



Full wwPDB EM Validation Report ⓘ

Nov 15, 2022 – 01:22 AM JST

PDB ID : 6JO6
EMDB ID : EMD-9854
Title : Structure of the green algal photosystem I supercomplex with light-harvesting complex I
Authors : Suga, M.; Miyazaki, N.; Takahashi, Y.
Deposited on : 2019-03-20
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

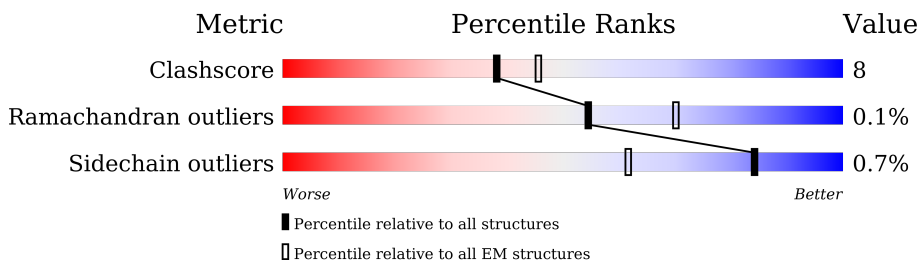
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	751	
2	B	755	
3	C	81	
4	D	161	
5	E	73	
6	F	165	
7	G	94	
8	I	106	

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Mol	Chain	Length	Quality of chain
9	J	41	
10	K	87	
11	L	156	
12	1	194	
12	Z	194	
13	3	268	
14	7	215	
15	8	217	
16	4	236	
17	5	229	
18	6	232	

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
19	CL0	A	801	X	-	-	-
20	CLA	1	602	X	-	-	-
20	CLA	1	603	X	-	-	-
20	CLA	1	604	X	-	-	-
20	CLA	1	606	X	-	-	-
20	CLA	1	608	X	-	-	-
20	CLA	1	609	X	-	-	-
20	CLA	1	610	X	-	-	-
20	CLA	1	611	X	-	-	-
20	CLA	1	612	X	-	-	-
20	CLA	1	613	X	-	-	-
20	CLA	1	614	X	-	-	-
20	CLA	1	616	X	-	-	-
20	CLA	3	602	X	-	-	-
20	CLA	3	603	X	-	-	-
20	CLA	3	604	X	-	-	-
20	CLA	3	606	X	-	-	-
20	CLA	3	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	3	609	X	-	-	-
20	CLA	3	610	X	-	-	-
20	CLA	3	611	X	-	-	-
20	CLA	3	612	X	-	-	-
20	CLA	3	617	X	-	-	-
20	CLA	3	620	X	-	-	-
20	CLA	4	601	X	-	-	-
20	CLA	4	603	X	-	-	-
20	CLA	4	609	X	-	-	-
20	CLA	4	610	X	-	-	-
20	CLA	4	611	X	-	-	-
20	CLA	4	612	X	-	-	-
20	CLA	4	614	X	-	-	-
20	CLA	4	616	X	-	-	-
20	CLA	5	601	X	-	-	-
20	CLA	5	603	X	-	-	-
20	CLA	5	606	X	-	-	-
20	CLA	5	609	X	-	-	-
20	CLA	5	610	X	-	-	-
20	CLA	5	611	X	-	-	-
20	CLA	5	612	X	-	-	-
20	CLA	5	613	X	-	-	-
20	CLA	5	614	X	-	-	-
20	CLA	5	616	X	-	-	-
20	CLA	5	617	X	-	-	-
20	CLA	5	621	X	-	-	-
20	CLA	6	601	X	-	-	-
20	CLA	6	602	X	-	-	-
20	CLA	6	603	X	-	-	-
20	CLA	6	604	X	-	-	-
20	CLA	6	609	X	-	-	-
20	CLA	6	610	X	-	-	-
20	CLA	6	611	X	-	-	-
20	CLA	6	612	X	-	-	-
20	CLA	6	613	X	-	-	-
20	CLA	6	614	X	-	-	-
20	CLA	6	616	X	-	-	-
20	CLA	6	617	X	-	-	-
20	CLA	6	622	X	-	-	-
20	CLA	7	601	X	-	-	-
20	CLA	7	602	X	-	-	-
20	CLA	7	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	7	604	X	-	-	-
20	CLA	7	606	X	-	-	-
20	CLA	7	609	X	-	-	-
20	CLA	7	610	X	-	-	-
20	CLA	7	611	X	-	-	-
20	CLA	7	612	X	-	-	-
20	CLA	7	613	X	-	-	-
20	CLA	7	614	X	-	-	-
20	CLA	7	616	X	-	-	-
20	CLA	7	620	X	-	-	-
20	CLA	8	601	X	-	-	-
20	CLA	8	602	X	-	-	-
20	CLA	8	603	X	-	-	-
20	CLA	8	604	X	-	-	-
20	CLA	8	606	X	-	-	-
20	CLA	8	608	X	-	-	-
20	CLA	8	609	X	-	-	-
20	CLA	8	610	X	-	-	-
20	CLA	8	611	X	-	-	-
20	CLA	8	612	X	-	-	-
20	CLA	8	613	X	-	-	-
20	CLA	8	614	X	-	-	-
20	CLA	8	616	X	-	-	-
20	CLA	A	802	X	-	-	-
20	CLA	A	803	X	-	-	-
20	CLA	A	804	X	-	-	-
20	CLA	A	805	X	-	-	-
20	CLA	A	806	X	-	-	-
20	CLA	A	807	X	-	-	-
20	CLA	A	808	X	-	-	-
20	CLA	A	809	X	-	-	-
20	CLA	A	810	X	-	-	-
20	CLA	A	811	X	-	-	-
20	CLA	A	812	X	-	-	-
20	CLA	A	813	X	-	-	-
20	CLA	A	814	X	-	-	-
20	CLA	A	815	X	-	-	-
20	CLA	A	816	X	-	-	-
20	CLA	A	817	X	-	-	-
20	CLA	A	820	X	-	-	-
20	CLA	A	821	X	-	-	-
20	CLA	A	822	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	A	824	X	-	-	-
20	CLA	A	826	X	-	-	-
20	CLA	A	827	X	-	-	-
20	CLA	A	828	X	-	-	-
20	CLA	A	829	X	-	-	-
20	CLA	A	830	X	-	-	-
20	CLA	A	831	X	-	-	-
20	CLA	A	832	X	-	-	-
20	CLA	A	833	X	-	-	-
20	CLA	A	834	X	-	-	-
20	CLA	A	835	X	-	-	-
20	CLA	A	837	X	-	-	-
20	CLA	A	838	X	-	-	-
20	CLA	A	839	X	-	-	-
20	CLA	A	840	X	-	-	-
20	CLA	A	841	X	-	-	-
20	CLA	A	842	X	-	-	-
20	CLA	A	843	X	-	-	-
20	CLA	A	854	X	-	-	-
20	CLA	B	802	X	-	-	-
20	CLA	B	803	X	-	-	-
20	CLA	B	804	X	-	-	-
20	CLA	B	805	X	-	-	-
20	CLA	B	806	X	-	-	-
20	CLA	B	807	X	-	-	-
20	CLA	B	808	X	-	-	-
20	CLA	B	809	X	-	-	-
20	CLA	B	810	X	-	-	-
20	CLA	B	811	X	-	-	-
20	CLA	B	812	X	-	-	-
20	CLA	B	813	X	-	-	-
20	CLA	B	814	X	-	-	-
20	CLA	B	815	X	-	-	-
20	CLA	B	816	X	-	-	-
20	CLA	B	817	X	-	-	-
20	CLA	B	818	X	-	-	-
20	CLA	B	819	X	-	-	-
20	CLA	B	820	X	-	-	-
20	CLA	B	822	X	-	-	-
20	CLA	B	823	X	-	-	-
20	CLA	B	824	X	-	-	-
20	CLA	B	825	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	B	826	X	-	-	-
20	CLA	B	827	X	-	-	-
20	CLA	B	828	X	-	-	-
20	CLA	B	829	X	-	-	-
20	CLA	B	831	X	-	-	-
20	CLA	B	832	X	-	-	-
20	CLA	B	833	X	-	-	-
20	CLA	B	834	X	-	-	-
20	CLA	B	835	X	-	-	-
20	CLA	B	836	X	-	-	-
20	CLA	B	837	X	-	-	-
20	CLA	B	838	X	-	-	-
20	CLA	B	839	X	-	-	-
20	CLA	B	841	X	-	-	-
20	CLA	B	852	X	-	-	-
20	CLA	F	301	X	-	-	-
20	CLA	F	303	X	-	-	-
20	CLA	F	304	X	-	-	-
20	CLA	G	203	X	-	-	-
20	CLA	G	204	X	-	-	-
20	CLA	J	3002	X	-	-	-
20	CLA	K	4003	X	-	-	-
20	CLA	Z	602	X	-	-	-
20	CLA	Z	603	X	-	-	-
20	CLA	Z	604	X	-	-	-
20	CLA	Z	606	X	-	-	-
20	CLA	Z	608	X	-	-	-
20	CLA	Z	609	X	-	-	-
20	CLA	Z	610	X	-	-	-
20	CLA	Z	611	X	-	-	-
20	CLA	Z	612	X	-	-	-
20	CLA	Z	613	X	-	-	-
20	CLA	Z	614	X	-	-	-
20	CLA	Z	616	X	-	-	-
27	CHL	1	601	X	-	-	-
27	CHL	1	607	X	-	-	-
27	CHL	3	608	X	-	-	-
27	CHL	4	606	X	-	-	-
27	CHL	4	607	X	-	-	-
27	CHL	4	608	X	-	-	-
27	CHL	4	618	X	-	-	-
27	CHL	5	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CHL	5	608	X	-	-	-
27	CHL	5	618	X	-	-	-
27	CHL	6	606	X	-	-	-
27	CHL	6	607	X	-	-	-
27	CHL	6	608	X	-	-	-
27	CHL	6	618	X	-	-	-
27	CHL	7	607	X	-	-	-
27	CHL	8	607	X	-	-	-
27	CHL	Z	601	X	-	-	-
27	CHL	Z	607	X	-	-	-

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 45099 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	738	5800	3793	989	996	22	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	732	5822	3824	978	1002	18	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	insertion	UNP P09144
B	-15	HIS	-	insertion	UNP P09144
B	-14	HIS	-	insertion	UNP P09144
B	-13	HIS	-	insertion	UNP P09144
B	-12	HIS	-	insertion	UNP P09144
B	-11	HIS	-	insertion	UNP P09144
B	-10	HIS	-	insertion	UNP P09144
B	-9	HIS	-	insertion	UNP P09144
B	-8	HIS	-	insertion	UNP P09144
B	-7	HIS	-	insertion	UNP P09144
B	-6	HIS	-	insertion	UNP P09144
B	-5	HIS	-	insertion	UNP P09144
B	-4	HIS	-	insertion	UNP P09144
B	-3	HIS	-	insertion	UNP P09144
B	-2	HIS	-	insertion	UNP P09144
B	-1	HIS	-	insertion	UNP P09144
B	0	HIS	-	insertion	UNP P09144
B	1	HIS	-	insertion	UNP P09144
B	2	HIS	-	insertion	UNP P09144
B	3	HIS	-	insertion	UNP P09144

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	144	1132	725	200	200	7	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	61	480	306	85	89	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	165	1265	817	213	232	3	0	0

- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	G	68	503	327	87	89	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	37	281	195	39	46	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	39	320	219	45	55	1	0	0

- Molecule 10 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	45	Total	C	N	O	S	0	0
			297	190	49	56	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	118	Total	C	N	O	S	0	0
			853	561	136	153	3		

- Molecule 12 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1	194	Total	C	N	O	S	0	0
			1444	941	240	260	3		
12	Z	192	Total	C	N	O	S	0	0
			1436	937	238	258	3		

- Molecule 13 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	3	202	Total	C	N	O	S	0	0
			1555	1018	252	277	8		

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	7	212	Total	C	N	O	S	0	0
			1644	1069	273	296	6		

- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	8	217	Total	C	N	O	S	0	0
			1649	1073	280	292	4		

- Molecule 16 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	4	203	Total	C	N	O	S	0	0
			1570	1029	254	282	5		

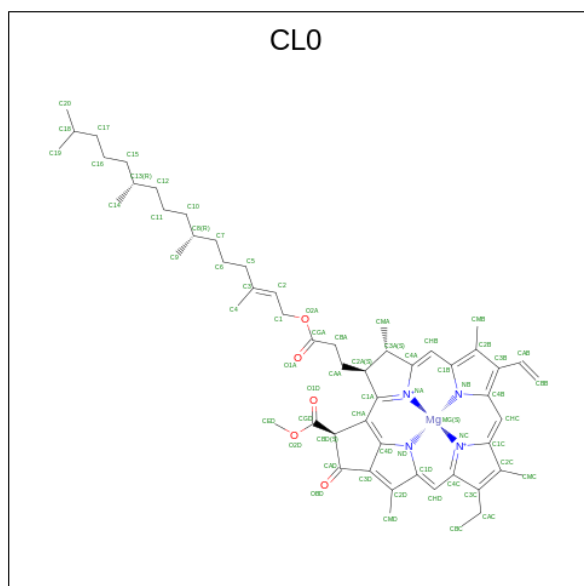
- Molecule 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	5	223	1744	1137	291	308	8	0	0

- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

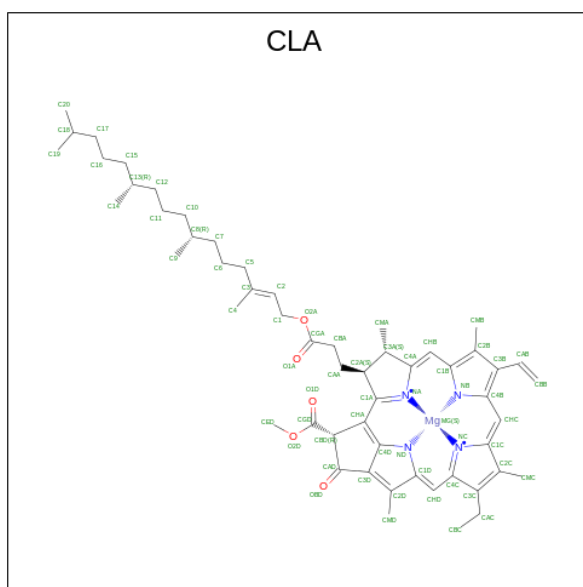
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	6	229	1765	1164	292	303	6	0	0

- Molecule 19 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



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

- Molecule 20 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
20	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
20	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
20	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
20	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
20	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
20	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
20	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
20	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
20	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
20	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
20	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
20	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
20	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
20	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	B	1	2480	2070	41	164	205	0
20	B	1	2480	2070	41	164	205	0
20	B	1	2480	2070	41	164	205	0
20	B	1	2480	2070	41	164	205	0
20	B	1	2480	2070	41	164	205	0
20	B	1	2480	2070	41	164	205	0
20	B	1	2480	2070	41	164	205	0
20	B	1	2480	2070	41	164	205	0
20	B	1	2480	2070	41	164	205	0
20	B	1	2480	2070	41	164	205	0
20	B	1	2480	2070	41	164	205	0
20	B	1	2480	2070	41	164	205	0
20	B	1	2480	2070	41	164	205	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
20	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
20	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
20	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
20	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
20	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
20	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
20	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
20	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
20	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
20	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
20	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
20	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
20	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
20	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
20	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
20	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
20	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
20	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
20	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
20	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
20	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
20	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
20	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
20	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
20	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
20	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
20	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
20	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
20	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
20	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
20	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
20	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
20	F	1	Total 175	C 145	Mg 3	N 12	O 15	0
20	F	1	Total 175	C 145	Mg 3	N 12	O 15	0
20	F	1	Total 175	C 145	Mg 3	N 12	O 15	0
20	G	1	Total 96	C 76	Mg 2	N 8	O 10	0
20	G	1	Total 96	C 76	Mg 2	N 8	O 10	0
20	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
20	K	1	Total 91	C 71	Mg 2	N 8	O 10	0
20	K	1	Total 91	C 71	Mg 2	N 8	O 10	0
20	L	1	Total 115	C 95	Mg 2	N 8	O 10	0
20	L	1	Total 115	C 95	Mg 2	N 8	O 10	0
20	1	1	Total 722	C 602	Mg 12	N 48	O 60	0
20	1	1	Total 722	C 602	Mg 12	N 48	O 60	0
20	1	1	Total 722	C 602	Mg 12	N 48	O 60	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
20	1	1	722	602	12	48	60	0
20	1	1	722	602	12	48	60	0
20	1	1	722	602	12	48	60	0
20	1	1	722	602	12	48	60	0
20	1	1	722	602	12	48	60	0
20	1	1	722	602	12	48	60	0
20	1	1	722	602	12	48	60	0
20	1	1	722	602	12	48	60	0
20	1	1	722	602	12	48	60	0
20	3	1	696	570	13	52	61	0
20	3	1	696	570	13	52	61	0
20	3	1	696	570	13	52	61	0
20	3	1	696	570	13	52	61	0
20	3	1	696	570	13	52	61	0
20	3	1	696	570	13	52	61	0
20	3	1	696	570	13	52	61	0
20	3	1	696	570	13	52	61	0
20	3	1	696	570	13	52	61	0
20	3	1	696	570	13	52	61	0
20	3	1	696	570	13	52	61	0
20	3	1	696	570	13	52	61	0
20	3	1	696	570	13	52	61	0
20	3	1	696	570	13	52	61	0

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Mol	Chain	Residues	Atoms					AltConf
20	3	1	Total	C	Mg	N	O	0
			696	570	13	52	61	
20	7	1	Total	C	Mg	N	O	0
			741	607	14	56	64	
20	7	1	Total	C	Mg	N	O	0
			741	607	14	56	64	
20	7	1	Total	C	Mg	N	O	0
			741	607	14	56	64	
20	7	1	Total	C	Mg	N	O	0
			741	607	14	56	64	
20	7	1	Total	C	Mg	N	O	0
			741	607	14	56	64	
20	7	1	Total	C	Mg	N	O	0
			741	607	14	56	64	
20	7	1	Total	C	Mg	N	O	0
			741	607	14	56	64	
20	7	1	Total	C	Mg	N	O	0
			741	607	14	56	64	
20	7	1	Total	C	Mg	N	O	0
			741	607	14	56	64	
20	7	1	Total	C	Mg	N	O	0
			741	607	14	56	64	
20	7	1	Total	C	Mg	N	O	0
			741	607	14	56	64	
20	7	1	Total	C	Mg	N	O	0
			741	607	14	56	64	
20	7	1	Total	C	Mg	N	O	0
			741	607	14	56	64	
20	7	1	Total	C	Mg	N	O	0
			741	607	14	56	64	
20	8	1	Total	C	Mg	N	O	0
			680	552	13	52	63	
20	8	1	Total	C	Mg	N	O	0
			680	552	13	52	63	
20	8	1	Total	C	Mg	N	O	0
			680	552	13	52	63	
20	8	1	Total	C	Mg	N	O	0
			680	552	13	52	63	
20	8	1	Total	C	Mg	N	O	0
			680	552	13	52	63	
20	8	1	Total	C	Mg	N	O	0
			680	552	13	52	63	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
20	8	1	680	552	13	52	63	0
20	8	1	680	552	13	52	63	0
20	8	1	680	552	13	52	63	0
20	8	1	680	552	13	52	63	0
20	8	1	680	552	13	52	63	0
20	8	1	680	552	13	52	63	0
20	8	1	680	552	13	52	63	0
20	Z	1	714	594	12	48	60	0
20	Z	1	714	594	12	48	60	0
20	Z	1	714	594	12	48	60	0
20	Z	1	714	594	12	48	60	0
20	Z	1	714	594	12	48	60	0
20	Z	1	714	594	12	48	60	0
20	Z	1	714	594	12	48	60	0
20	Z	1	714	594	12	48	60	0
20	Z	1	714	594	12	48	60	0
20	Z	1	714	594	12	48	60	0
20	Z	1	714	594	12	48	60	0
20	Z	1	714	594	12	48	60	0
20	Z	1	714	594	12	48	60	0
20	4	1	576	468	11	44	53	0
20	4	1	576	468	11	44	53	0

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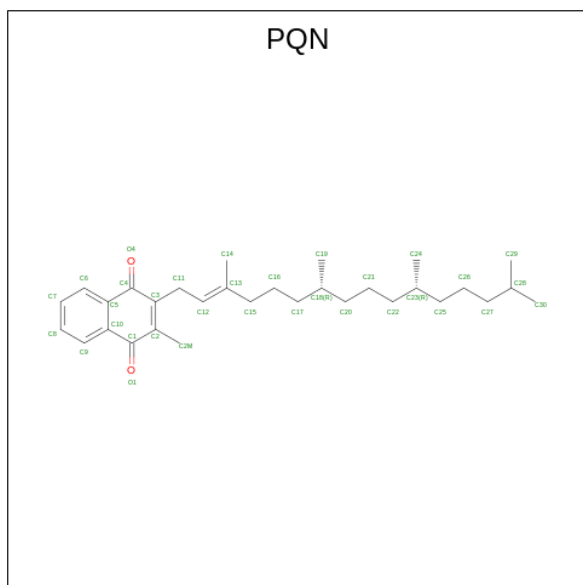
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
20	4	1	576	468	11	44	53	0
20	4	1	576	468	11	44	53	0
20	4	1	576	468	11	44	53	0
20	4	1	576	468	11	44	53	0
20	4	1	576	468	11	44	53	0
20	4	1	576	468	11	44	53	0
20	4	1	576	468	11	44	53	0
20	4	1	576	468	11	44	53	0
20	4	1	576	468	11	44	53	0
20	5	1	737	597	14	56	70	0
20	5	1	737	597	14	56	70	0
20	5	1	737	597	14	56	70	0
20	5	1	737	597	14	56	70	0
20	5	1	737	597	14	56	70	0
20	5	1	737	597	14	56	70	0
20	5	1	737	597	14	56	70	0
20	5	1	737	597	14	56	70	0
20	5	1	737	597	14	56	70	0
20	5	1	737	597	14	56	70	0
20	5	1	737	597	14	56	70	0
20	5	1	737	597	14	56	70	0
20	5	1	737	597	14	56	70	0

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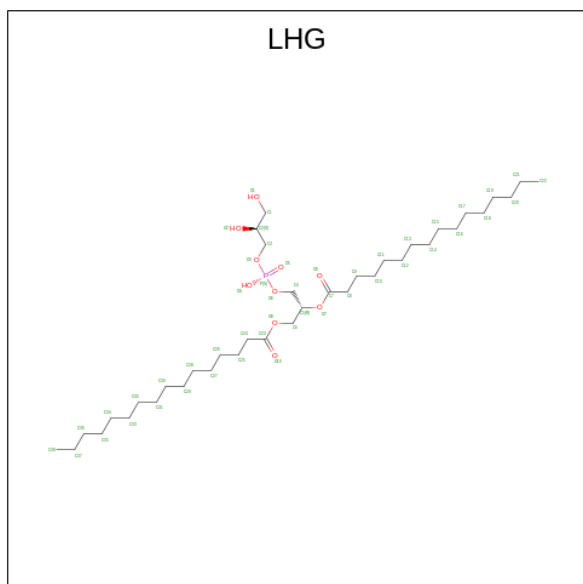
Mol	Chain	Residues	Atoms					AltConf
20	5	1	Total	C	Mg	N	O	0
			737	597	14	56	70	
20	5	1	Total	C	Mg	N	O	0
			737	597	14	56	70	
20	6	1	Total	C	Mg	N	O	0
			696	566	13	52	65	
20	6	1	Total	C	Mg	N	O	0
			696	566	13	52	65	
20	6	1	Total	C	Mg	N	O	0
			696	566	13	52	65	
20	6	1	Total	C	Mg	N	O	0
			696	566	13	52	65	
20	6	1	Total	C	Mg	N	O	0
			696	566	13	52	65	
20	6	1	Total	C	Mg	N	O	0
			696	566	13	52	65	
20	6	1	Total	C	Mg	N	O	0
			696	566	13	52	65	
20	6	1	Total	C	Mg	N	O	0
			696	566	13	52	65	
20	6	1	Total	C	Mg	N	O	0
			696	566	13	52	65	
20	6	1	Total	C	Mg	N	O	0
			696	566	13	52	65	
20	6	1	Total	C	Mg	N	O	0
			696	566	13	52	65	

- Molecule 21 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



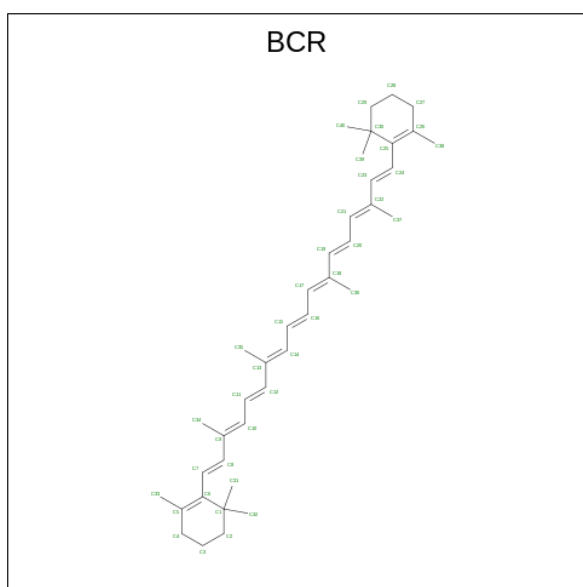
Mol	Chain	Residues	Atoms				AltConf
22	A	1	Total	C	O	P	0
			117	84	30	3	

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
22	A	1	Total 117	C 84	O 30	P 3	0
22	A	1	Total 117	C 84	O 30	P 3	0
22	B	1	Total 23	C 12	O 10	P 1	0
22	1	1	Total 43	C 32	O 10	P 1	0
22	7	1	Total 37	C 26	O 10	P 1	0
22	8	1	Total 37	C 26	O 10	P 1	0
22	Z	1	Total 43	C 32	O 10	P 1	0
22	4	1	Total 81	C 59	O 20	P 2	0
22	4	1	Total 81	C 59	O 20	P 2	0
22	5	1	Total 37	C 26	O 10	P 1	0
22	6	1	Total 49	C 38	O 10	P 1	0

- Molecule 23 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



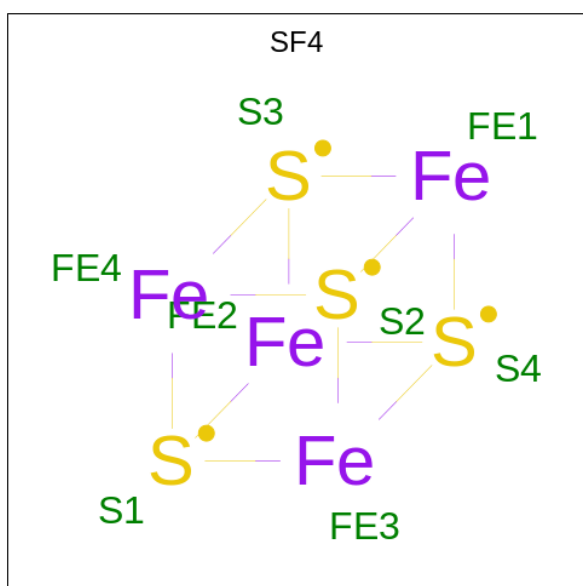
Mol	Chain	Residues	Atoms	AltConf
23	A	1	Total C 240 240	0
23	A	1	Total C 240 240	0
23	A	1	Total C 240 240	0
23	A	1	Total C 240 240	0
23	A	1	Total C 240 240	0
23	A	1	Total C 240 240	0
23	B	1	Total C 280 280	0
23	B	1	Total C 280 280	0
23	B	1	Total C 280 280	0
23	B	1	Total C 280 280	0
23	B	1	Total C 280 280	0
23	B	1	Total C 280 280	0
23	B	1	Total C 280 280	0
23	B	1	Total C 280 280	0
23	F	1	Total C 40 40	0
23	G	1	Total C 40 40	0
23	I	1	Total C 40 40	0
23	J	1	Total C 40 40	0
23	K	1	Total C 80 80	0
23	K	1	Total C 80 80	0
23	L	1	Total C 80 80	0
23	L	1	Total C 80 80	0
23	3	1	Total C 120 120	0

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Mol	Chain	Residues	Atoms		AltConf
23	3	1	Total	C	0
			120	120	
23	3	1	Total	C	0
			120	120	
23	7	1	Total	C	0
			80	80	
23	7	1	Total	C	0
			80	80	
23	8	1	Total	C	0
			40	40	
23	4	1	Total	C	0
			40	40	
23	5	1	Total	C	0
			80	80	
23	5	1	Total	C	0
			80	80	
23	6	1	Total	C	0
			80	80	
23	6	1	Total	C	0
			80	80	

- Molecule 24 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



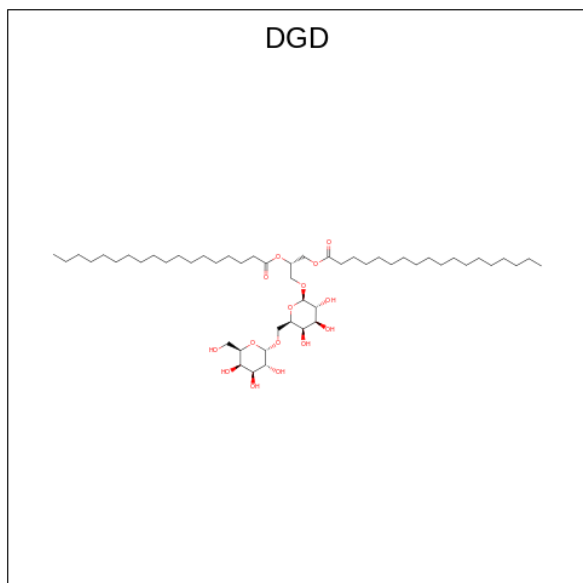
Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total	Fe	S	0
			8	4	4	

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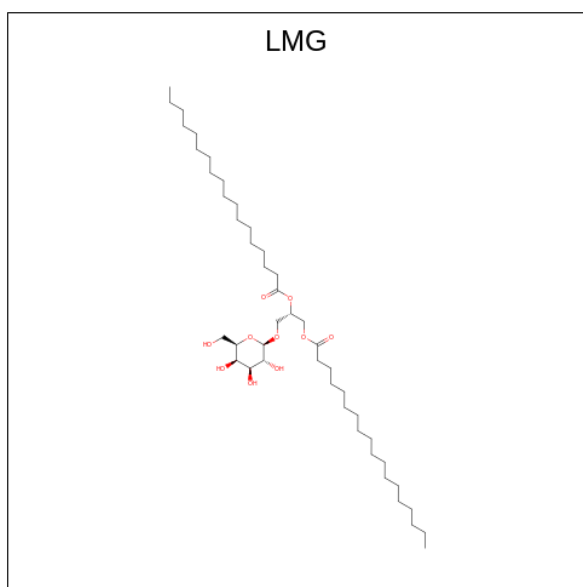
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
24	C	1	16	8	8	0
24	C	1	16	8	8	0

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



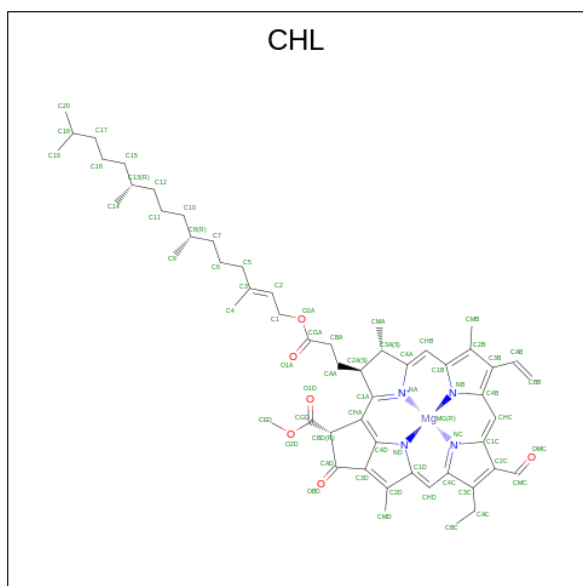
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
25	B	1	66	51	15	0

- Molecule 26 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
26	J	1	35	25	10	0

- Molecule 27 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



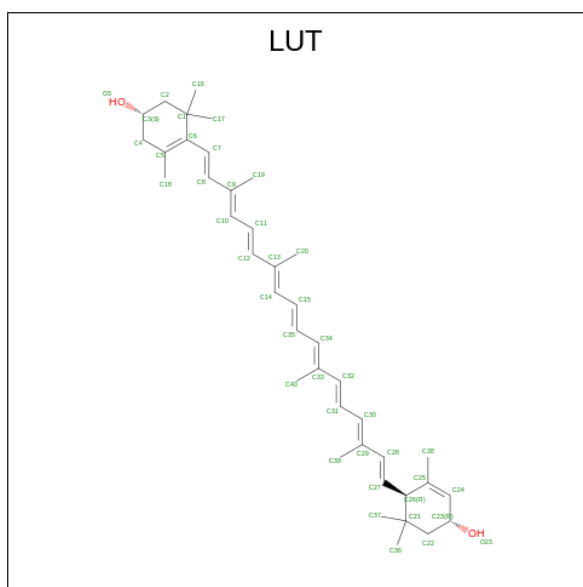
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
27	1	1	101	79	2	8	12	0
27	1	1	101	79	2	8	12	0
27	3	1	66	55	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
27	7	1	Total 54	C 43	Mg 1	N 4	O 6	0
27	8	1	Total 56	C 45	Mg 1	N 4	O 6	0
27	Z	1	Total 101	C 79	Mg 2	N 8	O 12	0
27	Z	1	Total 101	C 79	Mg 2	N 8	O 12	0
27	4	1	Total 201	C 159	Mg 4	N 16	O 22	0
27	4	1	Total 201	C 159	Mg 4	N 16	O 22	0
27	4	1	Total 201	C 159	Mg 4	N 16	O 22	0
27	4	1	Total 201	C 159	Mg 4	N 16	O 22	0
27	5	1	Total 145	C 114	Mg 3	N 12	O 16	0
27	5	1	Total 145	C 114	Mg 3	N 12	O 16	0
27	5	1	Total 145	C 114	Mg 3	N 12	O 16	0
27	6	1	Total 206	C 164	Mg 4	N 16	O 22	0
27	6	1	Total 206	C 164	Mg 4	N 16	O 22	0
27	6	1	Total 206	C 164	Mg 4	N 16	O 22	0
27	6	1	Total 206	C 164	Mg 4	N 16	O 22	0

- Molecule 28 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



Mol	Chain	Residues	Atoms			AltConf
28	1	1	Total	C	O	0
			126	120	6	
28	1	1	Total	C	O	0
			126	120	6	
28	1	1	Total	C	O	0
			126	120	6	
28	3	1	Total	C	O	0
			84	80	4	
28	3	1	Total	C	O	0
			84	80	4	
28	7	1	Total	C	O	0
			84	80	4	
28	7	1	Total	C	O	0
			84	80	4	
28	8	1	Total	C	O	0
			84	80	4	
28	8	1	Total	C	O	0
			84	80	4	
28	Z	1	Total	C	O	0
			126	120	6	
28	Z	1	Total	C	O	0
			126	120	6	
28	Z	1	Total	C	O	0
			126	120	6	
28	4	1	Total	C	O	0
			84	80	4	
28	4	1	Total	C	O	0
			84	80	4	

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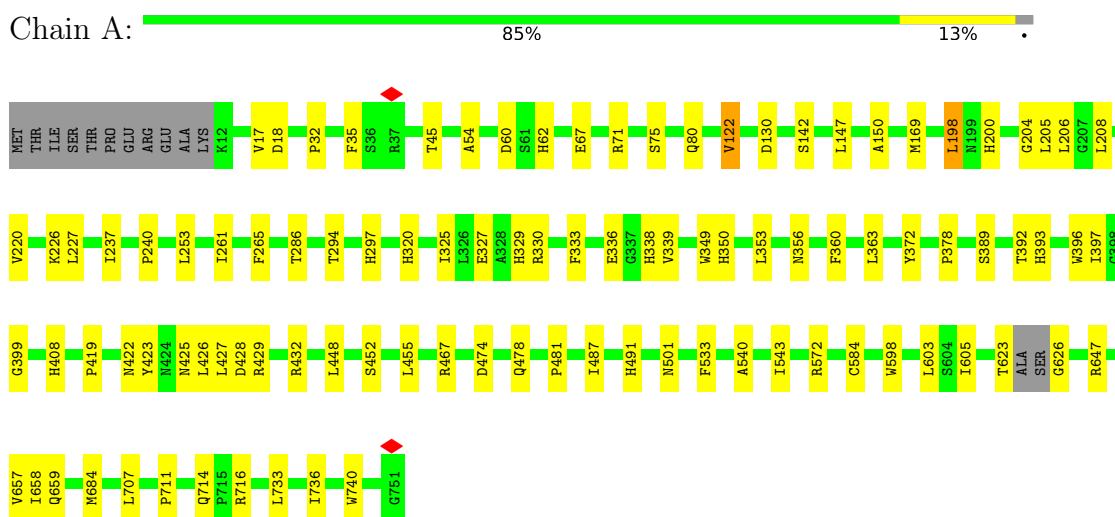
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Mol	Chain	Residues	Atoms			AltConf
28	5	1	Total	C	O	0
			84	80	4	
28	5	1	Total	C	O	0
			84	80	4	
28	6	1	Total	C	O	0
			84	80	4	
28	6	1	Total	C	O	0
			84	80	4	

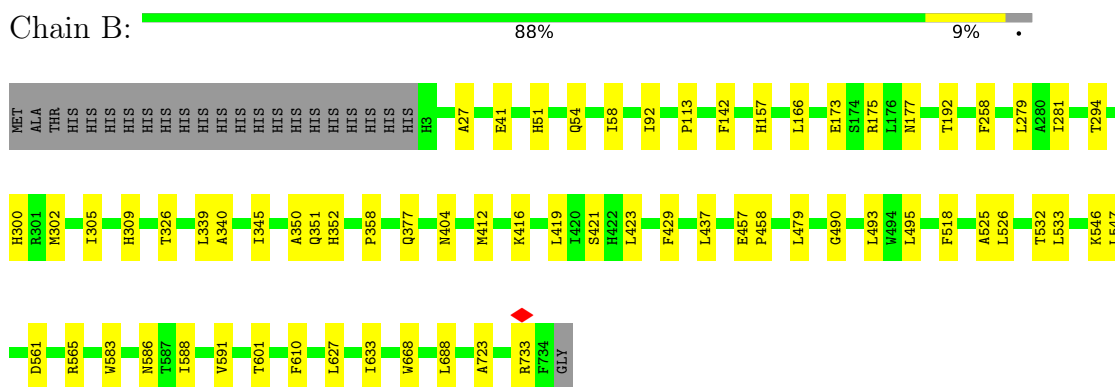
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

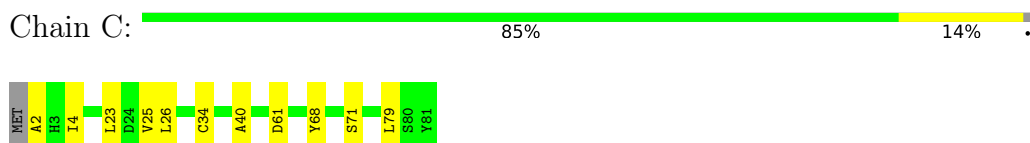
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



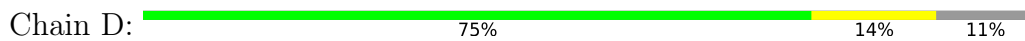
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



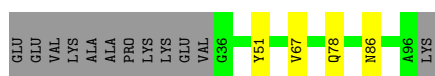
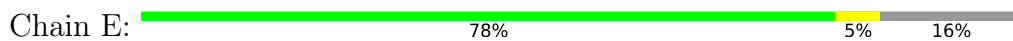
- Molecule 3: Photosystem I iron-sulfur center



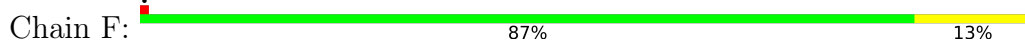
• Molecule 4: Photosystem I reaction center subunit II, chloroplastic



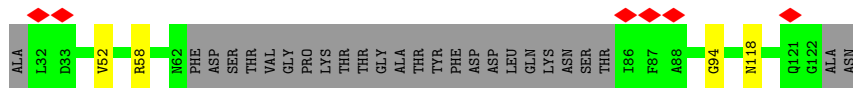
• Molecule 5: Photosystem I reaction center subunit IV, chloroplastic



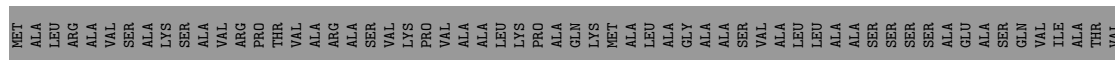
• Molecule 6: Photosystem I reaction center subunit F, Photosystem I reaction center subunit III, chloroplastic



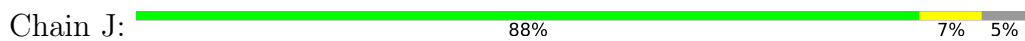
• Molecule 7: Photosystem I reaction center subunit V, chloroplastic



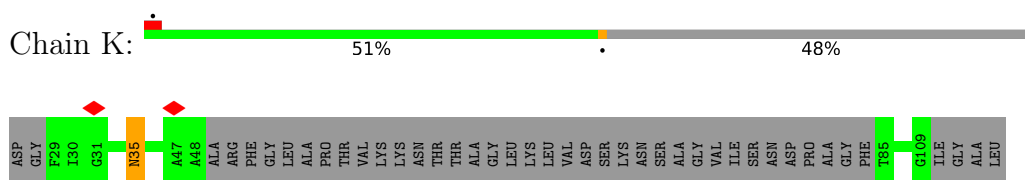
• Molecule 8: Photosystem I reaction center subunit VIII



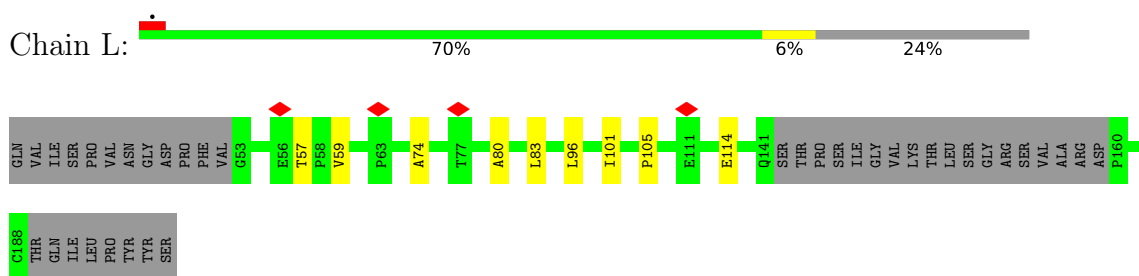
• Molecule 9: Photosystem I reaction center subunit IX



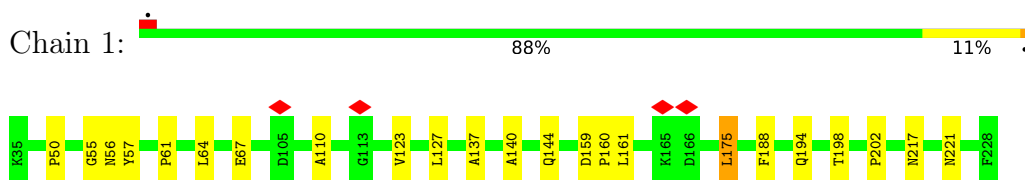
- Molecule 10: Photosystem I reaction center subunit psaK, chloroplactic



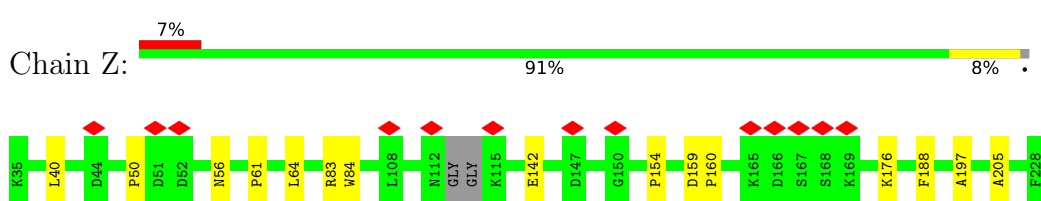
- Molecule 11: Photosystem I reaction center subunit XI



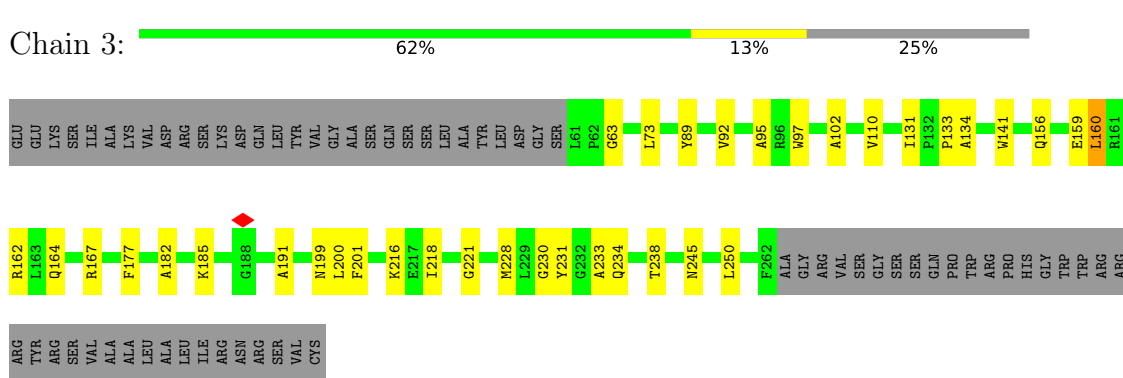
- Molecule 12: Chlorophyll a-b binding protein, chloroplactic



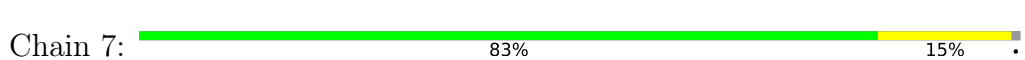
- Molecule 12: Chlorophyll a-b binding protein, chloroplactic

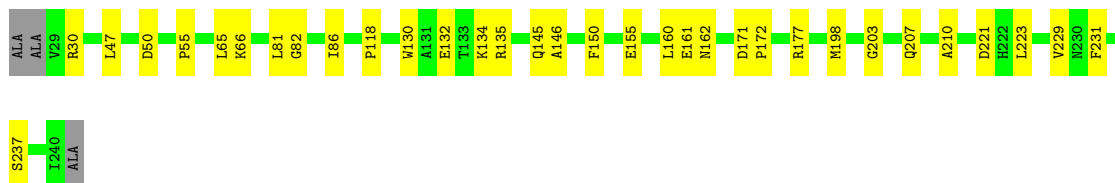


- Molecule 13: Chlorophyll a-b binding protein, chloroplactic

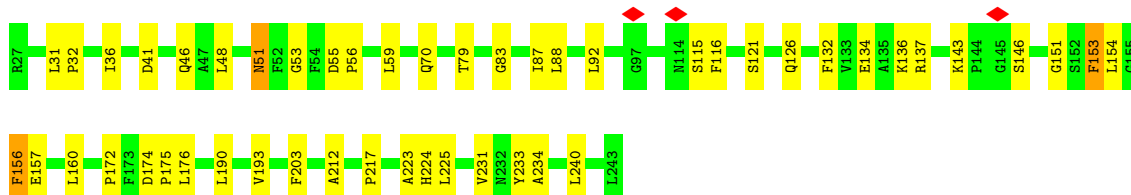
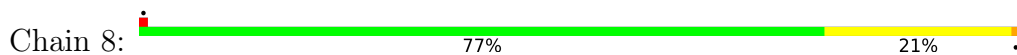


- Molecule 14: Chlorophyll a-b binding protein, chloroplactic

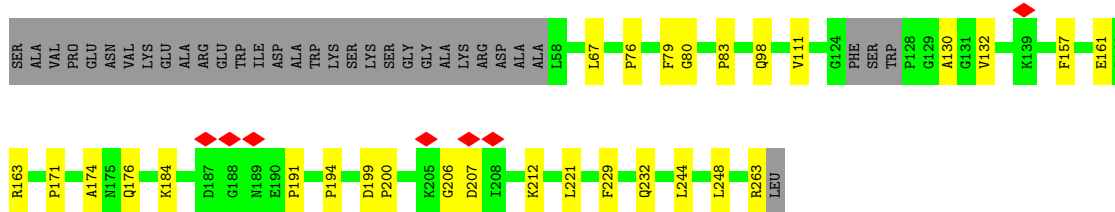




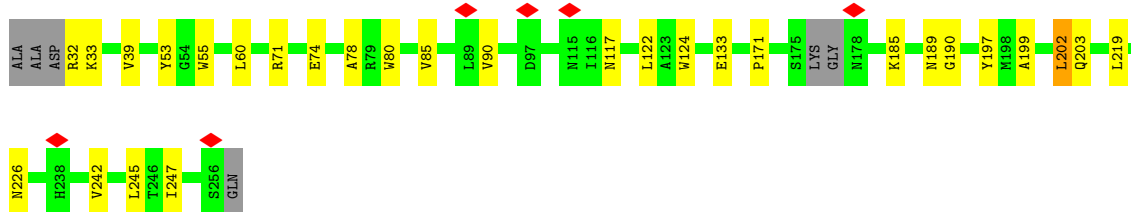
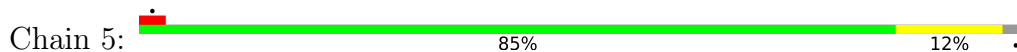
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic



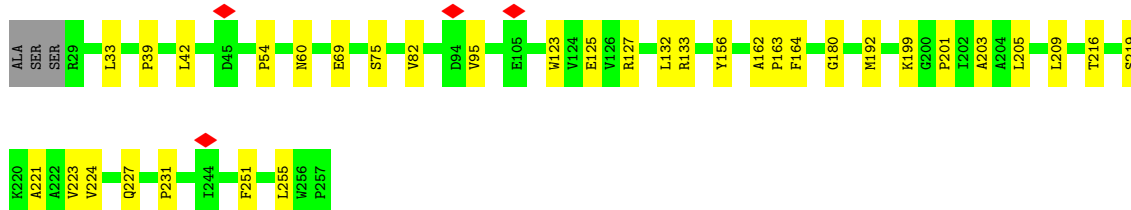
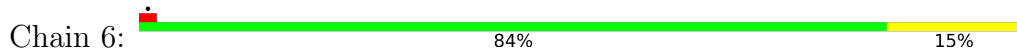
- Molecule 16: Chlorophyll a-b binding protein, chloroplastic



- Molecule 17: Chlorophyll a-b binding protein, chloroplastic



- Molecule 18: Chlorophyll a-b binding protein, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	379749	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.0	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	3750	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.460	Depositor
Minimum map value	-0.221	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.05	Depositor
Map size (\AA)	358.4, 358.4, 358.4	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.12, 1.12, 1.12	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: BCR, CLA, PQN, CL0, CHL, DGD, LHG, LMG, LUT, SF4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.35	0/5995	0.59	2/8172 (0.0%)
2	B	0.33	0/6035	0.54	2/8240 (0.0%)
3	C	0.32	0/610	0.60	1/826 (0.1%)
4	D	0.32	0/1160	0.53	0/1567
5	E	0.31	0/490	0.46	0/667
6	F	0.32	0/1291	0.58	0/1747
7	G	0.27	0/513	0.48	0/696
8	I	0.32	0/293	0.59	0/406
9	J	0.33	0/331	0.55	0/454
10	K	0.27	0/297	0.53	0/401
11	L	0.29	0/874	0.57	0/1194
12	1	0.30	0/1490	0.52	1/2028 (0.0%)
12	Z	0.30	0/1481	0.52	0/2015
13	3	0.35	0/1601	0.56	1/2173 (0.0%)
14	7	0.33	0/1696	0.55	0/2303
15	8	0.31	0/1700	0.61	1/2315 (0.0%)
16	4	0.33	0/1621	0.53	0/2209
17	5	0.30	0/1798	0.51	0/2450
18	6	0.30	0/1827	0.54	0/2497
All	All	0.32	0/31103	0.55	8/42360 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
14	7	0	1
16	4	0	1
All	All	0	3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	LEU	CA-CB-CG	7.63	132.85	115.30
15	8	240	LEU	CA-CB-CG	7.33	132.16	115.30
2	B	688	LEU	CA-CB-CG	5.74	128.49	115.30
1	A	455	LEU	CA-CB-CG	5.72	128.46	115.30
3	C	23	LEU	CB-CG-CD1	-5.46	101.72	111.00
13	3	200	LEU	CA-CB-CG	5.31	127.51	115.30
2	B	493	LEU	CA-CB-CG	5.16	127.18	115.30
12	1	175	LEU	CA-CB-CG	5.04	126.88	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	4	206	GLY	Peptide
14	7	150	PHE	Peptide
2	B	668	TRP	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	A	5800	0	5646	73	0
2	B	5822	0	5574	49	0
3	C	600	0	581	7	0
4	D	1132	0	1150	14	0
5	E	480	0	476	4	0
6	F	1265	0	1301	15	0
7	G	503	0	496	2	0
8	I	281	0	292	4	0
9	J	320	0	322	3	0
10	K	297	0	319	1	0
11	L	853	0	864	7	0
12	1	1444	0	1396	18	0
12	Z	1436	0	1389	15	0
13	3	1555	0	1522	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	7	1644	0	1584	28	0
15	8	1649	0	1629	48	0
16	4	1570	0	1527	22	0
17	5	1744	0	1717	32	0
18	6	1765	0	1767	29	0
19	A	65	0	72	1	0
20	1	722	0	735	23	0
20	3	696	0	631	20	0
20	4	576	0	495	22	0
20	5	737	0	638	27	0
20	6	696	0	622	21	0
20	7	741	0	665	22	0
20	8	680	0	593	21	0
20	A	2689	0	2798	122	0
20	B	2480	0	2545	99	0
20	F	175	0	177	8	0
20	G	96	0	72	0	0
20	J	42	0	31	0	0
20	K	91	0	66	3	0
20	L	115	0	111	1	0
20	Z	714	0	716	22	0
21	A	33	0	46	1	0
21	B	33	0	46	1	0
22	1	43	0	56	0	0
22	4	81	0	108	6	0
22	5	37	0	44	1	0
22	6	49	0	73	3	0
22	7	37	0	44	1	0
22	8	37	0	44	0	0
22	A	117	0	153	6	0
22	B	23	0	16	2	0
22	Z	43	0	56	3	0
23	3	120	0	168	15	0
23	4	40	0	56	2	0
23	5	80	0	112	10	0
23	6	80	0	112	9	0
23	7	80	0	112	6	0
23	8	40	0	56	5	0
23	A	240	0	336	20	0
23	B	280	0	392	22	0
23	F	40	0	56	6	0
23	G	40	0	56	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	I	40	0	56	2	0
23	J	40	0	56	3	0
23	K	80	0	112	3	0
23	L	80	0	112	4	0
24	A	8	0	0	0	0
24	C	16	0	0	0	0
25	B	66	0	96	2	0
26	J	35	0	40	0	0
27	1	101	0	74	3	0
27	3	66	0	70	5	0
27	4	201	0	150	1	0
27	5	145	0	103	5	0
27	6	206	0	160	7	0
27	7	54	0	43	0	0
27	8	56	0	47	1	0
27	Z	101	0	74	5	0
28	1	126	0	168	15	0
28	3	84	0	112	6	0
28	4	84	0	112	9	0
28	5	84	0	112	9	0
28	6	84	0	112	11	0
28	7	84	0	112	9	0
28	8	84	0	112	15	0
28	Z	126	0	168	11	0
All	All	45099	0	44862	716	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (716) 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)
15:8:156:PHE:CZ	15:8:172:PRO:HG3	1.95	0.99
17:5:185:LYS:O	17:5:189:ASN:ND2	2.01	0.94
15:8:156:PHE:CE1	15:8:172:PRO:HG3	2.06	0.90
17:5:199:ALA:O	17:5:203:GLN:HG3	1.85	0.77
20:3:610:CLA:HBB1	28:3:621:LUT:H32	1.66	0.77
13:3:156:GLN:O	13:3:160:LEU:HB2	1.84	0.77
14:7:203:GLY:O	14:7:207:GLN:HB2	1.86	0.76
20:A:815:CLA:H2	20:A:817:CLA:HMB2	1.69	0.75
20:A:806:CLA:H61	23:A:849:BCR:HC8	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:806:CLA:H11	20:A:807:CLA:HBB1	1.70	0.72
2:B:458:PRO:HG3	2:B:518:PHE:HB2	1.73	0.71
18:6:82:VAL:HG11	28:6:621:LUT:H12	1.72	0.71
20:3:609:CLA:HBB1	20:3:617:CLA:HBB1	1.76	0.68
20:Z:608:CLA:HBB1	20:Z:608:CLA:H151	1.76	0.68
20:B:812:CLA:HBB2	20:B:820:CLA:H72	1.77	0.67
20:F:304:CLA:HMC3	23:F:305:BCR:H24C	1.75	0.67
18:6:251:PHE:HB2	23:6:625:BCR:H282	1.76	0.66
20:6:602:CLA:H61	28:6:624:LUT:H28	1.77	0.66
13:3:238:THR:HG21	13:3:245:ASN:HD21	1.59	0.66
14:7:134:LYS:HG3	20:7:608:CLA:HBB1	1.78	0.65
20:A:816:CLA:H71	23:3:719:BCR:H12C	1.77	0.65
20:A:811:CLA:HBB2	20:A:814:CLA:HMA3	1.79	0.65
15:8:154:LEU:HB2	20:Z:603:CLA:H2	1.78	0.65
20:A:843:CLA:H143	23:L:201:BCR:H17C	1.79	0.65
2:B:339:LEU:HD21	20:B:829:CLA:HBB1	1.79	0.65
20:A:811:CLA:H12	20:A:813:CLA:H43	1.80	0.64
13:3:228:MET:HG2	28:3:622:LUT:H12	1.79	0.64
17:5:203:GLN:HG2	20:5:613:CLA:C1D	2.28	0.64
1:A:204:GLY:O	1:A:208:LEU:HB2	1.98	0.63
20:A:843:CLA:H202	11:L:96:LEU:HD21	1.79	0.63
22:4:622:LHG:H142	22:4:622:LHG:H292	1.79	0.63
15:8:156:PHE:O	15:8:160:LEU:HG	1.99	0.63
20:A:804:CLA:HBB2	20:A:812:CLA:H72	1.79	0.63
1:A:226:LYS:HD3	1:A:253:LEU:HD23	1.79	0.63
15:8:156:PHE:CZ	15:8:172:PRO:CG	2.78	0.62
1:A:327:GLU:HG2	1:A:339:VAL:HG22	1.80	0.62
20:4:613:CLA:H2	20:4:614:CLA:HMD1	1.82	0.61
15:8:136:LYS:HE2	20:8:608:CLA:HMC3	1.83	0.61
16:4:248:LEU:HD21	20:4:614:CLA:HMC3	1.82	0.61
1:A:714:GLN:OE1	1:A:716:ARG:NH2	2.34	0.61
15:8:134:GLU:OE1	15:8:137:ARG:NH2	2.34	0.61
15:8:156:PHE:CE1	15:8:160:LEU:HD21	2.37	0.60
20:A:805:CLA:H43	20:A:812:CLA:HMC2	1.83	0.60
2:B:92:ILE:HB	2:B:113:PRO:HB2	1.83	0.60
20:B:823:CLA:HBA1	23:B:846:BCR:H16C	1.83	0.60
15:8:41:ASP:OD1	15:8:46:GLN:NE2	2.35	0.60
20:A:828:CLA:HED1	20:A:836:CLA:HAB	1.83	0.60
1:A:572:ARG:NH1	22:A:846:LHG:O10	2.35	0.59
18:6:255:LEU:HD13	20:6:622:CLA:HMB3	1.83	0.59
11:L:57:THR:HG22	11:L:59:VAL:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:820:CLA:HAB	20:A:820:CLA:H8	1.83	0.59
20:1:608:CLA:HBB1	20:1:608:CLA:H121	1.83	0.59
6:F:179:LYS:HB2	6:F:182:ASP:HB2	1.84	0.59
1:A:501:ASN:HB2	20:A:837:CLA:HED2	1.84	0.59
1:A:736:ILE:HG21	20:A:829:CLA:HMC2	1.85	0.59
20:A:803:CLA:HED2	20:B:802:CLA:HBB1	1.84	0.58
2:B:41:GLU:HG2	2:B:166:LEU:HB2	1.84	0.58
1:A:265:PHE:HA	20:K:4003:CLA:HBC3	1.85	0.58
20:7:601:CLA:H171	20:7:613:CLA:HBC1	1.85	0.58
2:B:547:LEU:O	2:B:565:ARG:NH2	2.36	0.58
20:4:611:CLA:HAB	23:6:623:BCR:H312	1.84	0.58
14:7:55:PRO:HD2	28:7:622:LUT:H23	1.86	0.58
1:A:540:ALA:HB1	20:A:839:CLA:HMB3	1.84	0.58
15:8:156:PHE:CD1	15:8:160:LEU:HD21	2.39	0.58
20:7:620:CLA:HBB1	20:7:620:CLA:H93	1.86	0.58
16:4:111:VAL:HG11	28:4:619:LUT:H12	1.85	0.57
20:A:809:CLA:H71	20:A:831:CLA:H171	1.86	0.57
27:1:601:CHL:HBB2	20:1:602:CLA:HHD	1.87	0.57
20:A:841:CLA:HED2	2:B:421:SER:HB3	1.87	0.57
20:4:611:CLA:HBC3	22:4:622:LHG:HC62	1.85	0.57
20:A:823:CLA:HMD2	23:K:4001:BCR:H24C	1.86	0.57
15:8:156:PHE:HD1	15:8:160:LEU:HG	1.69	0.57
17:5:133:GLU:HG3	20:5:609:CLA:C4B	2.35	0.56
1:A:740:TRP:HB2	20:A:829:CLA:HBB1	1.87	0.56
9:J:28:GLU:OE1	9:J:31:ARG:NH2	2.38	0.56
20:3:620:CLA:HMC2	20:3:620:CLA:H92	1.87	0.56
2:B:416:LYS:HA	2:B:419:LEU:HD12	1.88	0.56
20:8:601:CLA:H93	20:8:613:CLA:H121	1.87	0.56
17:5:85:VAL:HG11	28:5:620:LUT:H12	1.87	0.56
23:B:801:BCR:H381	20:F:301:CLA:HMC2	1.87	0.56
14:7:146:ALA:HB1	14:7:155:GLU:H	1.71	0.56
13:3:245:ASN:HD22	20:3:613:CLA:HED3	1.71	0.56
20:B:825:CLA:H52	20:B:841:CLA:H201	1.88	0.56
17:5:219:LEU:HD21	20:5:614:CLA:HMC3	1.87	0.55
20:B:821:CLA:HMD2	23:B:843:BCR:HC7	1.89	0.55
13:3:102:ALA:HA	13:3:231:TYR:HE2	1.72	0.55
20:A:809:CLA:HBB2	20:A:829:CLA:H203	1.87	0.55
2:B:546:LYS:HD2	5:E:51:TYR:HA	1.87	0.55
14:7:47:LEU:HD11	14:7:65:LEU:HD21	1.87	0.55
20:A:803:CLA:H122	23:B:848:BCR:H12C	1.88	0.55
15:8:156:PHE:HD1	15:8:160:LEU:CG	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:6:54:PRO:HD2	28:6:624:LUT:H23	1.87	0.55
7:G:58:ARG:NH2	7:G:94:GLY:O	2.40	0.55
15:8:56:PRO:HD2	28:8:618:LUT:H23	1.88	0.55
13:3:159:GLU:OE2	13:3:162:ARG:NH2	2.33	0.55
13:3:164:GLN:OE1	13:3:167:ARG:NH2	2.39	0.55
20:7:610:CLA:HBB1	28:7:621:LUT:H32	1.88	0.55
6:F:189:VAL:HG13	20:F:301:CLA:H122	1.89	0.55
2:B:281:ILE:HD12	20:B:818:CLA:HBB1	1.90	0.54
14:7:207:GLN:NE2	28:7:621:LUT:O3	2.40	0.54
15:8:153:PHE:HB2	15:8:157:GLU:HB3	1.88	0.54
15:8:212:ALA:HB2	20:8:616:CLA:HED2	1.88	0.54
20:6:616:CLA:HBC3	20:6:622:CLA:HMC3	1.89	0.54
2:B:192:THR:HG21	2:B:279:LEU:HB2	1.89	0.54
12:1:160:PRO:HD2	28:1:617:LUT:H23	1.89	0.54
20:A:822:CLA:HBC3	20:A:828:CLA:H193	1.89	0.54
4:D:125:THR:HG23	4:D:136:PRO:HG2	1.90	0.54
20:4:613:CLA:HAB	20:4:613:CLA:H102	1.89	0.54
12:1:137:ALA:HB2	20:1:606:CLA:H52	1.89	0.54
1:A:353:LEU:HD11	20:A:831:CLA:HBB1	1.90	0.54
20:5:606:CLA:HMB2	23:5:622:BCR:H373	1.90	0.54
17:5:32:ARG:O	17:5:32:ARG:HG2	2.08	0.54
20:8:602:CLA:HBB1	20:8:602:CLA:H51	1.90	0.53
22:4:623:LHG:O2	18:6:133:ARG:NH2	2.40	0.53
13:3:250:LEU:HD21	20:3:614:CLA:HMC3	1.90	0.53
12:Z:142:GLU:HA	12:Z:142:GLU:OE1	2.07	0.53
20:B:805:CLA:H11	20:B:806:CLA:HBB1	1.91	0.53
10:K:35:ASN:ND2	20:K:4003:CLA:OBD	2.41	0.53
1:A:54:ALA:HB2	22:A:846:LHG:HC82	1.91	0.53
20:5:609:CLA:HBA1	20:5:621:CLA:HMD2	1.90	0.53
20:B:840:CLA:H191	8:I:89:ALA:HA	1.89	0.53
2:B:300:HIS:HB3	2:B:305:ILE:HD11	1.90	0.53
20:B:809:CLA:H102	20:B:827:CLA:H193	1.91	0.53
20:B:823:CLA:HAB	20:B:830:CLA:HMD2	1.91	0.53
14:7:134:LYS:HB3	20:7:608:CLA:HMC3	1.89	0.53
15:8:88:LEU:O	15:8:92:LEU:N	2.41	0.53
1:A:658:ILE:HG13	1:A:659:GLN:HG3	1.91	0.53
14:7:160:LEU:HD23	14:7:161:GLU:HG3	1.91	0.53
20:B:840:CLA:HBB1	23:B:848:BCR:H363	1.90	0.52
12:Z:64:LEU:HD13	20:Z:602:CLA:H42	1.91	0.52
20:B:805:CLA:NB	20:B:829:CLA:HMB2	2.25	0.52
20:B:809:CLA:H91	20:B:840:CLA:H12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:830:CLA:HBB2	20:B:838:CLA:HMC2	1.90	0.52
8:I:83:THR:HG22	8:I:87:LEU:HD12	1.91	0.52
20:1:602:CLA:H52	28:1:618:LUT:H28	1.92	0.52
20:3:604:CLA:HMC1	23:3:718:BCR:H19C	1.90	0.52
17:5:203:GLN:HG2	20:5:613:CLA:ND	2.24	0.52
2:B:437:LEU:HD12	20:B:833:CLA:HAB	1.92	0.52
20:B:832:CLA:H201	23:F:305:BCR:H15C	1.91	0.52
17:5:245:LEU:HD13	18:6:224:VAL:HG21	1.91	0.52
17:5:247:ILE:HD11	23:5:625:BCR:H351	1.91	0.52
1:A:399:GLY:HA3	1:A:603:LEU:HD11	1.91	0.52
20:A:816:CLA:H51	13:3:233:ALA:HA	1.91	0.52
20:A:827:CLA:H111	20:A:840:CLA:H71	1.91	0.52
2:B:352:HIS:ND1	20:B:817:CLA:OBD	2.42	0.52
20:B:839:CLA:HBB2	21:B:842:PQN:H141	1.92	0.52
20:B:826:CLA:H122	23:B:846:BCR:H373	1.92	0.52
3:C:61:ASP:O	5:E:86:ASN:ND2	2.40	0.52
1:A:75:SER:HB3	20:A:812:CLA:HHD	1.92	0.52
20:A:810:CLA:H102	23:J:3003:BCR:H332	1.91	0.52
20:4:609:CLA:HHC	20:4:609:CLA:HBB1	1.90	0.52
1:A:147:LEU:HD11	20:A:830:CLA:H42	1.92	0.52
20:F:303:CLA:HHC	20:F:303:CLA:HBB1	1.91	0.52
23:B:801:BCR:H323	20:B:832:CLA:HBB1	1.92	0.51
16:4:83:PRO:HD2	28:4:620:LUT:H23	1.93	0.51
20:A:854:CLA:HBB1	2:B:526:LEU:HD21	1.91	0.51
6:F:201:GLY:HA3	15:8:59:LEU:HD21	1.92	0.51
15:8:224:HIS:CD2	20:8:614:CLA:NC	2.78	0.51
17:5:78:ALA:HB1	17:5:190:GLY:HA3	1.92	0.51
1:A:320:HIS:HB3	1:A:325:ILE:HD11	1.93	0.51
20:B:837:CLA:H151	23:F:305:BCR:H21C	1.93	0.51
14:7:210:ALA:HB2	20:7:616:CLA:HED2	1.93	0.51
20:A:807:CLA:H151	20:A:830:CLA:HBB2	1.93	0.51
20:B:812:CLA:HHC	20:B:812:CLA:HBB1	1.91	0.51
20:A:802:CLA:H152	20:A:842:CLA:HBB1	1.92	0.51
2:B:340:ALA:HB2	23:B:847:BCR:H372	1.93	0.51
20:7:610:CLA:H13	28:7:621:LUT:H403	1.91	0.51
16:4:199:ASP:OD1	28:4:619:LUT:O23	2.28	0.51
22:4:622:LHG:HC91	23:6:623:BCR:HC41	1.92	0.51
15:8:51:ASN:ND2	20:8:602:CLA:O1D	2.44	0.51
27:5:607:CHL:H12	23:5:625:BCR:H383	1.92	0.51
14:7:221:ASP:HB3	14:7:229:VAL:HG11	1.91	0.51
20:B:839:CLA:H142	23:L:201:BCR:H21C	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:5:242:VAL:HG11	23:5:625:BCR:H353	1.91	0.51
1:A:130:ASP:OD2	6:F:93:GLN:NE2	2.45	0.50
1:A:356:ASN:O	1:A:360:PHE:HB2	2.11	0.50
20:B:818:CLA:HAB	20:B:818:CLA:H8	1.92	0.50
20:B:819:CLA:HMB2	20:B:824:CLA:HMA3	1.92	0.50
20:B:826:CLA:HHC	20:B:826:CLA:HBB1	1.93	0.50
14:7:66:LYS:O	14:7:162:ASN:ND2	2.43	0.50
12:Z:50:PRO:O	12:Z:56:ASN:ND2	2.43	0.50
20:B:823:CLA:H121	23:B:846:BCR:H352	1.93	0.50
3:C:34:CYS:HA	5:E:67:VAL:HG23	1.93	0.50
16:4:67:LEU:HD22	16:4:80:GLY:HA3	1.93	0.50
20:A:840:CLA:HBA2	22:A:847:LHG:H221	1.92	0.50
1:A:396:TRP:HB3	20:A:829:CLA:HMC3	1.92	0.50
20:1:606:CLA:HMB1	20:1:609:CLA:HBC2	1.93	0.50
18:6:75:SER:HB2	18:6:180:GLY:HA3	1.93	0.50
20:8:606:CLA:HHC	20:8:606:CLA:HBB1	1.94	0.50
12:Z:142:GLU:HG3	20:Z:609:CLA:C4B	2.41	0.50
16:4:232:GLN:HE22	28:4:619:LUT:C3	2.24	0.50
1:A:35:PHE:HB2	1:A:62:HIS:CD2	2.46	0.50
3:C:40:ALA:O	4:D:170:GLN:NE2	2.40	0.50
1:A:198:LEU:HD22	20:A:826:CLA:HMD3	1.94	0.50
1:A:605:ILE:HD12	19:A:801:CL0:H53	1.93	0.50
20:A:822:CLA:HMB2	20:A:826:CLA:HMA3	1.93	0.50
20:B:815:CLA:HBB1	23:B:843:BCR:H382	1.94	0.50
23:3:717:BCR:HC31	20:7:601:CLA:HBC2	1.93	0.50
20:7:601:CLA:H91	20:7:616:CLA:HMD2	1.93	0.50
18:6:205:LEU:HD22	28:6:621:LUT:H163	1.94	0.50
20:F:301:CLA:HHC	20:F:301:CLA:HBB1	1.94	0.50
20:3:617:CLA:HBA2	20:7:601:CLA:H72	1.94	0.50
20:1:603:CLA:HED2	20:1:603:CLA:H43	1.94	0.49
17:5:245:LEU:HD11	23:5:625:BCR:H352	1.94	0.49
18:6:163:PRO:HD2	28:6:621:LUT:H23	1.93	0.49
1:A:707:LEU:HD13	23:F:305:BCR:H321	1.93	0.49
20:A:806:CLA:H51	20:A:814:CLA:H12	1.94	0.49
20:B:839:CLA:H8	20:B:840:CLA:H121	1.93	0.49
6:F:223:THR:OG1	6:F:227:ARG:NH2	2.45	0.49
15:8:55:ASP:OD1	28:8:618:LUT:O23	2.30	0.49
20:5:617:CLA:HED1	22:6:619:LHG:H302	1.92	0.49
20:A:815:CLA:HBA1	20:A:817:CLA:HMB3	1.94	0.49
27:1:601:CHL:HMD2	23:8:619:BCR:H323	1.95	0.49
18:6:95:VAL:HG11	20:6:604:CLA:HED2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:805:CLA:H42	20:A:812:CLA:HBB1	1.94	0.49
20:A:807:CLA:HBB	20:A:831:CLA:HAB	1.94	0.49
2:B:627:LEU:O	2:B:733:ARG:NH2	2.43	0.49
15:8:154:LEU:HD12	20:Z:603:CLA:H43	1.95	0.49
15:8:160:LEU:HD22	20:8:608:CLA:HMC2	1.94	0.49
27:6:606:CHL:HHC	27:6:606:CHL:HBB1	1.94	0.49
1:A:333:PHE:HD2	22:A:847:LHG:HC42	1.78	0.49
3:C:2:ALA:N	3:C:71:SER:O	2.46	0.49
1:A:363:LEU:HD11	20:A:820:CLA:H71	1.95	0.49
20:B:833:CLA:HBA1	9:J:36:PRO:HG2	1.94	0.49
27:3:608:CHL:H43	23:3:718:BCR:H14C	1.93	0.49
17:5:60:LEU:HD13	20:5:602:CLA:H42	1.93	0.49
18:6:69:GLU:HG2	18:6:132:LEU:HD12	1.93	0.49
2:B:258:PHE:CZ	20:B:817:CLA:H2	2.48	0.49
20:B:822:CLA:HHC	20:B:841:CLA:HED1	1.95	0.49
14:7:135:ARG:NH2	20:7:609:CLA:O1D	2.45	0.49
20:3:612:CLA:HHC	20:3:612:CLA:HBB1	1.94	0.48
20:Z:610:CLA:H13	28:Z:617:LUT:H403	1.95	0.48
20:B:813:CLA:H42	23:B:844:BCR:H21C	1.96	0.48
20:B:825:CLA:H92	20:B:836:CLA:H41	1.95	0.48
14:7:171:ASP:OD1	28:7:621:LUT:O23	2.31	0.48
27:Z:601:CHL:HBB2	20:Z:602:CLA:HHD	1.94	0.48
20:A:802:CLA:H122	23:A:852:BCR:H23C	1.95	0.48
20:A:805:CLA:H2	20:A:812:CLA:H92	1.95	0.48
23:A:856:BCR:HC22	9:J:31:ARG:HH11	1.78	0.48
2:B:258:PHE:HZ	20:B:817:CLA:H2	1.78	0.48
4:D:88:TRP:HB3	4:D:136:PRO:HB3	1.95	0.48
20:7:601:CLA:H62	20:7:601:CLA:H41	1.69	0.48
15:8:225:LEU:HD21	20:8:614:CLA:HMC3	1.96	0.48
20:B:807:CLA:H12	8:I:83:THR:HG21	1.96	0.48
2:B:525:ALA:HB2	20:B:837:CLA:HMA1	1.95	0.48
17:5:133:GLU:HG3	20:5:609:CLA:NB	2.29	0.48
14:7:223:LEU:HD21	20:7:614:CLA:HMC3	1.96	0.48
20:B:832:CLA:H152	6:F:157:LEU:HD22	1.94	0.48
12:1:217:ASN:HD21	15:8:121:SER:HB2	1.77	0.48
13:3:216:LYS:HD3	20:3:612:CLA:HAA2	1.95	0.48
20:A:841:CLA:H121	20:F:303:CLA:HAC1	1.94	0.48
20:1:606:CLA:H41	20:1:606:CLA:H61	1.63	0.48
17:5:197:TYR:CD2	28:5:624:LUT:H12	2.49	0.48
2:B:54:GLN:HE21	2:B:58:ILE:HG13	1.79	0.48
20:B:806:CLA:HAB	20:B:828:CLA:HMC2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:828:CLA:H52	23:B:844:BCR:H24C	1.94	0.47
4:D:140:ARG:HB3	4:D:148:GLN:HB3	1.96	0.47
23:F:305:BCR:H341	23:F:305:BCR:H11C	1.73	0.47
16:4:157:PHE:HZ	23:4:621:BCR:H373	1.79	0.47
18:6:123:TRP:CE2	23:6:623:BCR:H10C	2.48	0.47
20:A:841:CLA:H18	20:F:301:CLA:H61	1.95	0.47
23:A:852:BCR:H20C	23:A:852:BCR:H361	1.61	0.47
18:6:156:TYR:HB3	20:6:610:CLA:HED2	1.96	0.47
20:A:818:CLA:CHD	20:A:819:CLA:HBB2	2.45	0.47
20:B:835:CLA:HMB1	23:B:847:BCR:HC31	1.96	0.47
20:7:612:CLA:HAC2	20:7:613:CLA:H193	1.95	0.47
4:D:97:GLU:H	4:D:127:GLN:HE22	1.62	0.47
13:3:95:ALA:HB1	13:3:221:GLY:HA3	1.96	0.47
15:8:36:ILE:HD12	15:8:53:GLY:HA3	1.96	0.47
17:5:247:ILE:HD11	23:5:625:BCR:H15C	1.96	0.47
18:6:127:ARG:HH21	27:6:618:CHL:HMC	1.79	0.47
20:A:808:CLA:H41	20:A:808:CLA:H61	1.59	0.47
23:A:848:BCR:H362	23:A:849:BCR:H21C	1.96	0.47
6:F:224:VAL:HG12	6:F:226:PRO:HD2	1.96	0.47
14:7:30:ARG:NH1	14:7:50:ASP:O	2.47	0.47
14:7:132:GLU:HG2	20:7:609:CLA:NB	2.30	0.47
1:A:169:MET:HG3	23:A:848:BCR:H322	1.96	0.47
20:A:854:CLA:HBC2	2:B:586:ASN:HB2	1.96	0.47
20:B:807:CLA:HAA1	8:I:80:VAL:HG22	1.95	0.47
1:A:429:ARG:HG2	1:A:432:ARG:HH22	1.79	0.47
2:B:173:GLU:HG3	2:B:302:MET:HE3	1.97	0.47
14:7:81:LEU:HD23	20:7:604:CLA:HHC	1.96	0.47
20:B:818:CLA:H3A	20:B:818:CLA:HBA2	1.75	0.47
14:7:203:GLY:O	14:7:207:GLN:CB	2.59	0.47
16:4:161:GLU:HG3	20:4:609:CLA:C4B	2.44	0.47
17:5:245:LEU:HA	18:6:227:GLN:HE21	1.80	0.47
23:5:625:BCR:H351	23:5:625:BCR:H15C	1.64	0.47
20:A:841:CLA:H92	23:B:801:BCR:H15C	1.97	0.47
2:B:429:PHE:CD2	20:B:837:CLA:HAB	2.50	0.47
20:8:613:CLA:H2	20:8:614:CLA:HMD1	1.95	0.47
27:Z:601:CHL:H61	27:Z:601:CHL:H41	1.72	0.47
2:B:423:LEU:HD13	2:B:533:LEU:HA	1.96	0.47
13:3:141:TRP:NE1	20:3:606:CLA:OBD	2.37	0.47
15:8:156:PHE:HZ	15:8:172:PRO:CG	2.27	0.47
20:A:829:CLA:H3A	20:A:829:CLA:HBA2	1.70	0.46
20:1:604:CLA:H62	20:1:604:CLA:H41	1.72	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:8:613:CLA:HMB3	28:8:617:LUT:H162	1.97	0.46
12:1:202:PRO:O	28:1:617:LUT:O3	2.33	0.46
20:3:607:CLA:H143	23:3:719:BCR:H391	1.96	0.46
27:3:608:CHL:HMB3	23:3:717:BCR:H362	1.97	0.46
27:6:607:CHL:H62	27:6:607:CHL:H41	1.64	0.46
12:1:50:PRO:O	12:1:56:ASN:ND2	2.48	0.46
13:3:182:ALA:HA	13:3:185:LYS:HE2	1.97	0.46
20:A:843:CLA:H193	11:L:96:LEU:HD11	1.97	0.46
17:5:133:GLU:OE1	17:5:133:GLU:HA	2.15	0.46
1:A:422:ASN:HD21	1:A:427:LEU:HD23	1.81	0.46
1:A:491:HIS:HE1	20:A:836:CLA:NB	2.11	0.46
20:A:816:CLA:H101	23:3:719:BCR:H14C	1.98	0.46
2:B:588:ILE:HA	2:B:591:VAL:HG22	1.97	0.46
23:B:801:BCR:H11C	23:B:801:BCR:H341	1.83	0.46
3:C:79:LEU:O	4:D:77:LYS:NZ	2.41	0.46
16:4:79:PHE:HB2	20:4:602:CLA:HMD1	1.97	0.46
20:5:609:CLA:H3A	20:5:609:CLA:HBA2	1.47	0.46
1:A:80:GLN:HB2	20:A:806:CLA:HMB2	1.97	0.46
1:A:330:ARG:HE	1:A:336:GLU:HA	1.80	0.46
1:A:356:ASN:ND2	20:A:806:CLA:OBD	2.46	0.46
20:A:814:CLA:HMB3	20:A:814:CLA:H112	1.97	0.46
20:1:602:CLA:H61	20:1:602:CLA:H41	1.72	0.46
23:7:623:BCR:H15C	23:7:623:BCR:H351	1.82	0.46
22:5:623:LHG:H112	22:5:623:LHG:H311	1.96	0.46
2:B:490:GLY:HA3	2:B:495:LEU:HD13	1.98	0.46
1:A:261:ILE:HD11	20:A:816:CLA:HBA2	1.97	0.46
20:A:818:CLA:H2	20:K:4002:CLA:HED1	1.97	0.46
23:L:201:BCR:H15C	23:L:201:BCR:H351	1.83	0.46
12:1:159:ASP:OD1	28:1:617:LUT:O23	2.29	0.46
20:8:604:CLA:HBB1	23:8:619:BCR:H393	1.97	0.46
20:4:612:CLA:HED3	20:4:612:CLA:H12	1.98	0.46
20:5:606:CLA:H62	27:5:608:CHL:HMB2	1.97	0.46
20:3:603:CLA:H2	20:3:603:CLA:H61	1.70	0.46
15:8:190:LEU:HA	15:8:193:VAL:HG12	1.98	0.46
20:Z:613:CLA:HMB1	20:Z:613:CLA:H18	1.98	0.46
20:4:602:CLA:CBB	28:4:620:LUT:H32	2.46	0.46
23:A:850:BCR:H24C	23:A:850:BCR:H371	1.79	0.46
2:B:27:ALA:HA	20:B:829:CLA:H42	1.98	0.46
2:B:175:ARG:HB2	20:B:813:CLA:HBC2	1.98	0.46
20:1:611:CLA:H92	20:1:611:CLA:H62	1.82	0.46
14:7:145:GLN:NE2	15:8:32:PRO:O	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:7:198:MET:SD	20:7:602:CLA:HBB1	2.55	0.46
17:5:122:LEU:HD11	20:6:616:CLA:HBA2	1.97	0.46
2:B:51:HIS:CE1	20:B:805:CLA:ND	2.84	0.45
2:B:309:HIS:HA	20:B:841:CLA:HMD1	1.98	0.45
23:B:843:BCR:H372	23:G:205:BCR:HC42	1.98	0.45
23:7:624:BCR:H11C	23:7:624:BCR:H341	1.85	0.45
20:Z:602:CLA:H61	20:Z:602:CLA:H41	1.61	0.45
16:4:76:PRO:HB3	16:4:212:LYS:HB3	1.98	0.45
1:A:481:PRO:HG3	1:A:533:PHE:HB2	1.97	0.45
14:7:130:TRP:CZ2	23:7:623:BCR:HC8	2.51	0.45
12:Z:40:LEU:HD12	27:Z:601:CHL:HMA3	1.97	0.45
16:4:200:PRO:HD2	28:4:619:LUT:H23	1.97	0.45
17:5:133:GLU:HG3	20:5:609:CLA:C1B	2.45	0.45
1:A:733:LEU:HD22	20:A:842:CLA:HMA1	1.98	0.45
20:A:821:CLA:HBB1	23:K:4001:BCR:H14C	1.99	0.45
20:A:825:CLA:H2	23:A:850:BCR:H363	1.98	0.45
2:B:412:MET:HG3	23:B:846:BCR:H402	1.99	0.45
20:4:601:CLA:HBB1	22:4:622:LHG:H272	1.99	0.45
20:A:805:CLA:O1A	20:A:812:CLA:ND	2.49	0.45
20:B:805:CLA:HBA1	20:B:805:CLA:H3A	1.65	0.45
12:Z:159:ASP:OD1	28:Z:617:LUT:O23	2.30	0.45
16:4:171:PRO:HB3	16:4:191:PRO:HG3	1.97	0.45
20:A:812:CLA:H142	20:A:812:CLA:H112	1.67	0.45
20:A:815:CLA:H122	20:3:607:CLA:HMC2	1.99	0.45
20:1:602:CLA:CBB	28:1:618:LUT:H32	2.46	0.45
15:8:48:LEU:HD21	15:8:70:GLN:HG3	1.98	0.45
20:8:606:CLA:HMB2	23:8:619:BCR:H373	1.98	0.45
16:4:194:PRO:HB3	27:4:608:CHL:HBC2	1.99	0.45
20:A:810:CLA:H93	23:A:856:BCR:H373	1.99	0.45
20:B:819:CLA:H41	20:B:819:CLA:H61	1.76	0.45
1:A:18:ASP:OD2	1:A:71:ARG:NH2	2.44	0.45
20:B:820:CLA:HBB1	23:B:843:BCR:H17C	1.98	0.45
13:3:199:ASN:OD1	28:3:621:LUT:O23	2.35	0.45
20:8:610:CLA:CBB	28:8:617:LUT:H32	2.47	0.45
28:8:618:LUT:H35	28:8:618:LUT:H401	1.82	0.45
12:Z:197:ALA:HB2	20:Z:616:CLA:HED2	1.99	0.45
20:A:817:CLA:HHD	13:3:133:PRO:HG2	1.99	0.45
20:A:823:CLA:H3A	20:A:823:CLA:HBA2	1.59	0.45
20:A:841:CLA:HBC1	21:A:844:PQN:H201	1.97	0.45
20:B:805:CLA:HHC	20:B:805:CLA:HBB1	1.99	0.45
6:F:158:TYR:HA	6:F:202:TRP:HZ2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1:608:CLA:HMA1	28:1:619:LUT:H203	1.99	0.45
15:8:31:LEU:HD21	20:8:601:CLA:HMA3	1.99	0.45
20:Z:610:CLA:CBB	28:Z:617:LUT:H32	2.47	0.45
1:A:422:ASN:OD1	1:A:425:ASN:ND2	2.48	0.45
20:A:843:CLA:H62	20:A:843:CLA:H41	1.67	0.45
4:D:128:LEU:HA	4:D:132:PHE:HD2	1.82	0.45
20:5:611:CLA:H41	20:5:611:CLA:H61	1.67	0.45
23:6:625:BCR:H11C	23:6:625:BCR:H341	1.80	0.45
1:A:393:HIS:HE1	20:A:829:CLA:ND	2.11	0.45
20:A:829:CLA:H202	23:J:3003:BCR:H17C	1.98	0.45
2:B:723:ALA:HB2	20:B:827:CLA:HBB1	1.98	0.45
28:Z:619:LUT:H15	28:Z:619:LUT:H201	1.84	0.45
1:A:448:LEU:O	1:A:452:SER:OG	2.22	0.44
2:B:27:ALA:HB2	25:B:850:DGD:HA51	2.00	0.44
20:B:823:CLA:HMD1	20:B:824:CLA:HHC	1.97	0.44
20:B:829:CLA:H62	20:B:829:CLA:H41	1.79	0.44
12:Z:61:PRO:HD2	28:Z:618:LUT:H23	1.99	0.44
17:5:202:LEU:HG	20:5:613:CLA:HAC2	1.99	0.44
18:6:33:LEU:HD21	20:6:601:CLA:HMA3	1.98	0.44
18:6:39:PRO:HD2	18:6:42:LEU:HD12	1.99	0.44
20:6:610:CLA:CBB	28:6:621:LUT:H32	2.48	0.44
20:A:802:CLA:C1D	2:B:583:TRP:HE1	2.30	0.44
28:3:621:LUT:H15	28:3:621:LUT:H201	1.87	0.44
14:7:132:GLU:HG2	20:7:609:CLA:C1B	2.47	0.44
12:Z:188:PHE:CD2	28:Z:618:LUT:H12	2.52	0.44
20:4:601:CLA:OBD	18:6:127:ARG:NH1	2.50	0.44
12:Z:83:ARG:NH1	20:Z:608:CLA:OBD	2.42	0.44
16:4:111:VAL:HG22	16:4:229:PHE:HE2	1.82	0.44
20:4:612:CLA:H62	20:4:612:CLA:H41	1.80	0.44
17:5:32:ARG:O	17:5:33:LYS:C	2.56	0.44
20:5:604:CLA:HMB3	28:5:624:LUT:H162	2.00	0.44
28:6:624:LUT:H15	28:6:624:LUT:H201	1.85	0.44
1:A:150:ALA:HB2	1:A:378:PRO:HD2	1.99	0.44
20:7:601:CLA:H92	20:7:613:CLA:H51	2.00	0.44
15:8:115:SER:OG	15:8:116:PHE:N	2.48	0.44
27:Z:601:CHL:H52	22:Z:620:LHG:H181	2.00	0.44
20:Z:604:CLA:H62	20:Z:604:CLA:H41	1.71	0.44
28:5:624:LUT:H15	28:5:624:LUT:H201	1.89	0.44
23:B:843:BCR:H11C	23:B:843:BCR:H341	1.83	0.44
28:1:619:LUT:H15	28:1:619:LUT:H201	1.81	0.44
28:8:617:LUT:H35	28:8:617:LUT:H401	1.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:6:199:LYS:HE2	18:6:203:ALA:HB1	2.00	0.44
18:6:209:LEU:HD21	20:6:614:CLA:HMC3	2.00	0.44
1:A:45:THR:HG23	5:E:78:GLN:HE21	1.83	0.44
1:A:419:PRO:HB2	4:D:103:ALA:HB2	1.98	0.44
20:A:833:CLA:H143	20:A:833:CLA:H111	1.85	0.44
23:A:852:BCR:H362	20:A:854:CLA:H42	1.99	0.44
2:B:142:PHE:HZ	20:B:814:CLA:H101	1.82	0.44
20:8:610:CLA:H52	28:8:617:LUT:H30	1.99	0.44
27:Z:601:CHL:H11	22:Z:620:LHG:H161	2.00	0.44
18:6:162:ALA:HB2	20:6:610:CLA:HBD	1.99	0.44
1:A:297:HIS:HE1	20:A:819:CLA:ND	2.15	0.44
20:A:822:CLA:H111	20:A:822:CLA:H152	1.66	0.44
4:D:117:LYS:HE2	4:D:119:GLU:HB3	1.99	0.44
13:3:63:GLY:HA3	13:3:218:ILE:HG21	1.99	0.44
13:3:97:TRP:CE2	27:3:608:CHL:HED2	2.52	0.44
20:Z:602:CLA:H72	28:Z:618:LUT:H28	2.00	0.44
27:6:607:CHL:HBA1	23:6:625:BCR:H21C	2.00	0.44
1:A:623:THR:HG1	1:A:626:GLY:N	2.16	0.44
2:B:351:GLN:HE21	20:B:826:CLA:HMD2	1.82	0.44
20:B:812:CLA:H2	20:B:812:CLA:H61	1.66	0.44
20:B:815:CLA:H51	20:B:815:CLA:H11	1.76	0.44
23:J:3003:BCR:H24C	23:J:3003:BCR:H371	1.73	0.44
11:L:80:ALA:HB3	11:L:83:LEU:HD23	2.00	0.44
15:8:217:PRO:O	28:8:617:LUT:O3	2.33	0.44
20:4:601:CLA:C1C	22:4:622:LHG:H102	2.12	0.44
20:A:804:CLA:H2	20:A:804:CLA:HED2	1.98	0.44
20:B:806:CLA:H43	25:B:850:DGD:HB51	1.98	0.44
20:B:831:CLA:HAC1	20:B:838:CLA:HBC3	2.00	0.44
15:8:176:LEU:HD12	28:8:617:LUT:H222	1.99	0.44
18:6:127:ARG:NH2	27:6:618:CHL:HMC	2.33	0.44
20:B:832:CLA:H2	20:B:832:CLA:H62	1.78	0.43
12:1:61:PRO:HD2	28:1:618:LUT:H23	2.00	0.43
12:1:161:LEU:HD12	28:1:617:LUT:H222	1.99	0.43
13:3:131:ILE:HG22	13:3:134:ALA:H	1.83	0.43
14:7:172:PRO:HD2	28:7:621:LUT:H23	2.00	0.43
16:4:98:GLN:NE2	16:4:191:PRO:O	2.48	0.43
23:A:851:BCR:H15C	23:A:851:BCR:H351	1.82	0.43
20:B:825:CLA:HBA2	20:B:825:CLA:H3A	1.79	0.43
20:A:826:CLA:H141	20:A:826:CLA:H161	1.87	0.43
20:A:828:CLA:H61	20:A:828:CLA:H2	1.85	0.43
20:A:854:CLA:HBB	20:B:802:CLA:H202	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:833:CLA:H102	20:B:833:CLA:H61	1.82	0.43
23:B:843:BCR:H362	23:G:205:BCR:H312	1.99	0.43
3:C:4:ILE:HB	3:C:68:TYR:HB2	1.99	0.43
23:L:205:BCR:H11C	23:L:205:BCR:H341	1.88	0.43
20:4:611:CLA:H61	20:4:611:CLA:H41	1.61	0.43
20:6:612:CLA:H41	20:6:612:CLA:H62	1.80	0.43
1:A:32:PRO:HG2	6:F:185:ILE:HD11	2.00	0.43
1:A:122:VAL:HB	20:B:833:CLA:HMD1	2.00	0.43
23:A:848:BCR:H20C	23:A:848:BCR:H361	1.88	0.43
20:B:806:CLA:H72	20:B:806:CLA:H111	1.81	0.43
14:7:118:PRO:HB2	15:8:234:ALA:HB1	2.00	0.43
20:7:606:CLA:HHC	20:7:606:CLA:HBB1	2.00	0.43
15:8:79:THR:HG23	28:8:618:LUT:H202	2.01	0.43
20:6:610:CLA:H91	20:6:610:CLA:H112	1.88	0.43
1:A:227:LEU:HD22	1:A:237:ILE:HG23	1.99	0.43
1:A:426:LEU:HD13	20:A:825:CLA:C1C	2.48	0.43
1:A:647:ARG:NH1	2:B:633:ILE:O	2.51	0.43
20:A:834:CLA:HAB	20:A:835:CLA:HHB	2.01	0.43
2:B:258:PHE:CD1	20:B:817:CLA:HMB2	2.54	0.43
12:1:110:ALA:HB1	12:1:127:LEU:HD22	2.01	0.43
12:1:144:GLN:HB3	20:1:608:CLA:HMC3	2.00	0.43
28:7:622:LUT:H35	28:7:622:LUT:H401	1.87	0.43
12:Z:160:PRO:HD2	28:Z:617:LUT:H23	2.00	0.43
12:Z:205:ALA:HB1	20:Z:613:CLA:HED3	2.01	0.43
20:Z:612:CLA:H51	20:Z:612:CLA:H11	1.81	0.43
2:B:177:ASN:HD22	2:B:294:THR:HG23	1.83	0.43
11:L:74:ALA:HB2	20:L:203:CLA:HMD1	2.00	0.43
23:7:623:BCR:H24C	23:7:623:BCR:H371	1.86	0.43
1:A:60:ASP:OD2	1:A:350:HIS:NE2	2.49	0.43
20:A:841:CLA:H2	20:B:832:CLA:H42	1.99	0.43
13:3:92:VAL:HG21	13:3:191:ALA:HB1	2.00	0.43
17:5:71:ARG:NH1	17:5:74:GLU:OE1	2.52	0.43
17:5:80:TRP:CE2	27:5:608:CHL:HED2	2.53	0.43
20:5:602:CLA:H102	20:5:603:CLA:HMB3	2.01	0.43
1:A:200:HIS:CG	20:A:814:CLA:HMC2	2.54	0.43
20:A:834:CLA:H61	20:A:834:CLA:H41	1.77	0.43
23:G:205:BCR:H361	23:G:205:BCR:H20C	1.81	0.43
23:3:718:BCR:H15C	23:3:718:BCR:H351	1.81	0.43
20:Z:608:CLA:H203	20:Z:608:CLA:H162	1.90	0.43
28:Z:619:LUT:H35	28:Z:619:LUT:H401	1.78	0.43
17:5:171:PRO:HD2	28:5:620:LUT:H23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:SER:HB3	20:A:829:CLA:HAA2	2.00	0.43
20:A:811:CLA:H111	20:A:811:CLA:H152	1.75	0.43
20:A:831:CLA:H142	20:A:831:CLA:H111	1.82	0.43
4:D:182:ILE:HD12	4:D:185:LYS:HD3	2.00	0.43
15:8:126:GLN:HE22	27:8:607:CHL:CMC	2.32	0.43
15:8:175:PRO:HD2	28:8:617:LUT:H23	2.00	0.43
16:4:163:ARG:HE	16:4:174:ALA:HB1	1.82	0.43
18:6:223:VAL:HB	20:6:616:CLA:C1C	2.48	0.43
23:A:849:BCR:H15C	23:A:849:BCR:H351	1.81	0.43
2:B:561:ASP:OD2	2:B:565:ARG:NH1	2.50	0.43
20:B:805:CLA:C4B	20:B:829:CLA:HMB2	2.49	0.43
20:B:834:CLA:H61	20:B:834:CLA:H2	1.70	0.43
6:F:204:LEU:HD11	20:8:602:CLA:H92	2.01	0.43
14:7:231:PHE:O	14:7:237:SER:OG	2.35	0.43
16:4:244:LEU:HD22	28:4:619:LUT:H163	2.00	0.43
17:5:90:VAL:HG11	20:5:604:CLA:HAC2	2.00	0.43
23:6:625:BCR:H15C	23:6:625:BCR:H351	1.78	0.43
1:A:408:HIS:HE1	20:A:831:CLA:NA	2.17	0.42
20:A:817:CLA:H62	20:3:607:CLA:H62	2.01	0.42
13:3:156:GLN:O	13:3:160:LEU:CB	2.62	0.42
15:8:156:PHE:CD1	15:8:160:LEU:CD2	3.01	0.42
23:3:718:BCR:H322	20:5:601:CLA:H101	2.01	0.42
15:8:174:ASP:OD1	28:8:617:LUT:O23	2.33	0.42
12:Z:176:LYS:HD3	20:Z:612:CLA:HBA1	2.01	0.42
28:Z:619:LUT:H31	28:Z:619:LUT:H391	1.78	0.42
12:1:123:VAL:HG11	20:1:606:CLA:HMD1	2.01	0.42
22:Z:620:LHG:H101	22:Z:620:LHG:H132	1.88	0.42
16:4:221:LEU:HD11	20:4:611:CLA:HAC1	2.00	0.42
28:5:620:LUT:H35	28:5:620:LUT:H401	1.86	0.42
28:6:624:LUT:H35	28:6:624:LUT:H401	1.92	0.42
20:A:833:CLA:H41	20:A:833:CLA:H61	1.60	0.42
20:A:841:CLA:H2	20:A:841:CLA:H61	1.81	0.42
20:3:603:CLA:H92	20:3:603:CLA:H62	1.89	0.42
20:Z:610:CLA:H52	28:Z:617:LUT:H30	2.01	0.42
20:6:611:CLA:H61	20:6:611:CLA:H41	1.69	0.42
20:A:839:CLA:H62	20:A:839:CLA:H41	1.76	0.42
20:1:606:CLA:HBB2	27:1:607:CHL:CBB	2.49	0.42
22:7:625:LHG:H291	22:7:625:LHG:H321	1.89	0.42
1:A:487:ILE:HD11	20:A:838:CLA:H2	2.01	0.42
20:A:802:CLA:H18	20:A:854:CLA:H193	2.01	0.42
20:A:824:CLA:H3A	20:A:824:CLA:HBA2	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:8:151:GLY:N	15:8:157:GLU:OE1	2.53	0.42
16:4:176:GLN:HA	16:4:184:LYS:HA	2.01	0.42
20:4:610:CLA:CBB	28:4:619:LUT:H32	2.48	0.42
20:5:609:CLA:HBA2	20:5:617:CLA:HMC1	2.01	0.42
18:6:201:PRO:HB2	28:6:621:LUT:H173	2.01	0.42
1:A:349:TRP:HB3	20:A:806:CLA:HAC1	2.02	0.42
1:A:423:TYR:CE1	4:D:105:ILE:HG13	2.54	0.42
20:A:833:CLA:HMB1	20:A:843:CLA:HAA2	2.01	0.42
27:3:608:CHL:HMB2	23:3:718:BCR:HC7	2.01	0.42
20:8:601:CLA:HBA1	20:8:601:CLA:H3A	1.78	0.42
1:A:294:THR:HG23	20:A:820:CLA:HMA3	2.01	0.42
20:B:802:CLA:H122	20:B:802:CLA:H161	1.88	0.42
20:B:823:CLA:H61	20:B:823:CLA:H41	1.70	0.42
4:D:62:THR:HB	4:D:112:LEU:HD22	2.02	0.42
12:1:188:PHE:CD2	28:1:618:LUT:H12	2.55	0.42
20:3:609:CLA:HBA2	20:3:609:CLA:H3A	1.80	0.42
28:3:622:LUT:H15	28:3:622:LUT:H201	1.87	0.42
1:A:338:HIS:HE1	22:A:847:LHG:HC11	1.84	0.42
1:A:598:TRP:HE1	20:B:803:CLA:C1D	2.33	0.42
20:A:806:CLA:HBA1	20:A:806:CLA:H3A	1.78	0.42
20:A:816:CLA:H62	20:A:816:CLA:H41	1.67	0.42
2:B:532:THR:HG21	20:B:838:CLA:HMB3	2.02	0.42
20:B:838:CLA:HHC	20:B:838:CLA:HBB1	2.01	0.42
12:1:194:GLN:NE2	12:1:198:THR:OG1	2.53	0.42
14:7:82:GLY:HA2	20:7:604:CLA:HAB	2.02	0.42
1:A:428:ASP:O	1:A:432:ARG:HB2	2.19	0.42
2:B:350:ALA:HB3	2:B:377:GLN:HE21	1.85	0.42
12:1:55:GLY:H	12:1:175:LEU:HD23	1.85	0.42
20:6:611:CLA:HBC3	22:6:619:LHG:HC62	2.02	0.42
20:A:834:CLA:H72	20:A:834:CLA:H111	1.91	0.41
20:A:840:CLA:H72	23:A:851:BCR:H373	2.02	0.41
23:A:849:BCR:H24C	23:A:849:BCR:H371	1.85	0.41
2:B:157:HIS:HE1	20:B:811:CLA:NA	2.17	0.41
2:B:358:PRO:HG3	20:B:818:CLA:HBA1	2.02	0.41
20:B:813:CLA:H92	20:B:824:CLA:H42	2.02	0.41
20:B:836:CLA:H41	20:B:836:CLA:H62	1.70	0.41
6:F:133:LEU:HD22	6:F:148:GLU:HB2	2.02	0.41
23:G:205:BCR:H11C	23:G:205:BCR:H341	1.91	0.41
13:3:201:PHE:HA	17:5:39:VAL:HG22	2.02	0.41
20:3:610:CLA:H72	20:3:610:CLA:H112	1.88	0.41
18:6:125:GLU:HG3	20:6:609:CLA:C4B	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:GLU:OE2	1:A:71:ARG:NH2	2.53	0.41
1:A:389:SER:HB3	20:A:829:CLA:HMA1	2.01	0.41
20:B:813:CLA:H112	20:B:813:CLA:H151	1.81	0.41
20:B:835:CLA:H3A	20:B:835:CLA:HBA2	1.70	0.41
20:1:613:CLA:H2	20:1:614:CLA:OBD	2.19	0.41
15:8:143:LYS:HB2	15:8:146:SER:HB2	2.01	0.41
20:A:841:CLA:H62	20:A:841:CLA:H102	1.92	0.41
23:A:850:BCR:H11C	23:A:850:BCR:H341	1.84	0.41
20:B:813:CLA:H43	23:B:844:BCR:H19C	2.02	0.41
20:B:825:CLA:H42	20:B:837:CLA:HBA1	2.02	0.41
20:B:834:CLA:H161	20:B:834:CLA:H122	1.73	0.41
6:F:137:PRO:HG3	23:F:305:BCR:H281	2.03	0.41
20:1:610:CLA:CBB	28:1:617:LUT:H32	2.49	0.41
20:1:614:CLA:H142	20:1:614:CLA:H112	1.87	0.41
12:Z:154:PRO:HB3	20:Z:608:CLA:HBC2	2.01	0.41
1:A:474:ASP:O	1:A:478:GLN:NE2	2.54	0.41
20:A:806:CLA:H152	20:A:806:CLA:H112	1.79	0.41
20:A:831:CLA:H61	20:A:831:CLA:H41	1.65	0.41
2:B:345:ILE:HG23	20:B:818:CLA:H61	2.02	0.41
20:B:841:CLA:HBA1	22:B:851:LHG:HC62	2.01	0.41
4:D:151:HIS:HA	4:D:152:PRO:HA	1.88	0.41
20:1:614:CLA:HBC1	28:1:617:LUT:H162	2.02	0.41
23:8:619:BCR:H15C	23:8:619:BCR:H351	1.81	0.41
20:B:807:CLA:H91	20:B:807:CLA:H112	1.91	0.41
20:B:840:CLA:HHD	20:B:840:CLA:HAC1	1.91	0.41
23:B:848:BCR:H15C	23:B:848:BCR:H351	1.86	0.41
13:3:73:LEU:HG	20:3:602:CLA:HAA2	2.02	0.41
14:7:82:GLY:O	14:7:86:ILE:HG12	2.20	0.41
12:Z:84:TRP:CE2	20:Z:608:CLA:HED2	2.56	0.41
16:4:130:ALA:HB1	16:4:132:VAL:HG23	2.01	0.41
20:5:602:CLA:CBB	28:5:624:LUT:H32	2.50	0.41
6:F:123:LEU:HD13	6:F:131:PRO:HB3	2.03	0.41
28:1:619:LUT:H401	28:1:619:LUT:H35	1.82	0.41
23:3:719:BCR:H11C	23:3:719:BCR:H341	1.97	0.41
23:3:719:BCR:H20C	23:3:719:BCR:H361	1.87	0.41
20:8:613:CLA:H91	20:8:613:CLA:H111	1.90	0.41
28:8:617:LUT:H15	28:8:617:LUT:H201	1.92	0.41
20:4:601:CLA:H142	20:4:601:CLA:H111	1.80	0.41
28:5:620:LUT:H15	28:5:620:LUT:H201	1.90	0.41
20:B:824:CLA:H143	20:B:824:CLA:H161	1.96	0.41
20:B:830:CLA:HMC2	20:B:841:CLA:H143	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:3:89:TYR:HD1	13:3:191:ALA:HB2	1.85	0.41
28:7:622:LUT:H15	28:7:622:LUT:H201	1.86	0.41
15:8:83:GLY:O	15:8:87:ILE:HG12	2.21	0.41
20:Z:611:CLA:H203	20:Z:611:CLA:H161	1.89	0.41
18:6:221:ALA:HB2	18:6:231:PRO:HD3	2.03	0.41
20:6:610:CLA:H52	28:6:621:LUT:H30	2.02	0.41
1:A:711:PRO:HA	6:F:171:LEU:HD11	2.02	0.41
20:A:808:CLA:HMB3	20:A:809:CLA:HHB	2.03	0.41
20:A:843:CLA:H13	20:A:843:CLA:H101	1.90	0.41
2:B:326:THR:HG21	2:B:404:ASN:HD21	1.85	0.41
4:D:66:ILE:HB	4:D:105:ILE:HB	2.03	0.41
13:3:177:PHE:CE2	27:3:608:CHL:HBB2	2.56	0.41
28:3:622:LUT:H35	28:3:622:LUT:H401	1.97	0.41
18:6:164:PHE:O	28:6:621:LUT:O23	2.33	0.41
27:6:606:CHL:H51	27:6:608:CHL:HMB2	2.02	0.41
1:A:220:VAL:HG13	1:A:240:PRO:HB3	2.02	0.41
1:A:397:ILE:HG23	20:A:807:CLA:H143	2.03	0.41
1:A:684:MET:HB2	20:A:802:CLA:C1C	2.50	0.41
20:A:818:CLA:H41	20:A:818:CLA:H62	1.61	0.41
23:A:851:BCR:H24C	23:A:851:BCR:H371	1.90	0.41
23:A:856:BCR:H361	23:A:856:BCR:H20C	1.84	0.41
2:B:54:GLN:HB2	20:B:805:CLA:HMB2	2.02	0.41
2:B:601:THR:HG21	2:B:610:PHE:HB2	2.02	0.41
20:B:828:CLA:HBA2	20:B:828:CLA:H3A	1.67	0.41
20:B:839:CLA:H193	23:I:172:BCR:H362	2.02	0.41
6:F:139:LEU:HD13	20:F:304:CLA:HED3	2.03	0.41
7:G:52:VAL:HG11	12:1:140:ALA:HA	2.02	0.41
12:1:57:TYR:HB2	20:1:602:CLA:HMD1	2.03	0.41
28:1:617:LUT:H15	28:1:617:LUT:H201	1.97	0.41
20:3:604:CLA:C4B	23:3:717:BCR:H281	2.34	0.41
20:7:610:CLA:CBB	28:7:621:LUT:H32	2.50	0.41
20:5:602:CLA:H122	28:5:624:LUT:H371	2.03	0.41
18:6:216:THR:H	18:6:219:SER:HB2	1.85	0.41
20:6:604:CLA:H122	23:6:623:BCR:H403	2.03	0.41
1:A:543:ILE:HG12	20:A:827:CLA:HBC2	2.02	0.41
20:A:829:CLA:O1D	20:A:830:CLA:HHB	2.21	0.41
23:A:851:BCR:H11C	23:A:851:BCR:H341	1.85	0.41
20:1:612:CLA:H51	20:1:612:CLA:H11	1.81	0.41
28:1:618:LUT:H35	28:1:618:LUT:H401	1.93	0.41
13:3:110:VAL:HG21	23:3:718:BCR:H272	2.03	0.41
20:4:612:CLA:H52	20:4:612:CLA:H11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:5:622:BCR:H11C	23:5:622:BCR:H341	1.97	0.41
20:6:613:CLA:H52	22:6:619:LHG:H202	2.03	0.41
1:A:392:THR:HG22	20:A:829:CLA:HAB	2.04	0.40
20:A:842:CLA:H61	20:A:842:CLA:H102	1.51	0.40
16:4:232:GLN:HG2	20:4:613:CLA:ND	2.37	0.40
17:5:53:TYR:HB2	20:5:602:CLA:HMD1	2.02	0.40
27:5:608:CHL:HBB2	27:5:618:CHL:CHC	2.52	0.40
20:A:814:CLA:H41	20:A:814:CLA:H61	1.66	0.40
20:B:816:CLA:CHD	20:B:817:CLA:HBB2	2.51	0.40
11:L:101:ILE:HG12	11:L:114:GLU:HA	2.03	0.40
20:1:609:CLA:H143	20:1:609:CLA:H161	1.88	0.40
23:7:623:BCR:H342	20:8:614:CLA:H62	2.03	0.40
15:8:88:LEU:HD11	28:8:617:LUT:H10	2.02	0.40
15:8:203:PHE:CD2	28:8:618:LUT:H12	2.57	0.40
15:8:223:ALA:HB1	15:8:231:VAL:HG11	2.03	0.40
20:A:809:CLA:H3A	20:A:809:CLA:HBA2	1.63	0.40
20:B:805:CLA:H72	20:B:805:CLA:H111	1.90	0.40
22:B:851:LHG:O2	12:1:67:GLU:OE1	2.39	0.40
3:C:25:VAL:HG23	3:C:26:LEU:HG	2.04	0.40
13:3:230:GLY:O	13:3:234:GLN:HB2	2.22	0.40
15:8:132:PHE:CE2	23:8:619:BCR:H10C	2.57	0.40
20:4:602:CLA:H142	20:4:602:CLA:H111	1.96	0.40
20:4:602:CLA:H71	20:4:603:CLA:HMA1	2.03	0.40
23:4:621:BCR:H15C	23:4:621:BCR:H351	1.86	0.40
17:5:55:TRP:CZ2	20:5:601:CLA:HBA1	2.56	0.40
1:A:397:ILE:HG21	20:A:830:CLA:HHC	2.02	0.40
1:A:467:ARG:HH22	11:L:105:PRO:HB3	1.85	0.40
20:A:831:CLA:H13	22:A:846:LHG:H211	2.04	0.40
23:A:850:BCR:H20C	23:A:850:BCR:H361	1.85	0.40
23:I:172:BCR:H11C	23:I:172:BCR:H341	1.97	0.40
23:3:719:BCR:H15C	23:3:719:BCR:H351	1.87	0.40
15:8:233:TYR:CD1	20:8:613:CLA:H12	2.56	0.40
16:4:111:VAL:HG11	28:4:619:LUT:H10	2.04	0.40
17:5:124:TRP:CE2	20:6:614:CLA:H3A	2.57	0.40
20:5:606:CLA:HBA2	23:5:622:BCR:H19C	2.02	0.40
27:5:607:CHL:HBB2	20:5:609:CLA:HAC2	2.04	0.40
23:5:622:BCR:H15C	23:5:622:BCR:H351	1.87	0.40
18:6:192:MET:HG3	20:6:613:CLA:HAC2	2.03	0.40
27:6:606:CHL:HMB2	23:6:623:BCR:H373	2.03	0.40
1:A:329:HIS:HA	20:A:845:CLA:HBC2	2.04	0.40
20:A:810:CLA:H61	20:A:810:CLA:H41	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:457:GLU:HA	2:B:458:PRO:HD3	1.95	0.40
20:B:825:CLA:H71	20:B:836:CLA:H62	2.03	0.40
20:B:837:CLA:H102	20:B:837:CLA:H62	1.77	0.40
23:K:4004:BCR:H361	23:K:4004:BCR:H20C	1.87	0.40
12:1:64:LEU:HD13	20:1:602:CLA:H42	2.04	0.40
20:3:606:CLA:HMB1	20:3:609:CLA:HBC2	2.04	0.40
14:7:130:TRP:CD1	23:7:623:BCR:H12C	2.57	0.40
15:8:156:PHE:HZ	15:8:172:PRO:CB	2.34	0.40
17:5:55:TRP:HZ2	20:5:601:CLA:H12	1.86	0.40
20:5:610:CLA:H112	20:5:610:CLA:H91	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	734/751 (98%)	712 (97%)	21 (3%)	1 (0%)	51	82
2	B	730/755 (97%)	706 (97%)	24 (3%)	0	100	100
3	C	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
4	D	142/161 (88%)	134 (94%)	8 (6%)	0	100	100
5	E	59/73 (81%)	54 (92%)	5 (8%)	0	100	100
6	F	163/165 (99%)	158 (97%)	5 (3%)	0	100	100
7	G	64/94 (68%)	63 (98%)	1 (2%)	0	100	100
8	I	35/106 (33%)	34 (97%)	1 (3%)	0	100	100
9	J	37/41 (90%)	35 (95%)	2 (5%)	0	100	100
10	K	41/87 (47%)	41 (100%)	0	0	100	100
11	L	114/156 (73%)	110 (96%)	4 (4%)	0	100	100
12	1	192/194 (99%)	186 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	Z	188/194 (97%)	180 (96%)	8 (4%)	0	100	100
13	3	200/268 (75%)	194 (97%)	6 (3%)	0	100	100
14	7	210/215 (98%)	198 (94%)	12 (6%)	0	100	100
15	8	215/217 (99%)	206 (96%)	9 (4%)	0	100	100
16	4	199/236 (84%)	184 (92%)	14 (7%)	1 (0%)	29	61
17	5	219/229 (96%)	201 (92%)	18 (8%)	0	100	100
18	6	227/232 (98%)	215 (95%)	12 (5%)	0	100	100
All	All	3847/4255 (90%)	3684 (96%)	161 (4%)	2 (0%)	54	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	VAL
16	4	207	ASP

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	A	599/610 (98%)	592 (99%)	7 (1%)	71	91
2	B	596/617 (97%)	595 (100%)	1 (0%)	93	98
3	C	69/70 (99%)	69 (100%)	0	100	100
4	D	121/129 (94%)	120 (99%)	1 (1%)	81	94
5	E	52/62 (84%)	52 (100%)	0	100	100
6	F	127/127 (100%)	126 (99%)	1 (1%)	81	94
7	G	48/69 (70%)	47 (98%)	1 (2%)	53	81
8	I	31/76 (41%)	31 (100%)	0	100	100
9	J	35/37 (95%)	35 (100%)	0	100	100
10	K	30/60 (50%)	29 (97%)	1 (3%)	38	72
11	L	85/119 (71%)	85 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	1	137/137 (100%)	136 (99%)	1 (1%)	84	95
12	Z	137/137 (100%)	137 (100%)	0	100	100
13	3	155/209 (74%)	154 (99%)	1 (1%)	86	96
14	7	164/164 (100%)	163 (99%)	1 (1%)	86	96
15	8	163/163 (100%)	160 (98%)	3 (2%)	59	85
16	4	159/185 (86%)	158 (99%)	1 (1%)	86	96
17	5	181/184 (98%)	178 (98%)	3 (2%)	60	86
18	6	183/185 (99%)	182 (100%)	1 (0%)	88	96
All	All	3072/3340 (92%)	3049 (99%)	23 (1%)	84	95

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	A	205	LEU
1	A	206	LEU
1	A	286	THR
1	A	372	TYR
1	A	584	CYS
1	A	657	VAL
2	B	479	LEU
4	D	59	ASN
6	F	168	ARG
7	G	118	ASN
10	K	35	ASN
12	1	221	ASN
13	3	160	LEU
14	7	177	ARG
15	8	51	ASN
15	8	153	PHE
15	8	156	PHE
16	4	263	ARG
17	5	117	ASN
17	5	202	LEU
17	5	226	ASN
18	6	60	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	ASN
2	B	276	HIS
3	C	38	GLN
4	D	59	ASN
4	D	127	GLN
7	G	118	ASN
12	1	194	GLN
12	1	221	ASN
13	3	245	ASN
14	7	207	GLN
15	8	51	ASN
15	8	126	GLN
12	Z	180	ASN
12	Z	221	ASN
17	5	142	ASN
17	5	147	ASN
17	5	226	ASN
18	6	227	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

