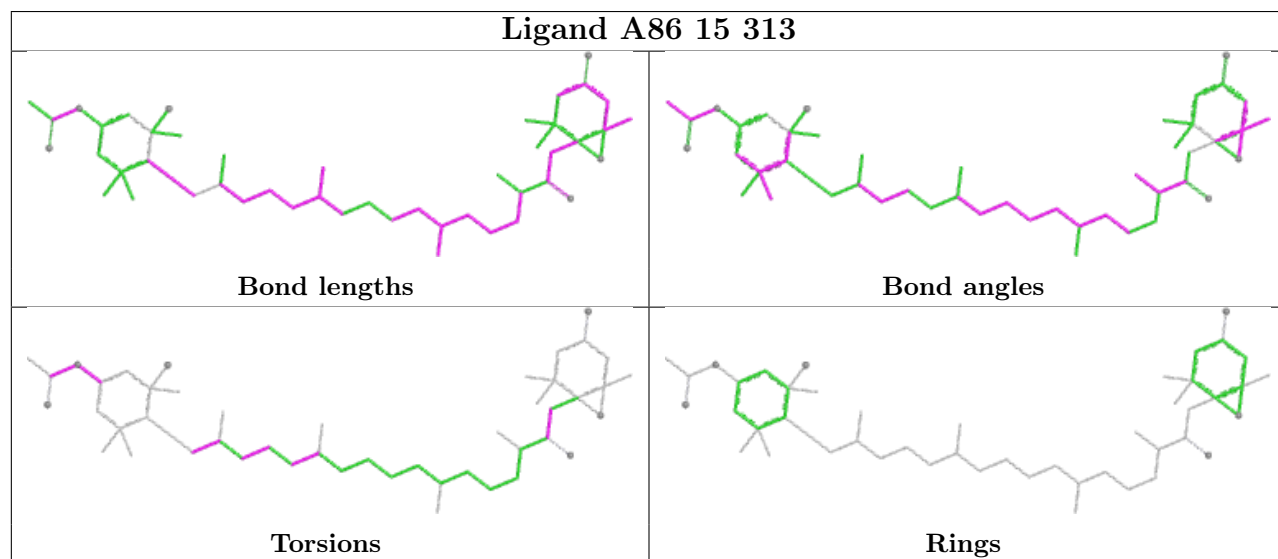
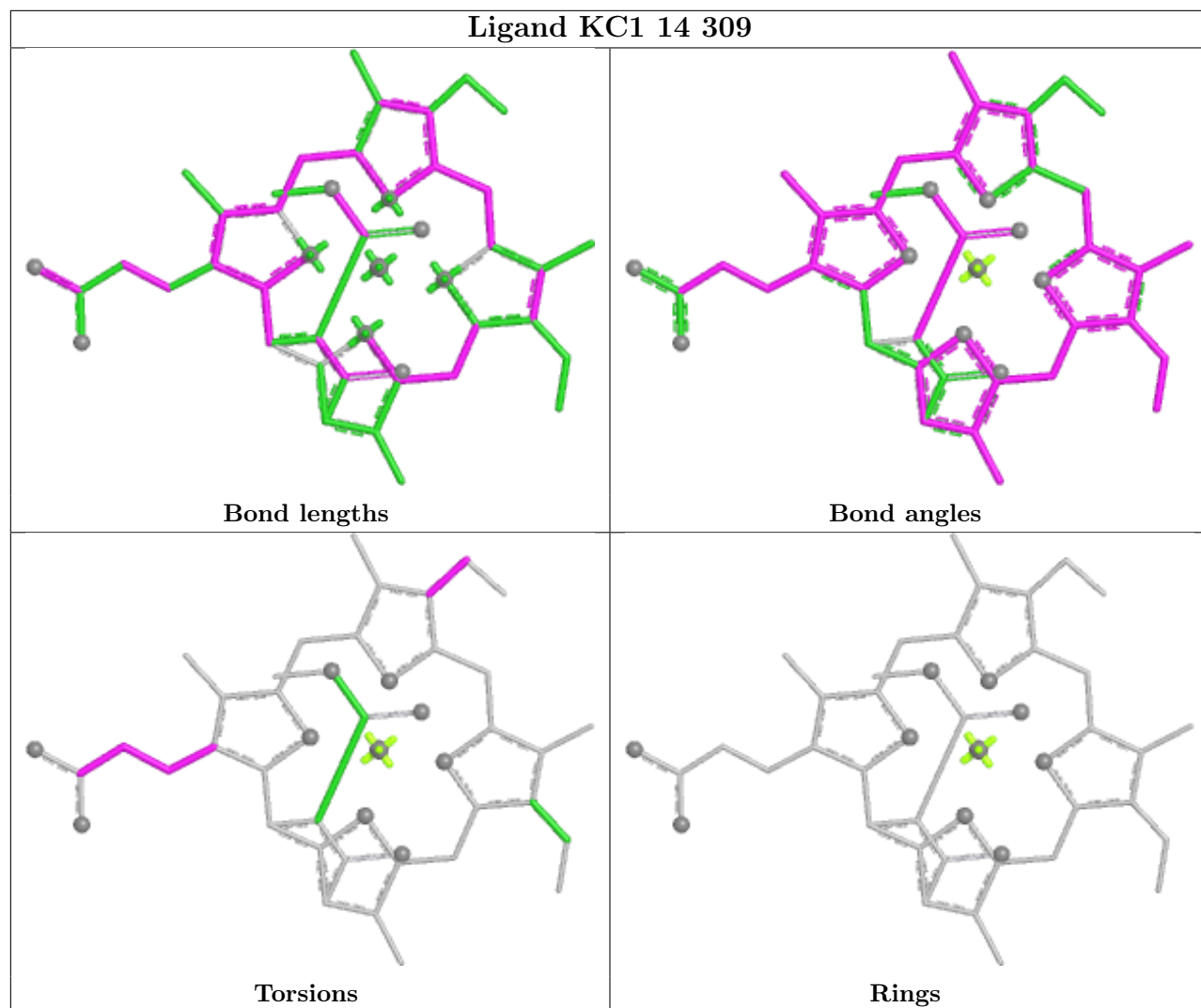