285 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	LHG	8	620	20	36,36,48	1.03	2 (5%)	39,42,54	1.13	2 (5%)
20	CLA	5	612	-	52,60,73	2.30	18 (34%)	60,97,113	3.01	26 (43%)
23	BCR	8	619	-	41,41,41	0.68	0	56,56,56	1.83	13 (23%)
20	CLA	B	811	-	54,62,73	2.13	16 (29%)	67,100,113	3.04	29 (43%)
20	CLA	F	304	6	65,73,73	2.02	17 (26%)	76,113,113	2.79	28 (36%)
20	CLA	K	4003	-	46,54,73	2.44	15 (32%)	53,90,113	3.15	23 (43%)
20	CLA	B	837	-	65,73,73	2.01	16 (24%)	76,113,113	2.75	30 (39%)
20	CLA	1	608	-	65,73,73	2.04	17 (26%)	76,113,113	2.65	27 (35%)
20	CLA	3	620	-	56,64,73	2.19	17 (30%)	65,102,113	2.86	25 (38%)
20	CLA	Z	613	-	65,73,73	2.05	17 (26%)	76,113,113	2.59	25 (32%)
20	CLA	A	829	-	65,73,73	1.98	16 (24%)	76,113,113	2.74	29 (38%)
20	CLA	A	806	-	65,73,73	1.99	15 (23%)	76,113,113	2.70	25 (32%)
20	CLA	5	603	-	46,54,73	2.40	17 (36%)	53,90,113	3.14	25 (47%)
20	CLA	5	604	17	50,58,73	2.32	15 (30%)	58,95,113	3.05	26 (44%)
21	PQN	A	844	-	34,34,34	1.57	2 (5%)	42,45,45	1.09	3 (7%)
20	CLA	B	813	-	65,73,73	2.01	17 (26%)	76,113,113	2.70	27 (35%)
20	CLA	5	602	17	65,73,73	2.01	15 (23%)	76,113,113	2.76	28 (36%)
20	CLA	B	802	-	65,73,73	1.95	17 (26%)	76,113,113	2.84	27 (35%)
23	BCR	B	801	-	41,41,41	0.73	0	56,56,56	1.93	16 (28%)
27	CHL	5	607	-	51,59,74	2.28	17 (33%)	55,96,114	3.33	30 (54%)
20	CLA	B	841	22	65,73,73	2.03	16 (24%)	76,113,113	2.72	28 (36%)
20	CLA	7	606	-	42,50,73	2.43	16 (38%)	48,85,113	3.43	24 (50%)
28	LUT	6	621	-	42,43,43	0.70	0	51,60,60	1.51	11 (21%)
20	CLA	6	616	18	46,54,73	2.46	16 (34%)	53,90,113	3.13	26 (49%)
23	BCR	A	851	-	41,41,41	0.80	1 (2%)	56,56,56	1.85	13 (23%)
20	CLA	7	612	14	52,60,73	2.25	16 (30%)	60,97,113	3.15	27 (45%)
27	CHL	3	608	-	66,74,74	1.91	16 (24%)	73,114,114	2.92	25 (34%)
26	LMG	J	3001	-	35,35,55	0.96	0	43,43,63	1.23	6 (13%)
20	CLA	8	610	15	60,68,73	2.09	14 (23%)	70,107,113	2.91	31 (44%)
20	CLA	4	613	16	56,64,73	2.20	16 (28%)	65,102,113	2.90	28 (43%)
20	CLA	G	204	7	46,54,73	2.46	16 (34%)	53,90,113	3.15	25 (47%)
20	CLA	B	814	-	60,68,73	2.09	16 (26%)	70,107,113	2.81	28 (40%)
20	CLA	4	616	16	41,49,73	2.55	16 (39%)	47,84,113	3.48	25 (53%)
20	CLA	6	604	-	65,73,73	2.05	17 (26%)	76,113,113	2.64	27 (35%)
20	CLA	B	839	-	65,73,73	2.04	17 (26%)	76,113,113	2.67	26 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	LHG	1	620	20	42,42,48	0.99	2 (4%)	45,48,54	1.08	3 (6%)
20	CLA	8	612	15	52,60,73	2.25	17 (32%)	60,97,113	3.03	30 (50%)
28	LUT	3	622	-	42,43,43	0.79	0	51,60,60	1.71	14 (27%)
20	CLA	A	810	1	65,73,73	1.99	18 (27%)	76,113,113	2.66	27 (35%)
20	CLA	Z	610	12	60,68,73	2.10	15 (25%)	70,107,113	2.88	29 (41%)
20	CLA	A	805	20	55,63,73	2.16	15 (27%)	64,101,113	2.91	26 (40%)
20	CLA	4	614	-	45,53,73	2.44	16 (35%)	52,89,113	3.14	25 (48%)
23	BCR	K	4001	-	41,41,41	0.69	0	56,56,56	2.00	15 (26%)
20	CLA	B	817	-	59,67,73	2.11	16 (27%)	68,105,113	2.84	26 (38%)
20	CLA	8	604	-	46,54,73	2.43	16 (34%)	53,90,113	3.10	25 (47%)
20	CLA	4	612	16	52,60,73	2.26	17 (32%)	60,97,113	3.05	27 (45%)
20	CLA	5	611	22	55,63,73	2.23	18 (32%)	64,101,113	2.87	27 (42%)
23	BCR	B	845	-	41,41,41	0.71	0	56,56,56	1.85	13 (23%)
23	BCR	B	846	-	41,41,41	0.78	0	56,56,56	1.87	15 (26%)
23	BCR	B	843	-	41,41,41	0.71	0	56,56,56	1.59	9 (16%)
20	CLA	B	834	-	65,73,73	2.07	18 (27%)	76,113,113	2.68	28 (36%)
20	CLA	B	804	-	45,53,73	2.43	16 (35%)	52,89,113	3.30	27 (51%)
23	BCR	I	172	-	41,41,41	0.66	0	56,56,56	2.08	15 (26%)
28	LUT	7	622	-	42,43,43	0.74	0	51,60,60	1.58	10 (19%)
20	CLA	8	608	-	50,58,73	2.27	16 (32%)	58,95,113	3.10	26 (44%)
20	CLA	B	832	-	65,73,73	1.98	15 (23%)	76,113,113	2.76	26 (34%)
20	CLA	B	807	-	65,73,73	2.05	16 (24%)	76,113,113	2.74	27 (35%)
20	CLA	L	204	-	50,58,73	2.36	16 (32%)	58,95,113	3.09	25 (43%)
23	BCR	J	3003	-	41,41,41	0.72	0	56,56,56	1.73	12 (21%)
23	BCR	F	305	-	41,41,41	0.70	0	56,56,56	1.92	17 (30%)
20	CLA	7	610	14	60,68,73	2.09	15 (25%)	70,107,113	2.90	29 (41%)
20	CLA	A	838	-	51,59,73	2.30	16 (31%)	59,96,113	3.08	29 (49%)
20	CLA	L	203	-	65,73,73	2.01	16 (24%)	76,113,113	2.73	26 (34%)
27	CHL	4	607	-	51,59,74	2.28	16 (31%)	55,96,114	3.32	24 (43%)
23	BCR	B	847	-	41,41,41	0.77	0	56,56,56	1.92	14 (25%)
20	CLA	A	814	-	65,73,73	1.99	17 (26%)	76,113,113	2.78	27 (35%)
20	CLA	A	831	-	65,73,73	2.00	15 (23%)	76,113,113	2.77	27 (35%)
20	CLA	7	614	-	43,51,73	2.40	15 (34%)	49,86,113	3.33	26 (53%)
20	CLA	8	601	15	65,73,73	2.02	18 (27%)	76,113,113	2.67	28 (36%)
22	LHG	6	619	20	48,48,48	0.93	2 (4%)	51,54,54	1.04	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	1	604	-	57,65,73	2.20	16 (28%)	66,103,113	2.85	30 (45%)
20	CLA	A	821	-	45,53,73	2.43	16 (35%)	52,89,113	3.15	25 (48%)
22	LHG	B	851	20	22,22,48	1.15	2 (9%)	25,28,54	1.24	2 (8%)
20	CLA	6	602	18	65,73,73	2.03	16 (24%)	76,113,113	2.71	27 (35%)
23	BCR	3	717	-	41,41,41	0.73	0	56,56,56	1.82	14 (25%)
28	LUT	Z	618	-	42,43,43	0.75	0	51,60,60	1.59	14 (27%)
23	BCR	L	201	-	41,41,41	0.71	0	56,56,56	1.72	10 (17%)
23	BCR	5	625	-	41,41,41	0.69	0	56,56,56	2.33	20 (35%)
20	CLA	3	614	-	45,53,73	2.48	16 (35%)	52,89,113	3.25	25 (48%)
28	LUT	4	619	-	42,43,43	0.73	0	51,60,60	1.61	13 (25%)
27	CHL	8	607	-	56,64,74	2.15	18 (32%)	61,102,114	3.07	25 (40%)
20	CLA	5	601	17	65,73,73	2.06	17 (26%)	76,113,113	2.69	27 (35%)
20	CLA	5	617	-	46,54,73	2.33	17 (36%)	53,90,113	3.26	23 (43%)
20	CLA	3	607	13	60,68,73	2.14	16 (26%)	70,107,113	2.84	27 (38%)
20	CLA	5	614	-	45,53,73	2.47	16 (35%)	52,89,113	3.19	25 (48%)
23	BCR	A	856	-	41,41,41	0.78	0	56,56,56	1.88	14 (25%)
20	CLA	A	842	-	65,73,73	1.99	17 (26%)	76,113,113	2.82	28 (36%)
20	CLA	B	821	-	46,54,73	2.41	16 (34%)	53,90,113	3.19	23 (43%)
20	CLA	A	815	-	60,68,73	2.14	16 (26%)	70,107,113	2.80	27 (38%)
20	CLA	B	835	-	45,53,73	2.47	17 (37%)	52,89,113	3.07	25 (48%)
20	CLA	3	606	-	42,50,73	2.47	15 (35%)	48,85,113	3.28	23 (47%)
20	CLA	4	611	22	55,63,73	2.25	17 (30%)	64,101,113	2.80	27 (42%)
20	CLA	A	840	-	65,73,73	2.00	17 (26%)	76,113,113	2.84	28 (36%)
20	CLA	B	810	-	65,73,73	2.05	17 (26%)	76,113,113	2.73	27 (35%)
27	CHL	6	618	18	43,51,74	2.38	16 (37%)	45,86,114	3.59	23 (51%)
20	CLA	3	617	13	46,54,73	2.41	17 (36%)	53,90,113	3.18	25 (47%)
27	CHL	Z	601	12	53,61,74	2.25	18 (33%)	57,98,114	3.23	26 (45%)
27	CHL	1	607	-	48,56,74	2.37	19 (39%)	51,92,114	3.07	20 (39%)
20	CLA	A	826	-	65,73,73	1.97	16 (24%)	76,113,113	2.66	24 (31%)
23	BCR	7	623	-	41,41,41	0.70	0	56,56,56	1.99	15 (26%)
20	CLA	7	604	-	56,64,73	2.16	17 (30%)	65,102,113	2.97	26 (40%)
20	CLA	B	820	-	56,64,73	2.19	17 (30%)	65,102,113	2.91	28 (43%)
20	CLA	8	613	15	65,73,73	2.00	15 (23%)	76,113,113	2.68	27 (35%)
20	CLA	F	301	-	65,73,73	2.03	17 (26%)	76,113,113	2.74	28 (36%)
20	CLA	1	616	12	46,54,73	2.43	17 (36%)	53,90,113	3.01	25 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	A	833	-	65,73,73	2.01	16 (24%)	76,113,113	2.74	27 (35%)
20	CLA	5	621	-	46,54,73	2.40	17 (36%)	53,90,113	3.08	26 (49%)
23	BCR	K	4004	-	41,41,41	0.70	0	56,56,56	1.64	10 (17%)
20	CLA	5	609	17	50,58,73	2.31	17 (34%)	58,95,113	3.12	27 (46%)
20	CLA	A	845	22	52,60,73	2.30	17 (32%)	60,97,113	3.07	24 (40%)
27	CHL	7	607	-	54,62,74	2.20	17 (31%)	58,99,114	3.01	23 (39%)
20	CLA	B	831	-	49,57,73	2.33	16 (32%)	55,93,113	3.19	24 (43%)
28	LUT	7	621	-	42,43,43	0.74	0	51,60,60	1.55	11 (21%)
28	LUT	5	620	-	42,43,43	0.76	0	51,60,60	1.69	13 (25%)
20	CLA	G	203	-	50,58,73	2.34	16 (32%)	58,95,113	3.13	27 (46%)
20	CLA	F	303	-	45,53,73	2.44	18 (40%)	52,89,113	3.20	23 (44%)
20	CLA	3	610	13	65,73,73	2.01	14 (21%)	76,113,113	2.78	29 (38%)
20	CLA	7	608	-	50,58,73	2.29	16 (32%)	58,95,113	3.07	25 (43%)
21	PQN	B	842	-	34,34,34	1.55	2 (5%)	42,45,45	1.05	2 (4%)
20	CLA	3	611	-	41,49,73	2.56	16 (39%)	47,84,113	3.33	25 (53%)
22	LHG	4	623	-	31,31,48	1.15	2 (6%)	34,37,54	1.14	3 (8%)
27	CHL	6	606	-	56,64,74	2.13	16 (28%)	61,102,114	3.16	24 (39%)
28	LUT	3	621	-	42,43,43	0.77	0	51,60,60	1.61	12 (23%)
20	CLA	A	822	-	65,73,73	2.00	16 (24%)	76,113,113	2.56	27 (35%)
20	CLA	A	827	-	65,73,73	2.03	15 (23%)	76,113,113	2.74	27 (35%)
20	CLA	Z	616	12	46,54,73	2.44	17 (36%)	53,90,113	3.04	24 (45%)
27	CHL	6	608	-	51,59,74	2.22	17 (33%)	55,96,114	3.50	25 (45%)
20	CLA	A	818	-	65,73,73	2.00	15 (23%)	76,113,113	2.88	28 (36%)
20	CLA	B	805	-	65,73,73	2.04	17 (26%)	76,113,113	2.76	25 (32%)
23	BCR	L	205	-	41,41,41	0.71	0	56,56,56	1.69	11 (19%)
20	CLA	B	816	-	55,63,73	2.18	16 (29%)	64,101,113	2.97	26 (40%)
20	CLA	J	3002	9	42,50,73	2.45	15 (35%)	48,85,113	3.34	24 (50%)
28	LUT	Z	617	-	42,43,43	0.77	0	51,60,60	1.61	14 (27%)
20	CLA	7	613	14	65,73,73	2.00	18 (27%)	76,113,113	2.64	25 (32%)
28	LUT	Z	619	-	42,43,43	0.72	0	51,60,60	1.71	11 (21%)
20	CLA	5	610	17	60,68,73	2.11	15 (25%)	70,107,113	2.85	29 (41%)
22	LHG	5	623	20	36,36,48	1.06	2 (5%)	39,42,54	1.12	2 (5%)
20	CLA	3	612	13	46,54,73	2.41	17 (36%)	53,90,113	3.22	26 (49%)
27	CHL	6	607	-	56,64,74	2.12	16 (28%)	61,102,114	3.10	27 (44%)
20	CLA	6	617	-	46,54,73	2.42	18 (39%)	53,90,113	3.15	25 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CHL	5	618	17	43,51,74	2.39	16 (37%)	45,86,114	3.63	23 (51%)
20	CLA	A	837	1	45,53,73	2.48	17 (37%)	52,89,113	3.16	25 (48%)
20	CLA	A	823	-	49,57,73	2.33	17 (34%)	55,93,113	3.14	23 (41%)
20	CLA	B	836	-	60,68,73	2.14	18 (30%)	70,107,113	2.93	29 (41%)
20	CLA	A	843	-	65,73,73	2.01	16 (24%)	76,113,113	2.61	26 (34%)
28	LUT	8	618	-	42,43,43	0.76	0	51,60,60	1.68	13 (25%)
27	CHL	4	606	-	56,64,74	2.13	17 (30%)	61,102,114	3.05	23 (37%)
20	CLA	4	609	16	50,58,73	2.29	18 (36%)	58,95,113	3.16	28 (48%)
28	LUT	1	619	-	42,43,43	0.73	0	51,60,60	1.68	9 (17%)
20	CLA	A	813	-	54,62,73	2.23	16 (29%)	62,99,113	2.93	26 (41%)
20	CLA	8	609	15	46,54,73	2.39	16 (34%)	53,90,113	3.12	25 (47%)
20	CLA	Z	608	-	65,73,73	2.06	17 (26%)	76,113,113	2.64	27 (35%)
20	CLA	Z	603	-	57,65,73	2.18	17 (29%)	66,103,113	2.94	30 (45%)
20	CLA	4	601	16	61,69,73	2.09	16 (26%)	71,108,113	2.77	29 (40%)
23	BCR	3	719	-	41,41,41	0.71	0	56,56,56	1.75	12 (21%)
20	CLA	1	613	-	65,73,73	2.03	16 (24%)	76,113,113	2.62	26 (34%)
28	LUT	1	618	-	42,43,43	0.74	0	51,60,60	1.58	13 (25%)
20	CLA	6	611	22	55,63,73	2.24	18 (32%)	64,101,113	2.84	25 (39%)
20	CLA	6	614	-	45,53,73	2.45	17 (37%)	52,89,113	3.31	26 (50%)
24	SF4	A	853	1,2	0,12,12	-	-	-	-	-
20	CLA	A	811	-	65,73,73	2.00	17 (26%)	76,113,113	2.70	27 (35%)
20	CLA	1	602	12	65,73,73	2.03	16 (24%)	76,113,113	2.71	28 (36%)
22	LHG	4	622	20	48,48,48	0.97	2 (4%)	51,54,54	1.11	3 (5%)
20	CLA	A	828	-	65,73,73	1.96	17 (26%)	76,113,113	2.85	25 (32%)
20	CLA	6	610	18	60,68,73	2.16	16 (26%)	70,107,113	2.81	31 (44%)
23	BCR	B	844	-	41,41,41	0.69	0	56,56,56	1.72	12 (21%)
23	BCR	5	622	-	41,41,41	0.65	0	56,56,56	1.84	16 (28%)
20	CLA	1	609	12	65,73,73	2.05	17 (26%)	76,113,113	2.70	26 (34%)
23	BCR	3	718	-	41,41,41	0.72	0	56,56,56	1.92	16 (28%)
20	CLA	B	833	-	58,66,73	2.14	16 (27%)	67,104,113	2.97	30 (44%)
23	BCR	7	624	-	41,41,41	0.66	0	56,56,56	1.78	13 (23%)
27	CHL	5	608	-	51,59,74	2.20	16 (31%)	55,96,114	3.19	25 (45%)
20	CLA	B	808	-	65,73,73	1.99	18 (27%)	76,113,113	2.77	29 (38%)
20	CLA	A	854	-	65,73,73	1.98	14 (21%)	76,113,113	2.85	31 (40%)
20	CLA	B	818	-	60,68,73	2.08	17 (28%)	70,107,113	2.83	30 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	B	852	-	65,73,73	2.07	16 (24%)	76,113,113	2.62	27 (35%)
20	CLA	5	613	17	56,64,73	2.22	16 (28%)	65,102,113	2.77	26 (40%)
20	CLA	4	610	16	60,68,73	2.12	16 (26%)	70,107,113	2.82	29 (41%)
20	CLA	A	836	-	50,58,73	2.32	16 (32%)	58,95,113	3.03	29 (50%)
20	CLA	Z	611	22	65,73,73	2.07	16 (24%)	76,113,113	2.61	26 (34%)
20	CLA	A	817	-	57,65,73	2.16	17 (29%)	66,103,113	2.93	27 (40%)
20	CLA	B	803	-	65,73,73	2.00	17 (26%)	76,113,113	2.64	26 (34%)
20	CLA	K	4002	-	45,53,73	2.49	16 (35%)	52,89,113	3.20	25 (48%)
20	CLA	3	609	13	50,58,73	2.33	17 (34%)	58,95,113	3.02	29 (50%)
20	CLA	8	603	-	45,53,73	2.40	17 (37%)	52,89,113	3.29	24 (46%)
27	CHL	4	618	16	43,51,74	2.37	16 (37%)	45,86,114	3.61	22 (48%)
28	LUT	4	620	-	42,43,43	0.73	0	51,60,60	1.54	12 (23%)
20	CLA	A	804	-	65,73,73	1.98	17 (26%)	76,113,113	2.87	32 (42%)
23	BCR	4	621	-	41,41,41	0.68	0	56,56,56	1.77	13 (23%)
20	CLA	A	834	-	65,73,73	2.02	16 (24%)	76,113,113	2.79	29 (38%)
20	CLA	B	829	-	65,73,73	2.00	16 (24%)	76,113,113	2.81	30 (39%)
20	CLA	A	807	1	65,73,73	2.04	18 (27%)	76,113,113	2.77	28 (36%)
20	CLA	1	612	12	52,60,73	2.25	16 (30%)	60,97,113	3.08	29 (48%)
20	CLA	7	601	14	65,73,73	2.02	17 (26%)	76,113,113	2.75	26 (34%)
20	CLA	A	830	-	65,73,73	1.97	17 (26%)	76,113,113	2.63	25 (32%)
20	CLA	3	613	13	55,63,73	2.18	17 (30%)	64,101,113	2.88	26 (40%)
20	CLA	A	808	-	65,73,73	2.02	18 (27%)	76,113,113	2.80	28 (36%)
20	CLA	1	610	12	60,68,73	2.12	15 (25%)	70,107,113	2.90	31 (44%)
20	CLA	A	825	-	55,63,73	2.20	17 (30%)	64,101,113	2.86	25 (39%)
20	CLA	1	611	22	65,73,73	2.06	16 (24%)	76,113,113	2.64	28 (36%)
23	BCR	A	848	-	41,41,41	0.69	0	56,56,56	1.72	13 (23%)
23	BCR	6	625	-	41,41,41	0.66	0	56,56,56	1.99	14 (25%)
20	CLA	8	614	-	55,63,73	2.22	17 (30%)	64,101,113	2.91	29 (45%)
20	CLA	1	614	-	65,73,73	2.05	16 (24%)	76,113,113	2.71	26 (34%)
20	CLA	1	603	-	65,73,73	2.03	17 (26%)	76,113,113	2.74	27 (35%)
20	CLA	6	601	18	65,73,73	2.05	16 (24%)	76,113,113	2.68	28 (36%)
20	CLA	7	603	-	46,54,73	2.41	17 (36%)	53,90,113	3.25	24 (45%)
20	CLA	A	819	-	65,73,73	2.02	16 (24%)	76,113,113	2.70	27 (35%)
20	CLA	7	609	14	50,58,73	2.31	16 (32%)	58,95,113	3.20	30 (51%)
20	CLA	8	602	15	62,70,73	2.05	15 (24%)	72,109,113	2.83	27 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	BCR	A	850	-	41,41,41	0.72	0	56,56,56	1.90	10 (17%)
27	CHL	4	608	-	51,59,74	2.17	16 (31%)	55,96,114	3.22	25 (45%)
20	CLA	Z	614	-	65,73,73	2.06	16 (24%)	76,113,113	2.75	26 (34%)
20	CLA	4	603	16	46,54,73	2.37	16 (34%)	53,90,113	3.16	24 (45%)
20	CLA	3	603	-	65,73,73	1.99	17 (26%)	76,113,113	2.65	27 (35%)
22	LHG	A	847	20	37,37,48	1.05	2 (5%)	40,43,54	1.16	3 (7%)
20	CLA	B	838	-	47,55,73	2.32	17 (36%)	54,91,113	3.21	24 (44%)
25	DGD	B	850	-	67,67,67	0.80	2 (2%)	81,81,81	1.05	4 (4%)
20	CLA	1	606	-	52,60,73	2.29	17 (32%)	60,97,113	3.03	27 (45%)
28	LUT	5	624	-	42,43,43	0.77	0	51,60,60	1.55	13 (25%)
23	BCR	A	852	-	41,41,41	0.72	0	56,56,56	1.91	11 (19%)
20	CLA	A	824	-	51,59,73	2.29	18 (35%)	59,96,113	3.06	24 (40%)
22	LHG	Z	620	20	42,42,48	0.99	2 (4%)	45,48,54	1.12	4 (8%)
28	LUT	8	617	-	42,43,43	0.76	0	51,60,60	1.64	12 (23%)
28	LUT	6	624	-	42,43,43	0.72	0	51,60,60	1.50	12 (23%)
20	CLA	A	802	-	65,73,73	1.99	16 (24%)	76,113,113	2.67	30 (39%)
20	CLA	B	823	-	60,68,73	2.10	16 (26%)	70,107,113	2.71	28 (40%)
20	CLA	A	841	-	65,73,73	2.01	16 (24%)	76,113,113	2.76	29 (38%)
20	CLA	B	815	-	57,65,73	2.18	16 (28%)	66,103,113	2.94	26 (39%)
20	CLA	Z	606	-	52,60,73	2.30	17 (32%)	60,97,113	3.00	27 (45%)
27	CHL	1	601	12	53,61,74	2.20	18 (33%)	57,98,114	3.48	26 (45%)
20	CLA	A	839	-	65,73,73	2.01	17 (26%)	76,113,113	2.80	28 (36%)
20	CLA	4	602	16	60,68,73	2.12	17 (28%)	70,107,113	2.83	27 (38%)
20	CLA	B	840	-	65,73,73	2.06	16 (24%)	76,113,113	2.84	26 (34%)
20	CLA	8	616	15	46,54,73	2.41	18 (39%)	53,90,113	3.00	25 (47%)
20	CLA	5	606	-	55,63,73	2.24	17 (30%)	64,101,113	2.90	27 (42%)
20	CLA	6	612	18	52,60,73	2.25	17 (32%)	60,97,113	3.07	26 (43%)
20	CLA	B	806	2	65,73,73	1.98	15 (23%)	76,113,113	2.70	29 (38%)
20	CLA	B	809	2	65,73,73	1.98	16 (24%)	76,113,113	2.63	27 (35%)
20	CLA	6	613	-	56,64,73	2.20	17 (30%)	65,102,113	2.85	26 (40%)
20	CLA	B	826	-	65,73,73	2.00	17 (26%)	76,113,113	2.81	27 (35%)
20	CLA	8	611	22	46,54,73	2.43	17 (36%)	53,90,113	3.09	25 (47%)
20	CLA	Z	602	12	65,73,73	2.02	17 (26%)	76,113,113	2.72	27 (35%)
20	CLA	Z	609	12	65,73,73	2.04	16 (24%)	76,113,113	2.71	28 (36%)
23	BCR	B	848	-	41,41,41	0.71	0	56,56,56	1.58	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	SF4	C	101	3	0,12,12	-	-	-		
23	BCR	6	623	-	41,41,41	0.63	0	56,56,56	2.02	16 (28%)
20	CLA	7	620	-	60,68,73	2.16	16 (26%)	70,107,113	2.80	28 (40%)
20	CLA	6	609	18	50,58,73	2.34	17 (34%)	58,95,113	3.04	26 (44%)
22	LHG	7	625	20	36,36,48	1.03	2 (5%)	39,42,54	1.14	2 (5%)
23	BCR	A	849	-	41,41,41	0.75	0	56,56,56	1.74	14 (25%)
20	CLA	A	835	-	65,73,73	2.04	15 (23%)	76,113,113	2.77	24 (31%)
20	CLA	7	616	14	46,54,73	2.41	16 (34%)	53,90,113	3.05	24 (45%)
22	LHG	A	855	-	29,29,48	1.20	2 (6%)	32,35,54	1.19	3 (9%)
24	SF4	C	102	3	0,12,12	-	-	-		
20	CLA	Z	604	-	57,65,73	2.19	16 (28%)	66,103,113	2.83	28 (42%)
20	CLA	B	828	-	65,73,73	2.00	18 (27%)	76,113,113	2.61	25 (32%)
20	CLA	B	819	-	65,73,73	2.01	15 (23%)	76,113,113	2.59	26 (34%)
20	CLA	A	816	-	65,73,73	2.06	16 (24%)	76,113,113	2.70	27 (35%)
27	CHL	Z	607	-	48,56,74	2.36	17 (35%)	51,92,114	3.18	22 (43%)
28	LUT	1	617	-	42,43,43	0.75	0	51,60,60	1.57	12 (23%)
20	CLA	A	820	-	65,73,73	2.04	17 (26%)	76,113,113	2.79	26 (34%)
20	CLA	B	830	-	50,58,73	2.28	16 (32%)	58,95,113	3.12	28 (48%)
20	CLA	3	602	13	60,68,73	2.11	16 (26%)	70,107,113	2.86	30 (42%)
20	CLA	A	803	-	65,73,73	2.00	16 (24%)	76,113,113	2.85	29 (38%)
20	CLA	B	827	-	65,73,73	2.04	19 (29%)	76,113,113	2.74	27 (35%)
20	CLA	B	825	-	65,73,73	2.04	16 (24%)	76,113,113	2.62	26 (34%)
20	CLA	3	604	-	65,73,73	2.02	15 (23%)	76,113,113	2.65	24 (31%)
20	CLA	B	822	-	59,67,73	2.16	16 (27%)	68,105,113	2.85	27 (39%)
20	CLA	7	602	14	65,73,73	2.02	15 (23%)	76,113,113	2.75	29 (38%)
20	CLA	A	832	-	50,58,73	2.28	16 (32%)	58,95,113	2.98	28 (48%)
20	CLA	4	604	-	50,58,73	2.34	16 (32%)	58,95,113	3.02	27 (46%)
20	CLA	6	603	-	46,54,73	2.39	17 (36%)	53,90,113	3.20	25 (47%)
20	CLA	8	606	-	42,50,73	2.45	17 (40%)	48,85,113	3.26	22 (45%)
20	CLA	A	809	1	65,73,73	2.00	17 (26%)	76,113,113	2.79	27 (35%)
20	CLA	6	622	-	45,53,73	2.43	17 (37%)	52,89,113	3.20	25 (48%)
20	CLA	5	616	17	46,54,73	2.41	18 (39%)	53,90,113	3.11	26 (49%)
20	CLA	B	824	-	65,73,73	2.01	16 (24%)	76,113,113	2.68	30 (39%)
20	CLA	Z	612	-	52,60,73	2.29	17 (32%)	60,97,113	3.01	27 (45%)
20	CLA	B	812	-	65,73,73	2.04	18 (27%)	76,113,113	2.68	27 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	LHG	A	846	-	48,48,48	0.91	2 (4%)	51,54,54	1.03	3 (5%)
23	BCR	G	205	-	41,41,41	0.70	0	56,56,56	1.55	13 (23%)
20	CLA	7	611	22	41,49,73	2.50	18 (43%)	47,84,113	3.45	26 (55%)
19	CL0	A	801	-	65,73,73	1.95	16 (24%)	76,113,113	2.86	29 (38%)
20	CLA	A	812	20	65,73,73	2.00	16 (24%)	76,113,113	2.84	28 (36%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	LHG	8	620	20	-	12/41/41/53	-
20	CLA	5	612	-	1/1/12/20	3/22/100/115	-
23	BCR	8	619	-	-	8/29/63/63	0/2/2/2
20	CLA	B	811	-	1/1/13/20	7/25/101/115	-
20	CLA	F	304	6	1/1/15/20	8/37/115/115	-
20	CLA	K	4003	-	1/1/11/20	3/15/93/115	-
20	CLA	B	837	-	1/1/15/20	4/37/115/115	-
20	CLA	1	608	-	1/1/15/20	14/37/115/115	-
20	CLA	3	620	-	1/1/13/20	6/27/105/115	-
20	CLA	Z	613	-	1/1/15/20	11/37/115/115	-
20	CLA	A	829	-	1/1/15/20	22/37/115/115	-
20	CLA	A	806	-	1/1/15/20	17/37/115/115	-
20	CLA	5	603	-	1/1/11/20	4/15/93/115	-
20	CLA	5	604	17	-	2/19/97/115	-
21	PQN	A	844	-	-	7/23/43/43	0/2/2/2
20	CLA	B	813	-	1/1/15/20	13/37/115/115	-
20	CLA	5	602	17	-	11/37/115/115	-
20	CLA	B	802	-	1/1/15/20	14/37/115/115	-
27	CHL	5	607	-	3/3/17/26	8/21/119/137	-
23	BCR	B	801	-	-	6/29/63/63	0/2/2/2
20	CLA	B	841	22	1/1/15/20	8/37/115/115	-
20	CLA	7	606	-	1/1/10/20	7/10/88/115	-
28	LUT	6	621	-	-	4/29/67/67	0/2/2/2
20	CLA	6	616	18	1/1/11/20	4/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	A	851	-	-	4/29/63/63	0/2/2/2
20	CLA	7	612	14	1/1/12/20	5/22/100/115	-
27	CHL	3	608	-	3/3/20/26	17/39/137/137	-
26	LMG	J	3001	-	-	10/30/50/70	0/1/1/1
20	CLA	8	610	15	1/1/14/20	7/31/109/115	-
20	CLA	4	613	16	-	11/27/105/115	-
20	CLA	G	204	7	1/1/11/20	3/15/93/115	-
20	CLA	B	814	-	1/1/14/20	5/31/109/115	-
20	CLA	4	616	16	1/1/10/20	0/8/86/115	-
20	CLA	6	604	-	1/1/15/20	8/37/115/115	-
20	CLA	B	839	-	1/1/15/20	7/37/115/115	-
22	LHG	1	620	20	-	10/47/47/53	-
20	CLA	8	612	15	1/1/12/20	7/22/100/115	-
28	LUT	3	622	-	-	2/29/67/67	0/2/2/2
20	CLA	A	810	1	1/1/15/20	11/37/115/115	-
20	CLA	Z	610	12	1/1/14/20	12/31/109/115	-
20	CLA	A	805	20	1/1/13/20	7/25/103/115	-
20	CLA	4	614	-	1/1/11/20	2/13/91/115	-
23	BCR	K	4001	-	-	6/29/63/63	0/2/2/2
20	CLA	B	817	-	1/1/13/20	11/30/108/115	-
20	CLA	8	604	-	1/1/11/20	5/15/93/115	-
20	CLA	4	612	16	1/1/12/20	6/22/100/115	-
20	CLA	5	611	22	1/1/13/20	10/25/103/115	-
23	BCR	B	845	-	-	10/29/63/63	0/2/2/2
23	BCR	B	846	-	-	7/29/63/63	0/2/2/2
23	BCR	B	843	-	-	7/29/63/63	0/2/2/2
20	CLA	B	834	-	1/1/15/20	11/37/115/115	-
20	CLA	B	804	-	1/1/11/20	5/13/91/115	-
23	BCR	I	172	-	-	6/29/63/63	0/2/2/2
28	LUT	7	622	-	-	2/29/67/67	0/2/2/2
20	CLA	8	608	-	1/1/12/20	0/19/97/115	-
20	CLA	B	832	-	1/1/15/20	10/37/115/115	-
20	CLA	B	807	-	1/1/15/20	9/37/115/115	-
20	CLA	L	204	-	-	2/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	J	3003	-	-	8/29/63/63	0/2/2/2
20	CLA	7	610	14	1/1/14/20	5/31/109/115	-
20	CLA	A	838	-	1/1/12/20	2/21/99/115	-
20	CLA	L	203	-	-	11/37/115/115	-
27	CHL	4	607	-	3/3/17/26	10/21/119/137	-
23	BCR	B	847	-	-	9/29/63/63	0/2/2/2
20	CLA	A	814	-	1/1/15/20	17/37/115/115	-
20	CLA	A	831	-	1/1/15/20	14/37/115/115	-
20	CLA	7	614	-	1/1/10/20	2/11/89/115	-
20	CLA	8	601	15	1/1/15/20	13/37/115/115	-
22	LHG	6	619	20	-	17/53/53/53	-
20	CLA	1	604	-	1/1/13/20	8/28/106/115	-
20	CLA	A	821	-	1/1/11/20	3/13/91/115	-
22	LHG	B	851	20	-	10/26/26/53	-
20	CLA	6	602	18	1/1/15/20	15/37/115/115	-
23	BCR	3	717	-	-	8/29/63/63	0/2/2/2
28	LUT	Z	618	-	-	5/29/67/67	0/2/2/2
23	BCR	L	201	-	-	6/29/63/63	0/2/2/2
23	BCR	5	625	-	-	7/29/63/63	0/2/2/2
20	CLA	3	614	-	-	2/13/91/115	-
28	LUT	4	619	-	-	2/29/67/67	0/2/2/2
27	CHL	8	607	-	3/3/18/26	11/27/125/137	-
20	CLA	5	601	17	1/1/15/20	9/37/115/115	-
20	CLA	5	617	-	1/1/11/20	2/15/93/115	-
20	CLA	3	607	13	1/1/14/20	16/31/109/115	-
20	CLA	5	614	-	1/1/11/20	4/13/91/115	-
23	BCR	A	856	-	-	8/29/63/63	0/2/2/2
20	CLA	A	842	-	1/1/15/20	14/37/115/115	-
20	CLA	B	821	-	-	7/15/93/115	-
20	CLA	A	815	-	1/1/14/20	8/31/109/115	-
20	CLA	B	835	-	1/1/11/20	5/13/91/115	-
20	CLA	3	606	-	1/1/10/20	0/10/88/115	-
20	CLA	4	611	22	1/1/13/20	8/25/103/115	-
20	CLA	A	840	-	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	810	-	1/1/15/20	12/37/115/115	-
27	CHL	6	618	18	3/3/15/26	8/12/110/137	-
20	CLA	3	617	13	1/1/11/20	9/15/93/115	-
27	CHL	Z	601	12	3/3/17/26	10/24/122/137	-
27	CHL	1	607	-	3/3/16/26	7/18/116/137	-
20	CLA	A	826	-	1/1/15/20	16/37/115/115	-
23	BCR	7	623	-	-	8/29/63/63	0/2/2/2
20	CLA	7	604	-	1/1/13/20	6/27/105/115	-
20	CLA	B	820	-	1/1/13/20	8/27/105/115	-
20	CLA	8	613	15	1/1/15/20	12/37/115/115	-
20	CLA	B	830	-	-	4/19/97/115	-
20	CLA	F	301	-	1/1/15/20	10/37/115/115	-
20	CLA	1	616	12	1/1/11/20	2/15/93/115	-
20	CLA	A	833	-	1/1/15/20	8/37/115/115	-
20	CLA	5	621	-	1/1/11/20	3/15/93/115	-
23	BCR	K	4004	-	-	6/29/63/63	0/2/2/2
20	CLA	5	609	17	1/1/12/20	6/19/97/115	-
27	CHL	7	607	-	3/3/17/26	8/25/123/137	-
20	CLA	A	845	22	-	13/22/100/115	-
20	CLA	B	831	-	1/1/11/20	4/18/96/115	-
28	LUT	7	621	-	-	5/29/67/67	0/2/2/2
28	LUT	5	620	-	-	2/29/67/67	0/2/2/2
20	CLA	G	203	-	1/1/12/20	1/19/97/115	-
20	CLA	F	303	-	1/1/11/20	2/13/91/115	-
20	CLA	3	610	13	1/1/15/20	13/37/115/115	-
27	CHL	6	606	-	2/2/18/26	4/27/125/137	-
20	CLA	7	608	-	-	4/19/97/115	-
20	CLA	3	611	-	1/1/10/20	2/8/86/115	-
21	PQN	B	842	-	-	4/23/43/43	0/2/2/2
22	LHG	4	623	-	-	10/36/36/53	-
28	LUT	3	621	-	-	2/29/67/67	0/2/2/2
20	CLA	A	822	-	1/1/15/20	11/37/115/115	-
20	CLA	A	827	-	1/1/15/20	6/37/115/115	-
20	CLA	Z	616	12	1/1/11/20	3/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CHL	6	608	-	3/3/17/26	5/21/119/137	-
20	CLA	B	805	-	1/1/15/20	12/37/115/115	-
20	CLA	A	818	-	-	11/37/115/115	-
23	BCR	L	205	-	-	9/29/63/63	0/2/2/2
20	CLA	B	816	-	1/1/13/20	10/25/103/115	-
20	CLA	J	3002	9	1/1/10/20	5/10/88/115	-
28	LUT	Z	617	-	-	4/29/67/67	0/2/2/2
20	CLA	7	613	14	1/1/15/20	6/37/115/115	-
28	LUT	Z	619	-	-	4/29/67/67	0/2/2/2
20	CLA	5	610	17	1/1/14/20	10/31/109/115	-
22	LHG	5	623	20	-	13/41/41/53	-
20	CLA	3	612	13	1/1/11/20	2/15/93/115	-
27	CHL	6	607	-	2/2/18/26	12/27/125/137	-
20	CLA	6	617	-	1/1/11/20	0/15/93/115	-
27	CHL	5	618	17	3/3/15/26	4/12/110/137	-
20	CLA	A	837	1	1/1/11/20	9/13/91/115	-
20	CLA	A	823	-	-	11/18/96/115	-
20	CLA	B	836	-	1/1/14/20	7/31/109/115	-
20	CLA	A	843	-	1/1/15/20	18/37/115/115	-
28	LUT	8	618	-	-	2/29/67/67	0/2/2/2
27	CHL	4	606	-	3/3/18/26	7/27/125/137	-
20	CLA	4	609	16	1/1/12/20	6/19/97/115	-
28	LUT	1	619	-	-	2/29/67/67	0/2/2/2
20	CLA	A	813	-	1/1/12/20	8/24/102/115	-
20	CLA	8	609	15	1/1/11/20	1/15/93/115	-
20	CLA	Z	608	-	1/1/15/20	15/37/115/115	-
20	CLA	Z	603	-	1/1/13/20	9/28/106/115	-
20	CLA	4	601	16	1/1/14/20	10/33/111/115	-
23	BCR	3	719	-	-	8/29/63/63	0/2/2/2
20	CLA	1	613	-	1/1/15/20	12/37/115/115	-
28	LUT	1	618	-	-	2/29/67/67	0/2/2/2
20	CLA	6	611	22	1/1/13/20	7/25/103/115	-
20	CLA	6	614	-	1/1/11/20	4/13/91/115	-
24	SF4	A	853	1,2	-	-	0/6/5/5
20	CLA	A	811	-	1/1/15/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	1	602	12	1/1/15/20	12/37/115/115	-
22	LHG	4	622	20	-	13/53/53/53	-
20	CLA	A	828	-	1/1/15/20	13/37/115/115	-
20	CLA	6	610	18	1/1/14/20	9/31/109/115	-
23	BCR	B	844	-	-	8/29/63/63	0/2/2/2
23	BCR	5	622	-	-	6/29/63/63	0/2/2/2
24	SF4	C	101	3	-	-	0/6/5/5
20	CLA	1	609	12	1/1/15/20	9/37/115/115	-
23	BCR	3	718	-	-	2/29/63/63	0/2/2/2
20	CLA	B	833	-	1/1/13/20	7/29/107/115	-
27	CHL	5	608	-	2/2/17/26	7/21/119/137	-
23	BCR	7	624	-	-	6/29/63/63	0/2/2/2
20	CLA	B	808	-	1/1/15/20	8/37/115/115	-
20	CLA	A	854	-	1/1/15/20	10/37/115/115	-
20	CLA	B	818	-	1/1/14/20	11/31/109/115	-
20	CLA	B	852	-	1/1/15/20	9/37/115/115	-
20	CLA	5	613	17	1/1/13/20	7/27/105/115	-
20	CLA	4	610	16	1/1/14/20	7/31/109/115	-
20	CLA	A	836	-	-	2/19/97/115	-
20	CLA	Z	611	22	1/1/15/20	10/37/115/115	-
20	CLA	A	817	-	1/1/13/20	4/28/106/115	-
20	CLA	B	803	-	1/1/15/20	9/37/115/115	-
20	CLA	8	603	-	1/1/11/20	2/13/91/115	-
20	CLA	3	609	13	1/1/12/20	5/19/97/115	-
20	CLA	K	4002	-	-	5/13/91/115	-
27	CHL	4	618	16	3/3/15/26	4/12/110/137	-
28	LUT	4	620	-	-	2/29/67/67	0/2/2/2
20	CLA	A	804	-	1/1/15/20	10/37/115/115	-
23	BCR	4	621	-	-	11/29/63/63	0/2/2/2
20	CLA	A	834	-	1/1/15/20	10/37/115/115	-
20	CLA	B	829	-	1/1/15/20	8/37/115/115	-
20	CLA	A	807	1	1/1/15/20	17/37/115/115	-
20	CLA	1	612	12	1/1/12/20	6/22/100/115	-
20	CLA	7	601	14	1/1/15/20	17/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	830	-	1/1/15/20	9/37/115/115	-
20	CLA	3	613	13	-	16/25/103/115	-
20	CLA	A	808	-	1/1/15/20	10/37/115/115	-
20	CLA	1	610	12	1/1/14/20	7/31/109/115	-
20	CLA	A	825	-	-	7/25/103/115	-
20	CLA	1	611	22	1/1/15/20	10/37/115/115	-
23	BCR	A	848	-	-	4/29/63/63	0/2/2/2
23	BCR	6	625	-	-	7/29/63/63	0/2/2/2
20	CLA	8	614	-	1/1/13/20	6/25/103/115	-
20	CLA	1	614	-	1/1/15/20	9/37/115/115	-
20	CLA	1	603	-	1/1/15/20	7/37/115/115	-
20	CLA	6	601	18	1/1/15/20	12/37/115/115	-
20	CLA	7	603	-	1/1/11/20	3/15/93/115	-
20	CLA	7	609	14	1/1/12/20	5/19/97/115	-
20	CLA	A	819	-	-	11/37/115/115	-
20	CLA	8	602	15	1/1/14/20	9/34/112/115	-
23	BCR	A	850	-	-	4/29/63/63	0/2/2/2
27	CHL	4	608	-	3/3/17/26	4/21/119/137	-
20	CLA	Z	614	-	1/1/15/20	11/37/115/115	-
20	CLA	4	603	16	1/1/11/20	7/15/93/115	-
20	CLA	3	603	-	1/1/15/20	6/37/115/115	-
22	LHG	A	847	20	-	10/42/42/53	-
20	CLA	B	838	-	1/1/11/20	4/16/94/115	-
25	DGD	B	850	-	-	12/55/95/95	0/2/2/2
20	CLA	1	606	-	1/1/12/20	5/22/100/115	-
28	LUT	5	624	-	-	3/29/67/67	0/2/2/2
23	BCR	A	852	-	-	7/29/63/63	0/2/2/2
20	CLA	A	824	-	1/1/12/20	8/21/99/115	-
22	LHG	Z	620	20	-	17/47/47/53	-
28	LUT	8	617	-	-	3/29/67/67	0/2/2/2
28	LUT	6	624	-	-	3/29/67/67	0/2/2/2
20	CLA	A	802	-	1/1/15/20	7/37/115/115	-
20	CLA	B	823	-	1/1/14/20	7/31/109/115	-
20	CLA	A	841	-	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	815	-	1/1/13/20	4/28/106/115	-
20	CLA	Z	606	-	1/1/12/20	6/22/100/115	-
27	CHL	1	601	12	3/3/17/26	10/24/122/137	-
20	CLA	A	839	-	1/1/15/20	10/37/115/115	-
20	CLA	4	602	16	-	8/31/109/115	-
20	CLA	B	840	-	-	8/37/115/115	-
20	CLA	8	616	15	1/1/11/20	2/15/93/115	-
20	CLA	5	606	-	1/1/13/20	3/25/103/115	-
20	CLA	6	612	18	1/1/12/20	5/22/100/115	-
20	CLA	B	806	2	1/1/15/20	12/37/115/115	-
20	CLA	B	809	2	1/1/15/20	5/37/115/115	-
20	CLA	6	613	-	1/1/13/20	7/27/105/115	-
20	CLA	B	826	-	1/1/15/20	11/37/115/115	-
20	CLA	8	611	22	1/1/11/20	5/15/93/115	-
20	CLA	Z	602	12	1/1/15/20	12/37/115/115	-
20	CLA	Z	609	12	1/1/15/20	4/37/115/115	-
27	CHL	Z	607	-	3/3/16/26	6/18/116/137	-
23	BCR	B	848	-	-	4/29/63/63	0/2/2/2
23	BCR	6	623	-	-	9/29/63/63	0/2/2/2
20	CLA	7	620	-	1/1/14/20	8/31/109/115	-
20	CLA	6	609	18	1/1/12/20	4/19/97/115	-
22	LHG	7	625	20	-	9/41/41/53	-
23	BCR	A	849	-	-	3/29/63/63	0/2/2/2
20	CLA	A	835	-	1/1/15/20	12/37/115/115	-
20	CLA	7	616	14	1/1/11/20	3/15/93/115	-
22	LHG	A	855	-	-	11/34/34/53	-
24	SF4	C	102	3	-	-	0/6/5/5
20	CLA	Z	604	-	1/1/13/20	6/28/106/115	-
20	CLA	B	828	-	1/1/15/20	9/37/115/115	-
20	CLA	B	819	-	1/1/15/20	13/37/115/115	-
20	CLA	A	816	-	1/1/15/20	9/37/115/115	-
28	LUT	1	617	-	-	2/29/67/67	0/2/2/2
20	CLA	A	820	-	1/1/15/20	16/37/115/115	-
20	CLA	3	602	13	1/1/14/20	9/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	7	602	14	1/1/15/20	13/37/115/115	-
20	CLA	A	803	-	1/1/15/20	5/37/115/115	-
20	CLA	B	827	-	1/1/15/20	15/37/115/115	-
20	CLA	B	825	-	1/1/15/20	6/37/115/115	-
20	CLA	3	604	-	1/1/15/20	8/37/115/115	-
20	CLA	B	822	-	1/1/13/20	12/30/108/115	-
20	CLA	6	603	-	1/1/11/20	3/15/93/115	-
20	CLA	A	832	-	1/1/12/20	2/19/97/115	-
20	CLA	6	622	-	1/1/11/20	3/13/91/115	-
20	CLA	4	604	-	-	4/19/97/115	-
20	CLA	8	606	-	1/1/10/20	4/10/88/115	-
20	CLA	A	809	1	1/1/15/20	16/37/115/115	-
23	BCR	F	305	-	-	8/29/63/63	0/2/2/2
20	CLA	5	616	17	1/1/11/20	7/15/93/115	-
20	CLA	B	824	-	1/1/15/20	11/37/115/115	-
20	CLA	Z	612	-	1/1/12/20	8/22/100/115	-
20	CLA	B	812	-	1/1/15/20	13/37/115/115	-
22	LHG	A	846	-	-	14/53/53/53	-
23	BCR	G	205	-	-	4/29/63/63	0/2/2/2
20	CLA	7	611	22	1/1/10/20	2/8/86/115	-
19	CL0	A	801	-	2/2/20/25	7/37/135/135	-
20	CLA	A	812	20	1/1/15/20	14/37/115/115	-

All (3585) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	844	PQN	C3-C2	7.56	1.49	1.35
21	B	842	PQN	C3-C2	7.40	1.48	1.35
20	B	836	CLA	C3B-C2B	6.65	1.49	1.40
20	B	827	CLA	C3B-C2B	6.11	1.48	1.40
27	1	601	CHL	C3B-C2B	6.02	1.48	1.40
20	B	840	CLA	C3C-C2C	6.00	1.49	1.36
27	1	607	CHL	C3B-C2B	6.00	1.48	1.40
20	7	616	CLA	C3B-C2B	5.97	1.48	1.40
27	Z	601	CHL	C3B-C2B	5.96	1.48	1.40
20	G	204	CLA	C3B-C2B	5.94	1.48	1.40
20	7	601	CLA	C3B-C2B	5.94	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	5	621	CLA	C3B-C2B	5.94	1.48	1.40
27	4	607	CHL	C3B-C2B	5.93	1.48	1.40
20	7	620	CLA	C3B-C2B	5.93	1.48	1.40
20	A	806	CLA	C3B-C2B	5.93	1.48	1.40
20	G	203	CLA	C3B-C2B	5.92	1.48	1.40
20	8	616	CLA	C3B-C2B	5.92	1.48	1.40
27	Z	607	CHL	C3B-C2B	5.92	1.48	1.40
20	B	852	CLA	C3B-C2B	5.91	1.48	1.40
20	3	611	CLA	C3B-C2B	5.91	1.48	1.40
20	B	804	CLA	C3B-C2B	5.91	1.48	1.40
20	1	616	CLA	C3B-C2B	5.90	1.48	1.40
20	5	601	CLA	C3B-C2B	5.89	1.48	1.40
27	4	618	CHL	C3B-C2B	5.88	1.48	1.40
27	8	607	CHL	C3B-C2B	5.88	1.48	1.40
27	6	618	CHL	C3B-C2B	5.88	1.48	1.40
20	Z	608	CLA	C3B-C2B	5.87	1.48	1.40
20	8	614	CLA	C3B-C2B	5.87	1.48	1.40
27	5	618	CHL	C3B-C2B	5.87	1.48	1.40
20	B	834	CLA	C3B-C2B	5.87	1.48	1.40
20	K	4003	CLA	C3B-C2B	5.86	1.48	1.40
20	8	608	CLA	C3B-C2B	5.86	1.48	1.40
20	Z	616	CLA	C3B-C2B	5.86	1.48	1.40
20	Z	613	CLA	C3B-C2B	5.86	1.48	1.40
20	B	822	CLA	C3B-C2B	5.85	1.48	1.40
20	K	4002	CLA	C3B-C2B	5.85	1.48	1.40
20	5	612	CLA	C3B-C2B	5.84	1.48	1.40
20	5	611	CLA	C3B-C2B	5.84	1.48	1.40
20	Z	611	CLA	C3B-C2B	5.83	1.48	1.40
27	7	607	CHL	C3B-C2B	5.83	1.48	1.40
20	4	614	CLA	C3B-C2B	5.82	1.48	1.40
20	6	622	CLA	C3B-C2B	5.82	1.48	1.40
20	A	803	CLA	C3B-C2B	5.82	1.48	1.40
20	3	614	CLA	C3B-C2B	5.82	1.48	1.40
20	5	616	CLA	C3B-C2B	5.82	1.48	1.40
20	4	611	CLA	C3B-C2B	5.81	1.48	1.40
20	5	603	CLA	C3B-C2B	5.80	1.48	1.40
20	B	839	CLA	C3B-C2B	5.80	1.48	1.40
20	1	614	CLA	C3B-C2B	5.80	1.48	1.40
20	5	613	CLA	C3B-C2B	5.79	1.48	1.40
20	1	606	CLA	C3B-C2B	5.79	1.48	1.40
20	4	616	CLA	C3B-C2B	5.79	1.48	1.40
27	5	607	CHL	C3B-C2B	5.78	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	8	601	CLA	C3B-C2B	5.78	1.48	1.40
20	8	611	CLA	C3B-C2B	5.77	1.48	1.40
20	B	810	CLA	C3B-C2B	5.77	1.48	1.40
20	A	802	CLA	C3B-C2B	5.77	1.48	1.40
20	Z	612	CLA	C3B-C2B	5.77	1.48	1.40
20	B	825	CLA	C3B-C2B	5.77	1.48	1.40
20	8	613	CLA	C3B-C2B	5.76	1.48	1.40
20	6	611	CLA	C3B-C2B	5.76	1.48	1.40
20	6	613	CLA	C3B-C2B	5.75	1.48	1.40
20	5	614	CLA	C3B-C2B	5.74	1.48	1.40
20	B	841	CLA	C3B-C2B	5.74	1.48	1.40
20	Z	614	CLA	C3B-C2B	5.74	1.48	1.40
20	B	821	CLA	C3B-C2B	5.73	1.48	1.40
20	Z	603	CLA	C3B-C2B	5.73	1.48	1.40
20	6	616	CLA	C3B-C2B	5.73	1.48	1.40
20	A	833	CLA	C3B-C2B	5.73	1.48	1.40
20	Z	606	CLA	C3B-C2B	5.73	1.48	1.40
20	4	612	CLA	C3B-C2B	5.73	1.48	1.40
20	4	601	CLA	C3B-C2B	5.72	1.48	1.40
20	3	602	CLA	C3B-C2B	5.72	1.48	1.40
20	A	807	CLA	C3B-C2B	5.71	1.48	1.40
20	B	808	CLA	C3B-C2B	5.71	1.48	1.40
20	F	304	CLA	C3B-C2B	5.70	1.48	1.40
20	7	609	CLA	C3B-C2B	5.70	1.48	1.40
20	6	617	CLA	C3B-C2B	5.69	1.48	1.40
20	L	204	CLA	C3B-C2B	5.69	1.48	1.40
20	F	301	CLA	C3B-C2B	5.69	1.48	1.40
20	5	610	CLA	C3B-C2B	5.69	1.48	1.40
20	A	816	CLA	C3B-C2B	5.69	1.48	1.40
20	A	827	CLA	C3B-C2B	5.69	1.48	1.40
20	1	613	CLA	C3B-C2B	5.68	1.48	1.40
20	1	608	CLA	C3B-C2B	5.68	1.48	1.40
20	6	612	CLA	C3B-C2B	5.68	1.48	1.40
20	8	606	CLA	C3B-C2B	5.68	1.48	1.40
20	J	3002	CLA	C3B-C2B	5.67	1.48	1.40
20	3	617	CLA	C3B-C2B	5.66	1.48	1.40
20	7	603	CLA	C3B-C2B	5.65	1.48	1.40
20	B	807	CLA	C3B-C2B	5.65	1.48	1.40
20	Z	610	CLA	C3B-C2B	5.65	1.48	1.40
20	A	845	CLA	C3B-C2B	5.64	1.48	1.40
20	6	609	CLA	C3B-C2B	5.64	1.48	1.40
27	6	607	CHL	C3B-C2B	5.64	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	824	CLA	C3B-C2B	5.64	1.48	1.40
20	F	303	CLA	C3B-C2B	5.64	1.48	1.40
20	Z	609	CLA	C3B-C2B	5.64	1.48	1.40
20	6	610	CLA	C3B-C2B	5.64	1.48	1.40
20	7	614	CLA	C3B-C2B	5.63	1.48	1.40
20	A	843	CLA	C3B-C2B	5.62	1.48	1.40
20	6	601	CLA	C3B-C2B	5.62	1.48	1.40
20	A	832	CLA	C3B-C2B	5.61	1.48	1.40
20	B	820	CLA	C3B-C2B	5.61	1.48	1.40
20	A	821	CLA	C3B-C2B	5.61	1.48	1.40
20	6	603	CLA	C3B-C2B	5.61	1.48	1.40
20	B	805	CLA	C3B-C2B	5.61	1.48	1.40
20	A	823	CLA	C3B-C2B	5.61	1.48	1.40
20	8	609	CLA	C3B-C2B	5.61	1.48	1.40
20	5	606	CLA	C3B-C2B	5.61	1.48	1.40
20	8	602	CLA	C3B-C2B	5.61	1.48	1.40
20	B	833	CLA	C3B-C2B	5.61	1.48	1.40
20	A	814	CLA	C3B-C2B	5.60	1.48	1.40
20	3	609	CLA	C3B-C2B	5.60	1.48	1.40
27	6	606	CHL	C3B-C2B	5.60	1.48	1.40
20	A	836	CLA	C3B-C2B	5.60	1.48	1.40
20	A	820	CLA	C3B-C2B	5.60	1.48	1.40
20	A	809	CLA	C3B-C2B	5.60	1.48	1.40
20	B	813	CLA	C3B-C2B	5.59	1.48	1.40
20	7	606	CLA	C3B-C2B	5.59	1.48	1.40
20	B	831	CLA	C3B-C2B	5.59	1.48	1.40
20	B	835	CLA	C3B-C2B	5.59	1.48	1.40
20	3	612	CLA	C3B-C2B	5.59	1.48	1.40
20	Z	602	CLA	C3B-C2B	5.59	1.48	1.40
20	7	613	CLA	C3B-C2B	5.59	1.48	1.40
20	A	815	CLA	C3B-C2B	5.58	1.48	1.40
20	3	607	CLA	C3B-C2B	5.58	1.48	1.40
20	A	834	CLA	C3B-C2B	5.58	1.48	1.40
20	7	608	CLA	C3B-C2B	5.58	1.48	1.40
20	1	611	CLA	C3B-C2B	5.58	1.48	1.40
20	B	826	CLA	C3B-C2B	5.57	1.48	1.40
20	3	613	CLA	C3B-C2B	5.57	1.48	1.40
20	B	824	CLA	C3B-C2B	5.57	1.48	1.40
20	A	854	CLA	C3B-C2B	5.56	1.48	1.40
20	A	819	CLA	C3B-C2B	5.56	1.48	1.40
27	4	608	CHL	C3B-C2B	5.56	1.48	1.40
20	A	813	CLA	C3B-C2B	5.55	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	606	CLA	C3B-C2B	5.55	1.48	1.40
20	A	839	CLA	C3B-C2B	5.54	1.48	1.40
20	B	816	CLA	C3B-C2B	5.54	1.48	1.40
20	B	812	CLA	C3B-C2B	5.54	1.48	1.40
20	1	609	CLA	C3B-C2B	5.54	1.48	1.40
20	6	602	CLA	C3B-C2B	5.54	1.48	1.40
20	4	613	CLA	C3B-C2B	5.54	1.48	1.40
20	A	838	CLA	C3B-C2B	5.53	1.48	1.40
20	A	830	CLA	C3B-C2B	5.53	1.48	1.40
20	8	612	CLA	C3B-C2B	5.53	1.48	1.40
20	1	610	CLA	C3B-C2B	5.53	1.48	1.40
20	7	610	CLA	CHC-C1C	5.52	1.49	1.35
20	A	817	CLA	C1D-ND	5.52	1.44	1.37
20	7	612	CLA	C3B-C2B	5.52	1.48	1.40
20	4	603	CLA	C3B-C2B	5.52	1.48	1.40
20	A	808	CLA	C3B-C2B	5.52	1.48	1.40
20	1	603	CLA	C3B-C2B	5.52	1.48	1.40
20	8	604	CLA	C3B-C2B	5.51	1.48	1.40
20	8	603	CLA	C3B-C2B	5.51	1.48	1.40
20	A	811	CLA	C3B-C2B	5.51	1.48	1.40
20	B	802	CLA	C3B-C2B	5.51	1.48	1.40
20	1	602	CLA	C3B-C2B	5.51	1.48	1.40
20	B	805	CLA	CHC-C1C	5.50	1.49	1.35
20	1	612	CLA	C3B-C2B	5.49	1.48	1.40
20	L	204	CLA	C3C-C2C	5.49	1.48	1.36
20	6	614	CLA	C3B-C2B	5.48	1.48	1.40
20	5	604	CLA	C1D-ND	5.48	1.44	1.37
20	B	815	CLA	C3B-C2B	5.47	1.48	1.40
20	7	611	CLA	C3B-C2B	5.47	1.48	1.40
20	A	818	CLA	C3B-C2B	5.47	1.48	1.40
20	A	835	CLA	C3C-C2C	5.46	1.48	1.36
20	A	837	CLA	C3B-C2B	5.46	1.47	1.40
20	6	604	CLA	C3B-C2B	5.46	1.47	1.40
20	B	840	CLA	C3B-C2B	5.45	1.47	1.40
20	B	803	CLA	C3B-C2B	5.45	1.47	1.40
20	A	812	CLA	C3B-C2B	5.45	1.47	1.40
20	A	816	CLA	C3C-C2C	5.45	1.48	1.36
20	B	838	CLA	C3B-C2B	5.44	1.47	1.40
20	5	609	CLA	C3B-C2B	5.44	1.47	1.40
20	B	837	CLA	C3B-C2B	5.42	1.47	1.40
20	B	806	CLA	C3B-C2B	5.42	1.47	1.40
20	3	607	CLA	C3C-C2C	5.41	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	610	CLA	C3C-C2C	5.40	1.48	1.36
20	B	828	CLA	C3B-C2B	5.39	1.47	1.40
20	7	602	CLA	C3B-C2B	5.39	1.47	1.40
20	B	825	CLA	C3C-C2C	5.39	1.48	1.36
20	A	840	CLA	C3B-C2B	5.39	1.47	1.40
20	7	601	CLA	C3C-C2C	5.38	1.48	1.36
20	6	609	CLA	C3C-C2C	5.38	1.48	1.36
20	8	611	CLA	C1D-ND	5.38	1.44	1.37
20	3	620	CLA	C3B-C2B	5.38	1.47	1.40
20	8	609	CLA	C3C-C2C	5.38	1.48	1.36
20	1	611	CLA	C3C-C2C	5.37	1.48	1.36
20	7	604	CLA	C3B-C2B	5.37	1.47	1.40
20	A	845	CLA	C3C-C2C	5.36	1.48	1.36
20	A	815	CLA	C3C-C2C	5.36	1.48	1.36
20	A	831	CLA	C3B-C2B	5.36	1.47	1.40
20	F	301	CLA	C1D-ND	5.36	1.44	1.37
20	4	616	CLA	C1D-ND	5.35	1.44	1.37
20	B	852	CLA	C3C-C2C	5.35	1.48	1.36
20	G	204	CLA	C3C-C2C	5.35	1.48	1.36
20	3	610	CLA	CHC-C1C	5.35	1.48	1.35
20	B	814	CLA	C3B-C2B	5.35	1.47	1.40
20	A	809	CLA	C3C-C2C	5.35	1.48	1.36
20	B	805	CLA	C3C-C2C	5.35	1.48	1.36
20	Z	611	CLA	C3C-C2C	5.34	1.48	1.36
20	A	825	CLA	C3B-C2B	5.34	1.47	1.40
27	1	601	CHL	C2C-C3C	5.34	1.48	1.36
20	7	606	CLA	C3C-C2C	5.34	1.48	1.36
20	A	827	CLA	CHC-C1C	5.34	1.48	1.35
20	7	620	CLA	C3C-C2C	5.34	1.48	1.36
20	4	604	CLA	C3C-C2C	5.33	1.48	1.36
20	6	610	CLA	C3C-C2C	5.33	1.48	1.36
20	Z	614	CLA	C3C-C2C	5.33	1.48	1.36
20	5	609	CLA	C3C-C2C	5.33	1.48	1.36
27	Z	601	CHL	C2C-C3C	5.33	1.48	1.36
20	8	606	CLA	C3C-C2C	5.33	1.48	1.36
20	3	603	CLA	C3B-C2B	5.33	1.47	1.40
20	5	614	CLA	C3C-C2C	5.33	1.48	1.36
20	B	819	CLA	C3C-C2C	5.33	1.48	1.36
20	K	4002	CLA	C1D-ND	5.32	1.44	1.37
20	6	614	CLA	C3C-C2C	5.32	1.48	1.36
20	1	610	CLA	CHC-C1C	5.32	1.48	1.35
20	A	822	CLA	C3C-C2C	5.32	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	614	CLA	C3C-C2C	5.32	1.48	1.36
20	4	601	CLA	C3C-C2C	5.32	1.48	1.36
20	A	824	CLA	C3C-C2C	5.31	1.48	1.36
20	Z	614	CLA	C1D-ND	5.31	1.44	1.37
27	5	608	CHL	C3B-C2B	5.31	1.47	1.40
20	3	612	CLA	C3C-C2C	5.31	1.48	1.36
20	A	828	CLA	C3B-C2B	5.31	1.47	1.40
20	6	616	CLA	C3C-C2C	5.31	1.48	1.36
20	F	301	CLA	C3C-C2C	5.31	1.48	1.36
20	G	203	CLA	C3C-C2C	5.31	1.48	1.36
20	K	4002	CLA	C3C-C2C	5.31	1.48	1.36
20	B	835	CLA	C3C-C2C	5.31	1.48	1.36
20	7	609	CLA	C3C-C2C	5.31	1.48	1.36
20	3	610	CLA	C3B-C2B	5.30	1.47	1.40
20	Z	604	CLA	C3B-C2B	5.30	1.47	1.40
27	6	608	CHL	C3B-C2B	5.30	1.47	1.40
20	1	604	CLA	C3C-C2C	5.30	1.48	1.36
20	5	611	CLA	C3C-C2C	5.30	1.48	1.36
20	5	617	CLA	C3C-C2C	5.30	1.48	1.36
20	A	829	CLA	C3B-C2B	5.30	1.47	1.40
20	A	834	CLA	C3C-C2C	5.30	1.48	1.36
20	B	822	CLA	C3C-C2C	5.30	1.48	1.36
20	Z	608	CLA	C1D-ND	5.30	1.44	1.37
20	B	831	CLA	C3C-C2C	5.30	1.48	1.36
20	A	842	CLA	C3B-C2B	5.30	1.47	1.40
27	5	618	CHL	C2C-C3C	5.29	1.48	1.36
20	3	611	CLA	C3C-C2C	5.29	1.48	1.36
20	K	4003	CLA	C3C-C2C	5.29	1.48	1.36
20	B	823	CLA	C3B-C2B	5.29	1.47	1.40
20	A	810	CLA	C3C-C2C	5.29	1.48	1.36
20	B	820	CLA	C3C-C2C	5.29	1.48	1.36
20	4	610	CLA	C3B-C2B	5.28	1.47	1.40
20	J	3002	CLA	C3C-C2C	5.28	1.48	1.36
27	Z	607	CHL	C2C-C3C	5.28	1.48	1.36
20	B	829	CLA	C3C-C2C	5.28	1.48	1.36
20	3	606	CLA	C1D-ND	5.28	1.44	1.37
20	A	841	CLA	C3C-C2C	5.28	1.48	1.36
20	A	839	CLA	C3C-C2C	5.28	1.48	1.36
20	A	823	CLA	C3C-C2C	5.28	1.48	1.36
20	Z	604	CLA	C3C-C2C	5.28	1.47	1.36
27	7	607	CHL	C2C-C3C	5.28	1.48	1.36
20	5	612	CLA	C3C-C2C	5.28	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	7	614	CLA	C3C-C2C	5.28	1.47	1.36
20	B	821	CLA	C3C-C2C	5.28	1.47	1.36
20	B	826	CLA	C3C-C2C	5.28	1.47	1.36
20	7	620	CLA	C1D-ND	5.27	1.44	1.37
20	6	601	CLA	C3C-C2C	5.27	1.47	1.36
20	A	810	CLA	C3B-C2B	5.27	1.47	1.40
20	G	204	CLA	C1D-ND	5.27	1.44	1.37
20	1	604	CLA	C3B-C2B	5.27	1.47	1.40
20	A	838	CLA	C3C-C2C	5.27	1.47	1.36
20	6	604	CLA	C3C-C2C	5.27	1.47	1.36
20	A	821	CLA	C3C-C2C	5.27	1.47	1.36
20	7	602	CLA	CHC-C1C	5.27	1.48	1.35
20	Z	612	CLA	C3C-C2C	5.27	1.47	1.36
20	1	612	CLA	C3C-C2C	5.27	1.47	1.36
20	1	616	CLA	C3C-C2C	5.26	1.47	1.36
20	8	610	CLA	CHC-C1C	5.26	1.48	1.35
20	B	815	CLA	C3C-C2C	5.26	1.47	1.36
20	3	614	CLA	C1D-ND	5.26	1.44	1.37
20	4	602	CLA	C3C-C2C	5.26	1.47	1.36
20	B	810	CLA	C3C-C2C	5.26	1.47	1.36
20	B	818	CLA	C3B-C2B	5.26	1.47	1.40
20	A	827	CLA	C3C-C2C	5.26	1.47	1.36
20	A	826	CLA	C3C-C2C	5.26	1.47	1.36
20	8	610	CLA	C3B-C2B	5.26	1.47	1.40
27	4	606	CHL	C3B-C2B	5.26	1.47	1.40
20	L	203	CLA	C3C-C2C	5.25	1.47	1.36
20	B	827	CLA	C3C-C2C	5.25	1.47	1.36
20	A	820	CLA	C3C-C2C	5.25	1.47	1.36
20	8	614	CLA	C3C-C2C	5.25	1.47	1.36
20	3	606	CLA	C3C-C2C	5.25	1.47	1.36
20	7	608	CLA	C3C-C2C	5.25	1.47	1.36
20	5	606	CLA	C1D-ND	5.25	1.44	1.37
20	1	608	CLA	C3C-C2C	5.25	1.47	1.36
20	5	601	CLA	C3C-C2C	5.25	1.47	1.36
20	6	616	CLA	CHC-C1C	5.25	1.48	1.35
20	A	854	CLA	C3C-C2C	5.25	1.47	1.36
20	B	817	CLA	C1D-ND	5.25	1.44	1.37
20	A	831	CLA	C3C-C2C	5.25	1.47	1.36
20	7	603	CLA	C3C-C2C	5.24	1.47	1.36
20	A	837	CLA	C3C-C2C	5.24	1.47	1.36
20	A	816	CLA	C1D-ND	5.24	1.44	1.37
20	6	614	CLA	C1D-ND	5.24	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Z	603	CLA	C3C-C2C	5.24	1.47	1.36
20	Z	610	CLA	CHC-C1C	5.24	1.48	1.35
20	8	604	CLA	C3C-C2C	5.24	1.47	1.36
20	6	611	CLA	C3C-C2C	5.24	1.47	1.36
20	7	616	CLA	C3C-C2C	5.24	1.47	1.36
20	3	609	CLA	C3C-C2C	5.24	1.47	1.36
20	B	839	CLA	C3C-C2C	5.24	1.47	1.36
20	Z	616	CLA	C3C-C2C	5.24	1.47	1.36
20	B	837	CLA	C3C-C2C	5.24	1.47	1.36
20	5	616	CLA	C3C-C2C	5.24	1.47	1.36
20	1	609	CLA	C3C-C2C	5.24	1.47	1.36
20	A	854	CLA	CHC-C1C	5.23	1.48	1.35
20	A	845	CLA	C1D-ND	5.23	1.44	1.37
20	3	614	CLA	C3C-C2C	5.23	1.47	1.36
20	Z	608	CLA	C3C-C2C	5.23	1.47	1.36
20	1	609	CLA	C1D-ND	5.23	1.44	1.37
20	B	832	CLA	C3C-C2C	5.23	1.47	1.36
20	1	606	CLA	C3C-C2C	5.23	1.47	1.36
20	5	616	CLA	C1D-ND	5.23	1.44	1.37
20	5	606	CLA	C3C-C2C	5.23	1.47	1.36
20	3	611	CLA	C1D-ND	5.23	1.44	1.37
20	A	817	CLA	C3C-C2C	5.23	1.47	1.36
20	F	303	CLA	C3C-C2C	5.23	1.47	1.36
20	3	604	CLA	C3B-C2B	5.23	1.47	1.40
20	B	825	CLA	CHC-C1C	5.22	1.48	1.35
20	A	841	CLA	C3B-C2B	5.22	1.47	1.40
20	A	835	CLA	C1D-ND	5.22	1.44	1.37
20	6	611	CLA	C1D-ND	5.22	1.44	1.37
20	J	3002	CLA	C1D-ND	5.22	1.44	1.37
20	A	836	CLA	C3C-C2C	5.22	1.47	1.36
20	5	604	CLA	C3B-C2B	5.22	1.47	1.40
20	A	828	CLA	C1D-ND	5.22	1.44	1.37
20	A	828	CLA	C3C-C2C	5.22	1.47	1.36
20	F	304	CLA	C1D-ND	5.21	1.44	1.37
20	Z	613	CLA	C3C-C2C	5.21	1.47	1.36
20	5	602	CLA	C3B-C2B	5.21	1.47	1.40
20	B	807	CLA	C3C-C2C	5.21	1.47	1.36
20	4	616	CLA	C3C-C2C	5.21	1.47	1.36
20	1	608	CLA	C1D-ND	5.21	1.44	1.37
20	7	611	CLA	C1D-ND	5.21	1.44	1.37
27	1	607	CHL	C2C-C3C	5.21	1.47	1.36
20	B	811	CLA	C3C-C2C	5.21	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Z	606	CLA	C3C-C2C	5.21	1.47	1.36
20	5	602	CLA	CHC-C1C	5.21	1.48	1.35
20	4	604	CLA	C3B-C2B	5.21	1.47	1.40
20	7	603	CLA	C1D-ND	5.21	1.44	1.37
20	8	602	CLA	C3C-C2C	5.21	1.47	1.36
20	4	612	CLA	C3C-C2C	5.20	1.47	1.36
20	B	816	CLA	C1D-ND	5.20	1.44	1.37
20	Z	609	CLA	C3C-C2C	5.20	1.47	1.36
20	A	813	CLA	C3C-C2C	5.20	1.47	1.36
20	B	834	CLA	C3C-C2C	5.20	1.47	1.36
20	6	617	CLA	C3C-C2C	5.20	1.47	1.36
27	5	607	CHL	C2C-C3C	5.20	1.47	1.36
20	A	804	CLA	C3C-C2C	5.20	1.47	1.36
20	B	834	CLA	C1D-ND	5.20	1.44	1.37
20	Z	604	CLA	C1D-ND	5.20	1.44	1.37
20	B	829	CLA	CHC-C1C	5.20	1.48	1.35
20	3	604	CLA	C3C-C2C	5.20	1.47	1.36
20	4	611	CLA	C1D-ND	5.20	1.44	1.37
20	5	610	CLA	CHC-C1C	5.19	1.48	1.35
20	A	819	CLA	C3C-C2C	5.19	1.47	1.36
20	4	613	CLA	C1D-ND	5.19	1.44	1.37
20	3	612	CLA	C1D-ND	5.19	1.44	1.37
20	4	609	CLA	C3B-C2B	5.19	1.47	1.40
20	4	602	CLA	C3B-C2B	5.19	1.47	1.40
20	B	838	CLA	C3C-C2C	5.19	1.47	1.36
20	6	622	CLA	C3C-C2C	5.19	1.47	1.36
20	3	606	CLA	O2D-CGD	5.19	1.45	1.33
20	4	614	CLA	C3C-C2C	5.19	1.47	1.36
20	5	603	CLA	C3C-C2C	5.19	1.47	1.36
20	B	812	CLA	C3C-C2C	5.19	1.47	1.36
20	6	612	CLA	C3C-C2C	5.18	1.47	1.36
20	8	610	CLA	O2D-CGD	5.18	1.45	1.33
20	F	303	CLA	C1D-ND	5.18	1.44	1.37
20	Z	609	CLA	C1D-ND	5.18	1.44	1.37
20	A	804	CLA	C3B-C2B	5.18	1.47	1.40
20	4	603	CLA	C3C-C2C	5.18	1.47	1.36
20	6	602	CLA	CHC-C1C	5.17	1.48	1.35
20	A	808	CLA	C3C-C2C	5.17	1.47	1.36
20	7	602	CLA	C3C-C2C	5.17	1.47	1.36
20	Z	616	CLA	C1D-ND	5.17	1.44	1.37
20	A	833	CLA	C3C-C2C	5.17	1.47	1.36
20	8	603	CLA	C3C-C2C	5.17	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	816	CLA	CHC-C1C	5.17	1.48	1.35
20	3	617	CLA	C3C-C2C	5.17	1.47	1.36
20	A	802	CLA	O2D-CGD	5.17	1.45	1.33
20	A	845	CLA	O2D-CGD	5.16	1.45	1.33
20	K	4003	CLA	O2D-CGD	5.16	1.45	1.33
20	B	812	CLA	C1D-ND	5.16	1.44	1.37
20	6	602	CLA	C3C-C2C	5.16	1.47	1.36
20	Z	606	CLA	O2D-CGD	5.16	1.45	1.33
20	A	842	CLA	C3C-C2C	5.16	1.47	1.36
20	6	609	CLA	C1D-ND	5.16	1.44	1.37
20	B	828	CLA	C3C-C2C	5.16	1.47	1.36
20	A	835	CLA	C3B-C2B	5.16	1.47	1.40
20	4	611	CLA	C3C-C2C	5.16	1.47	1.36
20	1	602	CLA	CHC-C1C	5.16	1.48	1.35
20	B	830	CLA	C3B-C2B	5.16	1.47	1.40
20	A	840	CLA	C3C-C2C	5.16	1.47	1.36
20	5	613	CLA	C3C-C2C	5.16	1.47	1.36
20	4	616	CLA	CHC-C1C	5.16	1.48	1.35
20	B	841	CLA	C3C-C2C	5.16	1.47	1.36
20	B	852	CLA	O2D-CGD	5.16	1.45	1.33
20	B	814	CLA	C3C-C2C	5.16	1.47	1.36
20	4	614	CLA	O2D-CGD	5.16	1.45	1.33
20	B	833	CLA	C3C-C2C	5.16	1.47	1.36
20	L	204	CLA	O2D-CGD	5.16	1.45	1.33
20	B	830	CLA	C3C-C2C	5.15	1.47	1.36
20	7	611	CLA	C3C-C2C	5.15	1.47	1.36
20	B	803	CLA	CHC-C1C	5.15	1.48	1.35
20	B	832	CLA	C3B-C2B	5.15	1.47	1.40
20	8	610	CLA	C3C-C2C	5.15	1.47	1.36
20	A	807	CLA	C3C-C2C	5.15	1.47	1.36
27	1	607	CHL	CHC-C1C	5.15	1.48	1.35
20	4	604	CLA	C1D-ND	5.15	1.44	1.37
20	3	620	CLA	C3C-C2C	5.15	1.47	1.36
20	6	603	CLA	C3C-C2C	5.15	1.47	1.36
20	1	604	CLA	C1D-ND	5.15	1.44	1.37
20	6	603	CLA	C1D-ND	5.15	1.44	1.37
20	Z	610	CLA	O2D-CGD	5.14	1.45	1.33
20	8	616	CLA	C3C-C2C	5.14	1.47	1.36
20	B	814	CLA	CHC-C1C	5.14	1.48	1.35
27	4	607	CHL	C2C-C3C	5.14	1.47	1.36
20	B	829	CLA	C1D-ND	5.14	1.44	1.37
20	4	616	CLA	O2D-CGD	5.14	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	805	CLA	CHC-C1C	5.14	1.48	1.35
20	6	613	CLA	C3C-C2C	5.14	1.47	1.36
20	3	620	CLA	C1D-ND	5.14	1.44	1.37
20	7	612	CLA	C3C-C2C	5.14	1.47	1.36
27	6	618	CHL	O2D-CGD	5.14	1.45	1.33
20	7	604	CLA	C1D-ND	5.14	1.44	1.37
20	6	614	CLA	CHC-C1C	5.14	1.48	1.35
20	5	613	CLA	O2D-CGD	5.14	1.45	1.33
20	Z	606	CLA	C1D-ND	5.14	1.44	1.37
20	7	613	CLA	C3C-C2C	5.14	1.47	1.36
20	Z	604	CLA	O2D-CGD	5.13	1.45	1.33
20	B	815	CLA	C1D-ND	5.13	1.44	1.37
20	8	601	CLA	C3C-C2C	5.13	1.47	1.36
20	7	606	CLA	C1D-ND	5.13	1.44	1.37
20	Z	611	CLA	C1D-ND	5.13	1.44	1.37
20	A	822	CLA	CHC-C1C	5.13	1.48	1.35
20	5	614	CLA	C1D-ND	5.13	1.44	1.37
20	B	823	CLA	C3C-C2C	5.13	1.47	1.36
20	8	612	CLA	O2D-CGD	5.13	1.45	1.33
27	8	607	CHL	O2D-CGD	5.13	1.45	1.33
20	1	603	CLA	C3C-C2C	5.13	1.47	1.36
20	8	611	CLA	C3C-C2C	5.13	1.47	1.36
20	6	610	CLA	CHC-C1C	5.13	1.48	1.35
20	5	610	CLA	C3C-C2C	5.13	1.47	1.36
20	4	612	CLA	O2D-CGD	5.13	1.45	1.33
20	B	816	CLA	CHC-C1C	5.13	1.48	1.35
27	6	606	CHL	CHC-C1C	5.12	1.48	1.35
20	4	609	CLA	C3C-C2C	5.12	1.47	1.36
20	G	203	CLA	O2D-CGD	5.12	1.45	1.33
20	K	4003	CLA	C1D-ND	5.12	1.44	1.37
20	A	818	CLA	C1D-ND	5.12	1.44	1.37
20	8	608	CLA	C1D-ND	5.12	1.44	1.37
20	3	617	CLA	C1D-ND	5.12	1.44	1.37
20	B	817	CLA	C3C-C2C	5.12	1.47	1.36
20	3	612	CLA	O2D-CGD	5.12	1.45	1.33
27	4	607	CHL	O2D-CGD	5.12	1.45	1.33
20	Z	612	CLA	C1D-ND	5.12	1.44	1.37
20	A	841	CLA	O2D-CGD	5.12	1.45	1.33
27	4	608	CHL	O2D-CGD	5.12	1.45	1.33
20	B	813	CLA	C3C-C2C	5.11	1.47	1.36
20	A	840	CLA	C1D-ND	5.11	1.44	1.37
20	1	616	CLA	O2D-CGD	5.11	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	613	CLA	O2D-CGD	5.11	1.45	1.33
20	A	805	CLA	C3C-C2C	5.11	1.47	1.36
20	B	810	CLA	C1D-ND	5.11	1.44	1.37
20	A	843	CLA	O2D-CGD	5.11	1.45	1.33
20	6	603	CLA	O2D-CGD	5.11	1.45	1.33
20	1	613	CLA	O2D-CGD	5.11	1.45	1.33
20	B	824	CLA	CHC-C1C	5.11	1.48	1.35
20	1	603	CLA	C1D-ND	5.11	1.44	1.37
27	7	607	CHL	O2D-CGD	5.11	1.45	1.33
20	7	604	CLA	O2D-CGD	5.10	1.45	1.33
20	5	612	CLA	C1D-ND	5.10	1.44	1.37
27	6	618	CHL	C2C-C3C	5.10	1.47	1.36
20	8	610	CLA	C1D-ND	5.10	1.44	1.37
20	4	614	CLA	CHC-C1C	5.10	1.48	1.35
27	Z	607	CHL	CHC-C1C	5.10	1.48	1.35
20	5	612	CLA	O2D-CGD	5.10	1.45	1.33
20	L	203	CLA	C3B-C2B	5.10	1.47	1.40
20	1	614	CLA	C1D-ND	5.10	1.44	1.37
20	F	304	CLA	C3C-C2C	5.10	1.47	1.36
20	A	818	CLA	C3C-C2C	5.10	1.47	1.36
20	A	815	CLA	C1D-ND	5.10	1.44	1.37
20	Z	611	CLA	O2D-CGD	5.10	1.45	1.33
20	B	807	CLA	C1D-ND	5.10	1.44	1.37
20	B	837	CLA	CHC-C1C	5.10	1.48	1.35
20	Z	614	CLA	O2D-CGD	5.10	1.45	1.33
20	5	614	CLA	O2D-CGD	5.10	1.45	1.33
20	Z	612	CLA	O2D-CGD	5.10	1.45	1.33
20	5	617	CLA	C3B-C2B	5.09	1.47	1.40
20	G	203	CLA	C1D-ND	5.09	1.44	1.37
20	5	601	CLA	O2D-CGD	5.09	1.45	1.33
20	6	613	CLA	O2D-CGD	5.09	1.45	1.33
20	8	612	CLA	C3C-C2C	5.09	1.47	1.36
27	4	618	CHL	O2D-CGD	5.09	1.45	1.33
20	4	611	CLA	O2D-CGD	5.09	1.45	1.33
20	A	812	CLA	C3C-C2C	5.09	1.47	1.36
20	3	620	CLA	O2D-CGD	5.09	1.45	1.33
20	A	829	CLA	CHC-C1C	5.09	1.48	1.35
20	B	827	CLA	O2D-CGD	5.09	1.45	1.33
20	3	609	CLA	C1D-ND	5.09	1.44	1.37
20	A	825	CLA	C1D-ND	5.09	1.44	1.37
20	F	304	CLA	O2D-CGD	5.09	1.45	1.33
20	B	836	CLA	C3C-C2C	5.09	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	8	616	CLA	O2D-CGD	5.09	1.45	1.33
20	B	822	CLA	CHC-C1C	5.09	1.48	1.35
20	Z	613	CLA	O2D-CGD	5.09	1.45	1.33
20	Z	602	CLA	O2D-CGD	5.09	1.45	1.33
20	4	604	CLA	CHC-C1C	5.08	1.48	1.35
20	F	301	CLA	CHC-C1C	5.08	1.48	1.35
27	4	606	CHL	O2D-CGD	5.08	1.45	1.33
20	5	603	CLA	C1D-ND	5.08	1.44	1.37
20	Z	616	CLA	O2D-CGD	5.08	1.45	1.33
20	B	835	CLA	O2D-CGD	5.08	1.45	1.33
20	1	606	CLA	C1D-ND	5.08	1.44	1.37
20	A	802	CLA	C3C-C2C	5.08	1.47	1.36
20	A	825	CLA	C3C-C2C	5.08	1.47	1.36
20	A	815	CLA	CHC-C1C	5.08	1.48	1.35
20	6	612	CLA	O2D-CGD	5.08	1.45	1.33
27	1	601	CHL	CHC-C1C	5.08	1.48	1.35
20	8	602	CLA	CHC-C1C	5.08	1.48	1.35
20	4	604	CLA	O2D-CGD	5.08	1.45	1.33
20	Z	602	CLA	CHC-C1C	5.08	1.48	1.35
20	F	303	CLA	O2D-CGD	5.08	1.45	1.33
20	A	836	CLA	O2D-CGD	5.07	1.45	1.33
20	B	821	CLA	C1D-ND	5.07	1.44	1.37
20	3	602	CLA	C1D-ND	5.07	1.44	1.37
20	6	602	CLA	C1D-ND	5.07	1.44	1.37
20	5	611	CLA	O2D-CGD	5.07	1.45	1.33
20	3	614	CLA	O2D-CGD	5.07	1.45	1.33
20	A	811	CLA	C3C-C2C	5.07	1.47	1.36
20	B	816	CLA	C3C-C2C	5.07	1.47	1.36
20	A	839	CLA	C1D-ND	5.07	1.44	1.37
20	A	823	CLA	O2D-CGD	5.07	1.45	1.33
20	4	602	CLA	O2D-CGD	5.07	1.45	1.33
27	6	606	CHL	O2D-CGD	5.07	1.45	1.33
20	4	613	CLA	C3C-C2C	5.07	1.47	1.36
20	B	802	CLA	C3C-C2C	5.07	1.47	1.36
20	B	831	CLA	O2D-CGD	5.07	1.45	1.33
27	6	607	CHL	O2D-CGD	5.07	1.45	1.33
20	A	838	CLA	C1D-ND	5.07	1.44	1.37
20	B	830	CLA	CHC-C1C	5.07	1.48	1.35
27	8	607	CHL	C2C-C3C	5.07	1.47	1.36
20	6	616	CLA	O2D-CGD	5.07	1.45	1.33
20	B	820	CLA	O2D-CGD	5.07	1.45	1.33
20	7	614	CLA	C1D-ND	5.07	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	819	CLA	O2D-CGD	5.07	1.45	1.33
20	8	609	CLA	CHC-C1C	5.07	1.48	1.35
20	B	808	CLA	C3C-C2C	5.07	1.47	1.36
20	B	826	CLA	C1D-ND	5.06	1.44	1.37
20	L	204	CLA	C1D-ND	5.06	1.44	1.37
20	3	603	CLA	O2D-CGD	5.06	1.45	1.33
20	A	807	CLA	C1D-ND	5.06	1.44	1.37
20	6	617	CLA	C1D-ND	5.06	1.44	1.37
20	G	204	CLA	O2D-CGD	5.06	1.45	1.33
20	B	831	CLA	CHC-C1C	5.06	1.47	1.35
20	8	614	CLA	O2D-CGD	5.06	1.45	1.33
20	7	613	CLA	O2D-CGD	5.06	1.45	1.33
20	6	604	CLA	C1D-ND	5.06	1.44	1.37
20	8	614	CLA	CHC-C1C	5.06	1.47	1.35
20	5	604	CLA	O2D-CGD	5.06	1.45	1.33
20	A	832	CLA	C3C-C2C	5.06	1.47	1.36
20	B	811	CLA	C1D-ND	5.06	1.44	1.37
20	A	816	CLA	O2D-CGD	5.06	1.45	1.33
20	8	606	CLA	C1D-ND	5.06	1.44	1.37
20	7	616	CLA	O2D-CGD	5.06	1.45	1.33
20	3	611	CLA	O2D-CGD	5.06	1.45	1.33
20	4	603	CLA	O2D-CGD	5.06	1.45	1.33
27	Z	607	CHL	O2D-CGD	5.06	1.45	1.33
20	8	603	CLA	C1D-ND	5.06	1.44	1.37
20	1	614	CLA	O2D-CGD	5.06	1.45	1.33
20	7	610	CLA	C1D-ND	5.06	1.44	1.37
20	5	621	CLA	O2D-CGD	5.05	1.45	1.33
20	3	613	CLA	C3C-C2C	5.05	1.47	1.36
20	A	807	CLA	O2D-CGD	5.05	1.45	1.33
20	5	606	CLA	O2D-CGD	5.05	1.45	1.33
20	A	833	CLA	CHC-C1C	5.05	1.47	1.35
20	6	610	CLA	O2D-CGD	5.05	1.45	1.33
20	1	606	CLA	O2D-CGD	5.05	1.45	1.33
20	1	606	CLA	CHC-C1C	5.05	1.47	1.35
27	6	608	CHL	O2D-CGD	5.05	1.45	1.33
20	A	828	CLA	CHC-C1C	5.05	1.47	1.35
27	5	608	CHL	CHC-C1C	5.05	1.47	1.35
20	B	852	CLA	C1D-ND	5.05	1.44	1.37
27	5	618	CHL	O2D-CGD	5.05	1.45	1.33
20	B	811	CLA	O2D-CGD	5.05	1.45	1.33
20	8	611	CLA	O2D-CGD	5.05	1.45	1.33
20	1	613	CLA	C3C-C2C	5.05	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	823	CLA	CHC-C1C	5.05	1.47	1.35
20	5	611	CLA	C1D-ND	5.05	1.44	1.37
20	6	604	CLA	CHC-C1C	5.05	1.47	1.35
20	B	840	CLA	C1D-ND	5.05	1.44	1.37
20	B	817	CLA	O2D-CGD	5.05	1.45	1.33
20	B	819	CLA	O2D-CGD	5.05	1.45	1.33
20	B	822	CLA	O2D-CGD	5.05	1.45	1.33
20	1	602	CLA	C3C-C2C	5.05	1.47	1.36
20	1	612	CLA	O2D-CGD	5.05	1.45	1.33
20	3	604	CLA	O2D-CGD	5.04	1.45	1.33
20	B	822	CLA	C1D-ND	5.04	1.44	1.37
20	B	838	CLA	O2D-CGD	5.04	1.45	1.33
20	5	621	CLA	C3C-C2C	5.04	1.47	1.36
20	B	806	CLA	O2D-CGD	5.04	1.45	1.33
20	5	604	CLA	C3C-C2C	5.04	1.47	1.36
20	5	614	CLA	CHC-C1C	5.04	1.47	1.35
20	1	610	CLA	C3C-C2C	5.04	1.47	1.36
20	B	817	CLA	C3B-C2B	5.04	1.47	1.40
20	7	614	CLA	CHC-C1C	5.04	1.47	1.35
20	A	833	CLA	O2D-CGD	5.04	1.45	1.33
27	1	607	CHL	O2D-CGD	5.04	1.45	1.33
20	4	603	CLA	C1D-ND	5.04	1.44	1.37
20	J	3002	CLA	O2D-CGD	5.04	1.45	1.33
20	6	601	CLA	C1D-ND	5.04	1.44	1.37
20	B	804	CLA	C3C-C2C	5.04	1.47	1.36
20	8	601	CLA	C1D-ND	5.04	1.44	1.37
20	B	804	CLA	CHC-C1C	5.04	1.47	1.35
19	A	801	CL0	C3B-C2B	5.04	1.47	1.40
20	4	602	CLA	C1D-ND	5.04	1.44	1.37
20	Z	603	CLA	C1D-ND	5.03	1.44	1.37
20	A	817	CLA	O2D-CGD	5.03	1.45	1.33
20	7	611	CLA	O2D-CGD	5.03	1.45	1.33
20	4	602	CLA	CHC-C1C	5.03	1.47	1.35
20	K	4002	CLA	CHC-C1C	5.03	1.47	1.35
20	7	610	CLA	C3C-C2C	5.03	1.47	1.36
20	B	821	CLA	CHC-C1C	5.03	1.47	1.35
20	5	603	CLA	O2D-CGD	5.03	1.45	1.33
20	Z	606	CLA	CHC-C1C	5.03	1.47	1.35
20	B	839	CLA	O2D-CGD	5.03	1.45	1.33
20	Z	614	CLA	CHC-C1C	5.03	1.47	1.35
20	L	203	CLA	O2D-CGD	5.03	1.45	1.33
20	A	821	CLA	O2D-CGD	5.03	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	825	CLA	O2D-CGD	5.03	1.45	1.33
20	4	613	CLA	O2D-CGD	5.03	1.45	1.33
20	3	610	CLA	O2D-CGD	5.03	1.45	1.33
20	B	810	CLA	O2D-CGD	5.03	1.45	1.33
20	7	620	CLA	O2D-CGD	5.03	1.45	1.33
20	L	204	CLA	CHC-C1C	5.03	1.47	1.35
20	3	617	CLA	O2D-CGD	5.03	1.45	1.33
20	5	609	CLA	C1D-ND	5.03	1.44	1.37
20	7	612	CLA	O2D-CGD	5.02	1.45	1.33
20	8	604	CLA	O2D-CGD	5.02	1.45	1.33
27	Z	601	CHL	CHC-C1C	5.02	1.47	1.35
20	1	610	CLA	O2D-CGD	5.02	1.45	1.33
19	A	801	CL0	C3C-C2C	5.02	1.47	1.36
20	6	609	CLA	O2D-CGD	5.02	1.45	1.33
20	4	609	CLA	C1D-ND	5.02	1.44	1.37
20	3	603	CLA	C3C-C2C	5.02	1.47	1.36
20	8	608	CLA	O2D-CGD	5.02	1.45	1.33
20	A	824	CLA	O2D-CGD	5.02	1.45	1.33
20	3	607	CLA	C1D-ND	5.02	1.44	1.37
20	7	612	CLA	C1D-ND	5.02	1.44	1.37
20	Z	608	CLA	O2D-CGD	5.02	1.45	1.33
20	A	826	CLA	CHC-C1C	5.02	1.47	1.35
20	A	833	CLA	C1D-ND	5.02	1.44	1.37
20	6	610	CLA	C1D-ND	5.02	1.44	1.37
20	1	611	CLA	O2D-CGD	5.02	1.45	1.33
20	A	837	CLA	CHC-C1C	5.02	1.47	1.35
20	A	820	CLA	O2D-CGD	5.01	1.45	1.33
20	5	613	CLA	C1D-ND	5.01	1.43	1.37
20	1	604	CLA	O2D-CGD	5.01	1.45	1.33
20	7	604	CLA	CHC-C1C	5.01	1.47	1.35
20	6	617	CLA	O2D-CGD	5.01	1.45	1.33
20	B	820	CLA	C1D-ND	5.01	1.43	1.37
20	4	610	CLA	O2D-CGD	5.01	1.45	1.33
20	A	837	CLA	O2D-CGD	5.01	1.45	1.33
20	6	613	CLA	C1D-ND	5.01	1.43	1.37
20	1	614	CLA	CHC-C1C	5.01	1.47	1.35
20	B	806	CLA	C1D-ND	5.01	1.43	1.37
20	7	602	CLA	C1D-ND	5.01	1.43	1.37
20	8	604	CLA	CHC-C1C	5.01	1.47	1.35
27	4	608	CHL	CHC-C1C	5.01	1.47	1.35
20	A	830	CLA	O2D-CGD	5.01	1.45	1.33
20	3	611	CLA	CHC-C1C	5.01	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	5	602	CLA	C3C-C2C	5.01	1.47	1.36
20	4	609	CLA	O2D-CGD	5.01	1.45	1.33
20	B	807	CLA	O2D-CGD	5.01	1.45	1.33
20	A	814	CLA	C3C-C2C	5.00	1.47	1.36
20	1	608	CLA	O2D-CGD	5.00	1.45	1.33
20	6	611	CLA	O2D-CGD	5.00	1.45	1.33
20	5	606	CLA	CHC-C1C	5.00	1.47	1.35
20	B	823	CLA	O2D-CGD	5.00	1.45	1.33
20	A	819	CLA	CHC-C1C	5.00	1.47	1.35
20	B	816	CLA	O2D-CGD	5.00	1.45	1.33
20	B	839	CLA	CHC-C1C	5.00	1.47	1.35
20	3	606	CLA	CHC-C1C	5.00	1.47	1.35
20	8	613	CLA	C3C-C2C	5.00	1.47	1.36
20	Z	602	CLA	C3C-C2C	5.00	1.47	1.36
20	6	601	CLA	O2D-CGD	5.00	1.45	1.33
20	B	805	CLA	O2D-CGD	5.00	1.45	1.33
20	B	814	CLA	C1D-ND	5.00	1.43	1.37
20	1	604	CLA	CHC-C1C	5.00	1.47	1.35
20	Z	602	CLA	C1D-ND	5.00	1.43	1.37
20	B	832	CLA	C1D-ND	5.00	1.43	1.37
20	1	602	CLA	C1D-ND	5.00	1.43	1.37
27	6	607	CHL	C2C-C3C	4.99	1.47	1.36
20	Z	603	CLA	O2D-CGD	4.99	1.45	1.33
20	B	818	CLA	C1D-ND	4.99	1.43	1.37
20	Z	610	CLA	C3C-C2C	4.99	1.47	1.36
20	7	609	CLA	O2D-CGD	4.99	1.45	1.33
20	B	818	CLA	C3C-C2C	4.99	1.47	1.36
20	Z	613	CLA	C1D-ND	4.99	1.43	1.37
20	6	611	CLA	CHC-C1C	4.99	1.47	1.35
20	B	840	CLA	O2D-CGD	4.99	1.45	1.33
20	3	602	CLA	O2D-CGD	4.99	1.45	1.33
20	7	608	CLA	O2D-CGD	4.99	1.45	1.33
20	3	614	CLA	CHC-C1C	4.99	1.47	1.35
20	8	613	CLA	O2D-CGD	4.99	1.45	1.33
27	4	618	CHL	C2C-C3C	4.99	1.47	1.36
20	Z	613	CLA	CHC-C1C	4.99	1.47	1.35
20	1	612	CLA	C1D-ND	4.99	1.43	1.37
20	B	812	CLA	O2D-CGD	4.99	1.45	1.33
27	Z	601	CHL	O2D-CGD	4.99	1.45	1.33
20	7	616	CLA	CHC-C1C	4.99	1.47	1.35
20	A	813	CLA	CHC-C1C	4.99	1.47	1.35
20	4	612	CLA	C1D-ND	4.98	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	834	CLA	C1D-ND	4.98	1.43	1.37
20	A	837	CLA	C1D-ND	4.98	1.43	1.37
20	1	611	CLA	C1D-ND	4.98	1.43	1.37
20	A	843	CLA	C3C-C2C	4.98	1.47	1.36
20	8	606	CLA	O2D-CGD	4.98	1.45	1.33
20	6	604	CLA	O2D-CGD	4.98	1.45	1.33
20	4	610	CLA	CHC-C1C	4.98	1.47	1.35
20	A	805	CLA	C3B-C2B	4.98	1.47	1.40
20	K	4002	CLA	O2D-CGD	4.98	1.45	1.33
20	A	842	CLA	C1D-ND	4.98	1.43	1.37
20	A	830	CLA	C3C-C2C	4.98	1.47	1.36
20	B	804	CLA	C1D-ND	4.98	1.43	1.37
20	5	602	CLA	C1D-ND	4.98	1.43	1.37
20	A	826	CLA	O2D-CGD	4.98	1.45	1.33
20	A	810	CLA	CHC-C1C	4.97	1.47	1.35
20	B	841	CLA	CHC-C1C	4.97	1.47	1.35
20	A	817	CLA	C3B-C2B	4.97	1.47	1.40
20	7	603	CLA	O2D-CGD	4.97	1.45	1.33
20	Z	616	CLA	CHC-C1C	4.97	1.47	1.35
20	1	616	CLA	CHC-C1C	4.97	1.47	1.35
20	7	608	CLA	CHC-C1C	4.97	1.47	1.35
20	A	802	CLA	CHC-C1C	4.97	1.47	1.35
20	B	834	CLA	O2D-CGD	4.97	1.45	1.33
20	6	616	CLA	C1D-ND	4.97	1.43	1.37
20	B	818	CLA	O2D-CGD	4.97	1.45	1.33
20	3	607	CLA	O2D-CGD	4.97	1.45	1.33
20	7	620	CLA	CHC-C1C	4.97	1.47	1.35
20	A	812	CLA	O2D-CGD	4.97	1.45	1.33
27	5	607	CHL	CHC-C1C	4.97	1.47	1.35
20	6	622	CLA	O2D-CGD	4.97	1.45	1.33
19	A	801	CL0	O2D-CGD	4.97	1.45	1.33
20	B	836	CLA	O2D-CGD	4.96	1.45	1.33
20	B	841	CLA	C1D-ND	4.96	1.43	1.37
20	B	809	CLA	O2D-CGD	4.96	1.45	1.33
20	8	608	CLA	CHC-C1C	4.96	1.47	1.35
20	A	808	CLA	O2D-CGD	4.96	1.45	1.33
20	G	204	CLA	CHC-C1C	4.96	1.47	1.35
20	1	616	CLA	C1D-ND	4.96	1.43	1.37
20	B	806	CLA	C3C-C2C	4.96	1.47	1.36
20	L	203	CLA	CHC-C1C	4.96	1.47	1.35
27	5	608	CHL	O2D-CGD	4.96	1.45	1.33
20	A	835	CLA	O2D-CGD	4.96	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	841	CLA	C1D-ND	4.96	1.43	1.37
27	6	608	CHL	CHC-C1C	4.96	1.47	1.35
20	L	203	CLA	C1D-ND	4.96	1.43	1.37
20	B	824	CLA	C3C-C2C	4.96	1.47	1.36
20	B	838	CLA	CHC-C1C	4.96	1.47	1.35
20	6	602	CLA	O2D-CGD	4.96	1.45	1.33
20	K	4003	CLA	CHC-C1C	4.95	1.47	1.35
20	B	819	CLA	C1D-ND	4.95	1.43	1.37
20	6	622	CLA	CHC-C1C	4.95	1.47	1.35
20	8	603	CLA	O2D-CGD	4.95	1.45	1.33
20	A	834	CLA	O2D-CGD	4.95	1.45	1.33
20	F	303	CLA	CHC-C1C	4.95	1.47	1.35
27	6	618	CHL	CHC-C1C	4.95	1.47	1.35
20	B	836	CLA	CHC-C1C	4.95	1.47	1.35
20	Z	611	CLA	CHC-C1C	4.95	1.47	1.35
20	B	832	CLA	CHC-C1C	4.95	1.47	1.35
20	1	611	CLA	CHC-C1C	4.95	1.47	1.35
20	3	602	CLA	C3C-C2C	4.95	1.47	1.36
20	B	828	CLA	O2D-CGD	4.95	1.45	1.33
20	B	833	CLA	CHC-C1C	4.95	1.47	1.35
20	Z	609	CLA	O2D-CGD	4.95	1.45	1.33
20	6	612	CLA	C1D-ND	4.95	1.43	1.37
20	5	610	CLA	C1D-ND	4.95	1.43	1.37
20	8	601	CLA	O2D-CGD	4.95	1.45	1.33
20	B	803	CLA	C3C-C2C	4.95	1.47	1.36
20	7	602	CLA	O2D-CGD	4.95	1.45	1.33
20	A	836	CLA	C1D-ND	4.95	1.43	1.37
20	3	602	CLA	CHC-C1C	4.95	1.47	1.35
20	6	613	CLA	CHC-C1C	4.95	1.47	1.35
20	A	823	CLA	C1D-ND	4.95	1.43	1.37
20	8	604	CLA	C1D-ND	4.95	1.43	1.37
20	A	812	CLA	CHC-C1C	4.94	1.47	1.35
20	A	818	CLA	CHC-C1C	4.94	1.47	1.35
20	A	841	CLA	CHC-C1C	4.94	1.47	1.35
20	A	803	CLA	C3C-C2C	4.94	1.47	1.36
27	3	608	CHL	C3B-C2B	4.94	1.47	1.40
20	8	613	CLA	CHC-C1C	4.94	1.47	1.35
20	B	821	CLA	O2D-CGD	4.94	1.45	1.33
20	B	830	CLA	O2D-CGD	4.94	1.45	1.33
20	B	852	CLA	CHC-C1C	4.94	1.47	1.35
20	7	613	CLA	C1D-ND	4.94	1.43	1.37
20	B	808	CLA	O2D-CGD	4.94	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	613	CLA	CHC-C1C	4.94	1.47	1.35
20	8	616	CLA	CHC-C1C	4.94	1.47	1.35
20	A	805	CLA	C1D-ND	4.94	1.43	1.37
20	3	610	CLA	C3C-C2C	4.94	1.47	1.36
20	B	831	CLA	C1D-ND	4.94	1.43	1.37
20	B	813	CLA	CHC-C1C	4.94	1.47	1.35
20	A	818	CLA	O2D-CGD	4.93	1.45	1.33
20	5	609	CLA	O2D-CGD	4.93	1.45	1.33
20	5	601	CLA	C1D-ND	4.93	1.43	1.37
20	1	609	CLA	O2D-CGD	4.93	1.45	1.33
20	A	827	CLA	O2D-CGD	4.93	1.45	1.33
20	B	833	CLA	C1D-ND	4.93	1.43	1.37
20	B	835	CLA	CHC-C1C	4.93	1.47	1.35
20	A	804	CLA	CHC-C1C	4.93	1.47	1.35
20	Z	604	CLA	CHC-C1C	4.93	1.47	1.35
20	7	606	CLA	CHC-C1C	4.93	1.47	1.35
20	5	601	CLA	CHC-C1C	4.93	1.47	1.35
20	A	811	CLA	O2D-CGD	4.93	1.45	1.33
27	5	618	CHL	CHC-C1C	4.93	1.47	1.35
20	A	822	CLA	O2D-CGD	4.93	1.45	1.33
20	A	821	CLA	C1D-ND	4.93	1.43	1.37
20	A	814	CLA	CHC-C1C	4.93	1.47	1.35
20	3	604	CLA	C1D-ND	4.93	1.43	1.37
27	3	608	CHL	O2D-CGD	4.93	1.45	1.33
20	3	610	CLA	C1D-ND	4.92	1.43	1.37
20	A	829	CLA	C3C-C2C	4.92	1.47	1.36
20	7	609	CLA	CHC-C1C	4.92	1.47	1.35
20	Z	612	CLA	CHC-C1C	4.92	1.47	1.35
20	4	610	CLA	C1D-ND	4.92	1.43	1.37
20	6	612	CLA	CHC-C1C	4.92	1.47	1.35
20	3	609	CLA	CHC-C1C	4.92	1.47	1.35
20	A	808	CLA	C1D-ND	4.92	1.43	1.37
20	3	603	CLA	C1D-ND	4.92	1.43	1.37
27	6	607	CHL	CHC-C1C	4.92	1.47	1.35
27	5	607	CHL	O2D-CGD	4.92	1.45	1.33
20	A	811	CLA	CHC-C1C	4.92	1.47	1.35
20	6	617	CLA	CHC-C1C	4.92	1.47	1.35
20	8	612	CLA	C1D-ND	4.91	1.43	1.37
20	A	809	CLA	O2D-CGD	4.91	1.45	1.33
20	B	809	CLA	C3B-C2B	4.91	1.47	1.40
20	A	832	CLA	O2D-CGD	4.91	1.45	1.33
20	A	813	CLA	C1D-ND	4.91	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	5	617	CLA	O2D-CGD	4.91	1.45	1.33
20	A	824	CLA	C1D-ND	4.91	1.43	1.37
20	B	835	CLA	C1D-ND	4.91	1.43	1.37
20	5	612	CLA	CHC-C1C	4.91	1.47	1.35
20	3	617	CLA	CHC-C1C	4.91	1.47	1.35
20	A	820	CLA	CHC-C1C	4.91	1.47	1.35
20	B	819	CLA	CHC-C1C	4.91	1.47	1.35
20	A	809	CLA	CHC-C1C	4.90	1.47	1.35
20	Z	608	CLA	CHC-C1C	4.90	1.47	1.35
20	B	826	CLA	CHC-C1C	4.90	1.47	1.35
27	4	607	CHL	CHC-C1C	4.90	1.47	1.35
20	A	810	CLA	O2D-CGD	4.90	1.45	1.33
20	1	608	CLA	CHC-C1C	4.90	1.47	1.35
20	B	809	CLA	C3C-C2C	4.90	1.47	1.36
20	7	603	CLA	CHC-C1C	4.90	1.47	1.35
20	5	602	CLA	O2D-CGD	4.90	1.45	1.33
20	7	610	CLA	O2D-CGD	4.90	1.45	1.33
20	B	833	CLA	O2D-CGD	4.90	1.45	1.33
20	1	603	CLA	O2D-CGD	4.90	1.45	1.33
20	8	602	CLA	C1D-ND	4.89	1.43	1.37
20	7	610	CLA	C3B-C2B	4.89	1.47	1.40
20	B	836	CLA	C1D-ND	4.89	1.43	1.37
20	6	601	CLA	CHC-C1C	4.89	1.47	1.35
20	B	837	CLA	C1D-ND	4.89	1.43	1.37
20	1	613	CLA	C1D-ND	4.89	1.43	1.37
20	A	830	CLA	CHC-C1C	4.89	1.47	1.35
20	A	840	CLA	O2D-CGD	4.89	1.45	1.33
20	B	802	CLA	O2D-CGD	4.89	1.45	1.33
20	G	203	CLA	CHC-C1C	4.89	1.47	1.35
20	5	611	CLA	CHC-C1C	4.89	1.47	1.35
20	A	842	CLA	O2D-CGD	4.89	1.45	1.33
20	4	611	CLA	CHC-C1C	4.89	1.47	1.35
20	8	614	CLA	C1D-ND	4.89	1.43	1.37
20	A	811	CLA	C1D-ND	4.88	1.43	1.37
20	5	610	CLA	O2D-CGD	4.88	1.45	1.33
20	4	601	CLA	CHC-C1C	4.88	1.47	1.35
20	1	609	CLA	CHC-C1C	4.88	1.47	1.35
20	A	806	CLA	O2D-CGD	4.88	1.45	1.33
20	B	812	CLA	CHC-C1C	4.88	1.47	1.35
27	6	606	CHL	C2C-C3C	4.88	1.47	1.36
20	B	826	CLA	O2D-CGD	4.88	1.45	1.33
20	B	827	CLA	CHC-C1C	4.88	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	7	614	CLA	O2D-CGD	4.88	1.45	1.33
20	B	839	CLA	C1D-ND	4.88	1.43	1.37
20	A	832	CLA	CHC-C1C	4.88	1.47	1.35
20	B	813	CLA	C1D-ND	4.87	1.43	1.37
20	1	602	CLA	O2D-CGD	4.87	1.45	1.33
20	A	820	CLA	C1D-ND	4.87	1.43	1.37
20	B	834	CLA	CHC-C1C	4.87	1.47	1.35
20	7	601	CLA	C1D-ND	4.87	1.43	1.37
20	4	601	CLA	C1D-ND	4.87	1.43	1.37
27	3	608	CHL	C2C-C3C	4.87	1.47	1.36
20	A	843	CLA	CHC-C1C	4.87	1.47	1.35
20	4	612	CLA	CHC-C1C	4.87	1.47	1.35
20	8	611	CLA	CHC-C1C	4.86	1.47	1.35
20	5	613	CLA	CHC-C1C	4.86	1.47	1.35
20	5	609	CLA	CHC-C1C	4.86	1.47	1.35
20	A	823	CLA	CHC-C1C	4.86	1.47	1.35
20	7	601	CLA	CHC-C1C	4.86	1.47	1.35
20	A	842	CLA	CHC-C1C	4.86	1.47	1.35
20	B	814	CLA	O2D-CGD	4.86	1.45	1.33
20	B	823	CLA	C1D-ND	4.86	1.43	1.37
20	A	839	CLA	CHC-C1C	4.86	1.47	1.35
27	1	601	CHL	O2D-CGD	4.86	1.45	1.33
20	A	815	CLA	O2D-CGD	4.85	1.45	1.33
20	3	604	CLA	CHC-C1C	4.85	1.47	1.35
20	J	3002	CLA	CHC-C1C	4.85	1.47	1.35
27	6	608	CHL	C2C-C3C	4.85	1.47	1.36
20	A	827	CLA	C1D-ND	4.85	1.43	1.37
20	A	843	CLA	C1D-ND	4.85	1.43	1.37
20	7	609	CLA	C1D-ND	4.85	1.43	1.37
20	B	810	CLA	CHC-C1C	4.85	1.47	1.35
20	3	607	CLA	CHC-C1C	4.85	1.47	1.35
20	B	815	CLA	CHC-C1C	4.85	1.47	1.35
20	7	606	CLA	O2D-CGD	4.85	1.45	1.33
20	A	835	CLA	CHC-C1C	4.85	1.47	1.35
20	B	820	CLA	CHC-C1C	4.85	1.47	1.35
20	A	839	CLA	O2D-CGD	4.84	1.45	1.33
27	4	606	CHL	C2C-C3C	4.84	1.47	1.36
20	A	819	CLA	C1D-ND	4.84	1.43	1.37
20	8	616	CLA	C1D-ND	4.84	1.43	1.37
27	4	618	CHL	CHC-C1C	4.84	1.47	1.35
20	A	840	CLA	CHC-C1C	4.84	1.47	1.35
20	A	845	CLA	CHC-C1C	4.84	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	7	608	CLA	C1D-ND	4.84	1.43	1.37
20	3	620	CLA	CHC-C1C	4.83	1.47	1.35
20	A	829	CLA	O2D-CGD	4.83	1.45	1.33
20	B	841	CLA	O2D-CGD	4.83	1.45	1.33
20	A	831	CLA	O2D-CGD	4.83	1.45	1.33
20	B	804	CLA	O2D-CGD	4.83	1.45	1.33
20	8	603	CLA	CHC-C1C	4.83	1.47	1.35
20	B	815	CLA	O2D-CGD	4.83	1.45	1.33
20	7	604	CLA	C3C-C2C	4.83	1.47	1.36
27	7	607	CHL	CHC-C1C	4.83	1.47	1.35
20	B	806	CLA	CHC-C1C	4.83	1.47	1.35
20	B	829	CLA	O2D-CGD	4.83	1.45	1.33
20	8	601	CLA	CHC-C1C	4.82	1.47	1.35
20	8	608	CLA	C3C-C2C	4.82	1.47	1.36
20	B	811	CLA	CHC-C1C	4.82	1.47	1.35
20	8	606	CLA	CHC-C1C	4.82	1.47	1.35
20	A	828	CLA	O2D-CGD	4.82	1.45	1.33
20	A	814	CLA	C1D-ND	4.82	1.43	1.37
20	A	813	CLA	O2D-CGD	4.82	1.45	1.33
27	4	606	CHL	CHC-C1C	4.82	1.47	1.35
20	6	614	CLA	O2D-CGD	4.81	1.44	1.33
20	A	824	CLA	CHC-C1C	4.81	1.47	1.35
20	5	621	CLA	C1D-ND	4.81	1.43	1.37
20	Z	609	CLA	CHC-C1C	4.81	1.47	1.35
20	A	838	CLA	O2D-CGD	4.81	1.44	1.33
20	5	617	CLA	C1D-ND	4.80	1.43	1.37
20	6	622	CLA	C1D-ND	4.80	1.43	1.37
20	A	834	CLA	CHC-C1C	4.80	1.47	1.35
20	A	822	CLA	C3B-C2B	4.80	1.47	1.40
20	B	807	CLA	CHC-C1C	4.80	1.47	1.35
20	A	806	CLA	C3C-C2C	4.80	1.46	1.36
27	8	607	CHL	CHC-C1C	4.80	1.47	1.35
20	5	603	CLA	CHC-C1C	4.79	1.47	1.35
20	4	613	CLA	O2A-CGA	4.79	1.47	1.33
20	4	613	CLA	CHC-C1C	4.79	1.47	1.35
20	B	837	CLA	O2D-CGD	4.79	1.44	1.33
20	Z	603	CLA	CHC-C1C	4.79	1.47	1.35
20	4	601	CLA	O2D-CGD	4.79	1.44	1.33
20	7	601	CLA	O2D-CGD	4.78	1.44	1.33
20	6	609	CLA	CHC-C1C	4.78	1.47	1.35
20	1	603	CLA	CHC-C1C	4.78	1.47	1.35
20	A	803	CLA	C1D-ND	4.78	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	808	CLA	CHC-C1C	4.78	1.47	1.35
20	A	805	CLA	O2D-CGD	4.78	1.44	1.33
20	B	803	CLA	C1D-ND	4.78	1.43	1.37
20	A	806	CLA	CHC-C1C	4.78	1.47	1.35
20	8	609	CLA	C1D-ND	4.78	1.43	1.37
20	5	604	CLA	CHC-C1C	4.78	1.47	1.35
20	6	603	CLA	CHC-C1C	4.78	1.47	1.35
20	A	836	CLA	CHC-C1C	4.77	1.47	1.35
20	7	612	CLA	CHC-C1C	4.77	1.47	1.35
20	8	602	CLA	O2D-CGD	4.77	1.44	1.33
20	4	614	CLA	C1D-ND	4.77	1.43	1.37
20	F	301	CLA	O2D-CGD	4.77	1.44	1.33
20	8	609	CLA	O2D-CGD	4.77	1.44	1.33
20	B	828	CLA	CHC-C1C	4.77	1.47	1.35
20	A	829	CLA	C1D-ND	4.77	1.43	1.37
20	B	824	CLA	O2D-CGD	4.76	1.44	1.33
27	5	608	CHL	C2C-C3C	4.76	1.46	1.36
20	F	304	CLA	CHC-C1C	4.76	1.47	1.35
20	A	804	CLA	O2D-CGD	4.76	1.44	1.33
20	5	616	CLA	O2D-CGD	4.75	1.44	1.33
21	A	844	PQN	C10-C5	4.75	1.48	1.40
20	A	809	CLA	C1D-ND	4.75	1.43	1.37
20	8	612	CLA	CHC-C1C	4.75	1.47	1.35
20	7	611	CLA	CHC-C1C	4.75	1.47	1.35
20	A	822	CLA	C1D-ND	4.75	1.43	1.37
20	A	826	CLA	C3B-C2B	4.75	1.47	1.40
20	A	854	CLA	O2D-CGD	4.74	1.44	1.33
20	A	803	CLA	CHC-C1C	4.73	1.47	1.35
27	3	608	CHL	CHC-C1C	4.73	1.47	1.35
20	B	808	CLA	CHC-C1C	4.72	1.47	1.35
20	B	803	CLA	O2D-CGD	4.72	1.44	1.33
20	3	613	CLA	CHC-C1C	4.72	1.47	1.35
20	3	609	CLA	O2D-CGD	4.72	1.44	1.33
20	1	612	CLA	CHC-C1C	4.71	1.47	1.35
20	A	838	CLA	CHC-C1C	4.71	1.47	1.35
20	5	621	CLA	CHC-C1C	4.71	1.47	1.35
20	7	613	CLA	CHC-C1C	4.71	1.47	1.35
19	A	801	CL0	C1D-ND	4.71	1.43	1.37
20	B	838	CLA	C1D-ND	4.71	1.43	1.37
20	3	603	CLA	CHC-C1C	4.71	1.47	1.35
20	A	821	CLA	CHC-C1C	4.71	1.47	1.35
20	A	826	CLA	C1D-ND	4.70	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	5	616	CLA	CHC-C1C	4.70	1.47	1.35
20	A	814	CLA	O2D-CGD	4.70	1.44	1.33
20	A	825	CLA	CHC-C1C	4.69	1.47	1.35
20	3	613	CLA	C1D-ND	4.69	1.43	1.37
20	B	829	CLA	C3B-C2B	4.69	1.46	1.40
20	4	609	CLA	CHC-C1C	4.68	1.47	1.35
21	B	842	PQN	C10-C5	4.68	1.48	1.40
20	B	824	CLA	C1D-ND	4.67	1.43	1.37
20	B	830	CLA	C1D-ND	4.67	1.43	1.37
20	B	813	CLA	O2D-CGD	4.67	1.44	1.33
20	3	612	CLA	CHC-C1C	4.66	1.46	1.35
20	7	616	CLA	C1D-ND	4.66	1.43	1.37
20	A	812	CLA	C1D-ND	4.66	1.43	1.37
20	5	617	CLA	CHC-C1C	4.65	1.46	1.35
20	A	817	CLA	CHC-C1C	4.65	1.46	1.35
20	1	610	CLA	C1D-ND	4.65	1.43	1.37
27	4	608	CHL	C2C-C3C	4.65	1.46	1.36
20	8	613	CLA	C1D-ND	4.64	1.43	1.37
20	A	807	CLA	CHC-C1C	4.63	1.46	1.35
20	B	802	CLA	CHC-C1C	4.63	1.46	1.35
20	A	831	CLA	CHC-C1C	4.63	1.46	1.35
20	Z	610	CLA	C1D-ND	4.63	1.43	1.37
20	A	803	CLA	O2D-CGD	4.63	1.44	1.33
20	A	804	CLA	C1D-ND	4.62	1.43	1.37
20	B	805	CLA	C1D-ND	4.62	1.43	1.37
20	B	809	CLA	CHC-C1C	4.62	1.46	1.35
20	B	825	CLA	C1D-ND	4.61	1.43	1.37
20	A	806	CLA	C1D-ND	4.60	1.43	1.37
20	B	840	CLA	CHC-C1C	4.60	1.46	1.35
20	B	809	CLA	C1D-ND	4.59	1.43	1.37
20	B	818	CLA	CHC-C1C	4.58	1.46	1.35
20	A	810	CLA	C1D-ND	4.58	1.43	1.37
20	4	603	CLA	CHC-C1C	4.57	1.46	1.35
20	A	832	CLA	C1D-ND	4.55	1.43	1.37
20	B	808	CLA	C1D-ND	4.55	1.43	1.37
20	1	613	CLA	O2A-CGA	4.55	1.46	1.33
20	B	802	CLA	C1D-ND	4.54	1.43	1.37
20	5	613	CLA	O2A-CGA	4.54	1.46	1.33
20	B	827	CLA	C1D-ND	4.53	1.43	1.37
20	B	817	CLA	CHC-C1C	4.52	1.46	1.35
20	A	831	CLA	C1D-ND	4.52	1.43	1.37
20	B	825	CLA	O2D-CGD	4.52	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	832	CLA	O2D-CGD	4.51	1.44	1.33
20	B	835	CLA	O2A-CGA	4.51	1.45	1.30
20	A	854	CLA	O2A-CGA	4.51	1.46	1.33
20	4	604	CLA	CHD-C1D	4.50	1.47	1.38
20	A	837	CLA	CHD-C1D	4.50	1.47	1.38
20	1	604	CLA	CHD-C1D	4.50	1.47	1.38
20	6	610	CLA	CHD-C1D	4.50	1.47	1.38
20	K	4002	CLA	O2A-CGA	4.49	1.45	1.30
20	B	828	CLA	C1D-ND	4.49	1.43	1.37
20	A	821	CLA	O2A-CGA	4.48	1.45	1.30
20	3	614	CLA	O2A-CGA	4.48	1.45	1.30
22	4	622	LHG	O7-C7	4.46	1.46	1.34
20	5	614	CLA	O2A-CGA	4.46	1.45	1.30
20	B	819	CLA	C3B-C2B	4.46	1.46	1.40
20	6	622	CLA	O2A-CGA	4.46	1.45	1.30
20	8	603	CLA	O2A-CGA	4.44	1.45	1.30
20	A	838	CLA	CHD-C1D	4.43	1.47	1.38
20	A	835	CLA	CHD-C1D	4.43	1.47	1.38
20	8	611	CLA	CHD-C1D	4.43	1.47	1.38
27	4	606	CHL	O2A-CGA	4.43	1.46	1.33
20	4	611	CLA	CHD-C1D	4.43	1.47	1.38
20	B	828	CLA	O2A-CGA	4.43	1.46	1.33
20	B	819	CLA	CHD-C1D	4.42	1.47	1.38
20	K	4002	CLA	CHD-C1D	4.42	1.47	1.38
20	1	609	CLA	O2A-CGA	4.42	1.46	1.33
20	F	303	CLA	O2A-CGA	4.42	1.45	1.30
20	3	611	CLA	CHD-C1D	4.42	1.47	1.38
20	G	204	CLA	CHD-C1D	4.42	1.47	1.38
20	B	833	CLA	O2A-CGA	4.41	1.46	1.33
20	6	616	CLA	CHD-C1D	4.41	1.47	1.38
20	Z	604	CLA	CHD-C1D	4.41	1.47	1.38
20	K	4003	CLA	CHD-C1D	4.41	1.46	1.38
20	3	606	CLA	CHD-C1D	4.41	1.46	1.38
20	A	838	CLA	O2A-CGA	4.40	1.46	1.33
20	Z	613	CLA	O2A-CGA	4.40	1.46	1.33
20	A	810	CLA	O2A-CGA	4.40	1.46	1.33
20	Z	603	CLA	CHD-C1D	4.40	1.46	1.38
20	A	818	CLA	O2A-CGA	4.40	1.46	1.33
20	6	601	CLA	CHD-C1D	4.40	1.46	1.38
20	B	834	CLA	CHD-C1D	4.40	1.46	1.38
20	A	807	CLA	CHD-C1D	4.40	1.46	1.38
20	5	613	CLA	CHD-C1D	4.40	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	815	CLA	CHD-C1D	4.39	1.46	1.38
20	B	812	CLA	O2A-CGA	4.39	1.46	1.33
20	6	604	CLA	CHD-C1D	4.39	1.46	1.38
20	7	602	CLA	O2A-CGA	4.39	1.46	1.33
20	A	825	CLA	O2A-CGA	4.38	1.46	1.33
20	A	817	CLA	CHD-C1D	4.38	1.46	1.38
20	B	817	CLA	CHD-C1D	4.38	1.46	1.38
20	1	603	CLA	O2A-CGA	4.37	1.46	1.33
20	3	607	CLA	CHD-C1D	4.37	1.46	1.38
20	B	815	CLA	O2A-CGA	4.37	1.46	1.33
20	5	604	CLA	CHD-C1D	4.37	1.46	1.38
27	Z	607	CHL	O2A-CGA	4.37	1.46	1.33
20	Z	609	CLA	CHD-C1D	4.37	1.46	1.38
20	6	617	CLA	CHD-C1D	4.37	1.46	1.38
20	A	837	CLA	O2A-CGA	4.37	1.45	1.30
20	A	802	CLA	O2A-CGA	4.36	1.46	1.33
20	A	825	CLA	CHD-C1D	4.36	1.46	1.38
20	B	810	CLA	CHD-C1D	4.36	1.46	1.38
20	5	612	CLA	O2A-CGA	4.36	1.46	1.33
20	B	807	CLA	CHD-C1D	4.36	1.46	1.38
19	A	801	CL0	CHC-C1C	4.36	1.46	1.35
20	A	836	CLA	O2A-CGA	4.36	1.46	1.33
20	F	304	CLA	O2A-CGA	4.35	1.46	1.33
20	5	602	CLA	O2A-CGA	4.35	1.46	1.33
27	6	606	CHL	O2A-CGA	4.35	1.46	1.33
20	A	815	CLA	O2A-CGA	4.35	1.46	1.33
27	7	607	CHL	CHD-C1D	4.35	1.46	1.38
20	A	813	CLA	O2A-CGA	4.35	1.46	1.33
20	8	604	CLA	CHD-C1D	4.35	1.46	1.38
20	A	845	CLA	O2A-CGA	4.35	1.46	1.33
20	J	3002	CLA	CHD-C1D	4.34	1.46	1.38
20	5	601	CLA	O2A-CGA	4.34	1.46	1.33
20	6	613	CLA	O2A-CGA	4.34	1.46	1.33
20	Z	611	CLA	O2A-CGA	4.34	1.46	1.33
20	6	611	CLA	CHD-C1D	4.34	1.46	1.38
20	8	612	CLA	O2A-CGA	4.34	1.46	1.33
20	4	609	CLA	O2A-CGA	4.34	1.46	1.33
20	7	620	CLA	CHD-C1D	4.34	1.46	1.38
20	Z	609	CLA	O2A-CGA	4.34	1.46	1.33
20	B	822	CLA	O2A-CGA	4.34	1.46	1.33
20	3	613	CLA	O2A-CGA	4.34	1.46	1.33
20	A	840	CLA	O2A-CGA	4.34	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	6	611	CLA	O2A-CGA	4.34	1.46	1.33
20	4	614	CLA	O2A-CGA	4.33	1.45	1.30
20	Z	611	CLA	CHD-C1D	4.33	1.46	1.38
20	B	824	CLA	O2A-CGA	4.33	1.46	1.33
20	3	617	CLA	CHD-C1D	4.33	1.46	1.38
20	3	614	CLA	CHD-C1D	4.33	1.46	1.38
20	Z	608	CLA	CHD-C1D	4.33	1.46	1.38
20	3	607	CLA	O2A-CGA	4.33	1.46	1.33
20	B	852	CLA	O2A-CGA	4.33	1.46	1.33
20	1	602	CLA	O2A-CGA	4.33	1.46	1.33
20	1	606	CLA	O2A-CGA	4.33	1.46	1.33
20	Z	608	CLA	O2A-CGA	4.33	1.46	1.33
20	7	603	CLA	CHD-C1D	4.33	1.46	1.38
20	5	603	CLA	CHD-C1D	4.32	1.46	1.38
20	1	612	CLA	O2A-CGA	4.32	1.46	1.33
20	8	613	CLA	O2A-CGA	4.32	1.46	1.33
20	4	616	CLA	CHD-C1D	4.32	1.46	1.38
20	A	808	CLA	O2A-CGA	4.32	1.46	1.33
20	B	825	CLA	O2A-CGA	4.32	1.46	1.33
20	A	830	CLA	C1D-ND	4.32	1.43	1.37
20	3	609	CLA	O2A-CGA	4.32	1.46	1.33
20	1	610	CLA	O2A-CGA	4.31	1.45	1.33
20	B	852	CLA	CHD-C1D	4.31	1.46	1.38
20	A	823	CLA	O2A-CGA	4.31	1.45	1.33
27	1	601	CHL	O2A-CGA	4.31	1.45	1.33
20	1	609	CLA	CHD-C1D	4.31	1.46	1.38
20	A	824	CLA	O2A-CGA	4.31	1.45	1.33
20	B	811	CLA	CHD-C1D	4.31	1.46	1.38
20	5	606	CLA	CHD-C1D	4.31	1.46	1.38
20	B	814	CLA	O2A-CGA	4.31	1.45	1.33
20	3	604	CLA	CHD-C1D	4.31	1.46	1.38
20	3	620	CLA	CHD-C1D	4.31	1.46	1.38
20	5	606	CLA	O2A-CGA	4.31	1.45	1.33
20	B	840	CLA	O2A-CGA	4.31	1.45	1.33
20	1	614	CLA	O2A-CGA	4.30	1.45	1.33
27	Z	607	CHL	CHD-C1D	4.30	1.46	1.38
20	Z	612	CLA	O2A-CGA	4.30	1.45	1.33
20	8	606	CLA	CHD-C1D	4.30	1.46	1.38
20	B	811	CLA	O2A-CGA	4.30	1.45	1.33
27	4	607	CHL	O2A-CGA	4.30	1.45	1.33
20	B	830	CLA	O2A-CGA	4.30	1.45	1.33
27	5	607	CHL	O2A-CGA	4.30	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	6	612	CLA	O2A-CGA	4.30	1.45	1.33
20	5	616	CLA	CHD-C1D	4.30	1.46	1.38
20	4	602	CLA	CHD-C1D	4.30	1.46	1.38
20	Z	606	CLA	O2A-CGA	4.30	1.45	1.33
20	1	611	CLA	O2A-CGA	4.30	1.45	1.33
20	3	620	CLA	O2A-CGA	4.29	1.45	1.33
20	Z	603	CLA	O2A-CGA	4.29	1.45	1.33
20	4	612	CLA	O2A-CGA	4.29	1.45	1.33
20	5	614	CLA	CHD-C1D	4.29	1.46	1.38
20	B	813	CLA	CHD-C1D	4.29	1.46	1.38
20	Z	614	CLA	O2A-CGA	4.29	1.45	1.33
20	G	203	CLA	O2A-CGA	4.29	1.45	1.33
20	5	609	CLA	CHD-C1D	4.29	1.46	1.38
20	L	204	CLA	O2A-CGA	4.29	1.45	1.33
20	5	604	CLA	O2A-CGA	4.29	1.45	1.33
20	B	804	CLA	O2A-CGA	4.29	1.45	1.30
20	4	603	CLA	CHD-C1D	4.29	1.46	1.38
27	4	606	CHL	CHD-C1D	4.29	1.46	1.38
20	Z	614	CLA	CHD-C1D	4.28	1.46	1.38
20	6	614	CLA	O2A-CGA	4.28	1.45	1.30
20	A	836	CLA	CHD-C1D	4.28	1.46	1.38
20	B	807	CLA	O2A-CGA	4.28	1.45	1.33
20	7	608	CLA	O2A-CGA	4.28	1.45	1.33
20	Z	616	CLA	CHD-C1D	4.28	1.46	1.38
20	6	610	CLA	O2A-CGA	4.28	1.45	1.33
20	3	609	CLA	CHD-C1D	4.28	1.46	1.38
22	A	855	LHG	O8-C23	4.28	1.45	1.33
20	Z	604	CLA	O2A-CGA	4.27	1.45	1.33
20	B	809	CLA	CHD-C1D	4.27	1.46	1.38
20	B	840	CLA	CHD-C1D	4.27	1.46	1.38
20	3	612	CLA	CHD-C1D	4.27	1.46	1.38
27	Z	601	CHL	O2A-CGA	4.27	1.45	1.33
20	A	817	CLA	O2A-CGA	4.27	1.45	1.33
20	Z	606	CLA	CHD-C1D	4.27	1.46	1.38
20	1	603	CLA	CHD-C1D	4.27	1.46	1.38
20	6	614	CLA	CHD-C1D	4.27	1.46	1.38
20	5	611	CLA	O2A-CGA	4.27	1.45	1.33
20	A	822	CLA	O2A-CGA	4.27	1.45	1.33
20	B	836	CLA	O2A-CGA	4.27	1.45	1.33
20	7	604	CLA	O2A-CGA	4.27	1.45	1.33
20	4	611	CLA	O2A-CGA	4.27	1.45	1.33
27	1	607	CHL	O2A-CGA	4.27	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	820	CLA	O2A-CGA	4.27	1.45	1.33
20	A	835	CLA	O2A-CGA	4.27	1.45	1.33
20	7	614	CLA	CHD-C1D	4.27	1.46	1.38
20	A	807	CLA	O2A-CGA	4.27	1.45	1.33
20	B	829	CLA	CHD-C1D	4.26	1.46	1.38
20	1	614	CLA	CHD-C1D	4.26	1.46	1.38
20	5	611	CLA	CHD-C1D	4.26	1.46	1.38
20	4	604	CLA	O2A-CGA	4.26	1.45	1.33
20	B	820	CLA	CHD-C1D	4.26	1.46	1.38
20	8	614	CLA	O2A-CGA	4.26	1.45	1.33
27	5	608	CHL	CHD-C1D	4.26	1.46	1.38
20	B	835	CLA	CHD-C1D	4.26	1.46	1.38
20	5	612	CLA	CHD-C1D	4.26	1.46	1.38
20	L	203	CLA	O2A-CGA	4.26	1.45	1.33
20	Z	613	CLA	CHD-C1D	4.26	1.46	1.38
27	7	607	CHL	O2A-CGA	4.26	1.45	1.33
27	5	607	CHL	CHD-C1D	4.26	1.46	1.38
20	7	613	CLA	CHD-C1D	4.26	1.46	1.38
20	5	601	CLA	CHD-C1D	4.25	1.46	1.38
20	6	604	CLA	O2A-CGA	4.25	1.45	1.33
20	A	839	CLA	CHD-C1D	4.25	1.46	1.38
20	A	816	CLA	O2A-CGA	4.25	1.45	1.33
20	Z	612	CLA	CHD-C1D	4.25	1.46	1.38
20	B	822	CLA	CHD-C1D	4.25	1.46	1.38
20	1	608	CLA	CHD-C1D	4.25	1.46	1.38
27	5	608	CHL	O2A-CGA	4.25	1.45	1.33
20	A	815	CLA	CHD-C1D	4.25	1.46	1.38
20	L	204	CLA	CHD-C1D	4.25	1.46	1.38
20	B	839	CLA	O2A-CGA	4.25	1.45	1.33
20	3	602	CLA	CHD-C1D	4.25	1.46	1.38
20	4	613	CLA	CHD-C1D	4.25	1.46	1.38
27	1	607	CHL	CHD-C1D	4.25	1.46	1.38
20	B	837	CLA	CHD-C1D	4.25	1.46	1.38
27	8	607	CHL	O2A-CGA	4.24	1.45	1.33
20	B	816	CLA	O2A-CGA	4.24	1.45	1.33
20	B	833	CLA	CHD-C1D	4.24	1.46	1.38
20	A	805	CLA	O2A-CGA	4.24	1.45	1.33
20	5	609	CLA	O2A-CGA	4.24	1.45	1.33
20	3	602	CLA	O2A-CGA	4.24	1.45	1.33
27	4	607	CHL	CHD-C1D	4.24	1.46	1.38
27	5	618	CHL	CHD-C1D	4.24	1.46	1.38
20	A	821	CLA	CHD-C1D	4.23	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	6	609	CLA	CHD-C1D	4.23	1.46	1.38
20	1	608	CLA	O2A-CGA	4.23	1.45	1.33
20	7	601	CLA	O2A-CGA	4.23	1.45	1.33
20	4	610	CLA	O2A-CGA	4.23	1.45	1.33
20	6	602	CLA	O2A-CGA	4.23	1.45	1.33
27	4	608	CHL	O2A-CGA	4.23	1.45	1.33
20	B	830	CLA	CHD-C1D	4.23	1.46	1.38
27	6	608	CHL	O2A-CGA	4.23	1.45	1.33
20	A	808	CLA	CHD-C1D	4.23	1.46	1.38
20	1	611	CLA	CHD-C1D	4.23	1.46	1.38
20	6	601	CLA	O2A-CGA	4.23	1.45	1.33
20	4	602	CLA	O2A-CGA	4.23	1.45	1.33
20	6	603	CLA	CHD-C1D	4.22	1.46	1.38
20	Z	610	CLA	O2A-CGA	4.22	1.45	1.33
20	7	612	CLA	CHD-C1D	4.22	1.46	1.38
20	A	814	CLA	O2A-CGA	4.22	1.45	1.33
20	5	621	CLA	CHD-C1D	4.22	1.46	1.38
20	B	838	CLA	O2A-CGA	4.22	1.45	1.33
20	4	610	CLA	CHD-C1D	4.22	1.46	1.38
20	B	827	CLA	O2A-CGA	4.22	1.45	1.33
20	B	831	CLA	O2A-CGA	4.22	1.45	1.33
20	B	841	CLA	CHD-C1D	4.22	1.46	1.38
20	4	601	CLA	CHD-C1D	4.22	1.46	1.38
20	3	610	CLA	O2A-CGA	4.22	1.45	1.33
20	7	612	CLA	O2A-CGA	4.21	1.45	1.33
20	1	604	CLA	O2A-CGA	4.21	1.45	1.33
20	8	602	CLA	O2A-CGA	4.21	1.45	1.33
20	7	616	CLA	CHD-C1D	4.21	1.46	1.38
20	F	301	CLA	O2A-CGA	4.21	1.45	1.33
20	B	806	CLA	O2A-CGA	4.21	1.45	1.33
20	7	620	CLA	O2A-CGA	4.21	1.45	1.33
20	B	824	CLA	CHD-C1D	4.21	1.46	1.38
20	7	611	CLA	CHD-C1D	4.21	1.46	1.38
20	B	841	CLA	O2A-CGA	4.20	1.45	1.33
20	B	823	CLA	O2A-CGA	4.20	1.45	1.33
20	6	609	CLA	O2A-CGA	4.20	1.45	1.33
20	1	616	CLA	CHD-C1D	4.20	1.46	1.38
20	7	610	CLA	O2A-CGA	4.20	1.45	1.33
20	A	845	CLA	CHD-C1D	4.20	1.46	1.38
20	B	829	CLA	O2A-CGA	4.20	1.45	1.33
27	4	618	CHL	CHD-C1D	4.20	1.46	1.38
20	6	616	CLA	CHD-C4C	4.20	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	5	610	CLA	O2A-CGA	4.20	1.45	1.33
20	A	822	CLA	CHD-C1D	4.20	1.46	1.38
20	B	819	CLA	O2A-CGA	4.20	1.45	1.33
20	B	834	CLA	O2A-CGA	4.20	1.45	1.33
20	7	609	CLA	O2A-CGA	4.20	1.45	1.33
20	A	834	CLA	CHD-C1D	4.20	1.46	1.38
20	6	602	CLA	CHD-C1D	4.20	1.46	1.38
20	8	616	CLA	CHD-C1D	4.20	1.46	1.38
20	A	813	CLA	CHD-C1D	4.20	1.46	1.38
20	A	839	CLA	O2A-CGA	4.19	1.45	1.33
20	8	612	CLA	CHD-C1D	4.19	1.46	1.38
20	B	818	CLA	O2A-CGA	4.19	1.45	1.33
20	B	809	CLA	O2A-CGA	4.19	1.45	1.33
27	3	608	CHL	O2A-CGA	4.19	1.45	1.33
20	B	821	CLA	CHD-C1D	4.19	1.46	1.38
20	8	614	CLA	CHD-C1D	4.19	1.46	1.38
20	6	613	CLA	CHD-C1D	4.19	1.46	1.38
20	A	816	CLA	CHD-C1D	4.19	1.46	1.38
20	A	826	CLA	O2A-CGA	4.19	1.45	1.33
20	3	603	CLA	O2A-CGA	4.18	1.45	1.33
20	A	819	CLA	O2A-CGA	4.18	1.45	1.33
27	6	607	CHL	O2A-CGA	4.18	1.45	1.33
22	4	622	LHG	O8-C23	4.18	1.45	1.33
20	B	802	CLA	O2A-CGA	4.18	1.45	1.33
20	B	817	CLA	O2A-CGA	4.18	1.45	1.33
20	A	832	CLA	O2A-CGA	4.18	1.45	1.33
20	B	805	CLA	O2A-CGA	4.18	1.45	1.33
20	Z	602	CLA	O2A-CGA	4.17	1.45	1.33
20	1	604	CLA	CHD-C4C	4.17	1.48	1.39
20	A	804	CLA	CHD-C1D	4.17	1.46	1.38
20	B	812	CLA	CHD-C1D	4.17	1.46	1.38
20	B	810	CLA	O2A-CGA	4.17	1.45	1.33
20	4	601	CLA	O2A-CGA	4.17	1.45	1.33
20	G	203	CLA	CHD-C1D	4.17	1.46	1.38
20	B	820	CLA	O2A-CGA	4.16	1.45	1.33
27	6	606	CHL	CHD-C1D	4.16	1.46	1.38
20	3	604	CLA	O2A-CGA	4.16	1.45	1.33
22	6	619	LHG	O8-C23	4.16	1.45	1.33
20	5	602	CLA	CHD-C1D	4.16	1.46	1.38
20	A	820	CLA	CHD-C1D	4.16	1.46	1.38
22	Z	620	LHG	O7-C7	4.16	1.46	1.34
20	7	606	CLA	CHD-C1D	4.16	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	833	CLA	O2A-CGA	4.15	1.45	1.33
20	7	608	CLA	CHD-C1D	4.15	1.46	1.38
20	8	601	CLA	O2A-CGA	4.15	1.45	1.33
20	A	811	CLA	O2A-CGA	4.15	1.45	1.33
20	5	610	CLA	CHD-C1D	4.15	1.46	1.38
20	A	829	CLA	O2A-CGA	4.15	1.45	1.33
20	A	841	CLA	O2A-CGA	4.15	1.45	1.33
22	5	623	LHG	O8-C23	4.15	1.45	1.33
20	1	612	CLA	CHD-C1D	4.15	1.46	1.38
20	A	824	CLA	CHD-C1D	4.15	1.46	1.38
20	B	825	CLA	CHD-C1D	4.15	1.46	1.38
20	1	606	CLA	CHD-C1D	4.15	1.46	1.38
20	4	612	CLA	CHD-C1D	4.14	1.46	1.38
20	6	612	CLA	CHD-C1D	4.14	1.46	1.38
20	B	832	CLA	CHD-C1D	4.14	1.46	1.38
22	A	847	LHG	O8-C23	4.14	1.45	1.33
27	6	608	CHL	CHD-C1D	4.14	1.46	1.38
20	8	608	CLA	O2A-CGA	4.14	1.45	1.33
20	A	805	CLA	CHD-C1D	4.14	1.46	1.38
27	6	618	CHL	CHD-C1D	4.14	1.46	1.38
20	A	812	CLA	O2A-CGA	4.14	1.45	1.33
20	8	610	CLA	O2A-CGA	4.14	1.45	1.33
27	8	607	CHL	CHD-C1D	4.13	1.46	1.38
22	1	620	LHG	O8-C23	4.13	1.45	1.33
20	A	806	CLA	CHD-C1D	4.13	1.46	1.38
20	A	832	CLA	CHD-C1D	4.13	1.46	1.38
20	1	602	CLA	CHD-C1D	4.13	1.46	1.38
20	B	832	CLA	O2A-CGA	4.13	1.45	1.33
22	6	619	LHG	O7-C7	4.13	1.46	1.34
20	6	614	CLA	CHD-C4C	4.13	1.48	1.39
20	B	826	CLA	O2A-CGA	4.13	1.45	1.33
20	A	843	CLA	O2A-CGA	4.13	1.45	1.33
22	Z	620	LHG	O8-C23	4.13	1.45	1.33
22	4	623	LHG	O8-C23	4.13	1.45	1.33
19	A	801	CL0	O2A-CGA	4.13	1.45	1.33
20	A	806	CLA	O2A-CGA	4.13	1.45	1.33
20	8	609	CLA	CHD-C1D	4.13	1.46	1.38
20	3	617	CLA	O2A-CGA	4.13	1.46	1.33
20	B	816	CLA	CHD-C1D	4.13	1.46	1.38
20	L	203	CLA	CHD-C1D	4.12	1.46	1.38
20	B	804	CLA	CHD-C1D	4.12	1.46	1.38
20	B	810	CLA	CHD-C4C	4.12	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	620	LHG	O7-C7	4.12	1.45	1.34
20	B	839	CLA	CHD-C1D	4.12	1.46	1.38
20	A	826	CLA	CHD-C1D	4.12	1.46	1.38
20	8	601	CLA	CHD-C1D	4.12	1.46	1.38
27	6	607	CHL	CHD-C1D	4.12	1.46	1.38
20	B	831	CLA	CHD-C1D	4.11	1.46	1.38
20	A	828	CLA	O2A-CGA	4.11	1.45	1.33
22	4	623	LHG	O7-C7	4.11	1.45	1.34
20	B	808	CLA	O2A-CGA	4.10	1.45	1.33
20	B	806	CLA	CHD-C1D	4.10	1.46	1.38
20	Z	602	CLA	CHD-C1D	4.10	1.46	1.38
20	A	803	CLA	CHD-C1D	4.10	1.46	1.38
22	A	847	LHG	O7-C7	4.10	1.45	1.34
20	4	609	CLA	CHD-C1D	4.10	1.46	1.38
20	B	818	CLA	CHD-C1D	4.10	1.46	1.38
20	6	603	CLA	O2A-CGA	4.10	1.46	1.33
20	L	204	CLA	CHD-C4C	4.10	1.48	1.39
20	4	614	CLA	CHD-C1D	4.10	1.46	1.38
20	3	613	CLA	CHD-C1D	4.09	1.46	1.38
20	B	803	CLA	O2A-CGA	4.09	1.45	1.33
20	B	823	CLA	CHD-C1D	4.09	1.46	1.38
20	8	603	CLA	CHD-C1D	4.09	1.46	1.38
20	F	301	CLA	CHD-C1D	4.09	1.46	1.38
20	7	602	CLA	CHD-C1D	4.09	1.46	1.38
20	A	841	CLA	CHD-C1D	4.09	1.46	1.38
22	A	855	LHG	O7-C7	4.08	1.45	1.34
20	F	304	CLA	CHD-C1D	4.08	1.46	1.38
20	A	843	CLA	CHD-C1D	4.08	1.46	1.38
20	A	854	CLA	C1D-ND	4.08	1.42	1.37
20	6	601	CLA	CHD-C4C	4.08	1.48	1.39
20	B	814	CLA	CHD-C1D	4.08	1.46	1.38
20	L	203	CLA	CHD-C4C	4.08	1.48	1.39
20	A	837	CLA	CHD-C4C	4.08	1.48	1.39
20	8	611	CLA	O2A-CGA	4.07	1.46	1.33
20	3	603	CLA	CHD-C1D	4.07	1.46	1.38
20	G	204	CLA	O2A-CGA	4.07	1.46	1.33
20	7	603	CLA	O2A-CGA	4.07	1.46	1.33
20	7	616	CLA	O2A-CGA	4.07	1.46	1.33
20	1	613	CLA	CHD-C1D	4.07	1.46	1.38
22	5	623	LHG	O7-C7	4.07	1.45	1.34
20	A	831	CLA	O2A-CGA	4.06	1.45	1.33
20	8	604	CLA	O2A-CGA	4.06	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	6	610	CLA	CHD-C4C	4.06	1.48	1.39
20	A	834	CLA	O2A-CGA	4.06	1.45	1.33
20	B	819	CLA	CHD-C4C	4.06	1.48	1.39
20	A	827	CLA	CHD-C1D	4.06	1.46	1.38
20	A	842	CLA	O2A-CGA	4.06	1.45	1.33
20	B	821	CLA	O2A-CGA	4.06	1.45	1.33
20	3	610	CLA	CHD-C1D	4.05	1.46	1.38
22	B	851	LHG	O7-C7	4.05	1.45	1.34
20	A	819	CLA	CHD-C1D	4.05	1.46	1.38
20	B	837	CLA	O2A-CGA	4.05	1.45	1.33
20	7	604	CLA	CHD-C1D	4.05	1.46	1.38
22	A	846	LHG	O8-C23	4.04	1.45	1.33
20	4	601	CLA	CHD-C4C	4.04	1.48	1.39
20	B	803	CLA	CHD-C1D	4.04	1.46	1.38
20	B	808	CLA	CHD-C1D	4.04	1.46	1.38
20	A	815	CLA	CHD-C4C	4.04	1.48	1.39
20	A	823	CLA	CHD-C1D	4.04	1.46	1.38
20	8	616	CLA	O2A-CGA	4.04	1.45	1.33
20	B	834	CLA	CHD-C4C	4.04	1.48	1.39
20	A	835	CLA	CHD-C4C	4.03	1.48	1.39
20	B	828	CLA	CHD-C1D	4.03	1.46	1.38
20	G	204	CLA	CHD-C4C	4.03	1.48	1.39
20	B	836	CLA	CHD-C1D	4.03	1.46	1.38
20	B	815	CLA	CHD-C4C	4.03	1.48	1.39
20	4	604	CLA	CHD-C4C	4.03	1.48	1.39
20	3	614	CLA	CHD-C4C	4.03	1.48	1.39
20	B	826	CLA	CHD-C1D	4.03	1.46	1.38
20	7	603	CLA	CHD-C4C	4.03	1.48	1.39
20	A	817	CLA	CHD-C4C	4.02	1.48	1.39
20	4	602	CLA	CHD-C4C	4.02	1.48	1.39
20	7	613	CLA	O2A-CGA	4.02	1.45	1.33
20	8	604	CLA	CHD-C4C	4.02	1.48	1.39
20	K	4003	CLA	O2A-CGA	4.02	1.45	1.33
20	B	813	CLA	O2A-CGA	4.02	1.45	1.33
20	3	604	CLA	CHD-C4C	4.02	1.48	1.39
20	6	604	CLA	CHD-C4C	4.02	1.48	1.39
20	G	203	CLA	CHD-C4C	4.02	1.48	1.39
20	5	603	CLA	O2A-CGA	4.02	1.45	1.33
20	6	617	CLA	O2A-CGA	4.02	1.45	1.33
20	4	610	CLA	CHD-C4C	4.02	1.48	1.39
20	A	812	CLA	CHD-C1D	4.02	1.46	1.38
20	Z	604	CLA	CHD-C4C	4.02	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	817	CLA	CHD-C4C	4.02	1.48	1.39
20	A	854	CLA	C3D-C2D	4.02	1.50	1.39
20	3	606	CLA	CHD-C4C	4.02	1.48	1.39
20	5	617	CLA	O2A-CGA	4.01	1.45	1.33
20	A	830	CLA	O2A-CGA	4.01	1.45	1.33
20	A	842	CLA	CHD-C1D	4.01	1.46	1.38
20	1	616	CLA	O2A-CGA	4.01	1.45	1.33
20	A	802	CLA	C3D-C2D	4.01	1.50	1.39
20	5	616	CLA	O2A-CGA	4.01	1.45	1.33
20	A	829	CLA	CHD-C1D	4.01	1.46	1.38
20	6	617	CLA	CHD-C4C	4.01	1.48	1.39
20	3	607	CLA	CHD-C4C	4.00	1.48	1.39
20	K	4002	CLA	CHD-C4C	4.00	1.48	1.39
20	Z	614	CLA	CHD-C4C	4.00	1.48	1.39
20	A	811	CLA	CHD-C1D	4.00	1.46	1.38
20	5	621	CLA	O2A-CGA	4.00	1.45	1.33
20	A	814	CLA	CHD-C1D	4.00	1.46	1.38
20	7	610	CLA	CHD-C1D	4.00	1.46	1.38
20	Z	616	CLA	O2A-CGA	3.99	1.45	1.33
20	Z	609	CLA	CHD-C4C	3.99	1.48	1.39
25	B	850	DGD	O1G-C1A	3.99	1.45	1.33
20	7	620	CLA	CHD-C4C	3.99	1.48	1.39
22	7	625	LHG	O8-C23	3.99	1.45	1.33
20	K	4003	CLA	CHD-C4C	3.98	1.48	1.39
20	5	606	CLA	CHD-C4C	3.98	1.48	1.39
20	A	838	CLA	CHD-C4C	3.98	1.48	1.39
20	3	612	CLA	O2A-CGA	3.98	1.45	1.33
20	3	611	CLA	CHD-C4C	3.98	1.48	1.39
20	A	822	CLA	CHD-C4C	3.98	1.48	1.39
22	8	620	LHG	O7-C7	3.98	1.45	1.34
20	8	610	CLA	CHD-C1D	3.97	1.46	1.38
20	Z	616	CLA	CHD-C4C	3.97	1.48	1.39
20	8	613	CLA	CHD-C1D	3.97	1.46	1.38
20	B	805	CLA	CHD-C1D	3.97	1.46	1.38
20	Z	610	CLA	CHD-C1D	3.97	1.46	1.38
20	1	609	CLA	CHD-C4C	3.97	1.48	1.39
20	A	804	CLA	O2A-CGA	3.97	1.44	1.33
20	B	821	CLA	CHD-C4C	3.97	1.48	1.39
20	B	807	CLA	CHD-C4C	3.97	1.48	1.39
20	J	3002	CLA	CHD-C4C	3.97	1.48	1.39
20	4	616	CLA	CHD-C4C	3.96	1.48	1.39
20	6	616	CLA	O2A-CGA	3.96	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	840	CLA	CHD-C4C	3.96	1.48	1.39
20	1	603	CLA	CHD-C4C	3.96	1.48	1.39
20	3	620	CLA	CHD-C4C	3.96	1.48	1.39
20	6	622	CLA	CHD-C4C	3.96	1.48	1.39
20	A	803	CLA	O2A-CGA	3.96	1.44	1.33
20	4	611	CLA	CHD-C4C	3.96	1.48	1.39
20	A	809	CLA	O2A-CGA	3.96	1.44	1.33
20	5	610	CLA	CHD-C4C	3.96	1.48	1.39
20	B	820	CLA	CHD-C4C	3.96	1.48	1.39
27	1	601	CHL	CHD-C1D	3.96	1.46	1.38
20	1	610	CLA	CHD-C1D	3.96	1.46	1.38
20	Z	603	CLA	CHD-C4C	3.95	1.48	1.39
20	7	609	CLA	CHD-C1D	3.95	1.46	1.38
20	8	602	CLA	CHD-C1D	3.95	1.46	1.38
20	6	622	CLA	CHD-C1D	3.95	1.46	1.38
20	B	838	CLA	CHD-C1D	3.95	1.46	1.38
20	B	829	CLA	CHD-C4C	3.95	1.48	1.39
27	3	608	CHL	CHD-C1D	3.95	1.46	1.38
20	5	604	CLA	CHD-C4C	3.95	1.48	1.39
20	A	827	CLA	O2A-CGA	3.94	1.44	1.33
22	8	620	LHG	O8-C23	3.94	1.44	1.33
20	5	603	CLA	CHD-C4C	3.94	1.48	1.39
20	B	811	CLA	CHD-C4C	3.94	1.48	1.39
20	B	813	CLA	CHD-C4C	3.94	1.48	1.39
20	5	614	CLA	CHD-C4C	3.94	1.48	1.39
20	4	603	CLA	O2A-CGA	3.94	1.45	1.33
20	8	609	CLA	O2A-CGA	3.94	1.45	1.33
25	B	850	DGD	O2G-C1B	3.93	1.45	1.34
20	A	833	CLA	CHD-C1D	3.93	1.46	1.38
20	B	837	CLA	CHD-C4C	3.93	1.48	1.39
22	A	846	LHG	O7-C7	3.93	1.45	1.34
20	3	610	CLA	CHD-C4C	3.93	1.48	1.39
20	A	807	CLA	CHD-C4C	3.93	1.48	1.39
20	7	601	CLA	CHD-C1D	3.93	1.46	1.38
20	B	852	CLA	C3D-C2D	3.93	1.49	1.39
22	7	625	LHG	O7-C7	3.93	1.45	1.34
20	Z	611	CLA	CHD-C4C	3.92	1.48	1.39
20	1	611	CLA	CHD-C4C	3.92	1.48	1.39
20	8	608	CLA	CHD-C1D	3.92	1.46	1.38
20	8	611	CLA	CHD-C4C	3.92	1.48	1.39
20	5	613	CLA	CHD-C4C	3.92	1.48	1.39
20	Z	608	CLA	CHD-C4C	3.92	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	7	614	CLA	CHD-C4C	3.92	1.48	1.39
27	4	608	CHL	CHD-C1D	3.91	1.46	1.38
20	A	818	CLA	CHD-C1D	3.91	1.46	1.38
20	F	303	CLA	CHD-C1D	3.91	1.46	1.38
20	7	602	CLA	CHD-C4C	3.91	1.48	1.39
20	A	840	CLA	CHD-C1D	3.91	1.46	1.38
20	3	617	CLA	CHD-C4C	3.91	1.48	1.39
20	Z	606	CLA	CHD-C4C	3.91	1.48	1.39
20	8	614	CLA	CHD-C4C	3.91	1.48	1.39
19	A	801	CL0	CHD-C1D	3.91	1.46	1.38
20	B	825	CLA	CHD-C4C	3.90	1.48	1.39
20	A	839	CLA	CHD-C4C	3.90	1.48	1.39
20	5	601	CLA	CHD-C4C	3.90	1.48	1.39
20	6	611	CLA	CHD-C4C	3.90	1.48	1.39
20	A	831	CLA	CHD-C1D	3.90	1.46	1.38
20	4	611	CLA	C3D-C2D	3.90	1.49	1.39
20	3	609	CLA	CHD-C4C	3.89	1.48	1.39
20	A	821	CLA	CHD-C4C	3.89	1.48	1.39
20	A	810	CLA	CHD-C1D	3.89	1.45	1.38
20	6	609	CLA	CHD-C4C	3.89	1.48	1.39
20	6	603	CLA	CHD-C4C	3.89	1.48	1.39
27	Z	601	CHL	CHD-C1D	3.89	1.45	1.38
20	A	816	CLA	CHD-C4C	3.89	1.48	1.39
20	B	805	CLA	CHD-C4C	3.89	1.48	1.39
20	A	809	CLA	CHD-C1D	3.89	1.45	1.38
20	A	812	CLA	CHD-C4C	3.89	1.48	1.39
20	A	834	CLA	CHD-C4C	3.88	1.48	1.39
20	1	608	CLA	CHD-C4C	3.88	1.48	1.39
20	1	614	CLA	CHD-C4C	3.88	1.48	1.39
20	A	813	CLA	CHD-C4C	3.88	1.48	1.39
20	5	609	CLA	CHD-C4C	3.88	1.48	1.39
20	3	602	CLA	CHD-C4C	3.88	1.48	1.39
20	B	827	CLA	CHD-C1D	3.88	1.45	1.38
20	5	602	CLA	CHD-C4C	3.88	1.48	1.39
20	A	836	CLA	CHD-C4C	3.88	1.48	1.39
20	8	609	CLA	CHD-C4C	3.87	1.48	1.39
20	B	803	CLA	CHD-C4C	3.87	1.48	1.39
27	Z	601	CHL	C1D-ND	-3.87	1.33	1.37
20	4	603	CLA	CHD-C4C	3.87	1.48	1.39
20	A	825	CLA	CHD-C4C	3.87	1.48	1.39
20	A	845	CLA	CHD-C4C	3.87	1.48	1.39
20	5	616	CLA	CHD-C4C	3.87	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	7	609	CLA	C3D-C2D	3.86	1.49	1.39
20	B	814	CLA	CHD-C4C	3.86	1.48	1.39
20	5	601	CLA	C3D-C2D	3.86	1.49	1.39
20	A	831	CLA	C3D-C2D	3.86	1.49	1.39
20	F	301	CLA	CHD-C4C	3.86	1.48	1.39
20	8	606	CLA	CHD-C4C	3.86	1.48	1.39
20	3	612	CLA	CHD-C4C	3.86	1.48	1.39
20	7	610	CLA	CHD-C4C	3.86	1.48	1.39
20	B	831	CLA	CHD-C4C	3.86	1.48	1.39
20	A	825	CLA	C3D-C2D	3.86	1.49	1.39
20	A	840	CLA	CHD-C4C	3.86	1.48	1.39
20	A	806	CLA	CHD-C4C	3.85	1.48	1.39
20	6	602	CLA	CHD-C4C	3.85	1.48	1.39
20	A	823	CLA	CHD-C4C	3.85	1.48	1.39
20	B	822	CLA	CHD-C4C	3.85	1.48	1.39
20	B	839	CLA	CHD-C4C	3.85	1.48	1.39
20	A	805	CLA	CHD-C4C	3.85	1.48	1.39
20	A	832	CLA	CHD-C4C	3.85	1.48	1.39
20	4	613	CLA	CHD-C4C	3.85	1.48	1.39
20	3	613	CLA	CHD-C4C	3.85	1.48	1.39
20	7	606	CLA	CHD-C4C	3.85	1.48	1.39
20	B	832	CLA	CHD-C4C	3.84	1.48	1.39
20	5	621	CLA	CHD-C4C	3.84	1.48	1.39
20	A	827	CLA	CHD-C4C	3.84	1.48	1.39
20	7	611	CLA	CHD-C4C	3.84	1.48	1.39
20	5	617	CLA	CHD-C4C	3.84	1.48	1.39
20	Z	612	CLA	CHD-C4C	3.84	1.48	1.39
20	5	611	CLA	CHD-C4C	3.84	1.48	1.39
20	B	823	CLA	C3D-C2D	3.84	1.49	1.39
20	B	835	CLA	CHD-C4C	3.83	1.48	1.39
20	3	607	CLA	C3D-C2D	3.83	1.49	1.39
20	B	812	CLA	CHD-C4C	3.83	1.48	1.39
20	8	610	CLA	CHD-C4C	3.83	1.48	1.39
20	B	852	CLA	CHD-C4C	3.83	1.48	1.39
20	Z	613	CLA	CHD-C4C	3.83	1.48	1.39
20	A	809	CLA	CHD-C4C	3.82	1.48	1.39
20	A	841	CLA	CHD-C4C	3.82	1.48	1.39
20	B	809	CLA	CHD-C4C	3.82	1.48	1.39
20	A	833	CLA	CHD-C4C	3.82	1.48	1.39
20	1	606	CLA	CHD-C4C	3.82	1.48	1.39
20	6	610	CLA	C3D-C2D	3.82	1.49	1.39
20	1	602	CLA	CHD-C4C	3.82	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	5	617	CLA	CHD-C1D	3.82	1.45	1.38
20	7	616	CLA	CHD-C4C	3.82	1.47	1.39
20	K	4003	CLA	C3D-C2D	3.82	1.49	1.39
27	5	618	CHL	CHD-C4C	3.81	1.47	1.39
20	A	803	CLA	CHD-C4C	3.81	1.47	1.39
20	A	843	CLA	C3D-C2D	3.81	1.49	1.39
20	8	601	CLA	CHD-C4C	3.81	1.47	1.39
20	B	824	CLA	CHD-C4C	3.81	1.47	1.39
20	6	611	CLA	C3D-C2D	3.80	1.49	1.39
20	Z	611	CLA	C3D-C2D	3.80	1.49	1.39
20	A	820	CLA	CHD-C4C	3.80	1.47	1.39
20	4	610	CLA	C3D-C2D	3.80	1.49	1.39
20	6	613	CLA	CHD-C4C	3.80	1.47	1.39
20	B	816	CLA	CHD-C4C	3.80	1.47	1.39
20	1	614	CLA	C3D-C2D	3.80	1.49	1.39
20	3	603	CLA	CHD-C4C	3.80	1.47	1.39
20	1	613	CLA	CHD-C4C	3.79	1.47	1.39
20	5	612	CLA	CHD-C4C	3.79	1.47	1.39
20	B	818	CLA	CHD-C4C	3.79	1.47	1.39
27	4	618	CHL	CHD-C4C	3.79	1.47	1.39
20	7	609	CLA	CHD-C4C	3.79	1.47	1.39
20	7	612	CLA	CHD-C4C	3.79	1.47	1.39
20	7	601	CLA	CHD-C4C	3.79	1.47	1.39
20	B	830	CLA	CHD-C4C	3.78	1.47	1.39
20	B	826	CLA	CHD-C4C	3.78	1.47	1.39
20	1	610	CLA	CHD-C4C	3.78	1.47	1.39
20	4	613	CLA	OBD-CAD	3.78	1.29	1.22
27	1	607	CHL	CHD-C4C	3.78	1.47	1.39
20	7	614	CLA	C3D-C2D	3.78	1.49	1.39
20	B	841	CLA	CHD-C4C	3.78	1.47	1.39
20	1	616	CLA	CHD-C4C	3.78	1.47	1.39
20	4	614	CLA	CHD-C4C	3.78	1.47	1.39
20	4	609	CLA	CHD-C4C	3.78	1.47	1.39
20	8	603	CLA	CHD-C4C	3.77	1.47	1.39
20	Z	616	CLA	C3D-C2D	3.77	1.49	1.39
20	A	802	CLA	CHD-C4C	3.77	1.47	1.39
20	3	612	CLA	C3D-C2D	3.77	1.49	1.39
20	A	804	CLA	CHD-C4C	3.77	1.47	1.39
20	B	833	CLA	CHD-C4C	3.77	1.47	1.39
27	Z	607	CHL	CHD-C4C	3.77	1.47	1.39
20	A	841	CLA	C3D-C2D	3.77	1.49	1.39
20	L	203	CLA	C3D-C2D	3.77	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	612	CLA	C3D-C2D	3.77	1.49	1.39
20	8	612	CLA	CHD-C4C	3.77	1.47	1.39
20	B	827	CLA	CHD-C4C	3.77	1.47	1.39
20	8	614	CLA	C3D-C2D	3.77	1.49	1.39
20	5	611	CLA	C3D-C2D	3.77	1.49	1.39
20	6	601	CLA	C3D-C2D	3.77	1.49	1.39
20	F	303	CLA	CHD-C4C	3.76	1.47	1.39
20	A	836	CLA	C3D-C2D	3.76	1.49	1.39
20	Z	614	CLA	C3D-C2D	3.76	1.49	1.39
20	A	818	CLA	CHD-C4C	3.76	1.47	1.39
20	A	842	CLA	CHD-C4C	3.76	1.47	1.39
20	G	204	CLA	C3D-C2D	3.76	1.49	1.39
20	5	609	CLA	C3D-C2D	3.76	1.49	1.39
20	6	609	CLA	C3D-C2D	3.76	1.49	1.39
20	8	616	CLA	CHD-C4C	3.75	1.47	1.39
20	B	838	CLA	CHD-C4C	3.75	1.47	1.39
20	4	614	CLA	C3D-C2D	3.75	1.49	1.39
20	6	616	CLA	C3D-C2D	3.75	1.49	1.39
20	Z	602	CLA	CHD-C4C	3.75	1.47	1.39
20	1	611	CLA	C3D-C2D	3.75	1.49	1.39
20	8	604	CLA	C3D-C2D	3.75	1.49	1.39
20	B	803	CLA	C3D-C2D	3.75	1.49	1.39
20	1	610	CLA	C3D-C2D	3.75	1.49	1.39
20	A	843	CLA	CHD-C4C	3.75	1.47	1.39
27	5	607	CHL	CHD-C4C	3.74	1.47	1.39
20	B	806	CLA	CHD-C4C	3.74	1.47	1.39
20	B	823	CLA	CHD-C4C	3.74	1.47	1.39
20	F	304	CLA	CHD-C4C	3.74	1.47	1.39
20	8	604	CLA	OBD-CAD	3.74	1.28	1.22
20	4	603	CLA	C3D-C2D	3.74	1.49	1.39
20	B	841	CLA	C3D-C2D	3.74	1.49	1.39
20	3	606	CLA	C3D-C2D	3.74	1.49	1.39
20	7	611	CLA	C3D-C2D	3.74	1.49	1.39
20	G	203	CLA	C3D-C2D	3.74	1.49	1.39
20	A	837	CLA	C3D-C2D	3.74	1.49	1.39
20	3	611	CLA	C3D-C2D	3.74	1.49	1.39
20	A	803	CLA	C3D-C2D	3.74	1.49	1.39
20	B	835	CLA	C3D-C2D	3.74	1.49	1.39
20	A	819	CLA	CHD-C4C	3.74	1.47	1.39
20	B	836	CLA	CHD-C4C	3.74	1.47	1.39
20	B	807	CLA	C3D-C2D	3.74	1.49	1.39
20	8	609	CLA	C3D-C2D	3.74	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	5	604	CLA	C3D-C2D	3.74	1.49	1.39
20	8	616	CLA	C3D-C2D	3.74	1.49	1.39
20	Z	604	CLA	C3D-C2D	3.74	1.49	1.39
20	8	613	CLA	CHD-C4C	3.73	1.47	1.39
20	7	620	CLA	C3D-C2D	3.73	1.49	1.39
20	K	4002	CLA	C3D-C2D	3.73	1.49	1.39
20	1	603	CLA	C3D-C2D	3.73	1.49	1.39
20	4	612	CLA	CHD-C4C	3.73	1.47	1.39
20	Z	610	CLA	C3D-C2D	3.73	1.49	1.39
20	L	204	CLA	OBD-CAD	3.73	1.28	1.22
20	6	613	CLA	OBD-CAD	3.73	1.28	1.22
20	3	612	CLA	OBD-CAD	3.73	1.28	1.22
20	5	613	CLA	C3D-C2D	3.73	1.49	1.39
20	A	824	CLA	CHD-C4C	3.73	1.47	1.39
20	B	802	CLA	CHD-C1D	3.73	1.45	1.38
20	4	604	CLA	C3D-C2D	3.72	1.49	1.39
20	6	612	CLA	CHD-C4C	3.72	1.47	1.39
20	4	609	CLA	C3D-C2D	3.72	1.49	1.39
20	5	614	CLA	C3D-C2D	3.72	1.49	1.39
20	A	845	CLA	OBD-CAD	3.72	1.28	1.22
20	3	620	CLA	OBD-CAD	3.72	1.28	1.22
20	3	604	CLA	C3D-C2D	3.72	1.49	1.39
20	A	835	CLA	C3D-C2D	3.72	1.49	1.39
20	6	601	CLA	OBD-CAD	3.72	1.28	1.22
20	A	830	CLA	CHD-C1D	3.71	1.45	1.38
20	1	604	CLA	OBD-CAD	3.71	1.28	1.22
20	5	612	CLA	C3D-C2D	3.71	1.49	1.39
20	L	204	CLA	C3D-C2D	3.71	1.49	1.39
20	A	822	CLA	C3D-C2D	3.71	1.49	1.39
20	8	602	CLA	C3D-C2D	3.71	1.49	1.39
20	1	612	CLA	CHD-C4C	3.71	1.47	1.39
27	6	618	CHL	CHD-C4C	3.71	1.47	1.39
20	8	611	CLA	C3D-C2D	3.71	1.49	1.39
20	8	606	CLA	C3D-C2D	3.71	1.49	1.39
20	A	830	CLA	C3D-C2D	3.71	1.49	1.39
20	Z	606	CLA	C3D-C2D	3.71	1.49	1.39
20	B	817	CLA	C3D-C2D	3.71	1.49	1.39
20	3	603	CLA	C3D-C2D	3.71	1.49	1.39
20	7	604	CLA	CHD-C4C	3.71	1.47	1.39
20	1	616	CLA	C3D-C2D	3.71	1.49	1.39
20	3	614	CLA	OBD-CAD	3.70	1.28	1.22
20	3	614	CLA	C3D-C2D	3.70	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	804	CLA	CHD-C4C	3.70	1.47	1.39
27	Z	601	CHL	OBD-CAD	3.70	1.28	1.22
20	1	609	CLA	C3D-C2D	3.70	1.49	1.39
20	B	815	CLA	C3D-C2D	3.70	1.49	1.39
27	4	607	CHL	CHD-C4C	3.70	1.47	1.39
27	7	607	CHL	CHD-C4C	3.70	1.47	1.39
27	4	607	CHL	OBD-CAD	3.70	1.28	1.22
20	6	613	CLA	C3D-C2D	3.70	1.49	1.39
20	7	613	CLA	C3D-C2D	3.70	1.49	1.39
20	5	606	CLA	C3D-C2D	3.70	1.49	1.39
20	5	606	CLA	OBD-CAD	3.70	1.28	1.22
20	6	604	CLA	C3D-C2D	3.69	1.49	1.39
20	5	603	CLA	C3D-C2D	3.69	1.49	1.39
20	B	837	CLA	C3D-C2D	3.69	1.49	1.39
20	B	818	CLA	C3D-C2D	3.69	1.49	1.39
20	7	608	CLA	CHD-C4C	3.69	1.47	1.39
20	B	833	CLA	C3D-C2D	3.69	1.49	1.39
27	6	606	CHL	OBD-CAD	3.69	1.28	1.22
20	A	807	CLA	C3D-C2D	3.69	1.49	1.39
20	A	811	CLA	C3D-C2D	3.69	1.49	1.39
20	Z	610	CLA	CHD-C4C	3.69	1.47	1.39
20	A	826	CLA	C3D-C2D	3.69	1.49	1.39
27	7	607	CHL	OBD-CAD	3.69	1.28	1.22
20	A	820	CLA	C3D-C2D	3.69	1.49	1.39
20	A	816	CLA	C3D-C2D	3.69	1.49	1.39
27	6	607	CHL	OBD-CAD	3.69	1.28	1.22
27	5	618	CHL	OBD-CAD	3.69	1.28	1.22
20	6	614	CLA	OBD-CAD	3.69	1.28	1.22
20	Z	612	CLA	C3D-C2D	3.68	1.49	1.39
20	Z	603	CLA	C3D-C2D	3.68	1.49	1.39
20	B	834	CLA	C3D-C2D	3.68	1.49	1.39
20	3	611	CLA	OBD-CAD	3.68	1.28	1.22
20	4	616	CLA	C3D-C2D	3.68	1.49	1.39
20	6	612	CLA	C3D-C2D	3.68	1.49	1.39
20	B	804	CLA	C3D-C2D	3.68	1.49	1.39
27	8	607	CHL	OBD-CAD	3.68	1.28	1.22
20	A	805	CLA	C3D-C2D	3.68	1.49	1.39
20	3	620	CLA	C3D-C2D	3.68	1.49	1.39
20	4	604	CLA	OBD-CAD	3.68	1.28	1.22
27	4	606	CHL	OBD-CAD	3.68	1.28	1.22
20	Z	613	CLA	OBD-CAD	3.67	1.28	1.22
20	A	823	CLA	C3D-C2D	3.67	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	J	3002	CLA	C3D-C2D	3.67	1.49	1.39
20	7	613	CLA	CHD-C4C	3.67	1.47	1.39
20	A	835	CLA	OBD-CAD	3.67	1.28	1.22
20	B	821	CLA	C3D-C2D	3.67	1.49	1.39
27	6	618	CHL	OBD-CAD	3.67	1.28	1.22
20	Z	604	CLA	OBD-CAD	3.67	1.28	1.22
20	3	617	CLA	C3D-C2D	3.67	1.49	1.39
20	B	811	CLA	C3D-C2D	3.67	1.49	1.39
20	A	837	CLA	OBD-CAD	3.67	1.28	1.22
20	8	602	CLA	CHD-C4C	3.66	1.47	1.39
20	3	609	CLA	C3D-C2D	3.66	1.49	1.39
20	4	612	CLA	C3D-C2D	3.66	1.49	1.39
20	Z	609	CLA	C3D-C2D	3.66	1.49	1.39
20	J	3002	CLA	OBD-CAD	3.66	1.28	1.22
20	6	604	CLA	OBD-CAD	3.66	1.28	1.22
20	8	608	CLA	CHD-C4C	3.66	1.47	1.39
20	6	617	CLA	C3D-C2D	3.66	1.49	1.39
20	4	602	CLA	C3D-C2D	3.66	1.49	1.39
20	A	823	CLA	OBD-CAD	3.66	1.28	1.22
20	B	819	CLA	C3D-C2D	3.66	1.49	1.39
20	A	831	CLA	CHD-C4C	3.66	1.47	1.39
20	1	602	CLA	C3D-C2D	3.65	1.49	1.39
20	8	612	CLA	C3D-C2D	3.65	1.49	1.39
20	B	813	CLA	C3D-C2D	3.65	1.49	1.39
20	3	613	CLA	C3D-C2D	3.65	1.49	1.39
20	Z	602	CLA	C3D-C2D	3.65	1.49	1.39
20	A	824	CLA	OBD-CAD	3.65	1.28	1.22
20	B	834	CLA	OBD-CAD	3.65	1.28	1.22
20	1	604	CLA	C3D-C2D	3.65	1.49	1.39
20	7	612	CLA	C3D-C2D	3.65	1.49	1.39
20	5	621	CLA	OBD-CAD	3.65	1.28	1.22
20	1	606	CLA	OBD-CAD	3.65	1.28	1.22
20	B	835	CLA	OBD-CAD	3.65	1.28	1.22
20	7	612	CLA	OBD-CAD	3.65	1.28	1.22
20	4	613	CLA	C3D-C2D	3.64	1.49	1.39
20	7	616	CLA	C3D-C2D	3.64	1.49	1.39
20	B	820	CLA	C3D-C2D	3.64	1.49	1.39
20	K	4002	CLA	OBD-CAD	3.64	1.28	1.22
20	B	809	CLA	OBD-CAD	3.64	1.28	1.22
20	6	609	CLA	OBD-CAD	3.64	1.28	1.22
20	B	810	CLA	C3D-C2D	3.64	1.49	1.39
20	7	602	CLA	C3D-C2D	3.64	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	613	CLA	OBD-CAD	3.64	1.28	1.22
20	B	831	CLA	C3D-C2D	3.64	1.49	1.39
27	4	618	CHL	OBD-CAD	3.64	1.28	1.22
20	A	809	CLA	C3D-C2D	3.64	1.49	1.39
20	1	613	CLA	C3D-C2D	3.64	1.49	1.39
20	A	804	CLA	OBD-CAD	3.64	1.28	1.22
20	5	617	CLA	C3D-C2D	3.64	1.49	1.39
20	Z	612	CLA	OBD-CAD	3.64	1.28	1.22
20	Z	613	CLA	C3D-C2D	3.64	1.49	1.39
20	A	843	CLA	OBD-CAD	3.64	1.28	1.22
27	5	608	CHL	CHD-C4C	3.64	1.47	1.39
20	A	829	CLA	CHD-C4C	3.63	1.47	1.39
20	3	613	CLA	OBD-CAD	3.63	1.28	1.22
20	5	613	CLA	OBD-CAD	3.63	1.28	1.22
27	5	607	CHL	OBD-CAD	3.63	1.28	1.22
20	B	809	CLA	C3D-C2D	3.63	1.49	1.39
20	G	204	CLA	OBD-CAD	3.63	1.28	1.22
20	A	808	CLA	C3D-C2D	3.63	1.49	1.39
20	6	602	CLA	C3D-C2D	3.63	1.49	1.39
20	B	821	CLA	OBD-CAD	3.63	1.28	1.22
20	3	604	CLA	OBD-CAD	3.63	1.28	1.22
20	7	620	CLA	OBD-CAD	3.63	1.28	1.22
20	3	602	CLA	OBD-CAD	3.63	1.28	1.22
20	B	822	CLA	OBD-CAD	3.63	1.28	1.22
20	A	810	CLA	CHD-C4C	3.63	1.47	1.39
20	4	601	CLA	C3D-C2D	3.63	1.49	1.39
27	6	606	CHL	CHD-C4C	3.63	1.47	1.39
20	F	303	CLA	C3D-C2D	3.62	1.49	1.39
20	B	811	CLA	OBD-CAD	3.62	1.28	1.22
27	6	618	CHL	C3D-C2D	3.62	1.49	1.39
20	A	817	CLA	OBD-CAD	3.62	1.28	1.22
20	Z	606	CLA	OBD-CAD	3.62	1.28	1.22
20	A	826	CLA	CHD-C4C	3.62	1.47	1.39
20	5	616	CLA	C3D-C2D	3.62	1.49	1.39
20	A	813	CLA	C3D-C2D	3.62	1.49	1.39
20	Z	611	CLA	OBD-CAD	3.62	1.28	1.22
20	A	815	CLA	C3D-C2D	3.62	1.49	1.39
20	1	608	CLA	C3D-C2D	3.62	1.49	1.39
20	B	838	CLA	C3D-C2D	3.62	1.49	1.39
20	A	842	CLA	OBD-CAD	3.62	1.28	1.22
20	A	839	CLA	C3D-C2D	3.62	1.49	1.39
20	A	808	CLA	CHD-C4C	3.62	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	828	CLA	OBD-CAD	3.61	1.28	1.22
20	A	811	CLA	CHD-C4C	3.61	1.47	1.39
19	A	801	CL0	C3D-C2D	3.61	1.49	1.39
20	4	601	CLA	OBD-CAD	3.61	1.28	1.22
20	5	612	CLA	OBD-CAD	3.61	1.28	1.22
20	A	832	CLA	C3D-C2D	3.61	1.49	1.39
20	3	602	CLA	C3D-C2D	3.61	1.49	1.39
20	6	616	CLA	OBD-CAD	3.61	1.28	1.22
27	6	608	CHL	C1D-ND	-3.61	1.33	1.37
20	B	812	CLA	C3D-C2D	3.61	1.49	1.39
20	B	813	CLA	OBD-CAD	3.61	1.28	1.22
20	A	821	CLA	C3D-C2D	3.61	1.49	1.39
20	1	612	CLA	OBD-CAD	3.61	1.28	1.22
20	A	818	CLA	C3D-C2D	3.61	1.49	1.39
20	6	603	CLA	C3D-C2D	3.61	1.49	1.39
20	B	804	CLA	OBD-CAD	3.61	1.28	1.22
20	5	601	CLA	OBD-CAD	3.61	1.28	1.22
20	B	839	CLA	C3D-C2D	3.61	1.49	1.39
20	A	834	CLA	C3D-C2D	3.60	1.49	1.39
20	4	616	CLA	OBD-CAD	3.60	1.28	1.22
20	B	812	CLA	OBD-CAD	3.60	1.28	1.22
20	3	617	CLA	OBD-CAD	3.60	1.28	1.22
27	1	607	CHL	OBD-CAD	3.60	1.28	1.22
20	B	841	CLA	OBD-CAD	3.60	1.28	1.22
20	1	610	CLA	OBD-CAD	3.60	1.28	1.22
20	4	614	CLA	OBD-CAD	3.60	1.28	1.22
20	7	604	CLA	OBD-CAD	3.60	1.28	1.22
20	8	612	CLA	OBD-CAD	3.60	1.28	1.22
20	B	808	CLA	CHD-C4C	3.60	1.47	1.39
20	7	603	CLA	C3D-C2D	3.60	1.48	1.39
20	L	203	CLA	OBD-CAD	3.60	1.28	1.22
20	A	808	CLA	OBD-CAD	3.60	1.28	1.22
20	1	609	CLA	OBD-CAD	3.60	1.28	1.22
20	8	603	CLA	C3D-C2D	3.60	1.48	1.39
20	5	610	CLA	C3D-C2D	3.60	1.48	1.39
20	5	604	CLA	OBD-CAD	3.60	1.28	1.22
20	1	616	CLA	OBD-CAD	3.59	1.28	1.22
20	A	834	CLA	OBD-CAD	3.59	1.28	1.22
20	B	829	CLA	OBD-CAD	3.59	1.28	1.22
20	B	832	CLA	C3D-C2D	3.59	1.48	1.39
20	8	606	CLA	OBD-CAD	3.59	1.28	1.22
20	B	814	CLA	C3D-C2D	3.59	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	8	613	CLA	C3D-C2D	3.59	1.48	1.39
20	A	845	CLA	C3D-C2D	3.59	1.48	1.39
20	1	611	CLA	OBD-CAD	3.59	1.28	1.22
20	B	840	CLA	OBD-CAD	3.59	1.28	1.22
20	B	827	CLA	C3D-C2D	3.59	1.48	1.39
20	A	814	CLA	CHD-C4C	3.59	1.47	1.39
20	7	616	CLA	OBD-CAD	3.59	1.28	1.22
20	F	304	CLA	C3D-C2D	3.58	1.48	1.39
20	F	304	CLA	OBD-CAD	3.58	1.28	1.22
20	Z	610	CLA	OBD-CAD	3.58	1.28	1.22
20	K	4003	CLA	OBD-CAD	3.58	1.28	1.22
20	6	622	CLA	C3D-C2D	3.58	1.48	1.39
20	A	828	CLA	CHD-C1D	3.58	1.45	1.38
20	A	812	CLA	C3D-C2D	3.58	1.48	1.39
20	A	810	CLA	OBD-CAD	3.58	1.28	1.22
27	4	606	CHL	CHD-C4C	3.58	1.47	1.39
27	3	608	CHL	C1D-ND	-3.58	1.33	1.37
20	6	622	CLA	OBD-CAD	3.58	1.28	1.22
20	B	828	CLA	CHD-C4C	3.58	1.47	1.39
20	Z	608	CLA	C3D-C2D	3.57	1.48	1.39
20	A	829	CLA	C3D-C2D	3.57	1.48	1.39
27	5	618	CHL	C1D-ND	-3.57	1.33	1.37
20	A	819	CLA	C3D-C2D	3.57	1.48	1.39
20	B	828	CLA	C3D-C2D	3.57	1.48	1.39
20	6	617	CLA	OBD-CAD	3.57	1.28	1.22
20	A	814	CLA	OBD-CAD	3.57	1.28	1.22
20	B	852	CLA	OBD-CAD	3.57	1.28	1.22
20	4	611	CLA	OBD-CAD	3.57	1.28	1.22
27	6	608	CHL	CHD-C4C	3.57	1.47	1.39
20	A	830	CLA	OBD-CAD	3.56	1.28	1.22
20	7	606	CLA	OBD-CAD	3.56	1.28	1.22
20	A	813	CLA	OBD-CAD	3.56	1.28	1.22
20	B	836	CLA	C3D-C2D	3.56	1.48	1.39
20	6	611	CLA	OBD-CAD	3.56	1.28	1.22
20	B	818	CLA	OBD-CAD	3.56	1.28	1.22
20	A	827	CLA	C3D-C2D	3.56	1.48	1.39
20	5	621	CLA	C3D-C2D	3.56	1.48	1.39
20	A	842	CLA	C3D-C2D	3.56	1.48	1.39
20	A	841	CLA	OBD-CAD	3.55	1.28	1.22
20	B	823	CLA	OBD-CAD	3.55	1.28	1.22
27	4	618	CHL	C1D-ND	-3.55	1.33	1.37
20	5	617	CLA	OBD-CAD	3.55	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	816	CLA	OBD-CAD	3.55	1.28	1.22
20	8	608	CLA	C3D-C2D	3.55	1.48	1.39
20	5	616	CLA	OBD-CAD	3.55	1.28	1.22
20	B	824	CLA	OBD-CAD	3.55	1.28	1.22
20	A	838	CLA	C3D-C2D	3.55	1.48	1.39
20	B	802	CLA	OBD-CAD	3.55	1.28	1.22
20	4	610	CLA	OBD-CAD	3.55	1.28	1.22
20	6	602	CLA	OBD-CAD	3.55	1.28	1.22
20	5	602	CLA	OBD-CAD	3.54	1.28	1.22
20	A	824	CLA	C3D-C2D	3.54	1.48	1.39
20	B	816	CLA	C3D-C2D	3.54	1.48	1.39
20	A	818	CLA	OBD-CAD	3.54	1.28	1.22
20	4	609	CLA	OBD-CAD	3.54	1.28	1.22
20	7	601	CLA	C3D-C2D	3.54	1.48	1.39
20	A	802	CLA	C1B-NB	-3.54	1.32	1.35
20	B	808	CLA	OBD-CAD	3.54	1.28	1.22
20	B	805	CLA	C3D-C2D	3.54	1.48	1.39
20	A	854	CLA	CHD-C1D	3.54	1.45	1.38
20	Z	609	CLA	OBD-CAD	3.54	1.28	1.22
20	B	808	CLA	C3D-C2D	3.54	1.48	1.39
20	B	806	CLA	C3D-C2D	3.54	1.48	1.39
20	3	606	CLA	OBD-CAD	3.54	1.28	1.22
20	Z	616	CLA	OBD-CAD	3.53	1.28	1.22
20	A	840	CLA	C3D-C2D	3.53	1.48	1.39
20	5	611	CLA	OBD-CAD	3.53	1.28	1.22
20	A	820	CLA	OBD-CAD	3.53	1.28	1.22
27	6	608	CHL	OBD-CAD	3.53	1.28	1.22
27	Z	607	CHL	OBD-CAD	3.53	1.28	1.22
20	B	830	CLA	C3D-C2D	3.53	1.48	1.39
20	8	601	CLA	C3D-C2D	3.53	1.48	1.39
20	7	610	CLA	C3D-C2D	3.53	1.48	1.39
27	Z	601	CHL	CHD-C4C	3.53	1.47	1.39
20	1	602	CLA	OBD-CAD	3.53	1.28	1.22
20	1	606	CLA	C3D-C2D	3.53	1.48	1.39
20	8	611	CLA	OBD-CAD	3.52	1.28	1.22
27	6	618	CHL	C1D-ND	-3.52	1.33	1.37
20	B	822	CLA	C3D-C2D	3.52	1.48	1.39
20	B	805	CLA	OBD-CAD	3.52	1.28	1.22
20	A	806	CLA	C3D-C2D	3.52	1.48	1.39
20	B	832	CLA	OBD-CAD	3.52	1.28	1.22
27	8	607	CHL	CHD-C4C	3.52	1.47	1.39
20	B	827	CLA	OBD-CAD	3.52	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	836	CLA	OBD-CAD	3.52	1.28	1.22
19	A	801	CL0	OBD-CAD	3.52	1.28	1.22
20	5	609	CLA	OBD-CAD	3.52	1.28	1.22
20	A	825	CLA	OBD-CAD	3.51	1.28	1.22
20	B	810	CLA	OBD-CAD	3.51	1.28	1.22
20	8	613	CLA	OBD-CAD	3.51	1.28	1.22
20	A	838	CLA	OBD-CAD	3.51	1.28	1.22
20	A	826	CLA	OBD-CAD	3.51	1.28	1.22
20	3	609	CLA	OBD-CAD	3.51	1.28	1.22
20	A	811	CLA	OBD-CAD	3.51	1.28	1.22
27	6	607	CHL	C1D-ND	-3.50	1.33	1.37
20	A	810	CLA	C3D-C2D	3.50	1.48	1.39
20	A	814	CLA	C3D-C2D	3.50	1.48	1.39
20	A	819	CLA	OBD-CAD	3.50	1.28	1.22
20	8	602	CLA	OBD-CAD	3.50	1.28	1.22
20	7	601	CLA	OBD-CAD	3.49	1.28	1.22
20	B	830	CLA	OBD-CAD	3.49	1.28	1.22
20	8	616	CLA	OBD-CAD	3.49	1.28	1.22
20	B	840	CLA	C3D-C2D	3.49	1.48	1.39
20	B	819	CLA	OBD-CAD	3.49	1.28	1.22
20	7	610	CLA	OBD-CAD	3.49	1.28	1.22
27	5	608	CHL	OBD-CAD	3.49	1.28	1.22
27	4	608	CHL	CHD-C4C	3.49	1.47	1.39
20	B	815	CLA	OBD-CAD	3.49	1.28	1.22
20	A	817	CLA	C3D-C2D	3.49	1.48	1.39
27	1	601	CHL	C1D-ND	-3.49	1.33	1.37
27	1	601	CHL	CHD-C4C	3.49	1.47	1.39
20	4	612	CLA	OBD-CAD	3.49	1.28	1.22
20	B	825	CLA	OBD-CAD	3.49	1.28	1.22
27	3	608	CHL	CHD-C4C	3.49	1.47	1.39
20	3	610	CLA	C3D-C2D	3.48	1.48	1.39
27	8	607	CHL	C1D-ND	-3.48	1.33	1.37
20	B	833	CLA	OBD-CAD	3.48	1.28	1.22
20	5	610	CLA	OBD-CAD	3.48	1.28	1.22
20	7	606	CLA	C3D-C2D	3.47	1.48	1.39
20	7	608	CLA	C3D-C2D	3.47	1.48	1.39
20	A	805	CLA	OBD-CAD	3.47	1.28	1.22
19	A	801	CL0	CHD-C4C	3.47	1.47	1.39
20	7	614	CLA	OBD-CAD	3.47	1.28	1.22
20	5	614	CLA	OBD-CAD	3.46	1.28	1.22
20	B	802	CLA	CHD-C4C	3.46	1.47	1.39
20	A	815	CLA	OBD-CAD	3.46	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	854	CLA	CHD-C4C	3.46	1.47	1.39
20	Z	602	CLA	OBD-CAD	3.46	1.28	1.22
20	A	829	CLA	OBD-CAD	3.46	1.28	1.22
20	7	608	CLA	OBD-CAD	3.46	1.28	1.22
20	A	832	CLA	OBD-CAD	3.46	1.28	1.22
20	B	814	CLA	OBD-CAD	3.45	1.28	1.22
20	A	830	CLA	CHD-C4C	3.45	1.47	1.39
20	6	612	CLA	OBD-CAD	3.45	1.28	1.22
20	A	802	CLA	C1D-ND	3.45	1.42	1.37
27	1	607	CHL	C1D-ND	-3.45	1.33	1.37
20	B	825	CLA	C3D-C2D	3.45	1.48	1.39
20	A	806	CLA	OBD-CAD	3.45	1.28	1.22
20	8	609	CLA	OBD-CAD	3.45	1.28	1.22
27	4	618	CHL	C3D-C2D	3.45	1.48	1.39
27	4	607	CHL	C1D-ND	-3.44	1.33	1.37
20	A	821	CLA	OBD-CAD	3.44	1.28	1.22
27	5	607	CHL	C3D-C2D	3.44	1.48	1.39
20	B	817	CLA	OBD-CAD	3.44	1.28	1.22
27	6	607	CHL	CHD-C4C	3.44	1.47	1.39
27	4	606	CHL	C1D-ND	-3.44	1.33	1.37
20	A	802	CLA	OBD-CAD	3.44	1.28	1.22
20	4	602	CLA	OBD-CAD	3.44	1.28	1.22
20	A	809	CLA	OBD-CAD	3.43	1.28	1.22
20	7	609	CLA	OBD-CAD	3.43	1.28	1.22
20	B	839	CLA	OBD-CAD	3.43	1.28	1.22
20	B	831	CLA	OBD-CAD	3.43	1.28	1.22
20	B	802	CLA	C3D-C2D	3.43	1.48	1.39
20	7	611	CLA	OBD-CAD	3.42	1.28	1.22
20	3	603	CLA	OBD-CAD	3.42	1.28	1.22
20	B	807	CLA	OBD-CAD	3.42	1.28	1.22
20	8	610	CLA	C3D-C2D	3.42	1.48	1.39
20	A	831	CLA	OBD-CAD	3.42	1.28	1.22
20	A	828	CLA	C3D-C2D	3.42	1.48	1.39
27	1	607	CHL	C3D-C2D	3.42	1.48	1.39
27	4	607	CHL	C3D-C2D	3.42	1.48	1.39
20	5	602	CLA	C3D-C2D	3.41	1.48	1.39
20	A	840	CLA	OBD-CAD	3.41	1.28	1.22
20	Z	603	CLA	OBD-CAD	3.41	1.28	1.22
20	B	826	CLA	C3D-C2D	3.41	1.48	1.39
20	8	601	CLA	OBD-CAD	3.41	1.28	1.22
27	Z	607	CHL	C1D-ND	-3.41	1.33	1.37
27	5	618	CHL	C3D-C2D	3.41	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	607	CLA	OBD-CAD	3.41	1.28	1.22
20	7	604	CLA	C3D-C2D	3.40	1.48	1.39
20	7	611	CLA	C3A-C2A	-3.40	1.51	1.54
20	A	827	CLA	OBD-CAD	3.40	1.28	1.22
27	6	608	CHL	C3D-C2D	3.40	1.48	1.39
20	G	203	CLA	OBD-CAD	3.39	1.28	1.22
20	B	826	CLA	OBD-CAD	3.39	1.28	1.22
20	B	824	CLA	C3D-C2D	3.39	1.48	1.39
27	5	607	CHL	C1D-ND	-3.39	1.33	1.37
20	8	614	CLA	OBD-CAD	3.38	1.28	1.22
20	7	603	CLA	OBD-CAD	3.38	1.28	1.22
20	A	828	CLA	CHD-C4C	3.38	1.46	1.39
20	A	812	CLA	OBD-CAD	3.38	1.28	1.22
27	Z	607	CHL	C3D-C2D	3.38	1.48	1.39
20	A	833	CLA	C3D-C2D	3.36	1.48	1.39
20	6	610	CLA	OBD-CAD	3.36	1.28	1.22
20	7	613	CLA	OBD-CAD	3.36	1.28	1.22
20	B	820	CLA	OBD-CAD	3.35	1.28	1.22
20	F	303	CLA	OBD-CAD	3.35	1.28	1.22
20	B	803	CLA	OBD-CAD	3.34	1.28	1.22
20	Z	614	CLA	OBD-CAD	3.34	1.28	1.22
20	B	829	CLA	C3D-C2D	3.34	1.48	1.39
20	7	602	CLA	OBD-CAD	3.33	1.28	1.22
27	7	607	CHL	C1D-ND	-3.33	1.33	1.37
20	A	807	CLA	OBD-CAD	3.31	1.28	1.22
27	5	608	CHL	C1D-ND	-3.31	1.33	1.37
27	8	607	CHL	C3D-C2D	3.31	1.48	1.39
20	1	614	CLA	OBD-CAD	3.30	1.28	1.22
27	4	608	CHL	C1D-ND	-3.30	1.33	1.37
27	Z	601	CHL	C3D-C2D	3.30	1.48	1.39
27	4	606	CHL	C3D-C2D	3.29	1.48	1.39
20	Z	608	CLA	OBD-CAD	3.29	1.28	1.22
27	6	607	CHL	C3D-C2D	3.29	1.48	1.39
20	F	301	CLA	OBD-CAD	3.29	1.28	1.22
27	5	608	CHL	C3D-C2D	3.27	1.48	1.39
20	6	614	CLA	C3D-C2D	3.26	1.48	1.39
20	A	839	CLA	OBD-CAD	3.25	1.28	1.22
20	F	301	CLA	C3D-C2D	3.25	1.48	1.39
27	6	606	CHL	C3D-C2D	3.24	1.48	1.39
27	5	607	CHL	MG-NA	-3.23	1.98	2.06
27	3	608	CHL	OBD-CAD	3.21	1.28	1.22
20	4	603	CLA	OBD-CAD	3.20	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	4	608	CHL	OBD-CAD	3.20	1.28	1.22
20	1	608	CLA	OBD-CAD	3.19	1.28	1.22
27	1	601	CHL	C3D-C2D	3.19	1.47	1.39
27	7	607	CHL	C3D-C2D	3.18	1.47	1.39
20	A	822	CLA	OBD-CAD	3.18	1.28	1.22
27	3	608	CHL	C3D-C2D	3.17	1.47	1.39
20	A	803	CLA	OBD-CAD	3.17	1.27	1.22
20	6	603	CLA	OBD-CAD	3.16	1.27	1.22
27	4	608	CHL	C3D-C2D	3.15	1.47	1.39
20	4	616	CLA	C3A-C2A	-3.15	1.51	1.54
27	3	608	CHL	C1B-NB	-3.14	1.32	1.35
20	1	603	CLA	OBD-CAD	3.13	1.27	1.22
20	A	802	CLA	CHD-C1D	3.13	1.44	1.38
20	A	831	CLA	C1B-NB	-3.12	1.32	1.35
20	A	837	CLA	C1B-NB	-3.11	1.32	1.35
27	6	606	CHL	C1D-ND	-3.11	1.34	1.37
20	A	854	CLA	OBD-CAD	3.09	1.27	1.22
20	3	610	CLA	OBD-CAD	3.09	1.27	1.22
20	A	804	CLA	C3D-C2D	3.08	1.47	1.39
20	8	608	CLA	OBD-CAD	3.07	1.27	1.22
20	B	837	CLA	OBD-CAD	3.06	1.27	1.22
20	8	603	CLA	OBD-CAD	3.06	1.27	1.22
20	B	806	CLA	OBD-CAD	3.06	1.27	1.22
20	A	828	CLA	OBD-CAD	3.04	1.27	1.22
20	B	809	CLA	C1B-NB	-3.03	1.32	1.35
27	1	607	CHL	MG-NA	-3.01	1.99	2.06
20	B	816	CLA	OBD-CAD	3.01	1.27	1.22
20	B	838	CLA	OBD-CAD	2.96	1.27	1.22
27	4	607	CHL	MG-NA	-2.95	1.99	2.06
20	B	825	CLA	C1B-NB	-2.94	1.32	1.35
27	Z	607	CHL	MG-NA	-2.92	1.99	2.06
20	3	611	CLA	C3A-C2A	-2.92	1.51	1.54
20	B	828	CLA	C1B-NB	-2.90	1.32	1.35
27	6	607	CHL	MG-NA	-2.89	1.99	2.06
27	8	607	CHL	MG-NA	-2.87	1.99	2.06
27	1	601	CHL	C3D-C4D	-2.86	1.37	1.44
20	A	820	CLA	C1B-NB	-2.85	1.32	1.35
20	A	830	CLA	C1B-NB	-2.85	1.32	1.35
27	4	618	CHL	MG-NA	-2.85	1.99	2.06
20	B	805	CLA	C4B-CHC	2.84	1.48	1.41
27	5	618	CHL	MG-NA	-2.82	1.99	2.06
20	B	818	CLA	C1B-NB	-2.80	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	1	601	CHL	OBD-CAD	2.80	1.27	1.22
20	B	836	CLA	OBD-CAD	2.79	1.27	1.22
20	A	804	CLA	C3D-C4D	-2.79	1.37	1.44
20	A	837	CLA	C4D-CHA	2.79	1.48	1.38
20	B	835	CLA	C1B-NB	-2.78	1.32	1.35
27	6	608	CHL	MG-NA	-2.77	1.99	2.06
20	8	610	CLA	OBD-CAD	2.74	1.27	1.22
20	8	601	CLA	C4D-CHA	2.73	1.48	1.38
20	8	616	CLA	C4D-CHA	2.72	1.48	1.38
20	1	610	CLA	C1C-C2C	2.72	1.49	1.44
20	3	611	CLA	C4D-CHA	2.72	1.48	1.38
20	7	606	CLA	C1B-NB	-2.72	1.32	1.35
27	5	608	CHL	MG-NA	-2.72	1.99	2.06
20	B	835	CLA	C4D-CHA	2.72	1.48	1.38
20	7	610	CLA	C4B-CHC	2.72	1.48	1.41
20	A	833	CLA	OBD-CAD	2.71	1.27	1.22
20	3	610	CLA	C1C-C2C	2.71	1.49	1.44
20	7	611	CLA	C4D-CHA	2.71	1.48	1.38
27	6	608	CHL	C3D-C4D	-2.71	1.38	1.44
19	A	801	CL0	C1B-NB	-2.71	1.32	1.35
20	A	833	CLA	C1B-NB	-2.71	1.32	1.35
20	7	614	CLA	C4D-CHA	2.71	1.48	1.38
20	K	4002	CLA	C4D-CHA	2.71	1.48	1.38
20	5	611	CLA	C4D-CHA	2.70	1.48	1.38
20	3	603	CLA	C4D-CHA	2.70	1.48	1.38
27	8	607	CHL	C3D-C4D	-2.70	1.38	1.44
20	8	611	CLA	C4D-CHA	2.70	1.48	1.38
20	Z	609	CLA	C4D-CHA	2.70	1.48	1.38
20	Z	608	CLA	C4D-CHA	2.70	1.48	1.38
20	6	604	CLA	C4D-CHA	2.70	1.48	1.38
20	6	609	CLA	C4D-CHA	2.69	1.48	1.38
20	Z	610	CLA	C1C-C2C	2.69	1.49	1.44
20	B	823	CLA	C4D-CHA	2.69	1.48	1.38
20	4	611	CLA	C4D-CHA	2.69	1.48	1.38
20	5	616	CLA	C4D-CHA	2.69	1.48	1.38
20	6	616	CLA	C4D-CHA	2.69	1.48	1.38
27	7	607	CHL	MG-NA	-2.69	1.99	2.06
27	4	606	CHL	MG-NA	-2.68	1.99	2.06
20	G	204	CLA	C4D-CHA	2.68	1.47	1.38
20	B	815	CLA	C4D-CHA	2.68	1.47	1.38
20	B	852	CLA	C4D-CHA	2.68	1.47	1.38
20	B	806	CLA	C4D-CHA	2.68	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	3	608	CHL	C3D-C4D	-2.68	1.38	1.44
20	Z	616	CLA	C4D-CHA	2.68	1.47	1.38
20	3	606	CLA	C4D-CHA	2.67	1.47	1.38
20	B	809	CLA	C4D-CHA	2.67	1.47	1.38
20	A	831	CLA	C4D-CHA	2.67	1.47	1.38
20	B	841	CLA	C4D-CHA	2.67	1.47	1.38
20	A	840	CLA	C4D-CHA	2.67	1.47	1.38
20	5	603	CLA	C4D-CHA	2.67	1.47	1.38
20	1	616	CLA	C4D-CHA	2.66	1.47	1.38
20	A	822	CLA	C4D-CHA	2.66	1.47	1.38
20	Z	613	CLA	C4D-CHA	2.66	1.47	1.38
20	5	621	CLA	C4D-CHA	2.66	1.47	1.38
20	B	804	CLA	C4D-CHA	2.65	1.47	1.38
20	A	805	CLA	C1B-NB	-2.65	1.32	1.35
20	B	819	CLA	C4D-CHA	2.65	1.47	1.38
20	7	620	CLA	C4D-CHA	2.65	1.47	1.38
20	5	609	CLA	C4D-CHA	2.65	1.47	1.38
20	L	204	CLA	C4C-C3C	2.65	1.49	1.45
20	A	839	CLA	C4D-CHA	2.65	1.47	1.38
20	Z	614	CLA	C4D-CHA	2.65	1.47	1.38
20	3	609	CLA	C4D-CHA	2.65	1.47	1.38
27	3	608	CHL	MG-NA	-2.65	2.00	2.06
20	4	601	CLA	C4D-CHA	2.65	1.47	1.38
20	5	612	CLA	C4D-CHA	2.65	1.47	1.38
20	1	612	CLA	C4D-CHA	2.65	1.47	1.38
20	F	303	CLA	C4D-CHA	2.64	1.47	1.38
20	4	603	CLA	C4D-CHA	2.64	1.47	1.38
20	5	601	CLA	C4D-CHA	2.64	1.47	1.38
20	5	614	CLA	C4D-CHA	2.64	1.47	1.38
20	A	803	CLA	C1B-NB	-2.64	1.32	1.35
20	B	818	CLA	C4D-CHA	2.64	1.47	1.38
20	B	812	CLA	C4D-CHA	2.64	1.47	1.38
20	B	807	CLA	C4D-CHA	2.64	1.47	1.38
20	1	609	CLA	C4D-CHA	2.64	1.47	1.38
20	3	604	CLA	C4D-CHA	2.64	1.47	1.38
20	6	603	CLA	C4D-CHA	2.64	1.47	1.38
20	B	816	CLA	C4D-CHA	2.64	1.47	1.38
20	5	604	CLA	C4D-CHA	2.64	1.47	1.38
20	5	606	CLA	C4D-CHA	2.64	1.47	1.38
20	A	833	CLA	C4D-CHA	2.63	1.47	1.38
20	8	603	CLA	C3D-C4D	-2.63	1.38	1.44
20	6	610	CLA	C4D-CHA	2.63	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	6	606	CHL	C2C-C1C	2.63	1.50	1.44
20	8	612	CLA	C4D-CHA	2.63	1.47	1.38
27	6	618	CHL	MG-NA	-2.63	2.00	2.06
27	4	607	CHL	C3D-C4D	-2.63	1.38	1.44
20	3	620	CLA	C4D-CHA	2.63	1.47	1.38
20	A	816	CLA	C4D-CHA	2.63	1.47	1.38
20	1	603	CLA	C4D-CHA	2.63	1.47	1.38
20	7	609	CLA	C4D-CHA	2.63	1.47	1.38
20	J	3002	CLA	C4D-CHA	2.62	1.47	1.38
20	A	821	CLA	C4D-CHA	2.62	1.47	1.38
20	Z	604	CLA	C4D-CHA	2.62	1.47	1.38
20	7	613	CLA	C4D-CHA	2.62	1.47	1.38
20	6	611	CLA	C4D-CHA	2.62	1.47	1.38
20	A	819	CLA	C4D-CHA	2.62	1.47	1.38
20	A	842	CLA	C4D-CHA	2.62	1.47	1.38
20	Z	606	CLA	C4D-CHA	2.62	1.47	1.38
20	1	608	CLA	C4D-CHA	2.62	1.47	1.38
20	8	608	CLA	C4D-CHA	2.62	1.47	1.38
20	A	845	CLA	C4D-CHA	2.62	1.47	1.38
20	A	835	CLA	C4D-CHA	2.62	1.47	1.38
20	4	614	CLA	C4D-CHA	2.61	1.47	1.38
20	3	613	CLA	C4C-C3C	2.61	1.49	1.45
19	A	801	CL0	C4D-CHA	2.61	1.47	1.38
20	B	820	CLA	C4D-CHA	2.61	1.47	1.38
20	B	811	CLA	C4D-CHA	2.61	1.47	1.38
20	A	815	CLA	C4D-CHA	2.61	1.47	1.38
20	A	841	CLA	C4D-CHA	2.61	1.47	1.38
20	6	617	CLA	C4D-CHA	2.61	1.47	1.38
20	A	821	CLA	C1B-NB	-2.61	1.32	1.35
20	4	616	CLA	C4D-CHA	2.61	1.47	1.38
20	A	807	CLA	C3D-C4D	-2.61	1.38	1.44
20	3	614	CLA	C4D-CHA	2.60	1.47	1.38
20	B	833	CLA	C4D-CHA	2.60	1.47	1.38
20	A	833	CLA	C3D-C4D	-2.60	1.38	1.44
20	A	832	CLA	C4D-CHA	2.60	1.47	1.38
20	B	837	CLA	C4D-CHA	2.60	1.47	1.38
20	A	805	CLA	C4D-CHA	2.60	1.47	1.38
20	A	813	CLA	C4D-CHA	2.60	1.47	1.38
20	L	204	CLA	C4D-CHA	2.60	1.47	1.38
20	A	825	CLA	C4D-CHA	2.60	1.47	1.38
20	1	604	CLA	C4D-CHA	2.60	1.47	1.38
20	8	614	CLA	C4D-CHA	2.60	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	G	203	CLA	C4D-CHA	2.60	1.47	1.38
20	A	854	CLA	C1C-C2C	2.60	1.49	1.44
20	B	836	CLA	C3D-C4D	-2.59	1.38	1.44
20	3	613	CLA	C4D-CHA	2.59	1.47	1.38
20	5	613	CLA	C4D-CHA	2.59	1.47	1.38
20	5	603	CLA	OBD-CAD	2.59	1.26	1.22
20	1	606	CLA	C4D-CHA	2.59	1.47	1.38
20	3	607	CLA	C4D-CHA	2.59	1.47	1.38
20	A	836	CLA	C4D-CHA	2.59	1.47	1.38
20	Z	603	CLA	C4D-CHA	2.59	1.47	1.38
20	4	610	CLA	C4D-CHA	2.59	1.47	1.38
20	A	807	CLA	C4D-CHA	2.59	1.47	1.38
20	Z	602	CLA	C4D-CHA	2.59	1.47	1.38
20	F	301	CLA	C4B-CHC	2.59	1.48	1.41
20	B	834	CLA	C4D-CHA	2.59	1.47	1.38
20	A	834	CLA	C4D-CHA	2.59	1.47	1.38
20	B	824	CLA	C4D-CHA	2.59	1.47	1.38
27	4	618	CHL	C3D-C4D	-2.59	1.38	1.44
20	K	4003	CLA	C4D-CHA	2.58	1.47	1.38
20	6	602	CLA	C4D-CHA	2.58	1.47	1.38
20	6	622	CLA	C4D-CHA	2.58	1.47	1.38
20	6	601	CLA	C4D-CHA	2.58	1.47	1.38
20	B	839	CLA	C4D-CHA	2.58	1.47	1.38
20	A	802	CLA	C4D-CHA	2.58	1.47	1.38
20	A	843	CLA	C4D-CHA	2.58	1.47	1.38
20	1	613	CLA	C4D-CHA	2.58	1.47	1.38
20	F	301	CLA	C4D-CHA	2.58	1.47	1.38
20	A	824	CLA	C4D-CHA	2.58	1.47	1.38
20	B	822	CLA	C4D-CHA	2.58	1.47	1.38
20	7	606	CLA	C4D-CHA	2.58	1.47	1.38
20	B	836	CLA	C4D-CHA	2.58	1.47	1.38
20	A	828	CLA	C4D-CHA	2.58	1.47	1.38
27	Z	601	CHL	C2C-C1C	2.58	1.50	1.44
20	8	606	CLA	C4D-CHA	2.58	1.47	1.38
20	A	822	CLA	C1B-NB	-2.58	1.32	1.35
20	B	808	CLA	C4D-CHA	2.58	1.47	1.38
20	3	610	CLA	C4B-CHC	2.57	1.48	1.41
20	5	604	CLA	C4C-C3C	2.57	1.49	1.45
20	8	602	CLA	C4D-CHA	2.57	1.47	1.38
20	A	830	CLA	C4D-CHA	2.57	1.47	1.38
20	A	809	CLA	C4D-CHA	2.57	1.47	1.38
20	B	803	CLA	C4D-CHA	2.57	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	614	CLA	C4D-CHA	2.57	1.47	1.38
20	5	610	CLA	C4D-CHA	2.57	1.47	1.38
20	Z	611	CLA	C4D-CHA	2.57	1.47	1.38
20	8	610	CLA	C1C-C2C	2.57	1.49	1.44
20	4	609	CLA	C4D-CHA	2.57	1.47	1.38
20	A	854	CLA	C1B-NB	-2.57	1.32	1.35
20	1	611	CLA	C4D-CHA	2.57	1.47	1.38
20	4	612	CLA	C4D-CHA	2.57	1.47	1.38
20	A	823	CLA	C4D-CHA	2.57	1.47	1.38
20	B	840	CLA	C4D-CHA	2.57	1.47	1.38
20	1	602	CLA	C4D-CHA	2.57	1.47	1.38
20	A	810	CLA	C4D-CHA	2.56	1.47	1.38
20	B	821	CLA	C4D-CHA	2.56	1.47	1.38
20	3	610	CLA	C4D-CHA	2.56	1.47	1.38
20	8	610	CLA	C4D-CHA	2.56	1.47	1.38
27	4	606	CHL	C3D-C4D	-2.56	1.38	1.44
20	4	610	CLA	C1B-NB	-2.56	1.32	1.35
20	B	817	CLA	C4D-CHA	2.56	1.47	1.38
20	3	617	CLA	C4D-CHA	2.56	1.47	1.38
20	1	610	CLA	C4B-CHC	2.56	1.48	1.41
20	B	826	CLA	C4D-CHA	2.56	1.47	1.38
27	5	618	CHL	C3D-C4D	-2.56	1.38	1.44
20	8	609	CLA	C4D-CHA	2.56	1.47	1.38
20	A	814	CLA	C4D-CHA	2.56	1.47	1.38
27	Z	607	CHL	C3D-C4D	-2.55	1.38	1.44
20	A	838	CLA	C4D-CHA	2.55	1.47	1.38
20	A	813	CLA	C1B-NB	-2.55	1.32	1.35
20	6	613	CLA	C4D-CHA	2.55	1.47	1.38
20	Z	612	CLA	C4D-CHA	2.55	1.47	1.38
20	B	831	CLA	C4D-CHA	2.55	1.47	1.38
20	A	826	CLA	C4D-CHA	2.55	1.47	1.38
20	A	803	CLA	C4D-CHA	2.55	1.47	1.38
20	A	829	CLA	C4D-CHA	2.54	1.47	1.38
20	4	604	CLA	C4D-CHA	2.54	1.47	1.38
20	7	612	CLA	C4D-CHA	2.54	1.47	1.38
20	B	840	CLA	C3D-C4D	-2.54	1.38	1.44
20	A	808	CLA	C4D-CHA	2.54	1.47	1.38
20	4	613	CLA	C4D-CHA	2.54	1.47	1.38
20	7	603	CLA	C4D-CHA	2.54	1.47	1.38
27	1	601	CHL	MG-NA	-2.54	2.00	2.06
20	3	612	CLA	C4D-CHA	2.54	1.47	1.38
20	A	805	CLA	C4B-CHC	2.54	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	7	607	CHL	C3D-C4D	-2.53	1.38	1.44
20	B	832	CLA	C4D-CHA	2.53	1.47	1.38
20	5	617	CLA	C4D-CHA	2.53	1.47	1.38
20	4	601	CLA	C4C-C3C	2.53	1.49	1.45
27	5	607	CHL	C3D-C4D	-2.53	1.38	1.44
20	B	805	CLA	C4D-CHA	2.53	1.47	1.38
20	7	602	CLA	C4D-CHA	2.53	1.47	1.38
20	A	817	CLA	C4D-CHA	2.53	1.47	1.38
20	4	602	CLA	C4D-CHA	2.53	1.47	1.38
20	5	616	CLA	C4C-C3C	2.53	1.49	1.45
20	B	828	CLA	C4D-CHA	2.53	1.47	1.38
20	Z	610	CLA	C4B-CHC	2.53	1.48	1.41
20	1	610	CLA	C4D-CHA	2.53	1.47	1.38
20	7	604	CLA	C1C-C2C	2.53	1.49	1.44
27	6	606	CHL	MG-NA	-2.53	2.00	2.06
20	A	820	CLA	C4D-CHA	2.52	1.47	1.38
20	7	616	CLA	C4D-CHA	2.52	1.47	1.38
20	1	604	CLA	C4C-C3C	2.52	1.49	1.45
27	1	601	CHL	C2C-C1C	2.52	1.49	1.44
20	A	818	CLA	C4D-CHA	2.52	1.47	1.38
20	F	304	CLA	C4D-CHA	2.52	1.47	1.38
20	A	833	CLA	C4B-CHC	2.52	1.48	1.41
27	4	608	CHL	C2C-C1C	2.52	1.49	1.44
20	A	842	CLA	C3D-C4D	-2.52	1.38	1.44
20	1	603	CLA	C1B-NB	-2.52	1.33	1.35
20	7	601	CLA	C4D-CHA	2.52	1.47	1.38
20	Z	610	CLA	C4D-CHA	2.52	1.47	1.38
20	B	827	CLA	C4D-CHA	2.52	1.47	1.38
27	Z	601	CHL	MG-NA	-2.52	2.00	2.06
20	7	604	CLA	C4D-CHA	2.52	1.47	1.38
20	B	813	CLA	C4D-CHA	2.52	1.47	1.38
20	Z	602	CLA	C4B-CHC	2.52	1.48	1.41
20	F	303	CLA	C4B-CHC	2.51	1.48	1.41
20	7	610	CLA	C4D-CHA	2.51	1.47	1.38
20	7	608	CLA	C4D-CHA	2.51	1.47	1.38
20	1	611	CLA	C4C-C3C	2.51	1.49	1.45
20	Z	606	CLA	C4B-CHC	2.51	1.48	1.41
20	B	810	CLA	C4D-CHA	2.51	1.47	1.38
20	B	831	CLA	C1B-NB	-2.51	1.33	1.35
27	Z	601	CHL	C3D-C4D	-2.51	1.38	1.44
20	B	814	CLA	C4D-CHA	2.51	1.47	1.38
20	B	829	CLA	C3D-C4D	-2.51	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	8	612	CLA	C1B-NB	-2.51	1.33	1.35
27	6	618	CHL	C3D-C4D	-2.51	1.38	1.44
20	A	816	CLA	C4B-CHC	2.51	1.48	1.41
20	8	610	CLA	C3D-C4D	-2.50	1.38	1.44
20	5	603	CLA	C3D-C4D	-2.50	1.38	1.44
27	6	606	CHL	C3D-C4D	-2.50	1.38	1.44
20	3	602	CLA	C4D-CHA	2.50	1.47	1.38
20	8	604	CLA	C4D-CHA	2.50	1.47	1.38
20	6	616	CLA	C4B-CHC	2.50	1.47	1.41
20	5	602	CLA	C4B-CHC	2.50	1.47	1.41
20	7	602	CLA	C4B-CHC	2.50	1.47	1.41
27	4	608	CHL	MG-NA	-2.50	2.00	2.06
20	A	831	CLA	C4C-C3C	2.50	1.49	1.45
20	A	811	CLA	C4D-CHA	2.50	1.47	1.38
20	8	603	CLA	C4D-CHA	2.50	1.47	1.38
20	6	612	CLA	C4D-CHA	2.49	1.47	1.38
27	4	608	CHL	C3D-C4D	-2.49	1.38	1.44
27	6	608	CHL	C2C-C1C	2.49	1.49	1.44
20	A	812	CLA	C4D-CHA	2.49	1.47	1.38
20	B	825	CLA	C3D-C4D	-2.49	1.38	1.44
20	B	812	CLA	C4B-CHC	2.49	1.47	1.41
20	8	613	CLA	C4D-CHA	2.49	1.47	1.38
20	3	604	CLA	C1B-NB	-2.48	1.33	1.35
20	3	611	CLA	C4C-C3C	2.48	1.49	1.45
27	5	608	CHL	C3D-C4D	-2.48	1.38	1.44
20	5	602	CLA	C4D-CHA	2.48	1.47	1.38
20	5	617	CLA	C4C-C3C	2.48	1.49	1.45
20	4	602	CLA	C3D-C4D	-2.48	1.38	1.44
20	A	806	CLA	C4D-CHA	2.48	1.47	1.38
20	B	830	CLA	C4D-CHA	2.48	1.47	1.38
20	A	828	CLA	C3D-C4D	-2.48	1.38	1.44
20	4	611	CLA	C4C-C3C	2.47	1.49	1.45
27	4	606	CHL	C1B-NB	-2.47	1.33	1.35
20	A	854	CLA	C4D-CHA	2.47	1.47	1.38
20	A	819	CLA	C4B-CHC	2.47	1.47	1.41
27	4	608	CHL	C4D-CHA	2.47	1.47	1.38
20	B	807	CLA	C4C-C3C	2.47	1.49	1.45
20	B	839	CLA	C3D-C4D	-2.47	1.38	1.44
20	F	301	CLA	C3D-C4D	-2.47	1.38	1.44
20	6	602	CLA	C4B-CHC	2.47	1.47	1.41
20	B	816	CLA	C1C-C2C	2.47	1.49	1.44
20	B	808	CLA	C1B-NB	-2.47	1.33	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	851	LHG	O8-C23	2.46	1.45	1.33
20	A	827	CLA	C4D-CHA	2.46	1.47	1.38
20	A	827	CLA	C4B-CHC	2.46	1.47	1.41
20	B	830	CLA	C3D-C4D	-2.46	1.38	1.44
27	6	607	CHL	C3D-C4D	-2.46	1.38	1.44
20	A	806	CLA	C3D-C4D	-2.46	1.38	1.44
27	6	606	CHL	C4B-CHC	2.46	1.47	1.41
20	4	614	CLA	C1C-C2C	2.46	1.49	1.44
20	B	825	CLA	C4D-CHA	2.46	1.47	1.38
20	G	203	CLA	C4C-C3C	2.46	1.49	1.45
20	7	606	CLA	C4B-CHC	2.46	1.47	1.41
20	5	621	CLA	C4C-C3C	2.46	1.49	1.45
20	6	614	CLA	C4D-CHA	2.45	1.47	1.38
20	A	804	CLA	C4B-CHC	2.45	1.47	1.41
20	6	603	CLA	C3D-C4D	-2.45	1.38	1.44
20	4	602	CLA	C4C-C3C	2.45	1.49	1.45
20	A	826	CLA	C1C-C2C	2.45	1.49	1.44
20	1	606	CLA	C4B-CHC	2.45	1.47	1.41
20	8	606	CLA	C1B-NB	-2.45	1.33	1.35
20	A	819	CLA	C3D-C4D	-2.45	1.38	1.44
20	7	603	CLA	C3D-C4D	-2.45	1.38	1.44
20	A	838	CLA	C4C-C3C	2.45	1.49	1.45
20	L	203	CLA	C4D-CHA	2.45	1.47	1.38
20	A	828	CLA	C4B-CHC	2.45	1.47	1.41
20	7	608	CLA	C3D-C4D	-2.45	1.38	1.44
27	1	607	CHL	C3D-C4D	-2.44	1.38	1.44
20	4	613	CLA	C4C-C3C	2.44	1.49	1.45
20	B	826	CLA	C4B-CHC	2.44	1.47	1.41
20	4	616	CLA	C4B-CHC	2.44	1.47	1.41
20	5	602	CLA	C3D-C4D	-2.44	1.38	1.44
20	B	804	CLA	C1C-C2C	2.44	1.49	1.44
20	7	610	CLA	C1C-C2C	2.44	1.49	1.44
20	A	838	CLA	C3D-C4D	-2.44	1.38	1.44
20	B	802	CLA	C4D-CHA	2.44	1.47	1.38
20	Z	616	CLA	C4C-C3C	2.44	1.49	1.45
20	A	827	CLA	C1C-C2C	2.44	1.49	1.44
20	6	616	CLA	C1C-C2C	2.44	1.49	1.44
20	1	616	CLA	C4C-C3C	2.43	1.49	1.45
20	B	824	CLA	C1C-C2C	2.43	1.49	1.44
20	B	829	CLA	C4D-CHA	2.43	1.47	1.38
20	B	838	CLA	C4D-CHA	2.43	1.47	1.38
20	8	610	CLA	C4B-CHC	2.43	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	836	CLA	C4C-C3C	2.43	1.49	1.45
20	B	805	CLA	C3D-C4D	-2.43	1.38	1.44
20	A	825	CLA	C4C-C3C	2.43	1.49	1.45
20	B	806	CLA	C3D-C4D	-2.42	1.38	1.44
27	5	608	CHL	C4D-CHA	2.42	1.47	1.38
20	A	841	CLA	C4B-CHC	2.42	1.47	1.41
20	A	817	CLA	C3D-C4D	-2.42	1.38	1.44
20	Z	604	CLA	C4C-C3C	2.42	1.49	1.45
20	A	806	CLA	C1B-NB	-2.42	1.33	1.35
20	6	622	CLA	C4C-C3C	2.42	1.49	1.45
20	B	824	CLA	C3D-C4D	-2.42	1.38	1.44
20	1	602	CLA	C4B-CHC	2.42	1.47	1.41
27	6	618	CHL	C2C-C1C	2.42	1.49	1.44
20	B	834	CLA	C4C-C3C	2.42	1.49	1.45
27	1	601	CHL	C4B-CHC	2.41	1.47	1.41
20	A	835	CLA	C3D-C4D	-2.41	1.38	1.44
20	3	614	CLA	C4C-C3C	2.41	1.49	1.45
20	B	833	CLA	C3D-C4D	-2.41	1.38	1.44
20	G	204	CLA	C4C-C3C	2.41	1.49	1.45
20	8	614	CLA	C4B-CHC	2.41	1.47	1.41
20	B	830	CLA	C1C-C2C	2.41	1.49	1.44
20	A	817	CLA	C4C-C3C	2.40	1.49	1.45
20	B	819	CLA	C4C-C3C	2.40	1.49	1.45
20	7	611	CLA	C1B-NB	-2.40	1.33	1.35
20	8	608	CLA	C4B-CHC	2.40	1.47	1.41
20	7	616	CLA	C3D-C4D	-2.40	1.38	1.44
20	B	813	CLA	C4C-C3C	2.40	1.49	1.45
20	6	616	CLA	C4C-C3C	2.40	1.49	1.45
20	A	832	CLA	C3D-C4D	-2.40	1.38	1.44
20	B	817	CLA	C3D-C4D	-2.40	1.38	1.44
20	A	830	CLA	C4B-CHC	2.40	1.47	1.41
20	B	838	CLA	C4B-CHC	2.40	1.47	1.41
20	4	614	CLA	C4B-CHC	2.40	1.47	1.41
20	8	602	CLA	C4B-CHC	2.40	1.47	1.41
20	5	621	CLA	C1B-NB	-2.40	1.33	1.35
20	4	603	CLA	C3D-C4D	-2.40	1.38	1.44
20	F	301	CLA	C1C-C2C	2.40	1.49	1.44
20	6	609	CLA	C4C-C3C	2.39	1.49	1.45
20	4	616	CLA	C1C-C2C	2.39	1.49	1.44
20	8	604	CLA	C4C-C3C	2.39	1.49	1.45
20	B	807	CLA	C3D-C4D	-2.39	1.38	1.44
20	4	603	CLA	C4C-C3C	2.39	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	810	CLA	C4C-C3C	2.39	1.49	1.45
20	A	821	CLA	C3D-C4D	-2.39	1.38	1.44
20	7	616	CLA	C4B-CHC	2.39	1.47	1.41
20	A	829	CLA	C1C-C2C	2.39	1.49	1.44
20	1	611	CLA	C4B-CHC	2.39	1.47	1.41
20	8	613	CLA	C1C-C2C	2.39	1.49	1.44
20	6	613	CLA	C4B-CHC	2.39	1.47	1.41
20	B	816	CLA	C4B-CHC	2.39	1.47	1.41
20	B	840	CLA	C1C-NC	-2.39	1.34	1.37
20	8	608	CLA	C3D-C4D	-2.39	1.38	1.44
20	Z	612	CLA	C4B-CHC	2.38	1.47	1.41
20	B	826	CLA	C3D-C4D	-2.38	1.38	1.44
20	B	819	CLA	C1B-NB	-2.38	1.33	1.35
20	B	820	CLA	C3D-C4D	-2.38	1.38	1.44
20	B	829	CLA	C4B-CHC	2.38	1.47	1.41
20	B	824	CLA	C4B-CHC	2.38	1.47	1.41
20	A	835	CLA	C4C-C3C	2.38	1.49	1.45
20	6	602	CLA	C1C-C2C	2.38	1.49	1.44
20	1	603	CLA	C3D-C4D	-2.38	1.38	1.44
20	6	614	CLA	C3D-C4D	-2.38	1.38	1.44
20	K	4002	CLA	C4B-CHC	2.38	1.47	1.41
20	A	803	CLA	C4B-NB	-2.38	1.33	1.35
20	B	821	CLA	C4C-C3C	2.38	1.49	1.45
20	Z	611	CLA	C4C-C3C	2.38	1.49	1.45
20	5	613	CLA	C4C-C3C	2.38	1.49	1.45
20	B	838	CLA	C3D-C4D	-2.38	1.38	1.44
20	B	827	CLA	C1B-NB	-2.38	1.33	1.35
20	B	815	CLA	C4C-C3C	2.38	1.49	1.45
20	B	803	CLA	C4B-CHC	2.38	1.47	1.41
20	B	816	CLA	C3D-C4D	-2.38	1.38	1.44
20	1	602	CLA	C3D-C4D	-2.37	1.38	1.44
20	1	608	CLA	C3D-C4D	-2.37	1.38	1.44
20	A	815	CLA	C3D-C4D	-2.37	1.38	1.44
20	B	810	CLA	C3D-C4D	-2.37	1.38	1.44
20	5	610	CLA	C4B-CHC	2.37	1.47	1.41
27	7	607	CHL	C4C-C3C	2.37	1.49	1.45
20	A	810	CLA	C4B-CHC	2.37	1.47	1.41
20	B	837	CLA	C3D-C4D	-2.37	1.38	1.44
20	B	817	CLA	C4B-NB	-2.37	1.33	1.35
20	6	614	CLA	C4B-CHC	2.37	1.47	1.41
27	4	606	CHL	C2C-C1C	2.37	1.49	1.44
20	A	811	CLA	C4B-CHC	2.37	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	6	617	CLA	C4C-C3C	2.37	1.49	1.45
20	A	808	CLA	C3D-C4D	-2.37	1.38	1.44
20	A	809	CLA	C1C-C2C	2.36	1.49	1.44
20	7	601	CLA	C3D-C4D	-2.36	1.38	1.44
20	4	609	CLA	C4B-CHC	2.36	1.47	1.41
20	A	824	CLA	C4C-C3C	2.36	1.49	1.45
20	B	817	CLA	C4C-C3C	2.36	1.49	1.45
20	B	814	CLA	C4B-CHC	2.36	1.47	1.41
20	B	821	CLA	C4B-CHC	2.36	1.47	1.41
20	B	829	CLA	C1C-C2C	2.36	1.49	1.44
20	B	827	CLA	C4B-NB	-2.36	1.33	1.35
20	8	611	CLA	C4C-C3C	2.36	1.49	1.45
20	3	614	CLA	C4B-CHC	2.36	1.47	1.41
20	B	817	CLA	C1C-NC	-2.36	1.34	1.37
27	Z	601	CHL	C4B-CHC	2.36	1.47	1.41
20	7	604	CLA	C3D-C4D	-2.36	1.38	1.44
20	3	611	CLA	C4B-CHC	2.36	1.47	1.41
20	5	606	CLA	C4B-CHC	2.36	1.47	1.41
20	L	204	CLA	C4B-CHC	2.36	1.47	1.41
20	B	822	CLA	C3D-C4D	-2.36	1.38	1.44
20	6	614	CLA	C4C-C3C	2.36	1.49	1.45
20	7	620	CLA	C4C-C3C	2.36	1.49	1.45
20	B	822	CLA	C1C-C2C	2.36	1.49	1.44
20	A	827	CLA	C3D-C4D	-2.36	1.38	1.44
20	B	831	CLA	C4B-CHC	2.36	1.47	1.41
20	7	612	CLA	C3D-C4D	-2.36	1.38	1.44
20	A	822	CLA	C3D-C4D	-2.36	1.38	1.44
20	A	805	CLA	C3D-C4D	-2.36	1.38	1.44
20	B	813	CLA	C3D-C4D	-2.36	1.38	1.44
20	B	828	CLA	C3D-C4D	-2.36	1.38	1.44
20	L	203	CLA	C4C-C3C	2.36	1.49	1.45
20	A	826	CLA	C3D-C4D	-2.36	1.38	1.44
20	6	604	CLA	C1C-C2C	2.36	1.49	1.44
20	7	620	CLA	C4B-CHC	2.36	1.47	1.41
20	6	603	CLA	C4C-C3C	2.36	1.49	1.45
20	A	825	CLA	C3D-C4D	-2.36	1.38	1.44
20	5	617	CLA	C1C-NC	-2.36	1.34	1.37
20	Z	603	CLA	C4C-C3C	2.35	1.49	1.45
27	1	607	CHL	C4D-CHA	2.35	1.46	1.38
20	5	604	CLA	C3D-C4D	-2.35	1.38	1.44
20	B	809	CLA	C3D-C4D	-2.35	1.38	1.44
20	A	832	CLA	C4C-C3C	2.35	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	833	CLA	C1C-C2C	2.35	1.49	1.44
20	B	814	CLA	C3D-C4D	-2.35	1.38	1.44
20	B	831	CLA	C3D-C4D	-2.35	1.38	1.44
20	1	616	CLA	C3D-C4D	-2.35	1.38	1.44
20	Z	602	CLA	C3D-C4D	-2.35	1.38	1.44
20	1	613	CLA	C1C-C2C	2.35	1.49	1.44
27	Z	601	CHL	C4C-C3C	2.35	1.49	1.45
20	Z	616	CLA	C4B-CHC	2.35	1.47	1.41
20	A	809	CLA	C4B-CHC	2.35	1.47	1.41
20	6	611	CLA	C4B-CHC	2.35	1.47	1.41
20	Z	603	CLA	C3D-C4D	-2.35	1.38	1.44
20	B	805	CLA	C1C-C2C	2.35	1.49	1.44
20	6	614	CLA	C1C-C2C	2.35	1.49	1.44
20	B	803	CLA	C1B-NB	-2.35	1.33	1.35
20	A	814	CLA	C3D-C4D	-2.35	1.38	1.44
20	B	841	CLA	C1C-C2C	2.35	1.49	1.44
20	7	602	CLA	C3D-C4D	-2.34	1.38	1.44
20	8	606	CLA	C4B-CHC	2.34	1.47	1.41
20	B	824	CLA	C1B-NB	-2.34	1.33	1.35
20	A	812	CLA	C3D-C4D	-2.34	1.38	1.44
20	A	804	CLA	C1C-C2C	2.34	1.49	1.44
20	B	839	CLA	C1B-NB	-2.34	1.33	1.35
27	3	608	CHL	C2C-C1C	2.34	1.49	1.44
20	5	621	CLA	C3D-C4D	-2.34	1.38	1.44
20	A	808	CLA	C1B-NB	-2.34	1.33	1.35
27	6	606	CHL	C4D-CHA	2.34	1.46	1.38
20	A	808	CLA	C1C-C2C	2.34	1.49	1.44
20	A	826	CLA	C4B-CHC	2.34	1.47	1.41
20	B	834	CLA	C4B-CHC	2.34	1.47	1.41
27	5	618	CHL	C4C-C3C	2.34	1.49	1.45
20	A	832	CLA	C1B-NB	-2.34	1.33	1.35
20	A	822	CLA	C4B-CHC	2.34	1.47	1.41
20	7	616	CLA	C1C-C2C	2.34	1.49	1.44
20	7	608	CLA	C4B-CHC	2.34	1.47	1.41
20	6	622	CLA	C4B-CHC	2.34	1.47	1.41
20	8	604	CLA	C3D-C4D	-2.34	1.38	1.44
20	8	606	CLA	C3D-C4D	-2.34	1.38	1.44
20	B	832	CLA	C4B-CHC	2.34	1.47	1.41
20	A	810	CLA	C1B-NB	-2.34	1.33	1.35
20	1	604	CLA	C3D-C4D	-2.34	1.38	1.44
27	5	608	CHL	C2C-C1C	2.34	1.49	1.44
20	A	812	CLA	C1B-NB	-2.34	1.33	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	813	CLA	C4B-CHC	2.33	1.47	1.41
20	Z	609	CLA	C4C-C3C	2.33	1.49	1.45
20	7	609	CLA	C4C-C3C	2.33	1.49	1.45
20	6	610	CLA	C4B-CHC	2.33	1.47	1.41
20	5	601	CLA	C4B-CHC	2.33	1.47	1.41
20	A	840	CLA	C3D-C4D	-2.33	1.38	1.44
20	L	203	CLA	C3D-C4D	-2.33	1.38	1.44
20	B	836	CLA	C1B-NB	-2.33	1.33	1.35
20	B	819	CLA	C3D-C4D	-2.33	1.38	1.44
20	8	616	CLA	C4B-CHC	2.33	1.47	1.41
20	8	613	CLA	C4B-CHC	2.33	1.47	1.41
20	B	852	CLA	C4B-CHC	2.33	1.47	1.41
20	A	829	CLA	C4B-CHC	2.33	1.47	1.41
20	B	832	CLA	C3D-C4D	-2.33	1.38	1.44
20	5	614	CLA	C4B-CHC	2.33	1.47	1.41
20	A	818	CLA	C4B-CHC	2.33	1.47	1.41
20	B	841	CLA	C4B-CHC	2.33	1.47	1.41
20	K	4002	CLA	C4C-C3C	2.33	1.49	1.45
20	1	604	CLA	C1B-NB	-2.33	1.33	1.35
20	6	601	CLA	C4C-C3C	2.33	1.49	1.45
20	A	837	CLA	C4C-C3C	2.32	1.49	1.45
20	Z	611	CLA	C4B-CHC	2.32	1.47	1.41
20	B	822	CLA	C4B-CHC	2.32	1.47	1.41
20	A	810	CLA	C3D-C4D	-2.32	1.38	1.44
20	B	808	CLA	C3D-C4D	-2.32	1.38	1.44
20	3	611	CLA	C1C-C2C	2.32	1.49	1.44
20	4	609	CLA	C1B-NB	-2.32	1.33	1.35
20	1	614	CLA	C4B-CHC	2.32	1.47	1.41
20	B	852	CLA	C4C-C3C	2.32	1.49	1.45
20	J	3002	CLA	C4C-C3C	2.32	1.49	1.45
27	8	607	CHL	C4C-C3C	2.32	1.49	1.45
20	3	617	CLA	C4C-C3C	2.32	1.49	1.45
20	6	613	CLA	C4C-C3C	2.32	1.49	1.45
20	1	602	CLA	C1C-C2C	2.32	1.49	1.44
20	B	811	CLA	C3D-C4D	-2.32	1.38	1.44
20	Z	608	CLA	C3D-C4D	-2.32	1.38	1.44
20	4	604	CLA	C4B-CHC	2.32	1.47	1.41
20	7	606	CLA	C3D-C4D	-2.32	1.38	1.44
20	8	602	CLA	C1C-C2C	2.32	1.49	1.44
20	B	830	CLA	C4B-CHC	2.32	1.47	1.41
20	A	815	CLA	C4B-CHC	2.32	1.47	1.41
20	G	204	CLA	C4B-CHC	2.32	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	7	613	CLA	C4C-C3C	2.32	1.49	1.45
20	7	610	CLA	C3D-C4D	-2.32	1.38	1.44
20	3	612	CLA	C3D-C4D	-2.32	1.38	1.44
20	A	807	CLA	C4C-C3C	2.32	1.49	1.45
27	7	607	CHL	C4D-CHA	2.32	1.46	1.38
20	6	617	CLA	C3D-C4D	-2.32	1.38	1.44
20	B	839	CLA	C4B-CHC	2.32	1.47	1.41
27	4	606	CHL	C4D-CHA	2.31	1.46	1.38
20	6	604	CLA	C4B-CHC	2.31	1.47	1.41
20	B	834	CLA	C3D-C4D	-2.31	1.39	1.44
27	Z	607	CHL	C4B-CHC	2.31	1.47	1.41
20	7	601	CLA	C4B-CHC	2.31	1.47	1.41
20	6	612	CLA	C4B-CHC	2.31	1.47	1.41
20	B	804	CLA	C1B-NB	-2.31	1.33	1.35
20	8	601	CLA	C4B-CHC	2.31	1.47	1.41
20	4	604	CLA	C3D-C4D	-2.31	1.39	1.44
20	6	610	CLA	C1B-NB	-2.31	1.33	1.35
20	J	3002	CLA	C4B-CHC	2.31	1.47	1.41
20	B	829	CLA	C4C-C3C	2.31	1.49	1.45
20	A	834	CLA	C3D-C4D	-2.31	1.39	1.44
20	1	616	CLA	C4B-CHC	2.31	1.47	1.41
20	5	612	CLA	C3D-C4D	-2.31	1.39	1.44
20	5	614	CLA	C4C-C3C	2.31	1.49	1.45
20	B	840	CLA	C1B-NB	-2.31	1.33	1.35
20	3	606	CLA	C4C-C3C	2.31	1.49	1.45
20	K	4002	CLA	C1C-C2C	2.31	1.49	1.44
20	K	4003	CLA	C4C-C3C	2.31	1.49	1.45
20	Z	608	CLA	C4C-C3C	2.31	1.49	1.45
20	B	834	CLA	C1B-NB	-2.31	1.33	1.35
20	4	613	CLA	C1B-NB	-2.31	1.33	1.35
20	A	854	CLA	C4B-CHC	2.31	1.47	1.41
20	A	824	CLA	C3D-C4D	-2.31	1.39	1.44
20	7	616	CLA	C4C-C3C	2.30	1.49	1.45
20	4	616	CLA	C3D-C4D	-2.30	1.39	1.44
20	B	809	CLA	C4C-C3C	2.30	1.49	1.45
20	A	836	CLA	C3D-C4D	-2.30	1.39	1.44
20	B	818	CLA	C3D-C4D	-2.30	1.39	1.44
20	B	811	CLA	C4C-C3C	2.30	1.49	1.45
20	B	825	CLA	C4B-CHC	2.30	1.47	1.41
20	3	617	CLA	C3D-C4D	-2.30	1.39	1.44
20	A	845	CLA	C4C-C3C	2.30	1.49	1.45
20	8	603	CLA	C1B-NB	-2.30	1.33	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	5	611	CLA	C4B-CHC	2.30	1.47	1.41
20	A	842	CLA	C4B-CHC	2.30	1.47	1.41
20	B	836	CLA	C4B-CHC	2.30	1.47	1.41
20	A	841	CLA	C1C-C2C	2.30	1.49	1.44
20	Z	608	CLA	C4B-CHC	2.30	1.47	1.41
20	A	816	CLA	C4C-C3C	2.30	1.49	1.45
20	3	602	CLA	C3D-C4D	-2.30	1.39	1.44
20	B	836	CLA	C4C-C3C	2.30	1.49	1.45
20	8	601	CLA	C4C-C3C	2.30	1.49	1.45
20	L	203	CLA	C4B-CHC	2.29	1.47	1.41
20	3	607	CLA	C4C-C3C	2.29	1.49	1.45
20	G	203	CLA	C4B-CHC	2.29	1.47	1.41
20	6	611	CLA	C4C-C3C	2.29	1.49	1.45
20	A	828	CLA	C1C-NC	-2.29	1.34	1.37
20	A	820	CLA	C1C-C2C	2.29	1.49	1.44
20	Z	614	CLA	C1C-C2C	2.29	1.49	1.44
20	3	620	CLA	C4B-CHC	2.29	1.47	1.41
20	5	612	CLA	C4B-CHC	2.29	1.47	1.41
20	A	804	CLA	C4D-CHA	2.29	1.46	1.38
20	6	612	CLA	C1C-C2C	2.29	1.49	1.44
20	B	827	CLA	C3D-C4D	-2.29	1.39	1.44
20	8	608	CLA	C1C-C2C	2.29	1.49	1.44
20	A	820	CLA	C3D-C4D	-2.29	1.39	1.44
20	K	4003	CLA	C3D-C4D	-2.29	1.39	1.44
20	6	612	CLA	C3D-C4D	-2.29	1.39	1.44
20	6	610	CLA	C4C-C3C	2.29	1.49	1.45
20	G	203	CLA	C3D-C4D	-2.29	1.39	1.44
20	B	837	CLA	C4B-CHC	2.29	1.47	1.41
20	8	604	CLA	C4B-CHC	2.29	1.47	1.41
20	5	606	CLA	C4C-C3C	2.29	1.49	1.45
20	A	827	CLA	C1B-NB	-2.29	1.33	1.35
20	7	604	CLA	C4B-CHC	2.29	1.47	1.41
20	7	613	CLA	C3D-C4D	-2.29	1.39	1.44
20	B	823	CLA	C1B-NB	-2.28	1.33	1.35
20	A	837	CLA	C4B-CHC	2.28	1.47	1.41
20	B	804	CLA	C4B-CHC	2.28	1.47	1.41
20	B	835	CLA	C4B-CHC	2.28	1.47	1.41
20	1	606	CLA	C3D-C4D	-2.28	1.39	1.44
20	Z	613	CLA	C4B-CHC	2.28	1.47	1.41
20	3	606	CLA	C4B-CHC	2.28	1.47	1.41
27	5	607	CHL	C4D-CHA	2.28	1.46	1.38
20	5	610	CLA	C1C-C2C	2.28	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	8	613	CLA	C4C-C3C	2.28	1.49	1.45
20	8	613	CLA	C3D-C4D	-2.28	1.39	1.44
20	1	613	CLA	C4B-CHC	2.28	1.47	1.41
20	Z	614	CLA	C4B-CHC	2.28	1.47	1.41
20	7	612	CLA	C1B-NB	-2.28	1.33	1.35
20	J	3002	CLA	C1C-C2C	2.28	1.49	1.44
20	5	602	CLA	C1C-C2C	2.28	1.49	1.44
20	B	805	CLA	C1B-CHB	2.28	1.47	1.41
20	A	823	CLA	C4B-CHC	2.28	1.47	1.41
20	8	601	CLA	C1B-NB	-2.28	1.33	1.35
20	A	843	CLA	C4B-CHC	2.28	1.47	1.41
20	1	609	CLA	C4C-C3C	2.28	1.49	1.45
20	4	616	CLA	C4C-C3C	2.28	1.49	1.45
20	B	833	CLA	C4C-C3C	2.28	1.49	1.45
20	7	614	CLA	C4C-C3C	2.28	1.49	1.45
20	Z	604	CLA	C4B-CHC	2.27	1.47	1.41
20	3	613	CLA	C3D-C4D	-2.27	1.39	1.44
20	4	612	CLA	C3D-C4D	-2.27	1.39	1.44
20	A	840	CLA	C1B-NB	-2.27	1.33	1.35
20	Z	612	CLA	C1B-NB	-2.27	1.33	1.35
20	A	811	CLA	C3D-C4D	-2.27	1.39	1.44
20	8	616	CLA	C1C-C2C	2.27	1.49	1.44
27	1	601	CHL	C4D-CHA	2.27	1.46	1.38
20	A	843	CLA	C3D-C4D	-2.27	1.39	1.44
20	3	604	CLA	C3D-C4D	-2.27	1.39	1.44
20	A	816	CLA	C3D-C4D	-2.27	1.39	1.44
20	B	852	CLA	C1C-C2C	2.27	1.49	1.44
20	6	601	CLA	C4B-CHC	2.27	1.47	1.41
20	1	613	CLA	C4C-C3C	2.27	1.49	1.45
20	4	602	CLA	C4B-CHC	2.27	1.47	1.41
20	A	811	CLA	C1C-C2C	2.27	1.49	1.44
20	1	608	CLA	C4B-CHC	2.27	1.47	1.41
20	A	824	CLA	C4B-CHC	2.27	1.47	1.41
20	7	614	CLA	C4B-CHC	2.27	1.47	1.41
20	5	601	CLA	C3D-C4D	-2.27	1.39	1.44
20	3	612	CLA	C4B-CHC	2.27	1.47	1.41
20	3	612	CLA	C4C-C3C	2.27	1.48	1.45
20	7	608	CLA	C1B-NB	-2.27	1.33	1.35
20	F	303	CLA	C3D-C4D	-2.27	1.39	1.44
20	3	607	CLA	C3D-C4D	-2.27	1.39	1.44
27	Z	607	CHL	C4D-CHA	2.27	1.46	1.38
19	A	801	CL0	C3D-C4D	-2.27	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	841	CLA	C3D-C4D	-2.27	1.39	1.44
20	Z	612	CLA	C3D-C4D	-2.27	1.39	1.44
20	4	613	CLA	C3D-C4D	-2.27	1.39	1.44
20	B	814	CLA	C1C-C2C	2.27	1.49	1.44
20	A	813	CLA	C3D-C4D	-2.27	1.39	1.44
20	4	601	CLA	C3D-C4D	-2.27	1.39	1.44
20	5	614	CLA	C1C-C2C	2.27	1.49	1.44
20	B	820	CLA	C4C-C3C	2.27	1.48	1.45
20	7	603	CLA	C4C-C3C	2.27	1.48	1.45
20	A	812	CLA	C4B-CHC	2.26	1.47	1.41
20	7	603	CLA	C4B-CHC	2.26	1.47	1.41
20	A	802	CLA	C4B-CHC	2.26	1.47	1.41
20	Z	604	CLA	C3D-C4D	-2.26	1.39	1.44
20	4	604	CLA	C4C-C3C	2.26	1.48	1.45
20	A	832	CLA	C1C-C2C	2.26	1.48	1.44
20	1	606	CLA	C1B-NB	-2.26	1.33	1.35
20	Z	614	CLA	C4C-C3C	2.26	1.48	1.45
27	6	618	CHL	C4B-CHC	2.26	1.47	1.41
20	5	603	CLA	C4C-C3C	2.26	1.48	1.45
20	3	606	CLA	C3D-C4D	-2.26	1.39	1.44
20	1	614	CLA	C3D-C4D	-2.26	1.39	1.44
20	7	616	CLA	C1B-CHB	2.26	1.47	1.41
27	5	608	CHL	C4B-CHC	2.26	1.47	1.41
20	A	813	CLA	C1C-C2C	2.26	1.48	1.44
20	8	616	CLA	C1B-CHB	2.26	1.47	1.41
20	A	817	CLA	C1B-CHB	2.26	1.47	1.41
20	3	620	CLA	C4C-C3C	2.26	1.48	1.45
20	A	840	CLA	C1C-C2C	2.26	1.48	1.44
20	8	602	CLA	C3D-C4D	-2.26	1.39	1.44
20	F	304	CLA	C3D-C4D	-2.26	1.39	1.44
20	B	826	CLA	C1C-NC	-2.26	1.34	1.37
20	6	601	CLA	C3D-C4D	-2.26	1.39	1.44
20	6	622	CLA	C3D-C4D	-2.26	1.39	1.44
20	B	820	CLA	C4B-CHC	2.26	1.47	1.41
20	6	604	CLA	C4C-C3C	2.26	1.48	1.45
27	4	618	CHL	C4D-CHA	2.25	1.46	1.38
20	A	840	CLA	C4B-CHC	2.25	1.47	1.41
20	3	603	CLA	C3D-C4D	-2.25	1.39	1.44
27	8	607	CHL	C1B-NB	-2.25	1.33	1.35
20	Z	616	CLA	C1B-CHB	2.25	1.47	1.41
20	7	611	CLA	C4C-C3C	2.25	1.48	1.45
20	7	611	CLA	C4B-CHC	2.25	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	5	603	CLA	C1B-NB	-2.25	1.33	1.35
20	A	836	CLA	C4B-CHC	2.25	1.47	1.41
20	8	601	CLA	C1C-C2C	2.25	1.48	1.44
27	Z	607	CHL	C1B-CHB	2.25	1.47	1.41
20	1	608	CLA	C1C-C2C	2.25	1.48	1.44
27	5	607	CHL	C4B-CHC	2.25	1.47	1.41
20	8	609	CLA	C1C-C2C	2.25	1.48	1.44
20	Z	606	CLA	C1C-C2C	2.25	1.48	1.44
20	8	601	CLA	C3D-C4D	-2.25	1.39	1.44
20	A	845	CLA	C3D-C4D	-2.25	1.39	1.44
20	3	604	CLA	C4C-C3C	2.25	1.48	1.45
27	Z	607	CHL	C2C-C1C	2.25	1.49	1.44
20	B	838	CLA	C1C-C2C	2.25	1.48	1.44
20	B	810	CLA	C4B-CHC	2.25	1.47	1.41
20	8	612	CLA	C3D-C4D	-2.25	1.39	1.44
20	8	609	CLA	C4C-C3C	2.25	1.48	1.45
20	B	835	CLA	C3D-C4D	-2.25	1.39	1.44
20	A	841	CLA	C1B-NB	-2.25	1.33	1.35
20	B	832	CLA	C1B-NB	-2.25	1.33	1.35
20	B	822	CLA	C4C-C3C	2.25	1.48	1.45
20	G	204	CLA	C1C-C2C	2.25	1.48	1.44
20	8	611	CLA	C4B-CHC	2.25	1.47	1.41
20	A	810	CLA	C1C-C2C	2.25	1.48	1.44
20	A	815	CLA	C1B-NB	-2.25	1.33	1.35
20	A	839	CLA	C4B-CHC	2.25	1.47	1.41
20	A	813	CLA	C4C-C3C	2.25	1.48	1.45
20	F	303	CLA	C1C-C2C	2.24	1.48	1.44
20	5	611	CLA	C1C-C2C	2.24	1.48	1.44
20	F	303	CLA	C1C-NC	-2.24	1.34	1.37
20	A	815	CLA	C4C-C3C	2.24	1.48	1.45
20	4	611	CLA	C4B-CHC	2.24	1.47	1.41
27	4	608	CHL	C4B-CHC	2.24	1.47	1.41
20	B	828	CLA	C4C-C3C	2.24	1.48	1.45
20	Z	612	CLA	C4C-C3C	2.24	1.48	1.45
20	3	613	CLA	C1C-C2C	2.24	1.48	1.44
20	3	614	CLA	C1C-C2C	2.24	1.48	1.44
20	5	612	CLA	C1B-NB	-2.24	1.33	1.35
20	5	606	CLA	C3D-C4D	-2.24	1.39	1.44
20	K	4003	CLA	C4B-CHC	2.24	1.47	1.41
20	1	609	CLA	C3D-C4D	-2.24	1.39	1.44
20	3	609	CLA	C4C-C3C	2.24	1.48	1.45
20	B	821	CLA	C3D-C4D	-2.24	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	5	613	CLA	C3D-C4D	-2.24	1.39	1.44
20	A	839	CLA	C4C-C3C	2.24	1.48	1.45
20	A	816	CLA	C1C-C2C	2.24	1.48	1.44
20	1	611	CLA	C1B-NB	-2.24	1.33	1.35
20	A	829	CLA	C3D-C4D	-2.24	1.39	1.44
20	Z	616	CLA	C3D-C4D	-2.24	1.39	1.44
20	1	603	CLA	C4C-C3C	2.24	1.48	1.45
20	F	303	CLA	C1B-NB	-2.24	1.33	1.35
27	3	608	CHL	C4D-CHA	2.24	1.46	1.38
20	B	835	CLA	C4C-C3C	2.24	1.48	1.45
20	A	845	CLA	C4B-CHC	2.24	1.47	1.41
20	5	609	CLA	C4C-C3C	2.24	1.48	1.45
20	B	802	CLA	C1B-NB	-2.24	1.33	1.35
20	Z	603	CLA	C1B-NB	-2.24	1.33	1.35
20	7	609	CLA	C1C-C2C	2.24	1.48	1.44
20	1	616	CLA	C1B-CHB	2.24	1.47	1.41
20	8	606	CLA	C4C-C3C	2.24	1.48	1.45
20	4	612	CLA	C4B-CHC	2.23	1.47	1.41
20	4	603	CLA	C1B-NB	-2.23	1.33	1.35
20	B	840	CLA	C4C-C3C	2.23	1.48	1.45
20	7	608	CLA	C1C-C2C	2.23	1.48	1.44
20	B	812	CLA	C3D-C4D	-2.23	1.39	1.44
20	A	818	CLA	C3D-C4D	-2.23	1.39	1.44
20	6	610	CLA	C3D-C4D	-2.23	1.39	1.44
20	B	815	CLA	C3D-C4D	-2.23	1.39	1.44
20	A	828	CLA	C1C-C2C	2.23	1.48	1.44
20	1	606	CLA	C1C-C2C	2.23	1.48	1.44
20	8	611	CLA	C3D-C4D	-2.23	1.39	1.44
20	6	613	CLA	C3D-C4D	-2.23	1.39	1.44
20	A	819	CLA	C1C-C2C	2.23	1.48	1.44
20	L	204	CLA	C1C-C2C	2.23	1.48	1.44
20	Z	602	CLA	C1C-C2C	2.23	1.48	1.44
20	3	609	CLA	C4B-CHC	2.23	1.47	1.41
20	4	612	CLA	C1C-C2C	2.23	1.48	1.44
27	4	607	CHL	C4B-CHC	2.23	1.47	1.41
20	1	611	CLA	C3D-C4D	-2.23	1.39	1.44
20	Z	606	CLA	C3D-C4D	-2.23	1.39	1.44
20	B	812	CLA	C1C-C2C	2.23	1.48	1.44
20	A	845	CLA	C1C-NC	-2.23	1.34	1.37
20	A	823	CLA	C3D-C4D	-2.23	1.39	1.44
20	J	3002	CLA	C3D-C4D	-2.23	1.39	1.44
20	6	602	CLA	C3D-C4D	-2.23	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	823	CLA	C4C-C3C	2.23	1.48	1.45
20	A	840	CLA	C4C-C3C	2.23	1.48	1.45
27	4	618	CHL	C4B-CHC	2.23	1.47	1.41
20	1	609	CLA	C4B-CHC	2.23	1.47	1.41
20	5	617	CLA	C3D-C4D	-2.23	1.39	1.44
20	3	620	CLA	C3D-C4D	-2.22	1.39	1.44
20	1	611	CLA	C1C-C2C	2.22	1.48	1.44
20	7	620	CLA	C1C-C2C	2.22	1.48	1.44
20	A	843	CLA	C1B-NB	-2.22	1.33	1.35
20	A	837	CLA	C3D-C4D	-2.22	1.39	1.44
20	5	606	CLA	C1C-C2C	2.22	1.48	1.44
20	3	617	CLA	C4B-CHC	2.22	1.47	1.41
20	A	814	CLA	C1C-NC	-2.22	1.34	1.37
27	4	607	CHL	C1B-CHB	2.22	1.47	1.41
20	B	808	CLA	C4B-CHC	2.22	1.47	1.41
20	3	607	CLA	C4B-CHC	2.22	1.47	1.41
20	B	838	CLA	C4C-C3C	2.22	1.48	1.45
20	7	602	CLA	C1C-C2C	2.22	1.48	1.44
20	B	820	CLA	C1B-NB	-2.22	1.33	1.35
20	7	610	CLA	C1B-NB	-2.22	1.33	1.35
20	B	837	CLA	C1B-NB	-2.22	1.33	1.35
27	6	607	CHL	C4D-CHA	2.22	1.46	1.38
20	L	204	CLA	C3D-C4D	-2.22	1.39	1.44
20	1	612	CLA	C1B-NB	-2.22	1.33	1.35
27	6	618	CHL	C4D-CHA	2.22	1.46	1.38
20	7	601	CLA	C1B-CHB	2.22	1.47	1.41
20	G	204	CLA	C3D-C4D	-2.22	1.39	1.44
20	6	613	CLA	C1C-C2C	2.22	1.48	1.44
20	A	810	CLA	C1B-CHB	2.22	1.47	1.41
27	Z	601	CHL	C4D-CHA	2.22	1.46	1.38
20	Z	603	CLA	C4B-CHC	2.22	1.47	1.41
27	1	607	CHL	C4B-CHC	2.21	1.47	1.41
20	A	822	CLA	C1C-C2C	2.21	1.48	1.44
27	7	607	CHL	C1B-NB	-2.21	1.33	1.35
20	8	606	CLA	C1C-C2C	2.21	1.48	1.44
20	B	833	CLA	C1C-NC	-2.21	1.34	1.37
20	3	609	CLA	C3D-C4D	-2.21	1.39	1.44
20	A	809	CLA	C1B-NB	-2.21	1.33	1.35
20	B	839	CLA	C1C-C2C	2.21	1.48	1.44
20	5	613	CLA	C4B-CHC	2.21	1.47	1.41
20	5	601	CLA	C1C-C2C	2.21	1.48	1.44
20	A	839	CLA	C1C-C2C	2.21	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	614	CLA	C3D-C4D	-2.21	1.39	1.44
20	Z	613	CLA	C1C-C2C	2.21	1.48	1.44
20	6	616	CLA	C3D-C4D	-2.21	1.39	1.44
20	B	823	CLA	C4C-C3C	2.21	1.48	1.45
20	7	612	CLA	C4C-C3C	2.21	1.48	1.45
20	A	811	CLA	C1B-NB	-2.21	1.33	1.35
20	B	823	CLA	C3D-C4D	-2.21	1.39	1.44
20	A	824	CLA	C1B-NB	-2.21	1.33	1.35
20	6	610	CLA	C1C-C2C	2.21	1.48	1.44
20	8	603	CLA	C4B-CHC	2.21	1.47	1.41
20	A	832	CLA	C4B-CHC	2.21	1.47	1.41
20	L	203	CLA	C1C-C2C	2.21	1.48	1.44
20	1	610	CLA	C3D-C4D	-2.21	1.39	1.44
20	6	611	CLA	C3D-C4D	-2.21	1.39	1.44
20	8	612	CLA	C1C-C2C	2.21	1.48	1.44
20	6	611	CLA	C1C-C2C	2.21	1.48	1.44
20	5	601	CLA	C4C-C3C	2.21	1.48	1.45
27	4	607	CHL	C2C-C1C	2.21	1.49	1.44
20	A	809	CLA	C3D-C4D	-2.21	1.39	1.44
20	A	823	CLA	C1B-CHB	2.21	1.47	1.41
20	B	812	CLA	C4C-C3C	2.20	1.48	1.45
20	8	609	CLA	C4B-CHC	2.20	1.47	1.41
27	6	618	CHL	C4C-C3C	2.20	1.48	1.45
20	8	609	CLA	C3D-C4D	-2.20	1.39	1.44
20	5	616	CLA	C4B-CHC	2.20	1.47	1.41
20	3	610	CLA	C3D-C4D	-2.20	1.39	1.44
20	7	609	CLA	C3D-C4D	-2.20	1.39	1.44
20	1	604	CLA	C4B-CHC	2.20	1.47	1.41
20	5	614	CLA	C3D-C4D	-2.20	1.39	1.44
20	F	304	CLA	C4B-CHC	2.20	1.47	1.41
20	3	602	CLA	C4B-CHC	2.20	1.47	1.41
20	A	814	CLA	C4B-CHC	2.20	1.47	1.41
20	A	834	CLA	C4B-CHC	2.20	1.47	1.41
20	B	803	CLA	C3D-C4D	-2.20	1.39	1.44
20	Z	610	CLA	C3D-C4D	-2.20	1.39	1.44
20	5	612	CLA	C4C-C3C	2.20	1.48	1.45
20	7	612	CLA	C4B-CHC	2.20	1.47	1.41
20	A	804	CLA	C1B-NB	-2.20	1.33	1.35
20	A	845	CLA	C1B-NB	-2.20	1.33	1.35
20	B	812	CLA	C1B-NB	-2.20	1.33	1.35
20	B	813	CLA	C4B-CHC	2.20	1.47	1.41
20	4	612	CLA	C4C-C3C	2.20	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	L	204	CLA	C1B-CHB	2.20	1.47	1.41
20	7	606	CLA	C1C-C2C	2.20	1.48	1.44
20	6	617	CLA	C4B-CHC	2.20	1.47	1.41
20	4	610	CLA	C4C-C3C	2.20	1.48	1.45
20	5	609	CLA	C4B-CHC	2.20	1.47	1.41
20	B	828	CLA	C1C-NC	-2.20	1.34	1.37
20	6	604	CLA	C3D-C4D	-2.20	1.39	1.44
20	7	609	CLA	C4B-CHC	2.19	1.47	1.41
20	4	602	CLA	C1C-C2C	2.19	1.48	1.44
20	7	604	CLA	C1B-CHB	2.19	1.47	1.41
20	A	808	CLA	C4C-C3C	2.19	1.48	1.45
20	Z	614	CLA	C3D-C4D	-2.19	1.39	1.44
20	F	304	CLA	C4C-C3C	2.19	1.48	1.45
20	A	830	CLA	C3D-C4D	-2.19	1.39	1.44
20	B	831	CLA	C1C-C2C	2.19	1.48	1.44
20	5	610	CLA	C3D-C4D	-2.19	1.39	1.44
27	5	618	CHL	C4B-CHC	2.19	1.47	1.41
20	4	604	CLA	C1C-C2C	2.19	1.48	1.44
20	8	616	CLA	C3D-C4D	-2.19	1.39	1.44
20	B	852	CLA	C1B-CHB	2.19	1.47	1.41
20	8	616	CLA	C4C-C3C	2.19	1.48	1.45
20	B	811	CLA	C1B-NB	-2.19	1.33	1.35
20	1	616	CLA	C1B-NB	-2.19	1.33	1.35
20	8	608	CLA	C1B-CHB	2.19	1.47	1.41
20	B	837	CLA	C1C-C2C	2.19	1.48	1.44
20	B	822	CLA	C1B-NB	-2.19	1.33	1.35
20	G	204	CLA	C1B-CHB	2.19	1.47	1.41
20	B	827	CLA	C4C-C3C	2.19	1.48	1.45
27	5	618	CHL	C4D-CHA	2.19	1.46	1.38
20	B	813	CLA	C1B-NB	-2.19	1.33	1.35
20	3	611	CLA	C3D-C4D	-2.19	1.39	1.44
20	B	802	CLA	C1B-CHB	2.19	1.47	1.41
20	A	839	CLA	C3D-C4D	-2.19	1.39	1.44
20	A	831	CLA	C1B-CHB	2.19	1.47	1.41
20	1	612	CLA	C4C-C3C	2.19	1.48	1.45
20	Z	613	CLA	C4C-C3C	2.19	1.48	1.45
20	5	617	CLA	C1B-NB	-2.19	1.33	1.35
20	B	841	CLA	C4C-C3C	2.19	1.48	1.45
20	6	609	CLA	C3D-C4D	-2.19	1.39	1.44
20	B	825	CLA	C4C-C3C	2.18	1.48	1.45
20	B	839	CLA	C4C-C3C	2.18	1.48	1.45
20	6	622	CLA	C1C-C2C	2.18	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	5	621	CLA	C1B-CHB	2.18	1.47	1.41
20	B	838	CLA	C1B-NB	-2.18	1.33	1.35
20	6	604	CLA	C1B-NB	-2.18	1.33	1.35
20	B	810	CLA	C1B-CHB	2.18	1.47	1.41
20	A	803	CLA	C3D-C4D	-2.18	1.39	1.44
20	3	604	CLA	C4B-CHC	2.18	1.47	1.41
27	5	607	CHL	C1C-NC	-2.18	1.34	1.37
20	4	610	CLA	C3D-C4D	-2.18	1.39	1.44
27	4	606	CHL	C4B-CHC	2.18	1.47	1.41
20	B	830	CLA	C4C-C3C	2.18	1.48	1.45
27	8	607	CHL	C1B-CHB	2.18	1.47	1.41
20	B	830	CLA	C1B-NB	-2.18	1.33	1.35
20	7	613	CLA	C1B-NB	-2.18	1.33	1.35
20	4	601	CLA	C1B-CHB	2.18	1.47	1.41
20	B	835	CLA	C1C-C2C	2.18	1.48	1.44
20	8	614	CLA	C1C-C2C	2.18	1.48	1.44
20	A	818	CLA	C1B-NB	-2.18	1.33	1.35
20	Z	612	CLA	C1C-C2C	2.18	1.48	1.44
20	A	803	CLA	C4C-C3C	2.18	1.48	1.45
20	B	815	CLA	C4B-CHC	2.18	1.47	1.41
20	5	611	CLA	C4C-C3C	2.18	1.48	1.45
20	A	834	CLA	C4C-C3C	2.18	1.48	1.45
27	Z	601	CHL	C1B-NB	-2.18	1.33	1.35
20	7	614	CLA	C1C-C2C	2.18	1.48	1.44
20	8	603	CLA	C4C-C3C	2.18	1.48	1.45
20	Z	616	CLA	C1C-C2C	2.18	1.48	1.44
20	A	817	CLA	C4B-CHC	2.17	1.47	1.41
20	5	621	CLA	C4B-CHC	2.17	1.47	1.41
20	3	603	CLA	C4B-CHC	2.17	1.47	1.41
20	A	835	CLA	C4B-CHC	2.17	1.47	1.41
20	A	841	CLA	C4C-C3C	2.17	1.48	1.45
20	3	611	CLA	C1B-CHB	2.17	1.47	1.41
20	A	831	CLA	C3D-C4D	-2.17	1.39	1.44
20	8	614	CLA	C3D-C4D	-2.17	1.39	1.44
20	5	609	CLA	C3D-C4D	-2.17	1.39	1.44
20	8	604	CLA	C1C-C2C	2.17	1.48	1.44
20	1	612	CLA	C3D-C4D	-2.17	1.39	1.44
20	6	613	CLA	C1B-CHB	2.17	1.47	1.41
20	Z	609	CLA	C4B-CHC	2.17	1.47	1.41
20	B	836	CLA	C1C-C2C	2.17	1.48	1.44
20	F	304	CLA	C1C-C2C	2.17	1.48	1.44
20	1	614	CLA	C1C-C2C	2.17	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	803	CLA	C4B-NB	-2.17	1.33	1.35
20	3	617	CLA	C1C-C2C	2.17	1.48	1.44
20	K	4002	CLA	C1B-CHB	2.17	1.47	1.41
20	B	802	CLA	C1C-NC	-2.17	1.34	1.37
20	A	820	CLA	C4B-CHC	2.17	1.47	1.41
20	5	601	CLA	C1B-CHB	2.17	1.47	1.41
20	A	838	CLA	C1C-NC	-2.17	1.34	1.37
20	1	608	CLA	C4C-C3C	2.17	1.48	1.45
20	1	614	CLA	C4C-C3C	2.17	1.48	1.45
20	B	807	CLA	C4B-CHC	2.17	1.47	1.41
20	A	838	CLA	C4B-CHC	2.17	1.47	1.41
20	B	828	CLA	C4B-CHC	2.17	1.47	1.41
20	B	823	CLA	C1C-NC	-2.17	1.34	1.37
20	1	616	CLA	C1C-C2C	2.17	1.48	1.44
20	7	601	CLA	C1C-NC	-2.17	1.34	1.37
20	6	601	CLA	C1B-CHB	2.17	1.47	1.41
20	Z	608	CLA	C1B-CHB	2.17	1.47	1.41
20	5	612	CLA	C1B-CHB	2.17	1.47	1.41
20	3	603	CLA	C4C-C3C	2.17	1.48	1.45
20	B	811	CLA	C1B-CHB	2.17	1.47	1.41
20	A	823	CLA	C1C-C2C	2.16	1.48	1.44
20	6	616	CLA	C1B-NB	-2.16	1.33	1.35
20	A	809	CLA	C4C-C3C	2.16	1.48	1.45
20	Z	611	CLA	C3D-C4D	-2.16	1.39	1.44
20	A	843	CLA	C1B-CHB	2.16	1.47	1.41
27	1	607	CHL	C4C-C3C	2.16	1.48	1.45
20	3	620	CLA	C1B-CHB	2.16	1.47	1.41
20	B	823	CLA	C4B-CHC	2.16	1.47	1.41
20	A	806	CLA	C4C-C3C	2.16	1.48	1.45
27	8	607	CHL	C4D-CHA	2.16	1.46	1.38
20	1	613	CLA	C3D-C4D	-2.16	1.39	1.44
20	K	4003	CLA	C1B-CHB	2.16	1.47	1.41
20	1	606	CLA	C1B-CHB	2.16	1.47	1.41
20	A	828	CLA	C1B-NB	-2.16	1.33	1.35
20	8	603	CLA	C1C-C2C	2.16	1.48	1.44
20	1	603	CLA	C4B-CHC	2.16	1.47	1.41
20	B	819	CLA	C4B-CHC	2.16	1.47	1.41
20	K	4002	CLA	C3D-C4D	-2.16	1.39	1.44
20	A	842	CLA	C1B-CHB	2.16	1.47	1.41
20	3	602	CLA	C4C-C3C	2.16	1.48	1.45
20	A	826	CLA	C1B-NB	-2.16	1.33	1.35
20	6	609	CLA	C4B-CHC	2.16	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	821	CLA	C1C-C2C	2.16	1.48	1.44
20	7	611	CLA	C3D-C4D	-2.16	1.39	1.44
20	5	611	CLA	C3D-C4D	-2.16	1.39	1.44
20	B	841	CLA	C3D-C4D	-2.16	1.39	1.44
20	A	815	CLA	C1C-C2C	2.16	1.48	1.44
20	A	824	CLA	C1C-C2C	2.16	1.48	1.44
20	8	603	CLA	C1B-CHB	2.16	1.47	1.41
20	A	812	CLA	C4C-C3C	2.15	1.48	1.45
20	4	616	CLA	C1B-CHB	2.15	1.47	1.41
20	A	822	CLA	C4C-C3C	2.15	1.48	1.45
20	6	602	CLA	C4C-C3C	2.15	1.48	1.45
20	8	614	CLA	C1B-CHB	2.15	1.47	1.41
20	4	609	CLA	C1C-NC	-2.15	1.34	1.37
20	7	608	CLA	C1B-CHB	2.15	1.47	1.41
20	8	601	CLA	C1B-CHB	2.15	1.47	1.41
20	3	612	CLA	C1B-NB	-2.15	1.33	1.35
20	4	614	CLA	C3D-C4D	-2.15	1.39	1.44
20	5	616	CLA	C3D-C4D	-2.15	1.39	1.44
20	B	833	CLA	C4B-CHC	2.15	1.47	1.41
20	6	603	CLA	C4B-CHC	2.15	1.47	1.41
27	4	607	CHL	C4D-CHA	2.15	1.46	1.38
20	8	606	CLA	C1C-NC	-2.15	1.34	1.37
27	1	601	CHL	C1B-NB	-2.15	1.33	1.35
27	4	618	CHL	C4C-C3C	2.15	1.48	1.45
20	1	603	CLA	C1B-CHB	2.15	1.47	1.41
20	4	601	CLA	C4B-CHC	2.15	1.47	1.41
20	A	819	CLA	C4C-C3C	2.15	1.48	1.45
19	A	801	CLO	C1C-NC	-2.15	1.34	1.37
20	3	620	CLA	C1B-NB	-2.15	1.33	1.35
20	B	815	CLA	C1C-NC	-2.15	1.34	1.37
20	3	602	CLA	C1C-NC	-2.15	1.34	1.37
20	3	607	CLA	C1C-C2C	2.15	1.48	1.44
20	A	842	CLA	C1B-NB	-2.15	1.33	1.35
20	4	613	CLA	C4B-CHC	2.15	1.47	1.41
20	Z	609	CLA	C3D-C4D	-2.15	1.39	1.44
20	8	612	CLA	C4B-CHC	2.15	1.47	1.41
27	1	601	CHL	C4C-C3C	2.15	1.48	1.45
27	4	606	CHL	C1B-CHB	2.15	1.47	1.41
20	Z	613	CLA	C3D-C4D	-2.15	1.39	1.44
20	A	838	CLA	C1B-NB	-2.14	1.33	1.35
20	3	603	CLA	C1B-NB	-2.14	1.33	1.35
20	6	622	CLA	C1B-CHB	2.14	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	808	CLA	C4C-C3C	2.14	1.48	1.45
20	5	602	CLA	C1B-NB	-2.14	1.33	1.35
20	1	608	CLA	C1B-CHB	2.14	1.46	1.41
20	B	818	CLA	C4B-CHC	2.14	1.46	1.41
20	8	614	CLA	C4C-C3C	2.14	1.48	1.45
20	B	852	CLA	C3D-C4D	-2.14	1.39	1.44
20	Z	608	CLA	C1C-C2C	2.14	1.48	1.44
20	3	614	CLA	C1B-CHB	2.14	1.46	1.41
20	4	609	CLA	C4C-C3C	2.14	1.48	1.45
20	7	614	CLA	C1B-NB	-2.14	1.33	1.35
20	6	603	CLA	C1C-C2C	2.14	1.48	1.44
20	7	620	CLA	C3D-C4D	-2.14	1.39	1.44
20	8	608	CLA	C1B-NB	-2.14	1.33	1.35
20	5	617	CLA	C1B-CHB	2.14	1.46	1.41
20	A	830	CLA	C1C-C2C	2.14	1.48	1.44
27	1	607	CHL	C1B-CHB	2.14	1.46	1.41
27	6	607	CHL	C4B-CHC	2.14	1.46	1.41
20	A	821	CLA	C4B-CHC	2.14	1.46	1.41
27	Z	607	CHL	C4C-C3C	2.13	1.48	1.45
20	B	806	CLA	C4B-CHC	2.13	1.46	1.41
20	3	613	CLA	C4B-CHC	2.13	1.46	1.41
20	5	604	CLA	C4B-CHC	2.13	1.46	1.41
20	Z	611	CLA	C1B-CHB	2.13	1.46	1.41
20	A	839	CLA	C1B-NB	-2.13	1.33	1.35
20	Z	603	CLA	C1B-CHB	2.13	1.46	1.41
20	A	807	CLA	C4B-CHC	2.13	1.46	1.41
20	A	821	CLA	C1B-CHB	2.13	1.46	1.41
20	A	824	CLA	C1B-CHB	2.13	1.46	1.41
20	B	829	CLA	C1B-CHB	2.13	1.46	1.41
20	8	611	CLA	C1B-CHB	2.13	1.46	1.41
20	5	609	CLA	C1A-CHA	2.13	1.51	1.43
20	F	301	CLA	C4C-C3C	2.13	1.48	1.45
20	B	821	CLA	C1B-CHB	2.13	1.46	1.41
27	6	608	CHL	C4B-CHC	2.13	1.46	1.41
20	A	814	CLA	C1B-NB	-2.13	1.33	1.35
20	3	617	CLA	C1B-NB	-2.13	1.33	1.35
20	Z	606	CLA	C1B-CHB	2.13	1.46	1.41
20	A	837	CLA	C1C-C2C	2.13	1.48	1.44
27	6	608	CHL	C4D-CHA	2.13	1.46	1.38
20	Z	604	CLA	C1C-C2C	2.13	1.48	1.44
20	B	804	CLA	C3D-C4D	-2.13	1.39	1.44
20	1	609	CLA	C1B-NB	-2.13	1.33	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Z	613	CLA	C1B-CHB	2.13	1.46	1.41
20	A	812	CLA	C1C-C2C	2.13	1.48	1.44
20	A	808	CLA	C1C-NC	-2.12	1.34	1.37
20	A	811	CLA	C1C-NC	-2.12	1.34	1.37
20	Z	606	CLA	C4C-C3C	2.12	1.48	1.45
20	5	603	CLA	C4B-CHC	2.12	1.46	1.41
20	B	839	CLA	C1B-CHB	2.12	1.46	1.41
20	6	604	CLA	C1B-CHB	2.12	1.46	1.41
20	7	603	CLA	C1C-C2C	2.12	1.48	1.44
20	Z	602	CLA	C4C-C3C	2.12	1.48	1.45
20	4	609	CLA	C3D-C4D	-2.12	1.39	1.44
20	A	804	CLA	C1C-NC	-2.12	1.34	1.37
20	B	833	CLA	C1B-CHB	2.12	1.46	1.41
20	4	613	CLA	C1C-C2C	2.12	1.48	1.44
20	A	834	CLA	C1B-NB	-2.12	1.33	1.35
20	6	612	CLA	C4C-C3C	2.12	1.48	1.45
20	7	620	CLA	C1B-CHB	2.12	1.46	1.41
20	6	622	CLA	C1B-NB	-2.12	1.33	1.35
20	B	806	CLA	C1C-C2C	2.12	1.48	1.44
20	B	814	CLA	C1B-NB	-2.12	1.33	1.35
20	Z	611	CLA	C1C-C2C	2.12	1.48	1.44
20	A	824	CLA	C1C-NC	-2.11	1.34	1.37
20	5	616	CLA	C1C-NC	-2.11	1.34	1.37
20	A	825	CLA	C1B-CHB	2.11	1.46	1.41
20	6	611	CLA	C1B-NB	-2.11	1.33	1.35
27	5	608	CHL	C1B-NB	-2.11	1.33	1.35
20	1	609	CLA	C1C-C2C	2.11	1.48	1.44
20	5	613	CLA	C1C-C2C	2.11	1.48	1.44
20	B	826	CLA	C1B-NB	-2.11	1.33	1.35
20	B	836	CLA	C1B-CHB	2.11	1.46	1.41
20	F	303	CLA	C4C-C3C	2.11	1.48	1.45
20	3	609	CLA	C1B-NB	-2.11	1.33	1.35
20	G	203	CLA	C1C-C2C	2.11	1.48	1.44
20	A	821	CLA	C4C-C3C	2.11	1.48	1.45
20	4	611	CLA	C1C-C2C	2.11	1.48	1.44
20	5	611	CLA	C1B-CHB	2.11	1.46	1.41
20	A	807	CLA	C1C-NC	-2.11	1.34	1.37
20	Z	613	CLA	C1B-NB	-2.11	1.33	1.35
20	6	609	CLA	C1B-NB	-2.11	1.33	1.35
20	A	836	CLA	C1B-CHB	2.11	1.46	1.41
20	4	610	CLA	C4B-CHC	2.11	1.46	1.41
20	F	301	CLA	C1B-CHB	2.11	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	802	CLA	C4C-C3C	2.10	1.48	1.45
20	B	817	CLA	C1B-CHB	2.10	1.46	1.41
20	7	603	CLA	C1B-CHB	2.10	1.46	1.41
20	Z	608	CLA	C1B-NB	-2.10	1.33	1.35
27	4	618	CHL	C1B-CHB	2.10	1.46	1.41
20	A	828	CLA	C1B-CHB	2.10	1.46	1.41
20	6	613	CLA	C1B-NB	-2.10	1.33	1.35
20	8	609	CLA	C1B-NB	-2.10	1.33	1.35
19	A	801	CL0	C1B-CHB	2.10	1.46	1.41
20	A	843	CLA	C1C-C2C	2.10	1.48	1.44
20	B	827	CLA	C4B-CHC	2.10	1.46	1.41
20	3	612	CLA	C1C-NC	-2.10	1.34	1.37
20	Z	602	CLA	C1B-NB	-2.10	1.33	1.35
20	A	805	CLA	C1C-C2C	2.10	1.48	1.44
20	B	807	CLA	C1C-C2C	2.10	1.48	1.44
20	B	832	CLA	C1C-C2C	2.10	1.48	1.44
20	A	808	CLA	C4B-CHC	2.10	1.46	1.41
20	B	802	CLA	C4B-CHC	2.10	1.46	1.41
20	3	602	CLA	C1C-C2C	2.10	1.48	1.44
20	5	616	CLA	C1C-C2C	2.10	1.48	1.44
20	B	834	CLA	C1B-CHB	2.10	1.46	1.41
20	8	601	CLA	C1A-CHA	2.10	1.51	1.43
27	6	608	CHL	C1B-CHB	2.10	1.46	1.41
20	6	609	CLA	C1C-C2C	2.10	1.48	1.44
20	B	811	CLA	C4B-CHC	2.10	1.46	1.41
20	4	614	CLA	C1B-CHB	2.10	1.46	1.41
20	5	614	CLA	C1B-CHB	2.09	1.46	1.41
20	B	820	CLA	C1B-CHB	2.09	1.46	1.41
20	B	813	CLA	C1C-C2C	2.09	1.48	1.44
20	6	617	CLA	C1C-C2C	2.09	1.48	1.44
20	A	823	CLA	C1B-NB	-2.09	1.33	1.35
20	4	612	CLA	C1B-NB	-2.09	1.33	1.35
20	5	604	CLA	C1B-NB	-2.09	1.33	1.35
20	6	603	CLA	C1B-NB	-2.09	1.33	1.35
20	A	814	CLA	C1B-CHB	2.09	1.46	1.41
20	A	826	CLA	C1B-CHB	2.09	1.46	1.41
20	B	838	CLA	C1B-CHB	2.09	1.46	1.41
27	5	618	CHL	C2C-C1C	2.09	1.49	1.44
20	4	609	CLA	C1C-C2C	2.09	1.48	1.44
27	5	607	CHL	C4C-C3C	2.09	1.48	1.45
20	A	845	CLA	C1B-CHB	2.09	1.46	1.41
20	A	835	CLA	C1C-NC	-2.09	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	5	612	CLA	C1C-C2C	2.09	1.48	1.44
20	A	807	CLA	C1B-CHB	2.09	1.46	1.41
20	F	304	CLA	C1B-CHB	2.09	1.46	1.41
20	B	818	CLA	C1A-CHA	2.09	1.51	1.43
20	7	611	CLA	C1C-C2C	2.09	1.48	1.44
27	1	607	CHL	C1B-NB	-2.09	1.33	1.35
20	4	603	CLA	C1C-NC	-2.09	1.34	1.37
20	3	609	CLA	C1C-C2C	2.08	1.48	1.44
20	8	604	CLA	C1B-CHB	2.08	1.46	1.41
20	A	817	CLA	C1C-NC	-2.08	1.34	1.37
20	B	831	CLA	C4C-C3C	2.08	1.48	1.45
20	4	611	CLA	C3D-C4D	-2.08	1.39	1.44
20	5	612	CLA	C1C-NC	-2.08	1.34	1.37
20	5	610	CLA	C4C-C3C	2.08	1.48	1.45
20	1	612	CLA	C4B-CHC	2.08	1.46	1.41
27	Z	601	CHL	C1B-CHB	2.08	1.46	1.41
20	7	606	CLA	C1C-NC	-2.08	1.34	1.37
20	A	842	CLA	C1C-C2C	2.08	1.48	1.44
20	6	602	CLA	C1B-NB	-2.08	1.33	1.35
27	1	607	CHL	C4B-NB	-2.08	1.33	1.35
20	B	812	CLA	C1B-CHB	2.08	1.46	1.41
20	1	613	CLA	C1B-CHB	2.08	1.46	1.41
20	7	613	CLA	C1C-C2C	2.08	1.48	1.44
20	Z	609	CLA	C1C-C2C	2.08	1.48	1.44
20	B	824	CLA	C4C-C3C	2.08	1.48	1.45
20	A	806	CLA	C4B-CHC	2.08	1.46	1.41
27	8	607	CHL	C1C-NC	-2.08	1.34	1.37
20	1	614	CLA	C1B-NB	-2.08	1.33	1.35
20	A	820	CLA	C4C-C3C	2.08	1.48	1.45
20	1	602	CLA	C4C-C3C	2.08	1.48	1.45
20	B	808	CLA	C1C-C2C	2.08	1.48	1.44
20	B	805	CLA	C4C-C3C	2.08	1.48	1.45
20	A	807	CLA	C1B-NB	-2.08	1.33	1.35
20	F	304	CLA	C1A-CHA	2.07	1.51	1.43
20	A	829	CLA	C4B-NB	-2.07	1.33	1.35
20	1	610	CLA	C1B-NB	-2.07	1.33	1.35
20	B	827	CLA	C1A-CHA	2.07	1.51	1.43
27	6	607	CHL	C1C-NC	-2.07	1.34	1.37
20	3	606	CLA	C1B-CHB	2.07	1.46	1.41
20	3	620	CLA	C1C-C2C	2.07	1.48	1.44
20	B	810	CLA	C1B-NB	-2.07	1.33	1.35
20	5	611	CLA	C1A-CHA	2.07	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	5	601	CLA	C1B-NB	-2.07	1.33	1.35
20	B	834	CLA	C1C-NC	-2.07	1.34	1.37
20	7	613	CLA	C4B-CHC	2.07	1.46	1.41
20	B	827	CLA	C1C-C2C	2.07	1.48	1.44
20	A	809	CLA	C1C-NC	-2.07	1.34	1.37
27	3	608	CHL	C4B-CHC	2.07	1.46	1.41
20	5	609	CLA	C1C-C2C	2.07	1.48	1.44
20	A	833	CLA	C4C-C3C	2.07	1.48	1.45
20	3	603	CLA	C1C-NC	-2.07	1.34	1.37
20	5	616	CLA	C1B-NB	-2.07	1.33	1.35
20	8	611	CLA	C1C-C2C	2.07	1.48	1.44
20	8	614	CLA	C1B-NB	-2.06	1.33	1.35
20	7	609	CLA	C1A-CHA	2.06	1.51	1.43
20	A	803	CLA	C1C-C2C	2.06	1.48	1.44
20	6	612	CLA	C1B-CHB	2.06	1.46	1.41
20	B	837	CLA	C4C-C3C	2.06	1.48	1.45
20	6	609	CLA	C1A-CHA	2.06	1.51	1.43
20	1	602	CLA	C1B-CHB	2.06	1.46	1.41
27	1	601	CHL	C1B-CHB	2.06	1.46	1.41
20	4	612	CLA	C1B-CHB	2.06	1.46	1.41
20	8	612	CLA	C4C-C3C	2.06	1.48	1.45
23	A	851	BCR	C10-C9	-2.06	1.33	1.35
20	7	612	CLA	C1C-NC	-2.06	1.34	1.37
20	B	803	CLA	C1A-CHA	2.06	1.51	1.43
20	1	608	CLA	C1B-NB	-2.06	1.33	1.35
20	B	836	CLA	C1C-NC	-2.06	1.34	1.37
20	4	614	CLA	C4C-C3C	2.06	1.48	1.45
20	4	610	CLA	C1C-NC	-2.06	1.34	1.37
20	1	612	CLA	C1C-C2C	2.06	1.48	1.44
20	A	825	CLA	C4B-CHC	2.06	1.46	1.41
20	5	603	CLA	C1B-CHB	2.06	1.46	1.41
20	5	609	CLA	C1B-NB	-2.06	1.33	1.35
20	A	825	CLA	C1B-NB	-2.06	1.33	1.35
20	A	842	CLA	C4C-C3C	2.06	1.48	1.45
20	4	611	CLA	C1A-CHA	2.06	1.51	1.43
20	4	603	CLA	C4B-CHC	2.06	1.46	1.41
27	7	607	CHL	C4B-CHC	2.06	1.46	1.41
20	B	820	CLA	C1C-C2C	2.06	1.48	1.44
20	7	602	CLA	C4C-C3C	2.05	1.48	1.45
20	B	811	CLA	C1C-C2C	2.05	1.48	1.44
20	6	601	CLA	C1C-C2C	2.05	1.48	1.44
20	J	3002	CLA	C1B-CHB	2.05	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	816	CLA	C1B-CHB	2.05	1.46	1.41
20	5	606	CLA	C1B-CHB	2.05	1.46	1.41
20	A	820	CLA	C1A-CHA	2.05	1.51	1.43
20	B	818	CLA	C4C-C3C	2.05	1.48	1.45
20	B	802	CLA	C3D-C4D	-2.05	1.39	1.44
27	5	618	CHL	C1B-CHB	2.05	1.46	1.41
20	1	604	CLA	C1C-C2C	2.05	1.48	1.44
20	A	817	CLA	C1D-C2D	2.05	1.49	1.45
20	A	804	CLA	C4C-C3C	2.05	1.48	1.45
20	6	612	CLA	C1B-NB	-2.05	1.33	1.35
20	4	611	CLA	C1B-CHB	2.05	1.46	1.41
20	6	617	CLA	C1B-NB	-2.05	1.33	1.35
20	Z	610	CLA	C1B-CHB	2.05	1.46	1.41
20	Z	609	CLA	C1A-CHA	2.05	1.51	1.43
20	4	604	CLA	C1B-NB	-2.05	1.33	1.35
20	1	603	CLA	C1C-C2C	2.05	1.48	1.44
20	5	613	CLA	C1B-NB	-2.05	1.33	1.35
20	8	602	CLA	C1B-CHB	2.04	1.46	1.41
20	6	614	CLA	C1B-CHB	2.04	1.46	1.41
20	B	812	CLA	C1C-NC	-2.04	1.34	1.37
20	Z	602	CLA	C1C-NC	-2.04	1.34	1.37
20	A	836	CLA	C1C-C2C	2.04	1.48	1.44
20	B	805	CLA	C1B-NB	-2.04	1.33	1.35
20	F	301	CLA	C1B-NB	-2.04	1.33	1.35
20	8	606	CLA	C1B-CHB	2.04	1.46	1.41
20	B	827	CLA	C1C-NC	-2.04	1.34	1.37
20	G	203	CLA	C1B-CHB	2.04	1.46	1.41
20	7	601	CLA	C1B-NB	-2.04	1.33	1.35
27	6	608	CHL	C1B-NB	-2.04	1.33	1.35
20	F	303	CLA	C1B-CHB	2.04	1.46	1.41
27	6	607	CHL	C4C-C3C	2.04	1.48	1.45
20	3	617	CLA	C1B-CHB	2.04	1.46	1.41
20	B	816	CLA	C1B-CHB	2.04	1.46	1.41
20	7	613	CLA	C1B-CHB	2.04	1.46	1.41
20	Z	616	CLA	C1B-NB	-2.04	1.33	1.35
20	5	611	CLA	C1B-NB	-2.04	1.33	1.35
20	A	840	CLA	C1A-CHA	2.04	1.51	1.43
20	3	609	CLA	C1C-NC	-2.04	1.34	1.37
20	6	617	CLA	C1B-CHB	2.04	1.46	1.41
20	B	840	CLA	C1B-CHB	2.04	1.46	1.41
20	7	604	CLA	C4C-C3C	2.04	1.48	1.45
20	6	603	CLA	C1B-CHB	2.04	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	1	607	CHL	C2C-C1C	2.04	1.48	1.44
27	6	618	CHL	C1B-CHB	2.04	1.46	1.41
20	B	808	CLA	C1C-NC	-2.04	1.34	1.37
20	4	602	CLA	C1B-NB	-2.04	1.33	1.35
20	A	802	CLA	C1A-CHA	2.04	1.51	1.43
20	A	810	CLA	C4C-C3C	2.04	1.48	1.45
20	3	606	CLA	C1C-C2C	2.04	1.48	1.44
27	8	607	CHL	C4B-CHC	2.04	1.46	1.41
20	A	818	CLA	C1C-NC	-2.04	1.34	1.37
20	8	616	CLA	C1B-NB	-2.04	1.33	1.35
20	3	603	CLA	C1B-CHB	2.04	1.46	1.41
20	5	616	CLA	C1B-CHB	2.04	1.46	1.41
20	B	806	CLA	C1B-NB	-2.03	1.33	1.35
20	B	841	CLA	C1B-CHB	2.03	1.46	1.41
20	B	825	CLA	C1C-C2C	2.03	1.48	1.44
20	B	809	CLA	C1B-CHB	2.03	1.46	1.41
20	7	611	CLA	C1A-CHA	2.03	1.51	1.43
20	1	606	CLA	C4C-C3C	2.03	1.48	1.45
20	3	607	CLA	C1B-NB	-2.03	1.33	1.35
20	B	828	CLA	C1C-C2C	2.03	1.48	1.44
20	A	802	CLA	C1C-C2C	2.03	1.48	1.44
20	B	826	CLA	C4C-C3C	2.03	1.48	1.45
20	A	830	CLA	C1A-CHA	2.03	1.51	1.43
20	B	835	CLA	C1A-CHA	2.03	1.51	1.43
20	5	621	CLA	C1A-CHA	2.03	1.51	1.43
20	B	813	CLA	C1B-CHB	2.03	1.46	1.41
20	6	611	CLA	C1B-CHB	2.03	1.46	1.41
20	A	829	CLA	C1A-CHA	2.03	1.51	1.43
20	7	606	CLA	C4C-C3C	2.03	1.48	1.45
20	A	819	CLA	C1B-NB	-2.03	1.33	1.35
20	4	609	CLA	C1A-CHA	2.03	1.51	1.43
20	A	837	CLA	C1A-CHA	2.03	1.51	1.43
20	B	810	CLA	C1C-C2C	2.03	1.48	1.44
20	B	808	CLA	C1B-CHB	2.03	1.46	1.41
20	4	601	CLA	C1C-NC	-2.03	1.34	1.37
20	3	613	CLA	C1A-CHA	2.03	1.51	1.43
20	B	802	CLA	C1C-C2C	2.03	1.48	1.44
20	5	617	CLA	C1A-CHA	2.03	1.51	1.43
20	A	808	CLA	C1B-CHB	2.03	1.46	1.41
20	Z	612	CLA	C1B-CHB	2.03	1.46	1.41
20	B	804	CLA	C1A-CHA	2.03	1.51	1.43
20	7	604	CLA	C1B-NB	-2.02	1.33	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	830	CLA	C1C-NC	-2.02	1.34	1.37
20	6	617	CLA	C1C-NC	-2.02	1.34	1.37
20	5	606	CLA	C1B-NB	-2.02	1.33	1.35
20	L	203	CLA	C1B-CHB	2.02	1.46	1.41
20	8	611	CLA	C1A-CHA	2.02	1.51	1.43
20	5	603	CLA	C1C-C2C	2.02	1.48	1.44
20	B	834	CLA	C1C-C2C	2.02	1.48	1.44
20	A	807	CLA	C1C-C2C	2.02	1.48	1.44
20	A	811	CLA	C4C-C3C	2.02	1.48	1.45
20	B	814	CLA	C4C-C3C	2.02	1.48	1.45
20	6	614	CLA	C1D-C2D	2.02	1.49	1.45
20	B	807	CLA	C1B-NB	-2.02	1.33	1.35
20	B	826	CLA	C1B-CHB	2.02	1.46	1.41
20	4	602	CLA	C1B-CHB	2.02	1.46	1.41
27	5	607	CHL	C1B-CHB	2.02	1.46	1.41
20	3	612	CLA	C1C-C2C	2.02	1.48	1.44
20	A	810	CLA	C1C-NC	-2.02	1.34	1.37
27	7	607	CHL	C1B-CHB	2.02	1.46	1.41
20	7	611	CLA	C1B-CHB	2.02	1.46	1.41
20	B	815	CLA	C1C-C2C	2.02	1.48	1.44
20	7	603	CLA	C1B-NB	-2.01	1.33	1.35
20	A	814	CLA	C1C-C2C	2.01	1.48	1.44
27	4	608	CHL	C1B-CHB	2.01	1.46	1.41
20	8	612	CLA	C1C-NC	-2.01	1.34	1.37
27	4	618	CHL	C2C-C1C	2.01	1.48	1.44
20	B	816	CLA	C4C-C3C	2.01	1.48	1.45
20	A	839	CLA	C1A-CHA	2.01	1.51	1.43
27	6	606	CHL	C1B-CHB	2.01	1.46	1.41
20	6	611	CLA	C1A-CHA	2.01	1.51	1.43
20	7	613	CLA	C1A-CHA	2.01	1.51	1.43
20	B	828	CLA	C1B-CHB	2.01	1.46	1.41
20	B	803	CLA	C1C-NC	-2.01	1.34	1.37
20	3	613	CLA	C1B-CHB	2.01	1.46	1.41
20	B	818	CLA	C1C-NC	-2.01	1.34	1.37
20	7	614	CLA	C1A-CHA	2.01	1.51	1.43
20	1	609	CLA	C1A-CHA	2.00	1.51	1.43
20	A	825	CLA	C1C-NC	-2.00	1.34	1.37
20	7	601	CLA	C1C-C2C	2.00	1.48	1.44
19	A	801	CL0	C1A-CHA	2.00	1.51	1.43
20	B	809	CLA	C1A-CHA	2.00	1.51	1.43
20	Z	603	CLA	C1C-C2C	2.00	1.48	1.44
20	Z	606	CLA	C1B-NB	-2.00	1.33	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	834	CLA	C1B-CHB	2.00	1.46	1.41
20	Z	604	CLA	C1B-CHB	2.00	1.46	1.41
20	Z	614	CLA	C1B-CHB	2.00	1.46	1.41
20	8	616	CLA	C1A-CHA	2.00	1.51	1.43