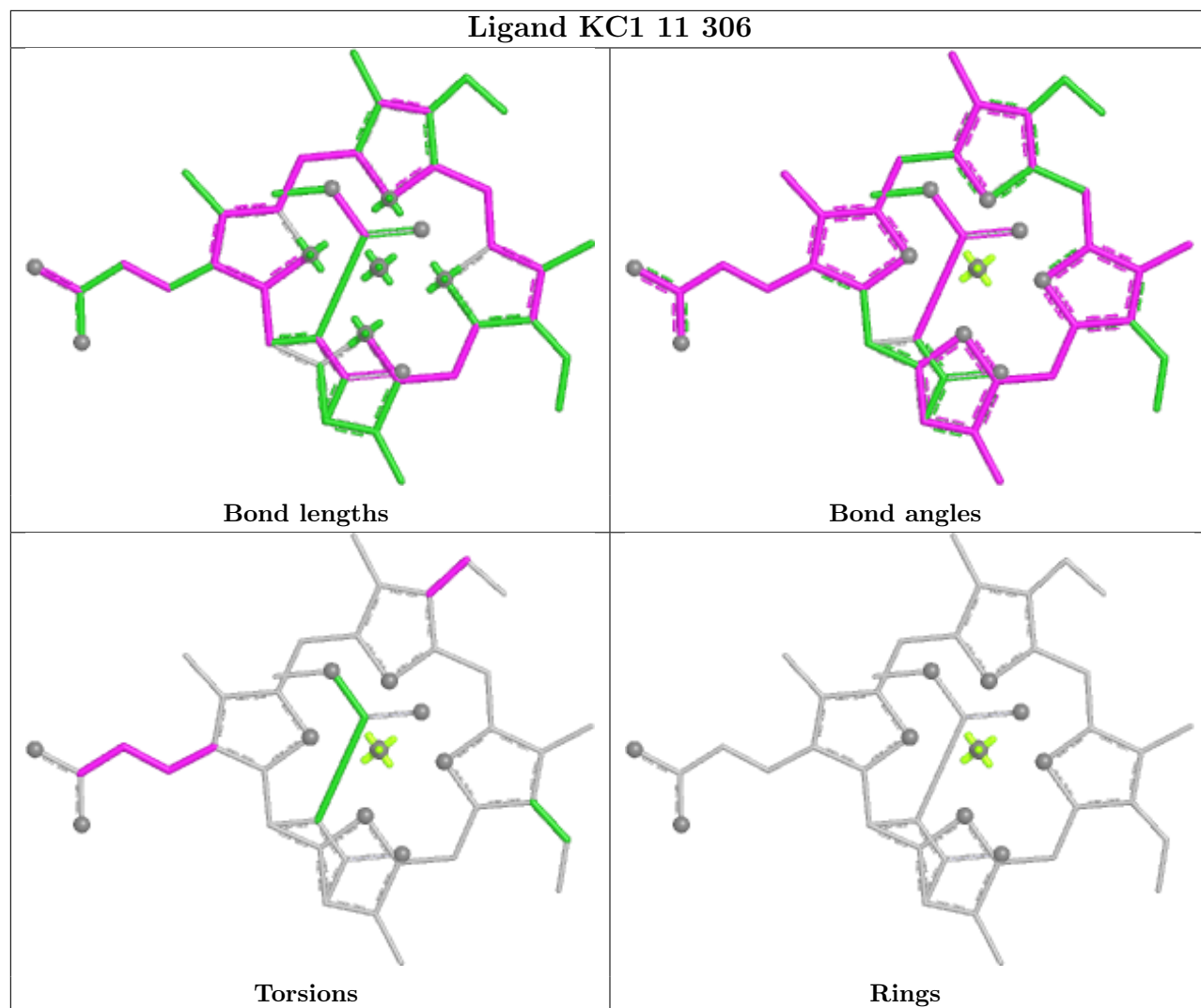


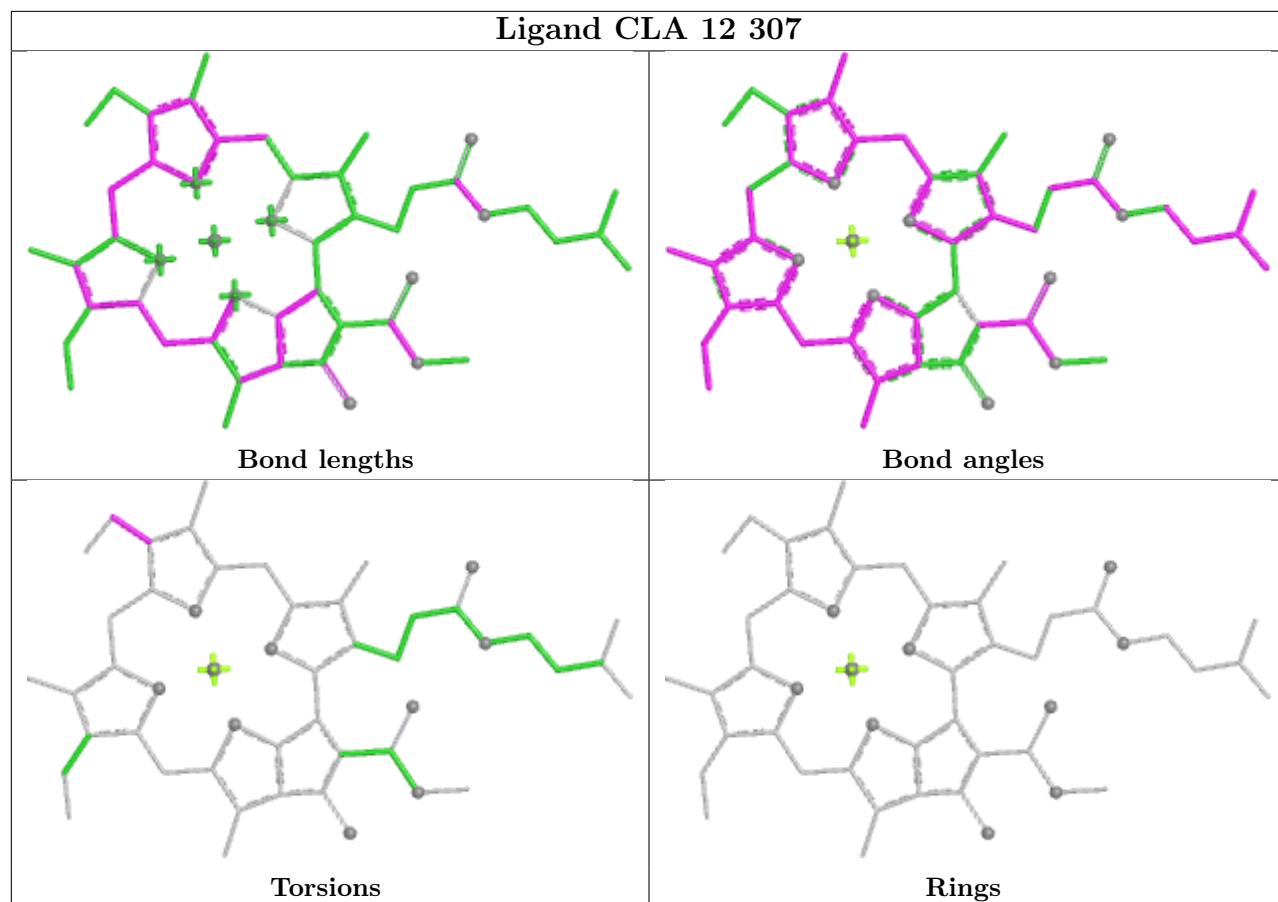


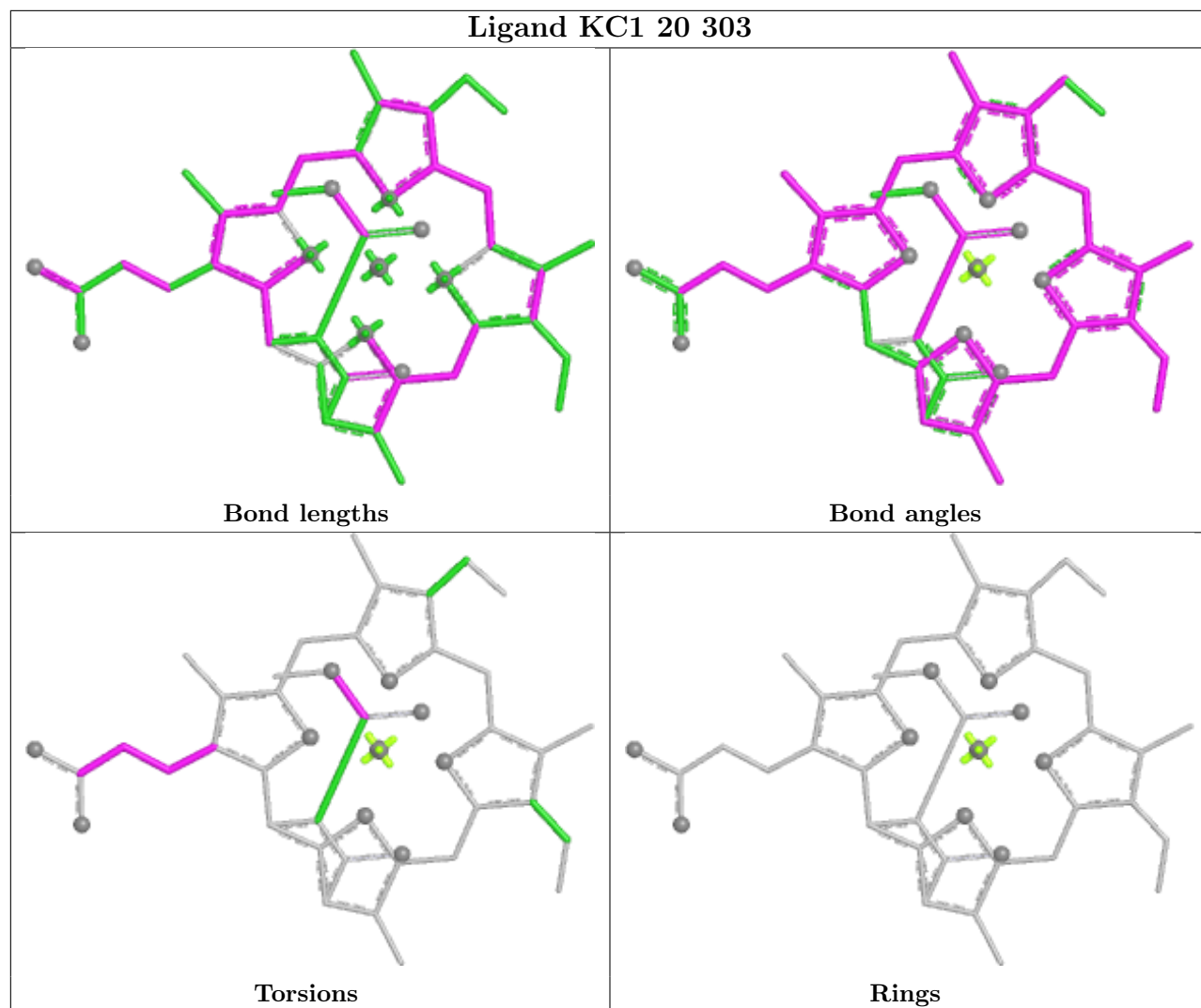


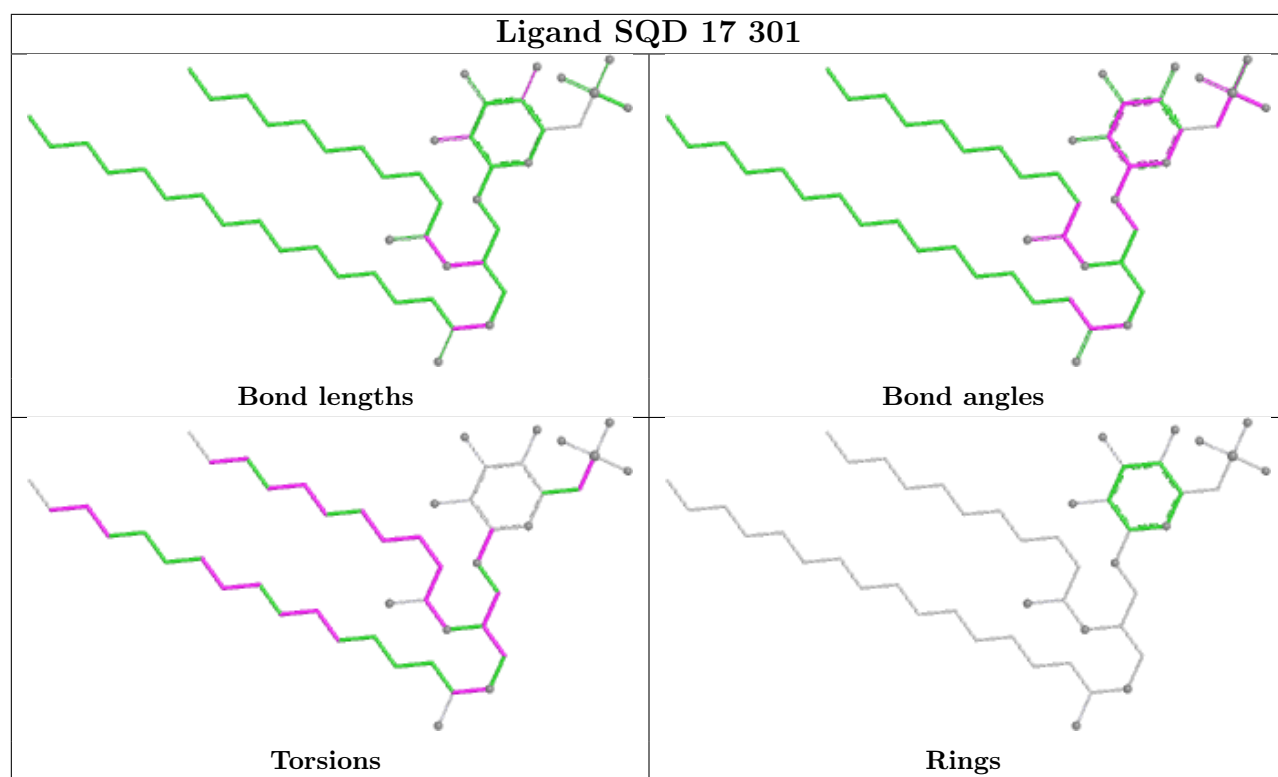