All (6430) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	6	608	CHL	C4A-NA-C1A	-12.36	101.15	106.71
27	1	601	CHL	C4A-NA-C1A	-11.60	101.49	106.71
27	4	608	CHL	C2D-C1D-ND	10.39	117.76	110.10
27	6	618	CHL	C2D-C1D-ND	10.27	117.67	110.10
20	A	818	CLA	C1D-ND-C4D	-10.24	99.06	106.33
27	Z	601	CHL	C2D-C1D-ND	10.21	117.63	110.10
27	4	618	CHL	C4A-NA-C1A	-10.15	102.14	106.71
27	5	618	CHL	C4A-NA-C1A	-10.12	102.16	106.71
27	1	601	CHL	C2D-C1D-ND	10.00	117.47	110.10
27	3	608	CHL	C2D-C1D-ND	9.96	117.44	110.10
27	6	606	CHL	C2D-C1D-ND	9.92	117.42	110.10
27	6	607	CHL	C2D-C1D-ND	9.90	117.40	110.10
20	B	805	CLA	C1D-ND-C4D	-9.87	99.32	106.33
20	L	203	CLA	C1D-ND-C4D	-9.82	99.36	106.33
27	6	618	CHL	C4A-NA-C1A	-9.81	102.30	106.71
27	4	607	CHL	C4A-NA-C1A	-9.78	102.31	106.71
20	A	823	CLA	C1D-ND-C4D	-9.73	99.43	106.33
20	B	821	CLA	C1D-ND-C4D	-9.72	99.43	106.33
27	5	618	CHL	C2D-C1D-ND	9.72	117.27	110.10
20	B	802	CLA	C1D-ND-C4D	-9.71	99.43	106.33
20	7	604	CLA	C1D-ND-C4D	-9.71	99.44	106.33
20	L	204	CLA	C1D-ND-C4D	-9.68	99.46	106.33
20	B	838	CLA	C1D-ND-C4D	-9.67	99.46	106.33
27	6	608	CHL	C2D-C1D-ND	9.67	117.23	110.10
27	4	618	CHL	C2D-C1D-ND	9.66	117.23	110.10
20	B	829	CLA	C1D-ND-C4D	-9.66	99.47	106.33
20	A	842	CLA	C1D-ND-C4D	-9.63	99.50	106.33
20	7	608	CLA	C1D-ND-C4D	-9.62	99.50	106.33
20	A	816	CLA	C1D-ND-C4D	-9.62	99.50	106.33
27	5	608	CHL	C2D-C1D-ND	9.62	117.19	110.10
20	6	614	CLA	C1D-ND-C4D	-9.61	99.50	106.33
20	5	602	CLA	C1D-ND-C4D	-9.61	99.51	106.33
20	7	602	CLA	C1D-ND-C4D	-9.59	99.52	106.33
20	A	841	CLA	C1D-ND-C4D	-9.57	99.54	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	F	304	CLA	C1D-ND-C4D	-9.54	99.56	106.33
20	A	828	CLA	C1D-ND-C4D	-9.54	99.56	106.33
20	A	802	CLA	C2D-C1D-ND	9.53	117.13	110.10
20	A	827	CLA	C1D-ND-C4D	-9.53	99.57	106.33
27	5	607	CHL	C2D-C1D-ND	9.52	117.12	110.10
20	A	845	CLA	C1D-ND-C4D	-9.51	99.58	106.33
20	4	616	CLA	C1D-ND-C4D	-9.47	99.61	106.33
27	4	607	CHL	C2D-C1D-ND	9.46	117.07	110.10
27	4	606	CHL	C2D-C1D-ND	9.46	117.07	110.10
20	8	614	CLA	C1D-ND-C4D	-9.45	99.62	106.33
20	A	812	CLA	C1D-ND-C4D	-9.44	99.63	106.33
20	A	808	CLA	C1D-ND-C4D	-9.44	99.63	106.33
20	B	826	CLA	C1D-ND-C4D	-9.43	99.64	106.33
20	B	831	CLA	C1D-ND-C4D	-9.43	99.64	106.33
27	1	607	CHL	C2D-C1D-ND	9.42	117.05	110.10
20	8	602	CLA	C1D-ND-C4D	-9.41	99.65	106.33
27	8	607	CHL	C2D-C1D-ND	9.41	117.04	110.10
27	Z	607	CHL	C2D-C1D-ND	9.41	117.04	110.10
20	7	606	CLA	C1D-ND-C4D	-9.41	99.65	106.33
20	A	809	CLA	C1D-ND-C4D	-9.41	99.65	106.33
20	5	617	CLA	C1D-ND-C4D	-9.41	99.65	106.33
20	7	610	CLA	C1D-ND-C4D	-9.39	99.67	106.33
20	A	854	CLA	C2D-C1D-ND	9.38	117.02	110.10
20	6	613	CLA	C1D-ND-C4D	-9.38	99.67	106.33
20	A	814	CLA	C1D-ND-C4D	-9.36	99.68	106.33
20	B	830	CLA	C1D-ND-C4D	-9.35	99.69	106.33
20	A	834	CLA	C1D-ND-C4D	-9.35	99.69	106.33
20	B	840	CLA	C1D-ND-C4D	-9.34	99.70	106.33
20	3	613	CLA	C1D-ND-C4D	-9.33	99.70	106.33
27	5	607	CHL	C4A-NA-C1A	-9.33	102.51	106.71
20	B	814	CLA	C1D-ND-C4D	-9.32	99.71	106.33
20	Z	602	CLA	C1D-ND-C4D	-9.32	99.71	106.33
20	4	614	CLA	C1D-ND-C4D	-9.32	99.71	106.33
20	8	613	CLA	C1D-ND-C4D	-9.31	99.72	106.33
20	3	602	CLA	C1D-ND-C4D	-9.30	99.73	106.33
20	3	614	CLA	C1D-ND-C4D	-9.29	99.73	106.33
20	1	602	CLA	C1D-ND-C4D	-9.29	99.74	106.33
20	6	602	CLA	C1D-ND-C4D	-9.29	99.74	106.33
20	B	812	CLA	C1D-ND-C4D	-9.29	99.74	106.33
20	1	610	CLA	C1D-ND-C4D	-9.28	99.74	106.33
20	7	612	CLA	C1D-ND-C4D	-9.28	99.74	106.33
20	Z	614	CLA	C1D-ND-C4D	-9.27	99.75	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	609	CLA	C1D-ND-C4D	-9.27	99.75	106.33
20	A	806	CLA	C1D-ND-C4D	-9.27	99.75	106.33
20	A	828	CLA	C2D-C1D-ND	9.26	116.93	110.10
20	Z	610	CLA	C1D-ND-C4D	-9.26	99.76	106.33
20	B	833	CLA	C1D-ND-C4D	-9.26	99.76	106.33
20	A	811	CLA	C1D-ND-C4D	-9.23	99.78	106.33
20	A	817	CLA	C1D-ND-C4D	-9.23	99.78	106.33
27	3	608	CHL	C4A-NA-C1A	-9.22	102.56	106.71
20	7	601	CLA	C1D-ND-C4D	-9.22	99.79	106.33
20	A	804	CLA	C1D-ND-C4D	-9.22	99.79	106.33
20	3	610	CLA	C1D-ND-C4D	-9.20	99.80	106.33
20	4	613	CLA	C1D-ND-C4D	-9.20	99.80	106.33
20	6	622	CLA	C1D-ND-C4D	-9.18	99.81	106.33
20	A	840	CLA	C1D-ND-C4D	-9.18	99.82	106.33
20	B	822	CLA	C1D-ND-C4D	-9.17	99.82	106.33
20	F	303	CLA	C1D-ND-C4D	-9.15	99.83	106.33
20	4	602	CLA	C1D-ND-C4D	-9.14	99.84	106.33
20	B	816	CLA	C1D-ND-C4D	-9.14	99.84	106.33
20	F	301	CLA	C1D-ND-C4D	-9.14	99.84	106.33
19	A	801	CL0	C1D-ND-C4D	-9.14	99.84	106.33
20	B	832	CLA	C1D-ND-C4D	-9.14	99.84	106.33
20	3	607	CLA	C1D-ND-C4D	-9.13	99.85	106.33
20	A	824	CLA	C1D-ND-C4D	-9.12	99.86	106.33
27	8	607	CHL	C4A-NA-C1A	-9.11	102.61	106.71
20	B	811	CLA	C1D-ND-C4D	-9.11	99.86	106.33
20	B	815	CLA	C1D-ND-C4D	-9.09	99.88	106.33
20	8	604	CLA	C1D-ND-C4D	-9.09	99.88	106.33
20	7	620	CLA	C1D-ND-C4D	-9.09	99.88	106.33
20	A	836	CLA	C1D-ND-C4D	-9.07	99.89	106.33
20	3	612	CLA	C1D-ND-C4D	-9.07	99.89	106.33
20	A	854	CLA	C1D-ND-C4D	-9.06	99.90	106.33
27	Z	601	CHL	C4A-NA-C1A	-9.06	102.63	106.71
20	A	830	CLA	C1D-ND-C4D	-9.06	99.90	106.33
20	Z	606	CLA	C1D-ND-C4D	-9.06	99.90	106.33
20	5	610	CLA	C1D-ND-C4D	-9.06	99.90	106.33
20	4	601	CLA	C1D-ND-C4D	-9.05	99.91	106.33
20	A	833	CLA	C1D-ND-C4D	-9.05	99.91	106.33
20	6	612	CLA	C1D-ND-C4D	-9.04	99.91	106.33
20	8	608	CLA	C1D-ND-C4D	-9.04	99.91	106.33
20	3	617	CLA	C1D-ND-C4D	-9.04	99.91	106.33
20	1	613	CLA	C1D-ND-C4D	-9.03	99.92	106.33
20	5	604	CLA	C1D-ND-C4D	-9.03	99.92	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	614	CLA	C1D-ND-C4D	-9.03	99.92	106.33
20	Z	612	CLA	C1D-ND-C4D	-9.03	99.92	106.33
20	8	610	CLA	C1D-ND-C4D	-9.02	99.93	106.33
20	8	612	CLA	C1D-ND-C4D	-9.02	99.93	106.33
20	K	4002	CLA	C1D-ND-C4D	-9.02	99.93	106.33
20	A	839	CLA	C1D-ND-C4D	-9.00	99.94	106.33
20	1	606	CLA	C1D-ND-C4D	-9.00	99.94	106.33
20	A	820	CLA	C1D-ND-C4D	-9.00	99.94	106.33
20	A	802	CLA	C1D-ND-C4D	-8.99	99.95	106.33
20	A	810	CLA	C1D-ND-C4D	-8.99	99.95	106.33
20	5	614	CLA	C1D-ND-C4D	-8.99	99.95	106.33
20	B	810	CLA	C1D-ND-C4D	-8.98	99.95	106.33
20	7	609	CLA	C1D-ND-C4D	-8.98	99.96	106.33
20	Z	611	CLA	C1D-ND-C4D	-8.97	99.96	106.33
20	B	827	CLA	C1D-ND-C4D	-8.97	99.96	106.33
20	G	203	CLA	C1D-ND-C4D	-8.97	99.96	106.33
20	J	3002	CLA	C1D-ND-C4D	-8.96	99.97	106.33
27	6	606	CHL	C4A-NA-C1A	-8.96	102.68	106.71
20	4	604	CLA	C1D-ND-C4D	-8.96	99.97	106.33
20	A	813	CLA	C1D-ND-C4D	-8.96	99.97	106.33
27	7	607	CHL	C2D-C1D-ND	8.95	116.70	110.10
20	8	603	CLA	C1D-ND-C4D	-8.94	99.99	106.33
20	Z	613	CLA	C1D-ND-C4D	-8.93	99.99	106.33
20	7	611	CLA	C1D-ND-C4D	-8.93	99.99	106.33
20	1	612	CLA	C1D-ND-C4D	-8.93	99.99	106.33
20	Z	604	CLA	C1D-ND-C4D	-8.93	99.99	106.33
20	5	612	CLA	C1D-ND-C4D	-8.91	100.01	106.33
20	B	834	CLA	C1D-ND-C4D	-8.90	100.01	106.33
20	A	829	CLA	C1D-ND-C4D	-8.89	100.02	106.33
20	3	620	CLA	C1D-ND-C4D	-8.88	100.02	106.33
20	B	807	CLA	C1D-ND-C4D	-8.88	100.03	106.33
20	B	820	CLA	C1D-ND-C4D	-8.87	100.03	106.33
20	3	604	CLA	C1D-ND-C4D	-8.87	100.03	106.33
20	B	808	CLA	C1D-ND-C4D	-8.86	100.04	106.33
20	5	606	CLA	C1D-ND-C4D	-8.86	100.04	106.33
20	B	852	CLA	C1D-ND-C4D	-8.85	100.05	106.33
20	A	818	CLA	C2D-C1D-ND	8.85	116.62	110.10
20	A	825	CLA	C1D-ND-C4D	-8.85	100.05	106.33
20	B	837	CLA	C1D-ND-C4D	-8.84	100.06	106.33
20	5	609	CLA	C1D-ND-C4D	-8.83	100.06	106.33
20	A	819	CLA	C1D-ND-C4D	-8.83	100.06	106.33
20	5	617	CLA	C2D-C1D-ND	8.83	116.61	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	6	601	CLA	C1D-ND-C4D	-8.81	100.07	106.33
20	Z	609	CLA	C1D-ND-C4D	-8.81	100.08	106.33
20	B	804	CLA	C1D-ND-C4D	-8.80	100.08	106.33
20	B	813	CLA	C1D-ND-C4D	-8.79	100.09	106.33
20	B	839	CLA	C1D-ND-C4D	-8.79	100.09	106.33
20	4	612	CLA	C1D-ND-C4D	-8.78	100.09	106.33
20	3	603	CLA	C1D-ND-C4D	-8.78	100.10	106.33
20	7	603	CLA	C1D-ND-C4D	-8.78	100.10	106.33
20	B	841	CLA	C1D-ND-C4D	-8.76	100.11	106.33
20	3	606	CLA	C1D-ND-C4D	-8.76	100.11	106.33
20	6	617	CLA	C1D-ND-C4D	-8.74	100.12	106.33
20	4	610	CLA	C1D-ND-C4D	-8.74	100.12	106.33
20	1	604	CLA	C1D-ND-C4D	-8.74	100.13	106.33
20	A	805	CLA	C1D-ND-C4D	-8.74	100.13	106.33
20	A	821	CLA	C1D-ND-C4D	-8.74	100.13	106.33
20	A	831	CLA	C1D-ND-C4D	-8.73	100.14	106.33
20	K	4003	CLA	C1D-ND-C4D	-8.72	100.14	106.33
20	G	204	CLA	C1D-ND-C4D	-8.72	100.14	106.33
20	8	606	CLA	C1D-ND-C4D	-8.71	100.14	106.33
20	B	836	CLA	C1D-ND-C4D	-8.70	100.15	106.33
20	B	802	CLA	C2D-C1D-ND	8.70	116.51	110.10
20	B	823	CLA	C1D-ND-C4D	-8.70	100.16	106.33
20	3	609	CLA	C1D-ND-C4D	-8.70	100.16	106.33
20	7	614	CLA	C1D-ND-C4D	-8.69	100.16	106.33
20	5	616	CLA	C1D-ND-C4D	-8.69	100.16	106.33
27	4	606	CHL	C4A-NA-C1A	-8.69	102.80	106.71
20	8	609	CLA	C1D-ND-C4D	-8.68	100.17	106.33
20	B	838	CLA	C2D-C1D-ND	8.68	116.50	110.10
20	1	609	CLA	C1D-ND-C4D	-8.66	100.18	106.33
20	6	611	CLA	C1D-ND-C4D	-8.66	100.18	106.33
20	6	603	CLA	C1D-ND-C4D	-8.66	100.18	106.33
20	5	601	CLA	C1D-ND-C4D	-8.66	100.18	106.33
20	6	609	CLA	C1D-ND-C4D	-8.66	100.19	106.33
20	A	826	CLA	C1D-ND-C4D	-8.65	100.19	106.33
20	3	611	CLA	C1D-ND-C4D	-8.65	100.19	106.33
20	A	809	CLA	C2D-C1D-ND	8.65	116.48	110.10
20	A	843	CLA	C1D-ND-C4D	-8.64	100.19	106.33
20	6	616	CLA	C1D-ND-C4D	-8.64	100.19	106.33
20	1	611	CLA	C1D-ND-C4D	-8.64	100.20	106.33
27	5	608	CHL	C4A-NA-C1A	-8.64	102.82	106.71
20	1	603	CLA	C1D-ND-C4D	-8.64	100.20	106.33
20	6	604	CLA	C1D-ND-C4D	-8.63	100.20	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	824	CLA	C1D-ND-C4D	-8.62	100.21	106.33
20	1	608	CLA	C1D-ND-C4D	-8.61	100.22	106.33
20	A	823	CLA	C2D-C1D-ND	8.61	116.45	110.10
20	B	825	CLA	C1D-ND-C4D	-8.60	100.22	106.33
20	5	611	CLA	C1D-ND-C4D	-8.59	100.23	106.33
20	6	610	CLA	C1D-ND-C4D	-8.58	100.24	106.33
20	7	616	CLA	C1D-ND-C4D	-8.57	100.25	106.33
20	B	805	CLA	C2D-C1D-ND	8.56	116.41	110.10
20	Z	608	CLA	C1D-ND-C4D	-8.56	100.25	106.33
20	7	613	CLA	C1D-ND-C4D	-8.56	100.26	106.33
20	A	803	CLA	C1D-ND-C4D	-8.55	100.26	106.33
20	B	818	CLA	C1D-ND-C4D	-8.54	100.27	106.33
20	A	838	CLA	C1D-ND-C4D	-8.53	100.28	106.33
20	A	835	CLA	C1D-ND-C4D	-8.52	100.28	106.33
20	1	616	CLA	C1D-ND-C4D	-8.52	100.28	106.33
20	B	828	CLA	C1D-ND-C4D	-8.51	100.29	106.33
20	B	803	CLA	C1D-ND-C4D	-8.51	100.29	106.33
20	7	609	CLA	C2D-C1D-ND	8.51	116.37	110.10
20	Z	603	CLA	C1D-ND-C4D	-8.50	100.29	106.33
20	B	817	CLA	C1D-ND-C4D	-8.50	100.30	106.33
20	8	602	CLA	C2D-C1D-ND	8.48	116.36	110.10
20	4	603	CLA	C1D-ND-C4D	-8.45	100.33	106.33
20	B	806	CLA	C1D-ND-C4D	-8.45	100.33	106.33
20	A	807	CLA	C1D-ND-C4D	-8.43	100.35	106.33
20	8	616	CLA	C1D-ND-C4D	-8.43	100.35	106.33
20	A	840	CLA	C2D-C1D-ND	8.42	116.31	110.10
20	8	611	CLA	C1D-ND-C4D	-8.42	100.36	106.33
20	8	601	CLA	C1D-ND-C4D	-8.40	100.36	106.33
20	B	835	CLA	C1D-ND-C4D	-8.40	100.37	106.33
20	A	841	CLA	C2D-C1D-ND	8.39	116.29	110.10
20	A	830	CLA	C2D-C1D-ND	8.39	116.28	110.10
20	B	819	CLA	C1D-ND-C4D	-8.38	100.38	106.33
20	Z	616	CLA	C1D-ND-C4D	-8.38	100.38	106.33
20	A	832	CLA	C1D-ND-C4D	-8.34	100.41	106.33
20	L	203	CLA	C2D-C1D-ND	8.33	116.25	110.10
20	A	814	CLA	C2D-C1D-ND	8.33	116.24	110.10
20	Z	610	CLA	C2D-C1D-ND	8.32	116.24	110.10
20	B	821	CLA	C2D-C1D-ND	8.31	116.23	110.10
20	L	204	CLA	C2D-C1D-ND	8.30	116.22	110.10
20	A	829	CLA	C2D-C1D-ND	8.29	116.21	110.10
20	B	831	CLA	C2D-C1D-ND	8.29	116.21	110.10
20	A	831	CLA	C2D-C1D-ND	8.28	116.21	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	F	303	CLA	C2D-C1D-ND	8.26	116.19	110.10
20	A	815	CLA	C1D-ND-C4D	-8.26	100.47	106.33
20	4	609	CLA	C2D-C1D-ND	8.25	116.18	110.10
20	4	614	CLA	C2D-C1D-ND	8.24	116.17	110.10
20	8	608	CLA	C2D-C1D-ND	8.23	116.17	110.10
20	A	833	CLA	C2D-C1D-ND	8.23	116.17	110.10
20	A	816	CLA	C2D-C1D-ND	8.22	116.16	110.10
20	6	614	CLA	CMD-C2D-C1D	8.22	139.19	124.71
20	A	845	CLA	C2D-C1D-ND	8.21	116.16	110.10
23	I	172	BCR	C24-C23-C22	-8.21	113.83	126.23
20	6	622	CLA	C2D-C1D-ND	8.21	116.15	110.10
20	F	304	CLA	C2D-C1D-ND	8.20	116.15	110.10
20	5	613	CLA	C1D-ND-C4D	-8.20	100.51	106.33
20	1	610	CLA	C2D-C1D-ND	8.19	116.14	110.10
20	4	611	CLA	C1D-ND-C4D	-8.19	100.52	106.33
20	8	613	CLA	C2D-C1D-ND	8.18	116.14	110.10
20	A	822	CLA	C1D-ND-C4D	-8.17	100.53	106.33
20	7	602	CLA	C2D-C1D-ND	8.15	116.11	110.10
20	A	842	CLA	C2D-C1D-ND	8.14	116.11	110.10
20	3	613	CLA	C2D-C1D-ND	8.14	116.10	110.10
20	B	809	CLA	C1D-ND-C4D	-8.13	100.56	106.33
20	A	820	CLA	C2D-C1D-ND	8.13	116.09	110.10
20	A	812	CLA	C2D-C1D-ND	8.13	116.09	110.10
20	B	803	CLA	C2D-C1D-ND	8.13	116.09	110.10
20	7	608	CLA	C2D-C1D-ND	8.13	116.09	110.10
20	5	603	CLA	C1D-ND-C4D	-8.11	100.57	106.33
20	B	827	CLA	C2D-C1D-ND	8.11	116.08	110.10
20	8	614	CLA	C2D-C1D-ND	8.11	116.08	110.10
20	B	826	CLA	C2D-C1D-ND	8.10	116.07	110.10
20	1	602	CLA	C2D-C1D-ND	8.09	116.06	110.10
20	B	804	CLA	C2D-C1D-ND	8.08	116.06	110.10
20	5	621	CLA	C1D-ND-C4D	-8.08	100.60	106.33
20	B	816	CLA	C2D-C1D-ND	8.06	116.05	110.10
20	Z	602	CLA	C2D-C1D-ND	8.06	116.04	110.10
20	6	613	CLA	C2D-C1D-ND	8.05	116.04	110.10
20	A	819	CLA	C2D-C1D-ND	8.05	116.03	110.10
20	B	836	CLA	C2D-C1D-ND	8.04	116.03	110.10
20	7	604	CLA	C2D-C1D-ND	8.04	116.03	110.10
20	B	812	CLA	C2D-C1D-ND	8.03	116.03	110.10
20	A	827	CLA	C2D-C1D-ND	8.03	116.02	110.10
19	A	801	CL0	C2D-C1D-ND	8.02	116.02	110.10
20	7	611	CLA	C2D-C1D-ND	8.01	116.01	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	808	CLA	C2D-C1D-ND	8.00	116.00	110.10
20	A	811	CLA	C2D-C1D-ND	8.00	116.00	110.10
27	6	607	CHL	C4A-NA-C1A	-7.98	103.12	106.71
20	Z	614	CLA	C2D-C1D-ND	7.98	115.98	110.10
20	7	601	CLA	C2D-C1D-ND	7.98	115.98	110.10
20	7	612	CLA	C2D-C1D-ND	7.98	115.98	110.10
20	4	616	CLA	C2D-C1D-ND	7.97	115.98	110.10
20	8	609	CLA	C2D-C1D-ND	7.96	115.97	110.10
20	6	602	CLA	C2D-C1D-ND	7.96	115.97	110.10
20	A	834	CLA	C2D-C1D-ND	7.95	115.96	110.10
20	7	606	CLA	C2D-C1D-ND	7.94	115.96	110.10
20	A	837	CLA	C1D-ND-C4D	-7.94	100.69	106.33
20	G	203	CLA	C2D-C1D-ND	7.93	115.95	110.10
20	Z	606	CLA	C2D-C1D-ND	7.93	115.95	110.10
20	4	601	CLA	C2D-C1D-ND	7.93	115.95	110.10
20	A	803	CLA	C2D-C1D-ND	7.93	115.94	110.10
20	B	823	CLA	C2D-C1D-ND	7.92	115.94	110.10
20	8	610	CLA	C2D-C1D-ND	7.91	115.93	110.10
20	5	609	CLA	C2D-C1D-ND	7.90	115.92	110.10
20	7	610	CLA	C2D-C1D-ND	7.89	115.92	110.10
20	B	832	CLA	C2D-C1D-ND	7.88	115.91	110.10
20	A	817	CLA	CMD-C2D-C1D	7.88	138.60	124.71
20	A	839	CLA	C2D-C1D-ND	7.88	115.91	110.10
20	3	603	CLA	C2D-C1D-ND	7.88	115.91	110.10
20	7	614	CLA	C2D-C1D-ND	7.87	115.91	110.10
20	5	610	CLA	C2D-C1D-ND	7.87	115.90	110.10
20	1	613	CLA	C2D-C1D-ND	7.86	115.90	110.10
20	1	612	CLA	C2D-C1D-ND	7.85	115.89	110.10
20	B	841	CLA	C2D-C1D-ND	7.85	115.89	110.10
20	A	813	CLA	C2D-C1D-ND	7.84	115.89	110.10
20	7	620	CLA	C2D-C1D-ND	7.84	115.88	110.10
20	5	611	CLA	C2D-C1D-ND	7.84	115.88	110.10
20	B	808	CLA	C2D-C1D-ND	7.82	115.86	110.10
20	B	814	CLA	C2D-C1D-ND	7.82	115.86	110.10
20	3	602	CLA	C2D-C1D-ND	7.82	115.86	110.10
20	B	806	CLA	C2D-C1D-ND	7.81	115.86	110.10
20	A	805	CLA	C2D-C1D-ND	7.81	115.86	110.10
20	8	603	CLA	C2D-C1D-ND	7.81	115.86	110.10
20	3	610	CLA	C2D-C1D-ND	7.78	115.84	110.10
20	5	616	CLA	C2D-C1D-ND	7.78	115.84	110.10
20	B	852	CLA	C2D-C1D-ND	7.78	115.84	110.10
20	3	614	CLA	C2D-C1D-ND	7.78	115.84	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	815	CLA	C2D-C1D-ND	7.78	115.84	110.10
20	A	843	CLA	C2D-C1D-ND	7.78	115.84	110.10
20	3	617	CLA	C2D-C1D-ND	7.78	115.84	110.10
20	B	833	CLA	C2D-C1D-ND	7.76	115.82	110.10
20	4	613	CLA	C2D-C1D-ND	7.76	115.82	110.10
20	5	602	CLA	C2D-C1D-ND	7.76	115.82	110.10
20	6	612	CLA	C2D-C1D-ND	7.76	115.82	110.10
20	3	604	CLA	C2D-C1D-ND	7.74	115.81	110.10
20	A	810	CLA	C2D-C1D-ND	7.74	115.81	110.10
20	3	607	CLA	C2D-C1D-ND	7.74	115.81	110.10
20	3	609	CLA	C2D-C1D-ND	7.74	115.81	110.10
20	A	826	CLA	C2D-C1D-ND	7.74	115.81	110.10
20	A	825	CLA	C2D-C1D-ND	7.73	115.80	110.10
20	A	824	CLA	C2D-C1D-ND	7.73	115.80	110.10
20	A	836	CLA	C2D-C1D-ND	7.72	115.79	110.10
20	5	612	CLA	C2D-C1D-ND	7.72	115.79	110.10
20	8	601	CLA	C2D-C1D-ND	7.72	115.79	110.10
20	5	614	CLA	C2D-C1D-ND	7.71	115.79	110.10
20	K	4002	CLA	C2D-C1D-ND	7.71	115.78	110.10
20	A	806	CLA	C2D-C1D-ND	7.70	115.78	110.10
20	6	609	CLA	C2D-C1D-ND	7.70	115.78	110.10
20	Z	611	CLA	C2D-C1D-ND	7.70	115.78	110.10
20	1	614	CLA	C2D-C1D-ND	7.70	115.78	110.10
20	Z	613	CLA	C2D-C1D-ND	7.68	115.76	110.10
20	4	602	CLA	C2D-C1D-ND	7.67	115.76	110.10
20	A	804	CLA	CMD-C2D-C1D	7.67	138.24	124.71
20	5	606	CLA	C2D-C1D-ND	7.67	115.75	110.10
20	B	818	CLA	C2D-C1D-ND	7.67	115.75	110.10
20	5	604	CLA	C2D-C1D-ND	7.67	115.75	110.10
20	B	811	CLA	C2D-C1D-ND	7.67	115.75	110.10
20	1	606	CLA	C2D-C1D-ND	7.66	115.75	110.10
20	3	612	CLA	C2D-C1D-ND	7.66	115.75	110.10
20	6	603	CLA	C2D-C1D-ND	7.66	115.75	110.10
20	B	807	CLA	C2D-C1D-ND	7.66	115.75	110.10
20	1	611	CLA	C2D-C1D-ND	7.65	115.74	110.10
20	J	3002	CLA	C2D-C1D-ND	7.65	115.74	110.10
20	Z	609	CLA	C2D-C1D-ND	7.64	115.74	110.10
20	8	612	CLA	C2D-C1D-ND	7.64	115.73	110.10
20	3	620	CLA	C2D-C1D-ND	7.64	115.73	110.10
20	B	830	CLA	C2D-C1D-ND	7.64	115.73	110.10
20	7	613	CLA	C2D-C1D-ND	7.63	115.73	110.10
20	4	610	CLA	C2D-C1D-ND	7.63	115.73	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Z	612	CLA	C2D-C1D-ND	7.63	115.73	110.10
20	F	301	CLA	CMD-C2D-C1D	7.61	138.13	124.71
20	8	606	CLA	C2D-C1D-ND	7.61	115.71	110.10
20	5	601	CLA	C2D-C1D-ND	7.60	115.71	110.10
20	B	837	CLA	C2D-C1D-ND	7.60	115.70	110.10
20	B	822	CLA	C2D-C1D-ND	7.60	115.70	110.10
20	1	608	CLA	C2D-C1D-ND	7.60	115.70	110.10
20	B	829	CLA	CMD-C2D-C1D	7.59	138.08	124.71
27	4	608	CHL	C4A-NA-C1A	-7.58	103.30	106.71
20	4	612	CLA	C2D-C1D-ND	7.55	115.67	110.10
20	6	611	CLA	C2D-C1D-ND	7.54	115.66	110.10
20	B	840	CLA	C2D-C1D-ND	7.53	115.65	110.10
20	K	4003	CLA	C2D-C1D-ND	7.53	115.65	110.10
20	3	611	CLA	C2D-C1D-ND	7.52	115.64	110.10
20	6	614	CLA	C2D-C1D-ND	7.51	115.64	110.10
20	6	601	CLA	C2D-C1D-ND	7.50	115.63	110.10
20	B	835	CLA	C2D-C1D-ND	7.50	115.63	110.10
20	B	839	CLA	C2D-C1D-ND	7.49	115.63	110.10
20	B	813	CLA	C2D-C1D-ND	7.49	115.62	110.10
20	A	821	CLA	C2D-C1D-ND	7.49	115.62	110.10
20	G	204	CLA	C2D-C1D-ND	7.48	115.62	110.10
20	1	603	CLA	C2D-C1D-ND	7.48	115.61	110.10
20	1	609	CLA	C2D-C1D-ND	7.48	115.61	110.10
20	Z	608	CLA	C2D-C1D-ND	7.47	115.61	110.10
20	B	834	CLA	C2D-C1D-ND	7.47	115.61	110.10
20	8	604	CLA	C2D-C1D-ND	7.46	115.60	110.10
20	A	815	CLA	CMD-C2D-C1D	7.46	137.86	124.71
20	6	616	CLA	C2D-C1D-ND	7.46	115.60	110.10
27	3	608	CHL	CMD-C2D-C1D	7.45	137.85	124.71
20	B	820	CLA	C2D-C1D-ND	7.45	115.59	110.10
20	8	611	CLA	C2D-C1D-ND	7.43	115.58	110.10
20	6	604	CLA	C2D-C1D-ND	7.42	115.58	110.10
20	6	617	CLA	C2D-C1D-ND	7.41	115.56	110.10
20	4	604	CLA	C2D-C1D-ND	7.41	115.56	110.10
20	8	616	CLA	C2D-C1D-ND	7.40	115.56	110.10
20	3	606	CLA	C2D-C1D-ND	7.40	115.56	110.10
20	B	826	CLA	CMD-C2D-C1D	7.39	137.74	124.71
20	B	828	CLA	C2D-C1D-ND	7.38	115.55	110.10
20	B	810	CLA	C2D-C1D-ND	7.38	115.54	110.10
20	F	301	CLA	C2D-C1D-ND	7.37	115.54	110.10
20	1	616	CLA	C2D-C1D-ND	7.37	115.53	110.10
23	B	801	BCR	C16-C15-C14	-7.36	108.39	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	822	CLA	C2D-C1D-ND	7.36	115.53	110.10
20	Z	616	CLA	C2D-C1D-ND	7.35	115.52	110.10
20	Z	604	CLA	C2D-C1D-ND	7.35	115.52	110.10
20	A	833	CLA	CMD-C2D-C1D	7.32	137.62	124.71
20	A	815	CLA	C2D-C1D-ND	7.32	115.50	110.10
20	7	603	CLA	C2D-C1D-ND	7.30	115.49	110.10
20	6	610	CLA	C2D-C1D-ND	7.30	115.48	110.10
27	7	607	CHL	CMD-C2D-C1D	7.29	137.57	124.71
20	B	817	CLA	C2D-C1D-ND	7.29	115.48	110.10
20	B	829	CLA	C2D-C1D-ND	7.29	115.48	110.10
20	A	832	CLA	C2D-C1D-ND	7.28	115.47	110.10
27	6	606	CHL	CMD-C2D-C1D	7.28	137.55	124.71
27	4	608	CHL	CMD-C2D-C1D	7.28	137.54	124.71
20	A	828	CLA	CHD-C4C-C3C	-7.28	114.15	124.84
20	4	611	CLA	C2D-C1D-ND	7.25	115.44	110.10
20	A	807	CLA	C2D-C1D-ND	7.25	115.44	110.10
20	5	603	CLA	C2D-C1D-ND	7.25	115.44	110.10
20	B	809	CLA	C2D-C1D-ND	7.24	115.44	110.10
20	4	603	CLA	C2D-C1D-ND	7.24	115.44	110.10
27	5	608	CHL	CMD-C2D-C1D	7.22	137.43	124.71
20	1	604	CLA	CMD-C2D-C1D	7.20	137.41	124.71
20	A	835	CLA	C2D-C1D-ND	7.20	115.41	110.10
20	A	817	CLA	C2D-C1D-ND	7.18	115.39	110.10
20	Z	603	CLA	C2D-C1D-ND	7.17	115.39	110.10
20	5	602	CLA	CMD-C2D-C1D	7.17	137.34	124.71
20	B	840	CLA	CMD-C2D-C1D	7.15	137.31	124.71
27	1	601	CHL	CMD-C2D-C1D	7.14	137.29	124.71
27	Z	607	CHL	CMD-C2D-C1D	7.13	137.28	124.71
20	7	614	CLA	O2D-CGD-CBD	7.12	123.92	111.27
20	A	837	CLA	C2D-C1D-ND	7.07	115.31	110.10
20	A	838	CLA	CMD-C2D-C1D	7.07	137.18	124.71
20	1	604	CLA	C2D-C1D-ND	7.06	115.31	110.10
27	4	606	CHL	CMD-C2D-C1D	7.06	137.15	124.71
27	3	608	CHL	C1C-C2C-C3C	-7.05	101.51	107.11
20	7	601	CLA	CMD-C2D-C1D	7.05	137.14	124.71
20	7	604	CLA	CMD-C2D-C1D	7.05	137.14	124.71
20	1	606	CLA	CMD-C2D-C1D	7.05	137.14	124.71
20	A	840	CLA	CMD-C2D-C1D	7.05	137.14	124.71
27	Z	607	CHL	C4A-NA-C1A	-7.04	103.54	106.71
20	A	835	CLA	CMD-C2D-C1D	7.04	137.11	124.71
20	7	603	CLA	CMD-C2D-C1D	7.03	137.11	124.71
20	B	819	CLA	C2D-C1D-ND	7.03	115.28	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	824	CLA	C2D-C1D-ND	7.02	115.28	110.10
20	5	613	CLA	C2D-C1D-ND	7.02	115.28	110.10
27	1	607	CHL	CMD-C2D-C1D	7.01	137.07	124.71
27	5	607	CHL	CMD-C2D-C1D	7.01	137.07	124.71
20	B	831	CLA	CMD-C2D-C1D	7.01	137.06	124.71
20	5	621	CLA	C2D-C1D-ND	6.99	115.25	110.10
20	8	610	CLA	CMD-C2D-C1D	6.98	137.01	124.71
20	8	603	CLA	CMD-C2D-C1D	6.98	137.01	124.71
20	6	602	CLA	CMD-C2D-C1D	6.97	136.99	124.71
27	5	618	CHL	CMD-C2D-C1D	6.97	136.99	124.71
27	7	607	CHL	C4A-NA-C1A	-6.96	103.58	106.71
27	4	607	CHL	CMD-C2D-C1D	6.96	136.98	124.71
20	B	816	CLA	CMD-C2D-C1D	6.96	136.97	124.71
20	7	606	CLA	CMD-C2D-C1D	6.96	136.97	124.71
20	A	827	CLA	CMD-C2D-C1D	6.95	136.96	124.71
20	7	616	CLA	C2D-C1D-ND	6.95	115.22	110.10
20	7	610	CLA	CMD-C2D-C1D	6.92	136.91	124.71
20	1	608	CLA	CMD-C2D-C1D	6.90	136.88	124.71
20	3	614	CLA	CMD-C2D-C1D	6.90	136.87	124.71
27	4	618	CHL	CMD-C2D-C1D	6.89	136.86	124.71
20	B	817	CLA	CMD-C2D-C1D	6.89	136.86	124.71
20	3	606	CLA	CMD-C2D-C1D	6.88	136.84	124.71
20	A	838	CLA	C2D-C1D-ND	6.87	115.17	110.10
20	3	610	CLA	CMD-C2D-C1D	6.87	136.83	124.71
20	A	819	CLA	CMD-C2D-C1D	6.87	136.82	124.71
20	B	834	CLA	CMD-C2D-C1D	6.87	136.82	124.71
20	4	602	CLA	CMD-C2D-C1D	6.86	136.81	124.71
20	J	3002	CLA	CMD-C2D-C1D	6.86	136.80	124.71
27	6	608	CHL	CMD-C2D-C1D	6.86	136.80	124.71
20	1	609	CLA	CMD-C2D-C1D	6.86	136.79	124.71
20	A	814	CLA	CMD-C2D-C1D	6.85	136.79	124.71
20	6	603	CLA	CMD-C2D-C1D	6.85	136.78	124.71
20	Z	604	CLA	CMD-C2D-C1D	6.85	136.78	124.71
20	B	806	CLA	CMD-C2D-C1D	6.85	136.78	124.71
20	B	810	CLA	CMD-C2D-C1D	6.84	136.77	124.71
20	B	825	CLA	C2D-C1D-ND	6.84	115.14	110.10
20	4	604	CLA	CMD-C2D-C1D	6.84	136.77	124.71
20	L	204	CLA	CMD-C2D-C1D	6.84	136.76	124.71
27	Z	601	CHL	C1D-ND-C4D	-6.84	101.48	106.33
20	A	845	CLA	CMD-C2D-C1D	6.83	136.74	124.71
20	8	601	CLA	CMD-C2D-C1D	6.82	136.73	124.71
20	B	811	CLA	CMD-C2D-C1D	6.81	136.71	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	822	CLA	CMD-C2D-C1D	6.80	136.71	124.71
20	Z	608	CLA	CMD-C2D-C1D	6.80	136.70	124.71
20	3	620	CLA	CMD-C2D-C1D	6.80	136.69	124.71
20	A	808	CLA	CMD-C2D-C1D	6.79	136.69	124.71
20	4	616	CLA	CMD-C2D-C1D	6.79	136.68	124.71
20	A	828	CLA	CMD-C2D-C1D	6.79	136.68	124.71
20	Z	609	CLA	CMD-C2D-C1D	6.79	136.68	124.71
20	5	610	CLA	CMD-C2D-C1D	6.79	136.68	124.71
20	6	616	CLA	CMD-C2D-C1D	6.79	136.68	124.71
20	F	304	CLA	CMD-C2D-C1D	6.78	136.67	124.71
20	A	839	CLA	CMD-C2D-C1D	6.78	136.66	124.71
20	5	616	CLA	CMD-C2D-C1D	6.78	136.66	124.71
20	B	803	CLA	CMD-C2D-C1D	6.78	136.66	124.71
20	5	621	CLA	C2C-C1C-NC	6.78	116.32	109.97
20	B	820	CLA	CMD-C2D-C1D	6.77	136.65	124.71
20	B	832	CLA	CMD-C2D-C1D	6.77	136.65	124.71
20	A	834	CLA	CMD-C2D-C1D	6.77	136.65	124.71
20	Z	614	CLA	CMD-C2D-C1D	6.76	136.63	124.71
20	G	203	CLA	CMD-C2D-C1D	6.76	136.63	124.71
20	Z	603	CLA	CMD-C2D-C1D	6.76	136.63	124.71
20	A	804	CLA	O2D-CGD-CBD	6.76	123.28	111.27
20	B	805	CLA	CMD-C2D-C1D	6.76	136.63	124.71
20	G	204	CLA	CMD-C2D-C1D	6.76	136.62	124.71
20	B	825	CLA	CMD-C2D-C1D	6.75	136.61	124.71
20	A	824	CLA	CMD-C2D-C1D	6.75	136.61	124.71
20	7	612	CLA	CMD-C2D-C1D	6.75	136.61	124.71
20	A	837	CLA	CMD-C2D-C1D	6.75	136.60	124.71
20	5	604	CLA	CMD-C2D-C1D	6.75	136.60	124.71
20	6	614	CLA	CHD-C1D-ND	-6.74	118.26	124.45
20	8	602	CLA	CHD-C4C-C3C	-6.73	114.95	124.84
20	A	812	CLA	CMD-C2D-C1D	6.72	136.56	124.71
20	B	812	CLA	CMD-C2D-C1D	6.72	136.56	124.71
20	B	804	CLA	CMD-C2D-C1D	6.71	136.53	124.71
27	6	607	CHL	CMD-C2D-C1D	6.70	136.53	124.71
20	B	815	CLA	CMD-C2D-C1D	6.70	136.52	124.71
20	A	842	CLA	CMD-C2D-C1D	6.70	136.51	124.71
20	8	608	CLA	CMD-C2D-C1D	6.69	136.51	124.71
20	3	602	CLA	CMD-C2D-C1D	6.69	136.50	124.71
20	7	620	CLA	CMD-C2D-C1D	6.69	136.50	124.71
20	7	608	CLA	CMD-C2D-C1D	6.68	136.49	124.71
20	K	4002	CLA	CMD-C2D-C1D	6.67	136.48	124.71
20	5	606	CLA	CMD-C2D-C1D	6.67	136.47	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	839	CLA	CMD-C2D-C1D	6.66	136.46	124.71
20	B	819	CLA	CMD-C2D-C1D	6.66	136.46	124.71
20	3	609	CLA	CMD-C2D-C1D	6.66	136.46	124.71
20	6	622	CLA	CMD-C2D-C1D	6.66	136.46	124.71
20	B	840	CLA	C2C-C1C-NC	6.66	116.21	109.97
20	5	614	CLA	CMD-C2D-C1D	6.66	136.44	124.71
20	8	608	CLA	CHD-C4C-C3C	-6.66	115.06	124.84
20	5	613	CLA	CMD-C2D-C1D	6.64	136.42	124.71
20	6	604	CLA	CMD-C2D-C1D	6.64	136.41	124.71
20	5	609	CLA	CMD-C2D-C1D	6.63	136.40	124.71
20	K	4003	CLA	CMD-C2D-C1D	6.63	136.40	124.71
20	B	841	CLA	O2D-CGD-CBD	6.63	123.04	111.27
27	6	618	CHL	C1D-ND-C4D	-6.62	101.63	106.33
20	B	813	CLA	CMD-C2D-C1D	6.62	136.38	124.71
20	5	603	CLA	CMD-C2D-C1D	6.62	136.38	124.71
20	A	807	CLA	CMD-C2D-C1D	6.62	136.38	124.71
20	A	813	CLA	CMD-C2D-C1D	6.62	136.37	124.71
20	6	610	CLA	CMD-C2D-C1D	6.61	136.37	124.71
20	B	836	CLA	CMD-C2D-C1D	6.61	136.36	124.71
20	7	602	CLA	CMD-C2D-C1D	6.60	136.35	124.71
20	A	818	CLA	CMD-C2D-C1D	6.60	136.35	124.71
20	B	818	CLA	CMD-C2D-C1D	6.60	136.34	124.71
20	Z	606	CLA	CMD-C2D-C1D	6.59	136.33	124.71
20	B	824	CLA	CMD-C2D-C1D	6.59	136.33	124.71
20	3	604	CLA	CMD-C2D-C1D	6.59	136.33	124.71
20	3	617	CLA	CMD-C2D-C1D	6.59	136.33	124.71
20	A	809	CLA	CMD-C2D-C1D	6.59	136.32	124.71
20	B	807	CLA	CMD-C2D-C1D	6.58	136.31	124.71
27	8	607	CHL	C1D-ND-C4D	-6.58	101.66	106.33
20	A	816	CLA	CMD-C2D-C1D	6.57	136.30	124.71
20	B	804	CLA	O2D-CGD-CBD	6.57	122.94	111.27
20	7	611	CLA	CMD-C2D-C1D	6.56	136.28	124.71
20	B	837	CLA	O2D-CGD-CBD	6.56	122.93	111.27
19	A	801	CL0	C2C-C1C-NC	6.56	116.12	109.97
27	8	607	CHL	CMD-C2D-C1D	6.56	136.28	124.71
20	A	804	CLA	C2D-C1D-ND	6.56	114.94	110.10
20	Z	602	CLA	CMD-C2D-C1D	6.55	136.26	124.71
20	A	812	CLA	CHD-C1D-ND	-6.55	118.44	124.45
20	B	837	CLA	CMD-C2D-C1D	6.55	136.25	124.71
20	6	601	CLA	CMD-C2D-C1D	6.54	136.25	124.71
20	6	612	CLA	C4A-NA-C1A	-6.54	103.77	106.71
20	8	606	CLA	CMD-C2D-C1D	6.54	136.24	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	4	607	CHL	C1D-ND-C4D	-6.53	101.69	106.33
20	F	303	CLA	CMD-C2D-C1D	6.53	136.22	124.71
20	A	831	CLA	C2C-C1C-NC	6.53	116.09	109.97
20	B	803	CLA	CHD-C1D-ND	-6.53	118.46	124.45
20	A	815	CLA	CHD-C1D-ND	-6.52	118.46	124.45
20	A	820	CLA	CMD-C2D-C1D	6.52	136.20	124.71
20	8	611	CLA	CMD-C2D-C1D	6.52	136.20	124.71
20	8	604	CLA	CMD-C2D-C1D	6.51	136.19	124.71
20	1	602	CLA	CMD-C2D-C1D	6.51	136.19	124.71
20	B	826	CLA	O2D-CGD-CBD	6.51	122.83	111.27
20	B	821	CLA	CMD-C2D-C1D	6.50	136.18	124.71
20	A	803	CLA	CMD-C2D-C1D	6.50	136.17	124.71
20	7	612	CLA	C4A-NA-C1A	-6.50	103.78	106.71
20	A	805	CLA	CMD-C2D-C1D	6.50	136.17	124.71
20	K	4002	CLA	O2D-CGD-CBD	6.50	122.81	111.27
20	3	611	CLA	CMD-C2D-C1D	6.49	136.15	124.71
20	B	833	CLA	CMD-C2D-C1D	6.49	136.15	124.71
23	5	625	BCR	C11-C10-C9	-6.48	118.06	127.31
20	1	603	CLA	CMD-C2D-C1D	6.48	136.13	124.71
20	6	617	CLA	CMD-C2D-C1D	6.48	136.13	124.71
20	5	612	CLA	CMD-C2D-C1D	6.48	136.13	124.71
20	4	601	CLA	CMD-C2D-C1D	6.45	136.09	124.71
20	A	823	CLA	CMD-C2D-C1D	6.45	136.08	124.71
20	A	803	CLA	CHD-C1D-ND	-6.45	118.53	124.45
20	A	822	CLA	CMD-C2D-C1D	6.44	136.07	124.71
27	6	606	CHL	C1D-ND-C4D	-6.44	101.76	106.33
20	A	806	CLA	CMD-C2D-C1D	6.44	136.06	124.71
27	5	618	CHL	C1D-ND-C4D	-6.43	101.77	106.33
20	7	614	CLA	CMD-C2D-C1D	6.43	136.04	124.71
20	3	612	CLA	CMD-C2D-C1D	6.43	136.04	124.71
20	B	829	CLA	CHD-C1D-ND	-6.41	118.56	124.45
20	B	802	CLA	CHD-C4C-C3C	-6.41	115.42	124.84
20	Z	616	CLA	CMD-C2D-C1D	6.40	136.00	124.71
20	6	613	CLA	CMD-C2D-C1D	6.40	135.99	124.71
20	A	817	CLA	CHD-C1D-ND	-6.40	118.58	124.45
20	7	604	CLA	CHD-C4C-C3C	-6.40	115.44	124.84
20	Z	612	CLA	CMD-C2D-C1D	6.39	135.98	124.71
20	B	816	CLA	CHD-C4C-C3C	-6.39	115.44	124.84
23	5	625	BCR	C15-C14-C13	-6.38	118.20	127.31
20	1	614	CLA	CMD-C2D-C1D	6.38	135.95	124.71
20	4	603	CLA	C2C-C1C-NC	6.37	115.94	109.97
20	A	818	CLA	CHD-C1D-ND	-6.37	118.60	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	829	CLA	CHD-C4C-C3C	-6.37	115.48	124.84
19	A	801	CL0	CHD-C4C-C3C	-6.37	115.48	124.84
20	A	808	CLA	CHD-C1D-ND	-6.36	118.61	124.45
20	5	617	CLA	CMD-C2D-C1D	6.36	135.92	124.71
20	B	833	CLA	O2D-CGD-CBD	6.36	122.57	111.27
20	4	612	CLA	CMD-C2D-C1D	6.36	135.92	124.71
20	A	827	CLA	CHD-C1D-ND	-6.36	118.61	124.45
20	1	611	CLA	CMD-C2D-C1D	6.35	135.91	124.71
27	6	608	CHL	C1D-ND-C4D	-6.35	101.82	106.33
20	7	603	CLA	CHD-C1D-ND	-6.35	118.62	124.45
20	B	815	CLA	O2D-CGD-CBD	6.35	122.56	111.27
20	4	603	CLA	C4A-NA-C1A	-6.35	103.85	106.71
20	Z	614	CLA	CHD-C1D-ND	-6.35	118.62	124.45
20	4	613	CLA	CMD-C2D-C1D	6.34	135.89	124.71
20	A	839	CLA	O2D-CGD-CBD	6.34	122.53	111.27
20	6	616	CLA	CHD-C1D-ND	-6.34	118.63	124.45
20	3	612	CLA	C4A-NA-C1A	-6.34	103.86	106.71
27	6	607	CHL	C1D-ND-C4D	-6.33	101.84	106.33
20	L	203	CLA	CHD-C1D-ND	-6.33	118.63	124.45
20	A	854	CLA	CHD-C4C-C3C	-6.33	115.54	124.84
20	B	836	CLA	C4A-NA-C1A	-6.33	103.86	106.71
20	1	604	CLA	CHD-C1D-ND	-6.33	118.64	124.45
20	A	854	CLA	O2D-CGD-CBD	6.32	122.50	111.27
20	L	203	CLA	CMD-C2D-C1D	6.32	135.85	124.71
20	B	830	CLA	CMD-C2D-C1D	6.32	135.85	124.71
20	1	609	CLA	CHD-C1D-ND	-6.32	118.65	124.45
20	B	814	CLA	CMD-C2D-C1D	6.31	135.83	124.71
27	4	608	CHL	C1D-ND-C4D	-6.31	101.85	106.33
20	B	808	CLA	CMD-C2D-C1D	6.30	135.82	124.71
27	1	601	CHL	C1D-ND-C4D	-6.30	101.86	106.33
20	6	609	CLA	CMD-C2D-C1D	6.30	135.82	124.71
20	B	838	CLA	CMD-C2D-C1D	6.30	135.82	124.71
20	8	612	CLA	CMD-C2D-C1D	6.30	135.81	124.71
27	6	607	CHL	C2C-C3C-C4C	-6.29	102.00	106.49
23	A	852	BCR	C20-C21-C22	-6.29	118.34	127.31
20	B	831	CLA	CHD-C1D-ND	-6.27	118.69	124.45
20	5	621	CLA	CMD-C2D-C1D	6.27	135.77	124.71
20	4	604	CLA	CHD-C1D-ND	-6.27	118.70	124.45
20	B	810	CLA	CHD-C1D-ND	-6.26	118.70	124.45
20	8	602	CLA	CMD-C2D-C1D	6.26	135.75	124.71
20	7	602	CLA	CHD-C1D-ND	-6.26	118.70	124.45
20	L	204	CLA	CHD-C1D-ND	-6.26	118.70	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	841	CLA	CMD-C2D-C1D	6.25	135.73	124.71
20	Z	610	CLA	CHD-C4C-C3C	-6.25	115.65	124.84
20	A	821	CLA	CMD-C2D-C1D	6.25	135.73	124.71
20	B	827	CLA	CMD-C2D-C1D	6.25	135.73	124.71
20	A	841	CLA	CHD-C1D-ND	-6.25	118.71	124.45
20	6	601	CLA	CHD-C1D-ND	-6.24	118.72	124.45
20	4	603	CLA	CMD-C2D-C1D	6.24	135.72	124.71
20	B	835	CLA	CMD-C2D-C1D	6.24	135.72	124.71
20	B	809	CLA	CMD-C2D-C1D	6.24	135.71	124.71
20	1	613	CLA	CMD-C2D-C1D	6.23	135.69	124.71
20	B	821	CLA	CHD-C1D-ND	-6.23	118.73	124.45
20	7	616	CLA	CMD-C2D-C1D	6.22	135.68	124.71
20	A	828	CLA	O2D-CGD-CBD	6.22	122.33	111.27
20	K	4003	CLA	CHD-C1D-ND	-6.22	118.73	124.45
20	A	835	CLA	CHD-C1D-ND	-6.22	118.74	124.45
20	1	616	CLA	CMD-C2D-C1D	6.22	135.67	124.71
27	8	607	CHL	C2C-C3C-C4C	-6.21	102.06	106.49
20	A	839	CLA	CHD-C1D-ND	-6.21	118.74	124.45
20	Z	609	CLA	CHD-C1D-ND	-6.21	118.75	124.45
20	4	609	CLA	CMD-C2D-C1D	6.21	135.66	124.71
20	Z	613	CLA	CMD-C2D-C1D	6.21	135.66	124.71
27	4	618	CHL	C1D-ND-C4D	-6.21	101.92	106.33
20	6	612	CLA	CMD-C2D-C1D	6.20	135.65	124.71
23	5	625	BCR	C7-C8-C9	-6.20	116.87	126.23
20	7	610	CLA	CHD-C4C-C3C	-6.19	115.74	124.84
20	4	609	CLA	CHD-C1D-ND	-6.19	118.77	124.45
27	3	608	CHL	C1D-ND-C4D	-6.19	101.94	106.33
20	3	607	CLA	CMD-C2D-C1D	6.18	135.61	124.71
20	A	838	CLA	C2C-C1C-NC	6.18	115.76	109.97
20	A	818	CLA	CHD-C4C-C3C	-6.18	115.75	124.84
20	A	831	CLA	O2D-CGD-CBD	6.18	122.25	111.27
20	4	612	CLA	C4A-NA-C1A	-6.17	103.93	106.71
20	A	817	CLA	C2C-C1C-NC	6.17	115.75	109.97
20	B	837	CLA	CHD-C1D-ND	-6.16	118.79	124.45
20	6	610	CLA	CHD-C1D-ND	-6.16	118.79	124.45
20	4	610	CLA	CMD-C2D-C1D	6.16	135.57	124.71
20	B	815	CLA	CHD-C1D-ND	-6.16	118.80	124.45
27	4	608	CHL	CHD-C4C-C3C	-6.16	115.79	124.84
20	Z	604	CLA	CHD-C1D-ND	-6.16	118.80	124.45
20	5	602	CLA	CHD-C1D-ND	-6.16	118.80	124.45
20	3	603	CLA	CMD-C2D-C1D	6.15	135.56	124.71
20	1	614	CLA	CHD-C1D-ND	-6.15	118.80	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	7	610	CLA	CHD-C1D-ND	-6.15	118.80	124.45
20	B	824	CLA	O2D-CGD-CBD	6.15	122.19	111.27
20	A	809	CLA	CHD-C1D-ND	-6.14	118.81	124.45
20	A	814	CLA	CHD-C1D-ND	-6.14	118.81	124.45
20	A	825	CLA	CMD-C2D-C1D	6.14	135.53	124.71
20	B	807	CLA	CHD-C1D-ND	-6.14	118.82	124.45
20	1	606	CLA	CHD-C4C-C3C	-6.13	115.83	124.84
20	B	840	CLA	CHD-C1D-ND	-6.13	118.82	124.45
20	4	609	CLA	C2C-C1C-NC	6.13	115.71	109.97
20	A	826	CLA	CHD-C4C-C3C	-6.13	115.83	124.84
20	7	608	CLA	CHD-C4C-C3C	-6.12	115.84	124.84
20	B	817	CLA	CHD-C1D-ND	-6.12	118.83	124.45
20	7	613	CLA	CMD-C2D-C1D	6.12	135.50	124.71
20	4	602	CLA	CHD-C1D-ND	-6.12	118.83	124.45
20	3	614	CLA	CHD-C1D-ND	-6.12	118.83	124.45
20	B	808	CLA	O2D-CGD-CBD	6.12	122.14	111.27
20	B	804	CLA	CHD-C4C-C3C	-6.11	115.86	124.84
20	5	609	CLA	CHD-C1D-ND	-6.11	118.84	124.45
20	A	814	CLA	CHD-C4C-C3C	-6.11	115.87	124.84
20	B	832	CLA	CHD-C1D-ND	-6.10	118.84	124.45
20	A	833	CLA	CHD-C4C-C3C	-6.10	115.87	124.84
20	A	834	CLA	CHD-C1D-ND	-6.10	118.84	124.45
27	6	618	CHL	CMD-C2D-C1D	6.10	135.47	124.71
20	A	818	CLA	O2D-CGD-CBD	6.10	122.11	111.27
27	6	608	CHL	C1C-C2C-C3C	-6.10	102.27	107.11
20	B	805	CLA	CHD-C1D-ND	-6.10	118.85	124.45
20	6	612	CLA	CHD-C4C-C3C	-6.09	115.89	124.84
20	A	840	CLA	O2D-CGD-CBD	6.09	122.09	111.27
20	Z	611	CLA	CMD-C2D-C1D	6.09	135.45	124.71
20	F	301	CLA	CHD-C4C-C3C	-6.09	115.89	124.84
20	3	604	CLA	CHD-C1D-ND	-6.09	118.86	124.45
27	1	601	CHL	O2D-CGD-CBD	6.08	122.08	111.27
20	7	612	CLA	CHD-C1D-ND	-6.08	118.86	124.45
27	6	608	CHL	CHD-C4C-C3C	-6.08	115.91	124.84
23	6	625	BCR	C15-C14-C13	-6.08	118.64	127.31
20	5	604	CLA	C2C-C1C-NC	6.07	115.66	109.97
20	A	830	CLA	CHD-C4C-C3C	-6.07	115.92	124.84
20	8	610	CLA	CHD-C4C-C3C	-6.07	115.92	124.84
20	B	818	CLA	C2C-C1C-NC	6.07	115.66	109.97
20	6	611	CLA	CMD-C2D-C1D	6.06	135.40	124.71
20	A	809	CLA	O2D-CGD-CBD	6.06	122.04	111.27
20	8	603	CLA	C4A-NA-C1A	-6.06	103.98	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	829	CLA	CMD-C2D-C1D	6.06	135.39	124.71
20	A	837	CLA	CHD-C1D-ND	-6.06	118.89	124.45
20	F	304	CLA	CHD-C4C-C3C	-6.06	115.93	124.84
20	7	603	CLA	C4A-NA-C1A	-6.06	103.98	106.71
20	3	613	CLA	C2C-C1C-NC	6.06	115.65	109.97
20	B	832	CLA	CHD-C4C-C3C	-6.05	115.94	124.84
20	4	611	CLA	CMD-C2D-C1D	6.05	135.38	124.71
20	8	604	CLA	CHD-C1D-ND	-6.05	118.90	124.45
20	B	807	CLA	C2C-C1C-NC	6.05	115.64	109.97
20	5	616	CLA	C2C-C1C-NC	6.04	115.64	109.97
20	A	840	CLA	CHD-C4C-C3C	-6.04	115.96	124.84
20	A	823	CLA	CHD-C1D-ND	-6.04	118.90	124.45
20	3	610	CLA	CHD-C4C-C3C	-6.04	115.97	124.84
20	1	602	CLA	CHD-C4C-C3C	-6.04	115.97	124.84
20	A	838	CLA	C4A-NA-C1A	-6.03	103.99	106.71
20	1	612	CLA	CMD-C2D-C1D	6.03	135.34	124.71
20	5	611	CLA	CMD-C2D-C1D	6.03	135.34	124.71
20	A	803	CLA	C2C-C1C-NC	6.03	115.62	109.97
20	6	609	CLA	C2C-C1C-NC	6.03	115.62	109.97
27	3	608	CHL	CHD-C4C-C3C	-6.03	115.98	124.84
20	B	841	CLA	CMD-C2D-C1D	6.02	135.33	124.71
20	B	809	CLA	C2C-C1C-NC	6.02	115.61	109.97
27	Z	607	CHL	C1D-ND-C4D	-6.02	102.06	106.33
20	G	203	CLA	CHD-C1D-ND	-6.02	118.92	124.45
20	5	610	CLA	CHD-C1D-ND	-6.02	118.92	124.45
20	Z	603	CLA	C2C-C1C-NC	6.02	115.61	109.97
27	1	601	CHL	C2C-C3C-C4C	-6.02	102.20	106.49
20	3	606	CLA	CHD-C1D-ND	-6.01	118.93	124.45
20	8	603	CLA	CHD-C1D-ND	-6.01	118.93	124.45
20	A	835	CLA	O2D-CGD-CBD	6.01	121.95	111.27
20	A	805	CLA	CHD-C4C-C3C	-6.01	116.01	124.84
20	7	620	CLA	CHD-C1D-ND	-6.01	118.93	124.45
20	1	612	CLA	C2C-C1C-NC	6.01	115.60	109.97
20	B	817	CLA	C2C-C1C-NC	6.01	115.60	109.97
20	B	836	CLA	CHD-C4C-C3C	-6.00	116.01	124.84
20	5	602	CLA	CHD-C4C-C3C	-6.00	116.02	124.84
20	B	805	CLA	CHD-C4C-C3C	-6.00	116.02	124.84
27	4	606	CHL	C1D-ND-C4D	-6.00	102.07	106.33
20	7	602	CLA	CHD-C4C-C3C	-6.00	116.02	124.84
20	B	826	CLA	CHD-C4C-C3C	-6.00	116.02	124.84
20	7	606	CLA	CHD-C4C-C3C	-6.00	116.02	124.84
20	B	811	CLA	C1B-C2B-C3B	-6.00	101.34	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	7	601	CLA	CHD-C4C-C3C	-5.99	116.03	124.84
27	5	607	CHL	C2C-C3C-C4C	-5.99	102.22	106.49
20	A	805	CLA	CHD-C1D-ND	-5.99	118.95	124.45
20	4	614	CLA	CHD-C4C-C3C	-5.99	116.04	124.84
20	A	811	CLA	CHD-C4C-C3C	-5.99	116.04	124.84
20	B	814	CLA	CHD-C4C-C3C	-5.99	116.04	124.84
20	1	610	CLA	CHD-C4C-C3C	-5.99	116.04	124.84
20	A	825	CLA	CHD-C1D-ND	-5.98	118.95	124.45
20	7	611	CLA	CAA-C2A-C3A	-5.98	102.14	116.10
20	7	613	CLA	C2C-C1C-NC	5.98	115.58	109.97
20	B	811	CLA	CHD-C1D-ND	-5.98	118.96	124.45
20	A	816	CLA	CHD-C1D-ND	-5.98	118.96	124.45
20	B	806	CLA	CHD-C4C-C3C	-5.97	116.06	124.84
20	A	836	CLA	CMD-C2D-C1D	5.96	135.22	124.71
20	8	612	CLA	CHD-C4C-C3C	-5.96	116.07	124.84
20	A	822	CLA	CHD-C1D-ND	-5.96	118.97	124.45
20	3	612	CLA	C2C-C1C-NC	5.96	115.56	109.97
20	Z	602	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
20	3	620	CLA	CHD-C1D-ND	-5.96	118.98	124.45
20	A	819	CLA	CHD-C4C-C3C	-5.96	116.09	124.84
20	A	841	CLA	CHD-C4C-C3C	-5.96	116.09	124.84
20	4	616	CLA	CHD-C1D-ND	-5.96	118.98	124.45
20	A	832	CLA	C2C-C1C-NC	5.96	115.55	109.97
27	Z	601	CHL	C2C-C3C-C4C	-5.95	102.25	106.49
20	8	616	CLA	CHD-C4C-C3C	-5.95	116.09	124.84
20	G	204	CLA	CHD-C1D-ND	-5.95	118.98	124.45
20	8	609	CLA	CMD-C2D-C1D	5.95	135.21	124.71
20	B	802	CLA	CMD-C2D-C1D	5.95	135.20	124.71
20	B	813	CLA	CHD-C1D-ND	-5.94	118.99	124.45
20	5	601	CLA	CMD-C2D-C1D	5.94	135.19	124.71
20	B	814	CLA	CHD-C1D-ND	-5.94	118.99	124.45
20	5	617	CLA	CHD-C1D-ND	-5.94	119.00	124.45
20	J	3002	CLA	CHD-C1D-ND	-5.94	119.00	124.45
20	8	614	CLA	CHD-C1D-ND	-5.93	119.00	124.45
20	A	835	CLA	C2C-C1C-NC	5.93	115.53	109.97
20	8	610	CLA	CHD-C1D-ND	-5.93	119.01	124.45
20	4	601	CLA	CHD-C1D-ND	-5.92	119.01	124.45
20	A	827	CLA	CHD-C4C-C3C	-5.92	116.13	124.84
20	4	616	CLA	CHD-C4C-C3C	-5.92	116.13	124.84
20	6	609	CLA	CHD-C1D-ND	-5.92	119.02	124.45
27	Z	601	CHL	CMD-C2D-C1D	5.92	135.14	124.71
20	6	601	CLA	O2D-CGD-CBD	5.92	121.78	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	836	CLA	C2C-C1C-NC	5.91	115.51	109.97
20	A	806	CLA	CHD-C1D-ND	-5.91	119.02	124.45
20	8	601	CLA	C2C-C1C-NC	5.91	115.51	109.97
20	8	603	CLA	CHD-C4C-C3C	-5.91	116.15	124.84
20	A	845	CLA	CHD-C1D-ND	-5.91	119.02	124.45
20	B	816	CLA	CHD-C1D-ND	-5.91	119.02	124.45
20	1	612	CLA	CHD-C4C-C3C	-5.91	116.16	124.84
20	7	614	CLA	CHD-C1D-ND	-5.91	119.03	124.45
20	A	810	CLA	CHD-C4C-C3C	-5.91	116.16	124.84
20	B	841	CLA	CHD-C4C-C3C	-5.91	116.16	124.84
20	B	834	CLA	CHD-C1D-ND	-5.91	119.03	124.45
20	3	607	CLA	CHD-C1D-ND	-5.91	119.03	124.45
20	3	602	CLA	CHD-C1D-ND	-5.90	119.03	124.45
20	7	609	CLA	CMD-C2D-C1D	5.90	135.12	124.71
20	A	821	CLA	C2C-C1C-NC	5.90	115.50	109.97
20	A	833	CLA	CHD-C1D-ND	-5.90	119.03	124.45
20	8	614	CLA	CMD-C2D-C1D	5.90	135.11	124.71
20	5	614	CLA	CHD-C1D-ND	-5.90	119.03	124.45
20	A	807	CLA	C4A-NA-C1A	-5.90	104.06	106.71
20	A	820	CLA	C4A-NA-C1A	-5.90	104.06	106.71
20	3	603	CLA	C2C-C1C-NC	5.90	115.50	109.97
20	3	610	CLA	CHD-C1D-ND	-5.89	119.04	124.45
27	4	607	CHL	C1C-C2C-C3C	-5.89	102.44	107.11
20	7	601	CLA	CHD-C1D-ND	-5.89	119.04	124.45
20	4	610	CLA	CHD-C1D-ND	-5.89	119.04	124.45
20	A	824	CLA	C2C-C1C-NC	5.89	115.49	109.97
20	G	203	CLA	C4A-NA-C1A	-5.89	104.06	106.71
20	B	837	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
20	7	609	CLA	CHD-C1D-ND	-5.88	119.05	124.45
20	1	602	CLA	CHD-C1D-ND	-5.88	119.05	124.45
20	B	808	CLA	CHD-C4C-C3C	-5.88	116.19	124.84
20	6	602	CLA	CHD-C4C-C3C	-5.88	116.20	124.84
20	5	617	CLA	C2C-C1C-NC	5.88	115.48	109.97
20	8	611	CLA	C2C-C1C-NC	5.88	115.48	109.97
20	A	804	CLA	C4A-NA-C1A	-5.87	104.06	106.71
20	F	303	CLA	CHD-C4C-C3C	-5.87	116.21	124.84
20	6	622	CLA	CHD-C1D-ND	-5.87	119.06	124.45
20	A	811	CLA	CMD-C2D-C1D	5.86	135.05	124.71
20	1	603	CLA	CHD-C1D-ND	-5.86	119.06	124.45
20	B	840	CLA	CHD-C4C-C3C	-5.86	116.22	124.84
20	3	612	CLA	CHD-C1D-ND	-5.86	119.07	124.45
20	A	842	CLA	CHD-C4C-C3C	-5.86	116.23	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	818	CLA	CHD-C1D-ND	-5.86	119.07	124.45
20	B	805	CLA	O2D-CGD-CBD	5.86	121.68	111.27
20	6	602	CLA	CHD-C1D-ND	-5.85	119.07	124.45
20	4	601	CLA	O2D-CGD-CBD	5.85	121.67	111.27
20	B	830	CLA	CHD-C4C-C3C	-5.85	116.24	124.84
20	3	617	CLA	CHD-C1D-ND	-5.85	119.08	124.45
20	6	603	CLA	C2C-C1C-NC	5.85	115.45	109.97
19	A	801	CL0	CMD-C2D-C1D	5.84	135.01	124.71
20	8	613	CLA	CMD-C2D-C1D	5.84	135.01	124.71
20	A	842	CLA	CHD-C1D-ND	-5.84	119.09	124.45
20	Z	612	CLA	CHD-C1D-ND	-5.84	119.09	124.45
20	B	830	CLA	CHD-C1D-ND	-5.83	119.09	124.45
20	K	4003	CLA	C2C-C1C-NC	5.83	115.43	109.97
20	B	826	CLA	CHD-C1D-ND	-5.83	119.10	124.45
20	B	824	CLA	CHD-C4C-C3C	-5.83	116.28	124.84
20	B	820	CLA	CHD-C1D-ND	-5.82	119.10	124.45
20	A	820	CLA	CHD-C4C-C3C	-5.82	116.28	124.84
20	3	609	CLA	CHD-C1D-ND	-5.82	119.11	124.45
20	7	608	CLA	CHD-C1D-ND	-5.82	119.11	124.45
20	4	612	CLA	CHD-C4C-C3C	-5.82	116.29	124.84
20	1	603	CLA	C2C-C1C-NC	5.82	115.42	109.97
20	B	811	CLA	C2C-C1C-NC	5.81	115.42	109.97
20	B	812	CLA	CHD-C4C-C3C	-5.81	116.30	124.84
20	B	819	CLA	CHD-C1D-ND	-5.81	119.11	124.45
20	A	843	CLA	CHD-C4C-C3C	-5.81	116.30	124.84
20	A	807	CLA	C2C-C1C-NC	5.81	115.42	109.97
20	Z	606	CLA	CHD-C4C-C3C	-5.81	116.30	124.84
20	B	804	CLA	CHD-C1D-ND	-5.81	119.11	124.45
27	5	607	CHL	C1D-ND-C4D	-5.81	102.21	106.33
20	B	827	CLA	C2C-C1C-NC	5.80	115.41	109.97
20	A	807	CLA	CHD-C1D-ND	-5.80	119.12	124.45
20	A	838	CLA	CHD-C1D-ND	-5.80	119.12	124.45
20	Z	603	CLA	CHD-C1D-ND	-5.80	119.12	124.45
20	5	606	CLA	CHD-C1D-ND	-5.80	119.12	124.45
20	A	832	CLA	CMD-C2D-C1D	5.80	134.94	124.71
20	A	816	CLA	CHD-C4C-C3C	-5.80	116.31	124.84
20	B	828	CLA	C2C-C1C-NC	5.80	115.41	109.97
20	B	822	CLA	CHD-C1D-ND	-5.80	119.13	124.45
20	A	826	CLA	CMD-C2D-C1D	5.80	134.93	124.71
20	B	827	CLA	CHD-C4C-C3C	-5.79	116.32	124.84
20	B	838	CLA	CHD-C1D-ND	-5.79	119.13	124.45
20	1	610	CLA	CMD-C2D-C1D	5.79	134.91	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	803	CLA	CHD-C4C-C3C	-5.79	116.33	124.84
20	A	824	CLA	CHD-C1D-ND	-5.79	119.14	124.45
20	K	4002	CLA	CHD-C1D-ND	-5.78	119.14	124.45
20	B	833	CLA	CHD-C1D-ND	-5.78	119.14	124.45
20	6	603	CLA	CHD-C1D-ND	-5.78	119.14	124.45
20	B	825	CLA	C4A-NA-C1A	-5.78	104.11	106.71
20	7	609	CLA	O2D-CGD-CBD	5.78	121.53	111.27
20	A	806	CLA	O2D-CGD-CBD	5.77	121.53	111.27
20	B	802	CLA	C2C-C1C-NC	5.77	115.38	109.97
20	A	843	CLA	CMD-C2D-C1D	5.77	134.89	124.71
20	7	612	CLA	C2C-C1C-NC	5.77	115.38	109.97
20	A	820	CLA	CHD-C1D-ND	-5.77	119.15	124.45
20	B	808	CLA	C2C-C1C-NC	5.77	115.38	109.97
20	8	602	CLA	CHD-C1D-ND	-5.77	119.15	124.45
20	B	822	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
20	B	820	CLA	O2D-CGD-CBD	5.77	121.52	111.27
20	F	301	CLA	CHD-C1D-ND	-5.77	119.16	124.45
20	3	604	CLA	C2C-C1C-NC	5.76	115.37	109.97
20	F	303	CLA	CHD-C1D-ND	-5.76	119.16	124.45
20	6	613	CLA	CHD-C1D-ND	-5.76	119.16	124.45
20	A	840	CLA	CHD-C1D-ND	-5.76	119.16	124.45
20	8	613	CLA	CHD-C4C-C3C	-5.76	116.38	124.84
20	F	304	CLA	CHD-C1D-ND	-5.76	119.16	124.45
20	1	606	CLA	CHD-C1D-ND	-5.76	119.16	124.45
27	5	608	CHL	C1D-ND-C4D	-5.76	102.25	106.33
20	5	613	CLA	C2C-C1C-NC	5.76	115.36	109.97
20	1	612	CLA	C4A-NA-C1A	-5.75	104.12	106.71
20	7	606	CLA	O2D-CGD-CBD	5.75	121.49	111.27
20	5	604	CLA	CHD-C1D-ND	-5.75	119.17	124.45
20	5	611	CLA	CHD-C4C-C3C	-5.75	116.39	124.84
20	8	601	CLA	O2D-CGD-CBD	5.75	121.48	111.27
20	Z	616	CLA	C2C-C1C-NC	5.74	115.35	109.97
20	6	604	CLA	CHD-C1D-ND	-5.74	119.18	124.45
20	Z	603	CLA	C4A-NA-C1A	-5.74	104.12	106.71
20	B	839	CLA	CHD-C4C-C3C	-5.74	116.41	124.84
20	8	614	CLA	CHD-C4C-C3C	-5.74	116.41	124.84
20	1	608	CLA	CHD-C1D-ND	-5.73	119.19	124.45
20	3	620	CLA	C2C-C1C-NC	5.73	115.34	109.97
20	5	601	CLA	CHD-C1D-ND	-5.72	119.20	124.45
20	8	608	CLA	CHD-C1D-ND	-5.72	119.20	124.45
20	1	616	CLA	C2C-C1C-NC	5.72	115.33	109.97
20	8	606	CLA	C2C-C1C-NC	5.72	115.33	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Z	606	CLA	CHD-C1D-ND	-5.72	119.20	124.45
20	B	830	CLA	O2D-CGD-CBD	5.71	121.42	111.27
20	B	813	CLA	CHD-C4C-C3C	-5.71	116.44	124.84
20	1	608	CLA	CHD-C4C-C3C	-5.71	116.44	124.84
20	Z	614	CLA	CHD-C4C-C3C	-5.71	116.44	124.84
20	A	804	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
27	4	608	CHL	C3D-C2D-C1D	-5.71	98.04	105.83
20	5	612	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
20	5	603	CLA	CHD-C1D-ND	-5.70	119.21	124.45
20	8	609	CLA	CHD-C1D-ND	-5.70	119.21	124.45
20	A	825	CLA	C2C-C1C-NC	5.70	115.31	109.97
20	5	614	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
20	3	610	CLA	C4A-NA-C1A	-5.70	104.14	106.71
20	1	614	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
20	4	613	CLA	C2C-C1C-NC	5.70	115.31	109.97
20	A	814	CLA	O2D-CGD-CBD	5.70	121.39	111.27
20	1	611	CLA	CHD-C1D-ND	-5.70	119.22	124.45
20	4	612	CLA	CHD-C1D-ND	-5.70	119.22	124.45
20	Z	610	CLA	CMD-C2D-C1D	5.70	134.75	124.71
20	7	613	CLA	CHD-C4C-C3C	-5.69	116.47	124.84
20	A	808	CLA	CHD-C4C-C3C	-5.69	116.48	124.84
20	8	616	CLA	CMD-C2D-C1D	5.69	134.74	124.71
20	A	810	CLA	CMD-C2D-C1D	5.69	134.74	124.71
20	B	806	CLA	C4A-NA-C1A	-5.69	104.15	106.71
20	B	815	CLA	C2C-C1C-NC	5.69	115.30	109.97
20	5	601	CLA	C2C-C1C-NC	5.68	115.29	109.97
27	1	601	CHL	CHD-C4C-C3C	-5.68	116.49	124.84
20	A	837	CLA	O2D-CGD-CBD	5.68	121.36	111.27
20	B	831	CLA	CHD-C4C-C3C	-5.67	116.50	124.84
27	4	606	CHL	C1C-C2C-C3C	-5.67	102.61	107.11
20	7	609	CLA	C2C-C1C-NC	5.67	115.29	109.97
20	6	604	CLA	CHD-C4C-C3C	-5.67	116.50	124.84
20	6	614	CLA	C4A-NA-C1A	-5.67	104.16	106.71
20	5	603	CLA	C2C-C1C-NC	5.67	115.28	109.97
20	B	828	CLA	CHD-C4C-C3C	-5.67	116.51	124.84
20	7	616	CLA	CHD-C4C-C3C	-5.67	116.51	124.84
20	A	813	CLA	CHD-C4C-C3C	-5.67	116.51	124.84
20	7	610	CLA	C4A-NA-C1A	-5.67	104.16	106.71
20	B	852	CLA	CHD-C4C-C3C	-5.66	116.52	124.84
20	5	610	CLA	CHD-C4C-C3C	-5.66	116.52	124.84
20	B	838	CLA	CHD-C4C-C3C	-5.66	116.52	124.84
20	A	839	CLA	C2C-C1C-NC	5.66	115.27	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Z	608	CLA	C2C-C1C-NC	5.66	115.27	109.97
20	7	603	CLA	O2D-CGD-CBD	5.65	121.32	111.27
20	1	611	CLA	C2C-C1C-NC	5.65	115.27	109.97
20	B	806	CLA	CHD-C1D-ND	-5.65	119.26	124.45
20	Z	613	CLA	CHD-C4C-C3C	-5.65	116.53	124.84
20	1	603	CLA	C4A-NA-C1A	-5.65	104.17	106.71
20	7	606	CLA	CHD-C1D-ND	-5.65	119.26	124.45
20	A	821	CLA	O2D-CGD-CBD	5.65	121.31	111.27
20	8	613	CLA	C2C-C1C-NC	5.65	115.27	109.97
20	G	204	CLA	O2D-CGD-CBD	5.65	121.31	111.27
20	A	845	CLA	C2C-C1C-NC	5.65	115.26	109.97
27	6	606	CHL	CHD-C4C-C3C	-5.65	116.54	124.84
20	A	819	CLA	CHD-C1D-ND	-5.65	119.26	124.45
20	B	852	CLA	CMD-C2D-C1D	5.65	134.67	124.71
20	5	609	CLA	C2C-C1C-NC	5.65	115.26	109.97
20	6	617	CLA	CHD-C1D-ND	-5.65	119.27	124.45
20	B	811	CLA	CHD-C4C-C3C	-5.65	116.54	124.84
20	8	606	CLA	CHD-C4C-C3C	-5.64	116.54	124.84
27	1	601	CHL	C3D-C2D-C1D	-5.64	98.13	105.83
20	B	812	CLA	CHD-C1D-ND	-5.64	119.27	124.45
20	7	603	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
20	A	808	CLA	C2C-C1C-NC	5.64	115.25	109.97
20	5	601	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
20	6	614	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
20	A	842	CLA	C2C-C1C-NC	5.64	115.25	109.97
20	8	601	CLA	CHD-C4C-C3C	-5.64	116.56	124.84
20	A	812	CLA	C2C-C1C-NC	5.64	115.25	109.97
20	4	612	CLA	C2C-C1C-NC	5.64	115.25	109.97
20	1	613	CLA	CHD-C4C-C3C	-5.64	116.56	124.84
20	7	612	CLA	CHD-C4C-C3C	-5.63	116.56	124.84
20	A	832	CLA	CHD-C4C-C3C	-5.63	116.56	124.84
20	7	614	CLA	CHD-C4C-C3C	-5.63	116.56	124.84
20	A	813	CLA	CHD-C1D-ND	-5.63	119.28	124.45
20	5	612	CLA	CHD-C1D-ND	-5.63	119.28	124.45
20	A	804	CLA	CHD-C1D-ND	-5.63	119.28	124.45
20	A	822	CLA	CHD-C4C-C3C	-5.63	116.56	124.84
20	B	836	CLA	O2D-CGD-CBD	5.63	121.27	111.27
20	4	611	CLA	C2C-C1C-NC	5.63	115.24	109.97
20	A	837	CLA	C2C-C1C-NC	5.62	115.24	109.97
20	B	835	CLA	CHD-C4C-C3C	-5.62	116.57	124.84
20	3	602	CLA	CHD-C4C-C3C	-5.62	116.57	124.84
20	Z	603	CLA	O2D-CGD-CBD	5.62	121.26	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	3	608	CHL	C3D-C2D-C1D	-5.62	98.16	105.83
20	8	606	CLA	CHD-C1D-ND	-5.62	119.29	124.45
20	3	607	CLA	C2C-C1C-NC	5.62	115.24	109.97
20	A	809	CLA	CHD-C4C-C3C	-5.62	116.58	124.84
20	B	810	CLA	C2C-C1C-NC	5.62	115.24	109.97
20	A	845	CLA	CHD-C4C-C3C	-5.62	116.58	124.84
20	7	611	CLA	CHD-C1D-ND	-5.62	119.29	124.45
20	5	616	CLA	CHD-C1D-ND	-5.62	119.29	124.45
20	A	834	CLA	C2C-C1C-NC	5.62	115.23	109.97
20	G	203	CLA	C2C-C1C-NC	5.61	115.22	109.97
20	A	839	CLA	CHD-C4C-C3C	-5.61	116.60	124.84
20	B	839	CLA	CHD-C1D-ND	-5.61	119.30	124.45
20	5	609	CLA	CHD-C4C-C3C	-5.61	116.60	124.84
20	B	825	CLA	CHD-C1D-ND	-5.60	119.30	124.45
20	A	840	CLA	C2C-C1C-NC	5.60	115.22	109.97
20	4	614	CLA	CMD-C2D-C1D	5.60	134.58	124.71
27	7	607	CHL	C1D-ND-C4D	-5.60	102.36	106.33
20	6	603	CLA	C4A-NA-C1A	-5.60	104.19	106.71
20	7	616	CLA	C2C-C1C-NC	5.60	115.22	109.97
20	Z	609	CLA	C2C-C1C-NC	5.60	115.22	109.97
20	5	612	CLA	C2C-C1C-NC	5.60	115.22	109.97
20	1	610	CLA	CHD-C1D-ND	-5.60	119.31	124.45
20	Z	608	CLA	CHD-C4C-C3C	-5.59	116.62	124.84
20	A	834	CLA	CHD-C4C-C3C	-5.59	116.62	124.84
20	Z	612	CLA	CHD-C4C-C3C	-5.59	116.62	124.84
20	A	829	CLA	C4A-NA-C1A	-5.59	104.19	106.71
20	B	825	CLA	CHD-C4C-C3C	-5.59	116.62	124.84
20	7	611	CLA	C2C-C1C-NC	5.59	115.21	109.97
20	7	620	CLA	CHD-C4C-C3C	-5.58	116.63	124.84
27	1	607	CHL	C4A-NA-C1A	-5.58	104.20	106.71
20	A	828	CLA	C3D-C2D-C1D	-5.58	98.21	105.83
20	7	604	CLA	CHD-C1D-ND	-5.58	119.32	124.45
20	5	601	CLA	O2D-CGD-CBD	5.58	121.18	111.27
27	1	607	CHL	C2C-C3C-C4C	-5.58	102.51	106.49
20	8	612	CLA	C2C-C1C-NC	5.58	115.20	109.97
20	A	824	CLA	CHD-C4C-C3C	-5.57	116.65	124.84
20	B	835	CLA	CHD-C1D-ND	-5.57	119.33	124.45
20	3	617	CLA	CHD-C4C-C3C	-5.57	116.65	124.84
20	B	823	CLA	CMD-C2D-C1D	5.57	134.53	124.71
20	6	613	CLA	CHD-C4C-C3C	-5.57	116.65	124.84
27	7	607	CHL	C2C-C3C-C4C	-5.57	102.52	106.49
20	B	820	CLA	C2C-C1C-NC	5.57	115.19	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	852	CLA	C2C-C1C-NC	5.57	115.19	109.97
20	8	616	CLA	C2C-C1C-NC	5.57	115.19	109.97
20	A	807	CLA	O2D-CGD-CBD	5.57	121.16	111.27
20	K	4002	CLA	CHD-C4C-C3C	-5.56	116.66	124.84
20	3	606	CLA	CHD-C4C-C3C	-5.56	116.67	124.84
20	3	611	CLA	CAA-C2A-C3A	-5.56	103.13	116.10
20	A	823	CLA	CHD-C4C-C3C	-5.56	116.67	124.84
20	7	609	CLA	CHD-C4C-C3C	-5.55	116.67	124.84
27	4	608	CHL	C1C-C2C-C3C	-5.55	102.70	107.11
20	4	616	CLA	CAA-C2A-C3A	-5.55	103.14	116.10
20	1	612	CLA	CHD-C1D-ND	-5.55	119.35	124.45
20	A	836	CLA	CHD-C1D-ND	-5.55	119.35	124.45
20	Z	602	CLA	CHD-C1D-ND	-5.55	119.35	124.45
20	A	805	CLA	C4A-NA-C1A	-5.55	104.21	106.71
20	B	818	CLA	CHD-C4C-C3C	-5.55	116.69	124.84
20	5	606	CLA	CHD-C4C-C3C	-5.55	116.69	124.84
20	3	603	CLA	CHD-C4C-C3C	-5.54	116.69	124.84
20	8	612	CLA	CHD-C1D-ND	-5.54	119.36	124.45
20	J	3002	CLA	CHD-C4C-C3C	-5.54	116.70	124.84
27	1	607	CHL	C1D-ND-C4D	-5.54	102.40	106.33
20	3	607	CLA	CHD-C4C-C3C	-5.54	116.70	124.84
20	B	811	CLA	C4A-NA-C1A	-5.54	104.22	106.71
20	6	617	CLA	CHD-C4C-C3C	-5.54	116.70	124.84
20	F	304	CLA	C2C-C1C-NC	5.54	115.16	109.97
20	3	611	CLA	CHD-C1D-ND	-5.54	119.37	124.45
20	1	616	CLA	CHD-C4C-C3C	-5.53	116.71	124.84
20	7	611	CLA	CHD-C4C-C3C	-5.53	116.71	124.84
20	8	609	CLA	CHD-C4C-C3C	-5.53	116.71	124.84
20	J	3002	CLA	C2C-C1C-NC	5.53	115.15	109.97
20	6	612	CLA	CHD-C1D-ND	-5.53	119.37	124.45
20	6	611	CLA	CHD-C4C-C3C	-5.53	116.71	124.84
20	Z	608	CLA	CHD-C1D-ND	-5.52	119.38	124.45
20	B	838	CLA	C2C-C1C-NC	5.52	115.14	109.97
20	5	606	CLA	C2C-C1C-NC	5.52	115.14	109.97
20	A	812	CLA	CHD-C4C-C3C	-5.52	116.73	124.84
20	3	617	CLA	C2C-C1C-NC	5.52	115.14	109.97
20	A	807	CLA	CHD-C4C-C3C	-5.52	116.73	124.84
20	G	204	CLA	CHD-C4C-C3C	-5.52	116.73	124.84
20	A	815	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
20	Z	611	CLA	C2C-C1C-NC	5.51	115.14	109.97
20	A	812	CLA	C4A-NA-C1A	-5.51	104.23	106.71
20	Z	611	CLA	CHD-C1D-ND	-5.51	119.39	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	5	602	CLA	C4A-NA-C1A	-5.51	104.23	106.71
20	8	611	CLA	CHD-C1D-ND	-5.50	119.40	124.45
20	7	603	CLA	C2C-C1C-NC	5.50	115.13	109.97
27	6	618	CHL	C1C-C2C-C3C	-5.50	102.75	107.11
20	Z	610	CLA	CHD-C1D-ND	-5.50	119.40	124.45
20	6	617	CLA	C2C-C1C-NC	5.50	115.12	109.97
20	F	301	CLA	C4A-NA-C1A	-5.50	104.23	106.71
20	B	820	CLA	CHD-C4C-C3C	-5.50	116.76	124.84
20	3	614	CLA	CHD-C4C-C3C	-5.50	116.76	124.84
20	1	613	CLA	CHD-C1D-ND	-5.50	119.40	124.45
20	B	833	CLA	CHD-C4C-C3C	-5.50	116.76	124.84
20	B	827	CLA	CHD-C1D-ND	-5.50	119.40	124.45
20	1	603	CLA	CHD-C4C-C3C	-5.49	116.76	124.84
20	B	823	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
20	3	609	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
20	3	611	CLA	C2C-C1C-NC	5.49	115.11	109.97
20	1	609	CLA	C2C-C1C-NC	5.49	115.11	109.97
20	8	612	CLA	C4A-NA-C1A	-5.48	104.24	106.71
20	6	603	CLA	CHD-C4C-C3C	-5.48	116.78	124.84
20	8	603	CLA	C2C-C1C-NC	5.48	115.11	109.97
20	6	617	CLA	C4A-NA-C1A	-5.48	104.24	106.71
20	K	4003	CLA	CHD-C4C-C3C	-5.48	116.78	124.84
20	3	609	CLA	C2C-C1C-NC	5.48	115.10	109.97
20	6	611	CLA	CHD-C1D-ND	-5.48	119.42	124.45
20	B	809	CLA	CHD-C1D-ND	-5.47	119.42	124.45
20	Z	616	CLA	CHD-C1D-ND	-5.47	119.42	124.45
20	4	613	CLA	CHD-C4C-C3C	-5.47	116.80	124.84
20	3	612	CLA	CHD-C4C-C3C	-5.47	116.80	124.84
20	5	603	CLA	C4A-NA-C1A	-5.47	104.25	106.71
20	B	835	CLA	C2C-C1C-NC	5.47	115.09	109.97
20	B	829	CLA	CHD-C4C-C3C	-5.47	116.81	124.84
20	4	611	CLA	CHD-C1D-ND	-5.46	119.43	124.45
20	G	204	CLA	C2C-C1C-NC	5.46	115.09	109.97
20	Z	603	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
20	5	611	CLA	O2D-CGD-CBD	5.46	120.97	111.27
20	1	608	CLA	C2C-C1C-NC	5.46	115.09	109.97
20	3	602	CLA	O2D-CGD-CBD	5.46	120.97	111.27
20	5	614	CLA	C4A-NA-C1A	-5.46	104.25	106.71
20	B	834	CLA	C2C-C1C-NC	5.45	115.08	109.97
20	7	616	CLA	CHD-C1D-ND	-5.45	119.44	124.45
20	6	609	CLA	CHD-C4C-C3C	-5.45	116.83	124.84
27	5	618	CHL	C1C-C2C-C3C	-5.45	102.79	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	5	603	CLA	CHD-C4C-C3C	-5.45	116.83	124.84
20	4	609	CLA	CHD-C4C-C3C	-5.45	116.84	124.84
20	6	612	CLA	C2C-C1C-NC	5.44	115.07	109.97
20	4	613	CLA	CHD-C1D-ND	-5.44	119.45	124.45
20	3	606	CLA	C2C-C1C-NC	5.44	115.07	109.97
20	B	831	CLA	C4A-NA-C1A	-5.44	104.26	106.71
20	5	611	CLA	C2C-C1C-NC	5.44	115.07	109.97
20	7	620	CLA	C2C-C1C-NC	5.44	115.06	109.97
20	A	808	CLA	O2D-CGD-CBD	5.43	120.92	111.27
20	4	604	CLA	CHD-C4C-C3C	-5.43	116.86	124.84
20	1	610	CLA	C4A-NA-C1A	-5.43	104.26	106.71
27	6	606	CHL	O2D-CGD-CBD	5.43	120.92	111.27
27	5	608	CHL	C1C-C2C-C3C	-5.43	102.80	107.11
27	6	606	CHL	C3D-C2D-C1D	-5.43	98.42	105.83
20	A	816	CLA	O2D-CGD-CBD	5.43	120.91	111.27
20	7	606	CLA	C4A-NA-C1A	-5.43	104.27	106.71
20	B	828	CLA	CMD-C2D-C1D	5.42	134.27	124.71
20	A	841	CLA	C2C-C1C-NC	5.42	115.05	109.97
20	A	820	CLA	C2C-C1C-NC	5.42	115.05	109.97
20	6	601	CLA	C2C-C1C-NC	5.41	115.04	109.97
20	B	810	CLA	C4A-NA-C1A	-5.41	104.27	106.71
20	B	836	CLA	CHD-C1D-ND	-5.41	119.48	124.45
20	A	821	CLA	CHD-C1D-ND	-5.41	119.48	124.45
20	5	613	CLA	CHD-C1D-ND	-5.41	119.48	124.45
27	5	618	CHL	O2D-CGD-CBD	5.41	120.88	111.27
27	5	608	CHL	C3D-C2D-C1D	-5.41	98.45	105.83
20	Z	611	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
27	4	607	CHL	CHD-C4C-C3C	-5.40	116.90	124.84
20	B	813	CLA	O2D-CGD-CBD	5.40	120.87	111.27
20	A	831	CLA	CMD-C2D-C1D	5.40	134.23	124.71
20	A	810	CLA	C2C-C1C-NC	5.40	115.03	109.97
20	6	604	CLA	C2C-C1C-NC	5.40	115.03	109.97
20	B	832	CLA	C2C-C1C-NC	5.40	115.03	109.97
20	Z	616	CLA	CHD-C4C-C3C	-5.40	116.91	124.84
20	F	303	CLA	C4A-NA-C1A	-5.39	104.28	106.71
20	5	603	CLA	O2D-CGD-CBD	5.39	120.85	111.27
20	5	621	CLA	O2D-CGD-CBD	5.39	120.85	111.27
20	B	828	CLA	C4A-NA-C1A	-5.39	104.28	106.71
20	8	611	CLA	O2D-CGD-CBD	5.39	120.84	111.27
20	1	609	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
20	K	4002	CLA	C2C-C1C-NC	5.38	115.02	109.97
20	6	622	CLA	C2C-C1C-NC	5.38	115.02	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	603	CLA	CHD-C4C-C3C	-5.38	116.93	124.84
20	4	601	CLA	C2C-C1C-NC	5.38	115.01	109.97
27	6	618	CHL	C3D-C2D-C1D	-5.38	98.49	105.83
20	B	832	CLA	O2D-CGD-CBD	5.38	120.83	111.27
20	6	611	CLA	C2C-C1C-NC	5.38	115.01	109.97
20	B	819	CLA	C2C-C1C-NC	5.37	115.01	109.97
20	Z	614	CLA	C2C-C1C-NC	5.37	115.01	109.97
20	A	826	CLA	CHD-C1D-ND	-5.37	119.52	124.45
20	3	603	CLA	CHD-C1D-ND	-5.37	119.52	124.45
20	A	826	CLA	O2D-CGD-CBD	5.37	120.82	111.27
20	B	824	CLA	CHD-C1D-ND	-5.37	119.52	124.45
20	3	617	CLA	C4A-NA-C1A	-5.37	104.29	106.71
20	6	616	CLA	C4A-NA-C1A	-5.37	104.29	106.71
20	A	826	CLA	C2C-C1C-NC	5.37	115.00	109.97
20	B	821	CLA	O2D-CGD-CBD	5.37	120.80	111.27
20	A	805	CLA	O2D-CGD-CBD	5.36	120.79	111.27
20	B	812	CLA	C2C-C1C-NC	5.36	114.99	109.97
20	8	604	CLA	C2C-C1C-NC	5.35	114.99	109.97
27	5	607	CHL	C3D-C2D-C1D	-5.35	98.53	105.83
27	Z	601	CHL	O2D-CGD-CBD	5.35	120.78	111.27
27	6	607	CHL	CHD-C4C-C3C	-5.35	116.98	124.84
20	A	828	CLA	CHD-C1D-ND	-5.35	119.54	124.45
20	B	821	CLA	CHD-C4C-C3C	-5.35	116.98	124.84
20	B	841	CLA	CHD-C1D-ND	-5.35	119.54	124.45
20	7	601	CLA	O2D-CGD-CBD	5.35	120.77	111.27
20	4	602	CLA	CHD-C4C-C3C	-5.34	116.99	124.84
20	A	826	CLA	C4A-NA-C1A	-5.34	104.31	106.71
20	8	606	CLA	C4A-NA-C1A	-5.34	104.31	106.71
20	4	602	CLA	C2C-C1C-NC	5.34	114.97	109.97
27	4	606	CHL	CHD-C4C-C3C	-5.34	116.99	124.84
20	3	614	CLA	C4A-NA-C1A	-5.34	104.31	106.71
20	A	821	CLA	CHD-C4C-C3C	-5.34	117.00	124.84
20	6	610	CLA	CHD-C4C-C3C	-5.33	117.00	124.84
20	A	854	CLA	CHD-C1D-ND	-5.33	119.56	124.45
20	A	842	CLA	O2D-CGD-CBD	5.33	120.74	111.27
20	B	806	CLA	C2C-C1C-NC	5.33	114.96	109.97
20	A	835	CLA	CHD-C4C-C3C	-5.33	117.01	124.84
20	A	803	CLA	O2D-CGD-CBD	5.33	120.73	111.27
20	Z	612	CLA	C2C-C1C-NC	5.32	114.96	109.97
20	3	613	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
20	3	611	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
20	3	614	CLA	C2C-C1C-NC	5.32	114.96	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	819	CLA	C4A-NA-C1A	-5.32	104.31	106.71
20	4	603	CLA	CHD-C1D-ND	-5.32	119.56	124.45
20	5	616	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
27	1	607	CHL	C3D-C2D-C1D	-5.32	98.57	105.83
23	A	852	BCR	C16-C17-C18	-5.32	119.72	127.31
20	A	809	CLA	C2C-C1C-NC	5.32	114.95	109.97
27	6	606	CHL	C1C-C2C-C3C	-5.32	102.89	107.11
20	1	614	CLA	C2C-C1C-NC	5.31	114.95	109.97
20	5	621	CLA	CHD-C4C-C3C	-5.31	117.03	124.84
20	A	823	CLA	C2C-C1C-NC	5.31	114.95	109.97
20	A	837	CLA	CHD-C4C-C3C	-5.31	117.04	124.84
27	Z	607	CHL	C2C-C3C-C4C	-5.31	102.70	106.49
20	A	813	CLA	C2C-C1C-NC	5.31	114.94	109.97
20	3	613	CLA	CMD-C2D-C1D	5.31	134.07	124.71
20	B	852	CLA	CHD-C1D-ND	-5.30	119.58	124.45
20	B	822	CLA	C2C-C1C-NC	5.30	114.94	109.97
20	B	821	CLA	C2C-C1C-NC	5.30	114.94	109.97
20	1	611	CLA	CHD-C4C-C3C	-5.30	117.05	124.84
20	L	203	CLA	C2C-C1C-NC	5.30	114.93	109.97
20	B	827	CLA	O2D-CGD-CBD	5.30	120.68	111.27
23	6	623	BCR	C7-C8-C9	-5.30	118.23	126.23
20	5	617	CLA	O2D-CGD-CBD	5.29	120.68	111.27
20	B	803	CLA	CHD-C4C-C3C	-5.29	117.06	124.84
20	4	614	CLA	CHD-C1D-ND	-5.29	119.59	124.45
27	4	618	CHL	C3D-C2D-C1D	-5.29	98.61	105.83
20	7	614	CLA	C2C-C1C-NC	5.29	114.92	109.97
20	Z	613	CLA	CHD-C1D-ND	-5.28	119.60	124.45
20	3	604	CLA	CHD-C4C-C3C	-5.28	117.08	124.84
20	8	604	CLA	CHD-C4C-C3C	-5.28	117.08	124.84
20	Z	604	CLA	C2C-C1C-NC	5.28	114.92	109.97
27	6	608	CHL	C3D-C2D-C1D	-5.27	98.63	105.83
20	8	613	CLA	CHD-C1D-ND	-5.27	119.61	124.45
23	B	845	BCR	C24-C23-C22	-5.27	118.27	126.23
20	4	602	CLA	C4A-NA-C1A	-5.27	104.33	106.71
20	A	811	CLA	CHD-C1D-ND	-5.27	119.61	124.45
20	A	829	CLA	CHD-C1D-ND	-5.27	119.61	124.45
20	5	614	CLA	C2C-C1C-NC	5.27	114.91	109.97
20	5	613	CLA	CHD-C4C-C3C	-5.27	117.10	124.84
20	1	604	CLA	C2C-C1C-NC	5.26	114.90	109.97
20	L	204	CLA	C2C-C1C-NC	5.26	114.90	109.97
20	6	616	CLA	CHD-C4C-C3C	-5.26	117.11	124.84
20	7	606	CLA	C2C-C1C-NC	5.26	114.90	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	8	610	CLA	C4A-NA-C1A	-5.25	104.34	106.71
20	A	802	CLA	CHD-C1D-ND	-5.25	119.63	124.45
20	1	616	CLA	CHD-C1D-ND	-5.25	119.63	124.45
20	B	836	CLA	C2C-C1C-NC	5.25	114.89	109.97
20	B	841	CLA	C2C-C1C-NC	5.25	114.89	109.97
20	3	614	CLA	O2D-CGD-CBD	5.25	120.59	111.27
20	B	818	CLA	O2D-CGD-CBD	5.24	120.59	111.27
27	4	618	CHL	O2D-CGD-CBD	5.24	120.59	111.27
20	8	611	CLA	CHD-C4C-C3C	-5.24	117.13	124.84
20	B	807	CLA	O2D-CGD-CBD	5.24	120.58	111.27
20	B	809	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
20	B	829	CLA	C2C-C1C-NC	5.24	114.88	109.97
27	4	618	CHL	C1C-C2C-C3C	-5.24	102.96	107.11
20	J	3002	CLA	O2D-CGD-CBD	5.24	120.58	111.27
20	B	834	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
20	1	614	CLA	C4A-NA-C1A	-5.24	104.35	106.71
27	5	608	CHL	CHD-C4C-C3C	-5.24	117.14	124.84
23	4	621	BCR	C15-C14-C13	-5.23	119.84	127.31
20	8	601	CLA	CHD-C1D-ND	-5.23	119.65	124.45
20	6	622	CLA	CHD-C4C-C3C	-5.23	117.15	124.84
20	Z	609	CLA	CHD-C4C-C3C	-5.23	117.15	124.84
20	5	611	CLA	CHD-C1D-ND	-5.23	119.65	124.45
27	6	608	CHL	CHD-C1D-ND	-5.23	119.65	124.45
20	A	854	CLA	C4A-NA-C1A	-5.23	104.36	106.71
20	A	843	CLA	CHD-C1D-ND	-5.23	119.65	124.45
20	B	814	CLA	O2D-CGD-CBD	5.23	120.56	111.27
19	A	801	CL0	O2D-CGD-CBD	5.23	120.56	111.27
20	L	204	CLA	CHD-C4C-C3C	-5.23	117.16	124.84
20	3	620	CLA	CHD-C4C-C3C	-5.22	117.16	124.84
27	5	618	CHL	CHD-C1D-ND	-5.22	119.65	124.45
20	7	604	CLA	C2C-C1C-NC	5.22	114.87	109.97
20	G	203	CLA	CHD-C4C-C3C	-5.22	117.16	124.84
20	3	611	CLA	O2D-CGD-CBD	5.22	120.55	111.27
27	5	618	CHL	C3D-C2D-C1D	-5.22	98.71	105.83
27	6	607	CHL	C3D-C2D-C1D	-5.22	98.71	105.83
27	Z	607	CHL	C3D-C2D-C1D	-5.22	98.71	105.83
20	4	610	CLA	CHD-C4C-C3C	-5.22	117.17	124.84
20	7	602	CLA	O2D-CGD-CBD	5.22	120.54	111.27
20	3	603	CLA	C4A-NA-C1A	-5.22	104.36	106.71
20	6	613	CLA	C2C-C1C-NC	5.22	114.86	109.97
27	5	607	CHL	CHD-C1D-ND	-5.21	119.66	124.45
20	5	617	CLA	CHD-C4C-C3C	-5.21	117.18	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	617	CLA	O2D-CGD-CBD	5.21	120.52	111.27
20	A	825	CLA	CHD-C4C-C3C	-5.21	117.19	124.84
20	5	604	CLA	CHD-C4C-C3C	-5.21	117.19	124.84
20	7	601	CLA	C2C-C1C-NC	5.20	114.85	109.97
27	5	618	CHL	C2C-C3C-C4C	-5.20	102.78	106.49
20	A	836	CLA	CHD-C4C-C3C	-5.20	117.20	124.84
27	7	607	CHL	C1C-C2C-C3C	-5.20	102.99	107.11
20	B	802	CLA	CHD-C1D-ND	-5.20	119.68	124.45
20	B	807	CLA	CHD-C4C-C3C	-5.20	117.20	124.84
27	4	606	CHL	C3D-C2D-C1D	-5.19	98.74	105.83
27	Z	601	CHL	C1C-C2C-C3C	-5.19	103.00	107.11
20	A	815	CLA	C2C-C1C-NC	5.18	114.83	109.97
20	A	838	CLA	O2D-CGD-CBD	5.18	120.47	111.27
23	I	172	BCR	C20-C21-C22	-5.18	119.92	127.31
20	6	601	CLA	CHD-C4C-C3C	-5.18	117.23	124.84
20	B	838	CLA	O2D-CGD-CBD	5.18	120.47	111.27
20	A	806	CLA	CHD-C4C-C3C	-5.18	117.23	124.84
20	4	611	CLA	CHD-C4C-C3C	-5.18	117.23	124.84
27	Z	607	CHL	CHD-C1D-ND	-5.17	119.70	124.45
23	L	201	BCR	C7-C8-C9	-5.17	118.42	126.23
20	6	610	CLA	O2D-CGD-CBD	5.17	120.45	111.27
20	B	819	CLA	CHD-C4C-C3C	-5.17	117.24	124.84
20	7	613	CLA	CHD-C1D-ND	-5.17	119.71	124.45
20	B	830	CLA	C2C-C1C-NC	5.16	114.81	109.97
20	7	608	CLA	C2C-C1C-NC	5.16	114.81	109.97
20	A	811	CLA	C2C-C1C-NC	5.16	114.80	109.97
27	6	618	CHL	CHD-C4C-C3C	-5.16	117.26	124.84
20	A	831	CLA	CHD-C4C-C3C	-5.15	117.26	124.84
20	4	609	CLA	C4A-NA-C1A	-5.15	104.39	106.71
20	B	811	CLA	O2D-CGD-CBD	5.15	120.43	111.27
20	L	203	CLA	CHD-C4C-C3C	-5.15	117.27	124.84
20	A	833	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
20	B	810	CLA	CHD-C4C-C3C	-5.15	117.27	124.84
20	A	832	CLA	O2D-CGD-CBD	5.14	120.41	111.27
20	6	603	CLA	O2D-CGD-CBD	5.14	120.41	111.27
20	Z	604	CLA	CHD-C4C-C3C	-5.14	117.29	124.84
20	Z	613	CLA	C2C-C1C-NC	5.14	114.78	109.97
20	A	831	CLA	CHD-C1D-ND	-5.14	119.73	124.45
20	B	830	CLA	C4A-NA-C1A	-5.13	104.40	106.71
20	8	610	CLA	O2D-CGD-CBD	5.13	120.38	111.27
20	A	827	CLA	C4A-NA-C1A	-5.12	104.40	106.71
27	5	607	CHL	O2D-CGD-CBD	5.12	120.37	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	813	CLA	C2C-C1C-NC	5.12	114.77	109.97
20	F	303	CLA	C2C-C1C-NC	5.12	114.77	109.97
20	1	603	CLA	O2D-CGD-CBD	5.12	120.37	111.27
20	B	823	CLA	CHD-C1D-ND	-5.12	119.75	124.45
20	6	622	CLA	O2D-CGD-CBD	5.12	120.36	111.27
20	A	829	CLA	C2C-C1C-NC	5.11	114.76	109.97
20	A	854	CLA	C3C-C4C-NC	5.11	116.30	110.57
20	B	815	CLA	CHD-C4C-C3C	-5.11	117.33	124.84
20	8	614	CLA	O2D-CGD-CBD	5.11	120.35	111.27
20	A	830	CLA	C2C-C1C-NC	5.10	114.75	109.97
27	6	618	CHL	C2C-C3C-C4C	-5.10	102.85	106.49
20	A	817	CLA	CHD-C4C-C3C	-5.10	117.34	124.84
27	3	608	CHL	CHD-C1D-ND	-5.10	119.77	124.45
20	A	818	CLA	C2C-C1C-NC	5.10	114.75	109.97
20	8	609	CLA	C2C-C1C-NC	5.10	114.75	109.97
20	A	832	CLA	CHD-C1D-ND	-5.08	119.78	124.45
23	B	848	BCR	C16-C17-C18	-5.08	120.06	127.31
20	Z	612	CLA	O2D-CGD-CBD	5.08	120.29	111.27
27	Z	607	CHL	C1C-C2C-C3C	-5.07	103.09	107.11
20	8	603	CLA	O2D-CGD-CBD	5.07	120.28	111.27
20	B	826	CLA	C4A-NA-C1A	-5.07	104.43	106.71
20	5	610	CLA	C4A-NA-C1A	-5.07	104.43	106.71
20	B	817	CLA	CHD-C4C-C3C	-5.07	117.39	124.84
23	K	4001	BCR	C11-C10-C9	-5.07	120.07	127.31
27	1	607	CHL	CHD-C1D-ND	-5.07	119.80	124.45
20	4	610	CLA	C2C-C1C-NC	5.06	114.72	109.97
20	A	840	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
20	B	813	CLA	C4A-NA-C1A	-5.06	104.43	106.71
20	7	614	CLA	C4A-NA-C1A	-5.06	104.43	106.71
20	A	838	CLA	CHD-C4C-C3C	-5.06	117.40	124.84
20	A	833	CLA	C2C-C1C-NC	5.06	114.71	109.97
20	A	843	CLA	C2C-C1C-NC	5.06	114.71	109.97
20	5	617	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
20	A	830	CLA	C4A-NA-C1A	-5.05	104.44	106.71
20	3	607	CLA	C4A-NA-C1A	-5.05	104.44	106.71
27	4	607	CHL	C3D-C2D-C1D	-5.05	98.94	105.83
20	B	836	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
20	B	824	CLA	C2C-C1C-NC	5.04	114.70	109.97
20	6	614	CLA	C2C-C1C-NC	5.04	114.69	109.97
20	8	614	CLA	C2C-C1C-NC	5.04	114.69	109.97
20	Z	602	CLA	C4A-NA-C1A	-5.04	104.44	106.71
20	F	301	CLA	C2C-C1C-NC	5.03	114.69	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	6	610	CLA	C2C-C1C-NC	5.03	114.69	109.97
20	6	604	CLA	O2D-CGD-CBD	5.03	120.21	111.27
20	7	611	CLA	O2D-CGD-CBD	5.03	120.21	111.27
20	6	610	CLA	C4A-NA-C1A	-5.03	104.44	106.71
27	7	607	CHL	C3D-C2D-C1D	-5.02	98.98	105.83
20	B	833	CLA	C2C-C1C-NC	5.02	114.68	109.97
27	8	607	CHL	CHD-C4C-C3C	-5.02	117.46	124.84
20	B	831	CLA	C2C-C1C-NC	5.02	114.67	109.97
20	B	839	CLA	C2C-C1C-NC	5.02	114.67	109.97
20	4	610	CLA	C4A-NA-C1A	-5.01	104.45	106.71
20	B	808	CLA	CHD-C1D-ND	-5.01	119.85	124.45
20	A	824	CLA	C4A-NA-C1A	-5.01	104.45	106.71
20	4	604	CLA	C2C-C1C-NC	5.01	114.66	109.97
20	4	614	CLA	C2C-C1C-NC	5.01	114.66	109.97
20	B	822	CLA	O2D-CGD-CBD	5.01	120.16	111.27
27	6	618	CHL	O2D-CGD-CBD	5.00	120.16	111.27
20	4	616	CLA	C2C-C1C-NC	5.00	114.66	109.97
27	4	618	CHL	C2C-C3C-C4C	-5.00	102.92	106.49
20	Z	609	CLA	C4A-NA-C1A	-5.00	104.46	106.71
20	A	820	CLA	O2D-CGD-CBD	5.00	120.15	111.27
27	4	618	CHL	CHD-C1D-ND	-5.00	119.86	124.45
20	8	608	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
27	Z	601	CHL	CHD-C4C-C3C	-4.99	117.50	124.84
20	B	828	CLA	O2D-CGD-CBD	4.99	120.14	111.27
20	3	602	CLA	C2C-C1C-NC	4.99	114.64	109.97
20	8	602	CLA	O2D-CGD-CBD	4.98	120.12	111.27
20	B	802	CLA	C3C-C4C-NC	4.98	116.16	110.57
23	B	847	BCR	C24-C23-C22	-4.98	118.71	126.23
20	4	616	CLA	C4A-NA-C1A	-4.98	104.47	106.71
20	A	802	CLA	CHD-C4C-C3C	-4.98	117.53	124.84
20	A	837	CLA	C4A-NA-C1A	-4.97	104.47	106.71
27	Z	601	CHL	C3D-C2D-C1D	-4.97	99.05	105.83
20	B	806	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
20	A	823	CLA	O2D-CGD-CBD	4.96	120.08	111.27
20	A	845	CLA	O2D-CGD-CBD	4.96	120.08	111.27
20	A	804	CLA	C2C-C1C-NC	4.96	114.62	109.97
20	B	837	CLA	C2C-C1C-NC	4.96	114.62	109.97
20	1	606	CLA	C2C-C1C-NC	4.96	114.62	109.97
20	6	611	CLA	O2D-CGD-CBD	4.96	120.08	111.27
20	A	806	CLA	C2C-C1C-NC	4.96	114.61	109.97
20	5	621	CLA	CHD-C1D-ND	-4.96	119.90	124.45
20	Z	616	CLA	O2D-CGD-CBD	4.95	120.06	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	8	603	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
20	B	826	CLA	C2C-C1C-NC	4.95	114.61	109.97
20	1	604	CLA	O2D-CGD-CBD	4.95	120.06	111.27
20	A	817	CLA	O2D-CGD-CBD	4.94	120.05	111.27
20	A	854	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
20	B	803	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
20	A	811	CLA	C4A-NA-C1A	-4.93	104.49	106.71
23	A	852	BCR	C7-C8-C9	-4.93	118.78	126.23
20	A	840	CLA	C4A-NA-C1A	-4.93	104.49	106.71
20	F	303	CLA	C3D-C2D-C1D	-4.93	99.11	105.83
20	1	613	CLA	C2C-C1C-NC	4.93	114.59	109.97
20	B	816	CLA	C3D-C2D-C1D	-4.92	99.11	105.83
20	5	606	CLA	C4A-NA-C1A	-4.91	104.50	106.71
20	1	604	CLA	CHD-C4C-C3C	-4.91	117.62	124.84
20	1	610	CLA	O2D-CGD-CBD	4.91	119.99	111.27
23	A	850	BCR	C16-C17-C18	-4.91	120.31	127.31
20	7	620	CLA	O2D-CGD-CBD	4.91	119.99	111.27
20	G	204	CLA	C4A-NA-C1A	-4.91	104.50	106.71
20	1	609	CLA	C4A-NA-C1A	-4.91	104.50	106.71
20	1	611	CLA	C4A-NA-C1A	-4.90	104.50	106.71
20	3	613	CLA	C4A-NA-C1A	-4.90	104.50	106.71
20	7	609	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
27	8	607	CHL	C3D-C2D-C1D	-4.90	99.15	105.83
20	Z	606	CLA	C2C-C1C-NC	4.90	114.56	109.97
27	7	607	CHL	O2D-CGD-CBD	4.89	119.96	111.27
20	A	815	CLA	O2D-CGD-CBD	4.89	119.95	111.27
20	6	602	CLA	C2C-C1C-NC	4.88	114.55	109.97
27	1	601	CHL	C1C-C2C-C3C	-4.88	103.24	107.11
20	A	813	CLA	C4A-NA-C1A	-4.88	104.51	106.71
20	B	838	CLA	C3D-C2D-C1D	-4.88	99.18	105.83
20	A	802	CLA	C2C-C1C-NC	4.88	114.54	109.97
20	8	610	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
20	B	829	CLA	O2D-CGD-CBD	4.87	119.92	111.27
27	4	607	CHL	O2D-CGD-CBD	4.87	119.92	111.27
20	G	203	CLA	O2D-CGD-CBD	4.87	119.92	111.27
20	B	816	CLA	C2C-C1C-NC	4.86	114.53	109.97
20	Z	602	CLA	C2C-C1C-NC	4.86	114.53	109.97
20	B	831	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
20	A	823	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
27	1	607	CHL	CHD-C4C-C3C	-4.86	117.70	124.84
20	4	616	CLA	O2D-CGD-CBD	4.86	119.90	111.27
20	A	819	CLA	C3D-C2D-C1D	-4.86	99.20	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	6	606	CHL	C2C-C3C-C4C	-4.86	103.03	106.49
20	B	829	CLA	C4A-NA-C1A	-4.86	104.52	106.71
20	8	616	CLA	CHD-C1D-ND	-4.86	119.99	124.45
20	7	610	CLA	O2D-CGD-CBD	4.85	119.89	111.27
20	A	809	CLA	C3D-C2D-C1D	-4.85	99.21	105.83
20	A	818	CLA	C3D-C2D-C1D	-4.85	99.21	105.83
19	A	801	CL0	CAA-C2A-C3A	-4.84	99.51	112.78
20	3	612	CLA	O2D-CGD-CBD	4.84	119.88	111.27
20	6	602	CLA	C4A-NA-C1A	-4.84	104.53	106.71
19	A	801	CL0	CHD-C1D-ND	-4.84	120.00	124.45
20	A	829	CLA	C3D-C2D-C1D	-4.84	99.22	105.83
27	4	618	CHL	CHD-C4C-C3C	-4.84	117.72	124.84
20	L	203	CLA	O2D-CGD-CBD	4.83	119.85	111.27
20	A	830	CLA	CMD-C2D-C1D	4.83	133.23	124.71
20	1	608	CLA	C4A-NA-C1A	-4.83	104.53	106.71
20	A	814	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
20	3	606	CLA	O2D-CGD-CBD	4.83	119.84	111.27
27	4	606	CHL	O2D-CGD-CBD	4.83	119.84	111.27
23	7	623	BCR	C16-C17-C18	-4.82	120.42	127.31
20	K	4003	CLA	O2D-CGD-CBD	4.82	119.84	111.27
20	8	608	CLA	C2C-C1C-NC	4.82	114.49	109.97
20	A	803	CLA	C4A-NA-C1A	-4.82	104.54	106.71
20	A	816	CLA	C2C-C1C-NC	4.82	114.48	109.97
20	B	831	CLA	O2D-CGD-CBD	4.81	119.82	111.27
20	4	610	CLA	O2D-CGD-CBD	4.81	119.82	111.27
23	A	848	BCR	C16-C17-C18	-4.81	120.44	127.31
20	8	609	CLA	O2D-CGD-CBD	4.81	119.81	111.27
20	A	812	CLA	O2D-CGD-CBD	4.80	119.80	111.27
20	A	835	CLA	C4A-NA-C1A	-4.80	104.55	106.71
20	8	602	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
20	L	204	CLA	O2D-CGD-CBD	4.80	119.80	111.27
20	6	617	CLA	O2D-CGD-CBD	4.80	119.80	111.27
20	5	614	CLA	O2D-CGD-CBD	4.80	119.79	111.27
20	A	814	CLA	C2C-C1C-NC	4.80	114.47	109.97
20	8	602	CLA	C2C-C1C-NC	4.80	114.47	109.97
20	A	822	CLA	C2C-C1C-NC	4.79	114.46	109.97
20	6	603	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
20	5	612	CLA	O2D-CGD-CBD	4.79	119.78	111.27
27	4	607	CHL	CHD-C1D-ND	-4.79	120.05	124.45
20	8	613	CLA	C4A-NA-C1A	-4.79	104.55	106.71
23	F	305	BCR	C11-C10-C9	-4.79	120.48	127.31
20	B	814	CLA	C2C-C1C-NC	4.78	114.45	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	820	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
20	A	854	CLA	C2C-C1C-NC	4.78	114.45	109.97
20	B	826	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
20	J	3002	CLA	C4A-NA-C1A	-4.78	104.56	106.71
20	Z	606	CLA	O2D-CGD-CBD	4.77	119.75	111.27
20	3	604	CLA	C4A-NA-C1A	-4.77	104.56	106.71
20	5	613	CLA	O2D-CGD-CBD	4.77	119.75	111.27
27	Z	607	CHL	CHD-C4C-C3C	-4.77	117.83	124.84
20	A	815	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
20	4	604	CLA	O2D-CGD-CBD	4.77	119.74	111.27
20	8	604	CLA	O2D-CGD-CBD	4.77	119.74	111.27
20	A	845	CLA	C3D-C2D-C1D	-4.77	99.33	105.83
20	3	613	CLA	CHD-C1D-ND	-4.77	120.08	124.45
20	1	608	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
20	F	304	CLA	O2D-CGD-CBD	4.76	119.73	111.27
20	A	803	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
20	B	804	CLA	C2C-C1C-NC	4.76	114.43	109.97
20	A	819	CLA	O2D-CGD-CBD	4.76	119.72	111.27
20	3	606	CLA	C4A-NA-C1A	-4.76	104.57	106.71
20	Z	610	CLA	O2D-CGD-CBD	4.76	119.72	111.27
23	B	844	BCR	C28-C27-C26	-4.76	105.59	114.08
20	G	203	CLA	C3D-C2D-C1D	-4.75	99.34	105.83
20	B	839	CLA	C4A-NA-C1A	-4.75	104.57	106.71
20	F	304	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
27	5	607	CHL	CHD-C4C-C3C	-4.75	117.86	124.84
20	1	602	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
20	B	832	CLA	C4A-NA-C1A	-4.75	104.57	106.71
20	5	603	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
20	Z	608	CLA	C4A-NA-C1A	-4.74	104.57	106.71
20	1	602	CLA	C2C-C1C-NC	4.74	114.42	109.97
20	5	610	CLA	O2D-CGD-CBD	4.74	119.70	111.27
20	4	611	CLA	O2D-CGD-CBD	4.74	119.69	111.27
20	A	828	CLA	C3C-C4C-NC	4.74	115.89	110.57
20	B	834	CLA	O2D-CGD-CBD	4.74	119.69	111.27
20	B	804	CLA	C3D-C2D-C1D	-4.74	99.37	105.83
27	5	608	CHL	O2D-CGD-CBD	4.74	119.68	111.27
20	A	819	CLA	C2C-C1C-NC	4.74	114.41	109.97
20	A	805	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
20	4	602	CLA	O2D-CGD-CBD	4.73	119.67	111.27
20	A	824	CLA	O2D-CGD-CBD	4.72	119.66	111.27
27	5	618	CHL	CHD-C4C-C3C	-4.72	117.90	124.84
20	5	616	CLA	C3D-C2D-C1D	-4.72	99.39	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Z	614	CLA	C4A-NA-C1A	-4.72	104.58	106.71
20	L	204	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
20	Z	614	CLA	O2D-CGD-CBD	4.72	119.65	111.27
20	A	833	CLA	O2D-CGD-CBD	4.71	119.65	111.27
20	A	813	CLA	O2D-CGD-CBD	4.71	119.64	111.27
20	7	616	CLA	O2D-CGD-CBD	4.71	119.64	111.27
20	Z	614	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
20	B	832	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
20	5	604	CLA	C3D-C2D-C1D	-4.70	99.41	105.83
20	A	816	CLA	C3D-C2D-C1D	-4.70	99.41	105.83
20	6	622	CLA	C3D-C2D-C1D	-4.70	99.41	105.83
23	B	847	BCR	C3-C4-C5	-4.70	105.68	114.08
20	4	612	CLA	O2D-CGD-CBD	4.70	119.62	111.27
20	K	4003	CLA	C4A-NA-C1A	-4.70	104.59	106.71
20	B	839	CLA	O2D-CGD-CBD	4.70	119.61	111.27
20	7	611	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
20	7	612	CLA	C3D-C2D-C1D	-4.69	99.42	105.83
20	6	609	CLA	C4A-NA-C1A	-4.69	104.60	106.71
20	4	609	CLA	O2D-CGD-CBD	4.69	119.61	111.27
20	4	616	CLA	C3D-C2D-C1D	-4.69	99.44	105.83
20	8	601	CLA	C3D-C2D-C1D	-4.69	99.44	105.83
20	B	833	CLA	C4A-NA-C1A	-4.68	104.60	106.71
20	5	609	CLA	O2D-CGD-CBD	4.68	119.59	111.27
23	6	625	BCR	C7-C8-C9	-4.68	119.17	126.23
20	5	610	CLA	C2C-C1C-NC	4.68	114.36	109.97
20	B	821	CLA	C3D-C2D-C1D	-4.68	99.45	105.83
20	Z	606	CLA	C3D-C2D-C1D	-4.67	99.45	105.83
20	A	842	CLA	C3D-C2D-C1D	-4.67	99.45	105.83
27	1	601	CHL	C3C-C4C-NC	4.67	115.81	110.57
20	A	832	CLA	C4A-NA-C1A	-4.67	104.61	106.71
23	5	622	BCR	C15-C14-C13	-4.67	120.64	127.31
23	6	623	BCR	C11-C10-C9	-4.67	120.64	127.31
20	B	809	CLA	O2D-CGD-CBD	4.67	119.56	111.27
20	B	818	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
20	B	819	CLA	O2D-CGD-CBD	4.66	119.56	111.27
20	B	852	CLA	O2D-CGD-CBD	4.66	119.56	111.27
20	B	807	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
20	Z	602	CLA	O2D-CGD-CBD	4.66	119.55	111.27
20	Z	608	CLA	C3D-C2D-C1D	-4.66	99.48	105.83
20	Z	602	CLA	C3D-C2D-C1D	-4.66	99.48	105.83
20	3	607	CLA	O2D-CGD-CBD	4.66	119.54	111.27
20	B	805	CLA	C3D-C2D-C1D	-4.65	99.48	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	7	602	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
20	Z	604	CLA	O2D-CGD-CBD	4.65	119.53	111.27
20	A	834	CLA	C4A-NA-C1A	-4.65	104.61	106.71
20	A	802	CLA	CMB-C2B-C3B	4.65	133.38	124.68
20	A	841	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
20	5	609	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
20	A	808	CLA	C4A-NA-C1A	-4.65	104.62	106.71
20	B	818	CLA	C4A-NA-C1A	-4.65	104.62	106.71
27	Z	601	CHL	C3C-C4C-NC	4.65	115.78	110.57
20	A	834	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
20	B	817	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
20	3	609	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
20	L	203	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
22	4	622	LHG	O7-C7-C8	4.64	121.50	111.50
20	6	613	CLA	O2D-CGD-CBD	4.64	119.51	111.27
20	7	611	CLA	C4A-NA-C1A	-4.64	104.62	106.71
20	7	603	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
20	5	606	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
20	B	812	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
20	4	602	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
20	1	613	CLA	O2D-CGD-CBD	4.64	119.51	111.27
20	6	616	CLA	C2C-C1C-NC	4.63	114.31	109.97
20	6	602	CLA	C3D-C2D-C1D	-4.63	99.52	105.83
20	7	602	CLA	C4A-NA-C1A	-4.63	104.63	106.71
20	A	805	CLA	C2C-C1C-NC	4.63	114.31	109.97
27	7	607	CHL	CHD-C4C-C3C	-4.62	118.04	124.84
20	1	606	CLA	O2D-CGD-CBD	4.62	119.48	111.27
20	5	602	CLA	O2D-CGD-CBD	4.62	119.48	111.27
20	A	839	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
20	A	815	CLA	C4A-NA-C1A	-4.62	104.63	106.71
20	B	827	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
20	7	601	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
23	F	305	BCR	C15-C14-C13	-4.62	120.72	127.31
20	7	620	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
20	A	808	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
20	B	824	CLA	C4A-NA-C1A	-4.61	104.63	106.71
20	8	609	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
20	A	835	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
20	1	602	CLA	C4A-NA-C1A	-4.61	104.64	106.71
20	7	606	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
20	A	807	CLA	C3D-C2D-C1D	-4.61	99.55	105.83
20	A	826	CLA	C3C-C4C-NC	4.60	115.73	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Z	612	CLA	C4A-NA-C1A	-4.60	104.64	106.71
20	4	609	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
27	8	607	CHL	C1C-C2C-C3C	-4.60	103.46	107.11
20	7	608	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
20	A	814	CLA	C3C-C4C-NC	4.59	115.72	110.57
20	Z	609	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
20	A	831	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
20	K	4003	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
20	B	817	CLA	O2D-CGD-CBD	4.59	119.42	111.27
20	1	603	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
20	B	825	CLA	C2C-C1C-NC	4.58	114.27	109.97
20	B	822	CLA	C4A-NA-C1A	-4.58	104.65	106.71
20	4	601	CLA	CHD-C4C-C3C	-4.58	118.11	124.84
20	3	604	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
20	8	606	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
27	6	606	CHL	CHD-C1D-ND	-4.58	120.25	124.45
27	4	606	CHL	C2C-C3C-C4C	-4.58	103.22	106.49
20	A	803	CLA	CAA-C2A-C3A	-4.58	100.24	112.78
23	5	625	BCR	C16-C17-C18	-4.58	120.78	127.31
23	6	623	BCR	C15-C14-C13	-4.58	120.78	127.31
20	B	840	CLA	O2D-CGD-CBD	4.58	119.40	111.27
20	6	612	CLA	O2D-CGD-CBD	4.58	119.40	111.27
20	B	841	CLA	C4A-NA-C1A	-4.58	104.65	106.71
20	B	852	CLA	C4A-NA-C1A	-4.58	104.65	106.71
20	5	601	CLA	C4A-NA-C1A	-4.58	104.65	106.71
20	4	601	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
20	6	609	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
20	B	840	CLA	C4A-NA-C1A	-4.57	104.65	106.71
20	L	203	CLA	C4A-NA-C1A	-4.57	104.65	106.71
20	1	611	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
20	8	608	CLA	O2D-CGD-CBD	4.57	119.39	111.27
20	A	833	CLA	C4A-NA-C1A	-4.57	104.65	106.71
20	B	820	CLA	C4A-NA-C1A	-4.57	104.65	106.71
20	7	614	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
20	5	612	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
23	7	623	BCR	C21-C20-C19	-4.57	108.96	123.22
20	1	609	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
20	3	617	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
27	4	607	CHL	C2C-C3C-C4C	-4.57	103.23	106.49
20	7	613	CLA	O2D-CGD-CBD	4.56	119.38	111.27
20	Z	606	CLA	C4A-NA-C1A	-4.56	104.65	106.71
20	8	611	CLA	C3D-C2D-C1D	-4.56	99.60	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	602	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
20	5	611	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
20	1	606	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
20	8	616	CLA	O2D-CGD-CBD	4.56	119.37	111.27
20	B	815	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
20	7	610	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
19	A	801	CL0	C3C-C4C-NC	4.56	115.68	110.57
20	B	838	CLA	C4A-NA-C1A	-4.56	104.66	106.71
20	F	304	CLA	C4A-NA-C1A	-4.56	104.66	106.71
20	B	823	CLA	C3D-C2D-C1D	-4.55	99.61	105.83
20	L	203	CLA	C3D-C4D-ND	4.55	117.61	110.24
20	A	825	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
20	A	822	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
27	4	608	CHL	O2D-CGD-CBD	4.55	119.36	111.27
20	7	604	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
20	A	827	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
20	A	813	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
20	3	620	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
20	5	604	CLA	O2D-CGD-CBD	4.55	119.35	111.27
20	B	808	CLA	C3C-C4C-NC	4.55	115.67	110.57
20	A	822	CLA	C4A-NA-C1A	-4.54	104.66	106.71
20	Z	610	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
20	6	613	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
20	B	837	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
20	8	609	CLA	C4A-NA-C1A	-4.54	104.66	106.71
27	1	607	CHL	C1C-C2C-C3C	-4.54	103.51	107.11
20	4	603	CLA	O2D-CGD-CBD	4.54	119.34	111.27
20	3	603	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
20	8	602	CLA	C4A-NA-C1A	-4.54	104.67	106.71
20	4	601	CLA	C4A-NA-C1A	-4.54	104.67	106.71
20	5	612	CLA	C4A-NA-C1A	-4.54	104.67	106.71
20	J	3002	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
20	5	610	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
20	G	204	CLA	C3D-C2D-C1D	-4.53	99.64	105.83
20	5	614	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
20	B	840	CLA	C1C-C2C-C3C	-4.53	102.19	106.96
20	3	606	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
20	B	835	CLA	O2D-CGD-CBD	4.53	119.31	111.27
20	B	823	CLA	C2C-C1C-NC	4.53	114.21	109.97
20	A	812	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
20	7	616	CLA	C4A-NA-C1A	-4.53	104.67	106.71
20	7	612	CLA	O2D-CGD-CBD	4.53	119.31	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	611	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
20	B	841	CLA	C3D-C2D-C1D	-4.52	99.67	105.83
23	B	845	BCR	C7-C8-C9	-4.52	119.41	126.23
20	4	614	CLA	O2D-CGD-CBD	4.52	119.29	111.27
20	B	840	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
20	B	835	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
20	A	828	CLA	C1D-CHD-C4C	-4.51	116.32	126.06
20	3	614	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
20	B	811	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
27	Z	607	CHL	O2D-CGD-CBD	4.51	119.29	111.27
20	A	829	CLA	C3C-C4C-NC	4.51	115.63	110.57
20	A	802	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
20	B	814	CLA	C4A-NA-C1A	-4.51	104.68	106.71
20	K	4002	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
27	6	618	CHL	CHD-C1D-ND	-4.50	120.32	124.45
20	B	829	CLA	C3D-C4D-ND	4.50	117.52	110.24
20	B	828	CLA	CHD-C1D-ND	-4.50	120.32	124.45
20	3	620	CLA	C4A-NA-C1A	-4.50	104.68	106.71
20	1	614	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
20	5	606	CLA	O2D-CGD-CBD	4.50	119.26	111.27
20	7	613	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
20	5	602	CLA	C2C-C1C-NC	4.49	114.18	109.97
27	4	606	CHL	CHD-C1D-ND	-4.49	120.32	124.45
20	1	614	CLA	O2D-CGD-CBD	4.49	119.25	111.27
20	F	301	CLA	O2D-CGD-CBD	4.49	119.25	111.27
20	5	609	CLA	C4A-NA-C1A	-4.49	104.69	106.71
20	A	830	CLA	CHD-C1D-ND	-4.49	120.33	124.45
28	Z	619	LUT	C35-C34-C33	-4.49	120.90	127.31
20	B	810	CLA	CAA-C2A-C3A	-4.49	100.49	112.78
20	B	816	CLA	C4A-NA-C1A	-4.49	104.69	106.71
20	6	614	CLA	O2D-CGD-CBD	4.49	119.24	111.27
20	A	843	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
20	6	616	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
20	5	601	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
20	6	614	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
20	3	612	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
20	B	802	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
23	J	3003	BCR	C24-C23-C22	-4.48	119.47	126.23
20	B	813	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
27	6	608	CHL	O2D-CGD-CBD	4.48	119.22	111.27
19	A	801	CL0	C1C-C2C-C3C	-4.47	102.25	106.96
20	A	818	CLA	C3D-C4D-ND	4.47	117.47	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	4	608	CHL	CHD-C1D-ND	-4.47	120.34	124.45
20	1	612	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
20	B	833	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
20	A	826	CLA	C3D-C2D-C1D	-4.47	99.74	105.83
20	6	611	CLA	C3D-C2D-C1D	-4.47	99.74	105.83
20	5	616	CLA	C4A-NA-C1A	-4.47	104.70	106.71
23	A	850	BCR	C3-C4-C5	-4.47	106.10	114.08
20	B	816	CLA	O2D-CGD-CBD	4.47	119.20	111.27
20	Z	616	CLA	C3D-C2D-C1D	-4.47	99.74	105.83
20	A	804	CLA	C3D-C4D-ND	4.46	117.46	110.24
20	A	818	CLA	C4A-NA-C1A	-4.46	104.70	106.71
20	A	811	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
20	Z	612	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
20	8	613	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
20	A	837	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
20	1	606	CLA	C4A-NA-C1A	-4.46	104.70	106.71
20	A	817	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
20	3	607	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
20	6	601	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
20	Z	611	CLA	O2D-CGD-CBD	4.46	119.19	111.27
20	B	810	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
20	4	609	CLA	C1D-CHD-C4C	-4.45	116.45	126.06
23	A	856	BCR	C20-C21-C22	-4.45	120.95	127.31
20	A	811	CLA	C1D-CHD-C4C	-4.45	116.46	126.06
20	5	602	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
20	B	834	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
27	5	608	CHL	CHD-C1D-ND	-4.45	120.37	124.45
20	4	604	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
20	F	301	CLA	C1D-CHD-C4C	-4.44	116.47	126.06
20	B	805	CLA	C3C-C4C-NC	4.44	115.55	110.57
20	1	610	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
20	B	815	CLA	C4A-NA-C1A	-4.44	104.71	106.71
20	4	614	CLA	C4A-NA-C1A	-4.44	104.71	106.71
20	A	830	CLA	C3C-C4C-NC	4.44	115.55	110.57
20	Z	603	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
20	6	612	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
20	A	810	CLA	CHD-C1D-ND	-4.43	120.38	124.45
20	4	612	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
20	L	204	CLA	C3D-C4D-ND	4.43	117.40	110.24
20	B	839	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
23	3	718	BCR	C16-C17-C18	-4.43	120.99	127.31
20	A	810	CLA	C3C-C4C-NC	4.43	115.54	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	613	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
20	F	301	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
20	6	604	CLA	C3D-C2D-C1D	-4.42	99.79	105.83
20	4	613	CLA	O2D-CGD-CBD	4.42	119.12	111.27
27	6	607	CHL	O2D-CGD-CBD	4.42	119.12	111.27
20	A	824	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
20	4	614	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
20	4	610	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
20	B	818	CLA	C1C-C2C-C3C	-4.42	102.31	106.96
20	4	603	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
23	A	856	BCR	C15-C16-C17	-4.41	114.44	123.47
20	B	820	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
20	B	852	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
20	B	803	CLA	C1D-CHD-C4C	-4.41	116.54	126.06
20	3	620	CLA	O2D-CGD-CBD	4.41	119.11	111.27
20	8	614	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
23	6	623	BCR	C28-C27-C26	-4.41	106.20	114.08
23	3	719	BCR	C16-C17-C18	-4.41	121.02	127.31
20	4	612	CLA	C1D-CHD-C4C	-4.41	116.55	126.06
23	7	623	BCR	C3-C4-C5	-4.41	106.20	114.08
20	A	839	CLA	C4A-NA-C1A	-4.41	104.72	106.71
20	3	607	CLA	C3D-C4D-ND	4.41	117.37	110.24
20	A	831	CLA	C3C-C4C-NC	4.41	115.51	110.57
23	A	851	BCR	C15-C14-C13	-4.40	121.03	127.31
27	1	601	CHL	CHD-C1D-ND	-4.40	120.41	124.45
20	7	609	CLA	C3C-C4C-NC	4.40	115.51	110.57
20	B	814	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
20	5	602	CLA	C3D-C4D-ND	4.40	117.36	110.24
20	1	613	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
23	B	843	BCR	C16-C17-C18	-4.40	121.03	127.31
27	5	607	CHL	C1D-CHD-C4C	-4.40	116.57	126.06
20	8	610	CLA	C1D-CHD-C4C	-4.40	116.57	126.06
20	B	821	CLA	C3D-C4D-ND	4.40	117.35	110.24
20	B	809	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
20	8	614	CLA	C3D-C4D-ND	4.40	117.35	110.24
20	A	828	CLA	C4A-NA-C1A	-4.40	104.73	106.71
20	6	610	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
20	Z	604	CLA	C3D-C2D-C1D	-4.39	99.83	105.83
20	7	602	CLA	C3D-C4D-ND	4.39	117.34	110.24
27	7	607	CHL	CHD-C1D-ND	-4.39	120.42	124.45
20	B	822	CLA	C3D-C2D-C1D	-4.39	99.84	105.83
20	B	819	CLA	C4A-NA-C1A	-4.39	104.73	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	827	CLA	C3D-C4D-ND	4.39	117.34	110.24
20	6	609	CLA	O2D-CGD-CBD	4.39	119.07	111.27
20	6	617	CLA	C3D-C2D-C1D	-4.39	99.85	105.83
20	6	614	CLA	C3D-C4D-ND	4.39	117.33	110.24
20	B	830	CLA	C3D-C4D-ND	4.38	117.33	110.24
20	8	606	CLA	CAA-C2A-C3A	-4.38	103.32	114.26
20	6	601	CLA	C4A-NA-C1A	-4.38	104.74	106.71
20	6	611	CLA	C4A-NA-C1A	-4.38	104.74	106.71
20	8	604	CLA	C3D-C4D-ND	4.38	117.32	110.24
23	A	851	BCR	C16-C17-C18	-4.38	121.06	127.31
20	A	836	CLA	C3D-C2D-C1D	-4.38	99.86	105.83
27	1	607	CHL	C1D-CHD-C4C	-4.37	116.62	126.06
20	B	807	CLA	C4A-NA-C1A	-4.37	104.74	106.71
20	Z	610	CLA	C4A-NA-C1A	-4.37	104.74	106.71
20	8	612	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
23	6	625	BCR	C3-C4-C5	-4.37	106.28	114.08
20	B	809	CLA	C4A-NA-C1A	-4.37	104.74	106.71
20	6	604	CLA	C4A-NA-C1A	-4.37	104.74	106.71
20	4	611	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
20	B	808	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
20	1	611	CLA	O2D-CGD-CBD	4.36	119.02	111.27
20	A	836	CLA	O2D-CGD-CBD	4.36	119.02	111.27
20	Z	611	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
23	L	205	BCR	C24-C23-C22	4.36	132.82	126.23
20	A	854	CLA	CAA-C2A-C3A	-4.36	100.85	112.78
20	B	840	CLA	C3D-C4D-ND	4.35	117.28	110.24
23	A	850	BCR	C15-C14-C13	-4.35	121.10	127.31
23	5	625	BCR	C3-C4-C5	-4.35	106.30	114.08
20	1	616	CLA	C3D-C2D-C1D	-4.35	99.89	105.83
28	Z	619	LUT	C31-C30-C29	-4.35	121.10	127.31
20	3	613	CLA	O2D-CGD-CBD	4.35	119.00	111.27
20	A	808	CLA	C3D-C4D-ND	4.35	117.28	110.24
20	1	612	CLA	O2D-CGD-CBD	4.35	119.00	111.27
20	3	610	CLA	C3D-C2D-C1D	-4.35	99.89	105.83
20	A	806	CLA	C3D-C2D-C1D	-4.35	99.89	105.83
20	8	613	CLA	O2D-CGD-CBD	4.35	118.99	111.27
20	B	819	CLA	C3D-C2D-C1D	-4.34	99.90	105.83
23	7	624	BCR	C16-C17-C18	-4.34	121.11	127.31
20	A	817	CLA	C3D-C4D-ND	4.34	117.26	110.24
20	A	821	CLA	C3D-C2D-C1D	-4.34	99.91	105.83
20	7	609	CLA	CMA-C3A-C4A	-4.34	100.11	111.77
20	3	602	CLA	C3D-C4D-ND	4.34	117.25	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	836	CLA	C3C-C4C-NC	4.33	115.43	110.57
20	A	819	CLA	C3C-C4C-NC	4.33	115.43	110.57
23	K	4001	BCR	C28-C27-C26	-4.33	106.34	114.08
20	A	830	CLA	C3D-C2D-C1D	-4.33	99.92	105.83
27	6	607	CHL	C3C-C4C-NC	4.33	115.42	110.57
20	Z	613	CLA	C3D-C2D-C1D	-4.33	99.93	105.83
20	7	612	CLA	C1D-CHD-C4C	-4.32	116.73	126.06
20	A	823	CLA	C3D-C4D-ND	4.32	117.23	110.24
23	B	847	BCR	C11-C10-C9	-4.32	121.14	127.31
20	B	833	CLA	C3D-C4D-ND	4.32	117.23	110.24
20	A	841	CLA	C4A-NA-C1A	-4.32	104.77	106.71
20	A	806	CLA	C3D-C4D-ND	4.31	117.22	110.24
20	6	613	CLA	C3D-C4D-ND	4.31	117.21	110.24
20	3	614	CLA	C3D-C4D-ND	4.31	117.21	110.24
20	Z	613	CLA	O2D-CGD-CBD	4.31	118.92	111.27
20	7	608	CLA	C3D-C4D-ND	4.31	117.21	110.24
20	8	604	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
20	A	812	CLA	C3D-C4D-ND	4.30	117.20	110.24
20	B	840	CLA	C3C-C4C-NC	4.30	115.40	110.57
27	6	607	CHL	C1C-C2C-C3C	-4.30	103.70	107.11
20	7	613	CLA	C1D-CHD-C4C	-4.30	116.78	126.06
20	B	816	CLA	C3C-C4C-NC	4.30	115.39	110.57
20	A	810	CLA	O2D-CGD-CBD	4.30	118.91	111.27
20	4	602	CLA	C3D-C4D-ND	4.30	117.19	110.24
20	4	616	CLA	C3D-C4D-ND	4.30	117.19	110.24
20	A	803	CLA	C3C-C4C-NC	4.30	115.39	110.57
20	7	604	CLA	C3D-C4D-ND	4.30	117.19	110.24
20	6	612	CLA	C1D-CHD-C4C	-4.30	116.79	126.06
20	A	816	CLA	C3D-C4D-ND	4.29	117.18	110.24
20	B	827	CLA	C3C-C4C-NC	4.29	115.38	110.57
20	Z	604	CLA	C3D-C4D-ND	4.29	117.18	110.24
20	A	831	CLA	C4A-NA-C1A	-4.29	104.78	106.71
20	A	817	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
20	A	842	CLA	C3D-C4D-ND	4.29	117.17	110.24
20	A	842	CLA	C4A-NA-C1A	-4.29	104.78	106.71
23	3	718	BCR	C15-C14-C13	-4.28	121.19	127.31
20	1	602	CLA	O2D-CGD-CBD	4.28	118.88	111.27
20	A	834	CLA	C3D-C4D-ND	4.28	117.17	110.24
20	1	614	CLA	C3D-C4D-ND	4.28	117.17	110.24
20	A	832	CLA	C3C-C4C-NC	4.28	115.37	110.57
27	5	608	CHL	C2C-C3C-C4C	-4.28	103.44	106.49
20	B	837	CLA	C4A-NA-C1A	-4.28	104.78	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	801	CL0	C3D-C2D-C1D	-4.28	99.99	105.83
20	A	840	CLA	C3C-C4C-NC	4.28	115.37	110.57
20	8	602	CLA	C3C-C4C-NC	4.28	115.37	110.57
20	B	802	CLA	O2D-CGD-CBD	4.28	118.87	111.27
20	A	841	CLA	C3D-C4D-ND	4.28	117.16	110.24
20	4	604	CLA	C3D-C4D-ND	4.28	117.16	110.24
20	B	835	CLA	C4A-NA-C1A	-4.28	104.78	106.71
23	7	624	BCR	C3-C4-C5	-4.27	106.44	114.08
20	B	810	CLA	C3D-C4D-ND	4.27	117.15	110.24
27	Z	607	CHL	C1D-CHD-C4C	-4.27	116.84	126.06
20	3	610	CLA	CMC-C2C-C1C	4.27	131.54	125.04
20	B	838	CLA	C3D-C4D-ND	4.27	117.15	110.24
20	5	621	CLA	C3C-C4C-NC	4.27	115.36	110.57
20	Z	610	CLA	C1D-CHD-C4C	-4.27	116.85	126.06
27	8	607	CHL	O2D-CGD-CBD	4.27	118.85	111.27
20	1	604	CLA	C3D-C2D-C1D	-4.27	100.01	105.83
20	3	610	CLA	O2D-CGD-CBD	4.27	118.85	111.27
20	3	613	CLA	C3D-C2D-C1D	-4.26	100.01	105.83
20	1	610	CLA	C2C-C1C-NC	4.26	113.97	109.97
20	7	604	CLA	C3C-C4C-NC	4.26	115.35	110.57
20	B	805	CLA	C3D-C4D-ND	4.26	117.13	110.24
20	B	814	CLA	C3D-C4D-ND	4.26	117.13	110.24
20	5	612	CLA	C1D-CHD-C4C	-4.26	116.86	126.06
20	1	612	CLA	C3C-C4C-NC	4.26	115.35	110.57
20	A	836	CLA	C3D-C4D-ND	4.26	117.13	110.24
20	7	612	CLA	C3D-C4D-ND	4.26	117.13	110.24
27	5	607	CHL	C1C-C2C-C3C	-4.26	103.73	107.11
20	6	602	CLA	O2D-CGD-CBD	4.26	118.83	111.27
20	8	612	CLA	C1D-CHD-C4C	-4.26	116.88	126.06
20	5	613	CLA	C3D-C2D-C1D	-4.25	100.03	105.83
20	1	612	CLA	C1D-CHD-C4C	-4.25	116.88	126.06
20	B	812	CLA	C4A-NA-C1A	-4.25	104.79	106.71
20	F	303	CLA	O2D-CGD-CBD	4.25	118.82	111.27
23	A	856	BCR	C16-C17-C18	-4.25	121.24	127.31
20	A	827	CLA	C2C-C1C-NC	4.25	113.95	109.97
27	6	607	CHL	C1D-CHD-C4C	-4.25	116.89	126.06
23	B	843	BCR	C20-C21-C22	-4.25	121.25	127.31
20	3	612	CLA	C3D-C4D-ND	4.25	117.11	110.24
20	Z	614	CLA	C3D-C4D-ND	4.25	117.11	110.24
20	5	609	CLA	C1D-CHD-C4C	-4.24	116.90	126.06
20	A	806	CLA	CAC-C3C-C4C	4.24	130.31	124.81
20	3	612	CLA	C1D-CHD-C4C	-4.24	116.91	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	850	DGD	O2G-C1B-C2B	4.24	120.64	111.50
23	6	623	BCR	C3-C4-C5	-4.24	106.51	114.08
20	6	612	CLA	C3C-C4C-NC	4.24	115.32	110.57
23	B	844	BCR	C24-C23-C22	-4.23	119.84	126.23
20	4	613	CLA	C3D-C4D-ND	4.23	117.09	110.24
20	A	829	CLA	C1D-CHD-C4C	-4.23	116.92	126.06
20	7	616	CLA	C3C-C4C-NC	4.23	115.32	110.57
20	A	807	CLA	CAA-C2A-C3A	-4.23	101.19	112.78
20	8	613	CLA	C3C-C4C-NC	4.23	115.32	110.57
20	B	831	CLA	C3D-C4D-ND	4.23	117.08	110.24
20	A	828	CLA	C2C-C1C-NC	4.23	113.93	109.97
23	4	621	BCR	C11-C10-C9	-4.23	121.28	127.31
20	F	304	CLA	C3D-C4D-ND	4.23	117.07	110.24
20	8	608	CLA	C1D-CHD-C4C	-4.23	116.94	126.06
20	B	830	CLA	C3D-C2D-C1D	-4.22	100.07	105.83
20	B	804	CLA	C4A-NA-C1A	-4.22	104.81	106.71
20	4	614	CLA	C3D-C4D-ND	4.22	117.07	110.24
20	6	602	CLA	C3D-C4D-ND	4.22	117.07	110.24
20	8	616	CLA	C3C-C4C-NC	4.22	115.31	110.57
20	7	613	CLA	C4A-NA-C1A	-4.22	104.81	106.71
20	B	811	CLA	C3D-C4D-ND	4.22	117.07	110.24
20	7	616	CLA	C3D-C4D-ND	4.22	117.07	110.24
20	A	811	CLA	C3D-C4D-ND	4.22	117.06	110.24
20	B	809	CLA	C1C-C2C-C3C	-4.22	102.52	106.96
20	A	832	CLA	C3D-C2D-C1D	-4.22	100.07	105.83
20	8	612	CLA	C3D-C4D-ND	4.22	117.06	110.24
20	A	809	CLA	C4A-NA-C1A	-4.22	104.81	106.71
20	Z	612	CLA	C3D-C4D-ND	4.22	117.06	110.24
20	Z	602	CLA	C3D-C4D-ND	4.21	117.06	110.24
28	8	617	LUT	C7-C8-C9	-4.21	119.87	126.23
20	B	825	CLA	C3D-C4D-ND	4.21	117.05	110.24
20	A	838	CLA	C3D-C2D-C1D	-4.21	100.09	105.83
20	A	854	CLA	CMD-C2D-C1D	4.21	132.13	124.71
20	7	608	CLA	O2D-CGD-CBD	4.21	118.75	111.27
20	1	604	CLA	C3D-C4D-ND	4.21	117.05	110.24
20	5	616	CLA	C1D-CHD-C4C	-4.21	116.98	126.06
28	1	619	LUT	C15-C14-C13	-4.21	121.30	127.31
20	A	812	CLA	C3C-C4C-NC	4.21	115.29	110.57
20	8	610	CLA	C2C-C1C-NC	4.21	113.91	109.97
27	3	608	CHL	O2D-CGD-CBD	4.21	118.74	111.27
20	A	811	CLA	O2D-CGD-CBD	4.20	118.74	111.27
20	7	610	CLA	C3D-C4D-ND	4.20	117.04	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	845	CLA	C4A-NA-C1A	-4.20	104.82	106.71
20	B	810	CLA	O2D-CGD-CBD	4.20	118.74	111.27
27	6	607	CHL	CHD-C1D-ND	-4.20	120.59	124.45
20	B	804	CLA	C1D-CHD-C4C	-4.20	117.00	126.06
23	L	201	BCR	C15-C14-C13	-4.20	121.32	127.31
28	4	619	LUT	C35-C34-C33	-4.20	121.32	127.31
20	A	821	CLA	C1C-C2C-C3C	-4.20	102.54	106.96
20	8	616	CLA	C3D-C2D-C1D	-4.20	100.11	105.83
20	A	804	CLA	CAA-C2A-C3A	-4.19	101.29	112.78
20	B	822	CLA	C3D-C4D-ND	4.19	117.02	110.24
20	1	609	CLA	O2D-CGD-CBD	4.19	118.72	111.27
20	B	805	CLA	C2C-C1C-NC	4.19	113.90	109.97
20	5	604	CLA	C3D-C4D-ND	4.19	117.02	110.24
20	L	204	CLA	C4A-NA-C1A	-4.19	104.82	106.71
20	A	841	CLA	C3C-C4C-NC	4.19	115.27	110.57
20	1	616	CLA	O2D-CGD-CBD	4.19	118.72	111.27
20	1	610	CLA	C3D-C4D-ND	4.19	117.01	110.24
20	8	602	CLA	C3D-C4D-ND	4.18	117.01	110.24
20	1	602	CLA	C3D-C4D-ND	4.18	117.00	110.24
20	A	854	CLA	C1D-CHD-C4C	-4.18	117.03	126.06
23	A	849	BCR	C16-C17-C18	-4.18	121.34	127.31
20	A	845	CLA	C3D-C4D-ND	4.18	117.00	110.24
20	7	606	CLA	C3D-C4D-ND	4.18	117.00	110.24
20	A	831	CLA	C3B-C4B-NB	4.18	114.62	109.21
20	7	602	CLA	C2C-C1C-NC	4.18	113.89	109.97
20	A	811	CLA	C3C-C4C-NC	4.18	115.26	110.57
22	1	620	LHG	O7-C7-C8	4.18	120.51	111.50
20	B	823	CLA	O2D-CGD-CBD	4.18	118.69	111.27
20	3	613	CLA	C3D-C4D-ND	4.18	117.00	110.24
23	3	717	BCR	C28-C27-C26	-4.18	106.62	114.08
27	6	606	CHL	C3C-C4C-NC	4.18	115.26	110.57
20	8	613	CLA	C3D-C4D-ND	4.18	117.00	110.24
20	6	612	CLA	C3D-C4D-ND	4.18	117.00	110.24
20	7	604	CLA	C4A-NA-C1A	-4.18	104.83	106.71
20	B	815	CLA	C3D-C4D-ND	4.18	117.00	110.24
20	6	609	CLA	C1D-CHD-C4C	-4.17	117.05	126.06
20	K	4002	CLA	C4A-NA-C1A	-4.17	104.83	106.71
20	B	813	CLA	C3D-C4D-ND	4.17	116.99	110.24
20	A	833	CLA	C3C-C4C-NC	4.17	115.25	110.57
27	8	607	CHL	C3C-C4C-NC	4.17	115.25	110.57
20	B	852	CLA	C3D-C4D-ND	4.17	116.98	110.24
27	4	608	CHL	C2C-C3C-C4C	-4.17	103.52	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	836	CLA	C1D-CHD-C4C	-4.17	117.07	126.06
20	F	301	CLA	C3C-C4C-NC	4.17	115.25	110.57
27	4	608	CHL	C3C-C4C-NC	4.17	115.25	110.57
20	Z	612	CLA	C1D-CHD-C4C	-4.17	117.07	126.06
20	4	603	CLA	C1C-C2C-C3C	-4.17	102.58	106.96
20	Z	610	CLA	C3D-C4D-ND	4.17	116.98	110.24
20	Z	611	CLA	C3D-C4D-ND	4.17	116.98	110.24
20	B	828	CLA	C3C-C4C-NC	4.17	115.24	110.57
20	B	829	CLA	C3C-C4C-NC	4.17	115.24	110.57
20	B	808	CLA	C1D-CHD-C4C	-4.16	117.07	126.06
28	8	618	LUT	C15-C14-C13	-4.16	121.37	127.31
20	A	843	CLA	O2D-CGD-CBD	4.16	118.67	111.27
20	5	621	CLA	C3D-C2D-C1D	-4.16	100.15	105.83
20	B	830	CLA	C3C-C4C-NC	4.16	115.24	110.57
20	7	620	CLA	C3D-C4D-ND	4.16	116.97	110.24
20	A	830	CLA	O2D-CGD-CBD	4.16	118.66	111.27
20	6	601	CLA	C3D-C4D-ND	4.16	116.97	110.24
27	6	618	CHL	C3C-C4C-NC	4.16	115.24	110.57
20	B	813	CLA	C3C-C4C-NC	4.16	115.23	110.57
23	7	623	BCR	C15-C14-C13	-4.16	121.38	127.31
19	A	801	CL0	C1D-CHD-C4C	-4.16	117.09	126.06
20	5	614	CLA	C3D-C4D-ND	4.16	116.96	110.24
20	K	4003	CLA	C3D-C4D-ND	4.15	116.95	110.24
20	4	604	CLA	C4A-NA-C1A	-4.15	104.84	106.71
23	K	4001	BCR	C16-C17-C18	-4.15	121.39	127.31
28	1	619	LUT	C35-C34-C33	-4.15	121.39	127.31
20	A	806	CLA	C4A-NA-C1A	-4.15	104.84	106.71
20	A	825	CLA	C4A-NA-C1A	-4.15	104.84	106.71
20	B	829	CLA	C3D-C2D-C1D	-4.15	100.17	105.83
20	A	824	CLA	C3D-C4D-ND	4.15	116.94	110.24
20	6	610	CLA	C3D-C4D-ND	4.14	116.94	110.24
20	8	612	CLA	C3C-C4C-NC	4.14	115.22	110.57
20	Z	610	CLA	CMC-C2C-C1C	4.14	131.35	125.04
20	B	820	CLA	C3D-C4D-ND	4.14	116.94	110.24
20	7	603	CLA	C3D-C4D-ND	4.14	116.94	110.24
20	3	617	CLA	C3D-C4D-ND	4.14	116.93	110.24
20	5	621	CLA	C1C-C2C-C3C	-4.14	102.61	106.96
23	3	718	BCR	C3-C4-C5	-4.14	106.69	114.08
20	3	613	CLA	C1D-CHD-C4C	-4.14	117.13	126.06
20	8	608	CLA	C3C-C4C-NC	4.14	115.21	110.57
20	6	609	CLA	C3C-C4C-NC	4.13	115.21	110.57
20	A	822	CLA	O2D-CGD-CBD	4.13	118.61	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	810	CLA	C3D-C2D-C1D	-4.13	100.19	105.83
20	B	832	CLA	C3D-C4D-ND	4.13	116.92	110.24
20	B	837	CLA	C3D-C4D-ND	4.13	116.92	110.24
20	B	836	CLA	CMB-C2B-C3B	4.13	132.41	124.68
20	A	825	CLA	C3D-C4D-ND	4.13	116.92	110.24
20	J	3002	CLA	CAA-C2A-C3A	-4.13	103.94	114.26
20	4	612	CLA	C3C-C4C-NC	4.13	115.20	110.57
20	7	601	CLA	C3D-C4D-ND	4.13	116.91	110.24
23	3	719	BCR	C3-C4-C5	-4.12	106.71	114.08
20	1	610	CLA	CAA-C2A-C3A	-4.12	101.49	112.78
20	3	606	CLA	C3D-C4D-ND	4.12	116.91	110.24
20	3	604	CLA	O2D-CGD-CBD	4.12	118.59	111.27
20	A	808	CLA	C3C-C4C-NC	4.12	115.19	110.57
20	B	812	CLA	C3D-C4D-ND	4.12	116.90	110.24
20	1	612	CLA	C3D-C4D-ND	4.12	116.90	110.24
20	K	4002	CLA	C3D-C4D-ND	4.11	116.89	110.24
20	A	824	CLA	C3C-C4C-NC	4.11	115.18	110.57
20	5	617	CLA	C3C-C4C-NC	4.11	115.18	110.57
20	8	602	CLA	C1D-CHD-C4C	-4.11	117.19	126.06
20	B	803	CLA	C2C-C1C-NC	4.11	113.82	109.97
20	4	609	CLA	C3C-C4C-NC	4.11	115.18	110.57
20	1	604	CLA	C4A-NA-C1A	-4.11	104.86	106.71
23	B	843	BCR	C15-C16-C17	-4.11	115.06	123.47
20	B	804	CLA	C3C-C4C-NC	4.11	115.18	110.57
20	Z	610	CLA	C2C-C1C-NC	4.11	113.82	109.97
20	6	616	CLA	C3D-C4D-ND	4.11	116.88	110.24
20	B	807	CLA	C3D-C4D-ND	4.10	116.88	110.24
20	J	3002	CLA	C3D-C4D-ND	4.10	116.88	110.24
20	5	601	CLA	C3D-C4D-ND	4.10	116.88	110.24
20	6	613	CLA	C4A-NA-C1A	-4.10	104.86	106.71
20	B	812	CLA	O2D-CGD-CBD	4.10	118.56	111.27
22	Z	620	LHG	O7-C7-C8	4.10	120.34	111.50
23	I	172	BCR	C3-C4-C5	-4.10	106.75	114.08
20	Z	609	CLA	C1D-CHD-C4C	-4.10	117.21	126.06
20	5	612	CLA	C3D-C4D-ND	4.10	116.87	110.24
27	7	607	CHL	C1D-CHD-C4C	-4.10	117.22	126.06
20	8	601	CLA	C3C-C4C-NC	4.10	115.17	110.57
23	6	625	BCR	C28-C27-C26	-4.10	106.76	114.08
20	A	845	CLA	C3C-C4C-NC	4.10	115.16	110.57
20	3	610	CLA	C3D-C4D-ND	4.09	116.86	110.24
20	A	838	CLA	C3D-C4D-ND	4.09	116.86	110.24
20	3	613	CLA	CAC-C3C-C4C	4.09	130.12	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	604	CLA	C3D-C4D-ND	4.09	116.86	110.24
20	1	603	CLA	C1C-C2C-C3C	-4.09	102.66	106.96
20	B	832	CLA	C1D-CHD-C4C	-4.09	117.23	126.06
23	J	3003	BCR	C20-C21-C22	-4.09	121.47	127.31
20	B	816	CLA	C1D-CHD-C4C	-4.09	117.24	126.06
20	B	834	CLA	C3D-C4D-ND	4.09	116.85	110.24
20	3	620	CLA	C3D-C4D-ND	4.09	116.85	110.24
20	A	831	CLA	C1D-CHD-C4C	-4.09	117.24	126.06
20	A	803	CLA	C3B-C4B-NB	4.09	114.49	109.21
20	4	603	CLA	C1D-CHD-C4C	-4.09	117.24	126.06
20	4	609	CLA	C1C-C2C-C3C	-4.09	102.66	106.96
20	B	828	CLA	C3D-C2D-C1D	-4.08	100.26	105.83
20	Z	603	CLA	C3D-C4D-ND	4.08	116.84	110.24
20	A	835	CLA	C3D-C4D-ND	4.08	116.84	110.24
20	4	609	CLA	C3D-C4D-ND	4.08	116.84	110.24
23	B	846	BCR	C15-C14-C13	-4.08	121.48	127.31
20	1	610	CLA	C1D-CHD-C4C	-4.08	117.25	126.06
20	4	601	CLA	C3D-C4D-ND	4.08	116.84	110.24
20	B	826	CLA	C3D-C4D-ND	4.08	116.84	110.24
20	5	609	CLA	C3C-C4C-NC	4.08	115.15	110.57
20	1	613	CLA	C3D-C4D-ND	4.08	116.84	110.24
20	A	810	CLA	C3D-C4D-ND	4.08	116.84	110.24
20	Z	606	CLA	C3D-C4D-ND	4.08	116.84	110.24
20	A	842	CLA	C3C-C4C-NC	4.08	115.15	110.57
23	3	718	BCR	C7-C8-C9	-4.08	120.07	126.23
20	6	617	CLA	C3D-C4D-ND	4.08	116.83	110.24
20	A	818	CLA	C3C-C4C-NC	4.08	115.14	110.57
20	Z	602	CLA	C3C-C4C-NC	4.08	115.14	110.57
20	A	803	CLA	C1D-CHD-C4C	-4.08	117.27	126.06
20	A	825	CLA	O2D-CGD-CBD	4.08	118.51	111.27
20	4	612	CLA	C3D-C4D-ND	4.08	116.83	110.24
20	A	814	CLA	C3D-C4D-ND	4.07	116.83	110.24
23	8	619	BCR	C15-C14-C13	-4.07	121.50	127.31
20	A	810	CLA	O2A-CGA-CBA	4.07	124.69	111.91
20	A	802	CLA	C4A-NA-C1A	-4.07	104.88	106.71
20	A	836	CLA	C1C-C2C-C3C	-4.07	102.68	106.96
20	G	203	CLA	C3D-C4D-ND	4.07	116.82	110.24
20	Z	613	CLA	C3D-C4D-ND	4.07	116.82	110.24
20	A	818	CLA	C1D-CHD-C4C	-4.07	117.28	126.06
20	B	802	CLA	C3D-C4D-ND	4.07	116.82	110.24
20	A	812	CLA	C1D-CHD-C4C	-4.07	117.28	126.06
20	4	610	CLA	C3D-C4D-ND	4.07	116.82	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	606	CLA	C3D-C4D-ND	4.07	116.82	110.24
20	8	609	CLA	C3C-C4C-NC	4.07	115.13	110.57
20	A	813	CLA	C3D-C4D-ND	4.07	116.82	110.24
20	B	839	CLA	C3C-C4C-NC	4.07	115.13	110.57
20	7	610	CLA	C1D-CHD-C4C	-4.07	117.29	126.06
20	B	833	CLA	C1D-CHD-C4C	-4.06	117.29	126.06
20	A	820	CLA	C3D-C4D-ND	4.06	116.81	110.24
20	5	610	CLA	C3D-C4D-ND	4.06	116.81	110.24
20	A	809	CLA	C3D-C4D-ND	4.06	116.81	110.24
20	B	819	CLA	C3D-C4D-ND	4.06	116.81	110.24
20	B	839	CLA	C3D-C4D-ND	4.06	116.81	110.24
20	B	802	CLA	CMA-C3A-C4A	-4.06	100.86	111.77
20	F	303	CLA	C3C-C4C-NC	4.06	115.12	110.57
20	5	606	CLA	C3D-C4D-ND	4.06	116.81	110.24
27	4	606	CHL	C3C-C4C-NC	4.06	115.12	110.57
20	1	611	CLA	C3C-C4C-NC	4.06	115.12	110.57
22	A	847	LHG	O7-C7-C8	4.06	120.25	111.50
20	Z	613	CLA	C1D-CHD-C4C	-4.06	117.31	126.06
20	4	603	CLA	C3B-C4B-NB	4.05	114.45	109.21
22	5	623	LHG	O7-C7-C8	4.05	120.24	111.50
20	F	304	CLA	C3C-C4C-NC	4.05	115.11	110.57
20	3	620	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
20	F	304	CLA	C1D-CHD-C4C	-4.05	117.32	126.06
20	K	4003	CLA	C1D-CHD-C4C	-4.05	117.32	126.06
20	5	621	CLA	C1D-CHD-C4C	-4.05	117.32	126.06
20	3	611	CLA	C4A-NA-C1A	-4.05	104.89	106.71
20	4	610	CLA	C1D-CHD-C4C	-4.05	117.33	126.06
20	3	606	CLA	CAA-C2A-C3A	-4.05	104.15	114.26
20	7	601	CLA	C3C-C4C-NC	4.05	115.11	110.57
20	7	608	CLA	C1C-C2C-C3C	-4.04	102.70	106.96
20	Z	603	CLA	C1C-C2C-C3C	-4.04	102.70	106.96
27	6	608	CHL	C3C-C4C-NC	4.04	115.11	110.57
20	G	204	CLA	C3D-C4D-ND	4.04	116.78	110.24
20	A	839	CLA	C3D-C4D-ND	4.04	116.78	110.24
20	B	827	CLA	C4A-NA-C1A	-4.04	104.89	106.71
20	B	802	CLA	C1D-CHD-C4C	-4.04	117.34	126.06
20	B	825	CLA	CAA-C2A-C3A	-4.04	101.72	112.78
27	3	608	CHL	C1D-CHD-C4C	-4.04	117.35	126.06
20	B	827	CLA	C3D-C4D-ND	4.03	116.76	110.24
20	4	614	CLA	C3C-C4C-NC	4.03	115.09	110.57
20	B	817	CLA	C3D-C4D-ND	4.03	116.76	110.24
20	A	838	CLA	C1C-C2C-C3C	-4.03	102.72	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	834	CLA	O2D-CGD-CBD	4.03	118.43	111.27
20	B	824	CLA	C3D-C2D-C1D	-4.03	100.33	105.83
20	A	842	CLA	C1D-CHD-C4C	-4.03	117.37	126.06
20	7	606	CLA	C3C-C4C-NC	4.03	115.09	110.57
20	B	826	CLA	C1D-CHD-C4C	-4.03	117.37	126.06
20	F	303	CLA	C1D-CHD-C4C	-4.03	117.37	126.06
23	F	305	BCR	C7-C8-C9	-4.03	120.15	126.23
20	7	604	CLA	C1D-CHD-C4C	-4.02	117.38	126.06
20	1	606	CLA	C3C-C4C-NC	4.02	115.08	110.57
23	5	625	BCR	C11-C12-C13	-4.02	115.11	126.42
20	6	604	CLA	C3D-C4D-ND	4.02	116.74	110.24
23	K	4001	BCR	C15-C16-C17	-4.02	115.24	123.47
20	A	810	CLA	C1D-CHD-C4C	-4.02	117.39	126.06
20	8	606	CLA	C3D-C4D-ND	4.02	116.74	110.24
20	Z	602	CLA	C1D-CHD-C4C	-4.02	117.39	126.06
20	A	826	CLA	C1D-CHD-C4C	-4.02	117.39	126.06
20	B	852	CLA	C3C-C4C-NC	4.02	115.08	110.57
20	A	830	CLA	C3D-C4D-ND	4.02	116.73	110.24
20	4	603	CLA	C3D-C4D-ND	4.02	116.73	110.24
27	6	606	CHL	C1D-CHD-C4C	-4.02	117.40	126.06
20	6	622	CLA	C3D-C4D-ND	4.02	116.73	110.24
20	A	843	CLA	C3C-C4C-NC	4.01	115.07	110.57
20	B	824	CLA	C3D-C4D-ND	4.01	116.73	110.24
20	8	616	CLA	C1D-CHD-C4C	-4.01	117.41	126.06
23	4	621	BCR	C28-C27-C26	-4.01	106.92	114.08
20	7	613	CLA	C3C-C4C-NC	4.01	115.07	110.57
20	A	821	CLA	C3D-C4D-ND	4.01	116.72	110.24
20	B	841	CLA	C3D-C4D-ND	4.01	116.72	110.24
20	8	603	CLA	C3D-C4D-ND	4.01	116.72	110.24
23	A	852	BCR	C20-C19-C18	-4.01	115.16	126.42
20	B	810	CLA	C1D-CHD-C4C	-4.01	117.42	126.06
20	B	814	CLA	C1D-CHD-C4C	-4.00	117.42	126.06
23	A	851	BCR	C20-C21-C22	-4.00	121.60	127.31
20	1	616	CLA	C4A-NA-C1A	-4.00	104.91	106.71
27	8	607	CHL	CHD-C1D-ND	-4.00	120.78	124.45
20	A	843	CLA	C1D-CHD-C4C	-4.00	117.43	126.06
19	A	801	CL0	C3D-C4D-ND	4.00	116.71	110.24
20	B	837	CLA	C3C-C4C-NC	4.00	115.05	110.57
20	1	610	CLA	O2A-CGA-CBA	4.00	124.45	111.91
20	1	611	CLA	C3D-C4D-ND	4.00	116.70	110.24
20	A	838	CLA	C1D-CHD-C4C	-4.00	117.44	126.06
20	8	603	CLA	C3C-C4C-NC	4.00	115.05	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Z	610	CLA	C3C-C4C-NC	3.99	115.05	110.57
20	Z	609	CLA	C3D-C4D-ND	3.99	116.69	110.24
20	B	824	CLA	C3C-C4C-NC	3.99	115.05	110.57
20	B	808	CLA	C3D-C4D-ND	3.99	116.69	110.24
27	4	608	CHL	C1D-CHD-C4C	-3.99	117.45	126.06
20	B	832	CLA	C1C-C2C-C3C	-3.99	102.76	106.96
20	B	828	CLA	C3D-C4D-ND	3.99	116.69	110.24
20	A	816	CLA	C3C-C4C-NC	3.99	115.04	110.57
20	1	603	CLA	C3D-C4D-ND	3.99	116.69	110.24
20	5	617	CLA	C3D-C4D-ND	3.99	116.69	110.24
20	B	826	CLA	C3C-C4C-NC	3.99	115.04	110.57
20	3	610	CLA	O2A-CGA-CBA	3.99	124.42	111.91
20	B	828	CLA	C1D-CHD-C4C	-3.99	117.46	126.06
20	6	601	CLA	C1C-C2C-C3C	-3.98	102.77	106.96
20	B	816	CLA	C3D-C4D-ND	3.98	116.68	110.24
20	6	611	CLA	C3D-C4D-ND	3.98	116.68	110.24
23	L	205	BCR	C16-C17-C18	-3.98	121.62	127.31
20	F	303	CLA	C3D-C4D-ND	3.98	116.68	110.24
20	A	845	CLA	C1D-CHD-C4C	-3.98	117.47	126.06
20	F	301	CLA	C3D-C4D-ND	3.98	116.68	110.24
20	1	614	CLA	C1D-CHD-C4C	-3.98	117.47	126.06
20	4	613	CLA	C1D-CHD-C4C	-3.98	117.47	126.06
20	B	811	CLA	C1D-CHD-C4C	-3.98	117.47	126.06
20	A	843	CLA	C3D-C4D-ND	3.98	116.68	110.24
20	8	604	CLA	C4A-NA-C1A	-3.98	104.92	106.71
20	1	602	CLA	C3C-C4C-NC	3.98	115.03	110.57
23	8	619	BCR	C16-C17-C18	-3.98	121.63	127.31
20	1	611	CLA	C1D-CHD-C4C	-3.98	117.48	126.06
20	7	612	CLA	C3C-C4C-NC	3.98	115.03	110.57
20	6	613	CLA	C3C-C4C-NC	3.98	115.03	110.57
20	5	617	CLA	C4A-NA-C1A	-3.98	104.92	106.71
20	6	616	CLA	O2D-CGD-CBD	3.98	118.33	111.27
20	B	823	CLA	C3D-C4D-ND	3.98	116.67	110.24
20	1	606	CLA	C1D-CHD-C4C	-3.98	117.48	126.06
20	3	610	CLA	C2C-C1C-NC	3.97	113.69	109.97
20	3	612	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
27	8	607	CHL	C1D-CHD-C4C	-3.97	117.50	126.06
20	B	805	CLA	C4A-NA-C1A	-3.97	104.92	106.71
23	3	717	BCR	C11-C10-C9	-3.96	121.65	127.31
20	6	603	CLA	C1C-C2C-C3C	-3.96	102.79	106.96
20	A	841	CLA	C1D-CHD-C4C	-3.96	117.51	126.06
22	6	619	LHG	O7-C7-C8	3.96	120.04	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	820	CLA	C3C-C4C-NC	3.96	115.01	110.57
20	B	823	CLA	C3C-C4C-NC	3.96	115.01	110.57
20	3	611	CLA	C3D-C4D-ND	3.96	116.64	110.24
20	B	814	CLA	C3C-C4C-NC	3.96	115.01	110.57
27	3	608	CHL	CBC-CAC-C3C	-3.96	101.52	112.43
20	1	608	CLA	C3C-C4C-NC	3.96	115.01	110.57
20	3	613	CLA	C3C-C4C-NC	3.96	115.01	110.57
20	7	601	CLA	C1D-CHD-C4C	-3.96	117.52	126.06
20	5	617	CLA	C1D-CHD-C4C	-3.96	117.52	126.06
20	K	4003	CLA	C3C-C4C-NC	3.96	115.01	110.57
20	A	839	CLA	C1C-C2C-C3C	-3.96	102.80	106.96
20	B	823	CLA	C1D-CHD-C4C	-3.95	117.53	126.06
20	B	821	CLA	C4A-NA-C1A	-3.95	104.93	106.71
23	A	849	BCR	C15-C14-C13	-3.95	121.67	127.31
20	B	825	CLA	C3D-C2D-C1D	-3.95	100.44	105.83
20	Z	611	CLA	C4A-NA-C1A	-3.95	104.93	106.71
20	B	841	CLA	C3C-C4C-NC	3.95	115.00	110.57
20	7	606	CLA	C1D-CHD-C4C	-3.95	117.53	126.06
20	B	834	CLA	C4A-NA-C1A	-3.95	104.93	106.71
20	6	617	CLA	C1D-CHD-C4C	-3.95	117.54	126.06
20	1	616	CLA	C3D-C4D-ND	3.95	116.62	110.24
20	7	606	CLA	CAA-C2A-C3A	-3.95	104.40	114.26
20	7	616	CLA	C3D-C2D-C1D	-3.95	100.45	105.83
20	3	603	CLA	C3D-C4D-ND	3.95	116.62	110.24
27	7	607	CHL	C3C-C4C-NC	3.95	115.00	110.57
20	A	807	CLA	C3D-C4D-ND	3.95	116.62	110.24
20	1	609	CLA	C3D-C4D-ND	3.95	116.62	110.24
20	8	613	CLA	C1D-CHD-C4C	-3.94	117.55	126.06
23	B	847	BCR	C15-C16-C17	-3.94	115.39	123.47
20	5	613	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
20	B	807	CLA	C3C-C4C-NC	3.94	114.99	110.57
20	A	826	CLA	C3D-C4D-ND	3.94	116.61	110.24
20	B	822	CLA	C3C-C4C-NC	3.94	114.99	110.57
20	5	601	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
20	B	818	CLA	C1D-CHD-C4C	-3.94	117.56	126.06
20	Z	608	CLA	O2D-CGD-CBD	3.94	118.27	111.27
20	1	609	CLA	C1D-CHD-C4C	-3.94	117.56	126.06
20	5	613	CLA	C1D-CHD-C4C	-3.94	117.56	126.06
20	A	827	CLA	CAA-C2A-C3A	-3.94	102.00	112.78
20	4	616	CLA	C3C-C4C-NC	3.94	114.98	110.57
20	B	829	CLA	C1D-CHD-C4C	-3.94	117.57	126.06
20	7	609	CLA	C1D-CHD-C4C	-3.94	117.57	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	820	CLA	C1C-C2C-C3C	-3.93	102.82	106.96
20	B	811	CLA	C3C-C4C-NC	3.93	114.98	110.57
20	A	843	CLA	C4A-NA-C1A	-3.93	104.94	106.71
20	3	609	CLA	C1D-CHD-C4C	-3.93	117.58	126.06
20	7	614	CLA	C3D-C4D-ND	3.93	116.60	110.24
20	B	802	CLA	CAA-C2A-C3A	-3.93	102.02	112.78
20	A	803	CLA	C3D-C4D-ND	3.93	116.59	110.24
20	B	802	CLA	C4A-NA-C1A	-3.93	104.94	106.71
20	3	604	CLA	C1C-C2C-C3C	-3.93	102.83	106.96
20	8	603	CLA	C1D-CHD-C4C	-3.93	117.58	126.06
20	A	831	CLA	C3D-C4D-ND	3.93	116.59	110.24
20	A	809	CLA	C1C-C2C-C3C	-3.92	102.83	106.96
20	5	609	CLA	C3D-C4D-ND	3.92	116.59	110.24
20	5	613	CLA	C3D-C4D-ND	3.92	116.59	110.24
20	7	604	CLA	CMC-C2C-C1C	3.92	131.01	125.04
20	A	805	CLA	C3D-C4D-ND	3.92	116.58	110.24
20	A	832	CLA	C3D-C4D-ND	3.92	116.58	110.24
23	K	4001	BCR	C3-C4-C5	-3.92	107.08	114.08
20	8	606	CLA	C1C-C2C-C3C	-3.92	102.83	106.96
20	1	616	CLA	C3C-C4C-NC	3.92	114.97	110.57
20	8	606	CLA	C3C-C4C-NC	3.92	114.97	110.57
20	7	611	CLA	C3D-C4D-ND	3.92	116.58	110.24
20	6	604	CLA	C3C-C4C-NC	3.92	114.97	110.57
20	5	606	CLA	C1C-C2C-C3C	-3.92	102.84	106.96
20	A	830	CLA	C1D-CHD-C4C	-3.92	117.61	126.06
23	L	201	BCR	C16-C17-C18	-3.92	121.72	127.31
27	6	608	CHL	C2C-C3C-C4C	-3.92	103.70	106.49
20	Z	610	CLA	O2A-CGA-CBA	3.91	124.19	111.91
20	3	603	CLA	C1C-C2C-C3C	-3.91	102.84	106.96
20	5	603	CLA	C1C-C2C-C3C	-3.91	102.84	106.96
20	A	821	CLA	C4A-NA-C1A	-3.91	104.95	106.71
20	3	609	CLA	C4A-NA-C1A	-3.91	104.95	106.71
27	1	607	CHL	O2D-CGD-CBD	3.91	118.22	111.27
20	Z	613	CLA	C4A-NA-C1A	-3.91	104.95	106.71
20	A	821	CLA	C1D-CHD-C4C	-3.91	117.62	126.06
20	A	815	CLA	C3C-C4C-NC	3.91	114.96	110.57
20	1	612	CLA	C1C-C2C-C3C	-3.91	102.85	106.96
20	Z	608	CLA	C3C-C4C-NC	3.91	114.95	110.57
23	A	850	BCR	C28-C27-C26	-3.91	107.10	114.08
23	K	4001	BCR	C7-C8-C9	-3.91	120.33	126.23
20	B	841	CLA	C1D-CHD-C4C	-3.91	117.63	126.06
20	8	610	CLA	CAA-C2A-C3A	-3.91	102.08	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	813	CLA	C3C-C4C-NC	3.91	114.95	110.57
20	5	616	CLA	C1C-C2C-C3C	-3.90	102.85	106.96
20	3	610	CLA	C1D-CHD-C4C	-3.90	117.64	126.06
20	7	609	CLA	C3D-C4D-ND	3.90	116.55	110.24
20	B	815	CLA	C1D-CHD-C4C	-3.90	117.64	126.06
27	5	607	CHL	C2A-C3A-C4A	-3.90	95.56	101.87
20	3	609	CLA	C3D-C4D-ND	3.90	116.55	110.24
20	5	611	CLA	C1D-CHD-C4C	-3.90	117.64	126.06
20	A	804	CLA	C3C-C4C-NC	3.90	114.95	110.57
22	B	851	LHG	O7-C7-C8	3.90	119.91	111.50
20	B	812	CLA	C1D-CHD-C4C	-3.90	117.64	126.06
20	4	611	CLA	C1D-CHD-C4C	-3.90	117.64	126.06
20	8	612	CLA	O2D-CGD-CBD	3.90	118.20	111.27
20	7	613	CLA	C3D-C4D-ND	3.90	116.55	110.24
20	8	616	CLA	C3D-C4D-ND	3.90	116.55	110.24
20	6	609	CLA	C1C-C2C-C3C	-3.90	102.86	106.96
20	A	839	CLA	C1D-CHD-C4C	-3.90	117.65	126.06
20	5	601	CLA	C3C-C4C-NC	3.90	114.94	110.57
20	6	602	CLA	C3C-C4C-NC	3.90	114.94	110.57
20	3	607	CLA	CAA-C2A-C3A	-3.90	102.11	112.78
20	B	807	CLA	C1C-C2C-C3C	-3.90	102.86	106.96
20	Z	614	CLA	C1D-CHD-C4C	-3.90	117.66	126.06
20	B	817	CLA	C4A-NA-C1A	-3.89	104.95	106.71
20	1	613	CLA	C1D-CHD-C4C	-3.89	117.66	126.06
20	A	808	CLA	C1C-C2C-C3C	-3.89	102.86	106.96
20	B	833	CLA	C3C-C4C-NC	3.89	114.94	110.57
22	7	625	LHG	O7-C7-C8	3.89	119.89	111.50
20	A	839	CLA	C3C-C4C-NC	3.89	114.93	110.57
20	B	812	CLA	C3C-C4C-NC	3.89	114.93	110.57
20	A	833	CLA	C1D-CHD-C4C	-3.89	117.67	126.06
20	A	817	CLA	C1D-CHD-C4C	-3.89	117.67	126.06
20	B	806	CLA	C3C-C4C-NC	3.89	114.93	110.57
20	Z	610	CLA	CAA-C2A-C3A	-3.89	102.13	112.78
22	4	623	LHG	O7-C7-C8	3.89	119.88	111.50
20	5	604	CLA	C1C-C2C-C3C	-3.89	102.87	106.96
20	A	809	CLA	C3C-C4C-NC	3.89	114.93	110.57
20	8	601	CLA	C1C-C2C-C3C	-3.89	102.87	106.96
20	A	820	CLA	C1C-C2C-C3C	-3.89	102.87	106.96
20	3	602	CLA	C1D-CHD-C4C	-3.89	117.68	126.06
20	5	603	CLA	C1D-CHD-C4C	-3.89	117.68	126.06
20	7	608	CLA	C1D-CHD-C4C	-3.88	117.68	126.06
20	B	823	CLA	C4A-NA-C1A	-3.88	104.96	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	5	612	CLA	C3C-C4C-NC	3.88	114.93	110.57
20	B	835	CLA	C3D-C4D-ND	3.88	116.52	110.24
20	1	612	CLA	C3B-C4B-NB	3.88	114.23	109.21
27	6	608	CHL	C1D-CHD-C4C	-3.88	117.68	126.06
20	3	606	CLA	C3C-C4C-NC	3.88	114.92	110.57
28	4	620	LUT	C35-C34-C33	-3.88	121.77	127.31
20	A	831	CLA	C1C-C2C-C3C	-3.88	102.88	106.96
20	B	810	CLA	C1C-C2C-C3C	-3.88	102.88	106.96
19	A	801	CL0	C3B-C4B-NB	3.88	114.22	109.21
20	A	836	CLA	C1D-CHD-C4C	-3.88	117.69	126.06
20	B	839	CLA	C1D-CHD-C4C	-3.88	117.69	126.06
20	8	609	CLA	C1D-CHD-C4C	-3.88	117.69	126.06
20	6	609	CLA	C3D-C4D-ND	3.88	116.51	110.24
20	A	825	CLA	C3B-C4B-NB	3.88	114.22	109.21
20	A	835	CLA	C1D-CHD-C4C	-3.88	117.69	126.06
20	B	838	CLA	C1C-C2C-C3C	-3.88	102.88	106.96
20	3	607	CLA	C1D-CHD-C4C	-3.88	117.70	126.06
20	A	827	CLA	O2D-CGD-CBD	3.88	118.16	111.27
20	8	611	CLA	C1C-C2C-C3C	-3.87	102.88	106.96
20	A	807	CLA	C1C-C2C-C3C	-3.87	102.88	106.96
20	B	806	CLA	C1D-CHD-C4C	-3.87	117.70	126.06
20	B	838	CLA	C3C-C4C-NC	3.87	114.91	110.57
20	B	818	CLA	C3D-C4D-ND	3.87	116.50	110.24
20	6	603	CLA	C1D-CHD-C4C	-3.87	117.71	126.06
20	A	802	CLA	C3D-C4D-ND	3.87	116.50	110.24
27	4	618	CHL	C1D-CHD-C4C	-3.87	117.71	126.06
20	7	620	CLA	C4A-NA-C1A	-3.87	104.97	106.71
20	3	603	CLA	C3C-C4C-NC	3.87	114.91	110.57
20	7	601	CLA	O2A-CGA-CBA	3.87	124.05	111.91
20	A	815	CLA	C1D-CHD-C4C	-3.87	117.71	126.06
20	8	608	CLA	C4A-NA-C1A	-3.87	104.97	106.71
20	Z	608	CLA	C1D-CHD-C4C	-3.87	117.72	126.06
20	5	604	CLA	C1D-CHD-C4C	-3.87	117.72	126.06
20	B	809	CLA	C3B-C4B-NB	3.87	114.21	109.21
20	B	840	CLA	C3B-C4B-NB	3.87	114.21	109.21
20	Z	606	CLA	C1D-CHD-C4C	-3.87	117.72	126.06
20	5	610	CLA	C1D-CHD-C4C	-3.87	117.72	126.06
20	A	817	CLA	C4A-NA-C1A	-3.86	104.97	106.71
20	3	613	CLA	C1C-C2C-C3C	-3.86	102.89	106.96
20	8	606	CLA	C1D-CHD-C4C	-3.86	117.72	126.06
20	A	832	CLA	C1D-CHD-C4C	-3.86	117.73	126.06
20	A	834	CLA	C1C-C2C-C3C	-3.86	102.90	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	5	616	CLA	C3C-C4C-NC	3.86	114.90	110.57
28	5	620	LUT	C35-C34-C33	-3.86	121.80	127.31
20	Z	611	CLA	C1D-CHD-C4C	-3.86	117.73	126.06
20	L	203	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
20	B	825	CLA	C1D-CHD-C4C	-3.86	117.73	126.06
20	A	819	CLA	C3D-C4D-ND	3.86	116.48	110.24
20	5	611	CLA	C3C-C4C-NC	3.86	114.90	110.57
20	1	610	CLA	CMC-C2C-C1C	3.86	130.92	125.04
20	5	602	CLA	C1D-CHD-C4C	-3.86	117.73	126.06
20	6	616	CLA	CMB-C2B-C3B	3.86	131.89	124.68
20	7	613	CLA	C1C-C2C-C3C	-3.85	102.90	106.96
27	5	618	CHL	C3C-C4C-NC	3.85	114.89	110.57
20	B	804	CLA	C3D-C4D-ND	3.85	116.47	110.24
20	6	603	CLA	C3D-C4D-ND	3.85	116.47	110.24
20	8	608	CLA	C3D-C4D-ND	3.85	116.47	110.24
20	5	616	CLA	C3D-C4D-ND	3.85	116.47	110.24
22	8	620	LHG	O7-C7-C8	3.85	119.80	111.50
20	5	604	CLA	CAC-C3C-C4C	3.85	129.81	124.81
20	Z	604	CLA	C4A-NA-C1A	-3.85	104.97	106.71
20	B	835	CLA	C3C-C4C-NC	3.85	114.89	110.57
20	1	614	CLA	C3C-C4C-NC	3.85	114.89	110.57
20	1	602	CLA	C1D-CHD-C4C	-3.85	117.75	126.06
20	3	607	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
20	5	611	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
23	B	845	BCR	C16-C17-C18	-3.85	121.82	127.31
23	5	622	BCR	C28-C27-C26	-3.85	107.21	114.08
20	A	837	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
20	A	822	CLA	C3D-C4D-ND	3.85	116.46	110.24
20	A	840	CLA	C3D-C4D-ND	3.85	116.46	110.24
20	4	611	CLA	C3D-C4D-ND	3.85	116.46	110.24
20	Z	609	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
20	6	617	CLA	C3C-C4C-NC	3.84	114.88	110.57
27	Z	601	CHL	C1D-CHD-C4C	-3.84	117.77	126.06
20	1	610	CLA	C3C-C4C-NC	3.84	114.88	110.57
20	A	829	CLA	O2D-CGD-CBD	3.84	118.10	111.27
20	1	608	CLA	C3D-C4D-ND	3.84	116.45	110.24
20	A	802	CLA	O2D-CGD-CBD	3.84	118.10	111.27
27	3	608	CHL	C3C-C4C-NC	3.84	114.88	110.57
20	J	3002	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
20	7	608	CLA	C3C-C4C-NC	3.84	114.88	110.57
20	1	608	CLA	O2D-CGD-CBD	3.84	118.09	111.27
20	A	824	CLA	C1C-C2C-C3C	-3.84	102.92	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Z	616	CLA	C3D-C4D-ND	3.84	116.45	110.24
20	Z	616	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
23	K	4004	BCR	C15-C14-C13	-3.84	121.84	127.31
23	3	717	BCR	C21-C20-C19	-3.83	111.25	123.22
27	4	607	CHL	C3C-C4C-NC	3.83	114.87	110.57
20	B	803	CLA	CAA-C2A-C3A	-3.83	102.29	112.78
23	3	719	BCR	C39-C30-C25	-3.83	104.09	110.30
20	4	611	CLA	C4A-NA-C1A	-3.83	104.98	106.71
20	Z	609	CLA	O2D-CGD-CBD	3.83	118.07	111.27
20	7	611	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
20	8	609	CLA	C3D-C4D-ND	3.83	116.43	110.24
20	Z	606	CLA	C3C-C4C-NC	3.83	114.86	110.57
20	A	832	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
20	8	610	CLA	C3D-C4D-ND	3.83	116.43	110.24
20	B	811	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
23	B	846	BCR	C3-C4-C5	-3.83	107.25	114.08
20	3	612	CLA	C3C-C4C-NC	3.83	114.86	110.57
20	B	835	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
20	1	609	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
20	4	611	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
20	B	829	CLA	CMB-C2B-C1B	3.82	134.34	128.46
20	8	601	CLA	C1D-CHD-C4C	-3.82	117.81	126.06
20	B	803	CLA	O2D-CGD-CBD	3.82	118.06	111.27
20	4	614	CLA	C1D-CHD-C4C	-3.82	117.81	126.06
20	1	608	CLA	C1D-CHD-C4C	-3.82	117.81	126.06
20	3	602	CLA	C4A-NA-C1A	-3.82	104.99	106.71
20	8	614	CLA	C3C-C4C-NC	3.82	114.85	110.57
20	Z	613	CLA	C3C-C4C-NC	3.82	114.85	110.57
20	5	617	CLA	C3B-C4B-NB	3.82	114.15	109.21
20	7	611	CLA	C1D-CHD-C4C	-3.82	117.82	126.06
27	6	618	CHL	C1D-CHD-C4C	-3.82	117.83	126.06
20	A	807	CLA	C1D-CHD-C4C	-3.82	117.83	126.06
20	Z	614	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
23	A	849	BCR	C20-C21-C22	-3.81	121.87	127.31
20	7	614	CLA	C3C-C4C-NC	3.81	114.84	110.57
20	4	616	CLA	C1D-CHD-C4C	-3.81	117.84	126.06
20	7	603	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
23	F	305	BCR	C3-C4-C5	-3.81	107.28	114.08
20	A	813	CLA	C1D-CHD-C4C	-3.81	117.84	126.06
20	B	825	CLA	C3C-C4C-NC	3.81	114.84	110.57
20	Z	608	CLA	C3D-C4D-ND	3.81	116.39	110.24
20	8	611	CLA	C1D-CHD-C4C	-3.80	117.85	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	8	619	BCR	C3-C4-C5	-3.80	107.29	114.08
28	8	618	LUT	C35-C34-C33	-3.80	121.89	127.31
20	8	611	CLA	C3C-C4C-NC	3.80	114.83	110.57
27	4	606	CHL	C1D-CHD-C4C	-3.80	117.86	126.06
20	Z	616	CLA	C1D-CHD-C4C	-3.80	117.86	126.06
20	A	842	CLA	C1C-C2C-C3C	-3.80	102.96	106.96
20	G	204	CLA	C1C-C2C-C3C	-3.80	102.96	106.96
20	3	611	CLA	C1D-CHD-C4C	-3.80	117.86	126.06
20	A	854	CLA	C3D-C4D-ND	3.80	116.38	110.24
20	6	617	CLA	CAA-C2A-C3A	-3.80	102.38	112.78
20	B	852	CLA	C1D-CHD-C4C	-3.80	117.87	126.06
20	1	616	CLA	C1D-CHD-C4C	-3.80	117.87	126.06
23	K	4004	BCR	C24-C23-C22	-3.80	120.50	126.23
20	B	824	CLA	C1D-CHD-C4C	-3.80	117.87	126.06
20	5	606	CLA	C1D-CHD-C4C	-3.80	117.87	126.06
20	A	829	CLA	C3D-C4D-ND	3.79	116.38	110.24
20	Z	614	CLA	C3C-C4C-NC	3.79	114.82	110.57
20	A	807	CLA	C3C-C4C-NC	3.79	114.82	110.57
20	3	606	CLA	C1D-CHD-C4C	-3.79	117.88	126.06
20	Z	611	CLA	C3C-C4C-NC	3.79	114.82	110.57
20	A	835	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
20	Z	616	CLA	C3C-C4C-NC	3.79	114.82	110.57
23	5	622	BCR	C3-C4-C5	-3.79	107.31	114.08
23	6	625	BCR	C11-C10-C9	-3.79	121.90	127.31
20	Z	604	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
20	A	806	CLA	C1D-CHD-C4C	-3.79	117.89	126.06
20	6	602	CLA	C1D-CHD-C4C	-3.79	117.89	126.06
20	K	4002	CLA	C3C-C4C-NC	3.79	114.82	110.57
20	1	613	CLA	C3C-C4C-NC	3.79	114.82	110.57
22	A	855	LHG	O7-C7-C8	3.78	119.66	111.50
27	Z	607	CHL	C3C-C4C-NC	3.78	114.81	110.57
20	J	3002	CLA	C1D-CHD-C4C	-3.78	117.89	126.06
27	4	607	CHL	C1D-CHD-C4C	-3.78	117.89	126.06
20	5	601	CLA	C1D-CHD-C4C	-3.78	117.90	126.06
20	A	822	CLA	C3C-C4C-NC	3.78	114.81	110.57
20	1	616	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
23	B	846	BCR	C16-C17-C18	-3.78	121.91	127.31
20	3	609	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
20	6	611	CLA	C3C-C4C-NC	3.78	114.81	110.57
20	A	805	CLA	C1D-CHD-C4C	-3.78	117.90	126.06
20	L	204	CLA	C3C-C4C-NC	3.78	114.81	110.57
20	3	617	CLA	C3C-C4C-NC	3.78	114.81	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	603	CLA	C3C-C4C-NC	3.78	114.81	110.57
20	7	602	CLA	C1D-CHD-C4C	-3.78	117.90	126.06
20	B	809	CLA	C3D-C4D-ND	3.78	116.35	110.24
20	B	817	CLA	C1C-C2C-C3C	-3.78	102.99	106.96
20	3	611	CLA	C3C-C4C-NC	3.78	114.81	110.57
20	5	614	CLA	C3C-C4C-NC	3.78	114.81	110.57
23	B	843	BCR	C11-C10-C9	-3.78	121.92	127.31
20	7	602	CLA	C3C-C4C-NC	3.77	114.80	110.57
20	5	609	CLA	C3B-C4B-NB	3.77	114.09	109.21
20	3	607	CLA	C3C-C4C-NC	3.77	114.80	110.57
20	A	804	CLA	C1D-CHD-C4C	-3.77	117.92	126.06
20	7	610	CLA	O2A-CGA-CBA	3.77	123.75	111.91
20	3	617	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
20	A	819	CLA	C1D-CHD-C4C	-3.77	117.92	126.06
20	B	820	CLA	C1D-CHD-C4C	-3.77	117.92	126.06
23	5	622	BCR	C16-C17-C18	-3.77	121.93	127.31
20	4	613	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
20	A	827	CLA	C1D-CHD-C4C	-3.77	117.93	126.06
20	5	611	CLA	C3D-C4D-ND	3.77	116.33	110.24
20	8	612	CLA	C3B-C4B-NB	3.77	114.08	109.21
20	A	834	CLA	CAA-C2A-C3A	-3.77	102.46	112.78
23	8	619	BCR	C21-C20-C19	-3.77	111.46	123.22
20	A	840	CLA	C1D-CHD-C4C	-3.77	117.93	126.06
27	1	601	CHL	C1D-CHD-C4C	-3.77	117.93	126.06
20	6	622	CLA	C4A-NA-C1A	-3.77	105.01	106.71
20	A	812	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
20	7	609	CLA	C4A-NA-C1A	-3.76	105.01	106.71
20	A	834	CLA	C1D-CHD-C4C	-3.76	117.94	126.06
20	5	614	CLA	C1D-CHD-C4C	-3.76	117.94	126.06
20	8	613	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
20	6	604	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
20	Z	612	CLA	C3C-C4C-NC	3.76	114.79	110.57
20	A	802	CLA	C3C-C4C-NC	3.76	114.79	110.57
20	B	815	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
20	8	612	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
20	4	610	CLA	CAA-C2A-C3A	-3.76	102.48	112.78
20	A	803	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
20	K	4002	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
20	B	821	CLA	C3C-C4C-NC	3.75	114.78	110.57
27	5	607	CHL	C3C-C4C-NC	3.75	114.78	110.57
20	A	806	CLA	C3B-C4B-NB	3.75	114.06	109.21
20	4	610	CLA	O2A-CGA-CBA	3.75	123.68	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	5	612	CLA	C1C-C2C-C3C	-3.75	103.01	106.96
23	A	856	BCR	C15-C14-C13	-3.75	121.96	127.31
20	B	836	CLA	C3D-C4D-ND	3.75	116.31	110.24
23	A	849	BCR	C11-C10-C9	-3.75	121.96	127.31
20	B	808	CLA	C4A-NA-C1A	-3.75	105.02	106.71
20	B	802	CLA	C3B-C4B-NB	3.75	114.06	109.21
20	3	611	CLA	C1C-C2C-C3C	-3.75	103.01	106.96
20	7	620	CLA	C3C-C4C-NC	3.75	114.78	110.57
20	5	609	CLA	C1C-C2C-C3C	-3.75	103.02	106.96
20	3	603	CLA	C1D-CHD-C4C	-3.75	117.97	126.06
20	7	614	CLA	C1D-CHD-C4C	-3.75	117.97	126.06
20	A	837	CLA	C3C-C4C-NC	3.75	114.77	110.57
20	B	817	CLA	C1D-CHD-C4C	-3.75	117.97	126.06
20	J	3002	CLA	C3C-C4C-NC	3.75	114.77	110.57
20	6	611	CLA	C1D-CHD-C4C	-3.75	117.98	126.06
20	5	621	CLA	C3D-C4D-ND	3.75	116.30	110.24
20	B	827	CLA	C3B-C4B-NB	3.75	114.05	109.21
20	B	840	CLA	C1D-CHD-C4C	-3.74	117.98	126.06
20	8	604	CLA	C1C-C2C-C3C	-3.74	103.02	106.96
28	8	617	LUT	C35-C34-C33	-3.74	121.97	127.31
20	K	4002	CLA	C1D-CHD-C4C	-3.74	117.98	126.06
20	7	603	CLA	C1D-CHD-C4C	-3.74	117.98	126.06
23	A	851	BCR	C11-C10-C9	-3.74	121.97	127.31
20	1	603	CLA	C1D-CHD-C4C	-3.74	117.99	126.06
20	B	809	CLA	C1D-CHD-C4C	-3.74	117.99	126.06
20	3	614	CLA	C1D-CHD-C4C	-3.74	117.99	126.06
20	3	603	CLA	C3B-C4B-NB	3.74	114.04	109.21
20	B	817	CLA	CAA-C2A-C3A	-3.74	102.55	112.78
20	1	604	CLA	C1C-C2C-C3C	-3.74	103.03	106.96
20	4	612	CLA	C1C-C2C-C3C	-3.74	103.03	106.96
20	A	804	CLA	C3D-C2D-C1D	-3.74	100.73	105.83
20	Z	603	CLA	C1D-CHD-C4C	-3.74	118.00	126.06
20	6	610	CLA	C1C-C2C-C3C	-3.73	103.03	106.96
20	5	603	CLA	C3D-C4D-ND	3.73	116.28	110.24
20	A	835	CLA	C3C-C4C-NC	3.73	114.76	110.57
20	A	814	CLA	C4A-NA-C1A	-3.73	105.03	106.71
20	A	823	CLA	C1C-C2C-C3C	-3.73	103.03	106.96
20	A	823	CLA	C1D-CHD-C4C	-3.73	118.01	126.06
20	8	611	CLA	C3D-C4D-ND	3.73	116.27	110.24
20	7	611	CLA	C3C-C4C-NC	3.73	114.75	110.57
20	B	827	CLA	C1D-CHD-C4C	-3.73	118.01	126.06
20	A	833	CLA	C3D-C4D-ND	3.73	116.27	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	852	CLA	C1C-C2C-C3C	-3.73	103.03	106.96
20	Z	603	CLA	C3C-C4C-NC	3.73	114.75	110.57
20	7	620	CLA	C1D-CHD-C4C	-3.73	118.01	126.06
20	A	841	CLA	C1C-C2C-C3C	-3.73	103.04	106.96
23	A	848	BCR	C7-C8-C9	-3.73	120.60	126.23
20	B	804	CLA	CMB-C2B-C3B	3.73	131.65	124.68
23	I	172	BCR	C16-C17-C18	-3.73	121.99	127.31
20	3	617	CLA	C1D-CHD-C4C	-3.73	118.02	126.06
28	7	622	LUT	C7-C8-C9	-3.73	120.60	126.23
20	B	827	CLA	C1C-C2C-C3C	-3.73	103.04	106.96
20	8	610	CLA	CMC-C2C-C1C	3.72	130.71	125.04
20	7	612	CLA	C1C-C2C-C3C	-3.72	103.04	106.96
23	G	205	BCR	C16-C17-C18	-3.72	122.00	127.31
20	B	802	CLA	CMA-C3A-C2A	-3.72	98.82	113.83
27	4	618	CHL	C3C-C4C-NC	3.72	114.74	110.57
20	A	837	CLA	C3D-C4D-ND	3.72	116.26	110.24
20	Z	608	CLA	C1C-C2C-C3C	-3.72	103.05	106.96
20	B	828	CLA	C1C-C2C-C3C	-3.72	103.05	106.96
20	3	602	CLA	C3C-C4C-NC	3.72	114.74	110.57
20	A	837	CLA	CMB-C2B-C3B	3.72	131.64	124.68
20	G	203	CLA	C3C-C4C-NC	3.72	114.74	110.57
20	B	834	CLA	C1D-CHD-C4C	-3.72	118.04	126.06
20	B	817	CLA	C3B-C4B-NB	3.72	114.02	109.21
20	6	603	CLA	C3C-C4C-NC	3.72	114.74	110.57
20	B	803	CLA	C3D-C4D-ND	3.72	116.25	110.24
20	7	616	CLA	C1C-C2C-C3C	-3.71	103.05	106.96
20	B	803	CLA	C4A-NA-C1A	-3.71	105.04	106.71
20	B	822	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
20	B	835	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
20	5	613	CLA	C3C-C4C-NC	3.71	114.73	110.57
20	A	815	CLA	C3D-C4D-ND	3.71	116.24	110.24
20	6	613	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
20	A	841	CLA	O2D-CGD-CBD	3.71	117.86	111.27
20	7	620	CLA	C1C-C2C-C3C	-3.71	103.05	106.96
19	A	801	CL0	C4A-NA-C1A	-3.71	105.04	106.71
20	A	825	CLA	C3C-C4C-NC	3.71	114.73	110.57
20	3	614	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
20	B	838	CLA	C1D-CHD-C4C	-3.71	118.06	126.06
28	6	621	LUT	C35-C34-C33	-3.71	122.02	127.31
20	1	608	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
20	A	822	CLA	C1D-CHD-C4C	-3.70	118.07	126.06
20	8	616	CLA	C1C-C2C-C3C	-3.70	103.06	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	827	CLA	C3C-C4C-NC	3.70	114.72	110.57
20	5	617	CLA	CAA-C2A-C3A	-3.70	102.64	112.78
20	4	602	CLA	C1D-CHD-C4C	-3.70	118.07	126.06
20	6	622	CLA	C1C-C2C-C3C	-3.70	103.06	106.96
20	A	823	CLA	C3C-C4C-NC	3.70	114.72	110.57
20	B	821	CLA	C1D-CHD-C4C	-3.70	118.08	126.06
23	B	847	BCR	C21-C20-C19	-3.70	111.68	123.22
20	6	609	CLA	C3B-C4B-NB	3.70	113.99	109.21
20	5	613	CLA	C4A-NA-C1A	-3.70	105.04	106.71
20	B	831	CLA	C1C-C2C-C3C	-3.69	103.07	106.96
20	G	203	CLA	C1C-C2C-C3C	-3.69	103.07	106.96
20	4	613	CLA	CAC-C3C-C4C	3.69	129.60	124.81
20	B	834	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
20	B	806	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
20	1	609	CLA	C3B-C4B-NB	3.69	113.98	109.21
20	4	604	CLA	C1D-CHD-C4C	-3.69	118.10	126.06
20	Z	611	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
28	Z	619	LUT	C15-C14-C13	-3.69	122.05	127.31
23	B	846	BCR	C39-C30-C25	-3.69	104.32	110.30
20	G	204	CLA	C3C-C4C-NC	3.69	114.71	110.57
27	5	608	CHL	C3C-C4C-NC	3.69	114.70	110.57
20	B	822	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
20	7	616	CLA	C1D-CHD-C4C	-3.69	118.11	126.06
20	B	840	CLA	CAC-C3C-C2C	3.69	133.83	127.53
23	3	717	BCR	C16-C17-C18	-3.69	122.05	127.31
23	B	844	BCR	C7-C8-C9	-3.69	120.67	126.23
20	3	620	CLA	C1D-CHD-C4C	-3.68	118.11	126.06
20	A	841	CLA	O2A-CGA-CBA	3.68	123.47	111.91
20	B	815	CLA	C3C-C4C-NC	3.68	114.70	110.57
27	1	607	CHL	C3C-C4C-NC	3.68	114.70	110.57
27	5	608	CHL	C1D-CHD-C4C	-3.68	118.12	126.06
20	5	602	CLA	C3C-C4C-NC	3.68	114.70	110.57
20	G	203	CLA	C1D-CHD-C4C	-3.68	118.12	126.06
20	A	808	CLA	C3B-C4B-NB	3.68	113.97	109.21
20	A	838	CLA	C3C-C4C-NC	3.68	114.70	110.57
20	A	820	CLA	C1D-CHD-C4C	-3.68	118.12	126.06
23	L	205	BCR	C20-C21-C22	-3.68	122.06	127.31
23	7	624	BCR	C7-C8-C9	-3.68	120.68	126.23
20	7	610	CLA	CAA-C2A-C3A	-3.68	102.71	112.78
20	6	611	CLA	C1C-C2C-C3C	-3.67	103.09	106.96
23	8	619	BCR	C28-C27-C26	-3.67	107.52	114.08
23	A	850	BCR	C24-C23-C22	-3.67	120.69	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	6	622	CLA	C3C-C4C-NC	3.67	114.69	110.57
20	1	603	CLA	C3B-C4B-NB	3.67	113.95	109.21
20	8	603	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
20	B	832	CLA	C3C-C4C-NC	3.67	114.69	110.57
19	A	801	CL0	CMA-C3A-C4A	-3.67	101.92	111.77
20	Z	609	CLA	C3B-C4B-NB	3.67	113.95	109.21
20	B	831	CLA	C3C-C4C-NC	3.67	114.68	110.57
20	Z	616	CLA	C4A-NA-C1A	-3.67	105.06	106.71
20	4	613	CLA	O2A-CGA-CBA	3.67	123.41	111.91
20	6	612	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
20	8	606	CLA	O2D-CGD-CBD	3.67	117.78	111.27
20	1	609	CLA	C3C-C4C-NC	3.66	114.68	110.57
20	3	609	CLA	C3C-C4C-NC	3.66	114.68	110.57
23	K	4004	BCR	C16-C17-C18	-3.66	122.08	127.31
20	B	837	CLA	C1D-CHD-C4C	-3.66	118.16	126.06
23	K	4001	BCR	C2-C3-C4	-3.66	103.19	111.38
20	4	604	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
20	A	836	CLA	C4A-NA-C1A	-3.66	105.06	106.71
20	A	803	CLA	CMB-C2B-C3B	3.66	131.52	124.68
28	8	618	LUT	C7-C8-C9	-3.66	120.71	126.23
20	B	823	CLA	CAC-C3C-C4C	3.66	129.56	124.81
20	A	828	CLA	CHD-C4C-NC	3.66	129.97	124.20
20	1	614	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
20	4	601	CLA	C3B-C4B-NB	3.66	113.94	109.21
20	G	204	CLA	C1D-CHD-C4C	-3.65	118.18	126.06
20	5	610	CLA	C3C-C4C-NC	3.65	114.67	110.57
23	6	623	BCR	C11-C12-C13	-3.65	116.16	126.42
20	B	806	CLA	C3D-C4D-ND	3.65	116.14	110.24
20	8	610	CLA	C3C-C4C-NC	3.65	114.67	110.57
20	A	816	CLA	C1D-CHD-C4C	-3.65	118.18	126.06
20	Z	612	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
20	7	609	CLA	CHB-C4A-NA	3.65	129.56	124.51
20	4	602	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
20	7	603	CLA	C3C-C4C-NC	3.65	114.66	110.57
20	4	613	CLA	C3C-C4C-NC	3.64	114.66	110.57
20	3	602	CLA	CAC-C3C-C4C	3.64	129.54	124.81
20	8	614	CLA	C1D-CHD-C4C	-3.64	118.20	126.06
20	7	610	CLA	C3C-C4C-NC	3.64	114.66	110.57
28	4	619	LUT	C35-C15-C14	-3.64	116.02	123.47
20	A	823	CLA	C4A-NA-C1A	-3.64	105.07	106.71
20	A	820	CLA	C3B-C4B-NB	3.64	113.91	109.21
20	B	819	CLA	C1D-CHD-C4C	-3.64	118.21	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	836	CLA	C3B-C4B-NB	3.64	113.91	109.21
20	B	841	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
20	6	614	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
28	3	622	LUT	C7-C8-C9	-3.63	120.74	126.23
27	5	618	CHL	C1D-CHD-C4C	-3.63	118.22	126.06
27	6	607	CHL	C4-C3-C5	3.63	121.38	115.27
20	B	812	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
20	F	304	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
20	5	621	CLA	C3B-C4B-NB	3.63	113.90	109.21
20	6	610	CLA	C1D-CHD-C4C	-3.63	118.23	126.06
20	A	802	CLA	CHB-C4A-NA	3.63	129.53	124.51
20	1	611	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
20	A	821	CLA	C3C-C4C-NC	3.62	114.64	110.57
20	7	606	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
20	5	614	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
20	6	614	CLA	C1D-CHD-C4C	-3.62	118.24	126.06
20	8	614	CLA	C4A-NA-C1A	-3.62	105.08	106.71
20	F	304	CLA	C3B-C4B-NB	3.62	113.89	109.21
20	7	609	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
20	A	814	CLA	C4C-C3C-C2C	-3.62	101.62	106.90
20	A	813	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
20	A	810	CLA	C4A-NA-C1A	-3.61	105.08	106.71
20	5	611	CLA	C4A-NA-C1A	-3.61	105.08	106.71
23	B	801	BCR	C11-C10-C9	-3.61	122.15	127.31
27	4	606	CHL	CAC-C3C-C4C	3.61	129.50	124.81
20	A	817	CLA	C3B-C4B-NB	3.61	113.88	109.21
20	7	612	CLA	C3B-C4B-NB	3.61	113.88	109.21
20	3	610	CLA	C3C-C4C-NC	3.61	114.62	110.57
20	A	826	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
20	B	830	CLA	C1D-CHD-C4C	-3.61	118.27	126.06
20	5	604	CLA	C3C-C4C-NC	3.61	114.62	110.57
20	6	604	CLA	C1D-CHD-C4C	-3.61	118.27	126.06
20	7	601	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
20	B	813	CLA	C1D-CHD-C4C	-3.61	118.28	126.06
20	B	819	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
23	6	623	BCR	C16-C17-C18	-3.61	122.16	127.31
20	A	840	CLA	C1C-C2C-C3C	-3.61	103.17	106.96
20	6	622	CLA	C1D-CHD-C4C	-3.60	118.28	126.06
23	A	848	BCR	C11-C10-C9	-3.60	122.17	127.31
20	8	604	CLA	C1D-CHD-C4C	-3.60	118.29	126.06
20	7	614	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
20	8	614	CLA	C1C-C2C-C3C	-3.60	103.17	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	8	601	CLA	C4A-NA-C1A	-3.60	105.09	106.71
20	4	614	CLA	C1C-C2C-C3C	-3.60	103.18	106.96
20	A	834	CLA	C3C-C4C-NC	3.59	114.60	110.57
20	Z	609	CLA	C3C-C4C-NC	3.59	114.60	110.57
20	B	823	CLA	C4C-C3C-C2C	-3.59	101.66	106.90
20	B	811	CLA	C4B-C3B-C2B	-3.59	103.58	106.92
20	A	825	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
20	B	824	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
20	A	836	CLA	C3C-C4C-NC	3.59	114.59	110.57
20	6	616	CLA	C3C-C4C-NC	3.59	114.59	110.57
20	A	825	CLA	C1D-CHD-C4C	-3.59	118.32	126.06
20	5	604	CLA	C3B-C4B-NB	3.59	113.85	109.21
20	A	828	CLA	C3D-C4D-ND	3.59	116.04	110.24
20	B	821	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
20	3	614	CLA	C3C-C4C-NC	3.58	114.59	110.57
23	3	718	BCR	C28-C27-C26	-3.58	107.68	114.08
20	7	613	CLA	C3B-C4B-NB	3.58	113.84	109.21
20	8	601	CLA	C3D-C4D-ND	3.58	116.03	110.24
20	7	604	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
20	5	621	CLA	CAC-C3C-C4C	3.58	129.46	124.81
20	A	821	CLA	C3B-C4B-NB	3.58	113.84	109.21
20	B	815	CLA	C3B-C4B-NB	3.58	113.84	109.21
20	7	608	CLA	C4A-NA-C1A	-3.58	105.10	106.71
20	A	809	CLA	C1D-CHD-C4C	-3.58	118.34	126.06
20	A	805	CLA	C3C-C4C-NC	3.58	114.58	110.57
20	A	807	CLA	C3B-C4B-NB	3.58	113.83	109.21
20	6	603	CLA	C3B-C4B-NB	3.58	113.83	109.21
20	A	802	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
20	B	831	CLA	C1D-CHD-C4C	-3.57	118.35	126.06
20	5	609	CLA	O2A-CGA-CBA	3.57	123.12	111.91
23	7	624	BCR	C15-C14-C13	-3.57	122.21	127.31
20	A	814	CLA	C1D-CHD-C4C	-3.57	118.35	126.06
20	A	828	CLA	C4C-C3C-C2C	-3.57	101.69	106.90
23	A	850	BCR	C11-C10-C9	-3.57	122.22	127.31
20	6	614	CLA	C3C-C4C-NC	3.57	114.57	110.57
20	K	4003	CLA	C1C-C2C-C3C	-3.57	103.21	106.96
20	1	603	CLA	C3C-C4C-NC	3.57	114.57	110.57
27	4	607	CHL	C3D-C4D-ND	3.57	116.01	110.24
20	8	608	CLA	CMC-C2C-C1C	3.56	130.47	125.04
20	F	304	CLA	CAA-C2A-C3A	-3.56	103.02	112.78
20	6	614	CLA	CAA-C2A-C3A	-3.56	103.03	112.78
20	1	609	CLA	CAA-C2A-C3A	-3.56	103.03	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	8	611	CLA	CAC-C3C-C4C	3.56	129.43	124.81
20	B	803	CLA	C3C-C4C-NC	3.56	114.56	110.57
20	4	612	CLA	C3B-C4B-NB	3.56	113.81	109.21
20	B	830	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
20	7	601	CLA	C3B-C4B-NB	3.56	113.81	109.21
20	Z	603	CLA	C3B-C4B-NB	3.56	113.81	109.21
20	A	810	CLA	C1C-C2C-C3C	-3.56	103.22	106.96
20	B	817	CLA	C3C-C4C-NC	3.56	114.56	110.57
23	K	4004	BCR	C20-C21-C22	-3.56	122.23	127.31
23	A	850	BCR	C20-C21-C22	-3.56	122.23	127.31
20	A	824	CLA	C3B-C4B-NB	3.55	113.81	109.21
20	L	203	CLA	C1D-CHD-C4C	-3.55	118.39	126.06
20	3	604	CLA	C3C-C4C-NC	3.55	114.56	110.57
20	5	606	CLA	C3C-C4C-NC	3.55	114.56	110.57
20	8	602	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
20	B	807	CLA	C1D-CHD-C4C	-3.55	118.40	126.06
20	A	804	CLA	C1C-C2C-C3C	-3.55	103.23	106.96
20	6	617	CLA	C1C-C2C-C3C	-3.55	103.23	106.96
28	6	624	LUT	C15-C14-C13	-3.55	122.25	127.31
20	A	820	CLA	CMB-C2B-C3B	3.55	131.31	124.68
23	4	621	BCR	C16-C17-C18	-3.55	122.25	127.31
20	4	613	CLA	C3B-C4B-NB	3.54	113.79	109.21
20	Z	604	CLA	C1D-CHD-C4C	-3.54	118.41	126.06
27	8	607	CHL	C3D-C4D-ND	3.54	115.97	110.24
20	B	824	CLA	CAC-C3C-C4C	3.54	129.40	124.81
20	A	825	CLA	CAC-C3C-C4C	3.54	129.40	124.81
20	A	837	CLA	C1D-CHD-C4C	-3.54	118.42	126.06
23	J	3003	BCR	C15-C14-C13	-3.54	122.26	127.31
20	A	804	CLA	O2D-CGD-O1D	-3.54	116.92	123.84
20	A	839	CLA	C1-C2-C3	-3.54	119.92	126.04
20	7	611	CLA	C3B-C4B-NB	3.54	113.78	109.21
20	B	808	CLA	C1C-C2C-C3C	-3.53	103.24	106.96
20	A	834	CLA	C3B-C4B-NB	3.53	113.78	109.21
20	B	802	CLA	C4C-C3C-C2C	-3.53	101.75	106.90
20	A	824	CLA	C1D-CHD-C4C	-3.53	118.44	126.06
27	8	607	CHL	C3B-C4B-NB	3.53	113.77	109.21
20	4	611	CLA	C3C-C4C-NC	3.53	114.53	110.57
20	L	204	CLA	C1D-CHD-C4C	-3.53	118.44	126.06
20	B	805	CLA	C1D-CHD-C4C	-3.53	118.44	126.06
20	B	820	CLA	C3C-C4C-NC	3.53	114.53	110.57
20	4	602	CLA	C3C-C4C-NC	3.53	114.53	110.57
20	B	807	CLA	C3B-C4B-NB	3.53	113.77	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	K	4004	BCR	C3-C4-C5	-3.53	107.78	114.08
20	A	817	CLA	CHC-C1C-C2C	-3.52	116.98	126.72
20	B	805	CLA	C4C-C3C-C2C	-3.52	101.77	106.90
28	7	621	LUT	C7-C8-C9	-3.52	120.92	126.23
20	A	805	CLA	C1C-C2C-C3C	-3.52	103.25	106.96
23	B	845	BCR	C3-C4-C5	-3.52	107.79	114.08
20	8	604	CLA	C3C-C4C-NC	3.52	114.52	110.57
23	B	801	BCR	C15-C16-C17	3.52	130.68	123.47
20	5	603	CLA	C3C-C4C-NC	3.52	114.51	110.57
20	A	808	CLA	C1D-CHD-C4C	-3.51	118.48	126.06
20	3	604	CLA	C1D-CHD-C4C	-3.51	118.48	126.06
20	8	608	CLA	CHD-C4C-NC	3.51	129.73	124.20
23	3	717	BCR	C15-C14-C13	-3.51	122.30	127.31
20	Z	613	CLA	C1C-C2C-C3C	-3.51	103.27	106.96
20	4	601	CLA	C1C-C2C-C3C	-3.51	103.27	106.96
23	A	856	BCR	C33-C5-C6	-3.51	120.59	124.53
20	3	606	CLA	C1C-C2C-C3C	-3.51	103.27	106.96
20	A	806	CLA	C3C-C4C-NC	3.51	114.50	110.57
27	Z	601	CHL	CHD-C1D-ND	-3.50	121.23	124.45
23	A	848	BCR	C16-C15-C14	-3.50	116.30	123.47
23	I	172	BCR	C20-C19-C18	-3.50	116.58	126.42
20	A	813	CLA	C1-O2A-CGA	3.50	125.63	116.44
28	Z	617	LUT	C35-C34-C33	-3.50	122.31	127.31
20	A	854	CLA	C4C-C3C-C2C	-3.50	101.80	106.90
20	B	833	CLA	C3B-C4B-NB	3.50	113.73	109.21
28	Z	618	LUT	C7-C8-C9	-3.50	120.95	126.23
23	B	845	BCR	C11-C10-C9	-3.50	122.32	127.31
20	A	835	CLA	CAA-C2A-C3A	-3.50	103.20	112.78
20	A	842	CLA	O2A-C1-C2	3.50	117.83	108.64
20	3	609	CLA	CAA-C2A-C3A	-3.49	103.21	112.78
20	3	620	CLA	C3C-C4C-NC	3.49	114.49	110.57
20	8	608	CLA	C1C-C2C-C3C	-3.49	103.28	106.96
20	6	616	CLA	CAA-C2A-C3A	-3.49	103.22	112.78
20	8	603	CLA	C3B-C4B-NB	3.49	113.72	109.21
20	6	616	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
20	3	609	CLA	C3B-C4B-NB	3.49	113.72	109.21
20	3	609	CLA	O2D-CGD-CBD	3.49	117.47	111.27
20	A	840	CLA	C3B-C4B-NB	3.49	113.72	109.21
20	A	830	CLA	C1-C2-C3	-3.48	120.02	126.04
20	8	602	CLA	CHD-C4C-NC	3.48	129.69	124.20
20	1	606	CLA	CAA-C2A-C3A	-3.48	103.25	112.78
23	B	843	BCR	C15-C14-C13	-3.48	122.35	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	J	3003	BCR	C3-C4-C5	-3.48	107.87	114.08
20	A	814	CLA	C3B-C4B-NB	3.47	113.70	109.21
20	5	616	CLA	C3B-C4B-NB	3.47	113.70	109.21
20	5	617	CLA	CHC-C1C-C2C	-3.47	117.11	126.72
27	6	607	CHL	C3B-C4B-NB	3.47	113.70	109.21
27	7	607	CHL	C3B-C4B-NB	3.47	113.70	109.21
20	6	612	CLA	C3B-C4B-NB	3.47	113.70	109.21
20	1	613	CLA	CAC-C3C-C4C	3.47	129.31	124.81
20	5	621	CLA	CHC-C1C-C2C	-3.47	117.13	126.72
20	B	804	CLA	C1C-C2C-C3C	-3.46	103.31	106.96
20	B	810	CLA	C3B-C4B-NB	3.46	113.69	109.21
20	5	617	CLA	C4C-C3C-C2C	-3.46	101.85	106.90
27	Z	601	CHL	CAC-C3C-C4C	3.46	129.30	124.81
20	7	604	CLA	O2D-CGD-CBD	3.46	117.42	111.27
20	A	815	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
20	B	819	CLA	C3C-C4C-NC	3.46	114.45	110.57
20	A	845	CLA	C3B-C4B-NB	3.46	113.69	109.21
20	B	822	CLA	C3B-C4B-NB	3.46	113.69	109.21
20	B	805	CLA	O2A-CGA-CBA	3.46	122.77	111.91
20	A	811	CLA	C1-C2-C3	-3.46	120.06	126.04
20	B	837	CLA	O2D-CGD-O1D	-3.46	117.08	123.84
20	G	203	CLA	C3B-C4B-NB	3.46	113.68	109.21
23	B	844	BCR	C15-C14-C13	-3.46	122.38	127.31
20	A	820	CLA	CBA-CAA-C2A	3.45	124.06	113.86
28	3	622	LUT	C18-C5-C6	-3.45	120.65	124.53
20	8	613	CLA	CAC-C3C-C4C	3.45	129.29	124.81
23	J	3003	BCR	C16-C17-C18	-3.45	122.39	127.31
23	B	846	BCR	C21-C20-C19	-3.45	112.46	123.22
20	5	613	CLA	C3B-C4B-NB	3.45	113.67	109.21
20	B	837	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
23	B	845	BCR	C15-C14-C13	-3.45	122.39	127.31
20	5	617	CLA	CAC-C3C-C4C	3.45	129.28	124.81
20	B	809	CLA	C3C-C4C-NC	3.44	114.43	110.57
20	7	610	CLA	C2C-C1C-NC	3.44	113.20	109.97
20	B	824	CLA	CMC-C2C-C1C	3.44	130.28	125.04
20	B	803	CLA	CMB-C2B-C3B	3.44	131.12	124.68
20	1	613	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
20	F	303	CLA	CAA-C2A-C3A	-3.44	103.36	112.78
20	B	840	CLA	CHC-C1C-C2C	-3.44	117.21	126.72
23	F	305	BCR	C21-C20-C19	-3.44	112.49	123.22
20	A	842	CLA	C1-C2-C3	-3.43	120.10	126.04
20	A	831	CLA	CHC-C1C-C2C	-3.43	117.22	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	5	621	CLA	C4A-NA-C1A	-3.43	105.16	106.71
20	3	607	CLA	O2A-CGA-CBA	3.43	122.68	111.91
28	1	617	LUT	C35-C15-C14	-3.43	116.44	123.47
20	7	609	CLA	C3B-C4B-NB	3.43	113.64	109.21
20	7	610	CLA	CHD-C4C-NC	3.43	129.61	124.20
20	B	834	CLA	C3C-C4C-NC	3.43	114.42	110.57
20	A	819	CLA	C4C-C3C-C2C	-3.43	101.90	106.90
27	5	618	CHL	C3D-C4D-ND	3.43	115.78	110.24
20	A	835	CLA	CHC-C1C-C2C	-3.42	117.25	126.72
20	6	613	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
20	A	831	CLA	CAC-C3C-C4C	3.42	129.25	124.81
20	4	601	CLA	C1D-CHD-C4C	-3.42	118.67	126.06
20	5	609	CLA	C1-C2-C3	-3.42	121.21	126.75
20	B	802	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
27	6	618	CHL	C3D-C4D-ND	3.42	115.77	110.24
23	A	856	BCR	C7-C8-C9	-3.42	121.07	126.23
20	8	610	CLA	O2A-CGA-CBA	3.42	122.63	111.91
20	4	616	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
20	6	601	CLA	C1D-CHD-C4C	-3.41	118.69	126.06
19	A	801	CL0	CBC-CAC-C3C	-3.41	103.02	112.43
20	B	810	CLA	C3C-C4C-NC	3.41	114.40	110.57
20	A	829	CLA	C1C-C2C-C3C	-3.41	103.37	106.96
20	L	204	CLA	C1C-C2C-C3C	-3.41	103.37	106.96
27	4	607	CHL	CBC-CAC-C3C	-3.41	103.02	112.43
20	1	610	CLA	C1C-C2C-C3C	-3.41	103.37	106.96
23	7	624	BCR	C11-C10-C9	-3.41	122.44	127.31
20	1	604	CLA	CAC-C3C-C4C	3.41	129.23	124.81
27	6	607	CHL	CAC-C3C-C4C	3.41	129.23	124.81
23	6	625	BCR	C15-C16-C17	-3.41	116.49	123.47
20	6	616	CLA	CAC-C3C-C4C	3.41	129.23	124.81
20	B	829	CLA	C1C-C2C-C3C	-3.41	103.37	106.96
20	4	604	CLA	C3C-C4C-NC	3.41	114.39	110.57
20	K	4003	CLA	CHC-C1C-C2C	-3.41	117.30	126.72
20	1	604	CLA	C1D-CHD-C4C	-3.41	118.71	126.06
28	3	621	LUT	C15-C14-C13	-3.41	122.45	127.31
27	6	608	CHL	C3D-C4D-ND	3.40	115.75	110.24
20	G	203	CLA	CAC-C3C-C4C	3.40	129.22	124.81
20	B	833	CLA	C4C-C3C-C2C	-3.40	101.94	106.90
20	A	835	CLA	C4-C3-C5	3.40	120.99	115.27
20	8	609	CLA	C1C-C2C-C3C	-3.40	103.38	106.96
20	A	811	CLA	C1C-C2C-C3C	-3.40	103.38	106.96
27	8	607	CHL	CAC-C3C-C4C	3.40	129.22	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	5	607	CHL	C3B-C4B-NB	3.39	113.60	109.21
20	B	836	CLA	C4C-C3C-C2C	-3.39	101.95	106.90
20	A	833	CLA	C1C-C2C-C3C	-3.39	103.39	106.96
20	B	826	CLA	C4C-C3C-C2C	-3.39	101.95	106.90
20	4	610	CLA	CHC-C1C-C2C	-3.39	117.34	126.72
20	B	806	CLA	C3B-C4B-NB	3.39	113.59	109.21
20	F	301	CLA	C1C-C2C-C3C	-3.39	103.39	106.96
20	L	203	CLA	C3C-C4C-NC	3.39	114.37	110.57
20	B	809	CLA	CAC-C3C-C4C	3.39	129.21	124.81
23	5	625	BCR	C28-C27-C26	-3.39	108.03	114.08
20	B	809	CLA	CHC-C1C-C2C	-3.39	117.35	126.72
20	G	204	CLA	C3B-C4B-NB	3.39	113.59	109.21
20	3	612	CLA	C3B-C4B-NB	3.39	113.59	109.21
20	B	817	CLA	CHC-C1C-C2C	-3.39	117.35	126.72
27	Z	601	CHL	C3D-C4D-ND	3.38	115.71	110.24
20	7	611	CLA	O2D-CGD-O1D	-3.38	117.22	123.84
20	3	602	CLA	O2A-CGA-CBA	3.38	122.52	111.91
20	B	807	CLA	CAC-C3C-C4C	3.38	129.20	124.81
20	6	622	CLA	CAC-C3C-C4C	3.38	129.20	124.81
20	4	611	CLA	C3B-C4B-NB	3.38	113.58	109.21
20	A	819	CLA	C1-C2-C3	-3.38	120.20	126.04
20	B	823	CLA	C3B-C4B-NB	3.38	113.58	109.21
27	3	608	CHL	C3B-C4B-NB	3.38	113.58	109.21
23	A	856	BCR	C38-C26-C25	-3.38	120.73	124.53
20	5	603	CLA	C3B-C4B-NB	3.38	113.58	109.21
22	A	846	LHG	O7-C7-C8	3.38	118.78	111.50
27	1	601	CHL	O2D-CGD-O1D	-3.37	117.24	123.84
20	7	610	CLA	CMC-C2C-C1C	3.37	130.18	125.04
20	B	818	CLA	CHC-C1C-C2C	-3.37	117.39	126.72
20	8	616	CLA	C4A-NA-C1A	-3.37	105.19	106.71
20	6	602	CLA	C1C-C2C-C3C	-3.37	103.41	106.96
20	J	3002	CLA	C3B-C4B-NB	3.37	113.57	109.21
20	4	610	CLA	C3C-C4C-NC	3.37	114.35	110.57
20	B	825	CLA	O2D-CGD-CBD	3.37	117.26	111.27
28	6	621	LUT	C35-C15-C14	-3.37	116.57	123.47
20	K	4003	CLA	C3B-C4B-NB	3.37	113.56	109.21
20	B	818	CLA	C3C-C4C-NC	3.37	114.35	110.57
20	4	603	CLA	CHC-C1C-C2C	-3.37	117.41	126.72
20	A	845	CLA	C4C-C3C-C2C	-3.36	101.99	106.90
20	1	606	CLA	C1C-C2C-C3C	-3.36	103.42	106.96
20	Z	606	CLA	C1C-C2C-C3C	-3.36	103.42	106.96
23	B	844	BCR	C16-C17-C18	-3.36	122.51	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	613	CLA	C4A-NA-C1A	-3.36	105.19	106.71
20	4	610	CLA	C3B-C4B-NB	3.36	113.56	109.21
20	B	813	CLA	C4C-C3C-C2C	-3.36	102.00	106.90
20	A	811	CLA	C3B-C4B-NB	3.36	113.56	109.21
20	5	604	CLA	CHC-C1C-C2C	-3.36	117.42	126.72
20	A	845	CLA	C1C-C2C-C3C	-3.36	103.42	106.96
20	A	843	CLA	C1C-C2C-C3C	-3.36	103.42	106.96
27	6	608	CHL	C2A-C3A-C4A	-3.36	96.44	101.87
20	6	617	CLA	C3B-C4B-NB	3.36	113.55	109.21
20	4	609	CLA	CHB-C4A-NA	3.36	129.16	124.51
20	Z	616	CLA	C3B-C4B-NB	3.36	113.55	109.21
20	1	608	CLA	C3B-C4B-NB	3.36	113.55	109.21
20	1	613	CLA	C3B-C4B-NB	3.36	113.55	109.21
20	4	610	CLA	C1C-C2C-C3C	-3.36	103.43	106.96
20	B	820	CLA	C3B-C4B-NB	3.35	113.55	109.21
28	3	622	LUT	C2-C3-C4	3.35	114.89	110.30
23	B	848	BCR	C15-C14-C13	-3.35	122.53	127.31
20	A	854	CLA	O2D-CGD-O1D	-3.35	117.28	123.84
20	A	809	CLA	C3B-C4B-NB	3.35	113.54	109.21
27	5	618	CHL	C3B-C4B-NB	3.35	113.54	109.21
20	A	827	CLA	C1C-C2C-C3C	-3.35	103.43	106.96
20	A	818	CLA	C1C-C2C-C3C	-3.35	103.43	106.96
20	A	822	CLA	C1C-C2C-C3C	-3.35	103.43	106.96
20	B	841	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
20	B	834	CLA	C3B-C4B-NB	3.35	113.54	109.21
20	8	611	CLA	C3B-C4B-NB	3.34	113.53	109.21
20	Z	604	CLA	C3C-C4C-NC	3.34	114.32	110.57
20	5	610	CLA	CAA-C2A-C3A	-3.34	103.63	112.78
20	5	610	CLA	C1C-C2C-C3C	-3.34	103.45	106.96
20	7	604	CLA	CAC-C3C-C4C	3.34	129.14	124.81
20	3	613	CLA	C3B-C4B-NB	3.34	113.53	109.21
20	5	612	CLA	C3B-C4B-NB	3.34	113.53	109.21
20	B	818	CLA	C3B-C4B-NB	3.34	113.52	109.21
20	Z	602	CLA	CAC-C3C-C4C	3.33	129.14	124.81
20	4	611	CLA	CAC-C3C-C4C	3.33	129.14	124.81
20	5	617	CLA	C1C-C2C-C3C	-3.33	103.45	106.96
20	6	601	CLA	C3C-C4C-NC	3.33	114.31	110.57
20	3	604	CLA	C3B-C4B-NB	3.33	113.51	109.21
20	B	852	CLA	C3B-C4B-NB	3.33	113.51	109.21
28	Z	618	LUT	C10-C11-C12	-3.33	112.83	123.22
20	B	808	CLA	CAA-C2A-C3A	-3.33	103.67	112.78
20	A	825	CLA	CHC-C1C-C2C	-3.33	117.52	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	5	608	CHL	CAC-C3C-C4C	3.33	129.13	124.81
20	3	611	CLA	C3B-C4B-NB	3.33	113.51	109.21
20	6	610	CLA	C3C-C4C-NC	3.32	114.30	110.57
20	8	609	CLA	C3B-C4B-NB	3.32	113.51	109.21
27	4	618	CHL	C3D-C4D-ND	3.32	115.61	110.24
20	A	803	CLA	CAC-C3C-C4C	3.32	129.12	124.81
20	8	610	CLA	C1C-C2C-C3C	-3.32	103.47	106.96
20	A	821	CLA	CHC-C1C-C2C	-3.32	117.54	126.72
27	5	608	CHL	C1B-CHB-C4A	-3.32	123.54	130.12
20	5	616	CLA	CAA-C2A-C3A	-3.32	103.69	112.78
20	F	301	CLA	CAA-C2A-C3A	-3.32	103.70	112.78
20	F	303	CLA	C1C-C2C-C3C	-3.31	103.47	106.96
20	5	606	CLA	CAA-C2A-C3A	-3.31	103.70	112.78
20	6	610	CLA	CMB-C2B-C3B	3.31	130.88	124.68
20	A	832	CLA	C3B-C4B-NB	3.31	113.49	109.21
28	8	617	LUT	C35-C15-C14	-3.31	116.69	123.47
20	A	823	CLA	C3B-C4B-NB	3.31	113.49	109.21
20	A	838	CLA	CHC-C1C-C2C	-3.31	117.56	126.72
20	B	827	CLA	CAA-C2A-C3A	-3.31	103.71	112.78
20	A	821	CLA	CBC-CAC-C3C	-3.31	103.30	112.43
20	8	610	CLA	CHD-C4C-NC	3.31	129.42	124.20
20	1	603	CLA	CBC-CAC-C3C	-3.31	103.31	112.43
20	B	804	CLA	C3B-C4B-NB	3.31	113.49	109.21
20	B	809	CLA	CAA-C2A-C3A	-3.31	103.72	112.78
20	A	830	CLA	CAC-C3C-C4C	3.31	129.10	124.81
27	6	608	CHL	C2A-C1A-CHA	-3.31	118.08	123.86
20	Z	604	CLA	C3B-C4B-NB	3.31	113.49	109.21
20	A	814	CLA	CAC-C3C-C4C	3.31	129.10	124.81
20	Z	608	CLA	C3B-C4B-NB	3.31	113.48	109.21
23	3	719	BCR	C15-C14-C13	-3.31	122.59	127.31
20	Z	611	CLA	C3B-C4B-NB	3.31	113.48	109.21
20	3	610	CLA	CHD-C4C-NC	3.31	129.41	124.20
20	6	609	CLA	CHC-C1C-C2C	-3.30	117.58	126.72
20	A	805	CLA	CHD-C4C-NC	3.30	129.41	124.20
20	B	817	CLA	CAC-C3C-C4C	3.30	129.10	124.81
20	A	835	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
20	B	833	CLA	CAA-C2A-C3A	-3.30	103.74	112.78
20	3	610	CLA	CAC-C3C-C4C	3.30	129.09	124.81
20	A	816	CLA	C4A-NA-C1A	-3.30	105.22	106.71
20	3	602	CLA	C3B-C4B-NB	3.30	113.47	109.21
20	Z	614	CLA	C3B-C4B-NB	3.30	113.47	109.21
20	3	614	CLA	C3B-C4B-NB	3.29	113.47	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	814	CLA	C1C-C2C-C3C	-3.29	103.49	106.96
20	B	833	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
20	1	612	CLA	CHC-C1C-C2C	-3.29	117.61	126.72