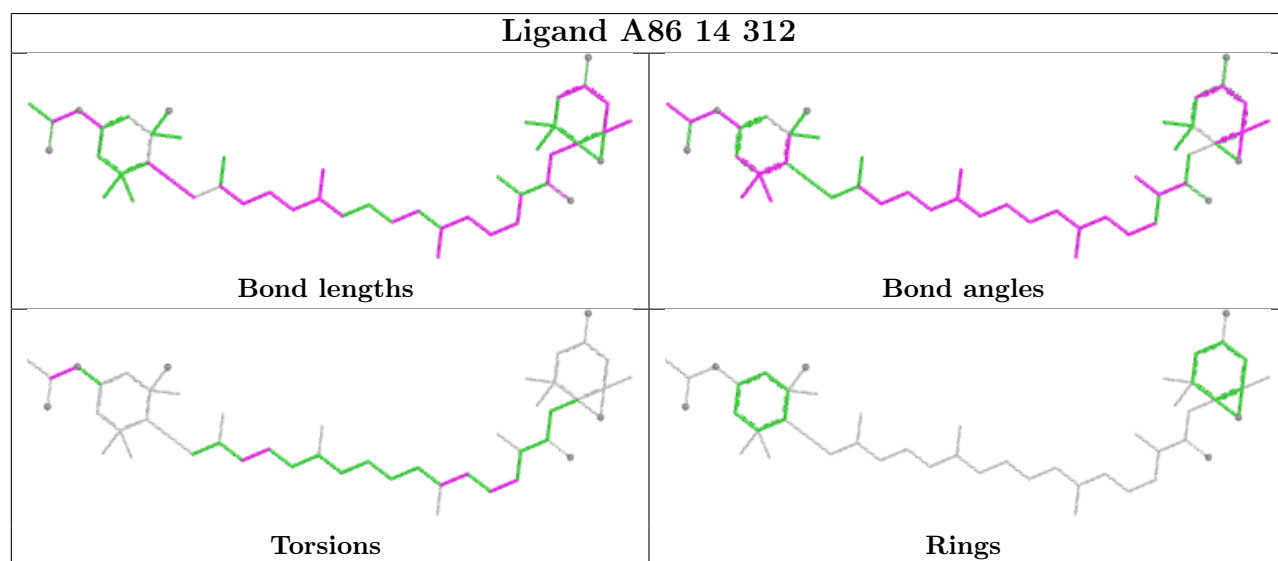
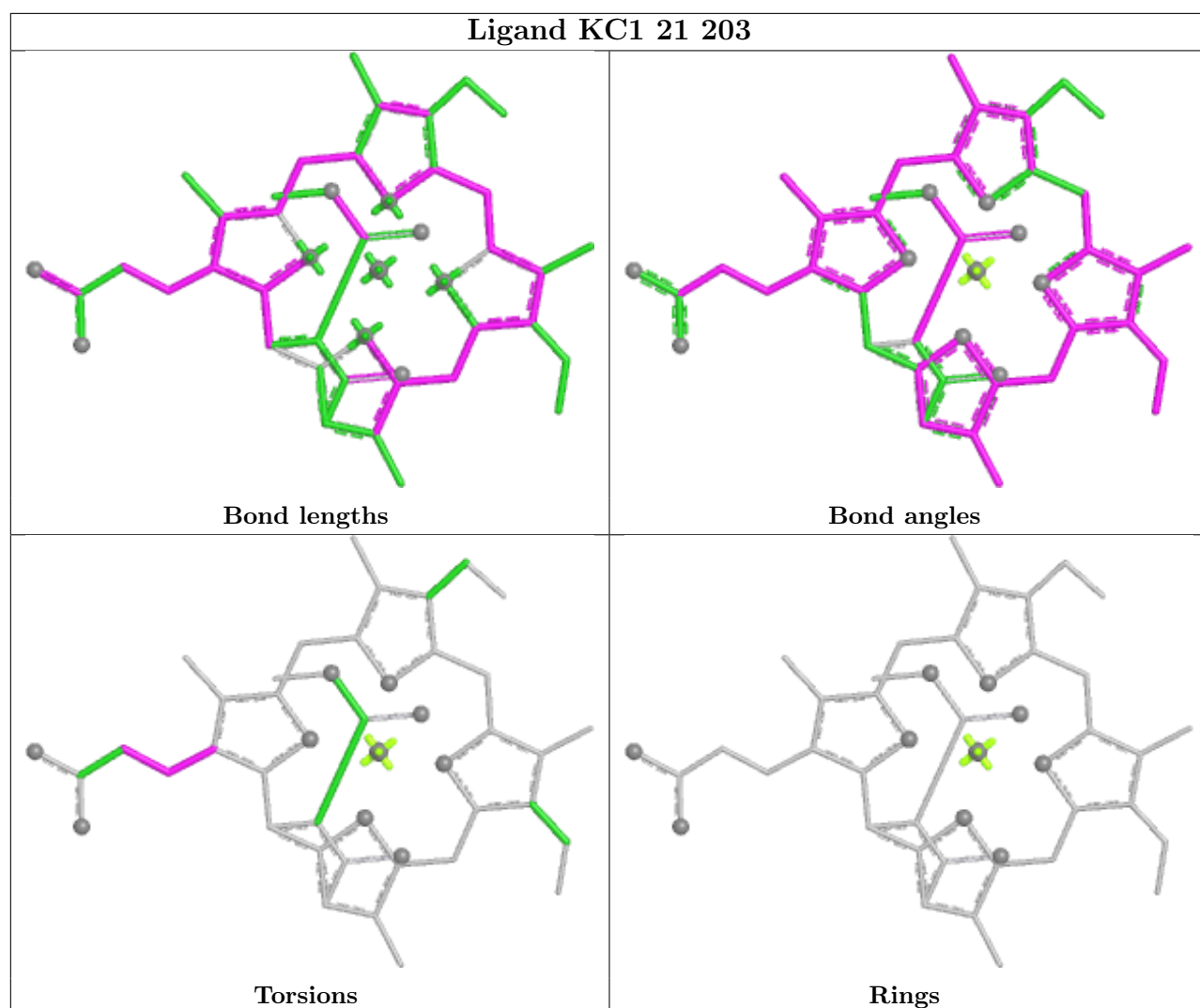


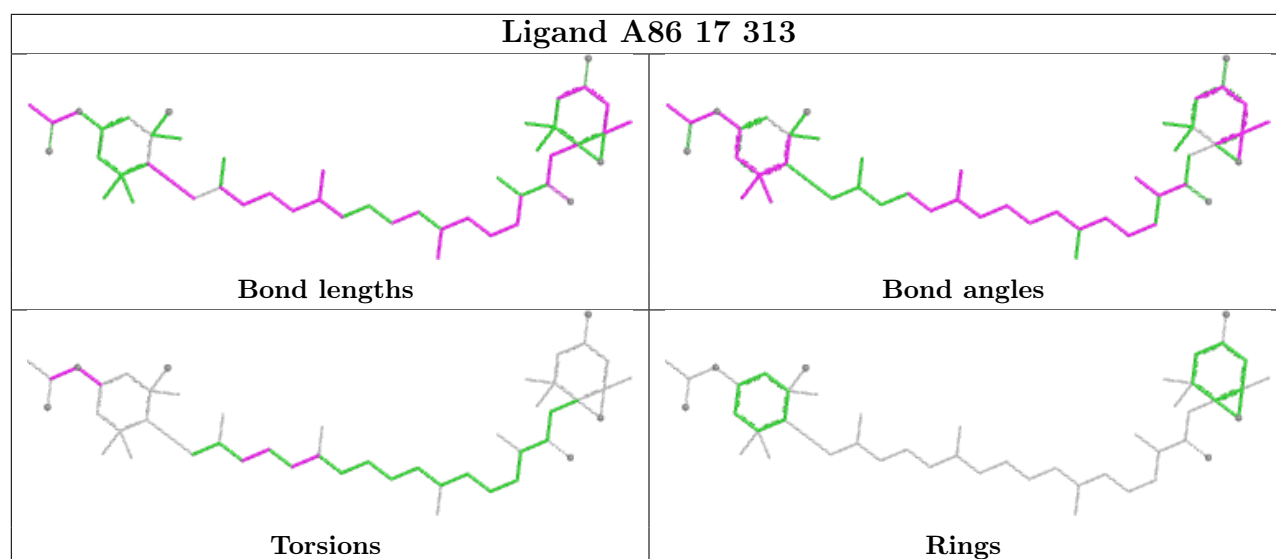












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31906. These allow visual inspection of the internal detail of the map and identification of artifacts.

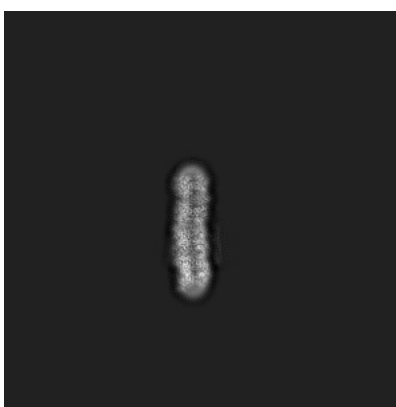
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

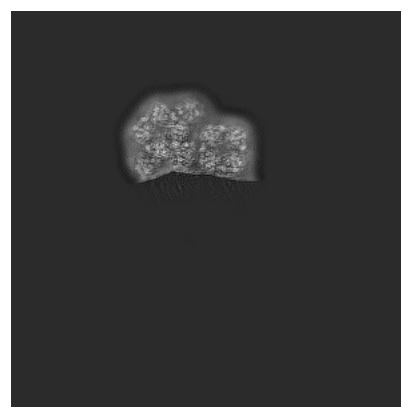
6.1.1 Primary map



X



Y

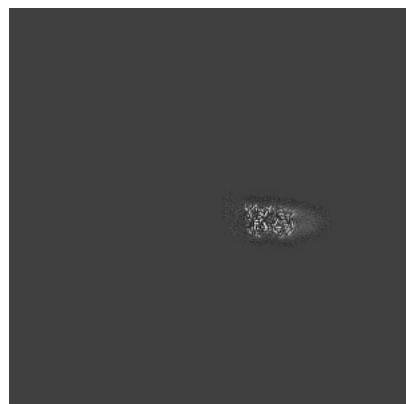


Z

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

6.2 Central slices [i](#)

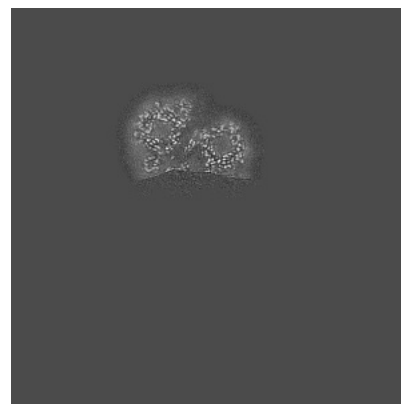
6.2.1 Primary map



X Index: 256



Y Index: 256

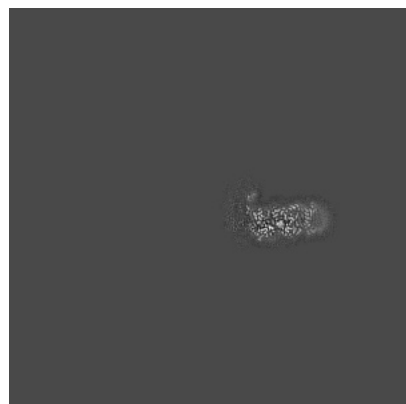


Z Index: 256

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

6.3 Largest variance slices [i](#)

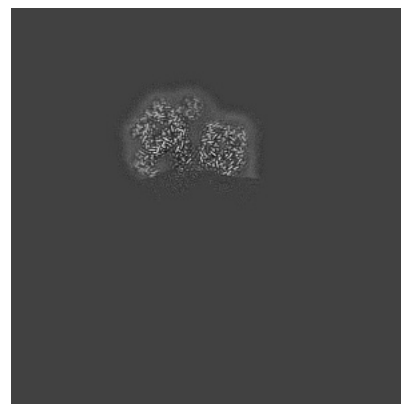
6.3.1 Primary map



X Index: 216



Y Index: 321

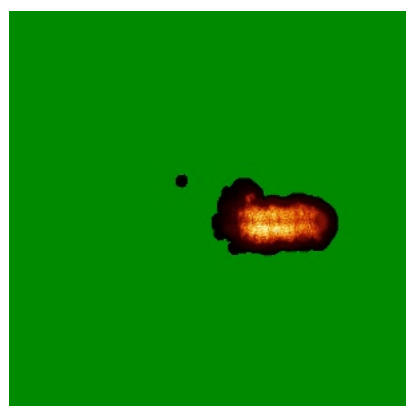


Z Index: 234

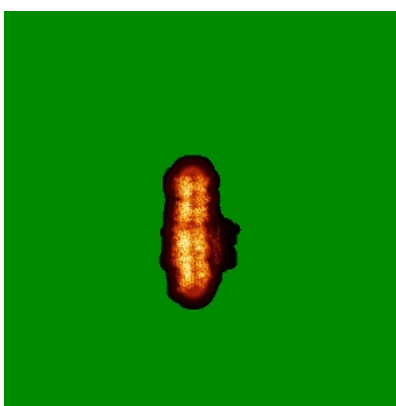
The images above show the largest variance slices of the map in three orthogonal directions.

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

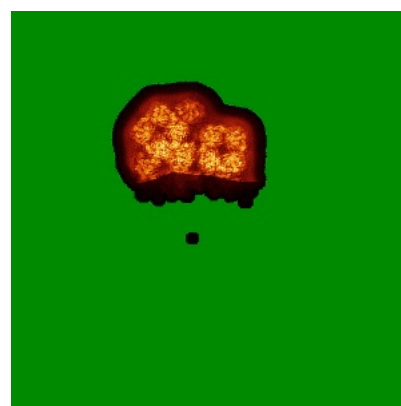
6.4.1 Primary map



X



Y

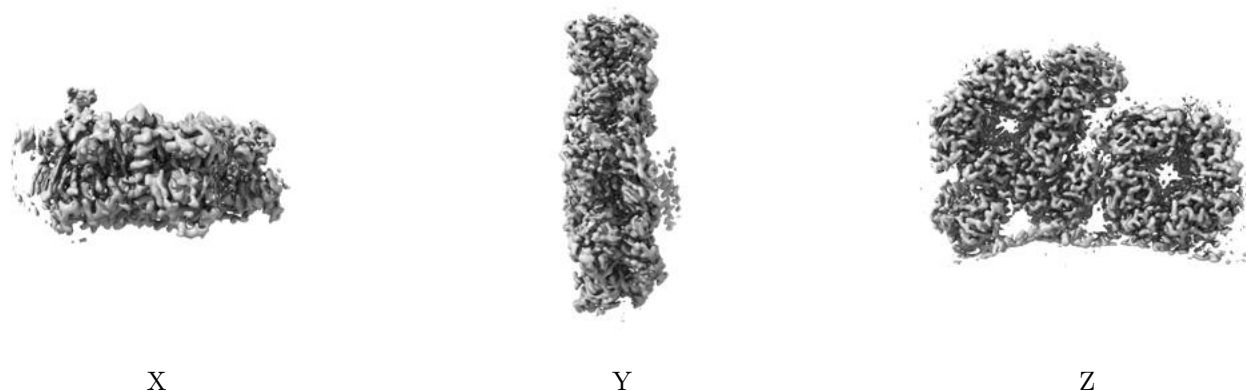


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.055. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

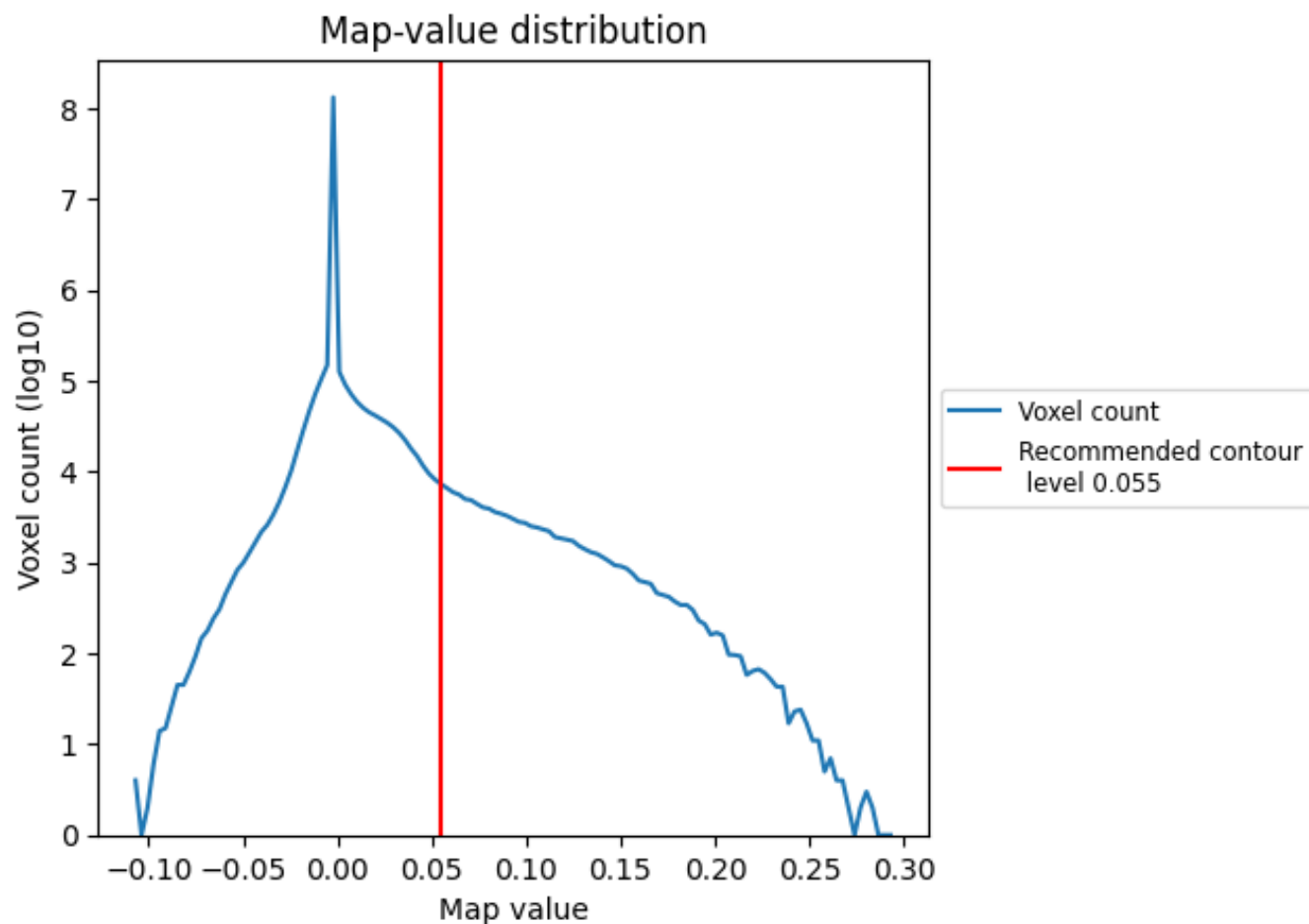
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