28	5	620	LUT	C28-C29-C30	-3.29	113.89	118.94
20	1	604	CLA	C3B-C4B-NB	3.29	113.47	109.21
19	A	801	CL0	CHC-C1C-C2C	-3.29	117.62	126.72
20	B	819	CLA	CHC-C1C-C2C	-3.29	117.62	126.72
20	A	830	CLA	C4C-C3C-C2C	-3.29	102.10	106.90
20	B	832	CLA	O2A-CGA-CBA	3.29	122.23	111.91
20	3	620	CLA	C3B-C4B-NB	3.29	113.46	109.21
28	1	617	LUT	C10-C11-C12	-3.29	112.96	123.22
20	A	838	CLA	C3B-C4B-NB	3.29	113.46	109.21
28	7	622	LUT	C35-C34-C33	-3.29	122.62	127.31
19	A	801	CL0	O2A-CGA-CBA	3.29	122.22	111.91
23	F	305	BCR	C15-C16-C17	-3.29	116.74	123.47
28	3	621	LUT	C35-C34-C33	-3.29	122.62	127.31
20	B	808	CLA	C4C-C3C-C2C	-3.29	102.11	106.90
28	8	618	LUT	C10-C11-C12	-3.29	112.97	123.22
20	3	604	CLA	CHC-C1C-C2C	-3.28	117.64	126.72
20	4	601	CLA	CHC-C1C-C2C	-3.28	117.64	126.72
19	A	801	CL0	C1-C2-C3	-3.28	120.36	126.04
20	A	837	CLA	CHC-C1C-C2C	-3.28	117.64	126.72
20	A	835	CLA	C3B-C4B-NB	3.28	113.45	109.21
20	B	803	CLA	CAC-C3C-C4C	3.28	129.07	124.81
20	B	832	CLA	CHD-C4C-NC	3.28	129.37	124.20
20	B	827	CLA	CMB-C2B-C3B	3.28	130.81	124.68
20	A	829	CLA	CMC-C2C-C1C	3.28	130.03	125.04
20	7	609	CLA	C1-C2-C3	-3.28	121.45	126.75
28	1	617	LUT	C35-C34-C33	-3.28	122.63	127.31
28	7	622	LUT	C15-C14-C13	-3.28	122.63	127.31
23	B	846	BCR	C7-C8-C9	-3.28	121.28	126.23
23	B	846	BCR	C40-C30-C25	3.28	115.61	110.30
20	A	840	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
20	B	825	CLA	CMB-C2B-C3B	3.28	130.81	124.68
20	7	603	CLA	C3B-C4B-NB	3.27	113.44	109.21
20	8	601	CLA	C3B-C4B-NB	3.27	113.44	109.21
28	5	620	LUT	C35-C15-C14	-3.27	116.77	123.47
20	B	839	CLA	CAC-C3C-C4C	3.27	129.06	124.81
20	6	616	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
20	B	813	CLA	CAC-C3C-C4C	3.27	129.05	124.81
20	B	806	CLA	O2D-CGD-CBD	3.27	117.08	111.27
27	4	618	CHL	C2A-C3A-C4A	-3.27	96.59	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	804	CLA	CMC-C2C-C1C	3.27	130.02	125.04
20	B	839	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
27	7	607	CHL	C4-C3-C5	3.27	120.77	115.27
20	B	836	CLA	CAC-C3C-C4C	3.26	129.05	124.81
20	B	811	CLA	CHC-C1C-C2C	-3.26	117.69	126.72
20	A	839	CLA	C4-C3-C5	3.26	120.76	115.27
27	4	607	CHL	C3B-C4B-NB	3.26	113.43	109.21
20	A	816	CLA	C4C-C3C-C2C	-3.26	102.14	106.90
20	A	812	CLA	C1-C2-C3	-3.26	120.40	126.04
27	3	608	CHL	O2A-CGA-CBA	3.26	122.15	111.91
20	B	810	CLA	CHC-C1C-C2C	-3.26	117.70	126.72
20	3	606	CLA	C3B-C4B-NB	3.26	113.42	109.21
27	5	607	CHL	CAC-C3C-C4C	3.26	129.04	124.81
20	A	830	CLA	C3B-C4B-NB	3.26	113.42	109.21
20	A	837	CLA	C3B-C4B-NB	3.26	113.42	109.21
20	5	616	CLA	O2D-CGD-CBD	3.26	117.06	111.27
20	8	611	CLA	CHC-C1C-C2C	-3.26	117.71	126.72
20	B	829	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
20	1	603	CLA	CHC-C1C-C2C	-3.26	117.72	126.72
20	A	831	CLA	O2D-CGD-O1D	-3.25	117.47	123.84
27	6	618	CHL	C3B-C4B-NB	3.25	113.42	109.21
23	J	3003	BCR	C38-C26-C25	-3.25	120.88	124.53
20	A	805	CLA	CMA-C3A-C4A	-3.25	103.03	111.77
20	A	842	CLA	C3B-C4B-NB	3.25	113.41	109.21
20	B	808	CLA	C3B-C4B-NB	3.25	113.41	109.21
23	B	847	BCR	C15-C14-C13	-3.25	122.68	127.31
20	A	831	CLA	C4C-C3C-C2C	-3.25	102.17	106.90
20	5	602	CLA	CMC-C2C-C1C	3.25	129.98	125.04
28	1	619	LUT	C31-C30-C29	-3.24	122.68	127.31
20	5	614	CLA	C3B-C4B-NB	3.24	113.41	109.21
20	4	609	CLA	C1-C2-C3	-3.24	121.50	126.75
20	5	602	CLA	CAC-C3C-C4C	3.24	129.02	124.81
20	A	839	CLA	C3B-C4B-NB	3.24	113.40	109.21
27	1	607	CHL	C1B-CHB-C4A	-3.24	123.70	130.12
20	A	843	CLA	CAC-C3C-C4C	3.24	129.02	124.81
20	6	610	CLA	CAA-C2A-C3A	-3.24	103.90	112.78
20	4	602	CLA	C3B-C4B-NB	3.24	113.40	109.21
20	A	815	CLA	C3B-C4B-NB	3.24	113.40	109.21
20	A	832	CLA	CAC-C3C-C4C	3.24	129.01	124.81
20	5	613	CLA	CAC-C3C-C4C	3.24	129.01	124.81
20	Z	603	CLA	CHC-C1C-C2C	-3.24	117.76	126.72
28	4	620	LUT	C35-C15-C14	-3.24	116.84	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	808	CLA	CAC-C3C-C4C	3.24	129.01	124.81
20	1	604	CLA	CHC-C1C-C2C	-3.24	117.77	126.72
28	5	620	LUT	C15-C14-C13	-3.24	122.69	127.31
23	7	623	BCR	C29-C30-C25	3.24	115.46	110.48
20	B	833	CLA	CAC-C3C-C4C	3.23	129.01	124.81
20	A	810	CLA	C4C-C3C-C2C	-3.23	102.19	106.90
20	A	825	CLA	O2A-CGA-CBA	3.23	122.05	111.91
20	A	809	CLA	C1-C2-C3	-3.23	120.45	126.04
20	B	828	CLA	C3B-C4B-NB	3.23	113.39	109.21
20	4	602	CLA	CAC-C3C-C4C	3.23	129.00	124.81
20	5	604	CLA	C4A-NA-C1A	-3.23	105.25	106.71
20	Z	610	CLA	CHD-C4C-NC	3.23	129.29	124.20
20	B	834	CLA	CMA-C3A-C4A	-3.23	103.10	111.77
20	B	821	CLA	C3B-C4B-NB	3.23	113.38	109.21
20	B	835	CLA	C3B-C4B-NB	3.23	113.38	109.21
20	6	601	CLA	C3B-C4B-NB	3.23	113.38	109.21
20	A	839	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
20	5	613	CLA	CHC-C1C-C2C	-3.23	117.80	126.72
20	5	611	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
20	8	616	CLA	C3B-C4B-NB	3.23	113.38	109.21
20	Z	616	CLA	CAC-C3C-C4C	3.23	129.00	124.81
20	A	843	CLA	C3B-C4B-NB	3.22	113.38	109.21
20	6	614	CLA	C3B-C4B-NB	3.22	113.38	109.21
20	5	602	CLA	CHD-C4C-NC	3.22	129.28	124.20
20	A	807	CLA	CHC-C1C-C2C	-3.22	117.80	126.72
20	B	825	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
20	A	812	CLA	O2A-CGA-CBA	3.22	122.02	111.91
20	7	608	CLA	CHD-C4C-NC	3.22	129.28	124.20
20	5	616	CLA	CHC-C1C-C2C	-3.22	117.81	126.72
20	A	834	CLA	C4-C3-C5	3.22	120.69	115.27
20	5	616	CLA	CAC-C3C-C4C	3.22	128.99	124.81
20	L	204	CLA	C3B-C4B-NB	3.22	113.37	109.21
20	Z	609	CLA	CHC-C1C-C2C	-3.22	117.81	126.72
20	7	613	CLA	CHC-C1C-C2C	-3.22	117.82	126.72
28	1	617	LUT	C30-C31-C32	-3.22	113.17	123.22
20	A	828	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
20	5	601	CLA	C3B-C4B-NB	3.22	113.37	109.21
20	1	602	CLA	C1C-C2C-C3C	-3.22	103.57	106.96
20	A	830	CLA	C1C-C2C-C3C	-3.22	103.58	106.96
20	6	611	CLA	CAA-C2A-C3A	-3.22	103.97	112.78
20	7	609	CLA	CMB-C2B-C3B	3.22	130.69	124.68
23	5	625	BCR	C40-C30-C25	3.22	115.52	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Z	613	CLA	C3B-C4B-NB	3.22	113.37	109.21
20	3	612	CLA	CHC-C1C-C2C	-3.22	117.83	126.72
20	7	609	CLA	C4C-C3C-C2C	-3.22	102.21	106.90
20	F	303	CLA	C4C-C3C-C2C	-3.21	102.21	106.90
20	Z	602	CLA	C4C-C3C-C2C	-3.21	102.21	106.90
20	8	609	CLA	CHB-C4A-NA	3.21	128.96	124.51
20	G	203	CLA	CAA-C2A-C3A	-3.21	103.98	112.78
20	Z	609	CLA	CAA-C2A-C3A	-3.21	103.98	112.78
21	B	842	PQN	C11-C12-C13	-3.21	121.44	126.79
27	4	618	CHL	CAC-C3C-C4C	3.21	128.98	124.81
20	B	828	CLA	CHC-C1C-C2C	-3.21	117.84	126.72
20	5	609	CLA	CHC-C1C-C2C	-3.21	117.84	126.72
20	4	613	CLA	CHC-C1C-C2C	-3.21	117.84	126.72
20	Z	606	CLA	CAA-C2A-C3A	-3.21	103.99	112.78
20	B	807	CLA	CHC-C1C-C2C	-3.21	117.85	126.72
20	5	602	CLA	C1C-C2C-C3C	-3.21	103.58	106.96
23	B	801	BCR	C2-C1-C6	3.21	115.42	110.48
20	A	840	CLA	CAC-C3C-C4C	3.21	128.97	124.81
20	A	845	CLA	CHC-C1C-C2C	-3.20	117.86	126.72
20	B	818	CLA	CBA-CAA-C2A	3.20	123.32	113.86
20	A	812	CLA	C3B-C4B-NB	3.20	113.35	109.21
28	1	618	LUT	C10-C11-C12	-3.20	113.22	123.22
20	A	802	CLA	C1D-CHD-C4C	-3.20	119.15	126.06
23	B	847	BCR	C7-C8-C9	-3.20	121.40	126.23
20	B	816	CLA	C1C-C2C-C3C	-3.20	103.59	106.96
20	4	601	CLA	CAC-C3C-C4C	3.20	128.96	124.81
20	3	602	CLA	C1C-C2C-C3C	-3.20	103.59	106.96
20	A	819	CLA	CAC-C3C-C4C	3.20	128.96	124.81
27	7	607	CHL	CAC-C3C-C4C	3.20	128.96	124.81
20	B	839	CLA	C4C-C3C-C2C	-3.20	102.24	106.90
20	B	834	CLA	CHC-C1C-C2C	-3.20	117.88	126.72
20	L	204	CLA	CAC-C3C-C4C	3.20	128.96	124.81
23	F	305	BCR	C35-C13-C14	-3.20	118.44	122.92
20	B	833	CLA	CHC-C1C-C2C	-3.20	117.88	126.72
28	Z	617	LUT	C35-C15-C14	-3.19	116.93	123.47
20	3	607	CLA	C3B-C4B-NB	3.19	113.34	109.21
21	A	844	PQN	C14-C13-C15	3.19	120.64	115.27
20	A	834	CLA	CHC-C1C-C2C	-3.19	117.89	126.72
23	3	718	BCR	C20-C21-C22	-3.19	122.76	127.31
20	3	613	CLA	CHC-C1C-C2C	-3.19	117.89	126.72
27	Z	607	CHL	C3D-C4D-ND	3.19	115.40	110.24
20	Z	616	CLA	CHC-C1C-C2C	-3.19	117.90	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	604	CLA	C1-C2-C3	-3.19	121.59	126.75
20	3	610	CLA	C1C-C2C-C3C	-3.19	103.60	106.96
20	B	812	CLA	CAC-C3C-C4C	3.19	128.95	124.81
27	3	608	CHL	C2C-C3C-C4C	-3.19	104.22	106.49
20	1	616	CLA	CHC-C1C-C2C	-3.19	117.91	126.72
20	1	604	CLA	C3C-C4C-NC	3.19	114.14	110.57
20	4	614	CLA	C3B-C4B-NB	3.19	113.33	109.21
20	B	829	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
20	3	620	CLA	CHC-C1C-C2C	-3.19	117.91	126.72
20	3	614	CLA	CAC-C3C-C4C	3.19	128.94	124.81
20	K	4002	CLA	C3B-C4B-NB	3.19	113.33	109.21
23	L	201	BCR	C11-C10-C9	-3.18	122.77	127.31
20	A	826	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
20	A	836	CLA	C1-C2-C3	-3.18	121.60	126.75
20	A	833	CLA	C4-C3-C5	3.18	120.62	115.27
20	A	818	CLA	C3B-C4B-NB	3.18	113.32	109.21
20	B	813	CLA	C3B-C4B-NB	3.18	113.32	109.21
20	B	840	CLA	C4C-C3C-C2C	-3.18	102.27	106.90
20	6	622	CLA	C3B-C4B-NB	3.18	113.32	109.21
20	A	836	CLA	CHC-C1C-C2C	-3.18	117.94	126.72
20	A	831	CLA	C4-C3-C5	3.17	120.61	115.27
20	3	609	CLA	C1-C2-C3	-3.17	121.62	126.75
20	7	604	CLA	CHD-C4C-NC	3.17	129.20	124.20
23	K	4001	BCR	C32-C1-C6	-3.17	105.15	110.30
20	3	614	CLA	CAA-C2A-C3A	-3.17	104.09	112.78
20	6	613	CLA	C3B-C4B-NB	3.17	113.31	109.21
28	1	618	LUT	C3-C4-C5	-3.17	105.54	111.85
20	4	603	CLA	CAC-C3C-C4C	3.17	128.92	124.81
20	7	614	CLA	C3B-C4B-NB	3.17	113.31	109.21
27	4	618	CHL	C3B-C4B-NB	3.17	113.31	109.21
20	B	830	CLA	CAC-C3C-C4C	3.17	128.92	124.81
28	7	621	LUT	C35-C15-C14	-3.17	116.98	123.47
27	6	618	CHL	CAC-C3C-C4C	3.17	128.92	124.81
28	5	620	LUT	C39-C29-C28	3.17	123.07	118.08
27	5	618	CHL	C2A-C3A-C4A	-3.17	96.75	101.87
20	B	834	CLA	CAC-C3C-C4C	3.17	128.92	124.81
23	L	201	BCR	C34-C9-C10	-3.17	118.49	122.92
20	A	854	CLA	C1C-C2C-C3C	-3.17	103.63	106.96
20	7	609	CLA	CHC-C1C-C2C	-3.17	117.97	126.72
20	B	829	CLA	CAC-C3C-C4C	3.17	128.92	124.81
20	4	616	CLA	CAC-C3C-C4C	3.17	128.92	124.81
20	A	834	CLA	C1-C2-C3	-3.17	120.57	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	808	CLA	O2A-CGA-CBA	3.16	121.84	111.91
20	Z	608	CLA	CAC-C3C-C4C	3.16	128.92	124.81
20	6	610	CLA	O2A-CGA-CBA	3.16	121.84	111.91
20	8	609	CLA	CAA-C2A-C3A	-3.16	104.11	112.78
20	7	614	CLA	O2D-CGD-O1D	-3.16	117.65	123.84
20	1	610	CLA	O2A-CGA-O1A	-3.16	115.61	123.59
20	3	603	CLA	CAC-C3C-C4C	3.16	128.91	124.81
20	3	611	CLA	CAC-C3C-C4C	3.16	128.91	124.81
28	5	624	LUT	C10-C11-C12	-3.16	113.35	123.22
23	A	856	BCR	C11-C10-C9	-3.16	122.80	127.31
20	1	614	CLA	C3B-C4B-NB	3.16	113.30	109.21
23	5	625	BCR	C23-C22-C21	-3.16	114.09	118.94
20	7	602	CLA	C4C-C3C-C2C	-3.16	102.29	106.90
20	8	609	CLA	C4C-C3C-C2C	-3.16	102.29	106.90
23	G	205	BCR	C11-C10-C9	-3.16	122.80	127.31
23	6	625	BCR	C11-C12-C13	-3.16	117.54	126.42
20	3	609	CLA	CHC-C1C-C2C	-3.16	117.98	126.72
20	A	817	CLA	C3C-C4C-NC	3.16	114.11	110.57
20	Z	610	CLA	C1C-C2C-C3C	-3.16	103.64	106.96
20	3	617	CLA	C3B-C4B-NB	3.16	113.29	109.21
20	B	827	CLA	C4C-C3C-C2C	-3.16	102.30	106.90
28	6	621	LUT	C7-C8-C9	-3.16	121.47	126.23
20	7	602	CLA	CHD-C4C-NC	3.16	129.18	124.20
20	A	816	CLA	C1C-C2C-C3C	-3.16	103.64	106.96
20	5	603	CLA	CMB-C2B-C3B	3.16	130.58	124.68
20	6	617	CLA	CAC-C3C-C4C	3.15	128.90	124.81
20	4	611	CLA	CAA-C2A-C3A	-3.15	104.14	112.78
20	A	807	CLA	CAC-C3C-C4C	3.15	128.90	124.81
20	3	609	CLA	CHB-C4A-NA	3.15	128.87	124.51
20	A	802	CLA	CMD-C2D-C1D	3.15	130.27	124.71
20	A	802	CLA	CAC-C3C-C4C	3.15	128.90	124.81
20	A	808	CLA	CAC-C3C-C4C	3.15	128.90	124.81
23	8	619	BCR	C11-C10-C9	-3.15	122.81	127.31
20	B	816	CLA	C4C-C3C-C2C	-3.15	102.30	106.90
20	3	610	CLA	CAA-C2A-C3A	-3.15	104.15	112.78
20	A	811	CLA	CAC-C3C-C4C	3.15	128.90	124.81
20	A	820	CLA	C1-C2-C3	-3.15	120.59	126.04
27	1	601	CHL	O2A-CGA-CBA	3.15	121.79	111.91
20	5	603	CLA	CHC-C1C-C2C	-3.15	118.01	126.72
20	F	301	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
20	A	829	CLA	CAC-C3C-C4C	3.15	128.89	124.81
20	3	606	CLA	CHC-C1C-C2C	-3.15	118.02	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	816	CLA	CHD-C4C-NC	3.15	129.16	124.20
23	A	848	BCR	C28-C27-C26	-3.15	108.46	114.08
20	5	611	CLA	C3B-C4B-NB	3.15	113.28	109.21
27	6	608	CHL	C3B-C4B-NB	3.15	113.28	109.21
20	1	611	CLA	CAC-C3C-C4C	3.15	128.89	124.81
20	4	611	CLA	CHC-C1C-C2C	-3.14	118.03	126.72
27	6	606	CHL	CAC-C3C-C4C	3.14	128.89	124.81
20	1	616	CLA	C3B-C4B-NB	3.14	113.27	109.21
20	L	203	CLA	C3B-C4B-NB	3.14	113.27	109.21
20	8	606	CLA	C3B-C4B-NB	3.14	113.27	109.21
20	8	611	CLA	CAA-C2A-C3A	-3.14	104.17	112.78
23	L	205	BCR	C28-C27-C26	-3.14	108.47	114.08
20	A	811	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
20	8	611	CLA	C4A-NA-C1A	-3.14	105.29	106.71
20	F	304	CLA	CAC-C3C-C4C	3.14	128.88	124.81
20	4	609	CLA	CHC-C1C-C2C	-3.14	118.04	126.72
28	3	622	LUT	C15-C14-C13	-3.14	122.83	127.31
20	7	620	CLA	C3B-C4B-NB	3.14	113.27	109.21
20	Z	612	CLA	C3B-C4B-NB	3.14	113.27	109.21
20	B	828	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
20	1	610	CLA	C1-C2-C3	-3.14	120.61	126.04
20	6	603	CLA	CHC-C1C-C2C	-3.14	118.04	126.72
20	7	601	CLA	C4A-NA-C1A	-3.14	105.30	106.71
20	Z	610	CLA	C1-C2-C3	-3.14	120.62	126.04
20	1	611	CLA	C4C-C3C-C2C	-3.13	102.33	106.90
20	B	823	CLA	CHC-C1C-C2C	-3.13	118.05	126.72
20	4	601	CLA	C3C-C4C-NC	3.13	114.08	110.57
20	A	837	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
20	B	830	CLA	C1-C2-C3	-3.13	121.68	126.75
23	B	801	BCR	C21-C20-C19	-3.13	113.44	123.22
27	6	607	CHL	C3D-C4D-ND	3.13	115.30	110.24
20	A	827	CLA	CHD-C4C-NC	3.13	129.14	124.20
20	A	810	CLA	C11-C10-C8	-3.13	105.80	115.92
20	B	816	CLA	C3B-C4B-NB	3.13	113.25	109.21
20	8	612	CLA	CHC-C1C-C2C	-3.13	118.07	126.72
20	Z	610	CLA	CAC-C3C-C4C	3.13	128.87	124.81
20	6	613	CLA	CAC-C3C-C4C	3.13	128.87	124.81
20	7	612	CLA	CHC-C1C-C2C	-3.13	118.08	126.72
20	B	824	CLA	O2A-CGA-CBA	3.13	121.72	111.91
20	1	609	CLA	CHC-C1C-C2C	-3.12	118.08	126.72
20	6	611	CLA	C3B-C4B-NB	3.12	113.25	109.21
20	A	840	CLA	C4C-C3C-C2C	-3.12	102.34	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	3	608	CHL	CHD-C4C-NC	3.12	129.12	124.20
20	A	839	CLA	CHC-C1C-C2C	-3.12	118.09	126.72
20	B	835	CLA	CHC-C1C-C2C	-3.12	118.09	126.72
20	A	832	CLA	CHC-C1C-C2C	-3.12	118.10	126.72
20	B	815	CLA	CAC-C3C-C4C	3.12	128.85	124.81
28	5	624	LUT	C38-C25-C24	-3.12	116.89	123.56
20	B	831	CLA	CMB-C2B-C3B	3.12	130.51	124.68
20	A	811	CLA	CAA-C2A-C3A	-3.12	104.25	112.78
20	B	838	CLA	C3B-C4B-NB	3.12	113.24	109.21
20	7	601	CLA	C4C-C3C-C2C	-3.12	102.36	106.90
20	3	603	CLA	CHC-C1C-C2C	-3.11	118.11	126.72
20	5	612	CLA	CHC-C1C-C2C	-3.11	118.11	126.72
23	7	623	BCR	C27-C26-C25	-3.11	118.21	122.73
20	A	836	CLA	CAC-C3C-C4C	3.11	128.85	124.81
20	Z	609	CLA	CAC-C3C-C4C	3.11	128.85	124.81
20	B	808	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
20	A	829	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
20	A	818	CLA	CHD-C4C-NC	3.11	129.10	124.20
27	4	606	CHL	C3B-C4B-NB	3.11	113.23	109.21
20	L	204	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
27	5	607	CHL	O2A-CGA-CBA	3.11	121.65	111.91
20	A	806	CLA	C1C-C2C-C3C	-3.10	103.69	106.96
20	A	838	CLA	CAC-C3C-C4C	3.10	128.84	124.81
20	B	818	CLA	C4-C3-C5	3.10	120.49	115.27
20	A	818	CLA	C4C-C3C-C2C	-3.10	102.37	106.90
27	Z	607	CHL	C3B-C4B-NB	3.10	113.22	109.21
20	Z	608	CLA	CHC-C1C-C2C	-3.10	118.14	126.72
20	6	617	CLA	CHC-C1C-C2C	-3.10	118.14	126.72
20	B	813	CLA	O2A-CGA-CBA	3.10	121.64	111.91
20	K	4003	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
20	A	812	CLA	CAC-C3C-C4C	3.10	128.83	124.81
20	1	606	CLA	CHD-C4C-NC	3.10	129.09	124.20
20	A	819	CLA	CMB-C2B-C3B	3.10	130.48	124.68
20	B	836	CLA	C1C-C2C-C3C	-3.10	103.70	106.96
20	8	602	CLA	C3B-C4B-NB	3.10	113.22	109.21
20	B	807	CLA	O2A-CGA-CBA	3.10	121.63	111.91
23	B	801	BCR	C3-C4-C5	-3.10	108.54	114.08
20	8	601	CLA	CHC-C1C-C2C	-3.10	118.15	126.72
20	B	821	CLA	CAC-C3C-C4C	3.10	128.83	124.81
28	5	620	LUT	C10-C11-C12	-3.09	113.56	123.22
27	1	607	CHL	CAC-C3C-C4C	3.09	128.82	124.81
20	B	832	CLA	C3B-C4B-NB	3.09	113.21	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	6	622	CLA	CHC-C1C-C2C	-3.09	118.17	126.72
23	B	846	BCR	C11-C10-C9	-3.09	122.90	127.31
22	4	622	LHG	C6-C5-C4	-3.09	104.47	111.79
20	B	832	CLA	CHC-C1C-C2C	-3.09	118.17	126.72
20	1	610	CLA	CHD-C4C-NC	3.09	129.08	124.20
20	B	820	CLA	CHC-C1C-C2C	-3.09	118.17	126.72
20	5	611	CLA	CAA-C2A-C3A	-3.09	104.31	112.78
28	Z	617	LUT	C30-C31-C32	-3.09	113.57	123.22
20	B	841	CLA	O2A-CGA-CBA	3.09	121.61	111.91
20	G	204	CLA	CAC-C3C-C4C	3.09	128.82	124.81
20	A	824	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
20	1	602	CLA	CAC-C3C-C4C	3.09	128.82	124.81
20	5	611	CLA	C4-C3-C5	3.09	120.47	115.27
20	5	601	CLA	CHC-C1C-C2C	-3.09	118.18	126.72
20	A	817	CLA	CBC-CAC-C3C	-3.09	103.92	112.43
20	3	603	CLA	CAA-C2A-C3A	-3.09	104.33	112.78
20	Z	604	CLA	CHC-C1C-C2C	-3.09	118.18	126.72
20	1	606	CLA	C4C-C3C-C2C	-3.09	102.40	106.90
20	Z	604	CLA	CAC-C3C-C4C	3.09	128.81	124.81
23	7	623	BCR	C11-C10-C9	-3.08	122.91	127.31
20	7	616	CLA	C3B-C4B-NB	3.08	113.20	109.21
20	B	815	CLA	CHC-C1C-C2C	-3.08	118.19	126.72
20	6	613	CLA	C4C-C3C-C2C	-3.08	102.40	106.90
28	3	621	LUT	C30-C31-C32	-3.08	113.59	123.22
20	Z	603	CLA	C1-O2A-CGA	3.08	124.53	116.44
20	B	803	CLA	C4C-C3C-C2C	-3.08	102.40	106.90
20	G	203	CLA	CHC-C1C-C2C	-3.08	118.19	126.72
27	4	606	CHL	C3D-C4D-ND	3.08	115.22	110.24
20	A	833	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
20	B	819	CLA	CAC-C3C-C4C	3.08	128.81	124.81
20	A	833	CLA	CMB-C2B-C3B	3.08	130.44	124.68
20	8	604	CLA	C3B-C4B-NB	3.08	113.19	109.21
20	3	617	CLA	CAA-C2A-C3A	-3.08	104.35	112.78
20	1	608	CLA	CHC-C1C-C2C	-3.08	118.20	126.72
20	1	611	CLA	CAA-C2A-C3A	-3.08	104.35	112.78
27	6	607	CHL	OMC-CMC-C2C	-3.08	118.73	125.69
20	A	841	CLA	CHB-C4A-NA	3.08	128.77	124.51
20	B	830	CLA	C3B-C4B-NB	3.08	113.19	109.21
28	Z	617	LUT	C10-C11-C12	-3.08	113.61	123.22
20	Z	611	CLA	CHC-C1C-C2C	-3.08	118.21	126.72
20	B	840	CLA	CAA-C2A-C3A	-3.08	104.36	112.78
20	J	3002	CLA	CHC-C1C-C2C	-3.08	118.21	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	806	CLA	CHC-C1C-C2C	-3.07	118.22	126.72
20	G	204	CLA	CHC-C1C-C2C	-3.07	118.23	126.72
27	4	608	CHL	C3B-C4B-NB	3.07	113.18	109.21
20	Z	602	CLA	C1C-C2C-C3C	-3.07	103.73	106.96
20	J	3002	CLA	CAC-C3C-C4C	3.07	128.79	124.81
20	7	606	CLA	CMB-C2B-C3B	3.07	130.42	124.68
20	B	808	CLA	CHC-C1C-C2C	-3.07	118.24	126.72
20	7	604	CLA	C3B-C4B-NB	3.07	113.17	109.21
20	6	602	CLA	CAC-C3C-C4C	3.07	128.79	124.81
20	B	833	CLA	O2A-CGA-CBA	3.07	121.53	111.91
27	5	607	CHL	C3D-C4D-ND	3.06	115.19	110.24
20	A	812	CLA	CAA-C2A-C3A	-3.06	104.39	112.78
20	B	829	CLA	C4-C3-C5	3.06	120.42	115.27
20	8	610	CLA	CAC-C3C-C4C	3.06	128.78	124.81
23	B	801	BCR	C20-C21-C22	-3.06	122.94	127.31
20	A	842	CLA	CHC-C1C-C2C	-3.06	118.25	126.72
20	7	602	CLA	CAC-C3C-C4C	3.06	128.78	124.81
20	5	606	CLA	CHC-C1C-C2C	-3.06	118.26	126.72
20	7	609	CLA	CAC-C3C-C4C	3.06	128.78	124.81
20	B	825	CLA	C1C-C2C-C3C	-3.06	103.74	106.96
20	5	610	CLA	O2A-CGA-CBA	3.06	121.51	111.91
20	7	606	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
20	6	609	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
20	6	601	CLA	CAA-C2A-C3A	-3.06	104.41	112.78
20	A	803	CLA	CHC-C1C-C2C	-3.06	118.27	126.72
20	8	606	CLA	CHC-C1C-C2C	-3.06	118.27	126.72
23	B	848	BCR	C10-C11-C12	-3.06	113.68	123.22
20	7	620	CLA	CHC-C1C-C2C	-3.06	118.27	126.72
20	A	841	CLA	C4C-C3C-C2C	-3.05	102.44	106.90
20	3	611	CLA	CHC-C1C-C2C	-3.05	118.27	126.72
23	5	625	BCR	C37-C22-C23	3.05	122.89	118.08
20	7	620	CLA	O2A-CGA-CBA	3.05	121.49	111.91
20	B	816	CLA	CAC-C3C-C4C	3.05	128.77	124.81
23	F	305	BCR	C28-C27-C26	-3.05	108.63	114.08
20	3	606	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
20	8	613	CLA	C3B-C4B-NB	3.05	113.16	109.21
20	B	820	CLA	O2A-CGA-CBA	3.05	121.48	111.91
20	B	826	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
20	1	616	CLA	CAC-C3C-C4C	3.05	128.77	124.81
20	A	815	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
28	7	621	LUT	C20-C13-C12	3.05	122.88	118.08
23	L	205	BCR	C29-C30-C25	3.05	115.17	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Z	612	CLA	CHC-C1C-C2C	-3.05	118.29	126.72
20	1	606	CLA	C4-C3-C5	3.04	120.39	115.27
20	B	806	CLA	CHD-C4C-NC	3.04	129.00	124.20
20	1	602	CLA	CHD-C4C-NC	3.04	129.00	124.20
20	3	617	CLA	CHC-C1C-C2C	-3.04	118.30	126.72
20	K	4002	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
20	5	611	CLA	CHC-C1C-C2C	-3.04	118.30	126.72
20	4	612	CLA	CHC-C1C-C2C	-3.04	118.30	126.72
28	3	622	LUT	C10-C11-C12	-3.04	113.72	123.22
20	7	606	CLA	C3B-C4B-NB	3.04	113.14	109.21
20	B	837	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
20	A	824	CLA	CHC-C1C-C2C	-3.04	118.31	126.72
20	B	813	CLA	C1C-C2C-C3C	-3.04	103.76	106.96
20	5	609	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
20	B	802	CLA	CHC-C1C-C2C	-3.04	118.32	126.72
20	B	810	CLA	CAC-C3C-C4C	3.04	128.75	124.81
20	B	839	CLA	C3B-C4B-NB	3.04	113.14	109.21
20	B	826	CLA	C1C-C2C-C3C	-3.04	103.76	106.96
27	6	606	CHL	C3D-C4D-ND	3.04	115.15	110.24
20	B	803	CLA	CHB-C4A-NA	3.04	128.71	124.51
20	6	617	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
20	7	611	CLA	CHC-C1C-C2C	-3.04	118.33	126.72
20	3	602	CLA	C4C-C3C-C2C	-3.03	102.47	106.90
20	B	825	CLA	O2A-CGA-CBA	3.03	121.43	111.91
27	6	608	CHL	CHD-C4C-NC	3.03	128.98	124.20
20	6	603	CLA	CAC-C3C-C4C	3.03	128.75	124.81
20	A	823	CLA	CHC-C1C-C2C	-3.03	118.33	126.72
20	A	854	CLA	C3B-C4B-NB	3.03	113.13	109.21
20	1	612	CLA	O2A-CGA-CBA	3.03	121.42	111.91
20	5	610	CLA	CAC-C3C-C4C	3.03	128.74	124.81
20	B	804	CLA	CHB-C4A-NA	3.03	128.70	124.51
20	7	603	CLA	CHC-C1C-C2C	-3.03	118.34	126.72
20	1	602	CLA	CMC-C2C-C1C	3.03	129.65	125.04
28	4	619	LUT	C30-C31-C32	-3.03	113.76	123.22
20	B	821	CLA	CHC-C1C-C2C	-3.03	118.34	126.72
20	3	607	CLA	CHC-C1C-C2C	-3.03	118.34	126.72
20	6	609	CLA	CMB-C2B-C3B	3.03	130.34	124.68
20	A	837	CLA	CAC-C3C-C4C	3.03	128.74	124.81
20	A	806	CLA	CMB-C2B-C3B	3.03	130.34	124.68
20	B	841	CLA	CAC-C3C-C4C	3.03	128.74	124.81
20	4	602	CLA	CHC-C1C-C2C	-3.03	118.35	126.72
20	7	613	CLA	CAC-C3C-C4C	3.03	128.74	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	7	616	CLA	C4C-C3C-C2C	-3.03	102.49	106.90
20	B	814	CLA	C4C-C3C-C2C	-3.03	102.49	106.90
20	4	616	CLA	C3B-C4B-NB	3.03	113.12	109.21
20	B	830	CLA	CAA-C2A-C3A	-3.02	104.50	112.78
20	1	612	CLA	C4C-C3C-C2C	-3.02	102.49	106.90
20	7	616	CLA	CAC-C3C-C4C	3.02	128.73	124.81
20	7	606	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
20	B	818	CLA	CHD-C4C-NC	3.02	128.97	124.20
20	1	602	CLA	O2A-CGA-CBA	3.02	121.39	111.91
20	7	601	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
20	B	820	CLA	CAA-C2A-C3A	-3.02	104.51	112.78
27	4	608	CHL	CHD-C4C-NC	3.02	128.96	124.20
20	A	843	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
20	1	602	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
20	F	304	CLA	CHC-C1C-C2C	-3.02	118.37	126.72
20	7	601	CLA	C4-C3-C5	3.02	120.35	115.27
20	6	611	CLA	CHC-C1C-C2C	-3.02	118.38	126.72
20	4	612	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
20	B	816	CLA	CMC-C2C-C1C	3.02	129.63	125.04
20	8	604	CLA	CHC-C1C-C2C	-3.02	118.38	126.72
20	A	835	CLA	C4C-C3C-C2C	-3.01	102.50	106.90
20	B	804	CLA	CHD-C4C-NC	3.01	128.95	124.20
20	8	616	CLA	CHC-C1C-C2C	-3.01	118.38	126.72
20	B	826	CLA	CHC-C1C-C2C	-3.01	118.39	126.72
20	F	304	CLA	CHD-C4C-NC	3.01	128.95	124.20
20	6	612	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
20	B	852	CLA	CHC-C1C-C2C	-3.01	118.39	126.72
20	7	614	CLA	CHC-C1C-C2C	-3.01	118.39	126.72
27	3	608	CHL	C3D-C4D-ND	3.01	115.11	110.24
27	1	607	CHL	C3B-C4B-NB	3.01	113.10	109.21
20	A	843	CLA	C4-C3-C5	3.01	120.34	115.27
20	7	616	CLA	CHC-C1C-C2C	-3.01	118.39	126.72
20	7	603	CLA	CAA-C2A-C3A	-3.01	104.54	112.78
20	B	814	CLA	CHD-C4C-NC	3.01	128.95	124.20
23	B	845	BCR	C37-C22-C21	-3.01	118.71	122.92
20	4	610	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
20	A	836	CLA	C3B-C4B-NB	3.01	113.10	109.21
20	B	826	CLA	CAA-C2A-C3A	-3.01	104.54	112.78
20	B	831	CLA	CHC-C1C-C2C	-3.01	118.41	126.72
20	1	602	CLA	C3B-C4B-NB	3.01	113.09	109.21
23	L	205	BCR	C23-C24-C25	-3.00	118.76	127.20
20	8	603	CLA	CAC-C3C-C4C	3.00	128.71	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	5	620	LUT	C30-C31-C32	-3.00	113.84	123.22
20	6	609	CLA	C1-C2-C3	-3.00	121.89	126.75
20	B	826	CLA	CHD-C4C-NC	3.00	128.93	124.20
20	B	830	CLA	C4C-C3C-C2C	-3.00	102.52	106.90
20	A	813	CLA	C3B-C4B-NB	3.00	113.09	109.21
20	B	839	CLA	CMB-C2B-C3B	3.00	130.29	124.68
20	A	812	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
20	7	612	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
20	1	609	CLA	CAC-C3C-C4C	3.00	128.70	124.81
23	6	623	BCR	C16-C15-C14	-3.00	117.33	123.47
20	B	814	CLA	C3B-C4B-NB	3.00	113.09	109.21
20	Z	606	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
20	4	604	CLA	CHC-C1C-C2C	-3.00	118.43	126.72
20	B	852	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
20	B	828	CLA	CAC-C3C-C4C	3.00	128.70	124.81
20	7	610	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
20	1	611	CLA	CHC-C1C-C2C	-3.00	118.44	126.72
20	A	818	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
23	5	622	BCR	C21-C20-C19	-3.00	113.87	123.22
20	5	606	CLA	C3B-C4B-NB	2.99	113.08	109.21
20	A	804	CLA	C4C-C3C-C2C	-2.99	102.53	106.90
20	G	203	CLA	C1-C2-C3	-2.99	121.91	126.75
20	4	609	CLA	C3B-C4B-NB	2.99	113.08	109.21
20	3	602	CLA	CAA-C2A-C3A	-2.99	104.58	112.78
20	B	835	CLA	CMB-C2B-C3B	2.99	130.28	124.68
20	6	601	CLA	CHC-C1C-C2C	-2.99	118.45	126.72
20	F	304	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
20	3	620	CLA	CBC-CAC-C3C	-2.99	104.18	112.43
20	A	803	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
20	A	803	CLA	C4-C3-C5	2.99	120.30	115.27
20	8	614	CLA	O2A-CGA-CBA	2.99	121.29	111.91
20	L	203	CLA	CHC-C1C-C2C	-2.99	118.45	126.72
23	6	625	BCR	C16-C17-C18	-2.99	123.04	127.31
20	5	603	CLA	CAC-C3C-C4C	2.99	128.69	124.81
20	5	614	CLA	CAC-C3C-C4C	2.99	128.69	124.81
20	7	608	CLA	C3B-C4B-NB	2.99	113.08	109.21
20	6	611	CLA	C4-C3-C5	2.99	120.30	115.27
20	7	602	CLA	O2A-CGA-CBA	2.99	121.29	111.91
20	6	604	CLA	C3B-C4B-NB	2.99	113.07	109.21
20	5	603	CLA	CAA-C2A-C3A	-2.99	104.60	112.78
27	1	601	CHL	C3D-C4D-ND	2.99	115.07	110.24
20	8	603	CLA	CHC-C1C-C2C	-2.99	118.46	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Z	613	CLA	CHC-C1C-C2C	-2.98	118.47	126.72
20	B	819	CLA	C3B-C4B-NB	2.98	113.07	109.21
27	4	618	CHL	CBC-CAC-C3C	-2.98	104.21	112.43
27	Z	607	CHL	CAC-C3C-C4C	2.98	128.68	124.81
20	A	829	CLA	C3B-C4B-NB	2.98	113.07	109.21
20	A	809	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
23	7	624	BCR	C28-C27-C26	-2.98	108.75	114.08
20	B	841	CLA	CMC-C2C-C1C	2.98	129.58	125.04
20	5	610	CLA	C3B-C4B-NB	2.98	113.06	109.21
20	7	612	CLA	O2A-CGA-CBA	2.98	121.25	111.91
23	4	621	BCR	C3-C4-C5	-2.98	108.76	114.08
20	1	602	CLA	CAA-C2A-C3A	-2.98	104.63	112.78
20	A	825	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
27	5	618	CHL	CAC-C3C-C4C	2.98	128.67	124.81
20	7	614	CLA	O1D-CGD-CBD	-2.98	118.39	124.48
20	A	822	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
20	5	612	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
20	B	804	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
20	K	4002	CLA	CHC-C1C-C2C	-2.97	118.49	126.72
20	8	616	CLA	C4C-C3C-C2C	-2.97	102.56	106.90
20	A	829	CLA	CHD-C4C-NC	2.97	128.89	124.20
20	B	812	CLA	C3B-C4B-NB	2.97	113.05	109.21
20	A	840	CLA	CHC-C1C-C2C	-2.97	118.50	126.72
20	B	821	CLA	C4C-C3C-C2C	-2.97	102.56	106.90
20	7	606	CLA	CHD-C4C-NC	2.97	128.89	124.20
20	A	808	CLA	C4C-C3C-C2C	-2.97	102.56	106.90
20	Z	603	CLA	CAC-C3C-C4C	2.97	128.67	124.81
20	8	608	CLA	C3B-C4B-NB	2.97	113.05	109.21
20	8	602	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
20	A	832	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
20	B	812	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
20	8	612	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
28	8	617	LUT	C30-C31-C32	-2.97	113.95	123.22
20	4	616	CLA	CHD-C4C-NC	2.97	128.88	124.20
20	5	604	CLA	C1-C2-C3	-2.97	121.95	126.75
20	6	602	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
20	7	602	CLA	CAA-C2A-C3A	-2.97	104.65	112.78
20	A	833	CLA	CHD-C4C-NC	2.97	128.88	124.20
20	3	610	CLA	CMA-C3A-C2A	-2.97	101.85	113.83
20	A	806	CLA	CHB-C4A-NA	2.97	128.62	124.51
20	7	601	CLA	CHC-C1C-C2C	-2.97	118.51	126.72
20	5	616	CLA	C4C-C3C-C2C	-2.97	102.57	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	827	CLA	CHC-C1C-C2C	-2.97	118.52	126.72
20	3	609	CLA	CAC-C3C-C4C	2.97	128.66	124.81
20	B	806	CLA	CHC-C1C-C2C	-2.97	118.52	126.72
20	8	609	CLA	CHC-C1C-C2C	-2.97	118.52	126.72
20	B	837	CLA	C3B-C4B-NB	2.96	113.04	109.21
20	3	603	CLA	O2D-CGD-CBD	2.96	116.53	111.27
20	6	614	CLA	CHD-C4C-NC	2.96	128.87	124.20
20	4	604	CLA	C3B-C4B-NB	2.96	113.04	109.21
20	A	813	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
20	A	805	CLA	CMC-C2C-C1C	2.96	129.55	125.04
23	3	718	BCR	C15-C16-C17	-2.96	117.41	123.47
20	1	603	CLA	CAC-C3C-C4C	2.96	128.65	124.81
20	6	601	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
20	A	841	CLA	CHC-C1C-C2C	-2.96	118.53	126.72
20	Z	608	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
20	Z	602	CLA	C4-C3-C5	2.96	120.25	115.27
20	6	611	CLA	CAC-C3C-C4C	2.96	128.65	124.81
20	7	610	CLA	CBC-CAC-C3C	-2.96	104.27	112.43
20	1	614	CLA	CAA-C2A-C3A	-2.96	104.68	112.78
20	B	824	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
20	4	614	CLA	CHD-C4C-NC	2.96	128.86	124.20
20	A	843	CLA	CHC-C1C-C2C	-2.96	118.54	126.72
20	7	601	CLA	CHD-C4C-NC	2.96	128.86	124.20
20	B	841	CLA	C3B-C4B-NB	2.96	113.03	109.21
20	8	603	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
20	6	602	CLA	CHD-C4C-NC	2.96	128.86	124.20
20	A	804	CLA	C1-C2-C3	-2.96	120.93	126.04
23	3	719	BCR	C20-C21-C22	-2.96	123.09	127.31
20	A	815	CLA	CHC-C1C-C2C	-2.95	118.55	126.72
20	F	301	CLA	CHD-C4C-NC	2.95	128.86	124.20
20	A	810	CLA	C3B-C4B-NB	2.95	113.03	109.21
20	B	817	CLA	C4C-C3C-C2C	-2.95	102.59	106.90
20	1	613	CLA	CMC-C2C-C1C	2.95	129.54	125.04
20	B	838	CLA	CAC-C3C-C4C	2.95	128.64	124.81
23	B	845	BCR	C2-C1-C6	2.95	115.03	110.48
20	7	616	CLA	CAA-C2A-C3A	-2.95	104.69	112.78
20	B	823	CLA	O2A-CGA-CBA	2.95	121.17	111.91
20	Z	611	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
20	B	822	CLA	CMB-C2B-C3B	2.95	130.20	124.68
20	Z	612	CLA	O2A-CGA-CBA	2.95	121.17	111.91
20	6	612	CLA	CHC-C1C-C2C	-2.95	118.56	126.72
20	B	812	CLA	CHC-C1C-C2C	-2.95	118.56	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	6	606	CHL	CBC-CAC-C3C	-2.95	104.30	112.43
20	8	610	CLA	C1-C2-C3	-2.95	120.94	126.04
20	Z	603	CLA	C4-C3-C5	2.95	120.23	115.27
20	5	601	CLA	O2A-CGA-CBA	2.95	121.16	111.91
20	B	832	CLA	CAA-C2A-C3A	-2.95	104.71	112.78
20	A	814	CLA	O2A-CGA-CBA	2.95	121.15	111.91
20	6	602	CLA	CMC-C2C-C1C	2.95	129.53	125.04
20	A	806	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
20	B	837	CLA	CHC-C1C-C2C	-2.95	118.57	126.72
20	A	854	CLA	CMA-C3A-C4A	-2.94	103.86	111.77
20	8	603	CLA	CAA-C2A-C3A	-2.94	104.72	112.78
19	A	801	CL0	CHB-C4A-NA	2.94	128.58	124.51
20	G	203	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
20	7	611	CLA	CAC-C3C-C4C	2.94	128.63	124.81
27	Z	601	CHL	C3B-C4B-NB	2.94	113.02	109.21
20	B	815	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
20	8	606	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
20	A	810	CLA	CHC-C1C-C2C	-2.94	118.58	126.72
20	Z	606	CLA	CHD-C4C-NC	2.94	128.84	124.20
20	B	808	CLA	O2A-CGA-O1A	-2.94	116.17	123.59
20	7	613	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
19	A	801	CL0	CHD-C4C-NC	2.94	128.84	124.20
20	B	841	CLA	CHD-C4C-NC	2.94	128.84	124.20
20	8	608	CLA	C1-C2-C3	-2.94	122.00	126.75
20	3	602	CLA	CMB-C2B-C3B	2.94	130.18	124.68
20	6	604	CLA	CHC-C1C-C2C	-2.94	118.59	126.72
20	Z	610	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
20	4	611	CLA	C4-C3-C5	2.94	120.21	115.27
20	B	807	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
20	B	837	CLA	C1-C2-C3	-2.94	120.96	126.04
27	5	608	CHL	C3B-C4B-NB	2.94	113.01	109.21
20	A	819	CLA	C1C-C2C-C3C	-2.94	103.87	106.96
20	A	827	CLA	CMC-C2C-C1C	2.94	129.51	125.04
20	A	805	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
27	6	606	CHL	O2A-CGA-CBA	2.94	121.12	111.91
20	A	842	CLA	C4C-C3C-C2C	-2.94	102.62	106.90
20	3	620	CLA	CAC-C3C-C4C	2.94	128.62	124.81
20	Z	614	CLA	CHC-C1C-C2C	-2.94	118.60	126.72
27	4	607	CHL	O2A-CGA-CBA	2.94	121.12	111.91
20	G	203	CLA	O2A-CGA-CBA	2.93	121.11	111.91
20	Z	606	CLA	C3B-C4B-NB	2.93	113.00	109.21
20	A	811	CLA	CHC-C1C-C2C	-2.93	118.61	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	852	BCR	C15-C14-C13	-2.93	123.12	127.31
20	B	810	CLA	O2A-CGA-CBA	2.93	121.11	111.91
20	B	822	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
20	1	616	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
20	A	807	CLA	O2A-CGA-CBA	2.93	121.10	111.91
20	8	616	CLA	CAC-C3C-C4C	2.93	128.61	124.81
20	8	612	CLA	C4-C3-C5	2.93	120.20	115.27
23	B	843	BCR	C20-C19-C18	-2.93	118.19	126.42
20	B	831	CLA	CHD-C4C-NC	2.93	128.82	124.20
20	B	802	CLA	C1-C2-C3	-2.93	120.98	126.04
20	B	813	CLA	CHC-C1C-C2C	-2.93	118.62	126.72
20	1	614	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
20	6	616	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
20	5	610	CLA	CHD-C4C-NC	2.93	128.82	124.20
20	B	811	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
20	L	204	CLA	CHC-C1C-C2C	-2.93	118.62	126.72
20	B	816	CLA	CAA-C2A-C3A	-2.93	104.76	112.78
20	7	620	CLA	CAC-C3C-C4C	2.93	128.61	124.81
20	F	301	CLA	O2A-CGA-CBA	2.93	121.09	111.91
20	6	610	CLA	C3B-C4B-NB	2.93	112.99	109.21
20	A	823	CLA	O2A-CGA-CBA	2.93	121.09	111.91
20	5	621	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
28	1	618	LUT	C35-C34-C33	-2.93	123.14	127.31
20	B	829	CLA	O2A-CGA-CBA	2.92	121.08	111.91
20	7	603	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
20	8	604	CLA	CAC-C3C-C4C	2.92	128.60	124.81
20	1	608	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
20	8	614	CLA	C3B-C4B-NB	2.92	112.99	109.21
20	B	825	CLA	CHC-C1C-C2C	-2.92	118.64	126.72
23	8	619	BCR	C7-C8-C9	-2.92	121.82	126.23
20	1	614	CLA	CHC-C1C-C2C	-2.92	118.65	126.72
20	6	610	CLA	CHC-C1C-C2C	-2.92	118.65	126.72
23	A	851	BCR	C16-C15-C14	-2.92	117.49	123.47
27	7	607	CHL	C3D-C4D-ND	2.92	114.96	110.24
20	1	609	CLA	O2A-CGA-CBA	2.92	121.07	111.91
27	Z	601	CHL	C4-C3-C5	2.92	120.18	115.27
20	4	601	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
20	Z	610	CLA	O2A-CGA-O1A	-2.92	116.23	123.59
20	Z	612	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
20	1	608	CLA	O2A-CGA-CBA	2.92	121.06	111.91
20	B	804	CLA	C4C-C3C-C2C	-2.92	102.65	106.90
20	A	804	CLA	O2A-CGA-CBA	2.92	121.06	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	813	CLA	CHC-C1C-C2C	-2.92	118.66	126.72
20	B	817	CLA	O2A-CGA-CBA	2.91	121.05	111.91
28	7	622	LUT	C10-C11-C12	-2.91	114.12	123.22
27	1	607	CHL	C3D-C4D-ND	2.91	114.95	110.24
20	B	834	CLA	CHB-C4A-NA	2.91	128.54	124.51
20	8	603	CLA	CHD-C4C-NC	2.91	128.79	124.20
28	5	620	LUT	C7-C8-C9	-2.91	121.83	126.23
20	4	616	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
20	7	614	CLA	CAC-C3C-C4C	2.91	128.59	124.81
20	8	613	CLA	CHC-C1C-C2C	-2.91	118.67	126.72
20	5	612	CLA	C4-C3-C5	2.91	120.17	115.27
20	8	613	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
20	7	603	CLA	CHD-C4C-NC	2.91	128.79	124.20
20	3	614	CLA	CHC-C1C-C2C	-2.91	118.67	126.72
20	A	818	CLA	C4-C3-C5	2.91	120.17	115.27
20	A	810	CLA	CAC-C3C-C4C	2.91	128.59	124.81
20	F	303	CLA	CAC-C3C-C4C	2.91	128.59	124.81
20	6	612	CLA	CHD-C4C-NC	2.91	128.79	124.20
20	Z	606	CLA	CHC-C1C-C2C	-2.91	118.68	126.72
20	8	614	CLA	CAA-C2A-C3A	-2.91	104.81	112.78
20	B	823	CLA	C4-C3-C5	2.91	120.16	115.27
27	6	606	CHL	C3B-C4B-NB	2.91	112.97	109.21
20	B	833	CLA	C1C-C2C-C3C	-2.91	103.90	106.96
20	Z	602	CLA	CHD-C4C-NC	2.91	128.78	124.20
20	4	613	CLA	O2A-C1-C2	2.91	116.27	108.64
20	B	824	CLA	C3B-C4B-NB	2.91	112.97	109.21
20	A	813	CLA	CAC-C3C-C4C	2.90	128.58	124.81
20	B	815	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
20	7	614	CLA	C4C-C3C-C2C	-2.90	102.66	106.90
20	A	854	CLA	O2A-CGA-CBA	2.90	121.02	111.91
20	A	842	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
20	3	607	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
20	4	614	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
27	4	606	CHL	O2A-CGA-CBA	2.90	121.02	111.91
25	B	850	DGD	C2G-O2G-C1B	-2.90	110.64	117.79
20	A	834	CLA	CHD-C4C-NC	2.90	128.78	124.20
20	Z	613	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
20	L	203	CLA	CAC-C3C-C4C	2.90	128.58	124.81
20	8	609	CLA	CAC-C3C-C4C	2.90	128.58	124.81
20	1	606	CLA	C3B-C4B-NB	2.90	112.96	109.21
27	5	607	CHL	C1B-CHB-C4A	-2.90	124.37	130.12
20	4	609	CLA	C4C-C3C-C2C	-2.90	102.67	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	841	CLA	C3B-C4B-NB	2.90	112.96	109.21
20	4	614	CLA	CMC-C2C-C1C	2.90	129.46	125.04
20	B	841	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
20	1	613	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
20	3	603	CLA	CBC-CAC-C3C	-2.90	104.44	112.43
20	6	613	CLA	CHC-C1C-C2C	-2.90	118.70	126.72
27	6	608	CHL	O2A-CGA-CBA	2.90	121.00	111.91
23	7	623	BCR	C15-C16-C17	-2.90	117.54	123.47
20	1	606	CLA	CHC-C1C-C2C	-2.90	118.71	126.72
20	B	812	CLA	CHD-C4C-NC	2.90	128.77	124.20
20	A	815	CLA	C4-C3-C5	2.90	120.14	115.27
20	Z	611	CLA	CAC-C3C-C4C	2.89	128.57	124.81
20	6	604	CLA	CAC-C3C-C4C	2.89	128.56	124.81
27	1	601	CHL	CAC-C3C-C4C	2.89	128.56	124.81
23	3	717	BCR	C16-C15-C14	-2.89	117.55	123.47
20	F	301	CLA	C1-C2-C3	-2.89	121.04	126.04
20	Z	613	CLA	CAC-C3C-C4C	2.89	128.56	124.81
23	B	848	BCR	C21-C20-C19	-2.89	114.19	123.22
20	B	837	CLA	CHD-C4C-NC	2.89	128.76	124.20
20	A	807	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
20	A	827	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
20	3	612	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
20	B	839	CLA	CHC-C1C-C2C	-2.89	118.72	126.72
20	5	606	CLA	CHD-C4C-NC	2.89	128.76	124.20
20	3	613	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
20	B	826	CLA	C3B-C4B-NB	2.89	112.95	109.21
20	8	614	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
28	8	618	LUT	C31-C30-C29	-2.89	123.19	127.31
23	5	622	BCR	C2-C1-C6	2.89	114.93	110.48
20	A	809	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
20	8	601	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
20	A	814	CLA	C1-O2A-CGA	2.89	124.02	116.44
23	3	718	BCR	C24-C23-C22	-2.89	121.87	126.23
20	B	825	CLA	CAC-C3C-C4C	2.89	128.56	124.81
20	7	608	CLA	CHC-C1C-C2C	-2.89	118.73	126.72
20	7	601	CLA	O2A-CGA-O1A	-2.89	116.30	123.59
23	A	851	BCR	C21-C20-C19	-2.89	114.20	123.22
23	F	305	BCR	C29-C30-C25	2.89	114.93	110.48
20	4	604	CLA	CHD-C4C-NC	2.89	128.75	124.20
20	A	805	CLA	CHC-C1C-C2C	-2.89	118.74	126.72
20	A	818	CLA	CHC-C1C-C2C	-2.89	118.74	126.72
20	7	620	CLA	C4C-C3C-C2C	-2.88	102.69	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	4	620	LUT	C10-C11-C12	-2.88	114.22	123.22
23	A	852	BCR	C11-C10-C9	-2.88	123.19	127.31
20	A	803	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
22	A	846	LHG	O8-C23-C24	2.88	120.95	111.91
20	4	604	CLA	CAC-C3C-C4C	2.88	128.55	124.81
20	F	303	CLA	CHC-C1C-C2C	-2.88	118.75	126.72
20	A	817	CLA	CAC-C3C-C4C	2.88	128.55	124.81
23	I	172	BCR	C28-C27-C26	-2.88	108.93	114.08
20	8	614	CLA	CHD-C4C-NC	2.88	128.74	124.20
20	A	803	CLA	CMC-C2C-C1C	2.88	129.42	125.04
20	4	610	CLA	CMB-C2B-C3B	2.88	130.06	124.68
20	B	831	CLA	C3B-C4B-NB	2.88	112.93	109.21
20	7	604	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
20	6	611	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
20	B	822	CLA	CAA-C2A-C3A	-2.88	104.90	112.78
20	B	838	CLA	CHC-C1C-C2C	-2.88	118.77	126.72
20	5	614	CLA	CHD-C4C-NC	2.88	128.74	124.20
23	B	848	BCR	C16-C15-C14	-2.88	117.58	123.47
20	B	835	CLA	C4C-C3C-C2C	-2.88	102.71	106.90
20	A	806	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
20	A	808	CLA	CMC-C2C-C1C	2.87	129.41	125.04
20	B	836	CLA	O2A-CGA-CBA	2.87	120.92	111.91
20	4	601	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
20	5	614	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
28	Z	617	LUT	C15-C14-C13	-2.87	123.21	127.31
20	Z	611	CLA	CAA-C2A-C3A	-2.87	104.92	112.78
20	1	613	CLA	C1-O2A-CGA	2.87	123.98	116.44
20	A	816	CLA	CHC-C1C-C2C	-2.87	118.78	126.72
20	1	610	CLA	CMB-C2B-C3B	2.87	130.05	124.68
20	4	616	CLA	CHC-C1C-C2C	-2.87	118.78	126.72
20	A	815	CLA	CAA-C2A-C1A	2.87	121.38	111.97
20	Z	614	CLA	CHD-C4C-NC	2.87	128.72	124.20
20	A	839	CLA	CAC-C3C-C4C	2.87	128.53	124.81
20	Z	602	CLA	C3B-C4B-NB	2.87	112.92	109.21
20	A	814	CLA	CHB-C4A-NA	2.87	128.48	124.51
20	7	606	CLA	CHC-C1C-C2C	-2.87	118.79	126.72
20	B	804	CLA	CAC-C3C-C4C	2.87	128.53	124.81
20	3	611	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
20	7	614	CLA	CAA-C2A-C3A	-2.86	104.93	112.78
20	A	823	CLA	C4C-C3C-C2C	-2.86	102.72	106.90
20	A	802	CLA	CHC-C1C-C2C	-2.86	118.80	126.72
20	1	611	CLA	C3B-C4B-NB	2.86	112.91	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	802	CLA	C4C-C3C-C2C	-2.86	102.72	106.90
20	A	822	CLA	CHC-C1C-C2C	-2.86	118.80	126.72
20	B	837	CLA	CHB-C4A-NA	2.86	128.47	124.51
20	A	804	CLA	CMD-C2D-C3D	-2.86	121.03	127.61
20	5	602	CLA	CAA-C2A-C3A	-2.86	104.94	112.78
20	8	609	CLA	CMA-C3A-C4A	-2.86	104.08	111.77
20	B	820	CLA	CHD-C4C-NC	2.86	128.71	124.20
20	5	601	CLA	CAA-C2A-C3A	-2.86	104.94	112.78
20	3	606	CLA	CAC-C3C-C4C	2.86	128.52	124.81
20	B	811	CLA	CAA-C2A-C3A	-2.86	104.94	112.78
20	7	604	CLA	C1-C2-C3	-2.86	121.10	126.04
23	B	801	BCR	C16-C17-C18	-2.86	123.23	127.31
20	A	814	CLA	C4-C3-C5	2.86	120.08	115.27
20	7	612	CLA	CAC-C3C-C4C	2.86	128.52	124.81
20	5	611	CLA	CHD-C4C-NC	2.86	128.71	124.20
20	5	602	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
20	5	610	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
20	A	840	CLA	O2A-CGA-CBA	2.86	120.88	111.91
20	B	825	CLA	C3B-C4B-NB	2.86	112.91	109.21
20	A	802	CLA	C3B-C4B-NB	2.86	112.90	109.21
20	1	614	CLA	C4-C3-C5	2.86	120.07	115.27
20	A	820	CLA	CHD-C4C-NC	2.85	128.70	124.20
27	1	601	CHL	C2A-C1A-CHA	-2.85	118.87	123.86
20	B	819	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
20	B	838	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
20	8	612	CLA	CHD-C4C-NC	2.85	128.70	124.20
20	4	610	CLA	C1-C2-C3	-2.85	121.11	126.04
20	8	608	CLA	CAC-C3C-C4C	2.85	128.51	124.81
27	Z	601	CHL	O2A-CGA-CBA	2.85	120.86	111.91
20	A	838	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
20	3	609	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
20	Z	614	CLA	O2A-CGA-CBA	2.85	120.86	111.91
20	4	602	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
20	6	610	CLA	CHD-C4C-NC	2.85	128.70	124.20
20	4	603	CLA	CBC-CAC-C3C	-2.85	104.57	112.43
27	1	601	CHL	O2A-C1-C2	2.85	116.13	108.64
20	8	601	CLA	CAC-C3C-C4C	2.85	128.51	124.81
20	5	614	CLA	CHC-C1C-C2C	-2.85	118.84	126.72
23	3	717	BCR	C24-C23-C22	-2.85	121.93	126.23
28	1	618	LUT	C38-C25-C24	-2.85	117.46	123.56
19	A	801	CL0	C4C-C3C-C2C	-2.85	102.74	106.90
20	4	613	CLA	C4A-NA-C1A	-2.85	105.42	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	811	CLA	CHD-C4C-NC	2.85	128.69	124.20
20	8	613	CLA	CMC-C2C-C1C	2.85	129.38	125.04
20	A	833	CLA	CHC-C1C-C2C	-2.85	118.84	126.72
20	A	829	CLA	C1-C2-C3	-2.85	121.12	126.04
23	B	844	BCR	C33-C5-C6	-2.85	121.33	124.53
20	3	617	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
20	8	612	CLA	O2A-CGA-CBA	2.85	120.84	111.91
23	B	847	BCR	C36-C18-C19	2.85	122.56	118.08
20	Z	616	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
20	A	805	CLA	CMB-C2B-C3B	2.85	130.00	124.68
20	A	820	CLA	CHC-C1C-C2C	-2.84	118.85	126.72
20	J	3002	CLA	C4C-C3C-C2C	-2.84	102.75	106.90
20	6	614	CLA	CAC-C3C-C4C	2.84	128.50	124.81
20	5	611	CLA	C4C-C3C-C2C	-2.84	102.75	106.90
20	3	602	CLA	CHD-C4C-NC	2.84	128.68	124.20
20	B	820	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
20	B	830	CLA	CHC-C1C-C2C	-2.84	118.86	126.72
28	4	619	LUT	C7-C8-C9	-2.84	121.94	126.23
20	6	610	CLA	CAC-C3C-C4C	2.84	128.50	124.81
20	A	811	CLA	CMC-C2C-C1C	2.84	129.37	125.04
20	8	604	CLA	CAA-C2A-C3A	-2.84	105.00	112.78
27	Z	601	CHL	C2A-C1A-CHA	-2.84	118.89	123.86
23	B	844	BCR	C11-C10-C9	-2.84	123.26	127.31
20	7	608	CLA	O2A-CGA-CBA	2.84	120.82	111.91
20	B	824	CLA	CHD-C4C-NC	2.84	128.68	124.20
20	A	828	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
20	7	611	CLA	CMA-C3A-C2A	-2.84	109.47	116.10
20	Z	604	CLA	C4-C3-C5	2.84	120.05	115.27
20	8	616	CLA	CAA-C2A-C3A	-2.84	105.01	112.78
20	B	837	CLA	CAA-C2A-C3A	-2.84	105.01	112.78
20	B	833	CLA	C4-C3-C5	2.84	120.04	115.27
20	B	824	CLA	CMB-C2B-C3B	2.84	129.99	124.68
20	6	614	CLA	CMD-C2D-C3D	-2.84	121.09	127.61
20	3	617	CLA	CAC-C3C-C4C	2.84	128.49	124.81
27	5	608	CHL	C2A-C3A-C4A	-2.84	97.29	101.87
20	1	604	CLA	C4-C3-C5	2.84	120.04	115.27
20	1	603	CLA	CAA-C2A-C3A	-2.83	105.02	112.78
20	A	827	CLA	C3B-C4B-NB	2.83	112.87	109.21
20	3	603	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
20	Z	614	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
20	7	602	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
20	A	840	CLA	CHD-C4C-NC	2.83	128.67	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	812	CLA	CHC-C1C-C2C	-2.83	118.89	126.72
20	1	603	CLA	CHD-C4C-NC	2.83	128.66	124.20
20	B	813	CLA	CAA-C2A-C3A	-2.83	105.03	112.78
20	F	303	CLA	CHD-C4C-NC	2.83	128.66	124.20
20	A	824	CLA	C1-C2-C3	-2.83	121.15	126.04
20	3	610	CLA	C1-C2-C3	-2.83	121.15	126.04
20	7	610	CLA	CAC-C3C-C4C	2.83	128.48	124.81
20	B	834	CLA	C4C-C3C-C2C	-2.83	102.78	106.90
20	A	822	CLA	CAA-C2A-C3A	-2.83	105.04	112.78
23	6	625	BCR	C21-C20-C19	-2.83	114.40	123.22
20	7	611	CLA	C4C-C3C-C2C	-2.83	102.78	106.90
20	B	838	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
20	Z	608	CLA	O2A-CGA-CBA	2.83	120.77	111.91
20	5	603	CLA	CHD-C4C-NC	2.83	128.66	124.20
20	8	608	CLA	C4C-C3C-C2C	-2.82	102.78	106.90
20	6	604	CLA	C4C-C3C-C2C	-2.82	102.78	106.90
20	4	613	CLA	CHB-C4A-NA	2.82	128.42	124.51
20	B	805	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
20	8	614	CLA	CHC-C1C-C2C	-2.82	118.91	126.72
20	A	814	CLA	CHC-C1C-C2C	-2.82	118.91	126.72
20	K	4002	CLA	C4C-C3C-C2C	-2.82	102.78	106.90
20	3	614	CLA	CHD-C4C-NC	2.82	128.65	124.20
20	B	822	CLA	CHC-C1C-C2C	-2.82	118.91	126.72
20	B	822	CLA	CHD-C4C-NC	2.82	128.65	124.20
20	B	802	CLA	O2A-CGA-CBA	2.82	120.76	111.91
20	B	807	CLA	C1-C2-C3	-2.82	121.16	126.04
20	A	808	CLA	C4-C3-C5	2.82	120.02	115.27
20	1	614	CLA	CHD-C4C-NC	2.82	128.65	124.20
20	6	612	CLA	CAC-C3C-C4C	2.82	128.47	124.81
23	J	3003	BCR	C11-C10-C9	-2.82	123.29	127.31
20	A	816	CLA	CHD-C4C-NC	2.82	128.65	124.20
23	4	621	BCR	C21-C20-C19	-2.82	114.42	123.22
20	A	823	CLA	CAC-C3C-C4C	2.82	128.47	124.81
20	5	606	CLA	O2A-CGA-CBA	2.82	120.75	111.91
20	F	301	CLA	CAC-C3C-C4C	2.82	128.47	124.81
20	5	603	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
28	7	622	LUT	C38-C25-C24	-2.82	117.53	123.56
20	A	841	CLA	CHD-C4C-NC	2.81	128.64	124.20
20	A	816	CLA	CAC-C3C-C4C	2.81	128.46	124.81
20	1	613	CLA	CHC-C1C-C2C	-2.81	118.94	126.72
20	8	611	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
27	1	601	CHL	CMB-C2B-C3B	2.81	129.94	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	3	719	BCR	C10-C11-C12	-2.81	114.44	123.22
20	5	610	CLA	CMB-C2B-C3B	2.81	129.94	124.68
20	6	616	CLA	C3B-C4B-NB	2.81	112.84	109.21
20	1	614	CLA	CMB-C2B-C3B	2.81	129.94	124.68
20	5	601	CLA	CBC-CAC-C3C	-2.81	104.68	112.43
20	5	604	CLA	CHB-C4A-NA	2.81	128.40	124.51
20	A	839	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
20	7	603	CLA	CAC-C3C-C4C	2.81	128.46	124.81
20	G	204	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
20	A	843	CLA	CHD-C4C-NC	2.81	128.63	124.20
20	B	811	CLA	CAC-C3C-C4C	2.81	128.45	124.81
20	5	602	CLA	O2A-CGA-CBA	2.81	120.72	111.91
20	A	809	CLA	CHB-C4A-NA	2.81	128.39	124.51
20	8	602	CLA	O2A-CGA-CBA	2.81	120.72	111.91
20	8	604	CLA	C4C-C3C-C2C	-2.81	102.81	106.90
28	7	621	LUT	C15-C14-C13	-2.81	123.31	127.31
20	B	827	CLA	O2A-CGA-CBA	2.81	120.71	111.91
20	B	836	CLA	CHC-C1C-C2C	-2.80	118.96	126.72
20	A	842	CLA	CHD-C4C-NC	2.80	128.62	124.20
20	4	613	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
20	A	822	CLA	CHD-C4C-NC	2.80	128.62	124.20
20	A	808	CLA	CAA-C2A-C3A	-2.80	105.10	112.78
20	1	613	CLA	CHD-C4C-NC	2.80	128.62	124.20
20	8	610	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
23	A	851	BCR	C15-C16-C17	-2.80	117.73	123.47
23	7	623	BCR	C24-C23-C22	-2.80	122.00	126.23
23	G	205	BCR	C28-C27-C26	-2.80	109.07	114.08
20	A	824	CLA	CAC-C3C-C4C	2.80	128.44	124.81
20	A	816	CLA	C4-C3-C5	2.80	119.98	115.27
20	1	610	CLA	CAC-C3C-C4C	2.80	128.44	124.81
20	B	823	CLA	CHB-C4A-NA	2.80	128.38	124.51
20	6	602	CLA	CHC-C1C-C2C	-2.80	118.97	126.72
20	8	602	CLA	CAA-C2A-C3A	-2.80	105.11	112.78
20	A	820	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
20	Z	613	CLA	CHD-C4C-NC	2.80	128.61	124.20
20	5	612	CLA	CHD-C4C-NC	2.80	128.61	124.20
20	A	830	CLA	CMC-C2C-C1C	2.80	129.30	125.04
20	A	854	CLA	CHA-C1A-NA	-2.80	119.99	126.40
27	6	606	CHL	C4-C3-C5	2.80	119.97	115.27
23	A	852	BCR	C16-C15-C14	-2.80	117.75	123.47
20	B	852	CLA	CAC-C3C-C4C	2.80	128.44	124.81
23	I	172	BCR	C10-C11-C12	-2.80	114.49	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	808	CLA	CHC-C1C-C2C	-2.80	118.99	126.72
20	B	829	CLA	CHC-C1C-C2C	-2.80	118.99	126.72
20	A	823	CLA	CHD-C4C-NC	2.80	128.61	124.20
20	4	612	CLA	C4-C3-C5	2.80	119.97	115.27
20	6	603	CLA	CAA-C2A-C3A	-2.79	105.12	112.78
20	4	609	CLA	CAC-C3C-C4C	2.79	128.44	124.81
20	A	804	CLA	CHD-C4C-NC	2.79	128.61	124.20
20	B	814	CLA	CHC-C1C-C2C	-2.79	118.99	126.72
20	5	602	CLA	C3B-C4B-NB	2.79	112.82	109.21
20	8	616	CLA	CHD-C4C-NC	2.79	128.60	124.20
20	6	622	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
20	1	604	CLA	CHB-C4A-NA	2.79	128.37	124.51
20	A	832	CLA	C1-C2-C3	-2.79	122.23	126.75
20	4	603	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
20	5	609	CLA	CMB-C2B-C3B	2.79	129.90	124.68
20	A	804	CLA	CHC-C1C-C2C	-2.79	119.00	126.72
23	I	172	BCR	C15-C14-C13	-2.79	123.33	127.31
20	Z	609	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
28	4	619	LUT	C39-C29-C28	2.79	122.47	118.08
20	1	611	CLA	CMB-C2B-C3B	2.79	129.90	124.68
20	7	614	CLA	CHD-C4C-NC	2.79	128.60	124.20
20	B	814	CLA	CMA-C3A-C4A	-2.79	104.28	111.77
20	B	802	CLA	CHB-C4A-NA	2.79	128.37	124.51
20	6	616	CLA	CHC-C1C-C2C	-2.79	119.02	126.72
20	B	836	CLA	C4-C3-C5	2.79	119.96	115.27
20	7	620	CLA	CHD-C4C-NC	2.79	128.59	124.20
20	1	608	CLA	CAC-C3C-C4C	2.78	128.42	124.81
20	B	806	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
20	7	603	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
20	B	820	CLA	C1-C2-C3	-2.78	121.23	126.04
20	A	826	CLA	C4-C3-C5	2.78	119.95	115.27
28	6	624	LUT	C16-C1-C6	-2.78	105.79	110.30
20	8	609	CLA	CMB-C2B-C3B	2.78	129.88	124.68
20	K	4003	CLA	CAA-C2A-C3A	-2.78	105.16	112.78
20	4	612	CLA	CAC-C3C-C4C	2.78	128.42	124.81
20	A	828	CLA	C3B-C4B-NB	2.78	112.80	109.21
20	B	819	CLA	C4-C3-C5	2.78	119.95	115.27
20	B	808	CLA	CBA-CAA-C2A	2.78	122.07	113.86
20	B	831	CLA	C4C-C3C-C2C	-2.78	102.85	106.90
20	5	601	CLA	C4C-C3C-C2C	-2.78	102.85	106.90
28	3	622	LUT	C15-C35-C34	-2.78	117.78	123.47
20	B	841	CLA	CMB-C2B-C3B	2.78	129.88	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Z	612	CLA	CHD-C4C-NC	2.78	128.58	124.20
20	Z	614	CLA	C4-C3-C5	2.78	119.94	115.27
20	Z	602	CLA	O2A-CGA-CBA	2.78	120.63	111.91
20	B	803	CLA	CHC-C1C-C2C	-2.78	119.04	126.72
20	B	805	CLA	CHC-C1C-C2C	-2.78	119.04	126.72
20	B	824	CLA	C4C-C3C-C2C	-2.78	102.85	106.90
20	A	843	CLA	CMC-C2C-C1C	2.78	129.27	125.04
20	B	827	CLA	CAC-C3C-C4C	2.78	128.41	124.81
20	6	604	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
20	A	843	CLA	CAA-C2A-C3A	-2.78	105.18	112.78
20	A	814	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
20	8	601	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
20	3	614	CLA	C4C-C3C-C2C	-2.77	102.85	106.90
20	L	203	CLA	CAA-C2A-C3A	-2.77	105.18	112.78
19	A	801	CL0	CMA-C3A-C2A	-2.77	102.64	113.83
20	3	602	CLA	CHC-C1C-C2C	-2.77	119.05	126.72
20	A	842	CLA	C4-C3-C5	2.77	119.94	115.27
20	A	816	CLA	C3B-C4B-NB	2.77	112.80	109.21
20	5	613	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
20	L	204	CLA	C1-C2-C3	-2.77	122.27	126.75
23	G	205	BCR	C10-C11-C12	-2.77	114.56	123.22
20	K	4002	CLA	CAC-C3C-C4C	2.77	128.41	124.81
20	B	836	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
20	A	815	CLA	CAC-C3C-C4C	2.77	128.41	124.81
20	A	836	CLA	CHB-C4A-NA	2.77	128.34	124.51
20	4	611	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
20	5	610	CLA	CMC-C2C-C1C	2.77	129.26	125.04
23	G	205	BCR	C7-C8-C9	-2.77	122.05	126.23
20	Z	602	CLA	CHC-C1C-C2C	-2.77	119.06	126.72
20	8	609	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
20	8	611	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
20	A	803	CLA	CHA-C1A-NA	-2.77	120.06	126.40
20	B	803	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
20	B	806	CLA	CMC-C2C-C1C	2.77	129.25	125.04
20	B	836	CLA	C1-C2-C3	-2.77	121.26	126.04
20	1	610	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
20	B	841	CLA	CHC-C1C-C2C	-2.77	119.07	126.72
20	Z	606	CLA	CAC-C3C-C4C	2.77	128.40	124.81
20	B	838	CLA	CHD-C4C-NC	2.77	128.56	124.20
20	A	818	CLA	O2A-CGA-CBA	2.77	120.59	111.91
20	G	204	CLA	CHD-C4C-NC	2.76	128.56	124.20
27	8	607	CHL	C2A-C1A-CHA	-2.76	119.03	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	8	611	CLA	CHB-C4A-NA	2.76	128.33	124.51
20	Z	609	CLA	O2A-CGA-CBA	2.76	120.58	111.91
20	5	610	CLA	CHC-C1C-C2C	-2.76	119.08	126.72
27	4	607	CHL	C1-C2-C3	-2.76	122.28	126.75
20	B	827	CLA	CHB-C4A-NA	2.76	128.33	124.51
20	3	612	CLA	CAC-C3C-C4C	2.76	128.39	124.81
20	B	836	CLA	CHD-C4C-NC	2.76	128.55	124.20
20	1	609	CLA	C4C-C3C-C2C	-2.76	102.87	106.90
20	Z	603	CLA	C4C-C3C-C2C	-2.76	102.87	106.90
20	A	804	CLA	CAC-C3C-C4C	2.76	128.39	124.81
20	A	834	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
20	3	609	CLA	CHD-C4C-NC	2.76	128.55	124.20
20	A	812	CLA	C11-C12-C13	-2.76	107.01	115.92
20	B	829	CLA	CMA-C3A-C2A	-2.76	102.71	113.83
27	5	608	CHL	C3D-C4D-ND	2.76	114.70	110.24
20	6	610	CLA	C4-C3-C5	2.76	119.91	115.27
20	B	840	CLA	O2A-CGA-CBA	2.76	120.56	111.91
20	1	608	CLA	CHD-C4C-NC	2.76	128.54	124.20
20	B	806	CLA	C1-C2-C3	-2.75	121.28	126.04
20	7	606	CLA	CBC-CAC-C3C	-2.75	104.84	112.43
28	3	621	LUT	C10-C11-C12	-2.75	114.62	123.22
23	F	305	BCR	C11-C12-C13	-2.75	118.68	126.42
20	B	841	CLA	C4-C3-C5	2.75	119.90	115.27
20	6	603	CLA	C4C-C3C-C2C	-2.75	102.88	106.90
20	A	831	CLA	CMB-C2B-C3B	2.75	129.83	124.68
20	5	603	CLA	CBC-CAC-C3C	-2.75	104.84	112.43
20	B	807	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
20	5	601	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
20	3	617	CLA	CHD-C4C-NC	2.75	128.54	124.20
20	4	613	CLA	CHD-C4C-NC	2.75	128.54	124.20
23	A	850	BCR	C7-C8-C9	-2.75	122.08	126.23
20	A	809	CLA	CHC-C1C-C2C	-2.75	119.11	126.72
20	6	612	CLA	C4-C3-C5	2.75	119.90	115.27
20	7	611	CLA	CHD-C4C-NC	2.75	128.54	124.20
20	B	802	CLA	CAC-C3C-C4C	2.75	128.38	124.81
20	A	830	CLA	CHD-C4C-NC	2.75	128.54	124.20
20	B	825	CLA	CHD-C4C-NC	2.75	128.54	124.20
20	B	835	CLA	CHD-C4C-NC	2.75	128.54	124.20
20	1	602	CLA	CHC-C1C-C2C	-2.75	119.12	126.72
20	5	609	CLA	CHB-C4A-NA	2.75	128.31	124.51
20	6	604	CLA	CHD-C4C-NC	2.75	128.53	124.20
20	A	843	CLA	O2A-CGA-CBA	2.75	120.53	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	827	CLA	CAC-C3C-C4C	2.75	128.37	124.81
20	B	822	CLA	CAC-C3C-C4C	2.75	128.37	124.81
23	L	205	BCR	C11-C10-C9	-2.75	123.39	127.31
20	B	829	CLA	C3B-C4B-NB	2.75	112.76	109.21
20	J	3002	CLA	CHD-C4C-NC	2.75	128.53	124.20
20	A	817	CLA	CHD-C4C-NC	2.75	128.53	124.20
22	A	847	LHG	O8-C23-C24	2.74	120.52	111.91
20	A	837	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
27	Z	601	CHL	CMB-C2B-C3B	2.74	129.81	124.68
20	3	604	CLA	CAC-C3C-C4C	2.74	128.37	124.81
20	A	808	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
28	5	624	LUT	C15-C14-C13	-2.74	123.39	127.31
23	A	849	BCR	C34-C9-C8	2.74	122.40	118.08
20	8	608	CLA	CHC-C1C-C2C	-2.74	119.13	126.72
20	A	833	CLA	C3B-C4B-NB	2.74	112.76	109.21
20	B	838	CLA	O2A-CGA-CBA	2.74	120.51	111.91
19	A	801	CL0	CMC-C2C-C1C	2.74	129.22	125.04
20	B	830	CLA	CHD-C4C-NC	2.74	128.52	124.20
20	A	813	CLA	CHD-C4C-NC	2.74	128.52	124.20
20	B	814	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
20	B	814	CLA	CHB-C4A-NA	2.74	128.30	124.51
20	K	4002	CLA	CHD-C4C-NC	2.74	128.52	124.20
20	Z	612	CLA	CAC-C3C-C4C	2.74	128.37	124.81
20	F	301	CLA	CHC-C1C-C2C	-2.74	119.14	126.72
20	B	816	CLA	CHC-C1C-C2C	-2.74	119.14	126.72
20	B	826	CLA	O2A-CGA-CBA	2.74	120.50	111.91
20	B	838	CLA	CAA-C2A-C3A	-2.74	105.28	112.78
20	A	843	CLA	CBC-CAC-C3C	-2.74	104.88	112.43
20	Z	602	CLA	CMC-C2C-C1C	2.74	129.21	125.04
20	B	824	CLA	CHC-C1C-C2C	-2.74	119.15	126.72
20	A	805	CLA	CAC-C3C-C4C	2.74	128.36	124.81
23	3	718	BCR	C29-C30-C25	2.74	114.69	110.48
20	5	614	CLA	CAA-C2A-C3A	-2.74	105.29	112.78
20	8	604	CLA	CHB-C4A-NA	2.73	128.29	124.51
20	4	609	CLA	CAA-C2A-C3A	-2.73	105.29	112.78
20	4	604	CLA	C4C-C3C-C2C	-2.73	102.91	106.90
20	5	604	CLA	C4C-C3C-C2C	-2.73	102.91	106.90
28	1	618	LUT	C35-C15-C14	-2.73	117.87	123.47
20	A	816	CLA	CHB-C4A-NA	2.73	128.29	124.51
20	6	614	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
20	6	614	CLA	CHC-C1C-C2C	-2.73	119.16	126.72
20	A	804	CLA	C3B-C4B-NB	2.73	112.74	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	5	601	CLA	CHD-C4C-NC	2.73	128.51	124.20
20	1	613	CLA	CAA-C2A-C3A	-2.73	105.30	112.78
20	Z	604	CLA	CHB-C4A-NA	2.73	128.29	124.51
20	B	816	CLA	C4-C3-C5	2.73	119.86	115.27
20	F	304	CLA	C4-C3-C5	2.73	119.86	115.27
20	B	816	CLA	O2A-CGA-CBA	2.73	120.47	111.91
20	A	826	CLA	CHC-C1C-C2C	-2.73	119.18	126.72
23	3	718	BCR	C11-C10-C9	-2.73	123.42	127.31
20	1	609	CLA	CHB-C4A-NA	2.73	128.28	124.51
20	4	616	CLA	CMA-C3A-C2A	-2.73	109.74	116.10
20	4	612	CLA	CHD-C4C-NC	2.73	128.50	124.20
20	3	610	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
23	8	619	BCR	C37-C22-C23	2.72	122.37	118.08
20	A	836	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
20	8	602	CLA	C4-C3-C5	2.72	119.85	115.27
20	3	607	CLA	CHD-C4C-NC	2.72	128.50	124.20
20	7	601	CLA	CAA-C2A-C3A	-2.72	105.32	112.78
20	3	611	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
25	B	850	DGD	O1G-C1A-C2A	2.72	120.45	111.91
27	4	618	CHL	CMB-C2B-C3B	2.72	129.77	124.68
20	A	814	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
20	4	614	CLA	CHC-C1C-C2C	-2.72	119.20	126.72
20	4	614	CLA	CAC-C3C-C4C	2.72	128.34	124.81
20	6	610	CLA	C1-C2-C3	-2.72	121.34	126.04
20	B	852	CLA	O2A-CGA-CBA	2.72	120.44	111.91
20	1	612	CLA	CHD-C4C-NC	2.72	128.49	124.20
20	A	809	CLA	CHD-C4C-NC	2.72	128.49	124.20
20	8	606	CLA	CHD-C4C-NC	2.72	128.49	124.20
28	1	619	LUT	C38-C25-C24	-2.72	117.74	123.56
22	4	623	LHG	O8-C23-C24	2.72	120.44	111.91
20	4	602	CLA	O2A-CGA-CBA	2.72	120.44	111.91
20	5	610	CLA	C1-C2-C3	-2.72	121.34	126.04
20	A	830	CLA	CHC-C1C-C2C	-2.72	119.20	126.72
20	B	837	CLA	O2A-CGA-CBA	2.72	120.44	111.91
27	8	607	CHL	C4-C3-C5	2.72	119.84	115.27
23	5	625	BCR	C20-C19-C18	-2.72	118.79	126.42
20	A	845	CLA	O2A-CGA-CBA	2.72	120.43	111.91
23	B	846	BCR	C29-C30-C25	2.72	114.66	110.48
28	8	617	LUT	C20-C13-C12	2.72	122.36	118.08
20	4	602	CLA	CHD-C4C-NC	2.72	128.48	124.20
27	4	608	CHL	CAC-C3C-C4C	2.72	128.33	124.81
20	A	838	CLA	C4-C3-C5	2.72	119.09	115.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	819	CLA	CHD-C4C-NC	2.71	128.48	124.20
20	A	803	CLA	O2A-CGA-CBA	2.71	120.43	111.91
20	6	603	CLA	CHD-C4C-NC	2.71	128.48	124.20
23	A	849	BCR	C24-C23-C22	-2.71	122.14	126.23
23	K	4001	BCR	C29-C30-C25	2.71	114.66	110.48
20	7	602	CLA	CHC-C1C-C2C	-2.71	119.22	126.72
20	A	832	CLA	CMB-C2B-C3B	2.71	129.75	124.68
20	B	811	CLA	CHD-C4C-NC	2.71	128.47	124.20
20	A	854	CLA	CMB-C2B-C3B	2.71	129.75	124.68
20	6	602	CLA	C3B-C4B-NB	2.71	112.71	109.21
27	1	601	CHL	C3B-C4B-NB	2.71	112.71	109.21
20	4	610	CLA	CHD-C4C-NC	2.71	128.47	124.20
20	6	611	CLA	CHD-C4C-NC	2.71	128.47	124.20
20	A	845	CLA	CAA-C2A-C3A	-2.71	105.36	112.78
28	7	622	LUT	C35-C15-C14	-2.71	117.93	123.47
20	8	614	CLA	CAC-C3C-C4C	2.71	128.32	124.81
20	1	612	CLA	CAC-C3C-C4C	2.71	128.32	124.81
20	B	805	CLA	CAC-C3C-C4C	2.70	128.32	124.81
20	B	813	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
20	B	839	CLA	CHD-C4C-NC	2.70	128.46	124.20
20	6	601	CLA	CHD-C4C-NC	2.70	128.46	124.20
20	A	839	CLA	CHD-C4C-NC	2.70	128.46	124.20
20	A	827	CLA	CMB-C2B-C3B	2.70	129.73	124.68
20	A	802	CLA	O2A-CGA-CBA	2.70	120.39	111.91
20	8	612	CLA	CAC-C3C-C4C	2.70	128.32	124.81
20	B	810	CLA	C4C-C3C-C2C	-2.70	102.96	106.90
20	7	610	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
27	4	618	CHL	C1B-CHB-C4A	-2.70	124.77	130.12
28	3	622	LUT	C20-C13-C12	2.70	122.33	118.08
20	B	815	CLA	CHB-C4A-NA	2.70	128.24	124.51
20	B	840	CLA	CMC-C2C-C3C	2.70	133.44	126.12
20	3	604	CLA	C4C-C3C-C2C	-2.70	102.97	106.90
20	B	816	CLA	CMB-C2B-C3B	2.70	129.72	124.68
28	Z	618	LUT	C15-C14-C13	-2.70	123.46	127.31
27	4	607	CHL	C2A-C3A-C4A	-2.70	97.51	101.87
20	B	816	CLA	CHB-C4A-NA	2.70	128.24	124.51
20	B	837	CLA	CAC-C3C-C4C	2.70	128.31	124.81
28	3	622	LUT	C30-C31-C32	-2.70	114.81	123.22
20	6	609	CLA	CHB-C4A-NA	2.70	128.24	124.51
20	B	806	CLA	CAA-C2A-C3A	-2.70	105.40	112.78
23	B	844	BCR	C20-C21-C22	-2.69	123.47	127.31
20	Z	609	CLA	CMB-C2B-C3B	2.69	129.72	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	808	CLA	C4-C3-C5	2.69	119.80	115.27
20	5	621	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
20	A	813	CLA	CMB-C2B-C3B	2.69	129.72	124.68
20	A	805	CLA	C4C-C3C-C2C	-2.69	102.97	106.90
20	8	608	CLA	CMB-C2B-C3B	2.69	129.71	124.68
20	A	827	CLA	C1-C2-C3	-2.69	121.39	126.04
20	A	807	CLA	CHD-C4C-NC	2.69	128.44	124.20
20	B	820	CLA	C4C-C3C-C2C	-2.69	102.97	106.90
27	4	608	CHL	C3D-C4D-ND	2.69	114.59	110.24
20	6	601	CLA	CBC-CAC-C3C	-2.69	105.02	112.43
20	6	616	CLA	CMC-C2C-C1C	2.69	129.13	125.04
20	A	835	CLA	CHB-C4A-NA	2.69	128.23	124.51
20	B	814	CLA	CAC-C3C-C4C	2.69	128.30	124.81
20	3	602	CLA	CMC-C2C-C1C	2.69	129.13	125.04
20	B	834	CLA	CHD-C4C-NC	2.69	128.44	124.20
20	A	810	CLA	C11-C12-C13	-2.69	107.23	115.92
23	3	717	BCR	C32-C1-C6	2.69	114.66	110.30
20	B	817	CLA	CHB-C4A-NA	2.69	128.23	124.51
20	3	613	CLA	CMC-C2C-C1C	2.69	129.13	125.04
23	B	843	BCR	C7-C8-C9	-2.69	122.17	126.23
20	B	807	CLA	CAA-C2A-C3A	-2.69	105.42	112.78
23	B	844	BCR	C29-C30-C25	2.69	114.62	110.48
20	B	803	CLA	O2A-CGA-CBA	2.69	120.34	111.91
20	7	608	CLA	C1-C2-C3	-2.69	122.41	126.75
20	B	830	CLA	CMC-C2C-C1C	2.69	129.13	125.04
20	Z	603	CLA	CHD-C4C-NC	2.69	128.44	124.20
23	K	4001	BCR	C2-C1-C6	2.69	114.61	110.48
20	B	807	CLA	CHB-C4A-NA	2.69	128.22	124.51
20	6	622	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
20	5	610	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
20	A	826	CLA	CHD-C4C-NC	2.68	128.43	124.20
20	F	303	CLA	CMB-C2B-C3B	2.68	129.70	124.68
20	B	809	CLA	CHD-C4C-NC	2.68	128.43	124.20
20	B	811	CLA	CAB-C3B-C2B	2.68	129.94	124.69
20	Z	604	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
20	A	810	CLA	O2A-CGA-O1A	-2.68	116.82	123.59
20	4	601	CLA	O2A-CGA-CBA	2.68	120.32	111.91
20	Z	608	CLA	CHD-C4C-NC	2.68	128.43	124.20
23	7	623	BCR	C38-C26-C27	2.68	118.77	113.62
20	A	810	CLA	C4-C3-C5	2.68	119.78	115.27
20	B	805	CLA	CHD-C4C-NC	2.68	128.43	124.20
20	B	822	CLA	O2A-CGA-CBA	2.68	120.32	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Z	614	CLA	CAA-C2A-C3A	-2.68	105.44	112.78
23	A	851	BCR	C24-C23-C22	-2.68	122.19	126.23
20	6	602	CLA	O2A-CGA-CBA	2.68	120.31	111.91
20	A	805	CLA	CBC-CAC-C3C	-2.68	105.05	112.43
20	B	806	CLA	CAC-C3C-C4C	2.68	128.28	124.81
23	8	619	BCR	C29-C30-C25	2.68	114.60	110.48
20	7	608	CLA	C4C-C3C-C2C	-2.68	103.00	106.90
20	B	802	CLA	CHD-C4C-NC	2.68	128.42	124.20
20	4	602	CLA	C1-C2-C3	-2.68	121.41	126.04
20	5	606	CLA	C4C-C3C-C2C	-2.68	103.00	106.90
20	B	835	CLA	CAC-C3C-C4C	2.68	128.28	124.81
20	A	815	CLA	O2A-CGA-CBA	2.68	120.30	111.91
20	B	813	CLA	C1-C2-C3	-2.67	121.42	126.04
23	A	851	BCR	C10-C11-C12	-2.67	114.87	123.22
20	L	203	CLA	C4C-C3C-C2C	-2.67	103.00	106.90
23	K	4001	BCR	C20-C21-C22	-2.67	123.49	127.31
20	5	621	CLA	CMB-C2B-C3B	2.67	129.68	124.68
20	A	840	CLA	C4-C3-C5	2.67	119.77	115.27
20	B	812	CLA	CMC-C2C-C1C	2.67	129.11	125.04
20	6	617	CLA	CHD-C4C-NC	2.67	128.41	124.20
20	G	204	CLA	CAA-C2A-C3A	-2.67	105.46	112.78
20	A	854	CLA	CMC-C2C-C1C	2.67	129.11	125.04
20	5	617	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
20	8	608	CLA	O2A-CGA-CBA	2.67	120.29	111.91
20	1	609	CLA	CMB-C2B-C3B	2.67	129.67	124.68
20	B	828	CLA	O2A-CGA-CBA	2.67	120.29	111.91
27	1	607	CHL	O2A-CGA-CBA	2.67	120.29	111.91
20	B	811	CLA	C4-C3-C5	2.67	119.76	115.27
20	A	814	CLA	CHD-C4C-NC	2.67	128.41	124.20
20	A	830	CLA	O2A-CGA-CBA	2.67	120.28	111.91
20	A	827	CLA	O2A-CGA-CBA	2.67	120.28	111.91
20	B	852	CLA	CHD-C4C-NC	2.67	128.41	124.20
20	Z	608	CLA	C4-C3-C5	2.67	119.76	115.27
20	A	805	CLA	CHB-C4A-NA	2.67	128.20	124.51
20	A	804	CLA	C7-C6-C5	-2.67	106.11	113.36
20	3	606	CLA	CHD-C4C-NC	2.67	128.41	124.20
27	Z	607	CHL	O2A-CGA-CBA	2.67	120.28	111.91
28	Z	617	LUT	C21-C26-C27	-2.67	109.33	112.70
20	B	818	CLA	CAC-C3C-C4C	2.67	128.27	124.81
20	7	612	CLA	CHD-C4C-NC	2.67	128.41	124.20
20	3	610	CLA	O2D-CGD-O1D	-2.67	118.63	123.84
20	8	604	CLA	CHD-C4C-NC	2.67	128.40	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	3	718	BCR	C2-C1-C6	2.66	114.58	110.48
20	1	604	CLA	C4C-C3C-C2C	-2.66	103.02	106.90
22	7	625	LHG	O8-C23-C24	2.66	120.27	111.91
20	B	804	CLA	O1D-CGD-CBD	-2.66	119.03	124.48
23	B	848	BCR	C3-C4-C5	-2.66	109.32	114.08
20	A	819	CLA	CHC-C1C-C2C	-2.66	119.36	126.72
27	5	618	CHL	CMB-C2B-C3B	2.66	129.66	124.68
20	3	603	CLA	CHD-C4C-NC	2.66	128.40	124.20
23	K	4004	BCR	C2-C1-C6	2.66	114.58	110.48
20	3	607	CLA	CMB-C2B-C3B	2.66	129.66	124.68
20	A	822	CLA	CAC-C3C-C4C	2.66	128.26	124.81
20	A	833	CLA	CAC-C3C-C4C	2.66	128.26	124.81
20	1	609	CLA	CHD-C4C-NC	2.66	128.39	124.20
28	6	624	LUT	C10-C11-C12	-2.66	114.92	123.22
20	5	602	CLA	CHC-C1C-C2C	-2.66	119.37	126.72
20	Z	604	CLA	CHD-C4C-NC	2.66	128.39	124.20
20	B	837	CLA	CMB-C2B-C3B	2.66	129.65	124.68
20	B	824	CLA	CHB-C4A-NA	2.66	128.19	124.51
20	5	613	CLA	CHB-C4A-NA	2.66	128.19	124.51
20	5	603	CLA	C4C-C3C-C2C	-2.66	103.03	106.90
28	Z	617	LUT	C17-C1-C6	2.66	114.61	110.30
20	4	616	CLA	CMC-C2C-C1C	2.65	129.08	125.04
20	B	805	CLA	C4-C3-C5	2.65	119.73	115.27
20	A	812	CLA	CMC-C2C-C1C	2.65	129.08	125.04
20	B	852	CLA	CAA-C2A-C3A	-2.65	105.51	112.78
20	1	606	CLA	CAC-C3C-C4C	2.65	128.25	124.81
20	A	828	CLA	CAA-C2A-C3A	-2.65	105.51	112.78
23	A	848	BCR	C31-C1-C6	-2.65	106.00	110.30
20	B	832	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
20	6	610	CLA	C4C-C3C-C2C	-2.65	103.03	106.90
20	B	840	CLA	CHD-C4C-NC	2.65	128.38	124.20
20	B	821	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
20	Z	610	CLA	C3B-C4B-NB	2.65	112.64	109.21
28	Z	619	LUT	C38-C25-C24	-2.65	117.89	123.56
20	4	612	CLA	O2A-CGA-CBA	2.65	120.22	111.91
20	7	613	CLA	CHD-C4C-NC	2.65	128.38	124.20
27	1	607	CHL	CMB-C2B-C3B	2.65	129.63	124.68
28	4	620	LUT	C15-C14-C13	-2.65	123.53	127.31
20	7	604	CLA	O2A-CGA-CBA	2.65	120.22	111.91
20	4	611	CLA	CMB-C2B-C3B	2.65	129.63	124.68
20	B	803	CLA	CHD-C4C-NC	2.65	128.37	124.20
20	A	821	CLA	CAA-C2A-C3A	-2.65	105.53	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	603	CLA	O2A-CGA-CBA	2.64	120.21	111.91
20	1	610	CLA	C3B-C4B-NB	2.64	112.63	109.21
28	3	621	LUT	C35-C15-C14	-2.64	118.06	123.47
20	3	604	CLA	CHD-C4C-NC	2.64	128.37	124.20
28	Z	618	LUT	C38-C25-C24	-2.64	117.90	123.56
20	A	836	CLA	O2A-CGA-CBA	2.64	120.20	111.91
20	G	204	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
20	B	819	CLA	CAA-C2A-C3A	-2.64	105.54	112.78
20	A	821	CLA	CHD-C4C-NC	2.64	128.37	124.20
20	A	821	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
20	8	616	CLA	CMC-C2C-C1C	2.64	129.06	125.04
20	4	616	CLA	CMB-C2B-C3B	2.64	129.62	124.68
20	J	3002	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
20	6	601	CLA	CAC-C3C-C4C	2.64	128.23	124.81
23	3	718	BCR	C21-C20-C19	-2.64	114.98	123.22
20	A	828	CLA	O2A-CGA-CBA	2.64	120.19	111.91
20	4	609	CLA	O2A-CGA-CBA	2.64	120.18	111.91
27	5	608	CHL	O2A-CGA-CBA	2.64	120.18	111.91
20	L	203	CLA	CHD-C4C-NC	2.64	128.36	124.20
20	B	820	CLA	CAC-C3C-C4C	2.64	128.23	124.81
27	6	618	CHL	C2A-C1A-CHA	-2.64	119.25	123.86
20	1	614	CLA	CAC-C3C-C4C	2.64	128.23	124.81
20	5	612	CLA	CAC-C3C-C4C	2.64	128.23	124.81
20	Z	616	CLA	CAA-C2A-C3A	-2.63	105.56	112.78
20	8	610	CLA	CMB-C2B-C3B	2.63	129.61	124.68
20	A	832	CLA	CHB-C4A-NA	2.63	128.15	124.51
20	B	804	CLA	CHC-C1C-C2C	-2.63	119.44	126.72
20	A	812	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
20	3	620	CLA	CHD-C4C-NC	2.63	128.35	124.20
20	7	602	CLA	C3B-C4B-NB	2.63	112.61	109.21
20	B	834	CLA	O2A-CGA-CBA	2.63	120.16	111.91
20	B	806	CLA	CBC-CAC-C3C	-2.63	105.18	112.43
20	A	802	CLA	C1-O2A-CGA	2.63	123.34	116.44
21	A	844	PQN	C11-C12-C13	-2.63	122.42	126.79
20	6	602	CLA	CBC-CAC-C3C	-2.63	105.19	112.43
20	8	610	CLA	C3B-C4B-NB	2.63	112.61	109.21
20	8	610	CLA	CHB-C4A-NA	2.63	128.15	124.51
28	7	621	LUT	C30-C31-C32	-2.63	115.02	123.22
20	B	826	CLA	C4-C3-C5	2.63	119.69	115.27
20	A	836	CLA	CAA-C2A-C3A	-2.63	105.58	112.78
20	B	811	CLA	O2A-CGA-CBA	2.63	120.15	111.91
20	A	806	CLA	CAA-CBA-CGA	-2.63	105.58	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	611	CLA	C1-C2-C3	-2.63	121.50	126.04
23	A	850	BCR	C16-C15-C14	-2.62	118.10	123.47
20	7	620	CLA	CMB-C2B-C3B	2.62	129.59	124.68
20	B	818	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
28	Z	618	LUT	C30-C31-C32	-2.62	115.03	123.22
20	8	610	CLA	O1D-CGD-CBD	-2.62	119.12	124.48
20	A	816	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
20	B	832	CLA	C4C-C3C-C2C	-2.62	103.08	106.90
20	8	614	CLA	CMB-C2B-C3B	2.62	129.58	124.68
20	A	808	CLA	C1-C2-C3	-2.62	121.51	126.04
20	B	806	CLA	O2A-CGA-CBA	2.62	120.13	111.91
20	3	612	CLA	CHD-C4C-NC	2.62	128.33	124.20
20	5	611	CLA	CHB-C4A-NA	2.62	128.13	124.51
20	6	622	CLA	CHB-C4A-NA	2.62	128.13	124.51
20	1	614	CLA	O2A-CGA-CBA	2.62	120.12	111.91
20	3	603	CLA	O2A-CGA-CBA	2.62	120.12	111.91
28	4	619	LUT	C12-C13-C14	-2.62	114.92	118.94
20	A	808	CLA	CHD-C4C-NC	2.62	128.33	124.20
20	5	606	CLA	CAC-C3C-C4C	2.62	128.21	124.81
20	1	616	CLA	CHD-C4C-NC	2.62	128.33	124.20
27	6	608	CHL	C1-C2-C3	-2.62	122.52	126.75
20	B	810	CLA	CHD-C4C-NC	2.62	128.32	124.20
20	6	601	CLA	CHB-C4A-NA	2.61	128.13	124.51
22	Z	620	LHG	O8-C23-C24	2.61	120.11	111.91
20	A	825	CLA	O2A-CGA-O1A	-2.61	117.00	123.59
20	B	830	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
20	B	813	CLA	CHD-C4C-NC	2.61	128.32	124.20
20	A	802	CLA	CMC-C2C-C1C	2.61	129.02	125.04
20	A	826	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
20	K	4003	CLA	CAC-C3C-C4C	2.61	128.20	124.81
20	B	815	CLA	CAA-C2A-C3A	-2.61	105.63	112.78
20	A	820	CLA	C2A-C3A-C4A	-2.61	97.65	101.87
23	A	848	BCR	C29-C30-C25	2.61	114.50	110.48
20	7	604	CLA	CHB-C4A-NA	2.61	128.12	124.51
20	A	826	CLA	CMC-C2C-C1C	2.61	129.01	125.04
19	A	801	CL0	O2D-CGD-O1D	-2.61	118.74	123.84
20	A	821	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
27	4	606	CHL	C2A-C3A-C4A	-2.61	97.66	101.87
20	A	824	CLA	O2A-CGA-CBA	2.61	120.09	111.91
20	6	604	CLA	O2A-CGA-CBA	2.61	120.09	111.91
20	7	610	CLA	C1-C2-C3	-2.61	121.53	126.04
20	B	822	CLA	CMC-C2C-C1C	2.61	129.01	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	6	613	CLA	CHD-C4C-NC	2.61	128.31	124.20
28	1	619	LUT	C10-C11-C12	-2.61	115.08	123.22
20	4	610	CLA	O2A-CGA-O1A	-2.61	117.02	123.59
20	Z	614	CLA	CHB-C4A-NA	2.61	128.12	124.51
20	A	836	CLA	CBC-CAC-C3C	-2.61	105.25	112.43
23	A	852	BCR	C29-C30-C25	2.61	114.49	110.48
20	B	812	CLA	O2A-CGA-CBA	2.61	120.08	111.91
23	4	621	BCR	C11-C12-C13	-2.61	119.10	126.42
20	3	604	CLA	CBC-CAC-C3C	-2.60	105.25	112.43
23	3	717	BCR	C38-C26-C25	-2.60	121.60	124.53
22	A	847	LHG	C5-O7-C7	-2.60	111.38	117.79
20	A	816	CLA	CAA-C2A-C3A	-2.60	105.65	112.78
20	6	602	CLA	CAA-C2A-C3A	-2.60	105.65	112.78
20	B	810	CLA	CBC-CAC-C3C	-2.60	105.26	112.43
20	1	603	CLA	C4C-C3C-C2C	-2.60	103.10	106.90
20	A	815	CLA	CHD-C4C-NC	2.60	128.30	124.20
20	F	303	CLA	C3B-C4B-NB	2.60	112.57	109.21
20	8	602	CLA	CHC-C1C-C2C	-2.60	119.53	126.72
28	1	618	LUT	C15-C14-C13	-2.60	123.60	127.31
20	4	614	CLA	CAA-C2A-C3A	-2.60	105.66	112.78
20	A	810	CLA	CHD-C4C-NC	2.60	128.30	124.20
20	B	833	CLA	CHD-C4C-NC	2.60	128.30	124.20
28	4	619	LUT	C20-C13-C12	2.60	122.17	118.08
20	5	610	CLA	C4-C3-C5	2.60	119.64	115.27
20	5	601	CLA	C1-C2-C3	-2.60	121.55	126.04
20	5	602	CLA	CBC-CAC-C3C	-2.60	105.26	112.43
20	A	815	CLA	CMB-C2B-C3B	2.60	129.54	124.68
20	B	819	CLA	CHD-C4C-NC	2.60	128.30	124.20
22	A	855	LHG	O8-C23-C24	2.60	120.06	111.91
20	3	604	CLA	CHB-C4A-NA	2.60	128.11	124.51
20	7	602	CLA	CHB-C4A-NA	2.60	128.11	124.51
28	8	618	LUT	C38-C25-C24	-2.60	118.00	123.56
20	6	616	CLA	CHD-C4C-NC	2.60	128.30	124.20
20	A	836	CLA	CMA-C3A-C4A	-2.60	104.79	111.77
27	6	618	CHL	C2A-C3A-C4A	-2.60	97.67	101.87
23	5	622	BCR	C37-C22-C23	2.60	122.17	118.08
20	B	814	CLA	CMC-C2C-C1C	2.60	128.99	125.04
20	A	829	CLA	CHC-C1C-C2C	-2.60	119.54	126.72
20	G	203	CLA	CMB-C2B-C3B	2.60	129.53	124.68
28	7	621	LUT	C10-C11-C12	-2.60	115.12	123.22
20	5	612	CLA	O2A-CGA-CBA	2.60	120.05	111.91
20	Z	611	CLA	O2A-CGA-CBA	2.60	120.05	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	829	CLA	CMB-C2B-C3B	2.60	129.53	124.68
23	5	622	BCR	C29-C30-C25	2.60	114.48	110.48
20	7	612	CLA	C4-C3-C5	2.59	119.63	115.27
20	A	812	CLA	C6-C7-C8	-2.59	107.54	115.92
20	B	827	CLA	CHD-C4C-NC	2.59	128.29	124.20
20	A	817	CLA	CMD-C2D-C3D	-2.59	121.65	127.61
28	Z	619	LUT	C11-C10-C9	-2.59	123.61	127.31
20	4	614	CLA	CHB-C4A-NA	2.59	128.10	124.51
20	5	613	CLA	O2A-CGA-CBA	2.59	120.04	111.91
20	A	804	CLA	CMC-C2C-C1C	2.59	128.98	125.04
20	B	827	CLA	C1-C2-C3	-2.59	121.56	126.04
20	8	613	CLA	CHD-C4C-NC	2.59	128.28	124.20
20	Z	611	CLA	CHD-C4C-NC	2.59	128.28	124.20
22	B	851	LHG	C5-O7-C7	-2.59	111.42	117.79
20	A	819	CLA	CMC-C2C-C1C	2.59	128.98	125.04
20	8	601	CLA	C4-C3-C5	2.59	119.62	115.27
20	4	611	CLA	CHB-C4A-NA	2.59	128.09	124.51
20	5	613	CLA	CAA-C2A-C3A	-2.59	105.69	112.78
20	A	809	CLA	CMB-C2B-C3B	2.59	129.52	124.68
28	1	618	LUT	C30-C31-C32	-2.59	115.14	123.22
20	8	601	CLA	CHD-C4C-NC	2.59	128.28	124.20
20	A	854	CLA	CHB-C4A-NA	2.59	128.09	124.51
20	8	604	CLA	CMB-C2B-C3B	2.58	129.51	124.68
20	A	808	CLA	CHB-C4A-NA	2.58	128.09	124.51
20	3	620	CLA	CAA-C2A-C3A	-2.58	105.70	112.78
20	Z	616	CLA	CHD-C4C-NC	2.58	128.27	124.20
20	A	828	CLA	CAC-C3C-C2C	2.58	131.94	127.53
20	7	604	CLA	CED-O2D-CGD	2.58	121.78	115.94
23	4	621	BCR	C29-C30-C25	2.58	114.45	110.48
28	8	617	LUT	C38-C25-C24	-2.58	118.04	123.56
20	B	811	CLA	CMA-C3A-C2A	-2.58	103.42	113.83
20	5	601	CLA	CAC-C3C-C4C	2.58	128.16	124.81
27	6	618	CHL	CMB-C2B-C3B	2.58	129.50	124.68
23	4	621	BCR	C23-C24-C25	-2.58	119.96	127.20
20	A	803	CLA	CHD-C4C-NC	2.58	128.27	124.20
20	A	806	CLA	CHD-C4C-NC	2.58	128.27	124.20
27	5	618	CHL	O2D-CGD-O1D	-2.58	118.80	123.84
20	Z	613	CLA	CAA-C2A-C3A	-2.58	105.72	112.78
20	3	610	CLA	O2A-CGA-O1A	-2.58	117.09	123.59
20	8	613	CLA	C1-O2A-CGA	2.58	123.20	116.44
20	1	604	CLA	O2A-CGA-CBA	2.58	119.99	111.91
20	A	817	CLA	O2A-CGA-CBA	2.58	119.99	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	L	203	CLA	CBC-CAC-C3C	-2.58	105.33	112.43
20	B	839	CLA	C1-C2-C3	-2.58	121.59	126.04
23	5	622	BCR	C31-C1-C6	-2.58	106.12	110.30
20	8	602	CLA	CHB-C4A-NA	2.58	128.07	124.51
20	B	809	CLA	O2D-CGD-O1D	-2.57	118.80	123.84
28	6	624	LUT	C35-C34-C33	-2.57	123.64	127.31
27	8	607	CHL	O2A-CGA-CBA	2.57	119.99	111.91
20	A	833	CLA	CMC-C2C-C1C	2.57	128.96	125.04
20	B	805	CLA	CHB-C4A-NA	2.57	128.07	124.51
28	4	619	LUT	C28-C29-C30	-2.57	114.99	118.94
20	A	813	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
20	3	607	CLA	CAC-C3C-C4C	2.57	128.15	124.81
20	3	620	CLA	C4C-C3C-C2C	-2.57	103.15	106.90
23	B	846	BCR	C2-C1-C6	2.57	114.44	110.48
20	A	822	CLA	C3B-C4B-NB	2.57	112.53	109.21
20	A	832	CLA	CMC-C2C-C1C	2.57	128.95	125.04
20	1	613	CLA	CHB-C4A-NA	2.57	128.07	124.51
28	3	622	LUT	C38-C25-C24	-2.57	118.06	123.56
20	4	603	CLA	CHD-C4C-NC	2.57	128.25	124.20
20	Z	609	CLA	CHB-C4A-NA	2.57	128.06	124.51
27	6	606	CHL	O2D-CGD-O1D	-2.57	118.81	123.84
20	Z	610	CLA	CMB-C2B-C3B	2.57	129.48	124.68
27	6	618	CHL	O2D-CGD-O1D	-2.57	118.82	123.84
20	A	845	CLA	CHD-C4C-NC	2.57	128.25	124.20
20	B	828	CLA	CHD-C4C-NC	2.57	128.25	124.20
20	A	817	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
20	3	613	CLA	O2A-CGA-CBA	2.57	119.96	111.91
23	A	856	BCR	C20-C19-C18	-2.57	119.21	126.42
28	Z	619	LUT	C10-C11-C12	-2.57	115.21	123.22
20	B	832	CLA	C1-C2-C3	-2.57	121.61	126.04
20	Z	610	CLA	C4-C3-C5	2.57	119.59	115.27
27	Z	601	CHL	C2A-C3A-C4A	-2.56	97.73	101.87
28	7	621	LUT	C38-C25-C24	-2.56	118.07	123.56
23	A	851	BCR	C23-C24-C25	-2.56	120.00	127.20
20	Z	609	CLA	CHD-C4C-NC	2.56	128.24	124.20
20	8	614	CLA	C4-C3-C5	2.56	119.58	115.27
20	8	603	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
20	5	609	CLA	CHD-C4C-NC	2.56	128.24	124.20
20	7	610	CLA	O2A-CGA-O1A	-2.56	117.13	123.59
27	6	618	CHL	CBC-CAC-C3C	-2.56	105.37	112.43
20	A	809	CLA	CMC-C2C-C1C	2.56	128.94	125.04
20	8	603	CLA	CMC-C2C-C1C	2.56	128.94	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	611	CLA	CHD-C4C-NC	2.56	128.24	124.20
28	4	620	LUT	C30-C31-C32	-2.56	115.22	123.22
28	5	624	LUT	C39-C29-C28	2.56	122.11	118.08
20	B	806	CLA	CHB-C4A-NA	2.56	128.05	124.51
20	1	614	CLA	CHB-C4A-NA	2.56	128.05	124.51
20	A	827	CLA	CHC-C1C-C2C	-2.56	119.64	126.72
20	B	821	CLA	CHD-C4C-NC	2.56	128.24	124.20
20	B	819	CLA	CHB-C4A-NA	2.56	128.05	124.51
28	1	617	LUT	C21-C26-C27	-2.56	109.47	112.70
23	4	621	BCR	C23-C22-C21	-2.56	115.01	118.94
20	A	822	CLA	C1-O2A-CGA	2.56	123.16	116.44
20	Z	604	CLA	O2A-CGA-CBA	2.56	119.94	111.91
23	5	625	BCR	C39-C30-C25	-2.56	106.15	110.30
27	4	607	CHL	CHD-C4C-NC	2.56	128.24	124.20
20	A	821	CLA	CAC-C3C-C4C	2.56	128.13	124.81
20	5	610	CLA	CHB-C4A-NA	2.56	128.05	124.51
20	1	604	CLA	CHD-C4C-NC	2.56	128.23	124.20
20	K	4002	CLA	O1D-CGD-CBD	-2.56	119.25	124.48
27	Z	601	CHL	O2D-CGD-O1D	-2.56	118.84	123.84
20	A	812	CLA	CHB-C4A-NA	2.56	128.05	124.51
20	4	604	CLA	CHB-C4A-NA	2.56	128.05	124.51
20	1	606	CLA	O2A-CGA-CBA	2.56	119.93	111.91
28	6	624	LUT	C38-C25-C24	-2.56	118.09	123.56
20	A	835	CLA	CHD-C4C-NC	2.56	128.23	124.20
23	A	856	BCR	C23-C24-C25	-2.56	120.03	127.20
20	1	602	CLA	C1-C2-C3	-2.55	121.62	126.04
20	7	610	CLA	CMB-C2B-C3B	2.55	129.46	124.68
20	B	805	CLA	C1C-C2C-C3C	-2.55	104.27	106.96
23	B	846	BCR	C37-C22-C23	2.55	122.10	118.08
20	Z	609	CLA	C1-C2-C3	-2.55	121.63	126.04
20	3	602	CLA	CHB-C4A-NA	2.55	128.04	124.51
28	1	619	LUT	C3-C4-C5	-2.55	106.77	111.85
20	8	614	CLA	CHB-C4A-NA	2.55	128.04	124.51
20	B	808	CLA	CMB-C2B-C3B	2.55	129.45	124.68
20	B	829	CLA	CMD-C2D-C3D	-2.55	121.74	127.61
20	A	845	CLA	C4-C3-C5	2.55	119.56	115.27
20	A	819	CLA	CHB-C4A-NA	2.55	128.04	124.51
20	B	840	CLA	CHB-C4A-NA	2.55	128.04	124.51
20	8	606	CLA	CAC-C3C-C4C	2.55	128.12	124.81
20	A	824	CLA	C4-C3-C5	2.55	118.90	115.98
20	6	612	CLA	CMC-C2C-C1C	2.55	128.92	125.04
20	3	609	CLA	CMB-C2B-C3B	2.55	129.45	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	829	CLA	C1-O2A-CGA	2.55	123.13	116.44
20	5	614	CLA	CMB-C2B-C3B	2.55	129.45	124.68
20	B	830	CLA	O2A-CGA-CBA	2.55	119.91	111.91
23	I	172	BCR	C29-C30-C25	2.55	114.40	110.48
20	B	815	CLA	O1D-CGD-CBD	-2.55	119.27	124.48
20	6	610	CLA	CHB-C4A-NA	2.55	128.03	124.51
20	B	823	CLA	CHD-C4C-NC	2.55	128.22	124.20
23	A	849	BCR	C32-C1-C6	2.55	114.43	110.30
20	A	804	CLA	CMA-C3A-C4A	-2.54	104.93	111.77
23	A	851	BCR	C34-C9-C8	2.54	122.09	118.08
20	A	839	CLA	CAA-C2A-C3A	-2.54	105.81	112.78
20	B	831	CLA	CAC-C3C-C4C	2.54	128.11	124.81
20	B	818	CLA	CMB-C2B-C3B	2.54	129.44	124.68
20	3	602	CLA	C1-C2-C3	-2.54	121.64	126.04
20	B	823	CLA	CMA-C3A-C2A	-2.54	103.57	113.83
20	A	830	CLA	CMB-C2B-C3B	2.54	129.44	124.68
20	5	609	CLA	CAC-C3C-C4C	2.54	128.11	124.81
20	6	610	CLA	CMA-C3A-C2A	-2.54	103.57	113.83
22	5	623	LHG	O8-C23-C24	2.54	119.89	111.91
20	B	815	CLA	C4-C3-C5	2.54	119.55	115.27
23	F	305	BCR	C2-C1-C6	2.54	114.39	110.48
20	7	604	CLA	CAA-C2A-C3A	-2.54	105.82	112.78
20	A	842	CLA	O2A-CGA-CBA	2.54	119.88	111.91
20	B	824	CLA	CAA-C2A-C3A	-2.54	105.82	112.78
23	3	719	BCR	C29-C30-C25	2.54	114.39	110.48
20	5	612	CLA	CMB-C2B-C3B	2.54	129.43	124.68
20	A	836	CLA	CHD-C4C-NC	2.54	128.21	124.20
20	B	826	CLA	O1D-CGD-CBD	-2.54	119.29	124.48
20	1	616	CLA	CAA-C2A-C3A	-2.54	105.83	112.78
20	Z	614	CLA	CAC-C3C-C4C	2.54	128.10	124.81
20	3	620	CLA	O2A-CGA-CBA	2.54	119.87	111.91
20	K	4003	CLA	CHD-C4C-NC	2.54	128.20	124.20
20	B	824	CLA	O2A-CGA-O1A	-2.54	117.19	123.59
23	J	3003	BCR	C10-C11-C12	-2.54	115.30	123.22
20	A	809	CLA	CAC-C3C-C4C	2.54	128.10	124.81
20	5	616	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
20	1	606	CLA	C1-C2-C3	-2.54	121.66	126.04
20	B	803	CLA	C3B-C4B-NB	2.54	112.49	109.21
20	5	611	CLA	CMB-C2B-C3B	2.54	129.42	124.68
23	A	848	BCR	C20-C21-C22	-2.54	123.69	127.31
27	6	606	CHL	CHD-C4C-NC	2.53	128.20	124.20
20	B	828	CLA	C1-C2-C3	-2.53	121.66	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	I	172	BCR	C15-C16-C17	-2.53	118.28	123.47
20	5	614	CLA	CMC-C2C-C1C	2.53	128.90	125.04
20	F	301	CLA	C3B-C4B-NB	2.53	112.48	109.21
20	B	813	CLA	C4-C3-C5	2.53	119.53	115.27
20	Z	614	CLA	CMB-C2B-C3B	2.53	129.42	124.68
20	A	815	CLA	CHA-C1A-NA	-2.53	120.60	126.40
20	8	611	CLA	CMB-C2B-C3B	2.53	129.41	124.68
28	8	617	LUT	C10-C11-C12	-2.53	115.32	123.22
20	6	602	CLA	CMB-C2B-C3B	2.53	129.41	124.68
28	8	618	LUT	C35-C15-C14	-2.53	118.29	123.47
28	6	621	LUT	C30-C31-C32	-2.53	115.32	123.22
20	3	604	CLA	C1-C2-C3	-2.53	121.67	126.04
23	K	4001	BCR	C35-C13-C12	2.53	122.06	118.08
20	A	834	CLA	CAC-C3C-C4C	2.53	128.09	124.81
20	B	818	CLA	O2A-CGA-CBA	2.53	119.84	111.91
20	5	604	CLA	CHD-C4C-NC	2.53	128.19	124.20
20	L	203	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
20	4	614	CLA	CMB-C2B-C3B	2.53	129.41	124.68
20	A	845	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
20	3	611	CLA	CMA-C3A-C2A	-2.53	110.20	116.10
27	6	607	CHL	CHB-C4A-NA	2.53	128.01	124.51
20	Z	608	CLA	CMB-C2B-C3B	2.53	129.41	124.68
20	A	837	CLA	CHD-C4C-NC	2.53	128.19	124.20
20	A	818	CLA	CAA-C2A-C3A	-2.53	105.86	112.78
20	A	807	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
20	1	604	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
20	5	616	CLA	CMB-C2B-C3B	2.52	129.40	124.68
20	A	822	CLA	C1-C2-C3	-2.52	121.68	126.04
20	Z	610	CLA	O1D-CGD-CBD	-2.52	119.32	124.48
20	3	610	CLA	CMB-C2B-C3B	2.52	129.40	124.68
20	3	611	CLA	CHD-C4C-NC	2.52	128.18	124.20
20	A	803	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
20	4	611	CLA	O2A-CGA-CBA	2.52	119.82	111.91
20	A	834	CLA	CHB-C4A-NA	2.52	128.00	124.51
20	7	616	CLA	CHD-C4C-NC	2.52	128.17	124.20
20	B	831	CLA	CMC-C2C-C1C	2.52	128.88	125.04
23	3	717	BCR	C7-C8-C9	-2.52	122.43	126.23
20	1	603	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
27	5	618	CHL	C1B-CHB-C4A	-2.52	125.13	130.12
20	5	604	CLA	CMC-C2C-C1C	2.52	128.87	125.04
20	7	608	CLA	CHB-C4A-NA	2.52	127.99	124.51
20	B	829	CLA	CHB-C4A-NA	2.52	127.99	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	3	621	LUT	C38-C25-C24	-2.52	118.17	123.56
20	A	824	CLA	CHD-C4C-NC	2.52	128.17	124.20
20	8	616	CLA	CHB-C4A-NA	2.52	127.99	124.51
20	Z	616	CLA	CMB-C2B-C3B	2.52	129.38	124.68
20	B	802	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
27	5	607	CHL	CMB-C2B-C3B	2.51	129.38	124.68
20	B	814	CLA	O2A-CGA-CBA	2.51	119.80	111.91
20	A	819	CLA	C3B-C4B-NB	2.51	112.46	109.21
20	B	809	CLA	C4-C3-C5	2.51	119.50	115.27
20	B	834	CLA	CMA-C3A-C2A	-2.51	103.69	113.83
20	1	604	CLA	CMA-C3A-C4A	-2.51	105.02	111.77
27	7	607	CHL	O2A-CGA-CBA	2.51	119.79	111.91
20	A	821	CLA	CHB-C4A-NA	2.51	127.99	124.51
20	5	613	CLA	C1-O2A-CGA	2.51	123.03	116.44
20	6	617	CLA	CMB-C2B-C3B	2.51	129.38	124.68
20	A	854	CLA	CHD-C4C-NC	2.51	128.16	124.20
20	K	4003	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
20	3	602	CLA	CBC-CAC-C3C	-2.51	105.51	112.43
20	8	609	CLA	CHD-C4C-NC	2.51	128.16	124.20
20	6	622	CLA	CHD-C4C-NC	2.51	128.16	124.20
20	A	811	CLA	CMB-C2B-C3B	2.51	129.37	124.68
20	4	613	CLA	CMC-C2C-C1C	2.51	128.86	125.04
20	5	613	CLA	CHD-C4C-NC	2.51	128.16	124.20
20	3	602	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
26	J	3001	LMG	O6-C1-O1	-2.51	104.03	109.97
20	B	822	CLA	CHB-C4A-NA	2.51	127.98	124.51
20	6	601	CLA	C4C-C3C-C2C	-2.51	103.24	106.90
20	A	804	CLA	C4-C3-C5	2.51	119.49	115.27
23	G	205	BCR	C20-C21-C22	-2.51	123.73	127.31
20	A	835	CLA	O2A-CGA-CBA	2.51	119.78	111.91
20	1	603	CLA	C4-C3-C5	2.51	119.49	115.27
20	1	612	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
27	5	608	CHL	CMB-C2B-C3B	2.51	129.37	124.68
28	3	621	LUT	C1-C2-C3	2.51	119.30	113.64
20	A	832	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
20	6	611	CLA	CMB-C2B-C3B	2.51	129.37	124.68
20	6	601	CLA	O2A-CGA-CBA	2.50	119.77	111.91
27	5	608	CHL	CHD-C4C-NC	2.50	128.15	124.20
20	A	838	CLA	CBA-CAA-C2A	-2.50	106.47	113.86
20	Z	606	CLA	O2A-CGA-CBA	2.50	119.77	111.91
23	6	623	BCR	C21-C20-C19	-2.50	115.40	123.22
20	B	814	CLA	CAA-C2A-C3A	-2.50	105.92	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	828	CLA	CHC-C1C-C2C	-2.50	119.80	126.72
23	4	621	BCR	C37-C22-C23	2.50	122.02	118.08
20	7	614	CLA	CMB-C2B-C3B	2.50	129.36	124.68
20	B	839	CLA	CMC-C2C-C1C	2.50	128.85	125.04
20	7	604	CLA	CHC-C1C-C2C	-2.50	119.80	126.72
20	7	613	CLA	CAA-C2A-C3A	-2.50	105.93	112.78
20	4	610	CLA	CAC-C3C-C4C	2.50	128.06	124.81
20	A	818	CLA	CHB-C4A-NA	2.50	127.97	124.51
20	A	838	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
20	A	822	CLA	CMB-C2B-C3B	2.50	129.35	124.68
20	B	819	CLA	O2A-CGA-CBA	2.50	119.74	111.91
20	3	614	CLA	CMB-C2B-C3B	2.50	129.35	124.68
20	B	804	CLA	CMA-C3A-C4A	-2.50	105.06	111.77
20	A	841	CLA	O2A-CGA-O1A	-2.50	117.29	123.59
20	B	808	CLA	CHD-C4C-NC	2.49	128.13	124.20
20	A	817	CLA	C4C-C3C-C2C	-2.49	103.26	106.90
20	6	611	CLA	O2A-CGA-CBA	2.49	119.73	111.91
23	7	623	BCR	C2-C1-C6	2.49	114.32	110.48
20	Z	612	CLA	C4-C3-C5	2.49	119.46	115.27
20	1	602	CLA	CMB-C2B-C3B	2.49	129.34	124.68
20	A	805	CLA	C3B-C4B-NB	2.49	112.43	109.21
20	B	815	CLA	CMB-C2B-C3B	2.49	129.34	124.68
23	J	3003	BCR	C16-C15-C14	-2.49	118.37	123.47
23	3	719	BCR	C16-C15-C14	-2.49	118.37	123.47
20	6	614	CLA	CMC-C2C-C1C	2.49	128.83	125.04
20	B	808	CLA	CHB-C4A-NA	2.49	127.95	124.51
20	B	839	CLA	O2A-CGA-CBA	2.49	119.72	111.91
20	L	204	CLA	O2A-CGA-CBA	2.49	119.72	111.91
20	6	622	CLA	CMC-C2C-C1C	2.49	128.83	125.04
20	Z	612	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
20	B	817	CLA	C4-C3-C5	2.49	119.45	115.27
20	A	820	CLA	CAC-C3C-C4C	2.49	128.04	124.81
20	Z	602	CLA	CMB-C2B-C3B	2.49	129.33	124.68
28	8	617	LUT	C39-C29-C28	2.49	122.00	118.08
20	3	611	CLA	CMB-C2B-C3B	2.48	129.33	124.68
20	Z	611	CLA	CMB-C2B-C3B	2.48	129.33	124.68
20	7	602	CLA	CMC-C2C-C1C	2.48	128.82	125.04
20	A	841	CLA	CAA-C2A-C3A	-2.48	105.98	112.78
20	B	809	CLA	CMC-C2C-C1C	2.48	128.82	125.04
20	1	606	CLA	CMC-C2C-C1C	2.48	128.82	125.04
20	6	622	CLA	CAA-C2A-C3A	-2.48	105.99	112.78
20	B	852	CLA	C4-C3-C5	2.48	119.44	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	841	CLA	CHB-C4A-NA	2.48	127.94	124.51
20	6	604	CLA	CMC-C2C-C1C	2.48	128.81	125.04
20	6	610	CLA	CMC-C2C-C1C	2.48	128.81	125.04
20	5	610	CLA	CBC-CAC-C3C	-2.48	105.60	112.43
20	A	815	CLA	CAA-C2A-C3A	-2.48	105.99	112.78
20	6	609	CLA	CAC-C3C-C4C	2.48	128.02	124.81
20	5	611	CLA	O2A-CGA-CBA	2.48	119.68	111.91
23	J	3003	BCR	C2-C1-C6	2.48	114.29	110.48
20	F	304	CLA	CMC-C2C-C1C	2.48	128.81	125.04
20	4	601	CLA	CAA-C2A-C3A	-2.48	106.00	112.78
20	3	610	CLA	C3B-C4B-NB	2.48	112.41	109.21
20	8	613	CLA	CMB-C2B-C3B	2.48	129.31	124.68
20	4	612	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
20	A	828	CLA	OBD-CAD-C3D	-2.48	122.56	128.52
20	Z	606	CLA	C1-C2-C3	-2.48	121.76	126.04
27	4	618	CHL	O2D-CGD-O1D	-2.47	119.00	123.84
23	B	801	BCR	C15-C14-C13	-2.47	123.78	127.31
20	7	616	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
20	6	611	CLA	CHB-C4A-NA	2.47	127.93	124.51
20	4	602	CLA	CBC-CAC-C3C	-2.47	105.62	112.43
21	B	842	PQN	C14-C13-C15	2.47	119.43	115.27
20	A	809	CLA	CBA-CAA-C2A	2.47	121.16	113.86
20	G	203	CLA	CHD-C4C-NC	2.47	128.10	124.20
28	Z	619	LUT	C7-C8-C9	-2.47	122.50	126.23
20	7	609	CLA	O1D-CGD-CBD	-2.47	119.43	124.48
20	6	614	CLA	CHB-C4A-NA	2.47	127.92	124.51
20	7	611	CLA	CMC-C2C-C1C	2.47	128.80	125.04
27	1	601	CHL	C4-C3-C2	-2.47	117.35	123.68
20	4	610	CLA	CHC-C1C-NC	2.47	127.95	124.20
20	B	809	CLA	C4C-C3C-C2C	-2.47	103.30	106.90
20	3	614	CLA	CMC-C2C-C1C	2.47	128.79	125.04
20	4	609	CLA	CMC-C2C-C1C	2.47	128.79	125.04
20	5	613	CLA	CMB-C2B-C3B	2.47	129.29	124.68
20	B	838	CLA	CMC-C2C-C1C	2.47	128.79	125.04
20	B	831	CLA	O2A-CGA-CBA	2.46	119.64	111.91
20	B	807	CLA	CMB-C2B-C3B	2.46	129.29	124.68
20	7	620	CLA	CHB-C4A-NA	2.46	127.92	124.51
20	B	809	CLA	O2A-CGA-CBA	2.46	119.64	111.91
20	7	609	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
20	3	613	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
20	A	825	CLA	CHD-C4C-NC	2.46	128.08	124.20
20	A	820	CLA	CMC-C2C-C1C	2.46	128.79	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	829	CLA	CHA-C1A-NA	-2.46	120.76	126.40
20	7	610	CLA	CHB-C4A-NA	2.46	127.92	124.51
23	A	852	BCR	C34-C9-C10	-2.46	119.47	122.92
20	8	616	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
20	A	807	CLA	C1-C2-C3	-2.46	121.79	126.04
20	5	616	CLA	CHB-C4A-NA	2.46	127.91	124.51
20	B	852	CLA	CMB-C2B-C3B	2.46	129.28	124.68
20	5	616	CLA	CHD-C4C-NC	2.46	128.07	124.20
23	B	801	BCR	C29-C30-C25	2.46	114.26	110.48
26	J	3001	LMG	O1-C7-C8	-2.46	104.97	110.90
20	A	839	CLA	CHB-C4A-NA	2.46	127.91	124.51
20	B	814	CLA	CMB-C2B-C3B	2.46	129.27	124.68
23	B	845	BCR	C34-C9-C10	-2.46	119.48	122.92
20	A	840	CLA	CHB-C4A-NA	2.46	127.91	124.51
27	4	608	CHL	CMB-C2B-C3B	2.45	129.27	124.68
28	Z	618	LUT	C35-C15-C14	-2.45	118.45	123.47
20	8	613	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
20	A	838	CLA	CHB-C4A-NA	2.45	127.90	124.51
20	1	611	CLA	O2A-CGA-CBA	2.45	119.60	111.91
20	1	606	CLA	CMB-C2B-C3B	2.45	129.26	124.68
20	A	804	CLA	CHB-C4A-NA	2.45	127.90	124.51
20	6	604	CLA	CHB-C4A-NA	2.45	127.90	124.51
20	Z	603	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
20	A	832	CLA	CHD-C4C-NC	2.45	128.06	124.20
20	3	604	CLA	C4-C3-C5	2.45	119.39	115.27
20	A	842	CLA	CAA-C2A-C3A	-2.45	106.07	112.78
28	5	620	LUT	C21-C26-C27	-2.45	109.61	112.70
20	Z	611	CLA	CHB-C4A-NA	2.45	127.90	124.51
27	4	606	CHL	C4-C3-C5	2.45	119.39	115.27
20	A	816	CLA	CMB-C2B-C3B	2.45	129.26	124.68
23	5	622	BCR	C8-C7-C6	-2.45	120.33	127.20
20	6	603	CLA	CBC-CAC-C3C	-2.45	105.69	112.43
20	1	613	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
23	G	205	BCR	C16-C15-C14	-2.45	118.46	123.47
20	3	607	CLA	C4-C3-C5	2.45	119.39	115.27
20	B	825	CLA	C4-C3-C5	2.44	119.38	115.27
19	A	801	CL0	CAC-C3C-C4C	2.44	127.98	124.81
20	A	834	CLA	O2A-CGA-CBA	2.44	119.58	111.91
20	7	620	CLA	CAA-C2A-C3A	-2.44	106.09	112.78
20	B	812	CLA	CHB-C4A-NA	2.44	127.89	124.51
20	Z	603	CLA	CBC-CAC-C3C	-2.44	105.70	112.43
20	B	834	CLA	CMB-C2B-C3B	2.44	129.25	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	603	CLA	CED-O2D-CGD	2.44	121.46	115.94
20	B	821	CLA	CHB-C4A-NA	2.44	127.89	124.51
20	A	823	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
27	6	607	CHL	C1B-CHB-C4A	-2.44	125.28	130.12
20	4	604	CLA	CMB-C2B-C3B	2.44	129.25	124.68
20	7	609	CLA	O2A-CGA-CBA	2.44	119.57	111.91
20	7	620	CLA	C4-C3-C5	2.44	119.38	115.27
20	B	831	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
20	5	611	CLA	CAC-C3C-C4C	2.44	127.98	124.81
20	7	608	CLA	CAA-C2A-C3A	-2.44	106.10	112.78
20	A	825	CLA	C1-C2-C3	-2.44	121.82	126.04
20	3	617	CLA	CMB-C2B-C3B	2.44	129.24	124.68
20	B	817	CLA	CHD-C4C-NC	2.44	128.05	124.20
28	Z	618	LUT	C31-C30-C29	-2.44	123.83	127.31
20	A	838	CLA	C1-C2-C3	-2.44	121.83	126.04
20	5	604	CLA	O2A-CGA-CBA	2.44	119.56	111.91
20	A	845	CLA	CHB-C4A-NA	2.44	127.88	124.51
20	A	814	CLA	C1-C2-C3	-2.44	121.83	126.04
20	4	604	CLA	CBC-CAC-C3C	-2.44	105.71	112.43
22	A	855	LHG	C5-O7-C7	-2.44	111.79	117.79
20	4	601	CLA	C1-C2-C3	-2.44	121.83	126.04
20	A	803	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
20	6	604	CLA	C1-C2-C3	-2.44	121.83	126.04
20	1	602	CLA	CBC-CAC-C3C	-2.44	105.71	112.43
20	B	835	CLA	CHB-C4A-NA	2.44	127.88	124.51
20	G	204	CLA	CMB-C2B-C3B	2.44	129.24	124.68
20	A	803	CLA	CBC-CAC-C3C	-2.44	105.72	112.43
20	3	609	CLA	CAA-CBA-CGA	-2.43	106.14	113.25
20	Z	616	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
20	B	817	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
20	Z	613	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
20	7	601	CLA	CMB-C2B-C3B	2.43	129.23	124.68
20	5	602	CLA	CHB-C4A-NA	2.43	127.88	124.51
20	6	616	CLA	CHB-C4A-NA	2.43	127.88	124.51
20	8	601	CLA	CHB-C4A-NA	2.43	127.88	124.51
20	3	603	CLA	C1-C2-C3	-2.43	121.84	126.04
28	4	619	LUT	C38-C25-C24	-2.43	118.36	123.56
20	B	837	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
20	3	614	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
20	5	609	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
20	Z	613	CLA	CMC-C2C-C1C	2.43	128.74	125.04
23	F	305	BCR	C37-C22-C23	2.43	121.91	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	1	618	LUT	C19-C9-C8	2.43	121.91	118.08
28	4	620	LUT	C38-C25-C24	-2.43	118.36	123.56
20	1	604	CLA	CMB-C2B-C3B	2.43	129.22	124.68
20	B	823	CLA	C1-C2-C3	-2.43	121.84	126.04
20	8	611	CLA	CHD-C4C-NC	2.43	128.03	124.20
27	5	618	CHL	CBC-CAC-C3C	-2.43	105.73	112.43
20	L	204	CLA	CHD-C4C-NC	2.43	128.03	124.20
20	4	610	CLA	CMA-C3A-C2A	-2.43	104.03	113.83
20	A	802	CLA	CAA-C2A-C3A	-2.43	106.13	112.78
20	6	609	CLA	CAA-C2A-C3A	-2.43	106.13	112.78
20	7	603	CLA	CMC-C2C-C1C	2.43	128.74	125.04
22	1	620	LHG	O8-C23-C24	2.42	119.52	111.91
27	6	607	CHL	CMB-C2B-C3B	2.42	129.21	124.68
20	1	603	CLA	C1-C2-C3	-2.42	121.85	126.04
20	Z	602	CLA	CAA-C2A-C3A	-2.42	106.14	112.78
20	A	854	CLA	CHC-C1C-C2C	-2.42	120.02	126.72
20	A	840	CLA	CMC-C2C-C1C	2.42	128.73	125.04
20	5	601	CLA	CMB-C2B-C3B	2.42	129.21	124.68
20	8	601	CLA	O2A-CGA-CBA	2.42	119.51	111.91
27	4	608	CHL	CBC-CAC-C3C	-2.42	105.75	112.43
20	1	611	CLA	CHB-C4A-NA	2.42	127.86	124.51
27	6	607	CHL	C2A-C3A-C4A	-2.42	97.96	101.87
20	A	813	CLA	CMC-C2C-C1C	2.42	128.73	125.04
20	Z	614	CLA	CBC-CAC-C3C	-2.42	105.76	112.43
20	8	604	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
20	A	834	CLA	CMA-C3A-C4A	-2.42	105.27	111.77
20	3	620	CLA	CMC-C2C-C1C	2.42	128.72	125.04
23	G	205	BCR	C29-C30-C25	2.42	114.21	110.48
20	B	827	CLA	O1D-CGD-CBD	-2.42	119.53	124.48
23	3	719	BCR	C34-C9-C8	2.42	121.89	118.08
23	5	622	BCR	C11-C12-C13	-2.42	119.62	126.42
20	B	805	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
23	L	205	BCR	C38-C26-C25	-2.42	121.81	124.53
20	A	829	CLA	CAA-C2A-C3A	-2.42	106.16	112.78
20	Z	609	CLA	CAA-CBA-CGA	-2.42	106.19	113.25
20	3	607	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
20	1	613	CLA	O2A-CGA-CBA	2.42	119.49	111.91
20	F	304	CLA	CHB-C4A-NA	2.42	127.85	124.51
20	B	804	CLA	CBC-CAC-C3C	-2.42	105.77	112.43
28	6	624	LUT	C3-C4-C5	-2.42	107.04	111.85
20	A	826	CLA	C3B-C4B-NB	2.42	112.33	109.21
28	5	624	LUT	C15-C35-C34	-2.42	118.53	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	6	603	CLA	CMC-C2C-C1C	2.42	128.72	125.04
20	A	826	CLA	CAC-C3C-C4C	2.41	127.94	124.81
20	A	829	CLA	CHB-C4A-NA	2.41	127.85	124.51
23	B	847	BCR	C16-C17-C18	-2.41	123.86	127.31
20	4	611	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
20	A	833	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
20	B	834	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
20	A	834	CLA	CBC-CAC-C3C	-2.41	105.78	112.43
20	5	611	CLA	CBC-CAC-C3C	-2.41	105.78	112.43
20	8	601	CLA	CMC-C2C-C1C	2.41	128.71	125.04
20	8	606	CLA	CMB-C2B-C3B	2.41	129.19	124.68
20	4	613	CLA	CAA-C2A-C3A	-2.41	106.17	112.78
20	A	802	CLA	CED-O2D-CGD	2.41	121.39	115.94
20	8	604	CLA	CMA-C3A-C2A	-2.41	104.10	113.83
20	B	810	CLA	C4-C3-C5	2.41	119.33	115.27
20	B	810	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
20	6	602	CLA	C1-C2-C3	-2.41	121.88	126.04
20	B	813	CLA	CHB-C4A-NA	2.41	127.84	124.51
27	4	607	CHL	O2D-CGD-O1D	-2.41	119.13	123.84
20	B	829	CLA	CAA-C2A-C3A	-2.41	106.19	112.78
20	7	613	CLA	CMC-C2C-C1C	2.41	128.71	125.04
20	F	301	CLA	CMD-C2D-C3D	-2.41	122.08	127.61
23	6	625	BCR	C37-C22-C23	2.41	121.87	118.08
27	3	608	CHL	C2A-C1A-CHA	-2.41	119.65	123.86
20	Z	613	CLA	CMB-C2B-C3B	2.41	129.18	124.68
20	6	622	CLA	CMB-C2B-C3B	2.41	129.18	124.68
28	3	621	LUT	C18-C5-C6	-2.41	121.83	124.53
20	G	203	CLA	O2D-CGD-O1D	-2.41	119.14	123.84
20	L	204	CLA	CHB-C4A-NA	2.41	127.84	124.51
26	J	3001	LMG	C1-C2-C3	-2.40	104.99	110.00
23	L	201	BCR	C33-C5-C6	-2.40	121.83	124.53
20	B	813	CLA	CMB-C2B-C3B	2.40	129.18	124.68
27	1	601	CHL	C2A-C3A-C4A	-2.40	97.99	101.87
20	4	612	CLA	CMC-C2C-C1C	2.40	128.70	125.04
20	B	821	CLA	CAA-C2A-C3A	-2.40	106.20	112.78
20	7	611	CLA	CHB-C4A-NA	2.40	127.83	124.51
20	5	606	CLA	C1-C2-C3	-2.40	121.89	126.04
27	Z	607	CHL	C1B-CHB-C4A	-2.40	125.36	130.12
20	J	3002	CLA	CHB-C4A-NA	2.40	127.83	124.51
20	B	823	CLA	C1C-C2C-C3C	-2.40	104.43	106.96
20	A	838	CLA	CBC-CAC-C3C	-2.40	105.82	112.43
20	1	614	CLA	CBC-CAC-C3C	-2.40	105.82	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	837	CLA	CHB-C4A-NA	2.40	127.83	124.51
20	K	4002	CLA	CMB-C2B-C3B	2.40	129.16	124.68
20	B	824	CLA	C4-C3-C5	2.40	119.30	115.27
27	5	607	CHL	C3A-C2A-C1A	-2.40	97.75	101.34
20	L	203	CLA	CHB-C4A-NA	2.40	127.83	124.51
20	A	822	CLA	CHB-C4A-NA	2.40	127.83	124.51
20	1	612	CLA	C4-C3-C5	2.40	119.30	115.27
23	A	856	BCR	C11-C12-C13	-2.39	119.69	126.42
20	4	609	CLA	CHD-C4C-NC	2.39	127.98	124.20
27	Z	607	CHL	CMB-C2B-C3B	2.39	129.16	124.68
20	4	601	CLA	CHB-C4A-NA	2.39	127.82	124.51
20	B	810	CLA	CMB-C2B-C3B	2.39	129.16	124.68
20	B	821	CLA	CMB-C2B-C3B	2.39	129.16	124.68
20	7	614	CLA	CHB-C4A-NA	2.39	127.82	124.51
20	6	603	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
20	A	838	CLA	O2A-CGA-CBA	2.39	119.42	111.91
27	3	608	CHL	C1-C2-C3	-2.39	121.91	126.04
28	6	621	LUT	C10-C11-C12	-2.39	115.75	123.22
20	3	613	CLA	CHD-C4C-NC	2.39	127.97	124.20
20	A	812	CLA	CMB-C2B-C3B	2.39	129.15	124.68
20	3	612	CLA	CBC-CAC-C3C	-2.39	105.84	112.43
20	A	812	CLA	C9-C8-C10	-2.39	102.63	111.29
20	A	835	CLA	CAC-C3C-C4C	2.39	127.91	124.81
27	4	608	CHL	O2A-CGA-CBA	2.39	119.41	111.91
20	8	614	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
20	6	622	CLA	CBC-CAC-C3C	-2.39	105.84	112.43
20	B	815	CLA	CHD-C4C-NC	2.39	127.97	124.20
19	A	801	CL0	O2A-CGA-O1A	-2.39	117.56	123.59
23	G	205	BCR	C20-C19-C18	-2.39	119.70	126.42
23	B	847	BCR	C10-C11-C12	-2.39	115.76	123.22
28	8	618	LUT	C16-C1-C6	-2.39	106.42	110.30
20	A	812	CLA	CHD-C4C-NC	2.39	127.97	124.20
20	B	840	CLA	C1-C2-C3	-2.39	121.91	126.04
20	5	613	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
20	5	603	CLA	CMC-C2C-C1C	2.39	128.68	125.04
20	A	818	CLA	CMB-C2B-C3B	2.39	129.15	124.68
20	B	826	CLA	C1-C2-C3	-2.39	121.91	126.04
20	L	203	CLA	O2A-CGA-CBA	2.39	119.40	111.91
23	6	625	BCR	C29-C30-C25	2.39	114.16	110.48
20	B	833	CLA	CAA-CBA-CGA	-2.39	106.28	113.25
23	A	849	BCR	C31-C1-C6	-2.39	106.43	110.30
20	6	611	CLA	CMC-C2C-C1C	2.38	128.67	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	4	622	LHG	O8-C23-C24	2.38	119.39	111.91
28	6	621	LUT	C20-C13-C12	2.38	121.83	118.08
20	B	840	CLA	C4-C3-C5	2.38	119.28	115.27
20	B	839	CLA	CAA-C2A-C3A	-2.38	106.25	112.78
27	3	608	CHL	O2A-CGA-O1A	-2.38	117.58	123.59
20	7	612	CLA	CMB-C2B-C3B	2.38	129.14	124.68
20	4	602	CLA	CAA-C2A-C3A	-2.38	106.25	112.78
20	A	843	CLA	CED-O2D-CGD	2.38	121.33	115.94
28	Z	619	LUT	C3-C4-C5	-2.38	107.11	111.85
20	1	616	CLA	CMB-C2B-C3B	2.38	129.13	124.68
20	6	609	CLA	CHD-C4C-NC	2.38	127.96	124.20
28	7	622	LUT	C20-C13-C12	2.38	121.83	118.08
20	5	614	CLA	CHB-C4A-NA	2.38	127.81	124.51
20	5	610	CLA	CMA-C3A-C2A	-2.38	104.22	113.83
20	1	610	CLA	CBC-CAC-C3C	-2.38	105.87	112.43
20	B	810	CLA	C1-C2-C3	-2.38	121.93	126.04
20	3	611	CLA	CMC-C2C-C1C	2.38	128.66	125.04
28	1	619	LUT	C19-C9-C8	2.38	121.83	118.08
20	8	616	CLA	CMB-C2B-C3B	2.38	129.13	124.68
20	B	830	CLA	CHB-C4A-NA	2.38	127.80	124.51
20	3	607	CLA	CHB-C4A-NA	2.38	127.80	124.51
20	A	842	CLA	CAC-C3C-C4C	2.38	127.90	124.81
20	B	829	CLA	CMC-C2C-C1C	2.38	128.66	125.04
20	B	837	CLA	C4-C3-C5	2.38	119.27	115.27
27	1	601	CHL	C6-C5-C3	-2.38	110.73	114.62
23	L	205	BCR	C15-C14-C13	-2.38	123.92	127.31
28	5	624	LUT	C7-C8-C9	-2.38	122.64	126.23
20	5	604	CLA	CAA-C2A-C3A	-2.38	106.27	112.78
23	7	624	BCR	C16-C15-C14	-2.37	118.61	123.47
20	B	818	CLA	C4C-C3C-C2C	-2.37	103.44	106.90
20	4	602	CLA	C4-C3-C5	2.37	119.27	115.27
20	8	612	CLA	CHB-C4A-NA	2.37	127.80	124.51
28	Z	619	LUT	C35-C15-C14	-2.37	118.61	123.47
28	8	618	LUT	C11-C10-C9	-2.37	123.92	127.31
20	3	617	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
20	7	609	CLA	CMA-C3A-C2A	-2.37	104.25	113.83
20	1	611	CLA	CED-O2D-CGD	2.37	121.31	115.94
23	K	4004	BCR	C11-C10-C9	-2.37	123.92	127.31
27	7	607	CHL	CMB-C2B-C3B	2.37	129.11	124.68
20	6	613	CLA	O2A-CGA-CBA	2.37	119.35	111.91
20	B	816	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
20	6	614	CLA	CMB-C2B-C3B	2.37	129.11	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	608	CLA	C4-C3-C5	2.37	119.26	115.27
20	A	802	CLA	CBA-CAA-C2A	2.37	120.86	113.86
28	4	620	LUT	C19-C9-C8	2.37	121.81	118.08
20	Z	604	CLA	CBC-CAC-C3C	-2.37	105.90	112.43
20	F	301	CLA	CMC-C2C-C1C	2.37	128.65	125.04
28	7	622	LUT	C30-C31-C32	-2.37	115.83	123.22
20	5	611	CLA	C1-C2-C3	-2.37	121.95	126.04
20	B	832	CLA	CHB-C4A-NA	2.37	127.78	124.51
20	6	613	CLA	CMC-C2C-C1C	2.37	128.64	125.04
20	B	841	CLA	O1D-CGD-CBD	-2.37	119.64	124.48
20	A	838	CLA	CAA-C2A-C3A	-2.37	106.30	112.78
20	4	616	CLA	CBC-CAC-C3C	-2.37	105.91	112.43
20	7	610	CLA	C4-C3-C5	2.37	119.25	115.27
20	Z	606	CLA	CBC-CAC-C3C	-2.36	105.91	112.43
20	4	609	CLA	CMB-C2B-C3B	2.36	129.10	124.68
20	A	837	CLA	CBC-CAC-C3C	-2.36	105.92	112.43
20	1	602	CLA	C4-C3-C5	2.36	119.25	115.27
20	B	829	CLA	CHD-C4C-NC	2.36	127.93	124.20
20	K	4003	CLA	CMB-C2B-C3B	2.36	129.10	124.68
20	3	620	CLA	C1-C2-C3	-2.36	121.96	126.04
20	5	617	CLA	CHB-C4A-NA	2.36	127.78	124.51
23	3	719	BCR	C2-C1-C6	2.36	114.12	110.48
20	B	812	CLA	CAA-C2A-C3A	-2.36	106.31	112.78
23	G	205	BCR	C15-C14-C13	-2.36	123.94	127.31
20	J	3002	CLA	CMB-C2B-C3B	2.36	129.09	124.68
22	6	619	LHG	O8-C23-C24	2.36	119.31	111.91
20	8	610	CLA	CED-O2D-CGD	2.36	121.28	115.94
27	5	608	CHL	CBC-CAC-C3C	-2.36	105.92	112.43
20	6	617	CLA	CHB-C4A-NA	2.36	127.78	124.51
20	Z	613	CLA	O2A-CGA-CBA	2.36	119.31	111.91
20	1	616	CLA	CHB-C4A-NA	2.36	127.77	124.51
20	A	829	CLA	C4-C3-C5	2.36	119.24	115.27
20	1	603	CLA	CMC-C2C-C1C	2.36	128.63	125.04
20	5	602	CLA	C4-C3-C5	2.36	119.24	115.27
20	A	811	CLA	CMA-C3A-C2A	-2.36	104.32	113.83
20	B	820	CLA	CMB-C2B-C3B	2.36	129.09	124.68
20	F	301	CLA	CMB-C2B-C3B	2.36	129.09	124.68
20	A	836	CLA	CMB-C2B-C3B	2.36	129.09	124.68
28	5	624	LUT	C18-C5-C6	-2.36	121.88	124.53
20	A	842	CLA	CBC-CAC-C3C	-2.36	105.94	112.43
20	G	203	CLA	CHB-C4A-NA	2.36	127.77	124.51
20	6	602	CLA	CHB-C4A-NA	2.36	127.77	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	7	613	CLA	O2A-CGA-CBA	2.36	119.30	111.91
20	5	616	CLA	CBC-CAC-C3C	-2.35	105.94	112.43
20	7	616	CLA	CMC-C2C-C1C	2.35	128.62	125.04
20	Z	603	CLA	O1D-CGD-CBD	-2.35	119.67	124.48
20	1	608	CLA	CBC-CAC-C3C	-2.35	105.94	112.43
20	B	803	CLA	C4-C3-C5	2.35	119.23	115.27
20	1	608	CLA	CMB-C2B-C3B	2.35	129.08	124.68
20	6	612	CLA	O2A-CGA-CBA	2.35	119.29	111.91
20	B	826	CLA	CMB-C2B-C3B	2.35	129.08	124.68
20	7	612	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
23	8	619	BCR	C23-C22-C21	-2.35	115.33	118.94
28	8	617	LUT	C15-C14-C13	-2.35	123.95	127.31
27	8	607	CHL	C1-C2-C3	-2.35	121.98	126.04
23	5	625	BCR	C15-C16-C17	-2.35	118.66	123.47
20	J	3002	CLA	CMC-C2C-C1C	2.35	128.62	125.04
20	Z	610	CLA	CBC-CAC-C3C	-2.35	105.95	112.43
20	A	820	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
20	3	611	CLA	CHB-C4A-NA	2.35	127.76	124.51
20	5	611	CLA	CMC-C2C-C1C	2.35	128.62	125.04
28	1	618	LUT	C31-C30-C29	-2.35	123.96	127.31
20	A	838	CLA	CMB-C2B-C3B	2.35	129.07	124.68
23	K	4004	BCR	C38-C26-C25	-2.35	121.89	124.53
20	B	823	CLA	CMA-C3A-C4A	-2.35	105.46	111.77
20	Z	606	CLA	C4-C3-C5	2.35	119.22	115.27
20	B	818	CLA	CBC-CAC-C3C	-2.35	105.95	112.43
23	A	849	BCR	C16-C15-C14	-2.35	118.66	123.47
20	6	610	CLA	CBC-CAC-C3C	-2.35	105.96	112.43
20	B	822	CLA	C1-C2-C3	-2.35	121.98	126.04
19	A	801	CL0	CGD-CBD-CAD	-2.35	103.13	110.73
28	7	621	LUT	C35-C34-C33	-2.35	123.96	127.31
20	B	815	CLA	C1-C2-C3	-2.35	121.98	126.04
20	6	604	CLA	CMB-C2B-C3B	2.35	129.07	124.68
23	7	624	BCR	C29-C30-C25	2.35	114.09	110.48
20	6	611	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
27	4	618	CHL	C2A-C1A-CHA	-2.35	119.76	123.86
28	1	617	LUT	C19-C9-C8	2.35	121.77	118.08
20	6	613	CLA	CMB-C2B-C3B	2.34	129.06	124.68
20	A	825	CLA	CHB-C4A-NA	2.34	127.75	124.51
20	5	602	CLA	CMB-C2B-C3B	2.34	129.06	124.68
23	B	845	BCR	C20-C21-C22	-2.34	123.97	127.31
20	B	836	CLA	CMC-C2C-C1C	2.34	128.61	125.04
20	7	610	CLA	CHC-C1C-C2C	-2.34	120.24	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	831	CLA	C1-C2-C3	-2.34	121.99	126.04
23	I	172	BCR	C2-C1-C6	2.34	114.09	110.48
20	Z	603	CLA	CMB-C2B-C3B	2.34	129.06	124.68
20	6	613	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
20	Z	608	CLA	CAA-C2A-C3A	-2.34	106.36	112.78
20	Z	606	CLA	CMC-C2C-C1C	2.34	128.60	125.04
27	8	607	CHL	CHB-C4A-NA	2.34	127.75	124.51
20	B	806	CLA	C4-C3-C5	2.34	119.21	115.27
20	5	612	CLA	CAA-C2A-C3A	-2.34	106.37	112.78
20	A	838	CLA	CHD-C4C-NC	2.34	127.89	124.20
20	5	621	CLA	CMC-C2C-C1C	2.34	128.60	125.04
28	1	618	LUT	C20-C13-C12	2.34	121.77	118.08
20	5	612	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
20	A	806	CLA	CAA-C2A-C3A	-2.34	106.37	112.78
20	A	815	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
20	3	610	CLA	CHC-C1C-C2C	-2.34	120.25	126.72
20	Z	602	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
20	A	819	CLA	C1-O2A-CGA	2.34	122.58	116.44
20	Z	608	CLA	CHB-C4A-NA	2.34	127.75	124.51
20	Z	616	CLA	CHB-C4A-NA	2.34	127.75	124.51
20	B	807	CLA	CBC-CAC-C3C	-2.34	105.98	112.43
27	5	607	CHL	O2D-CGD-O1D	-2.34	119.27	123.84
20	3	612	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
20	A	827	CLA	CHB-C4A-NA	2.34	127.74	124.51
20	F	304	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
20	B	826	CLA	CAC-C3C-C4C	2.34	127.84	124.81
20	A	834	CLA	CMB-C2B-C3B	2.34	129.05	124.68
20	Z	612	CLA	CMB-C2B-C3B	2.34	129.05	124.68
27	8	607	CHL	CMB-C2B-C3B	2.34	129.05	124.68
27	4	606	CHL	CHD-C4C-NC	2.34	127.88	124.20
20	1	610	CLA	CMA-C3A-C2A	-2.34	104.41	113.83
20	A	804	CLA	CMB-C2B-C3B	2.34	129.05	124.68
20	Z	610	CLA	CHB-C4A-NA	2.34	127.74	124.51
20	5	601	CLA	CMC-C2C-C1C	2.34	128.59	125.04
20	8	611	CLA	CMC-C2C-C1C	2.33	128.59	125.04
20	B	819	CLA	C1-C2-C3	-2.33	122.01	126.04
20	A	839	CLA	CMC-C2C-C1C	2.33	128.59	125.04
20	3	603	CLA	CMC-C2C-C1C	2.33	128.59	125.04
27	4	607	CHL	CAC-C3C-C4C	2.33	127.84	124.81
20	7	616	CLA	CMB-C2B-C3B	2.33	129.04	124.68
23	B	848	BCR	C34-C9-C8	2.33	121.75	118.08
20	A	825	CLA	CAA-C2A-C3A	-2.33	106.39	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	8	601	CLA	C1-C2-C3	-2.33	122.01	126.04
20	8	614	CLA	CMC-C2C-C1C	2.33	128.59	125.04
20	8	613	CLA	CHB-C4A-NA	2.33	127.74	124.51
20	4	611	CLA	C1-C2-C3	-2.33	122.01	126.04
20	A	842	CLA	CHB-C4A-NA	2.33	127.73	124.51
27	3	608	CHL	C4-C3-C5	2.33	119.19	115.27
20	7	620	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
20	4	616	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
20	B	813	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
20	Z	614	CLA	CMC-C2C-C1C	2.33	128.59	125.04
20	3	613	CLA	CAA-C2A-C3A	-2.33	106.40	112.78
20	B	811	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
20	L	204	CLA	CMB-C2B-C3B	2.33	129.03	124.68
27	Z	607	CHL	CBC-CAC-C3C	-2.33	106.01	112.43
20	B	823	CLA	CHC-C1C-NC	2.33	127.73	124.20
20	A	831	CLA	CMA-C3A-C2A	-2.33	104.44	113.83
20	8	610	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
20	Z	602	CLA	CHB-C4A-NA	2.33	127.73	124.51
20	Z	606	CLA	CHB-C4A-NA	2.33	127.73	124.51
20	B	804	CLA	CAA-C2A-C3A	-2.33	106.41	112.78
20	A	826	CLA	CHA-C1A-NA	-2.33	121.07	126.40
20	Z	613	CLA	CHB-C4A-NA	2.33	127.73	124.51
20	1	612	CLA	CBC-CAC-C3C	-2.33	106.02	112.43
20	6	609	CLA	O2A-CGA-CBA	2.33	119.20	111.91
20	B	831	CLA	CAA-C2A-C3A	-2.33	106.41	112.78
20	7	612	CLA	CHB-C4A-NA	2.32	127.73	124.51
27	Z	607	CHL	C2A-C1A-CHA	-2.32	119.79	123.86
20	4	604	CLA	CMC-C2C-C1C	2.32	128.58	125.04
20	3	606	CLA	O2D-CGD-O1D	-2.32	119.29	123.84
27	6	606	CHL	C2A-C3A-C4A	-2.32	98.12	101.87
20	K	4002	CLA	CHB-C4A-NA	2.32	127.72	124.51
20	5	603	CLA	CHB-C4A-NA	2.32	127.72	124.51
20	Z	603	CLA	O2A-CGA-CBA	2.32	119.20	111.91
20	B	840	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
28	5	624	LUT	C30-C31-C32	-2.32	115.97	123.22
20	4	603	CLA	CMB-C2B-C3B	2.32	129.02	124.68
27	1	607	CHL	CBC-CAC-C3C	-2.32	106.03	112.43
20	5	621	CLA	CHB-C4A-NA	2.32	127.72	124.51
20	A	802	CLA	C4-C3-C5	2.32	119.18	115.27
20	1	606	CLA	CBC-CAC-C3C	-2.32	106.03	112.43
20	Z	612	CLA	C1-C2-C3	-2.32	122.03	126.04
20	3	606	CLA	CHB-C4A-NA	2.32	127.72	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	606	CLA	CMB-C2B-C3B	2.32	129.02	124.68
23	A	848	BCR	C15-C14-C13	-2.32	124.00	127.31
28	Z	617	LUT	C20-C13-C12	2.32	121.73	118.08
23	3	718	BCR	C10-C11-C12	-2.32	115.98	123.22
20	A	806	CLA	CMC-C2C-C1C	2.32	128.57	125.04
20	A	845	CLA	CAC-C3C-C4C	2.32	127.82	124.81
23	8	619	BCR	C2-C1-C6	2.32	114.05	110.48
27	5	618	CHL	C2A-C1A-CHA	-2.32	119.80	123.86
20	7	610	CLA	CED-O2D-CGD	2.32	121.18	115.94
27	4	606	CHL	C1B-CHB-C4A	-2.32	125.53	130.12
23	4	621	BCR	C2-C3-C4	-2.32	106.20	111.38
28	Z	617	LUT	C39-C29-C28	2.32	121.73	118.08
20	B	818	CLA	CMC-C2C-C1C	2.32	128.57	125.04
20	6	612	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
20	B	824	CLA	O1D-CGD-CBD	-2.32	119.74	124.48
20	A	811	CLA	CHB-C4A-NA	2.32	127.71	124.51
20	5	606	CLA	CBC-CAC-C3C	-2.32	106.05	112.43
20	B	839	CLA	O2D-CGD-O1D	-2.31	119.31	123.84
20	A	813	CLA	CAA-C2A-C3A	-2.31	106.44	112.78
28	7	621	LUT	C31-C30-C29	-2.31	124.01	127.31
28	1	617	LUT	C8-C9-C10	-2.31	115.39	118.94
27	7	607	CHL	O2D-CGD-O1D	-2.31	119.31	123.84
20	A	843	CLA	CHB-C4A-NA	2.31	127.71	124.51
20	3	610	CLA	CHB-C4A-NA	2.31	127.71	124.51
20	7	606	CLA	CHB-C4A-NA	2.31	127.71	124.51
20	4	604	CLA	CAA-C2A-C3A	-2.31	106.44	112.78
20	B	818	CLA	CAA-C2A-C3A	-2.31	106.44	112.78
20	G	204	CLA	CHB-C4A-NA	2.31	127.71	124.51
20	8	610	CLA	CHC-C1C-C2C	-2.31	120.33	126.72
23	A	849	BCR	C15-C16-C17	-2.31	118.74	123.47
27	6	608	CHL	O2D-CGD-O1D	-2.31	119.32	123.84
28	5	624	LUT	C20-C13-C12	2.31	121.72	118.08
27	4	606	CHL	CBC-CAC-C3C	-2.31	106.06	112.43
20	4	616	CLA	CHB-C4A-NA	2.31	127.71	124.51
27	5	607	CHL	OMC-CMC-C2C	-2.31	120.46	125.69
20	8	609	CLA	CHA-C1A-NA	-2.31	121.10	126.40
20	4	613	CLA	C4-C3-C5	2.31	119.15	115.27
20	7	602	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
20	A	841	CLA	CAC-C3C-C4C	2.31	127.80	124.81
20	7	610	CLA	O1D-CGD-CBD	-2.31	119.76	124.48
20	6	617	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
20	Z	611	CLA	C1-C2-C3	-2.31	122.05	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	8	607	CHL	CHC-C1C-C2C	-2.31	117.75	126.11
20	B	828	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
23	5	622	BCR	C16-C15-C14	-2.31	118.75	123.47
20	7	601	CLA	CHB-C4A-NA	2.31	127.70	124.51
23	7	624	BCR	C37-C22-C23	2.31	121.71	118.08
20	1	604	CLA	C1-C2-C3	-2.30	122.06	126.04
23	K	4004	BCR	C10-C11-C12	-2.30	116.03	123.22
20	K	4002	CLA	CMC-C2C-C1C	2.30	128.55	125.04
20	B	838	CLA	CHB-C4A-NA	2.30	127.70	124.51
20	1	612	CLA	CMB-C2B-C3B	2.30	128.99	124.68
20	3	617	CLA	CHB-C4A-NA	2.30	127.70	124.51
23	I	172	BCR	C29-C28-C27	-2.30	106.23	111.38
20	B	807	CLA	CMC-C2C-C1C	2.30	128.54	125.04
20	6	604	CLA	CAA-C2A-C3A	-2.30	106.47	112.78
20	4	612	CLA	C1-C2-C3	-2.30	122.06	126.04
23	F	305	BCR	C16-C17-C18	-2.30	124.03	127.31
20	7	602	CLA	CMB-C2B-C3B	2.30	128.98	124.68
20	Z	606	CLA	CMB-C2B-C3B	2.30	128.98	124.68
20	A	813	CLA	CHB-C4A-NA	2.30	127.69	124.51
20	4	610	CLA	CHB-C4A-NA	2.30	127.69	124.51
27	7	607	CHL	CHB-C4A-NA	2.30	127.69	124.51
23	K	4001	BCR	C7-C6-C5	2.30	127.03	121.46
20	B	836	CLA	CAA-C2A-C3A	-2.30	106.48	112.78
20	A	854	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
20	8	608	CLA	CHB-C4A-NA	2.30	127.69	124.51
27	6	608	CHL	CHB-C4A-NA	2.30	127.69	124.51
20	7	613	CLA	C1-C2-C3	-2.30	122.07	126.04
28	3	621	LUT	C19-C9-C8	2.30	121.70	118.08
20	A	834	CLA	C11-C10-C8	-2.30	108.49	115.92
20	1	608	CLA	CMC-C2C-C1C	2.30	128.54	125.04
20	3	603	CLA	CHB-C4A-NA	2.30	127.69	124.51
20	5	621	CLA	CBC-CAC-C3C	-2.30	106.10	112.43
20	7	611	CLA	C2A-C3A-C4A	-2.30	98.85	101.78
23	7	624	BCR	C20-C21-C22	-2.30	124.03	127.31
20	8	610	CLA	CBC-CAC-C3C	-2.30	106.10	112.43
20	6	610	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
20	1	611	CLA	CHD-C4C-NC	2.30	127.82	124.20
20	F	304	CLA	CMB-C2B-C3B	2.30	128.97	124.68
27	6	607	CHL	C1-C2-C3	-2.30	122.07	126.04
20	L	203	CLA	CMC-C2C-C1C	2.29	128.53	125.04
20	Z	608	CLA	CMC-C2C-C1C	2.29	128.53	125.04
20	A	802	CLA	CBC-CAC-C3C	-2.29	106.11	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	8	613	CLA	CAA-C2A-C3A	-2.29	106.50	112.78
20	8	601	CLA	CMB-C2B-C3B	2.29	128.97	124.68
28	Z	617	LUT	C8-C9-C10	-2.29	115.42	118.94
27	6	608	CHL	CBC-CAC-C3C	-2.29	106.11	112.43
20	A	814	CLA	CMB-C2B-C3B	2.29	128.97	124.68
20	B	803	CLA	O2D-CGD-O1D	-2.29	119.35	123.84
20	A	818	CLA	CAC-C3C-C4C	2.29	127.78	124.81
20	A	807	CLA	CMC-C2C-C1C	2.29	128.53	125.04
20	7	612	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
20	7	609	CLA	CHD-C4C-NC	2.29	127.81	124.20
20	1	610	CLA	CHC-C1C-C2C	-2.29	120.39	126.72
20	B	828	CLA	CMB-C2B-C3B	2.29	128.96	124.68
22	A	846	LHG	C5-O7-C7	-2.29	112.15	117.79
20	A	804	CLA	O1D-CGD-CBD	-2.29	119.80	124.48
28	4	620	LUT	C18-C5-C6	-2.29	121.96	124.53
20	4	614	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
20	B	833	CLA	CMB-C2B-C3B	2.29	128.96	124.68
20	Z	616	CLA	CMC-C2C-C1C	2.29	128.53	125.04
20	7	602	CLA	CBC-CAC-C3C	-2.29	106.12	112.43
20	A	833	CLA	OBD-CAD-C3D	-2.29	123.01	128.52
20	A	826	CLA	C1-O2A-CGA	2.29	122.45	116.44
28	7	622	LUT	C16-C1-C6	-2.29	106.59	110.30
20	A	824	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
20	Z	603	CLA	CAA-C2A-C3A	-2.29	106.51	112.78
20	4	601	CLA	CHD-C4C-NC	2.29	127.81	124.20
20	Z	604	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
20	7	603	CLA	CBC-CAC-C3C	-2.29	106.13	112.43
27	5	608	CHL	O2D-CGD-O1D	-2.29	119.37	123.84
20	4	611	CLA	CMC-C2C-C1C	2.29	128.52	125.04
20	A	833	CLA	CHB-C4A-NA	2.29	127.67	124.51
20	3	609	CLA	C5-C3-C4	2.29	119.65	114.60
20	B	822	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
20	Z	608	CLA	CBC-CAC-C3C	-2.29	106.13	112.43
20	A	815	CLA	CHB-C4A-NA	2.29	127.67	124.51
20	B	830	CLA	CMB-C2B-C3B	2.28	128.95	124.68
20	A	841	CLA	CMA-C3A-C4A	-2.28	105.63	111.77
20	4	602	CLA	CMC-C2C-C1C	2.28	128.52	125.04
20	5	606	CLA	CHB-C4A-NA	2.28	127.67	124.51
20	A	841	CLA	C11-C10-C8	-2.28	108.53	115.92
20	1	603	CLA	CMB-C2B-C3B	2.28	128.95	124.68
20	8	602	CLA	O2D-CGD-O1D	-2.28	119.37	123.84
20	B	807	CLA	CHD-C4C-NC	2.28	127.80	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	852	BCR	C10-C11-C12	-2.28	116.09	123.22
20	A	832	CLA	O2A-CGA-CBA	2.28	119.07	111.91
20	A	854	CLA	O2A-C1-C2	2.28	114.63	108.64
20	7	608	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
23	7	624	BCR	C39-C30-C25	-2.28	106.60	110.30
20	L	204	CLA	CAA-C2A-C3A	-2.28	106.53	112.78
20	B	812	CLA	C1-O2A-CGA	2.28	122.43	116.44
20	6	602	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
20	5	612	CLA	CHB-C4A-NA	2.28	127.66	124.51
20	B	852	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
20	5	609	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
20	1	612	CLA	CHB-C4A-NA	2.28	127.66	124.51
20	4	601	CLA	CBC-CAC-C3C	-2.28	106.15	112.43
20	Z	614	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
20	1	612	CLA	C1-C2-C3	-2.28	122.11	126.04
20	3	617	CLA	CMC-C2C-C1C	2.28	128.51	125.04
20	A	831	CLA	CAA-C2A-C3A	-2.28	106.55	112.78
20	A	840	CLA	CMB-C2B-C3B	2.28	128.94	124.68
27	3	608	CHL	CHB-C4A-NA	2.28	127.66	124.51
20	1	610	CLA	CHB-C4A-NA	2.27	127.66	124.51
20	A	821	CLA	CMB-C2B-C3B	2.27	128.93	124.68
23	B	846	BCR	C23-C22-C21	-2.27	115.45	118.94
20	8	601	CLA	CBC-CAC-C3C	-2.27	106.16	112.43
28	6	624	LUT	C35-C15-C14	-2.27	118.82	123.47
20	B	841	CLA	C1-C2-C3	-2.27	122.11	126.04
20	A	819	CLA	O2A-CGA-CBA	2.27	119.04	111.91
20	G	204	CLA	CMC-C2C-C1C	2.27	128.50	125.04
20	7	608	CLA	CMC-C2C-C1C	2.27	128.50	125.04
28	4	619	LUT	C3-C4-C5	-2.27	107.33	111.85
20	B	830	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
20	8	612	CLA	CMC-C2C-C1C	2.27	128.50	125.04
20	B	820	CLA	C4-C3-C5	2.27	119.09	115.27
28	Z	618	LUT	C39-C29-C28	2.27	121.65	118.08
23	B	845	BCR	C16-C15-C14	-2.27	118.83	123.47
20	4	610	CLA	CBC-CAC-C3C	-2.27	106.18	112.43
20	L	203	CLA	C1-C2-C3	-2.27	122.12	126.04
20	A	841	CLA	CMB-C2B-C3B	2.27	128.92	124.68
20	Z	610	CLA	CED-O2D-CGD	2.27	121.06	115.94
20	8	602	CLA	CMC-C2C-C1C	2.27	128.49	125.04
20	6	601	CLA	C1-C2-C3	-2.27	122.12	126.04
23	5	622	BCR	C34-C9-C8	2.27	121.65	118.08
20	A	805	CLA	CHA-C1A-NA	-2.27	121.21	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	5	608	CHL	CHA-C1A-NA	-2.27	121.21	126.40
20	A	832	CLA	CAA-C2A-C3A	-2.27	106.57	112.78
20	A	811	CLA	O2D-CGD-O1D	-2.27	119.41	123.84
20	6	603	CLA	CMB-C2B-C3B	2.27	128.92	124.68
20	F	304	CLA	CBC-CAC-C3C	-2.26	106.19	112.43
20	8	611	CLA	CBC-CAC-C3C	-2.26	106.19	112.43
20	B	823	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
20	Z	611	CLA	C4-C3-C5	2.26	119.08	115.27
20	A	819	CLA	CBA-CAA-C2A	2.26	120.54	113.86
20	1	608	CLA	C1-C2-C3	-2.26	122.13	126.04
20	B	809	CLA	CHB-C4A-NA	2.26	127.64	124.51
20	B	825	CLA	CHB-C4A-NA	2.26	127.64	124.51
20	6	613	CLA	C1-C2-C3	-2.26	122.13	126.04
20	7	616	CLA	CHB-C4A-NA	2.26	127.64	124.51
20	4	602	CLA	CHB-C4A-NA	2.26	127.64	124.51
28	1	619	LUT	C8-C7-C6	-2.26	120.85	127.20
20	6	610	CLA	CMA-C3A-C4A	-2.26	105.70	111.77
20	B	818	CLA	CHB-C4A-NA	2.26	127.64	124.51
27	6	607	CHL	O2A-CGA-CBA	2.26	119.00	111.91
20	L	204	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
20	A	841	CLA	CMC-C2C-C1C	2.26	128.48	125.04
20	A	808	CLA	O2A-CGA-CBA	2.26	119.00	111.91
20	A	834	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
20	6	612	CLA	CBC-CAC-C3C	-2.26	106.20	112.43
20	A	807	CLA	CBC-CAC-C3C	-2.26	106.20	112.43
20	5	610	CLA	CMA-C3A-C4A	-2.26	105.70	111.77
27	4	606	CHL	O2D-CGD-O1D	-2.26	119.42	123.84
28	4	619	LUT	C10-C11-C12	-2.26	116.17	123.22
20	B	823	CLA	CAA-C2A-C3A	-2.26	106.60	112.78
20	G	204	CLA	CBC-CAC-C3C	-2.26	106.21	112.43
23	B	848	BCR	C35-C13-C12	2.26	121.63	118.08
20	B	832	CLA	CMC-C2C-C1C	2.26	128.47	125.04
23	B	801	BCR	C34-C9-C10	-2.26	119.76	122.92
20	Z	616	CLA	CBC-CAC-C3C	-2.26	106.21	112.43
27	5	608	CHL	C1-C2-C3	-2.26	123.10	126.75
20	7	620	CLA	CMC-C2C-C1C	2.26	128.47	125.04
20	B	835	CLA	CBC-CAC-C3C	-2.26	106.21	112.43
20	4	611	CLA	CBC-CAC-C3C	-2.26	106.21	112.43
20	4	610	CLA	O2D-CGD-O1D	-2.26	119.43	123.84
20	A	827	CLA	C4-C3-C5	2.25	119.06	115.27
26	J	3001	LMG	O3-C3-C2	-2.25	105.14	110.35
28	6	624	LUT	C39-C29-C28	2.25	121.63	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	5	625	BCR	C35-C13-C14	-2.25	119.77	122.92
20	Z	612	CLA	CBC-CAC-C3C	-2.25	106.22	112.43
20	A	836	CLA	O2D-CGD-O1D	-2.25	119.43	123.84
23	B	848	BCR	C37-C22-C23	2.25	121.63	118.08
20	3	613	CLA	CMB-C2B-C3B	2.25	128.89	124.68
20	A	841	CLA	C1-C2-C3	-2.25	122.15	126.04
20	7	602	CLA	CMA-C3A-C2A	-2.25	104.75	113.83
20	A	807	CLA	CMB-C2B-C3B	2.25	128.89	124.68
20	6	609	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
20	A	819	CLA	CHA-C1A-NA	-2.25	121.25	126.40
28	Z	618	LUT	C16-C1-C6	-2.25	106.65	110.30
20	A	832	CLA	C5-C3-C4	2.25	119.57	114.60
28	5	620	LUT	C20-C13-C12	2.25	121.62	118.08
28	6	621	LUT	C18-C5-C6	-2.25	122.00	124.53
20	7	606	CLA	CAC-C3C-C4C	2.25	127.73	124.81
20	B	819	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
20	4	612	CLA	CBC-CAC-C3C	-2.25	106.23	112.43
20	5	612	CLA	CBC-CAC-C3C	-2.25	106.23	112.43
20	3	610	CLA	C4-C3-C5	2.25	119.05	115.27
23	7	624	BCR	C2-C1-C6	2.25	113.94	110.48
20	8	604	CLA	CBC-CAC-C3C	-2.25	106.23	112.43
20	5	614	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
20	L	203	CLA	C4-C3-C5	2.25	119.05	115.27
23	3	718	BCR	C4-C5-C6	-2.25	119.47	122.73
20	1	606	CLA	O2D-CGD-O1D	-2.25	119.45	123.84
20	A	804	CLA	CBC-CAC-C3C	-2.25	106.24	112.43
28	6	621	LUT	C31-C30-C29	-2.25	124.11	127.31
20	B	831	CLA	CHB-C4A-NA	2.24	127.62	124.51
20	8	610	CLA	C4-C3-C5	2.24	119.05	115.27
20	A	810	CLA	CMC-C2C-C1C	2.24	128.46	125.04
28	Z	617	LUT	C19-C9-C8	2.24	121.61	118.08
20	7	603	CLA	CMB-C2B-C3B	2.24	128.88	124.68
28	4	620	LUT	C3-C4-C5	-2.24	107.39	111.85
20	6	610	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
28	1	617	LUT	C38-C25-C24	-2.24	118.76	123.56
20	B	820	CLA	CHB-C4A-NA	2.24	127.61	124.51
20	Z	610	CLA	CHC-C1C-C2C	-2.24	120.52	126.72
20	7	612	CLA	CBC-CAC-C3C	-2.24	106.25	112.43
20	A	818	CLA	O1D-CGD-CBD	-2.24	119.90	124.48
20	A	828	CLA	CHB-C4A-NA	2.24	127.61	124.51
20	A	843	CLA	CMB-C2B-C3B	2.24	128.87	124.68
20	7	604	CLA	CBC-CAC-C3C	-2.24	106.26	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	6	616	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
20	1	609	CLA	CMC-C2C-C1C	2.24	128.45	125.04
28	1	617	LUT	C20-C13-C12	2.24	121.61	118.08
20	B	812	CLA	C1-C2-C3	-2.24	122.17	126.04
20	5	602	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
20	3	620	CLA	CHB-C4A-NA	2.24	127.61	124.51
27	Z	601	CHL	C6-C5-C3	-2.24	110.96	114.62
20	B	806	CLA	CMB-C2B-C3B	2.24	128.86	124.68
20	Z	604	CLA	CMB-C2B-C3B	2.24	128.86	124.68
20	A	823	CLA	CHB-C4A-NA	2.24	127.60	124.51
20	1	608	CLA	CAA-C2A-C3A	-2.24	106.66	112.78
20	6	603	CLA	CHB-C4A-NA	2.24	127.60	124.51
20	B	803	CLA	CHA-C1A-NA	-2.24	121.28	126.40
27	4	607	CHL	CMB-C2B-C3B	2.24	128.86	124.68
20	1	609	CLA	C4-C3-C5	2.24	119.03	115.27
20	B	806	CLA	CHA-C1A-NA	-2.23	121.28	126.40
20	7	611	CLA	CBC-CAC-C3C	-2.23	106.27	112.43
20	A	819	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
23	K	4001	BCR	C4-C5-C6	-2.23	119.49	122.73
20	7	616	CLA	CBC-CAC-C3C	-2.23	106.28	112.43
20	8	603	CLA	CMB-C2B-C3B	2.23	128.85	124.68
23	K	4001	BCR	C1-C6-C5	-2.23	119.47	122.61
20	7	614	CLA	CMC-C2C-C1C	2.23	128.44	125.04
27	4	607	CHL	C2A-C1A-CHA	-2.23	119.96	123.86
20	8	602	CLA	CMB-C2B-C3B	2.23	128.85	124.68
23	5	625	BCR	C21-C20-C19	-2.23	116.26	123.22
20	1	604	CLA	CBC-CAC-C3C	-2.23	106.28	112.43
20	F	303	CLA	CMC-C2C-C1C	2.23	128.44	125.04
20	4	602	CLA	CMB-C2B-C3B	2.23	128.85	124.68
28	7	622	LUT	C39-C29-C28	2.23	121.59	118.08
20	1	602	CLA	CHB-C4A-NA	2.23	127.59	124.51
20	Z	602	CLA	CBC-CAC-C3C	-2.23	106.29	112.43
27	8	607	CHL	CBC-CAC-C3C	-2.23	106.29	112.43
23	G	205	BCR	C33-C5-C6	-2.23	122.03	124.53
20	J	3002	CLA	CBC-CAC-C3C	-2.23	106.29	112.43
20	7	620	CLA	CBC-CAC-C3C	-2.23	106.29	112.43
20	B	813	CLA	CMC-C2C-C1C	2.23	128.43	125.04
20	A	835	CLA	CMB-C2B-C3B	2.23	128.84	124.68
20	1	606	CLA	CHB-C4A-NA	2.23	127.59	124.51
20	7	601	CLA	C4-C3-C2	-2.23	117.97	123.68
20	B	811	CLA	CMB-C2B-C3B	2.23	129.04	124.69
20	7	613	CLA	CHB-C4A-NA	2.22	127.59	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Z	612	CLA	CHB-C4A-NA	2.22	127.59	124.51
20	A	809	CLA	O1D-CGD-CBD	-2.22	119.93	124.48
23	B	801	BCR	C11-C12-C13	-2.22	120.17	126.42
20	A	839	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
20	6	604	CLA	C4-C3-C5	2.22	119.01	115.27
20	3	614	CLA	CBC-CAC-C3C	-2.22	106.30	112.43
20	A	839	CLA	CMB-C2B-C3B	2.22	128.84	124.68
20	B	811	CLA	CHB-C4A-NA	2.22	127.58	124.51
20	A	823	CLA	CMC-C2C-C1C	2.22	128.42	125.04
27	5	607	CHL	C5-C3-C4	2.22	119.51	114.60
20	6	612	CLA	C1-C2-C3	-2.22	122.20	126.04
20	6	614	CLA	CBC-CAC-C3C	-2.22	106.31	112.43
20	A	807	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
20	A	817	CLA	C1-C2-C3	-2.22	122.20	126.04
20	3	613	CLA	CED-O2D-CGD	2.22	120.96	115.94
23	3	717	BCR	C37-C22-C23	2.22	121.58	118.08
20	7	613	CLA	CBC-CAC-C3C	-2.22	106.31	112.43
20	A	837	CLA	C2A-C3A-C4A	-2.22	98.28	101.87
20	3	611	CLA	CBC-CAC-C3C	-2.22	106.31	112.43
27	Z	601	CHL	C4-C3-C2	-2.22	117.98	123.68
20	B	837	CLA	CBC-CAC-C3C	-2.22	106.31	112.43
27	1	601	CHL	C4-C3-C5	2.22	119.00	115.27
20	B	834	CLA	CBC-CAC-C3C	-2.22	106.31	112.43
20	8	602	CLA	CBC-CAC-C3C	-2.22	106.31	112.43
20	3	617	CLA	CBC-CAC-C3C	-2.22	106.32	112.43
20	5	616	CLA	O2A-CGA-CBA	2.22	121.00	112.23
20	B	808	CLA	C1-C2-C3	-2.22	122.21	126.04
20	F	301	CLA	C4-C3-C5	2.22	119.00	115.27
20	B	833	CLA	CAA-C2A-C1A	-2.22	104.71	111.97
28	Z	617	LUT	C38-C25-C24	-2.22	118.82	123.56
20	Z	604	CLA	C1-C2-C3	-2.22	122.21	126.04
23	L	201	BCR	C20-C21-C22	-2.22	124.15	127.31
20	A	840	CLA	CAA-CBA-CGA	-2.22	106.78	113.25
20	4	604	CLA	O2D-CGD-O1D	-2.22	119.51	123.84
20	A	821	CLA	O1D-CGD-CBD	-2.21	119.95	124.48
28	8	618	LUT	C15-C35-C34	-2.21	118.94	123.47
20	3	610	CLA	CMA-C3A-C4A	-2.21	105.82	111.77
28	5	620	LUT	C8-C7-C6	-2.21	120.99	127.20
27	1	601	CHL	CHD-C4C-NC	2.21	127.69	124.20
20	7	613	CLA	CMB-C2B-C3B	2.21	128.82	124.68
20	1	608	CLA	CHB-C4A-NA	2.21	127.57	124.51
20	3	607	CLA	CBC-CAC-C3C	-2.21	106.33	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	831	CLA	CHB-C4A-NA	2.21	127.57	124.51
20	B	832	CLA	C4-C3-C5	2.21	118.99	115.27
20	B	805	CLA	C3B-C4B-NB	2.21	112.07	109.21
20	B	812	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
20	A	854	CLA	CAC-C3C-C4C	2.21	127.68	124.81
20	A	817	CLA	C4-C3-C5	2.21	118.99	115.27
20	3	614	CLA	CHB-C4A-NA	2.21	127.57	124.51
20	4	612	CLA	CMB-C2B-C3B	2.21	128.81	124.68
27	8	607	CHL	CED-O2D-CGD	2.21	120.93	115.94
20	A	802	CLA	CHD-C4C-NC	2.21	127.68	124.20
28	Z	619	LUT	C31-C32-C33	-2.21	120.21	126.42
20	8	616	CLA	CBC-CAC-C3C	-2.21	106.34	112.43
20	A	807	CLA	CHB-C4A-NA	2.21	127.56	124.51
20	A	831	CLA	O2A-CGA-CBA	2.21	118.83	111.91
22	1	620	LHG	C5-O7-C7	-2.21	112.36	117.79
20	7	609	CLA	C5-C3-C4	2.21	119.48	114.60
20	5	614	CLA	CBC-CAC-C3C	-2.21	106.35	112.43
23	L	201	BCR	C38-C26-C25	-2.21	122.05	124.53
23	7	623	BCR	C20-C21-C22	-2.21	124.16	127.31
20	3	609	CLA	O2A-CGA-CBA	2.21	118.83	111.91
20	8	609	CLA	O2A-CGA-CBA	2.20	120.94	112.23
20	Z	606	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
23	4	621	BCR	C15-C16-C17	-2.20	118.96	123.47
20	8	614	CLA	C1-C2-C3	-2.20	122.23	126.04
23	A	852	BCR	C28-C27-C26	-2.20	110.14	114.08
20	6	604	CLA	CBC-CAC-C3C	-2.20	106.36	112.43
20	A	841	CLA	CED-O2D-CGD	2.20	120.92	115.94
20	B	806	CLA	CED-O2D-CGD	2.20	120.92	115.94
20	B	835	CLA	CMC-C2C-C1C	2.20	128.39	125.04
20	A	854	CLA	C1-C2-C3	-2.20	122.24	126.04
20	7	608	CLA	CMB-C2B-C3B	2.20	128.79	124.68
20	B	837	CLA	CMC-C2C-C1C	2.20	128.39	125.04
28	1	617	LUT	C39-C29-C28	2.20	121.54	118.08
27	6	618	CHL	C1B-CHB-C4A	-2.20	125.76	130.12
20	5	613	CLA	CMC-C2C-C1C	2.20	128.39	125.04
23	8	619	BCR	C23-C24-C25	-2.20	121.03	127.20
20	B	820	CLA	CMC-C2C-C1C	2.20	128.39	125.04
27	6	607	CHL	CMA-C3A-C4A	-2.20	105.87	111.77
28	3	621	LUT	C40-C33-C32	2.20	121.54	118.08
20	B	832	CLA	CHA-C1A-NA	-2.20	121.37	126.40
20	4	603	CLA	CHA-C1A-NA	-2.20	121.37	126.40
20	B	837	CLA	O1D-CGD-CBD	-2.20	119.99	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	4	608	CHL	C1-C2-C3	-2.19	123.20	126.75
20	B	852	CLA	CHB-C4A-NA	2.19	127.54	124.51
20	A	809	CLA	C4-C3-C5	2.19	118.96	115.27
20	5	621	CLA	CAA-C2A-C1A	2.19	119.16	111.97
20	8	601	CLA	CHA-C1A-NA	-2.19	121.38	126.40
20	4	602	CLA	O2D-CGD-O1D	-2.19	119.55	123.84
20	3	609	CLA	CMA-C3A-C4A	-2.19	105.88	111.77
20	8	608	CLA	C5-C3-C4	2.19	119.44	114.60
20	6	609	CLA	C5-C3-C4	2.19	119.44	114.60
20	6	601	CLA	C4-C3-C5	2.19	118.95	115.27
20	7	614	CLA	CBC-CAC-C3C	-2.19	106.39	112.43
23	A	856	BCR	C31-C1-C6	-2.19	106.75	110.30
27	7	607	CHL	CHC-C1C-C2C	-2.19	118.17	126.11
20	B	817	CLA	C1-C2-C3	-2.19	122.26	126.04
20	K	4003	CLA	CHB-C4A-NA	2.19	127.54	124.51
23	A	849	BCR	C11-C12-C13	-2.19	120.27	126.42
20	7	611	CLA	CMB-C2B-C3B	2.19	128.77	124.68
20	1	616	CLA	CBC-CAC-C3C	-2.19	106.40	112.43
20	B	805	CLA	O1D-CGD-CBD	-2.19	120.01	124.48
20	1	604	CLA	CMD-C2D-C3D	-2.19	122.58	127.61
28	Z	618	LUT	C20-C13-C12	2.19	121.52	118.08
20	A	808	CLA	CMB-C2B-C3B	2.19	128.77	124.68
20	5	609	CLA	CHA-C1A-NA	-2.19	121.39	126.40
20	6	601	CLA	CMB-C2B-C3B	2.19	128.77	124.68
20	B	830	CLA	C5-C3-C4	2.19	119.43	114.60
20	A	817	CLA	CHB-C4A-NA	2.19	127.53	124.51
27	4	608	CHL	O2D-CGD-O1D	-2.19	119.56	123.84
20	A	804	CLA	C2A-C1A-CHA	-2.19	120.04	123.86
20	4	613	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
28	Z	618	LUT	C35-C34-C33	-2.19	124.19	127.31
20	3	612	CLA	CAA-C2A-C3A	-2.19	106.79	112.78
20	G	203	CLA	C5-C3-C4	2.18	119.43	114.60
20	F	304	CLA	O2A-CGA-CBA	2.18	118.76	111.91
20	A	836	CLA	CMC-C2C-C1C	2.18	128.37	125.04
20	3	609	CLA	CMC-C2C-C1C	2.18	128.37	125.04
23	8	619	BCR	C16-C15-C14	-2.18	119.00	123.47
20	3	604	CLA	O2D-CGD-O1D	-2.18	119.57	123.84
28	3	622	LUT	C40-C33-C32	2.18	121.52	118.08
20	A	840	CLA	CHA-C1A-NA	-2.18	121.40	126.40
23	3	719	BCR	C35-C13-C12	2.18	121.52	118.08
20	Z	613	CLA	C4-C3-C5	2.18	118.94	115.27
23	A	848	BCR	C32-C1-C6	2.18	113.84	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	G	204	CLA	O1D-CGD-CBD	-2.18	120.02	124.48
20	B	805	CLA	CMB-C2B-C3B	2.18	128.76	124.68
20	4	601	CLA	CMB-C2B-C3B	2.18	128.76	124.68
20	3	612	CLA	CMB-C2B-C3B	2.18	128.76	124.68
20	5	617	CLA	CHD-C4C-NC	2.18	127.64	124.20
20	B	802	CLA	CMC-C2C-C1C	2.18	128.36	125.04
23	3	718	BCR	C11-C12-C13	-2.18	120.30	126.42
20	6	616	CLA	O2A-CGA-CBA	2.18	120.84	112.23
22	8	620	LHG	O8-C23-C24	2.18	118.74	111.91
20	B	808	CLA	CBC-CAC-C3C	-2.18	106.43	112.43
27	6	606	CHL	CMB-C2B-C3B	2.18	128.75	124.68
20	1	609	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
20	Z	611	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
20	6	601	CLA	CMC-C2C-C1C	2.18	128.35	125.04
20	B	833	CLA	O1D-CGD-CBD	-2.18	120.03	124.48
20	A	837	CLA	CMC-C2C-C1C	2.18	128.35	125.04
28	6	621	LUT	C39-C29-C28	2.18	121.50	118.08
28	6	624	LUT	C18-C5-C6	-2.18	122.08	124.53
20	5	604	CLA	CBC-CAC-C3C	-2.17	106.44	112.43
20	A	841	CLA	C4-C3-C5	2.17	118.93	115.27
20	A	845	CLA	CMB-C2B-C3B	2.17	128.75	124.68
23	5	622	BCR	C11-C10-C9	-2.17	124.21	127.31
23	B	801	BCR	C36-C18-C19	2.17	121.50	118.08
28	5	620	LUT	C38-C25-C24	-2.17	118.92	123.56
20	3	612	CLA	CHB-C4A-NA	2.17	127.51	124.51
20	A	824	CLA	CMB-C2B-C3B	2.17	128.74	124.68
20	A	802	CLA	C1-C2-C3	-2.17	122.29	126.04
20	7	608	CLA	C5-C3-C4	2.17	119.39	114.60
20	B	832	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
20	3	620	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
20	A	820	CLA	C11-C10-C8	-2.17	108.91	115.92
20	4	603	CLA	CAA-C2A-C3A	-2.17	106.84	112.78
23	B	847	BCR	C19-C18-C17	-2.17	115.62	118.94
23	K	4004	BCR	C7-C8-C9	-2.17	122.96	126.23
20	5	601	CLA	CHB-C4A-NA	2.17	127.51	124.51
20	K	4002	CLA	CBC-CAC-C3C	-2.17	106.46	112.43
20	6	602	CLA	C4-C3-C5	2.17	118.91	115.27
20	B	836	CLA	CHA-C1A-NA	-2.16	121.44	126.40
20	1	609	CLA	CHA-C1A-NA	-2.16	121.44	126.40
20	5	604	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
28	3	621	LUT	C39-C29-C28	2.16	121.48	118.08
20	B	812	CLA	CMB-C2B-C3B	2.16	128.72	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	826	CLA	CHB-C4A-NA	2.16	127.50	124.51
23	J	3003	BCR	C7-C8-C9	-2.16	122.97	126.23
27	1	601	CHL	O2A-CGA-O1A	-2.16	118.14	123.59
20	A	818	CLA	C4-C3-C2	-2.16	118.13	123.68
20	8	612	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
20	3	602	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
20	A	825	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
20	B	814	CLA	C4-C3-C5	2.16	118.90	115.27
20	B	821	CLA	CMC-C2C-C1C	2.16	128.33	125.04
20	5	606	CLA	CMC-C2C-C1C	2.16	128.33	125.04
20	B	828	CLA	CBC-CAC-C3C	-2.16	106.48	112.43
20	6	613	CLA	CAA-C2A-C3A	-2.16	106.87	112.78
20	7	614	CLA	CHA-C1A-NA	-2.16	121.46	126.40
20	5	621	CLA	CHA-C1A-NA	-2.16	121.46	126.40
23	6	623	BCR	C29-C30-C25	2.16	113.80	110.48
20	5	606	CLA	CMB-C2B-C3B	2.16	128.71	124.68
23	B	846	BCR	C15-C16-C17	-2.16	119.06	123.47
20	6	609	CLA	CHA-C1A-NA	-2.16	121.46	126.40
20	5	621	CLA	CHD-C4C-NC	2.16	127.60	124.20
20	1	614	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
23	B	845	BCR	C23-C22-C21	2.16	122.25	118.94
27	1	607	CHL	CHD-C4C-NC	2.16	127.60	124.20
20	L	204	CLA	C5-C3-C4	2.15	119.36	114.60
20	1	610	CLA	CBA-CAA-C2A	2.15	120.22	113.86
20	A	822	CLA	C4-C3-C5	2.15	118.89	115.27
20	B	809	CLA	CBC-CAC-C3C	-2.15	106.49	112.43
20	B	824	CLA	CBC-CAC-C3C	-2.15	106.49	112.43
20	3	602	CLA	C1B-CHB-C4A	-2.15	125.85	130.12
20	B	818	CLA	CHA-C1A-NA	-2.15	121.47	126.40
27	4	607	CHL	C5-C3-C4	2.15	119.36	114.60
20	5	606	CLA	C4-C3-C5	2.15	118.89	115.27
20	F	301	CLA	CHB-C4A-NA	2.15	127.49	124.51
20	3	609	CLA	CBC-CAC-C3C	-2.15	106.50	112.43
27	Z	607	CHL	O2D-CGD-O1D	-2.15	119.63	123.84
27	6	608	CHL	C5-C3-C4	2.15	119.36	114.60
20	8	608	CLA	CAA-C2A-C3A	-2.15	106.89	112.78
20	5	609	CLA	C5-C3-C4	2.15	119.36	114.60
20	6	617	CLA	O2A-CGA-CBA	2.15	120.73	112.23
20	A	803	CLA	CHB-C4A-NA	2.15	127.49	124.51
27	6	607	CHL	CHD-C4C-NC	2.15	127.59	124.20
20	7	602	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
20	A	829	CLA	CMA-C3A-C2A	-2.15	105.16	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	814	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
23	B	845	BCR	C31-C1-C6	-2.15	106.81	110.30
20	B	814	CLA	C1-C2-C3	-2.15	122.33	126.04
23	B	801	BCR	C28-C27-C26	-2.15	110.24	114.08
20	A	831	CLA	CMA-C3A-C4A	-2.15	106.00	111.77
20	B	828	CLA	CHB-C4A-NA	2.15	127.48	124.51
20	8	604	CLA	CMC-C2C-C1C	2.15	128.31	125.04
23	A	849	BCR	C3-C4-C5	-2.15	110.24	114.08
23	B	843	BCR	C10-C11-C12	-2.15	116.52	123.22
20	B	841	CLA	CHA-C1A-NA	-2.15	121.48	126.40
20	1	602	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
23	3	719	BCR	C11-C10-C9	-2.15	124.25	127.31
23	L	201	BCR	C21-C20-C19	-2.15	116.52	123.22
28	8	617	LUT	C1-C2-C3	2.15	118.49	113.64
20	8	601	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
20	1	613	CLA	CMB-C2B-C3B	2.14	128.69	124.68
20	3	603	CLA	CHA-C1A-NA	-2.14	121.49	126.40
20	B	835	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
20	1	611	CLA	CMC-C2C-C1C	2.14	128.30	125.04
20	1	616	CLA	CMC-C2C-C1C	2.14	128.30	125.04
23	6	625	BCR	C2-C1-C6	2.14	113.78	110.48
20	A	817	CLA	CAA-C2A-C3A	-2.14	106.91	112.78
23	7	624	BCR	C21-C20-C19	-2.14	116.53	123.22
20	8	608	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
23	7	623	BCR	C37-C22-C23	2.14	121.45	118.08
20	B	822	CLA	C4-C3-C5	2.14	118.87	115.27
20	B	808	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
20	5	606	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
20	8	614	CLA	CBC-CAC-C3C	-2.14	106.53	112.43
20	3	602	CLA	C4-C3-C5	2.14	118.87	115.27
20	B	841	CLA	CBC-CAC-C3C	-2.14	106.54	112.43
23	5	622	BCR	C23-C24-C25	-2.14	121.20	127.20
23	5	625	BCR	C29-C30-C25	2.14	113.77	110.48
22	Z	620	LHG	C5-O7-C7	-2.14	112.53	117.79
20	5	609	CLA	CBC-CAC-C3C	-2.14	106.54	112.43
20	4	610	CLA	C4-C3-C5	2.14	118.86	115.27
20	B	833	CLA	CHC-C1C-NC	2.13	127.44	124.20
20	B	829	CLA	O2A-CGA-O1A	-2.13	118.20	123.59
23	B	847	BCR	C29-C28-C27	-2.13	106.61	111.38
20	A	810	CLA	CHB-C4A-NA	2.13	127.46	124.51
20	A	822	CLA	CMC-C2C-C1C	2.13	128.29	125.04
20	B	833	CLA	CHB-C4A-NA	2.13	127.46	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	839	CLA	CHB-C4A-NA	2.13	127.46	124.51
23	L	201	BCR	C11-C12-C13	-2.13	120.42	126.42
20	A	833	CLA	C1-O2A-CGA	2.13	122.04	116.44
20	A	827	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
20	3	607	CLA	C1-O2A-CGA	2.13	122.04	116.44
20	8	603	CLA	CBC-CAC-C3C	-2.13	106.55	112.43
20	8	612	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
20	7	609	CLA	CMC-C2C-C1C	2.13	128.28	125.04
20	A	839	CLA	O2A-CGA-CBA	2.13	118.60	111.91
20	A	823	CLA	CMB-C2B-C3B	2.13	128.66	124.68
23	3	717	BCR	C36-C18-C19	2.13	121.43	118.08
23	B	843	BCR	C23-C24-C25	-2.13	121.22	127.20
20	Z	612	CLA	CBA-CAA-C2A	-2.13	107.58	113.86
20	A	828	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
20	A	824	CLA	CHB-C4A-NA	2.13	127.46	124.51
20	B	824	CLA	C1-C2-C3	-2.13	122.36	126.04
23	F	305	BCR	C24-C23-C22	-2.13	123.02	126.23
20	6	612	CLA	CMB-C2B-C3B	2.13	128.66	124.68
20	B	814	CLA	CBC-CAC-C3C	-2.13	106.57	112.43
20	1	608	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
20	8	602	CLA	CAC-C3C-C2C	2.13	131.17	127.53
20	1	604	CLA	CAA-C2A-C3A	-2.13	106.95	112.78
20	4	604	CLA	C5-C3-C4	2.13	119.30	114.60
20	6	610	CLA	O1D-CGD-CBD	-2.13	120.14	124.48
20	3	613	CLA	CHB-C4A-NA	2.13	127.45	124.51
28	6	624	LUT	C19-C9-C8	2.12	121.42	118.08
20	B	819	CLA	CBC-CAC-C3C	-2.12	106.57	112.43
20	B	829	CLA	C2A-C1A-CHA	-2.12	120.14	123.86
20	3	604	CLA	CMB-C2B-C3B	2.12	128.65	124.68
20	7	609	CLA	CHA-C1A-NA	-2.12	121.53	126.40
28	1	618	LUT	C16-C1-C6	-2.12	106.86	110.30
28	6	621	LUT	C38-C25-C24	-2.12	119.02	123.56
20	4	601	CLA	C4-C3-C5	2.12	118.84	115.27
23	A	850	BCR	C21-C20-C19	-2.12	116.60	123.22
20	A	828	CLA	C4-C3-C5	2.12	118.84	115.27
28	Z	619	LUT	C18-C5-C6	-2.12	122.15	124.53
23	B	844	BCR	C21-C20-C19	-2.12	116.60	123.22
23	6	623	BCR	C24-C23-C22	-2.12	123.03	126.23
20	A	838	CLA	CMD-C2D-C3D	-2.12	122.74	127.61
23	B	847	BCR	C40-C30-C25	2.12	113.74	110.30
20	4	603	CLA	CHB-C4A-NA	2.12	127.44	124.51
23	3	717	BCR	C11-C12-C13	-2.12	120.46	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	610	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
23	7	623	BCR	C10-C11-C12	-2.12	116.61	123.22
23	B	846	BCR	C16-C15-C14	-2.12	119.14	123.47
20	A	810	CLA	CAA-CBA-CGA	-2.12	107.06	113.25
28	5	624	LUT	C28-C29-C30	-2.12	115.69	118.94
27	6	606	CHL	C2A-C1A-CHA	-2.12	120.16	123.86
28	7	621	LUT	C21-C26-C27	-2.12	110.03	112.70
20	A	822	CLA	O2D-CGD-O1D	-2.12	119.70	123.84
20	Z	603	CLA	CHA-C1A-NA	-2.12	121.55	126.40
23	I	172	BCR	C35-C13-C12	2.12	121.41	118.08
28	3	622	LUT	C35-C15-C14	-2.12	119.14	123.47
20	6	601	CLA	O1D-CGD-CBD	-2.12	120.16	124.48
20	Z	604	CLA	CMC-C2C-C1C	2.12	128.26	125.04
20	A	826	CLA	C1-C2-C3	-2.11	122.39	126.04
20	Z	603	CLA	O2A-C1-C2	2.11	114.19	108.64
26	J	3001	LMG	O2-C2-C1	-2.11	104.91	110.05
20	A	809	CLA	C6-C5-C3	-2.11	107.91	113.45
20	5	617	CLA	CHC-C1C-NC	2.11	127.41	124.20
20	A	802	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
27	4	618	CHL	CHD-C4C-NC	2.11	127.53	124.20
23	6	623	BCR	C38-C26-C25	-2.11	122.16	124.53
20	8	610	CLA	C1B-CHB-C4A	-2.11	125.94	130.12
20	4	609	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
20	7	609	CLA	CAA-C2A-C3A	-2.11	107.00	112.78
20	B	830	CLA	CBC-CAC-C3C	-2.11	106.62	112.43
20	A	840	CLA	C1-O2A-CGA	2.11	121.98	116.44
28	1	617	LUT	C15-C14-C13	-2.11	124.30	127.31
23	L	205	BCR	C21-C20-C19	-2.11	116.64	123.22
20	A	829	CLA	O2A-CGA-CBA	2.11	118.52	111.91
20	A	833	CLA	CHA-C1A-NA	-2.11	121.57	126.40
20	Z	609	CLA	CHA-C1A-NA	-2.11	121.57	126.40
20	B	852	CLA	CMC-C2C-C1C	2.11	128.25	125.04
20	8	612	CLA	CBC-CAC-C3C	-2.11	106.62	112.43
28	4	620	LUT	C21-C26-C27	-2.11	110.04	112.70
21	A	844	PQN	C21-C22-C23	-2.11	109.11	115.92
23	G	205	BCR	C37-C22-C23	2.11	121.40	118.08
20	B	852	CLA	CHA-C1A-NA	-2.11	121.57	126.40
23	F	305	BCR	C12-C13-C14	2.11	122.17	118.94
20	1	611	CLA	CHA-C1A-NA	-2.11	121.58	126.40
20	6	616	CLA	C2A-C3A-C4A	-2.11	98.47	101.87
20	B	827	CLA	CHA-C1A-NA	-2.11	121.58	126.40
20	4	613	CLA	O2A-CGA-O1A	-2.10	118.28	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	849	BCR	C8-C7-C6	-2.10	121.29	127.20
20	A	813	CLA	CHA-C1A-NA	-2.10	121.58	126.40
20	B	835	CLA	CHA-C1A-NA	-2.10	121.58	126.40
20	B	834	CLA	C4-C3-C5	2.10	118.81	115.27
20	4	612	CLA	CHB-C4A-NA	2.10	127.42	124.51
20	A	805	CLA	C4-C3-C5	2.10	118.81	115.27
20	A	854	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
20	B	803	CLA	C1B-CHB-C4A	-2.10	125.95	130.12
20	B	834	CLA	CMC-C2C-C1C	2.10	128.24	125.04
22	4	623	LHG	C5-O7-C7	-2.10	112.62	117.79
28	8	617	LUT	C18-C5-C6	-2.10	122.17	124.53
23	6	623	BCR	C37-C22-C23	2.10	121.39	118.08
27	6	618	CHL	CHB-C4A-NA	2.10	127.42	124.51
23	5	625	BCR	C23-C24-C25	-2.10	121.31	127.20
27	6	607	CHL	CBC-CAC-C3C	-2.10	106.64	112.43
20	Z	609	CLA	CBC-CAC-C3C	-2.10	106.64	112.43
20	8	613	CLA	C4-C3-C5	2.10	118.80	115.27
28	4	620	LUT	C39-C29-C28	2.10	121.38	118.08
20	Z	604	CLA	CMA-C3A-C4A	-2.10	106.13	111.77
20	8	614	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
20	5	617	CLA	O2A-CGA-CBA	2.10	120.52	112.23
28	7	621	LUT	C39-C29-C28	2.10	121.38	118.08
27	4	606	CHL	C1-C2-C3	-2.10	122.42	126.04
23	A	848	BCR	C21-C20-C19	-2.10	116.67	123.22
20	4	613	CLA	CMB-C2B-C3B	2.10	128.60	124.68
20	A	816	CLA	C1-C2-C3	-2.10	122.42	126.04
27	Z	601	CHL	CHB-C4A-NA	2.10	127.41	124.51
27	7	607	CHL	C1B-CHB-C4A	-2.10	125.97	130.12
20	8	606	CLA	CHB-C4A-NA	2.10	127.41	124.51
20	Z	608	CLA	O2D-CGD-O1D	-2.10	119.74	123.84
28	6	624	LUT	C30-C31-C32	-2.10	116.68	123.22
20	A	834	CLA	CMA-C3A-C2A	-2.10	105.38	113.83
23	3	717	BCR	C38-C26-C27	2.10	117.64	113.62
27	5	607	CHL	CBC-CAC-C3C	-2.10	106.66	112.43
27	3	608	CHL	O2D-CGD-O1D	-2.09	119.74	123.84
28	5	624	LUT	C35-C34-C33	-2.09	124.32	127.31
20	4	601	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
20	1	616	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
27	5	607	CHL	C1-C2-C3	-2.09	123.36	126.75
20	B	820	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
27	6	618	CHL	CHD-C4C-NC	2.09	127.50	124.20
20	1	612	CLA	CHA-C1A-NA	-2.09	121.61	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	819	CLA	CHC-C1C-NC	2.09	127.38	124.20
20	Z	609	CLA	CMC-C2C-C1C	2.09	128.22	125.04
20	5	616	CLA	CMC-C2C-C1C	2.09	128.22	125.04
20	8	612	CLA	CMB-C2B-C3B	2.09	128.59	124.68
23	5	625	BCR	C2-C1-C6	2.09	113.70	110.48
20	B	812	CLA	CBC-CAC-C3C	-2.09	106.67	112.43
20	5	613	CLA	CBC-CAC-C3C	-2.09	106.67	112.43
20	A	839	CLA	CBC-CAC-C3C	-2.09	106.67	112.43
28	6	621	LUT	C3-C4-C5	-2.09	107.69	111.85
25	B	850	DGD	O6D-C5D-C6D	2.09	110.88	106.67
28	5	620	LUT	C1-C2-C3	2.09	118.36	113.64
20	3	613	CLA	C1-C2-C3	-2.09	122.43	126.04
23	7	623	BCR	C28-C27-C26	-2.09	110.35	114.08
23	B	847	BCR	C20-C21-C22	-2.09	124.33	127.31
20	A	840	CLA	C1-C2-C3	-2.09	122.43	126.04
20	8	612	CLA	CED-O2D-CGD	2.09	120.66	115.94
23	6	625	BCR	C33-C5-C6	-2.09	122.19	124.53
23	L	205	BCR	C10-C11-C12	-2.09	116.71	123.22
28	8	618	LUT	C19-C9-C8	2.09	121.36	118.08
20	5	612	CLA	C1-C2-C3	-2.09	122.44	126.04
22	Z	620	LHG	C6-C5-C4	-2.09	106.86	111.79
20	7	601	CLA	C1-C2-C3	-2.08	122.44	126.04
23	5	625	BCR	C29-C28-C27	-2.08	106.72	111.38
20	7	606	CLA	CMC-C2C-C1C	2.08	128.21	125.04
20	A	815	CLA	CMD-C2D-C3D	-2.08	122.82	127.61
23	A	856	BCR	C35-C13-C12	2.08	121.35	118.08
20	8	606	CLA	CMC-C2C-C1C	2.08	128.21	125.04
27	4	608	CHL	C2A-C3A-C4A	-2.08	98.51	101.87
20	6	617	CLA	CHA-C1A-NA	-2.08	121.64	126.40
20	4	614	CLA	CED-O2D-CGD	2.08	120.64	115.94
20	4	609	CLA	CBA-CAA-C2A	2.08	120.00	113.86
28	Z	617	LUT	C16-C1-C6	-2.08	106.93	110.30
20	6	613	CLA	C1-O2A-CGA	2.08	121.89	116.44
20	3	609	CLA	CHA-C1A-NA	-2.08	121.64	126.40
20	4	612	CLA	CHA-C1A-NA	-2.08	121.64	126.40
20	3	612	CLA	O2A-CGA-CBA	2.08	120.44	112.23
23	6	623	BCR	C1-C6-C7	2.08	121.65	115.78
20	B	815	CLA	CBC-CAC-C3C	-2.08	106.71	112.43
20	3	602	CLA	C2A-C3A-C4A	-2.08	98.52	101.87
20	Z	604	CLA	CAA-C2A-C3A	-2.08	107.09	112.78
20	4	601	CLA	CHC-C1C-NC	2.08	127.35	124.20
20	A	832	CLA	CBC-CAC-C3C	-2.08	106.71	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	F	305	BCR	C2-C3-C4	-2.08	106.74	111.38
20	B	822	CLA	CBC-CAC-C3C	-2.07	106.71	112.43
20	B	818	CLA	C1-C2-C3	-2.07	122.45	126.04
20	B	809	CLA	CHA-C1A-NA	-2.07	121.65	126.40
27	5	608	CHL	C5-C3-C4	2.07	119.19	114.60
20	A	837	CLA	CAA-C2A-C3A	-2.07	107.10	112.78
20	A	816	CLA	O2A-CGA-CBA	2.07	118.42	111.91
20	A	808	CLA	C1-O2A-CGA	2.07	121.88	116.44
20	A	806	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
20	B	827	CLA	O2D-CGD-O1D	-2.07	119.79	123.84
20	A	829	CLA	C1B-CHB-C4A	-2.07	126.01	130.12
20	3	612	CLA	CMC-C2C-C1C	2.07	128.19	125.04
27	Z	601	CHL	CHD-C1D-C2D	-2.07	121.14	125.48
28	8	617	LUT	C28-C29-C30	-2.07	115.77	118.94
20	B	839	CLA	C4-C3-C5	2.07	118.75	115.27
20	5	614	CLA	CHA-C1A-NA	-2.07	121.66	126.40
20	A	854	CLA	C4-C3-C2	-2.07	118.37	123.68
27	5	607	CHL	CHB-C4A-NA	2.07	127.37	124.51
20	F	303	CLA	CHA-C1A-NA	-2.07	121.66	126.40
20	7	620	CLA	C1-C2-C3	-2.07	122.47	126.04
20	B	806	CLA	CMA-C3A-C4A	-2.07	106.22	111.77
20	6	614	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
27	6	608	CHL	CAA-C2A-C1A	-2.07	105.20	111.97
28	1	619	LUT	C15-C35-C34	-2.07	119.24	123.47
20	3	617	CLA	O1D-CGD-CBD	-2.07	120.26	124.48
20	7	602	CLA	C4-C3-C5	2.07	118.75	115.27
20	3	612	CLA	CHA-C1A-NA	-2.07	121.67	126.40
23	I	172	BCR	C34-C9-C8	2.07	121.33	118.08
20	A	818	CLA	CMC-C2C-C1C	2.07	128.18	125.04
20	1	604	CLA	CMC-C2C-C1C	2.07	128.18	125.04
20	4	604	CLA	O2A-CGA-CBA	2.07	118.39	111.91
20	7	604	CLA	C4-C3-C5	2.06	118.74	115.27
28	5	624	LUT	C3-C4-C5	-2.06	107.74	111.85
27	5	607	CHL	CGD-CBD-CAD	-2.06	104.05	110.73
20	1	610	CLA	O1D-CGD-CBD	-2.06	120.26	124.48
20	A	838	CLA	CHA-C1A-NA	-2.06	121.67	126.40
23	A	851	BCR	C29-C28-C27	-2.06	106.77	111.38
20	A	831	CLA	O1D-CGD-CBD	-2.06	120.26	124.48
27	6	606	CHL	O1D-CGD-CBD	-2.06	120.26	124.48
20	6	614	CLA	O2D-CGD-O1D	-2.06	119.81	123.84
20	7	612	CLA	CHA-C1A-NA	-2.06	121.67	126.40
20	B	809	CLA	C1-C2-C3	-2.06	122.48	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	603	CLA	CHB-C4A-NA	2.06	127.36	124.51
20	B	817	CLA	CBC-CAC-C3C	-2.06	106.75	112.43
20	6	603	CLA	CHA-C1A-NA	-2.06	121.68	126.40
20	B	811	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
20	5	603	CLA	CHA-C1A-NA	-2.06	121.68	126.40
20	A	836	CLA	C1-O2A-CGA	2.06	121.84	116.44
20	A	811	CLA	CBC-CAC-C3C	-2.06	106.76	112.43
20	1	604	CLA	CHC-C1C-NC	2.06	127.33	124.20
20	F	301	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
23	A	848	BCR	C39-C30-C25	-2.06	106.96	110.30
27	4	608	CHL	CHB-C4A-NA	2.06	127.36	124.51
20	B	834	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
20	3	607	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
28	1	618	LUT	C8-C7-C6	-2.06	121.43	127.20
20	4	614	CLA	CBC-CAC-C3C	-2.06	106.77	112.43
28	1	618	LUT	C39-C29-C28	2.06	121.31	118.08
20	Z	603	CLA	CMC-C2C-C1C	2.05	128.17	125.04
20	4	609	CLA	C5-C3-C4	2.05	119.14	114.60
23	6	623	BCR	C33-C5-C6	-2.05	122.22	124.53
20	A	821	CLA	O2A-CGA-CBA	2.05	120.63	114.03
20	Z	612	CLA	CMC-C2C-C1C	2.05	128.17	125.04
20	4	613	CLA	CBC-CAC-C3C	-2.05	106.77	112.43
20	4	601	CLA	C6-C7-C8	-2.05	109.28	115.92
20	A	814	CLA	CMC-C2C-C1C	2.05	128.16	125.04
20	7	610	CLA	C2A-C3A-C4A	-2.05	98.55	101.87
20	F	304	CLA	CHA-C1A-NA	-2.05	121.70	126.40
20	B	817	CLA	CMB-C2B-C1B	2.05	131.62	128.46
20	8	616	CLA	O2A-CGA-CBA	2.05	120.34	112.23
20	B	802	CLA	C4-C3-C5	2.05	118.72	115.27
20	Z	611	CLA	CMC-C2C-C1C	2.05	128.16	125.04
20	A	822	CLA	CBC-CAC-C3C	-2.05	106.78	112.43
20	A	820	CLA	CAA-C2A-C3A	-2.05	107.17	112.78
20	Z	609	CLA	O2D-CGD-O1D	-2.05	119.83	123.84
20	1	612	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
20	A	810	CLA	O2D-CGD-O1D	-2.05	119.83	123.84
20	5	602	CLA	CMD-C2D-C3D	-2.05	122.90	127.61
23	G	205	BCR	C35-C13-C12	2.05	121.31	118.08
20	7	612	CLA	CMC-C2C-C1C	2.05	128.16	125.04
20	A	836	CLA	CMA-C3A-C2A	-2.05	105.57	113.83
20	A	830	CLA	CHA-C1A-NA	-2.05	121.71	126.40
20	5	621	CLA	O2A-CGA-CBA	2.05	120.32	112.23
28	4	620	LUT	C20-C13-C12	2.05	121.30	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	849	BCR	C8-C9-C10	-2.05	115.80	118.94
23	3	718	BCR	C37-C22-C23	2.05	121.30	118.08
20	1	611	CLA	C4-C3-C5	2.05	118.71	115.27
27	4	608	CHL	C1B-CHB-C4A	-2.05	126.06	130.12
20	B	840	CLA	CMB-C2B-C3B	2.05	128.51	124.68
20	Z	603	CLA	C7-C6-C5	-2.04	107.81	113.36
20	B	833	CLA	CBC-CAC-C3C	-2.04	106.80	112.43
20	B	810	CLA	CHB-C4A-NA	2.04	127.34	124.51
20	A	842	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
20	A	816	CLA	C1-O2A-CGA	2.04	121.81	116.44
20	G	203	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
23	B	844	BCR	C10-C11-C12	-2.04	116.84	123.22
20	7	620	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
20	1	612	CLA	CMC-C2C-C1C	2.04	128.15	125.04
20	6	612	CLA	CHA-C1A-NA	-2.04	121.72	126.40
20	3	603	CLA	C4-C3-C5	2.04	118.71	115.27
20	1	614	CLA	CMC-C2C-C1C	2.04	128.15	125.04
20	B	836	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
28	8	618	LUT	C39-C29-C28	2.04	121.29	118.08
20	G	203	CLA	CMC-C2C-C1C	2.04	128.15	125.04
23	J	3003	BCR	C31-C1-C6	-2.04	106.99	110.30
28	1	617	LUT	C8-C7-C6	-2.04	121.47	127.20
20	1	612	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
20	A	807	CLA	C11-C12-C13	-2.04	109.33	115.92
20	5	616	CLA	CHA-C1A-NA	-2.04	121.73	126.40
20	A	813	CLA	C4-C3-C5	2.04	118.70	115.27
28	5	624	LUT	C19-C9-C8	2.04	121.29	118.08
23	F	305	BCR	C36-C18-C19	2.04	121.29	118.08
20	5	604	CLA	C5-C3-C4	2.04	119.10	114.60
23	A	851	BCR	C11-C12-C13	-2.04	120.69	126.42
20	K	4002	CLA	CAA-C2A-C3A	-2.04	107.20	112.78
20	F	304	CLA	C1-C2-C3	-2.04	122.52	126.04
20	Z	602	CLA	C1-C2-C3	-2.04	122.52	126.04
20	1	602	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
20	8	602	CLA	C1-O2A-CGA	2.04	121.78	116.44
20	8	614	CLA	CMA-C3A-C4A	-2.03	106.31	111.77
20	A	832	CLA	CHA-C1A-NA	-2.03	121.74	126.40
20	A	811	CLA	C4-C3-C5	2.03	118.69	115.27
20	3	614	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
28	3	622	LUT	C35-C34-C33	-2.03	124.41	127.31
27	5	618	CHL	O1D-CGD-CBD	-2.03	120.33	124.48
20	B	829	CLA	CMA-C3A-C4A	-2.03	106.31	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	6	623	BCR	C7-C6-C5	-2.03	116.54	121.46
20	8	612	CLA	CMA-C3A-C4A	-2.03	106.31	111.77
28	4	619	LUT	C21-C26-C27	-2.03	110.13	112.70
20	B	826	CLA	CMD-C2D-C3D	-2.03	122.94	127.61
23	A	848	BCR	C24-C23-C22	-2.03	123.17	126.23
27	8	607	CHL	O2D-CGD-O1D	-2.03	119.87	123.84
20	1	610	CLA	CMA-C3A-C4A	-2.03	106.32	111.77
20	B	825	CLA	CMD-C2D-C3D	-2.03	122.95	127.61
20	B	816	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
20	8	611	CLA	O2A-CGA-CBA	2.03	120.24	112.23
23	6	625	BCR	C39-C30-C25	-2.03	107.01	110.30
23	B	844	BCR	C16-C15-C14	-2.03	119.32	123.47
23	5	622	BCR	C23-C22-C21	-2.03	115.83	118.94
20	F	303	CLA	O2D-CGD-O1D	-2.03	119.88	123.84
20	8	613	CLA	C6-C7-C8	-2.03	109.37	115.92
27	5	607	CHL	O1D-CGD-CBD	-2.03	120.34	124.48
20	B	833	CLA	C1-O2A-CGA	2.03	121.76	116.44
28	3	621	LUT	C8-C7-C6	-2.02	121.52	127.20
23	5	625	BCR	C33-C5-C6	-2.02	122.25	124.53
20	B	837	CLA	CBA-CAA-C2A	2.02	119.84	113.86
28	Z	618	LUT	C19-C9-C8	2.02	121.27	118.08
27	3	608	CHL	CMB-C2B-C3B	2.02	128.46	124.68
28	Z	618	LUT	C15-C35-C34	-2.02	119.33	123.47
20	A	817	CLA	CHC-C1C-NC	2.02	127.27	124.20
20	1	611	CLA	O1D-CGD-CBD	-2.02	120.34	124.48
27	4	608	CHL	CED-O2D-CGD	2.02	120.51	115.94
28	Z	617	LUT	C31-C30-C29	-2.02	124.42	127.31
23	I	172	BCR	C7-C8-C9	-2.02	123.18	126.23
20	3	606	CLA	CED-O2D-CGD	2.02	120.51	115.94
20	5	602	CLA	C1-C2-C3	-2.02	122.55	126.04
20	6	622	CLA	CHA-C1A-NA	-2.02	121.77	126.40
28	3	622	LUT	C21-C26-C27	-2.02	110.15	112.70
20	7	603	CLA	O2A-CGA-CBA	2.02	120.21	112.23
20	B	836	CLA	CHB-C4A-NA	2.02	127.31	124.51
20	A	842	CLA	CMC-C2C-C1C	2.02	128.11	125.04
23	B	801	BCR	C34-C9-C8	2.02	121.26	118.08
20	A	830	CLA	CED-O2D-CGD	2.02	120.50	115.94
20	Z	608	CLA	CHA-C1A-NA	-2.02	121.78	126.40
23	B	801	BCR	C35-C13-C12	2.02	121.26	118.08
20	7	602	CLA	C1-C2-C3	-2.02	122.55	126.04
20	4	603	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
20	B	838	CLA	CMB-C2B-C3B	2.02	128.45	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	613	CLA	CBC-CAC-C3C	-2.01	106.88	112.43
20	K	4003	CLA	CHC-C1C-NC	2.01	127.26	124.20
20	5	601	CLA	O1D-CGD-CBD	-2.01	120.36	124.48
27	6	607	CHL	CHC-C1C-C2C	-2.01	118.81	126.11
20	8	612	CLA	C4-C3-C2	-2.01	118.51	123.68
20	4	609	CLA	C1B-CHB-C4A	-2.01	126.13	130.12
20	B	811	CLA	CBC-CAC-C3C	-2.01	106.88	112.43
20	B	824	CLA	CHA-C1A-NA	-2.01	121.79	126.40
27	6	608	CHL	C1B-CHB-C4A	-2.01	126.13	130.12
26	J	3001	LMG	C6-C5-C4	-2.01	108.29	113.00
20	8	612	CLA	CHA-C1A-NA	-2.01	121.79	126.40
28	8	618	LUT	C30-C31-C32	-2.01	116.94	123.22
27	5	618	CHL	CHC-C1C-C2C	-2.01	118.81	126.11
20	B	804	CLA	CHA-C1A-NA	-2.01	121.79	126.40
20	B	836	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
20	6	616	CLA	CAA-CBA-CGA	-2.01	107.38	113.25
20	A	833	CLA	CBC-CAC-C3C	-2.01	106.89	112.43
20	B	825	CLA	O2D-CGD-O1D	-2.01	119.91	123.84
20	B	825	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
20	B	828	CLA	CMA-C3A-C2A	-2.01	105.72	113.83
20	B	823	CLA	CMB-C2B-C3B	2.01	128.44	124.68
28	Z	618	LUT	C40-C33-C32	2.01	121.24	118.08
20	1	616	CLA	CHA-C1A-NA	-2.01	121.80	126.40
20	6	613	CLA	C4-C3-C5	2.01	118.65	115.27
20	6	617	CLA	CMC-C2C-C1C	2.01	128.10	125.04
23	B	848	BCR	C2-C1-C6	2.01	113.57	110.48
20	A	816	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
23	A	856	BCR	C34-C9-C8	2.01	121.24	118.08
27	3	608	CHL	C1B-CHB-C4A	-2.01	126.14	130.12
20	F	301	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
20	B	807	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
20	B	818	CLA	C2A-C3A-C4A	-2.01	98.63	101.87
20	B	827	CLA	C4-C3-C5	2.01	118.65	115.27
27	7	607	CHL	C2A-C1A-CHA	-2.01	120.35	123.86
20	A	808	CLA	CBC-CAC-C3C	-2.01	106.90	112.43
20	8	610	CLA	CMA-C3A-C2A	-2.01	105.73	113.83
20	B	835	CLA	CED-O2D-CGD	2.01	120.47	115.94
28	3	622	LUT	C39-C29-C28	2.01	121.24	118.08
28	4	619	LUT	C18-C5-C6	-2.00	122.28	124.53
20	A	818	CLA	CBC-CAC-C3C	-2.00	106.91	112.43
27	Z	601	CHL	O1D-CGD-CBD	-2.00	120.39	124.48
20	A	830	CLA	CHB-C4A-NA	2.00	127.28	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	820	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
23	B	846	BCR	C28-C27-C26	-2.00	110.50	114.08
20	8	603	CLA	CHA-C1A-NA	-2.00	121.81	126.40
28	6	624	LUT	C20-C13-C12	2.00	121.23	118.08
20	B	852	CLA	C1-C2-C3	-2.00	122.58	126.04
20	B	810	CLA	CHA-C1A-NA	-2.00	121.81	126.40
27	5	607	CHL	CHD-C4C-NC	2.00	127.36	124.20
20	A	825	CLA	C4-C3-C5	2.00	118.64	115.27
27	Z	607	CHL	CHD-C4C-NC	2.00	127.36	124.20
20	8	613	CLA	O2A-CGA-CBA	2.00	118.19	111.91
27	5	607	CHL	CMA-C3A-C4A	-2.00	106.39	111.77
20	A	827	CLA	CBC-CAC-C3C	-2.00	106.92	112.43