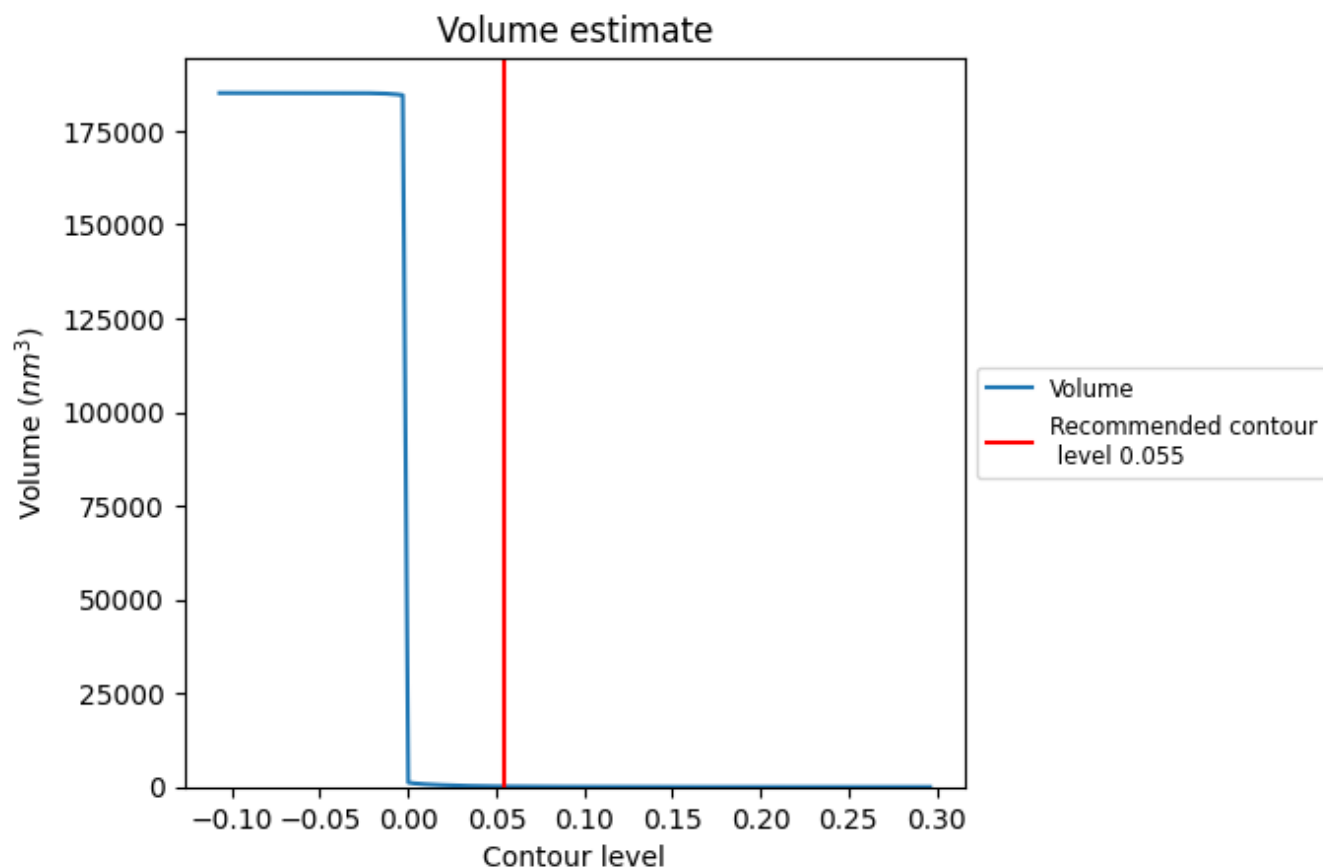
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

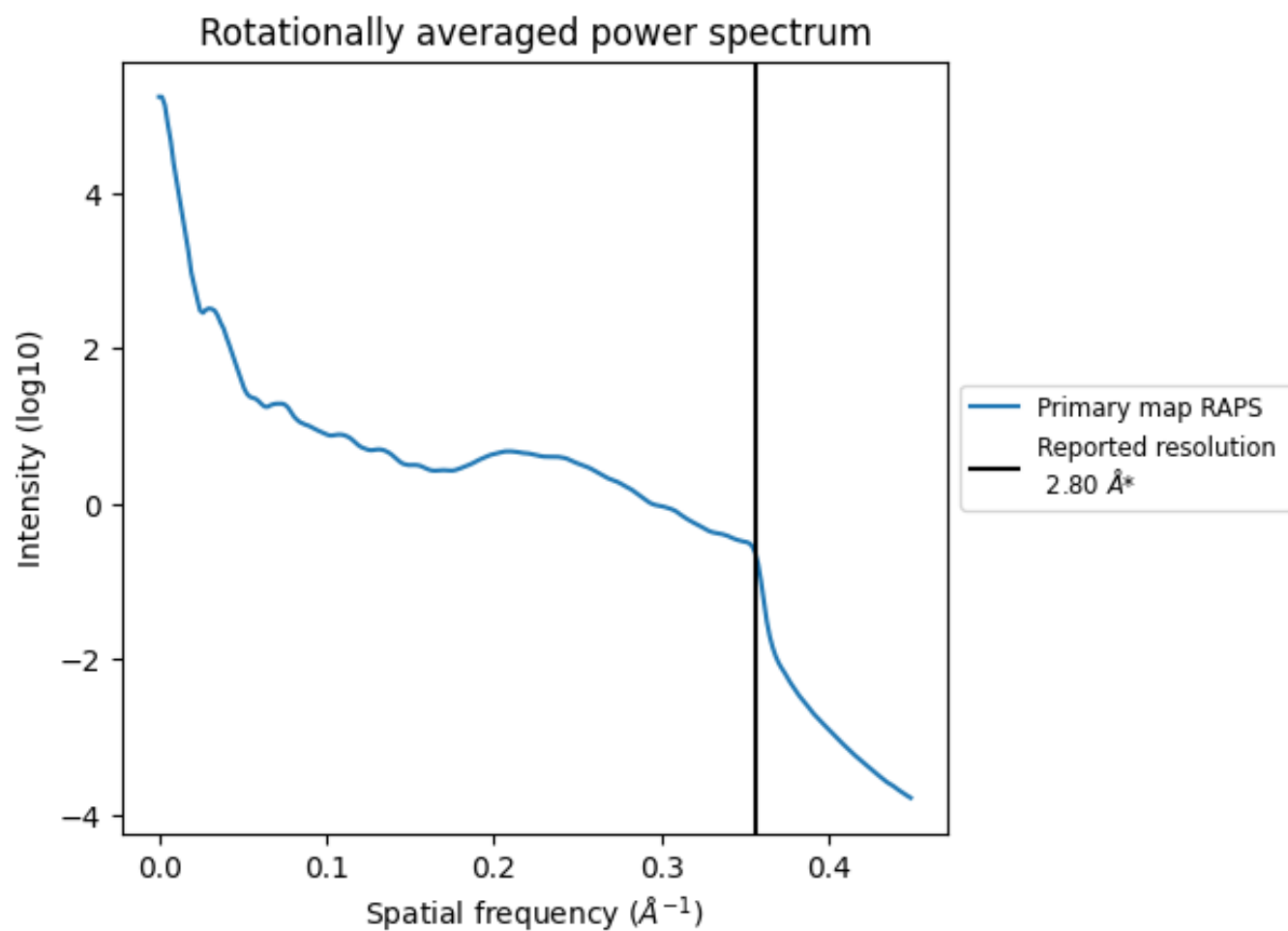
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 139 nm^3 ; this corresponds to an approximate mass of 126 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