All (230) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	A	801	CL0	ND
19	A	801	CL0	NC
20	A	802	CLA	ND
20	A	803	CLA	ND
20	A	804	CLA	ND
20	A	805	CLA	ND
20	A	806	CLA	ND
20	A	807	CLA	ND
20	A	808	CLA	ND
20	A	809	CLA	ND
20	A	810	CLA	ND
20	A	811	CLA	ND
20	A	812	CLA	ND
20	A	813	CLA	ND
20	A	814	CLA	ND
20	A	815	CLA	ND
20	A	816	CLA	ND
20	A	817	CLA	ND
20	A	820	CLA	ND
20	A	821	CLA	ND
20	A	822	CLA	ND
20	A	824	CLA	ND
20	A	826	CLA	ND
20	A	827	CLA	ND
20	A	828	CLA	ND
20	A	829	CLA	ND

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Mol	Chain	Res	Type	Atom
20	A	830	CLA	ND
20	A	831	CLA	ND
20	A	832	CLA	ND
20	A	833	CLA	ND
20	A	834	CLA	ND
20	A	835	CLA	ND
20	A	837	CLA	ND
20	A	838	CLA	ND
20	A	839	CLA	ND
20	A	840	CLA	ND
20	A	841	CLA	ND
20	A	842	CLA	ND
20	A	843	CLA	ND
20	A	854	CLA	ND
20	B	802	CLA	ND
20	B	803	CLA	ND
20	B	804	CLA	ND
20	B	805	CLA	ND
20	B	806	CLA	ND
20	B	807	CLA	ND
20	B	808	CLA	ND
20	B	809	CLA	ND
20	B	810	CLA	ND
20	B	811	CLA	ND
20	B	812	CLA	ND
20	B	813	CLA	ND
20	B	814	CLA	ND
20	B	815	CLA	ND
20	B	816	CLA	ND
20	B	817	CLA	ND
20	B	818	CLA	ND
20	B	819	CLA	ND
20	B	820	CLA	ND
20	B	822	CLA	ND
20	B	823	CLA	ND
20	B	824	CLA	ND
20	B	825	CLA	ND
20	B	826	CLA	ND
20	B	827	CLA	ND
20	B	828	CLA	ND
20	B	829	CLA	ND
20	B	831	CLA	ND