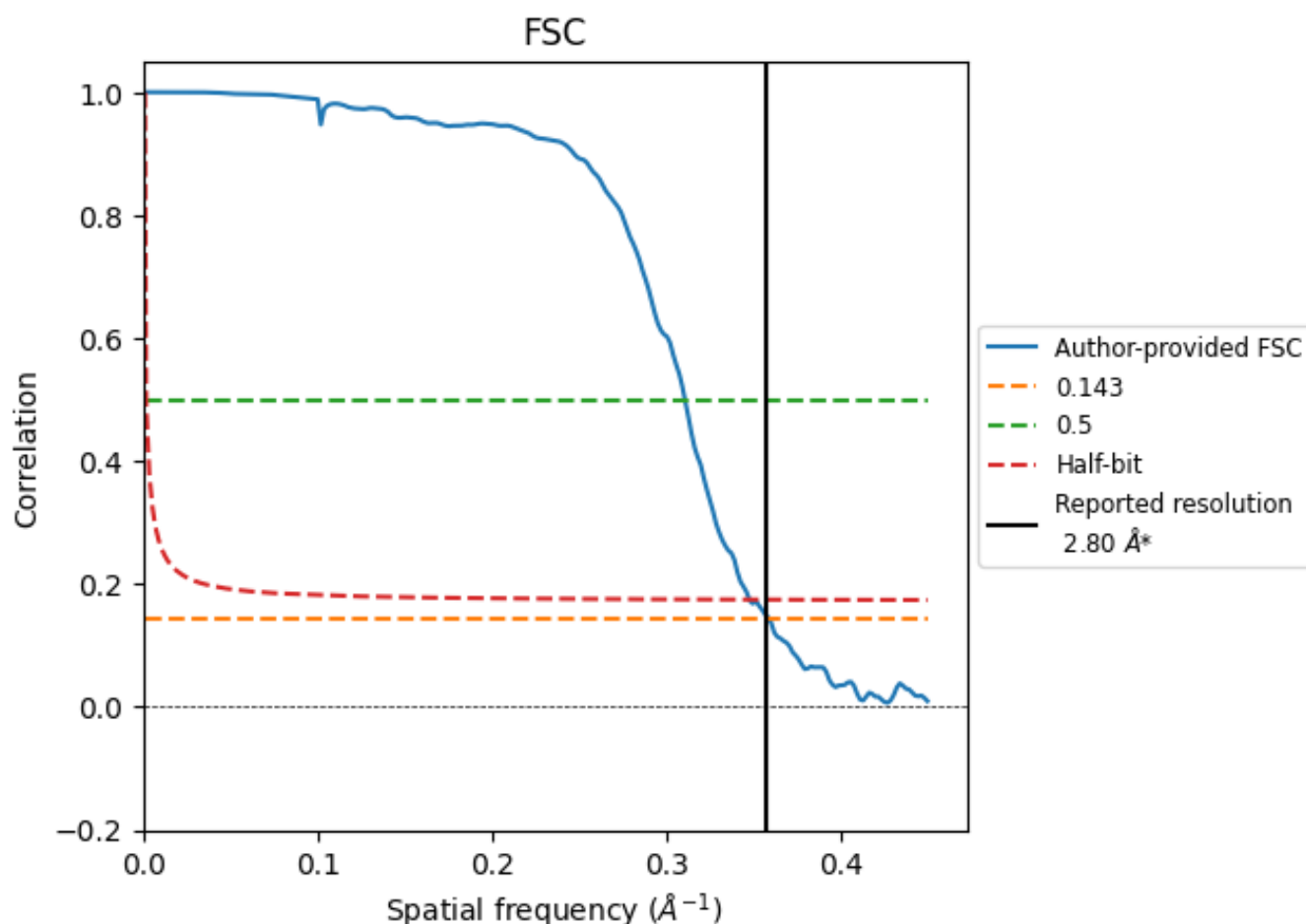


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

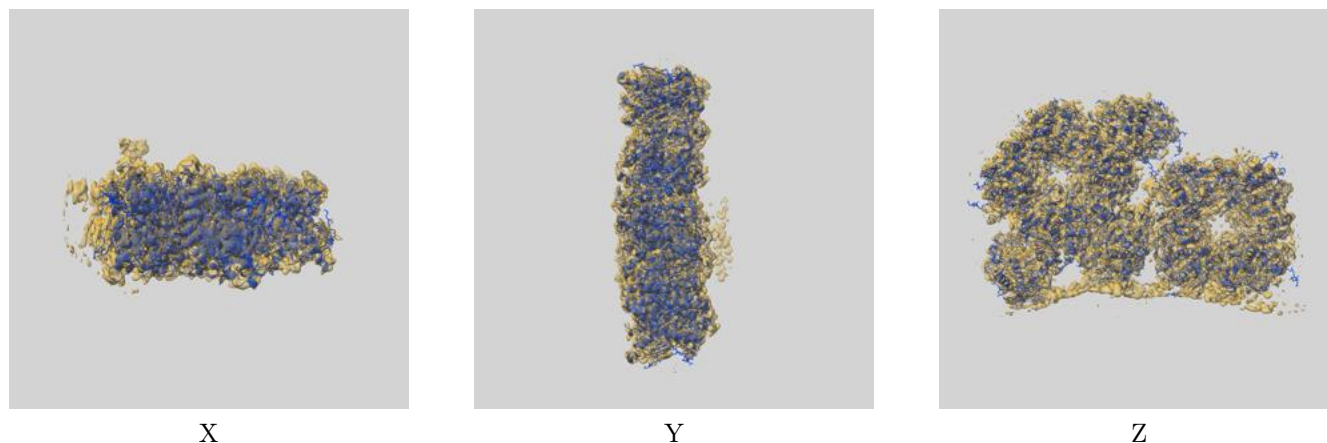
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.79	3.22	2.88
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

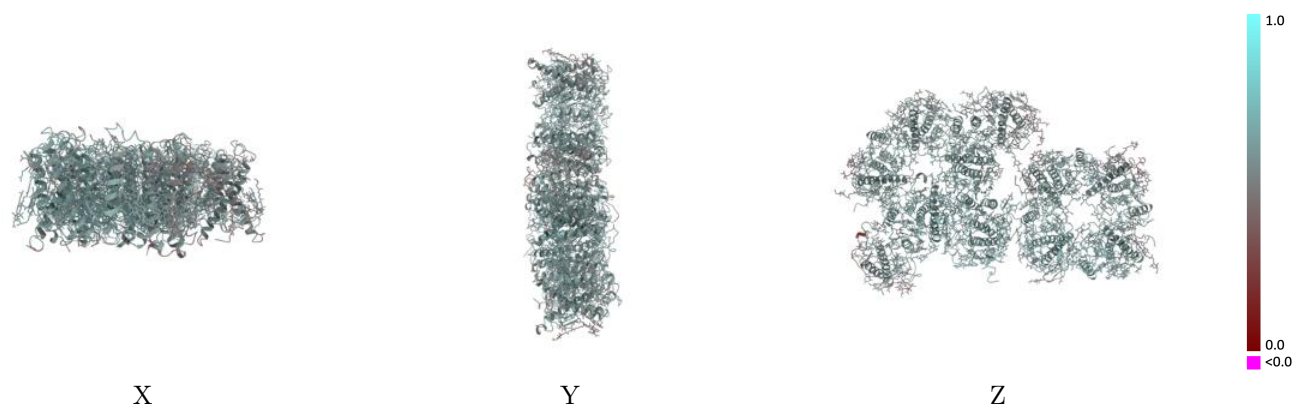
This section contains information regarding the fit between EMDB map EMD-31906 and PDB model 7VD6. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



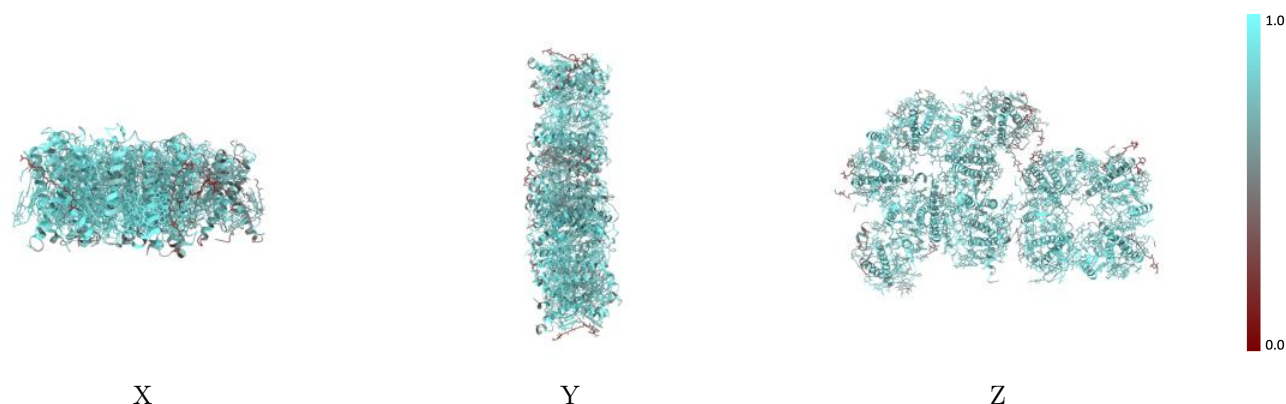
The images above show the 3D surface view of the map at the recommended contour level 0.055 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



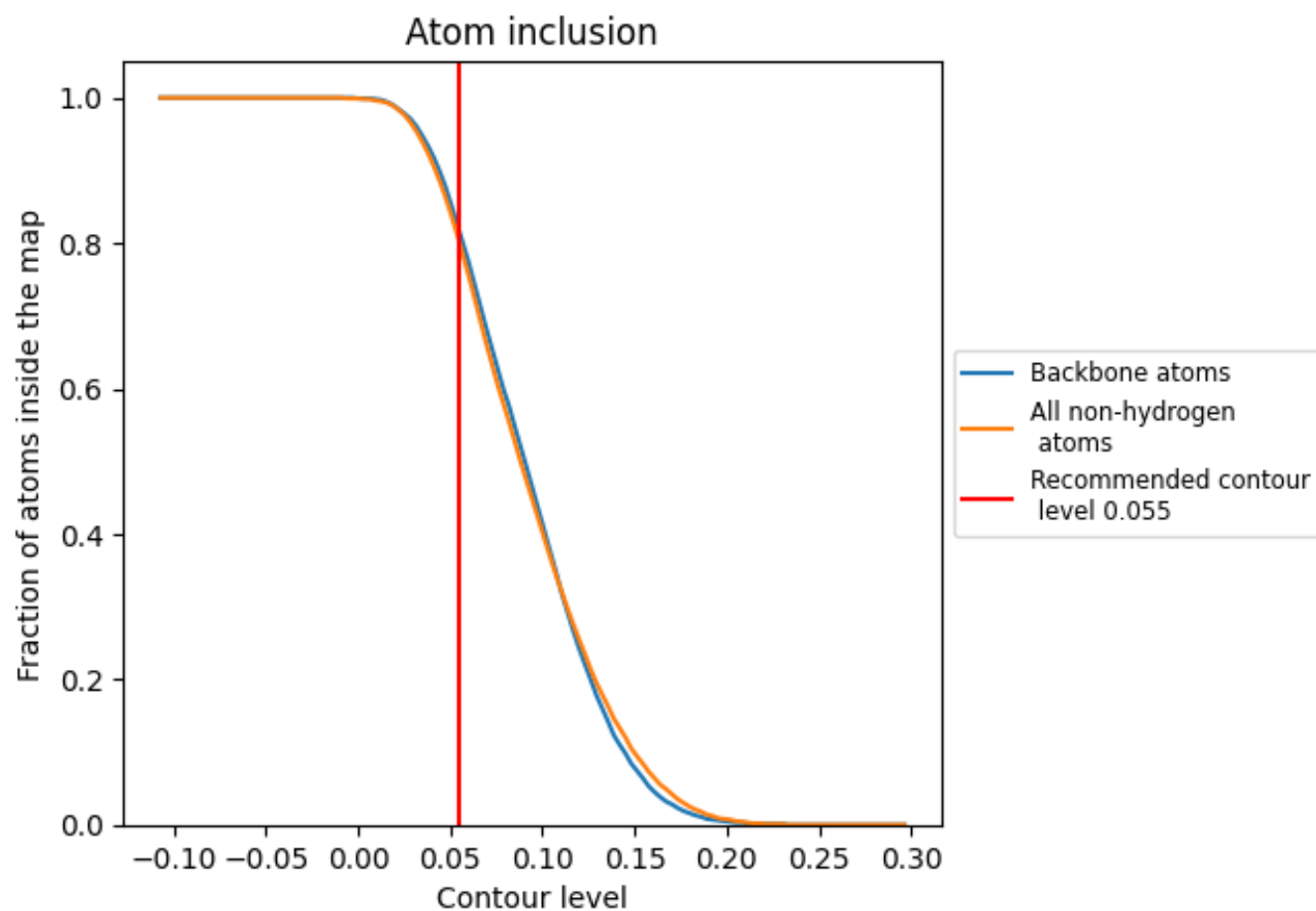
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.055).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8020	0.5650
11	0.8420	0.5920
12	0.8240	0.5710
13	0.7780	0.5400
14	0.7920	0.5550
15	0.7750	0.5530
16	0.8740	0.6000
17	0.8460	0.5940
18	0.7980	0.5550
19	0.8540	0.5990
20	0.7470	0.5190
21	0.6500	0.5210

1.0

0.0

<0.0