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Mol	Chain	Res	Type	Atom
20	B	832	CLA	ND
20	B	833	CLA	ND
20	B	834	CLA	ND
20	B	835	CLA	ND
20	B	836	CLA	ND
20	B	837	CLA	ND
20	B	838	CLA	ND
20	B	839	CLA	ND
20	B	841	CLA	ND
20	B	852	CLA	ND
20	F	301	CLA	ND
20	F	303	CLA	ND
20	F	304	CLA	ND
20	G	203	CLA	ND
20	G	204	CLA	ND
20	J	3002	CLA	ND
20	K	4003	CLA	ND
20	1	602	CLA	ND
20	1	603	CLA	ND
20	1	604	CLA	ND
20	1	606	CLA	ND
20	1	608	CLA	ND
20	1	609	CLA	ND
20	1	610	CLA	ND
20	1	611	CLA	ND
20	1	612	CLA	ND
20	1	613	CLA	ND
20	1	614	CLA	ND
20	1	616	CLA	ND
20	3	602	CLA	ND
20	3	603	CLA	ND
20	3	604	CLA	ND
20	3	606	CLA	ND
20	3	607	CLA	ND
20	3	609	CLA	ND
20	3	610	CLA	ND
20	3	611	CLA	ND
20	3	612	CLA	ND
20	3	617	CLA	ND
20	3	620	CLA	ND
20	7	601	CLA	ND
20	7	602	CLA	ND

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Mol	Chain	Res	Type	Atom
20	7	603	CLA	ND
20	7	604	CLA	ND
20	7	606	CLA	ND
20	7	609	CLA	ND
20	7	610	CLA	ND
20	7	611	CLA	ND
20	7	612	CLA	ND
20	7	613	CLA	ND
20	7	614	CLA	ND
20	7	616	CLA	ND
20	7	620	CLA	ND
20	8	601	CLA	ND
20	8	602	CLA	ND
20	8	603	CLA	ND
20	8	604	CLA	ND
20	8	606	CLA	ND
20	8	608	CLA	ND
20	8	609	CLA	ND
20	8	610	CLA	ND
20	8	611	CLA	ND
20	8	612	CLA	ND
20	8	613	CLA	ND
20	8	614	CLA	ND
20	8	616	CLA	ND
20	Z	602	CLA	ND
20	Z	603	CLA	ND
20	Z	604	CLA	ND
20	Z	606	CLA	ND
20	Z	608	CLA	ND
20	Z	609	CLA	ND
20	Z	610	CLA	ND
20	Z	611	CLA	ND
20	Z	612	CLA	ND
20	Z	613	CLA	ND
20	Z	614	CLA	ND
20	Z	616	CLA	ND
20	4	601	CLA	ND
20	4	603	CLA	ND
20	4	609	CLA	ND
20	4	610	CLA	ND
20	4	611	CLA	ND
20	4	612	CLA	ND

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Mol	Chain	Res	Type	Atom
20	4	614	CLA	ND
20	4	616	CLA	ND
20	5	601	CLA	ND
20	5	603	CLA	ND
20	5	606	CLA	ND
20	5	609	CLA	ND
20	5	610	CLA	ND
20	5	611	CLA	ND
20	5	612	CLA	ND
20	5	613	CLA	ND
20	5	614	CLA	ND
20	5	616	CLA	ND
20	5	617	CLA	ND
20	5	621	CLA	ND
20	6	601	CLA	ND
20	6	602	CLA	ND
20	6	603	CLA	ND
20	6	604	CLA	ND
20	6	609	CLA	ND
20	6	610	CLA	ND
20	6	611	CLA	ND
20	6	612	CLA	ND
20	6	613	CLA	ND
20	6	614	CLA	ND
20	6	616	CLA	ND
20	6	617	CLA	ND
20	6	622	CLA	ND
27	1	601	CHL	ND
27	1	601	CHL	NA
27	1	601	CHL	NC
27	1	607	CHL	ND
27	1	607	CHL	NA
27	1	607	CHL	NC
27	3	608	CHL	ND
27	3	608	CHL	NA
27	3	608	CHL	NC
27	7	607	CHL	ND
27	7	607	CHL	NA
27	7	607	CHL	NC
27	8	607	CHL	ND
27	8	607	CHL	NA
27	8	607	CHL	NC

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Mol	Chain	Res	Type	Atom
27	Z	601	CHL	ND
27	Z	601	CHL	NA
27	Z	601	CHL	NC
27	Z	607	CHL	ND
27	Z	607	CHL	NA
27	Z	607	CHL	NC
27	4	606	CHL	ND
27	4	606	CHL	NA
27	4	606	CHL	NC
27	4	607	CHL	ND
27	4	607	CHL	NA
27	4	607	CHL	NC
27	4	608	CHL	ND
27	4	608	CHL	NA
27	4	608	CHL	NC
27	4	618	CHL	ND
27	4	618	CHL	NA
27	4	618	CHL	NC
27	5	607	CHL	ND
27	5	607	CHL	NA
27	5	607	CHL	NC
27	5	608	CHL	ND
27	5	608	CHL	NC
27	5	618	CHL	ND
27	5	618	CHL	NA
27	5	618	CHL	NC
27	6	606	CHL	ND
27	6	606	CHL	NC
27	6	607	CHL	ND
27	6	607	CHL	NC
27	6	608	CHL	ND
27	6	608	CHL	NA
27	6	608	CHL	NC
27	6	618	CHL	ND
27	6	618	CHL	NA
27	6	618	CHL	NC

All (2144) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	804	CLA	CHA-CBD-CGD-O1D
20	A	804	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
20	A	807	CLA	C1A-C2A-CAA-CBA
20	A	809	CLA	C3A-C2A-CAA-CBA
20	A	812	CLA	C1A-C2A-CAA-CBA
20	A	814	CLA	C2-C3-C5-C6
20	A	814	CLA	C4-C3-C5-C6
20	A	815	CLA	C1A-C2A-CAA-CBA
20	A	816	CLA	C2-C3-C5-C6
20	A	816	CLA	C4-C3-C5-C6
20	A	818	CLA	CHA-CBD-CGD-O1D
20	A	818	CLA	CHA-CBD-CGD-O2D
20	A	818	CLA	C2-C3-C5-C6
20	A	818	CLA	C4-C3-C5-C6
20	A	819	CLA	C1A-C2A-CAA-CBA
20	A	819	CLA	C3A-C2A-CAA-CBA
20	A	820	CLA	C1A-C2A-CAA-CBA
20	A	820	CLA	C3A-C2A-CAA-CBA
20	A	822	CLA	CBD-CGD-O2D-CED
20	A	823	CLA	C1A-C2A-CAA-CBA
20	A	823	CLA	C3A-C2A-CAA-CBA
20	A	829	CLA	C1A-C2A-CAA-CBA
20	A	831	CLA	CHA-CBD-CGD-O1D
20	A	831	CLA	CHA-CBD-CGD-O2D
20	A	831	CLA	C4-C3-C5-C6
20	A	834	CLA	C2-C3-C5-C6
20	A	834	CLA	C4-C3-C5-C6
20	A	835	CLA	CHA-CBD-CGD-O1D
20	A	835	CLA	CHA-CBD-CGD-O2D
20	A	835	CLA	C2-C3-C5-C6
20	A	835	CLA	C4-C3-C5-C6
20	A	839	CLA	C14-C13-C15-C16
20	A	840	CLA	CHA-CBD-CGD-O1D
20	A	843	CLA	C4-C3-C5-C6
20	A	845	CLA	CHA-CBD-CGD-O2D
20	B	802	CLA	CHA-CBD-CGD-O1D
20	B	802	CLA	CHA-CBD-CGD-O2D
20	B	805	CLA	C1A-C2A-CAA-CBA
20	B	805	CLA	C3A-C2A-CAA-CBA
20	B	808	CLA	CHA-CBD-CGD-O1D
20	B	808	CLA	CHA-CBD-CGD-O2D
20	B	810	CLA	C1A-C2A-CAA-CBA
20	B	813	CLA	C1A-C2A-CAA-CBA
20	B	813	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	B	818	CLA	C1A-C2A-CAA-CBA
20	B	818	CLA	C3A-C2A-CAA-CBA
20	B	818	CLA	C4-C3-C5-C6
20	B	818	CLA	C6-C7-C8-C9
20	B	822	CLA	CHA-CBD-CGD-O1D
20	B	823	CLA	CBD-CGD-O2D-CED
20	B	823	CLA	C4-C3-C5-C6
20	B	828	CLA	C1A-C2A-CAA-CBA
20	B	828	CLA	C3A-C2A-CAA-CBA
20	B	829	CLA	C2-C3-C5-C6
20	B	829	CLA	C4-C3-C5-C6
20	B	833	CLA	CHA-CBD-CGD-O1D
20	B	833	CLA	CHA-CBD-CGD-O2D
20	B	835	CLA	C1A-C2A-CAA-CBA
20	B	836	CLA	C2-C3-C5-C6
20	B	836	CLA	C4-C3-C5-C6
20	F	301	CLA	CHA-CBD-CGD-O1D
20	F	301	CLA	CHA-CBD-CGD-O2D
20	F	301	CLA	CBD-CGD-O2D-CED
20	F	304	CLA	CHA-CBD-CGD-O1D
20	F	304	CLA	CHA-CBD-CGD-O2D
20	J	3002	CLA	C1A-C2A-CAA-CBA
20	J	3002	CLA	C3A-C2A-CAA-CBA
20	1	602	CLA	C2-C3-C5-C6
20	1	602	CLA	C4-C3-C5-C6
20	1	604	CLA	C2-C3-C5-C6
20	1	604	CLA	C4-C3-C5-C6
20	1	608	CLA	CBD-CGD-O2D-CED
20	1	613	CLA	CHA-CBD-CGD-O1D
20	1	613	CLA	CHA-CBD-CGD-O2D
20	3	607	CLA	C1A-C2A-CAA-CBA
20	3	607	CLA	C2-C1-O2A-CGA
20	3	611	CLA	CHA-CBD-CGD-O1D
20	3	611	CLA	CHA-CBD-CGD-O2D
20	3	613	CLA	CHA-CBD-CGD-O1D
20	3	613	CLA	CHA-CBD-CGD-O2D
20	7	601	CLA	C2A-CAA-CBA-CGA
20	7	601	CLA	C2-C3-C5-C6
20	7	601	CLA	C4-C3-C5-C6
20	7	603	CLA	CHA-CBD-CGD-O1D
20	7	603	CLA	CHA-CBD-CGD-O2D
20	7	606	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	7	606	CLA	C3A-C2A-CAA-CBA
20	7	606	CLA	CHA-CBD-CGD-O2D
20	7	608	CLA	CBD-CGD-O2D-CED
20	7	609	CLA	C1A-C2A-CAA-CBA
20	7	609	CLA	C3A-C2A-CAA-CBA
20	7	611	CLA	CHA-CBD-CGD-O1D
20	7	611	CLA	CHA-CBD-CGD-O2D
20	8	606	CLA	CBD-CGD-O2D-CED
20	8	612	CLA	C2-C3-C5-C6
20	8	612	CLA	C4-C3-C5-C6
20	8	612	CLA	C3-C5-C6-C7
20	Z	602	CLA	CBD-CGD-O2D-CED
20	Z	603	CLA	C4-C3-C5-C6
20	Z	604	CLA	C2-C3-C5-C6
20	Z	604	CLA	C4-C3-C5-C6
20	Z	609	CLA	C2A-CAA-CBA-CGA
20	Z	610	CLA	C1A-C2A-CAA-CBA
20	Z	610	CLA	C2-C3-C5-C6
20	Z	610	CLA	C4-C3-C5-C6
20	Z	613	CLA	CHA-CBD-CGD-O1D
20	Z	613	CLA	CHA-CBD-CGD-O2D
20	4	603	CLA	CBD-CGD-O2D-CED
20	4	609	CLA	C1A-C2A-CAA-CBA
20	4	609	CLA	C3A-C2A-CAA-CBA
20	5	609	CLA	C1A-C2A-CAA-CBA
20	5	609	CLA	C3A-C2A-CAA-CBA
20	5	612	CLA	C2-C3-C5-C6
20	5	612	CLA	C4-C3-C5-C6
20	5	621	CLA	CHA-CBD-CGD-O1D
20	5	621	CLA	CHA-CBD-CGD-O2D
20	6	610	CLA	C2-C3-C5-C6
20	6	610	CLA	C4-C3-C5-C6
20	6	611	CLA	C4-C3-C5-C6
20	6	614	CLA	CBD-CGD-O2D-CED
22	A	855	LHG	C4-O6-P-O4
22	B	851	LHG	C3-O3-P-O4
22	B	851	LHG	C4-O6-P-O5
22	B	851	LHG	O9-C7-O7-C5
22	Z	620	LHG	O10-C23-O8-C6
22	Z	620	LHG	C24-C23-O8-C6
22	4	622	LHG	O7-C5-C6-O8
22	4	623	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
22	5	623	LHG	C4-O6-P-O3
22	5	623	LHG	C4-O6-P-O4
22	5	623	LHG	C4-O6-P-O5
23	A	850	BCR	C23-C24-C25-C30
23	A	856	BCR	C21-C22-C23-C24
23	A	856	BCR	C37-C22-C23-C24
23	B	843	BCR	C7-C8-C9-C10
23	B	843	BCR	C7-C8-C9-C34
23	B	843	BCR	C21-C22-C23-C24
23	B	843	BCR	C37-C22-C23-C24
23	B	844	BCR	C7-C8-C9-C10
23	B	844	BCR	C7-C8-C9-C34
23	B	844	BCR	C21-C22-C23-C24
23	B	844	BCR	C37-C22-C23-C24
23	B	845	BCR	C7-C8-C9-C34
23	B	845	BCR	C21-C22-C23-C24
23	B	845	BCR	C37-C22-C23-C24
23	B	846	BCR	C1-C6-C7-C8
23	B	846	BCR	C7-C8-C9-C34
23	B	847	BCR	C1-C6-C7-C8
23	B	847	BCR	C7-C8-C9-C10
23	B	847	BCR	C7-C8-C9-C34
23	B	848	BCR	C1-C6-C7-C8
23	F	305	BCR	C21-C22-C23-C24
23	F	305	BCR	C37-C22-C23-C24
23	G	205	BCR	C1-C6-C7-C8
23	I	172	BCR	C1-C6-C7-C8
23	I	172	BCR	C17-C18-C19-C20
23	I	172	BCR	C36-C18-C19-C20
23	I	172	BCR	C21-C22-C23-C24
23	I	172	BCR	C37-C22-C23-C24
23	J	3003	BCR	C7-C8-C9-C34
23	J	3003	BCR	C17-C18-C19-C20
23	J	3003	BCR	C36-C18-C19-C20
23	K	4001	BCR	C21-C22-C23-C24
23	K	4001	BCR	C37-C22-C23-C24
23	K	4004	BCR	C23-C24-C25-C30
23	L	201	BCR	C23-C24-C25-C30
23	L	205	BCR	C7-C8-C9-C34
23	3	719	BCR	C1-C6-C7-C8
23	7	623	BCR	C23-C24-C25-C26
23	7	624	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
23	8	619	BCR	C17-C18-C19-C20
23	8	619	BCR	C36-C18-C19-C20
23	4	621	BCR	C7-C8-C9-C10
23	4	621	BCR	C7-C8-C9-C34
23	4	621	BCR	C11-C12-C13-C14
23	4	621	BCR	C11-C12-C13-C35
23	4	621	BCR	C17-C18-C19-C20
23	4	621	BCR	C36-C18-C19-C20
23	4	621	BCR	C23-C24-C25-C30
23	5	622	BCR	C11-C12-C13-C14
23	5	622	BCR	C11-C12-C13-C35
23	5	625	BCR	C7-C8-C9-C34
23	6	623	BCR	C7-C8-C9-C34
23	6	623	BCR	C11-C12-C13-C14
23	6	623	BCR	C11-C12-C13-C35
23	6	625	BCR	C11-C12-C13-C14
23	6	625	BCR	C11-C12-C13-C35
27	1	601	CHL	C1C-C2C-CMC-OMC
27	1	601	CHL	C3C-C2C-CMC-OMC
27	1	601	CHL	CHA-CBD-CGD-O1D
27	1	601	CHL	CHA-CBD-CGD-O2D
27	1	601	CHL	CAD-CBD-CGD-O1D
27	1	601	CHL	O2A-C1-C2-C3
27	1	607	CHL	C1C-C2C-CMC-OMC
27	1	607	CHL	C3C-C2C-CMC-OMC
27	1	607	CHL	CBD-CGD-O2D-CED
27	3	608	CHL	CBD-CGD-O2D-CED
27	3	608	CHL	C14-C13-C15-C16
27	7	607	CHL	C1C-C2C-CMC-OMC
27	7	607	CHL	C3C-C2C-CMC-OMC
27	7	607	CHL	C2-C3-C5-C6
27	7	607	CHL	C4-C3-C5-C6
27	8	607	CHL	C1A-C2A-CAA-CBA
27	8	607	CHL	C2A-CAA-CBA-CGA
27	8	607	CHL	C1C-C2C-CMC-OMC
27	8	607	CHL	C3C-C2C-CMC-OMC
27	Z	601	CHL	C3C-C2C-CMC-OMC
27	Z	607	CHL	C1C-C2C-CMC-OMC
27	Z	607	CHL	C3C-C2C-CMC-OMC
27	4	607	CHL	C1C-C2C-CMC-OMC
27	4	607	CHL	C3C-C2C-CMC-OMC
27	4	608	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	4	618	CHL	C1C-C2C-CMC-OMC
27	4	618	CHL	C3C-C2C-CMC-OMC
27	5	607	CHL	C1A-C2A-CAA-CBA
27	5	607	CHL	C1C-C2C-CMC-OMC
27	5	607	CHL	C3C-C2C-CMC-OMC
27	5	608	CHL	C1A-C2A-CAA-CBA
27	5	608	CHL	C3A-C2A-CAA-CBA
27	5	608	CHL	C1C-C2C-CMC-OMC
27	5	608	CHL	C3C-C2C-CMC-OMC
27	5	608	CHL	CBD-CGD-O2D-CED
27	5	618	CHL	C1C-C2C-CMC-OMC
27	5	618	CHL	C3C-C2C-CMC-OMC
27	6	607	CHL	C1A-C2A-CAA-CBA
27	6	607	CHL	C1C-C2C-CMC-OMC
27	6	607	CHL	C3C-C2C-CMC-OMC
27	6	607	CHL	CBD-CGD-O2D-CED
27	6	618	CHL	C1A-C2A-CAA-CBA
27	6	618	CHL	C3A-C2A-CAA-CBA
27	6	618	CHL	C3C-C2C-CMC-OMC
28	1	619	LUT	C1-C6-C7-C8
28	Z	619	LUT	C1-C6-C7-C8
28	Z	619	LUT	C27-C28-C29-C30
28	Z	619	LUT	C27-C28-C29-C39
28	4	619	LUT	C1-C6-C7-C8
28	5	620	LUT	C1-C6-C7-C8
27	1	607	CHL	O1D-CGD-O2D-CED
20	A	825	CLA	CBD-CGD-O2D-CED
20	A	829	CLA	CBD-CGD-O2D-CED
20	A	835	CLA	CBD-CGD-O2D-CED
20	B	803	CLA	CBD-CGD-O2D-CED
20	1	602	CLA	CBD-CGD-O2D-CED
20	5	606	CLA	CBD-CGD-O2D-CED
20	5	616	CLA	CBD-CGD-O2D-CED
27	6	608	CHL	CBD-CGD-O2D-CED
20	Z	611	CLA	O1A-CGA-O2A-C1
22	1	620	LHG	O10-C23-O8-C6
20	A	829	CLA	O1D-CGD-O2D-CED
20	B	803	CLA	O1D-CGD-O2D-CED
20	5	616	CLA	O1D-CGD-O2D-CED
27	6	608	CHL	O1D-CGD-O2D-CED
20	F	301	CLA	O1D-CGD-O2D-CED
20	8	606	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	6	614	CLA	O1D-CGD-O2D-CED
27	4	608	CHL	O1D-CGD-O2D-CED
27	6	607	CHL	O1D-CGD-O2D-CED
22	1	620	LHG	C24-C23-O8-C6
20	A	811	CLA	CBD-CGD-O2D-CED
20	A	837	CLA	CBD-CGD-O2D-CED
20	A	841	CLA	CBD-CGD-O2D-CED
20	B	810	CLA	CBD-CGD-O2D-CED
20	Z	608	CLA	CBD-CGD-O2D-CED
20	Z	611	CLA	CBD-CGD-O2D-CED
20	4	602	CLA	CBD-CGD-O2D-CED
20	4	613	CLA	CBD-CGD-O2D-CED
27	4	607	CHL	CBD-CGD-O2D-CED
20	A	806	CLA	O1A-CGA-O2A-C1
20	B	822	CLA	O1A-CGA-O2A-C1
20	1	611	CLA	O1A-CGA-O2A-C1
20	5	601	CLA	O1A-CGA-O2A-C1
20	1	608	CLA	O1D-CGD-O2D-CED
20	7	608	CLA	O1D-CGD-O2D-CED
27	3	608	CHL	O1D-CGD-O2D-CED
27	5	608	CHL	O1D-CGD-O2D-CED
20	3	613	CLA	CBD-CGD-O2D-CED
20	8	604	CLA	CBD-CGD-O2D-CED
20	6	602	CLA	CBD-CGD-O2D-CED
27	4	606	CHL	CBD-CGD-O2D-CED
20	A	822	CLA	O1D-CGD-O2D-CED
20	A	806	CLA	C3-C5-C6-C7
20	A	807	CLA	C3-C5-C6-C7
20	A	808	CLA	C3-C5-C6-C7
20	A	816	CLA	C3-C5-C6-C7
20	A	818	CLA	C3-C5-C6-C7
20	A	819	CLA	C3-C5-C6-C7
20	A	825	CLA	C3-C5-C6-C7
20	A	826	CLA	C3-C5-C6-C7
20	A	833	CLA	C3-C5-C6-C7
20	A	840	CLA	C3-C5-C6-C7
20	A	843	CLA	C3-C5-C6-C7
20	A	854	CLA	C3-C5-C6-C7
20	B	802	CLA	C3-C5-C6-C7
20	B	806	CLA	C3-C5-C6-C7
20	B	808	CLA	C3-C5-C6-C7
20	B	809	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
20	B	812	CLA	C3-C5-C6-C7
20	B	815	CLA	C3-C5-C6-C7
20	B	818	CLA	C3-C5-C6-C7
20	B	822	CLA	C3-C5-C6-C7
20	B	823	CLA	C3-C5-C6-C7
20	B	833	CLA	C3-C5-C6-C7
20	F	301	CLA	C3-C5-C6-C7
20	1	603	CLA	C3-C5-C6-C7
20	1	611	CLA	C3-C5-C6-C7
20	3	620	CLA	C3-C5-C6-C7
20	7	604	CLA	C3-C5-C6-C7
20	7	620	CLA	C3-C5-C6-C7
20	8	613	CLA	C3-C5-C6-C7
20	Z	608	CLA	C3-C5-C6-C7
20	4	611	CLA	C3-C5-C6-C7
20	5	613	CLA	C3-C5-C6-C7
20	6	604	CLA	C3-C5-C6-C7
27	3	608	CHL	C3-C5-C6-C7
20	B	822	CLA	CBA-CGA-O2A-C1
20	B	833	CLA	CBA-CGA-O2A-C1
20	Z	611	CLA	CBA-CGA-O2A-C1
22	B	851	LHG	C8-C7-O7-C5
20	B	823	CLA	O1D-CGD-O2D-CED
20	4	603	CLA	O1D-CGD-O2D-CED
20	1	613	CLA	CBD-CGD-O2D-CED
20	B	840	CLA	C2C-C3C-CAC-CBC
20	B	834	CLA	O1A-CGA-O2A-C1
20	A	845	CLA	C3-C5-C6-C7
20	1	606	CLA	C3-C5-C6-C7
20	7	612	CLA	C3-C5-C6-C7
20	5	612	CLA	C3-C5-C6-C7
20	B	840	CLA	C4C-C3C-CAC-CBC
20	B	819	CLA	C4-C3-C5-C6
20	1	603	CLA	C4-C3-C5-C6
27	Z	601	CHL	C4-C3-C5-C6
20	A	831	CLA	C2-C3-C5-C6
20	B	818	CLA	C2-C3-C5-C6
20	B	819	CLA	C2-C3-C5-C6
20	B	823	CLA	C2-C3-C5-C6
20	1	603	CLA	C2-C3-C5-C6
20	Z	603	CLA	C2-C3-C5-C6
20	6	611	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
27	Z	601	CHL	C2-C3-C5-C6
20	B	808	CLA	CBD-CGD-O2D-CED
20	A	815	CLA	C2A-CAA-CBA-CGA
20	A	825	CLA	C2A-CAA-CBA-CGA
20	A	837	CLA	C2A-CAA-CBA-CGA
20	A	845	CLA	C2A-CAA-CBA-CGA
20	B	824	CLA	C2A-CAA-CBA-CGA
20	B	839	CLA	C2A-CAA-CBA-CGA
20	B	852	CLA	C2A-CAA-CBA-CGA
20	3	607	CLA	C2A-CAA-CBA-CGA
20	5	601	CLA	C2A-CAA-CBA-CGA
20	5	609	CLA	C2A-CAA-CBA-CGA
27	Z	607	CHL	C2A-CAA-CBA-CGA
27	4	608	CHL	C2A-CAA-CBA-CGA
27	5	608	CHL	C2A-CAA-CBA-CGA
20	Z	602	CLA	O1D-CGD-O2D-CED
20	A	804	CLA	C3-C5-C6-C7
20	B	807	CLA	C3-C5-C6-C7
20	B	817	CLA	C3-C5-C6-C7
20	B	820	CLA	C3-C5-C6-C7
20	3	607	CLA	C3-C5-C6-C7
20	8	601	CLA	C3-C5-C6-C7
20	Z	602	CLA	C3-C5-C6-C7
20	Z	611	CLA	C3-C5-C6-C7
20	5	611	CLA	C3-C5-C6-C7
20	6	602	CLA	C3-C5-C6-C7
20	A	805	CLA	CBA-CGA-O2A-C1
20	A	806	CLA	CBA-CGA-O2A-C1
20	A	812	CLA	CBA-CGA-O2A-C1
20	A	820	CLA	CBA-CGA-O2A-C1
20	A	824	CLA	CBA-CGA-O2A-C1
20	A	829	CLA	CBA-CGA-O2A-C1
20	A	845	CLA	CBA-CGA-O2A-C1
20	B	818	CLA	CBA-CGA-O2A-C1
20	F	304	CLA	CBA-CGA-O2A-C1
20	1	611	CLA	CBA-CGA-O2A-C1
20	5	601	CLA	CBA-CGA-O2A-C1
20	5	606	CLA	O1D-CGD-O2D-CED
20	A	812	CLA	O1A-CGA-O2A-C1
20	A	845	CLA	O1A-CGA-O2A-C1
20	B	818	CLA	O1A-CGA-O2A-C1
20	B	833	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	F	304	CLA	O1A-CGA-O2A-C1
20	1	602	CLA	O1D-CGD-O2D-CED
20	A	809	CLA	CBD-CGD-O2D-CED
20	B	802	CLA	CBD-CGD-O2D-CED
20	B	822	CLA	CBD-CGD-O2D-CED
20	1	614	CLA	CBD-CGD-O2D-CED
20	7	602	CLA	CBD-CGD-O2D-CED
20	7	606	CLA	CBD-CGD-O2D-CED
20	8	614	CLA	CBD-CGD-O2D-CED
20	6	613	CLA	CBD-CGD-O2D-CED
20	6	616	CLA	CBD-CGD-O2D-CED
27	6	618	CHL	CBD-CGD-O2D-CED
20	A	805	CLA	C3-C5-C6-C7
20	A	809	CLA	C3-C5-C6-C7
20	A	831	CLA	C3-C5-C6-C7
20	A	839	CLA	C3-C5-C6-C7
20	B	852	CLA	C3-C5-C6-C7
20	8	614	CLA	C3-C5-C6-C7
20	5	606	CLA	C3-C5-C6-C7
20	3	607	CLA	CBA-CGA-O2A-C1
20	7	620	CLA	CBA-CGA-O2A-C1
20	8	602	CLA	CBA-CGA-O2A-C1
20	5	602	CLA	CBA-CGA-O2A-C1
20	6	611	CLA	CBA-CGA-O2A-C1
20	A	805	CLA	O1A-CGA-O2A-C1
20	A	829	CLA	O1A-CGA-O2A-C1
20	3	607	CLA	O1A-CGA-O2A-C1
20	A	835	CLA	O1D-CGD-O2D-CED
20	A	818	CLA	CBD-CGD-O2D-CED
20	8	611	CLA	CBD-CGD-O2D-CED
20	Z	614	CLA	CBD-CGD-O2D-CED
20	4	611	CLA	CBD-CGD-O2D-CED
20	3	604	CLA	C3-C5-C6-C7
20	Z	613	CLA	C3-C5-C6-C7
20	B	834	CLA	CBA-CGA-O2A-C1
20	6	602	CLA	CBA-CGA-O2A-C1
20	A	820	CLA	O1A-CGA-O2A-C1
20	A	808	CLA	C4-C3-C5-C6
20	A	833	CLA	C4-C3-C5-C6
20	A	839	CLA	C4-C3-C5-C6
20	A	842	CLA	C4-C3-C5-C6
20	1	606	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
20	Z	602	CLA	C4-C3-C5-C6
20	4	611	CLA	C4-C3-C5-C6
20	5	611	CLA	C4-C3-C5-C6
27	6	607	CHL	C4-C3-C5-C6
20	A	808	CLA	C2-C3-C5-C6
20	A	833	CLA	C2-C3-C5-C6
20	A	839	CLA	C2-C3-C5-C6
20	A	842	CLA	C2-C3-C5-C6
20	A	843	CLA	C2-C3-C5-C6
20	1	606	CLA	C2-C3-C5-C6
20	Z	602	CLA	C2-C3-C5-C6
20	4	611	CLA	C2-C3-C5-C6
20	5	611	CLA	C2-C3-C5-C6
27	6	607	CHL	C2-C3-C5-C6
20	B	840	CLA	CBD-CGD-O2D-CED
20	B	827	CLA	C2A-CAA-CBA-CGA
20	B	831	CLA	C2A-CAA-CBA-CGA
27	1	607	CHL	C2A-CAA-CBA-CGA
20	A	824	CLA	O1A-CGA-O2A-C1
20	7	620	CLA	O1A-CGA-O2A-C1
20	8	602	CLA	O1A-CGA-O2A-C1
20	8	612	CLA	O1A-CGA-O2A-C1
20	5	602	CLA	O1A-CGA-O2A-C1
20	6	611	CLA	O1A-CGA-O2A-C1
20	A	807	CLA	CBA-CGA-O2A-C1
20	8	612	CLA	CBA-CGA-O2A-C1
20	A	836	CLA	CBD-CGD-O2D-CED
20	Z	609	CLA	CBD-CGD-O2D-CED
20	4	613	CLA	O1D-CGD-O2D-CED
20	A	825	CLA	O1D-CGD-O2D-CED
20	Z	608	CLA	O1D-CGD-O2D-CED
20	6	602	CLA	O1A-CGA-O2A-C1
20	A	817	CLA	C3-C5-C6-C7
20	A	809	CLA	CBA-CGA-O2A-C1
20	A	814	CLA	CBA-CGA-O2A-C1
20	A	815	CLA	CBA-CGA-O2A-C1
20	A	818	CLA	CBA-CGA-O2A-C1
20	A	842	CLA	CBA-CGA-O2A-C1
20	A	843	CLA	CBA-CGA-O2A-C1
20	B	810	CLA	CBA-CGA-O2A-C1
20	B	814	CLA	CBA-CGA-O2A-C1
20	B	820	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	B	825	CLA	CBA-CGA-O2A-C1
20	B	829	CLA	CBA-CGA-O2A-C1
20	1	602	CLA	CBA-CGA-O2A-C1
20	1	604	CLA	CBA-CGA-O2A-C1
20	3	602	CLA	CBA-CGA-O2A-C1
20	3	620	CLA	CBA-CGA-O2A-C1
20	7	602	CLA	CBA-CGA-O2A-C1
20	7	604	CLA	CBA-CGA-O2A-C1
20	Z	602	CLA	CBA-CGA-O2A-C1
20	4	602	CLA	CBA-CGA-O2A-C1
20	4	611	CLA	CBA-CGA-O2A-C1
20	5	611	CLA	CBA-CGA-O2A-C1
20	6	609	CLA	CBA-CGA-O2A-C1
27	5	607	CHL	CBA-CGA-O2A-C1
27	6	607	CHL	CBA-CGA-O2A-C1
20	B	834	CLA	CBD-CGD-O2D-CED
22	Z	620	LHG	C7-C8-C9-C10
22	5	623	LHG	C23-C24-C25-C26
20	A	843	CLA	O1A-CGA-O2A-C1
20	Z	611	CLA	O1D-CGD-O2D-CED
20	4	601	CLA	C10-C11-C12-C13
22	4	623	LHG	O2-C2-C3-O3
20	Z	606	CLA	C3-C5-C6-C7
20	4	612	CLA	C3-C5-C6-C7
22	6	619	LHG	O7-C5-C6-O8
20	Z	604	CLA	CBA-CGA-O2A-C1
20	B	825	CLA	O1A-CGA-O2A-C1
20	4	602	CLA	O1A-CGA-O2A-C1
20	5	611	CLA	O1A-CGA-O2A-C1
20	4	612	CLA	C4-C3-C5-C6
20	A	812	CLA	C14-C13-C15-C16
20	A	819	CLA	C11-C10-C8-C9
20	A	822	CLA	C11-C10-C8-C9
20	A	827	CLA	C6-C7-C8-C9
20	A	843	CLA	C14-C13-C15-C16
20	1	602	CLA	C6-C7-C8-C9
20	3	610	CLA	C14-C13-C15-C16
20	7	601	CLA	C11-C12-C13-C14
20	Z	610	CLA	C6-C7-C8-C9
21	A	844	PQN	C24-C23-C25-C26
20	7	620	CLA	C5-C6-C7-C8
20	6	601	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
20	A	812	CLA	C2A-CAA-CBA-CGA
20	A	854	CLA	C2A-CAA-CBA-CGA
23	A	852	BCR	C7-C8-C9-C34
23	K	4004	BCR	C37-C22-C23-C24
23	3	719	BCR	C7-C8-C9-C34
23	3	719	BCR	C37-C22-C23-C24
23	7	623	BCR	C36-C18-C19-C20
28	6	621	LUT	C11-C12-C13-C20
23	7	623	BCR	C17-C18-C19-C20
22	1	620	LHG	C7-C8-C9-C10
22	6	619	LHG	C23-C24-C25-C26
26	J	3001	LMG	C28-C29-C30-C31
20	3	620	CLA	O1A-CGA-O2A-C1
20	7	604	CLA	O1A-CGA-O2A-C1
20	Z	602	CLA	O1A-CGA-O2A-C1
27	6	607	CHL	O1A-CGA-O2A-C1
20	B	807	CLA	C10-C11-C12-C13
20	8	601	CLA	C13-C15-C16-C17
21	B	842	PQN	C20-C21-C22-C23
20	B	836	CLA	C3-C5-C6-C7
20	B	840	CLA	C3-C5-C6-C7
20	3	603	CLA	C3-C5-C6-C7
20	8	602	CLA	C13-C15-C16-C17
20	7	612	CLA	CBA-CGA-O2A-C1
27	Z	601	CHL	CBA-CGA-O2A-C1
20	A	826	CLA	C10-C11-C12-C13
20	7	602	CLA	C15-C16-C17-C18
20	Z	611	CLA	C5-C6-C7-C8
20	A	837	CLA	O1D-CGD-O2D-CED
20	A	841	CLA	O1D-CGD-O2D-CED
20	K	4002	CLA	CBD-CGD-O2D-CED
20	A	808	CLA	C10-C11-C12-C13
20	A	814	CLA	C8-C10-C11-C12
20	A	814	CLA	C10-C11-C12-C13
20	A	829	CLA	C10-C11-C12-C13
20	B	818	CLA	C8-C10-C11-C12
20	B	827	CLA	C8-C10-C11-C12
20	B	829	CLA	C10-C11-C12-C13
20	B	837	CLA	C8-C10-C11-C12
20	6	610	CLA	C5-C6-C7-C8
20	A	809	CLA	O1A-CGA-O2A-C1
22	A	847	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
22	4	622	LHG	C23-C24-C25-C26
20	B	832	CLA	CBD-CGD-O2D-CED
20	4	602	CLA	O1D-CGD-O2D-CED
20	A	826	CLA	C13-C15-C16-C17
20	B	812	CLA	C10-C11-C12-C13
20	B	825	CLA	C13-C15-C16-C17
20	B	839	CLA	C15-C16-C17-C18
20	B	841	CLA	C10-C11-C12-C13
20	7	613	CLA	C5-C6-C7-C8
20	A	806	CLA	C2-C1-O2A-CGA
20	1	611	CLA	C8-C10-C11-C12
20	3	603	CLA	C13-C15-C16-C17
20	6	601	CLA	C10-C11-C12-C13
20	6	612	CLA	C3-C5-C6-C7
20	A	834	CLA	C5-C6-C7-C8
20	A	841	CLA	C11-C10-C8-C7
20	B	839	CLA	C6-C7-C8-C10
20	6	601	CLA	C11-C10-C8-C7
20	A	822	CLA	C3-C5-C6-C7
20	3	610	CLA	C3-C5-C6-C7
27	8	607	CHL	C3-C5-C6-C7
27	6	606	CHL	C3-C5-C6-C7
20	A	818	CLA	O1A-CGA-O2A-C1
20	B	810	CLA	O1A-CGA-O2A-C1
20	B	814	CLA	O1A-CGA-O2A-C1
20	B	820	CLA	O1A-CGA-O2A-C1
20	B	829	CLA	O1A-CGA-O2A-C1
20	1	604	CLA	O1A-CGA-O2A-C1
20	7	602	CLA	O1A-CGA-O2A-C1
20	7	612	CLA	O1A-CGA-O2A-C1
20	Z	604	CLA	O1A-CGA-O2A-C1
20	4	611	CLA	O1A-CGA-O2A-C1
20	6	609	CLA	O1A-CGA-O2A-C1
27	5	607	CHL	O1A-CGA-O2A-C1
20	A	814	CLA	C2A-CAA-CBA-CGA
20	B	804	CLA	C2A-CAA-CBA-CGA
20	B	810	CLA	O1D-CGD-O2D-CED
27	4	607	CHL	O1D-CGD-O2D-CED
20	B	802	CLA	C15-C16-C17-C18
20	B	834	CLA	C5-C6-C7-C8
20	6	602	CLA	C8-C10-C11-C12
20	6	604	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
20	1	602	CLA	O1A-CGA-O2A-C1
20	A	831	CLA	C8-C10-C11-C12
20	A	839	CLA	C13-C15-C16-C17
27	4	606	CHL	O1D-CGD-O2D-CED
20	B	805	CLA	C10-C11-C12-C13
20	Z	613	CLA	C5-C6-C7-C8
20	A	807	CLA	O1A-CGA-O2A-C1
20	A	814	CLA	O1A-CGA-O2A-C1
20	A	815	CLA	O1A-CGA-O2A-C1
20	A	842	CLA	O1A-CGA-O2A-C1
22	A	846	LHG	C23-C24-C25-C26
20	B	803	CLA	C10-C11-C12-C13
20	B	832	CLA	C13-C15-C16-C17
20	8	610	CLA	C10-C11-C12-C13
20	Z	602	CLA	C5-C6-C7-C8
27	3	608	CHL	C8-C10-C11-C12
20	A	811	CLA	O1D-CGD-O2D-CED
27	Z	601	CHL	O1A-CGA-O2A-C1
20	A	830	CLA	C13-C15-C16-C17
20	B	803	CLA	C8-C10-C11-C12
20	6	601	CLA	C8-C10-C11-C12
22	A	847	LHG	C4-O6-P-O3
22	A	855	LHG	C4-O6-P-O3
22	B	851	LHG	C3-O3-P-O6
22	7	625	LHG	C4-O6-P-O3
22	8	620	LHG	C3-O3-P-O6
22	8	620	LHG	C4-O6-P-O3
22	4	622	LHG	C3-O3-P-O6
22	4	623	LHG	C3-O3-P-O6
20	B	810	CLA	C3-C5-C6-C7
20	1	609	CLA	C3-C5-C6-C7
20	1	614	CLA	C3-C5-C6-C7
20	B	819	CLA	CBA-CGA-O2A-C1
20	B	810	CLA	C5-C6-C7-C8
27	3	608	CHL	C10-C11-C12-C13
20	B	811	CLA	C4-C3-C5-C6
20	B	819	CLA	C8-C10-C11-C12
20	A	803	CLA	C2A-CAA-CBA-CGA
20	A	809	CLA	C2A-CAA-CBA-CGA
20	A	834	CLA	C2A-CAA-CBA-CGA
20	8	602	CLA	C2A-CAA-CBA-CGA
20	Z	602	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
20	4	602	CLA	C2A-CAA-CBA-CGA
20	5	602	CLA	C2A-CAA-CBA-CGA
20	6	602	CLA	C2A-CAA-CBA-CGA
20	A	822	CLA	CBA-CGA-O2A-C1
20	B	811	CLA	CBA-CGA-O2A-C1
20	B	812	CLA	CBA-CGA-O2A-C1
20	B	813	CLA	CBA-CGA-O2A-C1
20	Z	613	CLA	C10-C11-C12-C13
20	6	602	CLA	C10-C11-C12-C13
23	B	801	BCR	C15-C16-C17-C18
23	7	623	BCR	C19-C20-C21-C22
20	Z	604	CLA	C5-C6-C7-C8
20	A	802	CLA	C3-C5-C6-C7
20	3	613	CLA	C3-C5-C6-C7
22	6	619	LHG	C27-C28-C29-C30
26	J	3001	LMG	C12-C13-C14-C15
20	3	613	CLA	O1D-CGD-O2D-CED
20	8	604	CLA	O1D-CGD-O2D-CED
20	6	602	CLA	O1D-CGD-O2D-CED
27	6	606	CHL	C6-C7-C8-C9
20	A	811	CLA	CBA-CGA-O2A-C1
20	A	825	CLA	CBA-CGA-O2A-C1
22	6	619	LHG	C14-C15-C16-C17
20	B	808	CLA	O1D-CGD-O2D-CED
20	F	301	CLA	C8-C10-C11-C12
20	A	823	CLA	CBD-CGD-O2D-CED
22	7	625	LHG	C25-C26-C27-C28
22	4	622	LHG	C12-C13-C14-C15
20	A	842	CLA	C5-C6-C7-C8
20	Z	608	CLA	C8-C10-C11-C12
25	B	850	DGD	C3B-C4B-C5B-C6B
20	B	824	CLA	C3-C5-C6-C7
25	B	850	DGD	C1B-C2B-C3B-C4B
22	6	619	LHG	C11-C10-C9-C8
22	6	619	LHG	C9-C10-C11-C12
22	6	619	LHG	C15-C16-C17-C18
20	A	831	CLA	C10-C11-C12-C13
20	B	812	CLA	C5-C6-C7-C8
20	3	613	CLA	C6-C7-C8-C9
27	3	608	CHL	C16-C17-C18-C19
20	3	607	CLA	C4-C3-C5-C6
20	4	613	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
20	4	613	CLA	C2-C3-C5-C6
20	A	829	CLA	C11-C10-C8-C9
20	B	815	CLA	C11-C10-C8-C9
20	1	610	CLA	C6-C7-C8-C9
20	3	607	CLA	C6-C7-C8-C9
22	Z	620	LHG	C23-C24-C25-C26
22	A	846	LHG	C28-C29-C30-C31
27	3	608	CHL	C5-C6-C7-C8
20	A	830	CLA	C2A-CAA-CBA-CGA
20	B	803	CLA	C2A-CAA-CBA-CGA
20	7	602	CLA	C2A-CAA-CBA-CGA
20	3	602	CLA	O1A-CGA-O2A-C1
23	L	205	BCR	C37-C22-C23-C24
22	7	625	LHG	C10-C11-C12-C13
23	J	3003	BCR	C7-C8-C9-C10
23	L	205	BCR	C21-C22-C23-C24
23	6	623	BCR	C7-C8-C9-C10
20	A	841	CLA	C8-C10-C11-C12
20	A	824	CLA	CBD-CGD-O2D-CED
20	1	613	CLA	O1D-CGD-O2D-CED
22	4	622	LHG	C10-C11-C12-C13
26	J	3001	LMG	C30-C31-C32-C33
20	B	811	CLA	O1A-CGA-O2A-C1
20	A	814	CLA	C16-C17-C18-C20
27	3	608	CHL	C16-C17-C18-C20
20	A	807	CLA	C5-C6-C7-C8
20	5	601	CLA	C13-C15-C16-C17
20	A	810	CLA	CBD-CGD-O2D-CED
20	A	826	CLA	CBD-CGD-O2D-CED
20	A	845	CLA	CBD-CGD-O2D-CED
20	B	841	CLA	CBD-CGD-O2D-CED
20	5	614	CLA	CBD-CGD-O2D-CED
27	6	618	CHL	O1D-CGD-O2D-CED
22	1	620	LHG	C24-C25-C26-C27
20	B	818	CLA	C5-C6-C7-C8
20	B	826	CLA	C10-C11-C12-C13
20	B	819	CLA	O1A-CGA-O2A-C1
20	1	614	CLA	CBA-CGA-O2A-C1
20	A	803	CLA	C3A-C2A-CAA-CBA
20	A	804	CLA	C3A-C2A-CAA-CBA
20	A	807	CLA	C3A-C2A-CAA-CBA
20	A	829	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	A	834	CLA	C3A-C2A-CAA-CBA
20	B	824	CLA	C3A-C2A-CAA-CBA
20	B	826	CLA	C3A-C2A-CAA-CBA
20	1	612	CLA	C3A-C2A-CAA-CBA
20	3	617	CLA	C3A-C2A-CAA-CBA
20	Z	612	CLA	C3A-C2A-CAA-CBA
20	5	601	CLA	C3A-C2A-CAA-CBA
27	6	607	CHL	C3A-C2A-CAA-CBA
20	Z	610	CLA	C5-C6-C7-C8
20	4	610	CLA	C5-C6-C7-C8
20	B	812	CLA	O1A-CGA-O2A-C1
20	A	814	CLA	C16-C17-C18-C19
20	3	613	CLA	C6-C7-C8-C10
27	6	606	CHL	C6-C7-C8-C10
20	A	820	CLA	C13-C15-C16-C17
20	A	834	CLA	C3-C5-C6-C7
20	6	611	CLA	C3-C5-C6-C7
20	A	825	CLA	O1A-CGA-O2A-C1
20	B	807	CLA	C4-C3-C5-C6
20	B	816	CLA	C4-C3-C5-C6
20	A	819	CLA	CBA-CGA-O2A-C1
20	B	831	CLA	CBA-CGA-O2A-C1
20	B	852	CLA	CBA-CGA-O2A-C1
20	B	807	CLA	C2-C3-C5-C6
22	A	847	LHG	C8-C7-O7-C5
22	4	623	LHG	C23-C24-C25-C26
20	6	616	CLA	O1D-CGD-O2D-CED
20	A	822	CLA	O1A-CGA-O2A-C1
22	Z	620	LHG	O2-C2-C3-O3
20	1	613	CLA	C10-C11-C12-C13
20	3	607	CLA	C8-C10-C11-C12
20	A	814	CLA	C3-C5-C6-C7
20	A	811	CLA	O1A-CGA-O2A-C1
20	B	813	CLA	O1A-CGA-O2A-C1
20	7	601	CLA	C8-C10-C11-C12
22	A	847	LHG	O9-C7-O7-C5
20	A	829	CLA	C2-C1-O2A-CGA
20	A	845	CLA	C2-C1-O2A-CGA
20	B	833	CLA	C2-C1-O2A-CGA
20	B	834	CLA	C2-C1-O2A-CGA
20	8	614	CLA	O1D-CGD-O2D-CED
23	A	848	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	A	848	BCR	C5-C6-C7-C8
23	A	850	BCR	C23-C24-C25-C26
23	A	856	BCR	C1-C6-C7-C8
23	A	856	BCR	C5-C6-C7-C8
23	A	856	BCR	C23-C24-C25-C26
23	A	856	BCR	C23-C24-C25-C30
23	B	844	BCR	C1-C6-C7-C8
23	B	844	BCR	C5-C6-C7-C8
23	B	846	BCR	C5-C6-C7-C8
23	B	847	BCR	C5-C6-C7-C8
23	B	848	BCR	C5-C6-C7-C8
23	G	205	BCR	C5-C6-C7-C8
23	I	172	BCR	C5-C6-C7-C8
23	J	3003	BCR	C23-C24-C25-C26
23	J	3003	BCR	C23-C24-C25-C30
23	K	4004	BCR	C23-C24-C25-C26
23	L	201	BCR	C1-C6-C7-C8
23	L	201	BCR	C5-C6-C7-C8
23	L	201	BCR	C23-C24-C25-C26
23	L	205	BCR	C23-C24-C25-C26
23	L	205	BCR	C23-C24-C25-C30
23	3	717	BCR	C23-C24-C25-C26
23	3	717	BCR	C23-C24-C25-C30
23	3	719	BCR	C5-C6-C7-C8
23	7	623	BCR	C1-C6-C7-C8
23	7	623	BCR	C5-C6-C7-C8
23	7	623	BCR	C23-C24-C25-C30
23	7	624	BCR	C1-C6-C7-C8
23	7	624	BCR	C5-C6-C7-C8
23	7	624	BCR	C23-C24-C25-C26
23	8	619	BCR	C1-C6-C7-C8
23	8	619	BCR	C5-C6-C7-C8
23	8	619	BCR	C23-C24-C25-C26
23	8	619	BCR	C23-C24-C25-C30
23	4	621	BCR	C23-C24-C25-C26
23	5	622	BCR	C1-C6-C7-C8
23	5	622	BCR	C5-C6-C7-C8
23	5	622	BCR	C23-C24-C25-C26
23	5	622	BCR	C23-C24-C25-C30
23	5	625	BCR	C1-C6-C7-C8
23	5	625	BCR	C5-C6-C7-C8
23	5	625	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
23	5	625	BCR	C23-C24-C25-C30
23	6	623	BCR	C1-C6-C7-C8
23	6	623	BCR	C5-C6-C7-C8
23	6	623	BCR	C23-C24-C25-C26
23	6	623	BCR	C23-C24-C25-C30
23	6	625	BCR	C1-C6-C7-C8
23	6	625	BCR	C5-C6-C7-C8
27	6	607	CHL	C3-C5-C6-C7
28	1	617	LUT	C1-C6-C7-C8
28	1	617	LUT	C5-C6-C7-C8
28	1	619	LUT	C5-C6-C7-C8
28	3	621	LUT	C1-C6-C7-C8
28	3	621	LUT	C5-C6-C7-C8
28	3	622	LUT	C1-C6-C7-C8
28	3	622	LUT	C5-C6-C7-C8
28	8	617	LUT	C1-C6-C7-C8
28	8	617	LUT	C5-C6-C7-C8
28	Z	619	LUT	C5-C6-C7-C8
28	4	619	LUT	C5-C6-C7-C8
28	4	620	LUT	C1-C6-C7-C8
28	4	620	LUT	C5-C6-C7-C8
28	6	621	LUT	C1-C6-C7-C8
28	6	621	LUT	C5-C6-C7-C8
27	8	607	CHL	CBA-CGA-O2A-C1
20	A	833	CLA	C10-C11-C12-C13
20	B	817	CLA	C5-C6-C7-C8
20	B	834	CLA	C10-C11-C12-C13
20	B	852	CLA	C10-C11-C12-C13
20	1	613	CLA	C5-C6-C7-C8
20	3	603	CLA	C5-C6-C7-C8
22	A	855	LHG	C8-C7-O7-C5
20	A	829	CLA	C13-C15-C16-C17
20	8	613	CLA	C5-C6-C7-C8
20	8	613	CLA	C15-C16-C17-C18
25	B	850	DGD	C7B-C8B-C9B-CAB
20	B	806	CLA	C4-C3-C5-C6
20	3	613	CLA	C4-C3-C5-C6
20	5	610	CLA	C4-C3-C5-C6
20	6	612	CLA	C4-C3-C5-C6
20	A	808	CLA	C11-C12-C13-C15
20	A	808	CLA	C12-C13-C15-C16
20	A	809	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
20	A	812	CLA	C12-C13-C15-C16
20	A	822	CLA	C2-C3-C5-C6
20	A	829	CLA	C6-C7-C8-C10
20	A	829	CLA	C11-C10-C8-C7
20	B	806	CLA	C2-C3-C5-C6
20	B	815	CLA	C11-C10-C8-C7
20	B	825	CLA	C6-C7-C8-C10
20	B	826	CLA	C11-C10-C8-C7
20	B	832	CLA	C2-C3-C5-C6
20	1	602	CLA	C6-C7-C8-C10
20	3	607	CLA	C2-C3-C5-C6
20	3	613	CLA	C2-C3-C5-C6
20	6	604	CLA	C6-C7-C8-C10
21	A	844	PQN	C22-C23-C25-C26
27	3	608	CHL	C11-C10-C8-C7
20	B	831	CLA	O1A-CGA-O2A-C1
20	B	852	CLA	O1A-CGA-O2A-C1
20	1	614	CLA	O1A-CGA-O2A-C1
20	A	818	CLA	C10-C11-C12-C13
20	B	806	CLA	C8-C10-C11-C12
20	B	827	CLA	C10-C11-C12-C13
20	Z	611	CLA	C10-C11-C12-C13
20	A	823	CLA	CBA-CGA-O2A-C1
20	A	839	CLA	CBA-CGA-O2A-C1
20	B	805	CLA	CBA-CGA-O2A-C1
20	B	828	CLA	CBA-CGA-O2A-C1
20	L	203	CLA	CBA-CGA-O2A-C1
20	3	613	CLA	CBA-CGA-O2A-C1
20	8	601	CLA	CBA-CGA-O2A-C1
20	Z	614	CLA	CBA-CGA-O2A-C1
20	4	604	CLA	CBA-CGA-O2A-C1
27	7	607	CHL	CBA-CGA-O2A-C1
20	1	602	CLA	C2A-CAA-CBA-CGA
20	3	602	CLA	C2A-CAA-CBA-CGA
20	5	610	CLA	C2A-CAA-CBA-CGA
20	A	840	CLA	C10-C11-C12-C13
20	3	607	CLA	C10-C11-C12-C13
20	7	620	CLA	C10-C11-C12-C13
20	6	613	CLA	O1D-CGD-O2D-CED
20	A	841	CLA	C15-C16-C17-C18
20	B	810	CLA	C10-C11-C12-C13
20	B	813	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
20	5	610	CLA	C5-C6-C7-C8
20	7	606	CLA	O1D-CGD-O2D-CED
22	A	847	LHG	O6-C4-C5-O7
20	A	806	CLA	C8-C10-C11-C12
20	B	823	CLA	C10-C11-C12-C13
20	1	608	CLA	C5-C6-C7-C8
20	Z	608	CLA	C15-C16-C17-C18
27	6	606	CHL	C5-C6-C7-C8
20	B	821	CLA	CBD-CGD-O2D-CED
20	3	617	CLA	CBD-CGD-O2D-CED
20	Z	613	CLA	CBD-CGD-O2D-CED
22	4	622	LHG	C13-C14-C15-C16
22	A	855	LHG	O9-C7-O7-C5
20	A	809	CLA	O1D-CGD-O2D-CED
26	J	3001	LMG	O6-C5-C6-O5
20	B	822	CLA	O1D-CGD-O2D-CED
20	A	822	CLA	C4-C3-C5-C6
20	B	832	CLA	C4-C3-C5-C6
20	B	811	CLA	C2-C3-C5-C6
20	B	816	CLA	C2-C3-C5-C6
20	4	612	CLA	C2-C3-C5-C6
20	A	808	CLA	C11-C12-C13-C14
20	A	808	CLA	C14-C13-C15-C16
20	A	809	CLA	C14-C13-C15-C16
20	A	829	CLA	C6-C7-C8-C9
20	A	829	CLA	C14-C13-C15-C16
20	A	841	CLA	C11-C10-C8-C9
20	B	825	CLA	C6-C7-C8-C9
20	B	826	CLA	C11-C10-C8-C9
20	B	839	CLA	C6-C7-C8-C9
20	5	602	CLA	C11-C10-C8-C9
20	6	601	CLA	C11-C10-C8-C9
20	6	604	CLA	C6-C7-C8-C9
27	3	608	CHL	C11-C10-C8-C9
20	A	818	CLA	O1D-CGD-O2D-CED
20	A	836	CLA	O1D-CGD-O2D-CED
20	B	834	CLA	C3-C5-C6-C7
20	A	819	CLA	C2A-CAA-CBA-CGA
20	B	817	CLA	C2A-CAA-CBA-CGA
20	1	604	CLA	C2A-CAA-CBA-CGA
20	5	621	CLA	C2A-CAA-CBA-CGA
20	6	610	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	B	850	DGD	O6E-C5E-C6E-O5E
23	A	856	BCR	C11-C12-C13-C35
23	B	801	BCR	C37-C22-C23-C24
23	B	847	BCR	C37-C22-C23-C24
28	8	618	LUT	C11-C12-C13-C20
20	A	819	CLA	O1A-CGA-O2A-C1
20	B	805	CLA	O1A-CGA-O2A-C1
27	8	607	CHL	O1A-CGA-O2A-C1
20	B	802	CLA	O1D-CGD-O2D-CED
20	A	804	CLA	C1A-C2A-CAA-CBA
20	A	809	CLA	C1A-C2A-CAA-CBA
20	A	810	CLA	C1A-C2A-CAA-CBA
20	A	811	CLA	C1A-C2A-CAA-CBA
20	A	821	CLA	C1A-C2A-CAA-CBA
20	A	824	CLA	C1A-C2A-CAA-CBA
20	A	825	CLA	C1A-C2A-CAA-CBA
20	A	834	CLA	C1A-C2A-CAA-CBA
20	A	835	CLA	C1A-C2A-CAA-CBA
20	B	804	CLA	C1A-C2A-CAA-CBA
20	B	811	CLA	C1A-C2A-CAA-CBA
20	B	815	CLA	C1A-C2A-CAA-CBA
20	B	820	CLA	C1A-C2A-CAA-CBA
20	B	821	CLA	C1A-C2A-CAA-CBA
20	B	822	CLA	C1A-C2A-CAA-CBA
20	B	824	CLA	C1A-C2A-CAA-CBA
20	B	832	CLA	C1A-C2A-CAA-CBA
20	B	838	CLA	C1A-C2A-CAA-CBA
20	B	852	CLA	C1A-C2A-CAA-CBA
20	F	304	CLA	C1A-C2A-CAA-CBA
20	L	203	CLA	C1A-C2A-CAA-CBA
20	1	602	CLA	C1A-C2A-CAA-CBA
20	1	610	CLA	C1A-C2A-CAA-CBA
20	1	611	CLA	C1A-C2A-CAA-CBA
20	1	612	CLA	C1A-C2A-CAA-CBA
20	1	614	CLA	C1A-C2A-CAA-CBA
20	3	602	CLA	C1A-C2A-CAA-CBA
20	3	604	CLA	C1A-C2A-CAA-CBA
20	3	610	CLA	C1A-C2A-CAA-CBA
20	3	617	CLA	C1A-C2A-CAA-CBA
20	7	604	CLA	C1A-C2A-CAA-CBA
20	7	610	CLA	C1A-C2A-CAA-CBA
20	7	614	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	8	604	CLA	C1A-C2A-CAA-CBA
20	8	610	CLA	C1A-C2A-CAA-CBA
20	8	614	CLA	C1A-C2A-CAA-CBA
20	Z	611	CLA	C1A-C2A-CAA-CBA
20	Z	612	CLA	C1A-C2A-CAA-CBA
20	4	602	CLA	C1A-C2A-CAA-CBA
20	4	610	CLA	C1A-C2A-CAA-CBA
20	4	611	CLA	C1A-C2A-CAA-CBA
20	5	601	CLA	C1A-C2A-CAA-CBA
20	5	610	CLA	C1A-C2A-CAA-CBA
20	5	611	CLA	C1A-C2A-CAA-CBA
20	5	616	CLA	C1A-C2A-CAA-CBA
20	6	610	CLA	C1A-C2A-CAA-CBA
20	6	611	CLA	C1A-C2A-CAA-CBA
20	6	614	CLA	C1A-C2A-CAA-CBA
27	7	607	CHL	C1A-C2A-CAA-CBA
27	Z	607	CHL	C1A-C2A-CAA-CBA
20	A	833	CLA	C8-C10-C11-C12
20	A	843	CLA	C13-C15-C16-C17
20	B	813	CLA	C15-C16-C17-C18
20	B	824	CLA	C13-C15-C16-C17
20	6	610	CLA	C10-C11-C12-C13
22	B	851	LHG	C4-O6-P-O3
22	6	619	LHG	C3-O3-P-O6
22	6	619	LHG	C4-O6-P-O3
20	Z	614	CLA	C3-C5-C6-C7
20	A	830	CLA	C5-C6-C7-C8
20	5	610	CLA	C10-C11-C12-C13
20	A	817	CLA	CBA-CGA-O2A-C1
20	B	827	CLA	CBA-CGA-O2A-C1
20	6	612	CLA	CBA-CGA-O2A-C1
22	5	623	LHG	O6-C4-C5-C6
20	B	832	CLA	O1D-CGD-O2D-CED
20	7	602	CLA	O1D-CGD-O2D-CED
22	8	620	LHG	C23-C24-C25-C26
20	B	834	CLA	O1D-CGD-O2D-CED
20	1	614	CLA	O1D-CGD-O2D-CED
20	4	604	CLA	O1A-CGA-O2A-C1
20	Z	614	CLA	O1D-CGD-O2D-CED
22	Z	620	LHG	C28-C29-C30-C31
20	B	827	CLA	C13-C15-C16-C17
20	3	604	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
20	7	601	CLA	C15-C16-C17-C18
20	1	608	CLA	CBA-CGA-O2A-C1
22	8	620	LHG	C24-C23-O8-C6
19	A	801	CL0	C15-C16-C17-C18
20	3	603	CLA	C10-C11-C12-C13
20	8	601	CLA	O1A-CGA-O2A-C1
27	7	607	CHL	O1A-CGA-O2A-C1
20	B	835	CLA	C2A-CAA-CBA-CGA
20	5	616	CLA	C2A-CAA-CBA-CGA
20	B	840	CLA	O1D-CGD-O2D-CED
20	B	819	CLA	C3-C5-C6-C7
22	6	619	LHG	C4-C5-C6-O8
26	J	3001	LMG	O1-C7-C8-C9
20	A	809	CLA	C13-C15-C16-C17
20	Z	608	CLA	C5-C6-C7-C8
27	3	608	CHL	C15-C16-C17-C18
20	3	613	CLA	O1A-CGA-O2A-C1
20	6	612	CLA	O1A-CGA-O2A-C1
20	6	611	CLA	C5-C6-C7-C8
22	A	846	LHG	C34-C35-C36-C37
20	L	203	CLA	O1A-CGA-O2A-C1
20	B	802	CLA	C10-C11-C12-C13
20	A	817	CLA	O1A-CGA-O2A-C1
20	A	843	CLA	C15-C16-C17-C18
20	A	826	CLA	C4-C3-C5-C6
20	A	829	CLA	C4-C3-C5-C6
20	B	808	CLA	C4-C3-C5-C6
20	1	608	CLA	C4-C3-C5-C6
20	Z	608	CLA	C4-C3-C5-C6
20	Z	614	CLA	C4-C3-C5-C6
20	6	613	CLA	C4-C3-C5-C6
20	5	613	CLA	C2-C3-C5-C6
20	A	826	CLA	CBA-CGA-O2A-C1
20	A	830	CLA	CBA-CGA-O2A-C1
20	B	836	CLA	CBA-CGA-O2A-C1
20	5	610	CLA	CBA-CGA-O2A-C1
20	B	817	CLA	C11-C12-C13-C14
20	5	602	CLA	CBD-CGD-O2D-CED
27	4	618	CHL	CBD-CGD-O2D-CED
20	A	835	CLA	C5-C6-C7-C8
20	B	816	CLA	C5-C6-C7-C8
25	B	850	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
20	A	810	CLA	C2A-CAA-CBA-CGA
20	6	601	CLA	C2A-CAA-CBA-CGA
20	3	610	CLA	C13-C15-C16-C17
20	A	840	CLA	C2-C1-O2A-CGA
20	B	831	CLA	C2-C1-O2A-CGA
20	3	613	CLA	C2-C1-O2A-CGA
20	Z	604	CLA	C2-C1-O2A-CGA
20	Z	608	CLA	C2-C1-O2A-CGA
20	A	807	CLA	C8-C10-C11-C12
20	A	823	CLA	O1A-CGA-O2A-C1
20	Z	614	CLA	O1A-CGA-O2A-C1
20	A	816	CLA	C5-C6-C7-C8
20	B	828	CLA	O1A-CGA-O2A-C1
25	B	850	DGD	C3A-C4A-C5A-C6A
20	1	612	CLA	C3-C5-C6-C7
20	Z	612	CLA	C3-C5-C6-C7
20	A	822	CLA	C10-C11-C12-C13
21	A	844	PQN	C23-C25-C26-C27
20	B	836	CLA	O1A-CGA-O2A-C1
20	1	608	CLA	O1A-CGA-O2A-C1
20	A	845	CLA	C4-C3-C5-C6
20	B	841	CLA	C4-C3-C5-C6
20	5	613	CLA	C4-C3-C5-C6
20	A	820	CLA	C11-C12-C13-C15
20	A	827	CLA	C6-C7-C8-C10
20	A	829	CLA	C2-C3-C5-C6
20	A	829	CLA	C12-C13-C15-C16
20	A	835	CLA	C6-C7-C8-C10
20	A	842	CLA	C6-C7-C8-C10
20	A	854	CLA	C12-C13-C15-C16
20	B	806	CLA	C11-C12-C13-C15
20	B	808	CLA	C2-C3-C5-C6
20	B	812	CLA	C6-C7-C8-C10
20	B	813	CLA	C11-C10-C8-C7
20	1	608	CLA	C2-C3-C5-C6
20	3	607	CLA	C6-C7-C8-C10
20	3	610	CLA	C12-C13-C15-C16
20	Z	610	CLA	C6-C7-C8-C10
20	Z	610	CLA	C11-C10-C8-C7
20	Z	614	CLA	C2-C3-C5-C6
20	5	602	CLA	C11-C10-C8-C7
20	5	602	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
20	6	602	CLA	C6-C7-C8-C10
20	6	602	CLA	C11-C10-C8-C7
20	6	613	CLA	C2-C3-C5-C6
21	A	844	PQN	C17-C18-C20-C21
20	B	806	CLA	C11-C12-C13-C14
20	B	813	CLA	C11-C10-C8-C9
20	B	827	CLA	C11-C10-C8-C9
20	B	834	CLA	C11-C10-C8-C9
20	B	840	CLA	C14-C13-C15-C16
20	1	610	CLA	C11-C10-C8-C9
20	7	602	CLA	C11-C10-C8-C9
20	7	604	CLA	C6-C7-C8-C9
20	Z	610	CLA	C11-C10-C8-C9
20	6	602	CLA	C6-C7-C8-C9
21	A	844	PQN	C19-C18-C20-C21
20	3	602	CLA	CBD-CGD-O2D-CED
22	8	620	LHG	C25-C26-C27-C28
22	Z	620	LHG	C24-C25-C26-C27
20	A	832	CLA	CBA-CGA-O2A-C1
20	7	601	CLA	CBA-CGA-O2A-C1
20	Z	603	CLA	CBA-CGA-O2A-C1
20	B	805	CLA	C15-C16-C17-C18
20	F	304	CLA	C5-C6-C7-C8
20	7	602	CLA	C13-C15-C16-C17
20	B	821	CLA	CBA-CGA-O2A-C1
20	B	828	CLA	C2A-CAA-CBA-CGA
20	7	616	CLA	C2A-CAA-CBA-CGA
22	8	620	LHG	C12-C13-C14-C15
20	A	826	CLA	O1A-CGA-O2A-C1
20	B	817	CLA	C10-C11-C12-C13
23	B	846	BCR	C7-C8-C9-C10
23	5	625	BCR	C7-C8-C9-C10
22	A	846	LHG	C10-C11-C12-C13
20	8	614	CLA	CBA-CGA-O2A-C1
20	6	610	CLA	CBA-CGA-O2A-C1
22	A	847	LHG	C15-C16-C17-C18
20	A	806	CLA	C10-C11-C12-C13
20	1	604	CLA	C5-C6-C7-C8
20	3	610	CLA	C8-C10-C11-C12
22	A	847	LHG	O6-C4-C5-C6
22	A	855	LHG	O6-C4-C5-C6
22	B	851	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
19	A	801	CL0	C3-C5-C6-C7
20	5	604	CLA	CBA-CGA-O2A-C1
27	1	601	CHL	CBA-CGA-O2A-C1
20	A	809	CLA	C5-C6-C7-C8
20	A	810	CLA	C4-C3-C5-C6
20	1	614	CLA	C4-C3-C5-C6
20	3	604	CLA	C4-C3-C5-C6
20	A	826	CLA	C2-C3-C5-C6
20	A	845	CLA	C2-C3-C5-C6
20	1	614	CLA	C2-C3-C5-C6
20	Z	608	CLA	C2-C3-C5-C6
20	5	610	CLA	C2-C3-C5-C6
20	6	612	CLA	C2-C3-C5-C6
22	6	619	LHG	C11-C12-C13-C14
20	B	819	CLA	C16-C17-C18-C20
27	8	607	CHL	C6-C7-C8-C10
20	Z	609	CLA	O1D-CGD-O2D-CED
20	4	610	CLA	CBA-CGA-O2A-C1
20	6	604	CLA	CBA-CGA-O2A-C1
20	A	824	CLA	C3A-C2A-CAA-CBA
20	A	837	CLA	C3A-C2A-CAA-CBA
20	B	804	CLA	C3A-C2A-CAA-CBA
20	B	835	CLA	C3A-C2A-CAA-CBA
20	3	604	CLA	C3A-C2A-CAA-CBA
20	4	613	CLA	C3A-C2A-CAA-CBA
20	6	609	CLA	C3A-C2A-CAA-CBA
23	B	846	BCR	C19-C20-C21-C22
20	7	601	CLA	C10-C11-C12-C13
20	A	839	CLA	O1A-CGA-O2A-C1
20	B	822	CLA	C11-C12-C13-C14
20	A	813	CLA	CBA-CGA-O2A-C1
20	8	610	CLA	CBA-CGA-O2A-C1
20	Z	608	CLA	CBA-CGA-O2A-C1
20	A	809	CLA	C8-C10-C11-C12
22	4	622	LHG	C4-C5-C6-O8
20	A	812	CLA	C3-C5-C6-C7
20	B	828	CLA	C3-C5-C6-C7
27	8	607	CHL	C6-C7-C8-C9
20	A	810	CLA	C2-C3-C5-C6
20	A	810	CLA	O1D-CGD-O2D-CED
27	4	606	CHL	C3C-C2C-CMC-OMC
20	B	827	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	8	620	LHG	O10-C23-O8-C6
20	1	610	CLA	C3-C5-C6-C7
20	3	602	CLA	C3-C5-C6-C7
20	4	613	CLA	C3-C5-C6-C7
20	4	601	CLA	C2A-CAA-CBA-CGA
20	A	831	CLA	CBA-CGA-O2A-C1
20	8	611	CLA	O1D-CGD-O2D-CED
20	A	830	CLA	O1A-CGA-O2A-C1
20	7	601	CLA	O1A-CGA-O2A-C1
20	5	610	CLA	O1A-CGA-O2A-C1
20	K	4003	CLA	CBA-CGA-O2A-C1
20	B	830	CLA	CAA-CBA-CGA-O2A
20	A	816	CLA	C13-C15-C16-C17
20	Z	603	CLA	O1A-CGA-O2A-C1
20	B	839	CLA	C13-C15-C16-C17
20	A	810	CLA	C2-C1-O2A-CGA
20	A	833	CLA	C2-C1-O2A-CGA
20	B	812	CLA	C2-C1-O2A-CGA
20	B	817	CLA	C2-C1-O2A-CGA
20	B	836	CLA	C2-C1-O2A-CGA
20	1	606	CLA	C2-C1-O2A-CGA
20	1	612	CLA	C2-C1-O2A-CGA
20	8	612	CLA	C2-C1-O2A-CGA
20	Z	602	CLA	C2-C1-O2A-CGA
20	4	609	CLA	C2-C1-O2A-CGA
20	4	613	CLA	C2-C1-O2A-CGA
20	3	604	CLA	C2-C3-C5-C6
20	A	802	CLA	C11-C10-C8-C9
20	A	807	CLA	C11-C12-C13-C14
20	A	815	CLA	C6-C7-C8-C9
20	A	820	CLA	C11-C12-C13-C14
20	1	613	CLA	C11-C10-C8-C9
20	3	607	CLA	C11-C10-C8-C9
20	Z	613	CLA	C6-C7-C8-C9
20	5	602	CLA	C14-C13-C15-C16
20	6	602	CLA	C11-C10-C8-C9
20	A	834	CLA	CBA-CGA-O2A-C1
20	A	813	CLA	O1A-CGA-O2A-C1
20	8	614	CLA	O1A-CGA-O2A-C1
20	3	620	CLA	C2A-CAA-CBA-CGA
20	8	610	CLA	C2A-CAA-CBA-CGA
20	A	843	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
23	A	848	BCR	C23-C24-C25-C26
23	A	850	BCR	C1-C6-C7-C8
23	A	850	BCR	C5-C6-C7-C8
23	A	851	BCR	C1-C6-C7-C8
23	A	851	BCR	C5-C6-C7-C8
23	A	851	BCR	C23-C24-C25-C26
23	A	851	BCR	C23-C24-C25-C30
23	B	801	BCR	C1-C6-C7-C8
23	B	801	BCR	C5-C6-C7-C8
23	B	844	BCR	C23-C24-C25-C30
23	B	846	BCR	C23-C24-C25-C26
23	B	846	BCR	C23-C24-C25-C30
23	B	847	BCR	C23-C24-C25-C26
23	B	847	BCR	C23-C24-C25-C30
23	F	305	BCR	C5-C6-C7-C8
23	F	305	BCR	C23-C24-C25-C26
23	F	305	BCR	C23-C24-C25-C30
23	J	3003	BCR	C1-C6-C7-C8
23	J	3003	BCR	C5-C6-C7-C8
23	K	4004	BCR	C1-C6-C7-C8
23	K	4004	BCR	C5-C6-C7-C8
23	3	717	BCR	C1-C6-C7-C8
23	4	621	BCR	C5-C6-C7-C8
23	6	625	BCR	C23-C24-C25-C26
23	6	625	BCR	C23-C24-C25-C30
28	7	621	LUT	C1-C6-C7-C8
28	7	621	LUT	C5-C6-C7-C8
28	Z	617	LUT	C1-C6-C7-C8
28	Z	617	LUT	C5-C6-C7-C8
28	5	620	LUT	C5-C6-C7-C8
28	5	624	LUT	C5-C6-C7-C8
28	6	624	LUT	C1-C6-C7-C8
28	6	624	LUT	C5-C6-C7-C8
20	1	608	CLA	C13-C15-C16-C17
20	4	611	CLA	O1D-CGD-O2D-CED
20	6	604	CLA	O1A-CGA-O2A-C1
20	A	827	CLA	CBA-CGA-O2A-C1
23	A	856	BCR	C11-C12-C13-C14
23	B	845	BCR	C7-C8-C9-C10
23	B	847	BCR	C21-C22-C23-C24
23	K	4004	BCR	C21-C22-C23-C24
23	L	205	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
23	3	719	BCR	C7-C8-C9-C10
23	3	719	BCR	C21-C22-C23-C24
28	6	621	LUT	C11-C12-C13-C14
22	A	846	LHG	C14-C15-C16-C17
22	6	619	LHG	C10-C11-C12-C13
20	A	832	CLA	O1A-CGA-O2A-C1
20	B	806	CLA	C10-C11-C12-C13
22	6	619	LHG	O6-C4-C5-C6
20	A	819	CLA	CAA-CBA-CGA-O2A
27	4	607	CHL	CAA-CBA-CGA-O2A
20	A	805	CLA	C4-C3-C5-C6
20	A	802	CLA	C11-C10-C8-C7
20	A	807	CLA	C11-C12-C13-C15
20	A	815	CLA	C6-C7-C8-C10
20	A	816	CLA	C12-C13-C15-C16
20	A	819	CLA	C6-C7-C8-C10
20	A	833	CLA	C11-C10-C8-C7
20	A	843	CLA	C6-C7-C8-C10
20	B	803	CLA	C11-C12-C13-C15
20	B	818	CLA	C6-C7-C8-C10
20	B	826	CLA	C11-C12-C13-C15
20	B	834	CLA	C11-C10-C8-C7
20	B	839	CLA	C12-C13-C15-C16
20	B	840	CLA	C12-C13-C15-C16
20	L	203	CLA	C11-C12-C13-C15
20	1	610	CLA	C11-C10-C8-C7
20	1	613	CLA	C11-C10-C8-C7
20	7	602	CLA	C11-C10-C8-C7
20	7	604	CLA	C6-C7-C8-C10
20	8	601	CLA	C6-C7-C8-C10
20	Z	613	CLA	C6-C7-C8-C10
27	3	608	CHL	C12-C13-C15-C16
20	5	601	CLA	C10-C11-C12-C13
23	B	801	BCR	C13-C14-C15-C16
23	K	4001	BCR	C13-C14-C15-C16
28	6	624	LUT	C29-C30-C31-C32
19	A	801	CL0	C16-C17-C18-C20
20	B	805	CLA	C13-C15-C16-C17
27	1	601	CHL	O1A-CGA-O2A-C1
20	G	203	CLA	C2A-CAA-CBA-CGA
20	Z	614	CLA	C2A-CAA-CBA-CGA
27	5	607	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	B	850	DGD	C2B-C1B-O2G-C2G
20	B	802	CLA	C13-C15-C16-C17
20	1	609	CLA	CBA-CGA-O2A-C1
20	A	803	CLA	CAD-CBD-CGD-O2D
20	A	812	CLA	CAD-CBD-CGD-O2D
20	A	813	CLA	CAD-CBD-CGD-O2D
20	A	815	CLA	CAD-CBD-CGD-O2D
20	A	821	CLA	CAD-CBD-CGD-O2D
20	A	842	CLA	CAD-CBD-CGD-O2D
20	B	803	CLA	CAD-CBD-CGD-O2D
20	B	812	CLA	CAD-CBD-CGD-O2D
20	B	816	CLA	CAD-CBD-CGD-O2D
20	B	820	CLA	CAD-CBD-CGD-O2D
20	B	821	CLA	CAD-CBD-CGD-O2D
20	B	829	CLA	CAD-CBD-CGD-O2D
20	F	303	CLA	CAD-CBD-CGD-O2D
20	K	4002	CLA	CAD-CBD-CGD-O2D
20	1	604	CLA	CAD-CBD-CGD-O2D
20	1	606	CLA	CAD-CBD-CGD-O2D
20	3	607	CLA	CAD-CBD-CGD-O2D
20	7	602	CLA	CAD-CBD-CGD-O2D
20	7	612	CLA	CAD-CBD-CGD-O2D
20	8	612	CLA	CAD-CBD-CGD-O2D
20	Z	606	CLA	CAD-CBD-CGD-O2D
20	4	601	CLA	CAD-CBD-CGD-O2D
20	4	603	CLA	CAD-CBD-CGD-O2D
20	4	610	CLA	CAD-CBD-CGD-O2D
20	4	612	CLA	CAD-CBD-CGD-O2D
20	4	614	CLA	CAD-CBD-CGD-O2D
20	6	604	CLA	CAD-CBD-CGD-O2D
20	6	614	CLA	CAD-CBD-CGD-O2D
20	A	842	CLA	C3-C5-C6-C7
20	A	806	CLA	C15-C16-C17-C18
20	1	611	CLA	C10-C11-C12-C13
20	3	613	CLA	C5-C6-C7-C8
20	8	601	CLA	C8-C10-C11-C12
20	5	604	CLA	O1A-CGA-O2A-C1
20	B	817	CLA	C4-C3-C5-C6
20	A	842	CLA	C16-C17-C18-C19
20	A	805	CLA	C2-C3-C5-C6
22	A	855	LHG	O6-C4-C5-O7
22	B	851	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
22	5	623	LHG	O6-C4-C5-O7
20	8	609	CLA	CAA-CBA-CGA-O2A
20	B	840	CLA	C2A-CAA-CBA-CGA
20	3	610	CLA	CBD-CGD-O2D-CED
20	7	601	CLA	CBD-CGD-O2D-CED
20	A	842	CLA	C16-C17-C18-C20
20	A	823	CLA	O1D-CGD-O2D-CED
27	4	618	CHL	O1D-CGD-O2D-CED
20	A	806	CLA	CHA-CBD-CGD-O1D
20	A	806	CLA	CHA-CBD-CGD-O2D
20	A	809	CLA	CHA-CBD-CGD-O1D
20	A	809	CLA	CHA-CBD-CGD-O2D
20	A	821	CLA	CHA-CBD-CGD-O1D
20	A	837	CLA	CHA-CBD-CGD-O1D
20	A	837	CLA	CHA-CBD-CGD-O2D
20	A	840	CLA	CHA-CBD-CGD-O2D
20	A	845	CLA	CHA-CBD-CGD-O1D
20	A	854	CLA	CHA-CBD-CGD-O1D
20	A	854	CLA	CHA-CBD-CGD-O2D
20	B	824	CLA	CHA-CBD-CGD-O1D
20	B	837	CLA	CHA-CBD-CGD-O1D
20	B	837	CLA	CHA-CBD-CGD-O2D
20	J	3002	CLA	CHA-CBD-CGD-O1D
20	J	3002	CLA	CHA-CBD-CGD-O2D
20	7	601	CLA	CHA-CBD-CGD-O1D
20	7	601	CLA	CHA-CBD-CGD-O2D
20	7	606	CLA	CHA-CBD-CGD-O1D
20	8	601	CLA	CHA-CBD-CGD-O1D
20	8	602	CLA	CHA-CBD-CGD-O2D
20	8	611	CLA	CHA-CBD-CGD-O1D
20	8	611	CLA	CHA-CBD-CGD-O2D
20	4	604	CLA	CHA-CBD-CGD-O1D
20	4	604	CLA	CHA-CBD-CGD-O2D
20	5	603	CLA	CHA-CBD-CGD-O1D
20	5	611	CLA	CHA-CBD-CGD-O1D
20	5	611	CLA	CHA-CBD-CGD-O2D
20	5	617	CLA	CHA-CBD-CGD-O1D
20	5	617	CLA	CHA-CBD-CGD-O2D
20	6	601	CLA	CHA-CBD-CGD-O1D
20	6	601	CLA	CHA-CBD-CGD-O2D
20	6	603	CLA	CHA-CBD-CGD-O1D
20	6	616	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
27	Z	601	CHL	CHA-CBD-CGD-O1D
27	Z	601	CHL	CHA-CBD-CGD-O2D
20	Z	606	CLA	CBD-CGD-O2D-CED
20	Z	608	CLA	O1A-CGA-O2A-C1
20	6	610	CLA	O1A-CGA-O2A-C1
22	A	855	LHG	O7-C5-C6-O8
20	1	612	CLA	CBA-CGA-O2A-C1
20	1	611	CLA	C5-C6-C7-C8
20	A	831	CLA	O1A-CGA-O2A-C1
22	7	625	LHG	C26-C27-C28-C29
20	B	828	CLA	C4-C3-C5-C6
20	A	834	CLA	O1A-CGA-O2A-C1
20	A	824	CLA	O1D-CGD-O2D-CED
20	K	4002	CLA	O1D-CGD-O2D-CED
20	B	805	CLA	C5-C6-C7-C8
20	B	809	CLA	C15-C16-C17-C18
20	A	819	CLA	C6-C7-C8-C9
20	A	828	CLA	C11-C12-C13-C14
20	A	831	CLA	C11-C10-C8-C9
20	F	304	CLA	C14-C13-C15-C16
20	A	826	CLA	O1D-CGD-O2D-CED
20	A	827	CLA	O1A-CGA-O2A-C1
20	B	819	CLA	C16-C17-C18-C19
20	5	614	CLA	O1D-CGD-O2D-CED
20	1	609	CLA	O1A-CGA-O2A-C1
23	K	4001	BCR	C7-C8-C9-C34
23	3	717	BCR	C7-C8-C9-C34
23	8	619	BCR	C11-C12-C13-C35
28	7	621	LUT	C11-C12-C13-C20
20	Z	614	CLA	C10-C11-C12-C13
27	7	607	CHL	C5-C6-C7-C8
20	A	808	CLA	C1A-C2A-CAA-CBA
20	A	831	CLA	C1A-C2A-CAA-CBA
20	A	845	CLA	C1A-C2A-CAA-CBA
20	B	814	CLA	C1A-C2A-CAA-CBA
20	B	823	CLA	C1A-C2A-CAA-CBA
20	B	826	CLA	C1A-C2A-CAA-CBA
20	B	829	CLA	C1A-C2A-CAA-CBA
20	1	608	CLA	C1A-C2A-CAA-CBA
20	7	602	CLA	C1A-C2A-CAA-CBA
20	8	611	CLA	C1A-C2A-CAA-CBA
20	6	602	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	A	808	CLA	C13-C15-C16-C17
20	7	613	CLA	C10-C11-C12-C13
20	1	608	CLA	C2-C1-O2A-CGA
20	8	613	CLA	C2-C1-O2A-CGA
20	Z	614	CLA	C2-C1-O2A-CGA
20	5	601	CLA	C2-C1-O2A-CGA
20	Z	606	CLA	CBA-CGA-O2A-C1
22	A	847	LHG	C3-O3-P-O6
22	4	622	LHG	C4-O6-P-O3
22	4	623	LHG	C4-O6-P-O3
22	5	623	LHG	C3-O3-P-O6
22	1	620	LHG	O2-C2-C3-O3
20	B	841	CLA	C2-C3-C5-C6
20	Z	606	CLA	O1A-CGA-O2A-C1
22	A	847	LHG	C4-O6-P-O5
22	B	851	LHG	C3-O3-P-O5
22	B	851	LHG	C4-O6-P-O4
22	7	625	LHG	C4-O6-P-O4
22	8	620	LHG	C3-O3-P-O5
22	8	620	LHG	C4-O6-P-O5
22	4	622	LHG	C3-O3-P-O4
22	6	619	LHG	C3-O3-P-O4
20	B	819	CLA	CBD-CGD-O2D-CED
20	6	601	CLA	C3-C5-C6-C7
20	B	822	CLA	C10-C11-C12-C13
20	A	806	CLA	CAD-CBD-CGD-O1D
20	A	816	CLA	CAD-CBD-CGD-O1D
20	A	845	CLA	CAD-CBD-CGD-O1D
20	A	854	CLA	CAD-CBD-CGD-O1D
20	B	837	CLA	CAD-CBD-CGD-O1D
20	J	3002	CLA	CAD-CBD-CGD-O1D
20	7	601	CLA	CAD-CBD-CGD-O1D
20	7	606	CLA	CAD-CBD-CGD-O1D
20	7	620	CLA	CAD-CBD-CGD-O1D
20	8	601	CLA	CAD-CBD-CGD-O1D
20	5	603	CLA	CAD-CBD-CGD-O1D
20	6	601	CLA	CAD-CBD-CGD-O1D
27	Z	601	CHL	CAD-CBD-CGD-O1D
20	3	609	CLA	CAA-CBA-CGA-O2A
20	A	804	CLA	C8-C10-C11-C12
20	B	808	CLA	C13-C15-C16-C17
20	B	819	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
20	1	608	CLA	C3-C5-C6-C7
20	3	610	CLA	CBA-CGA-O2A-C1
20	Z	613	CLA	O1D-CGD-O2D-CED
20	A	804	CLA	C13-C15-C16-C17
20	6	610	CLA	CBD-CGD-O2D-CED
20	A	820	CLA	C4-C3-C5-C6
20	A	807	CLA	C12-C13-C15-C16
20	A	810	CLA	C12-C13-C15-C16
20	A	812	CLA	C11-C10-C8-C7
20	A	814	CLA	C11-C12-C13-C15
20	A	831	CLA	C11-C10-C8-C7
20	A	835	CLA	C11-C12-C13-C15
20	A	839	CLA	C12-C13-C15-C16
20	B	802	CLA	C6-C7-C8-C10
20	B	805	CLA	C11-C12-C13-C15
20	B	810	CLA	C3A-C2A-CAA-CBA
20	B	819	CLA	C12-C13-C15-C16
20	F	304	CLA	C12-C13-C15-C16
20	8	601	CLA	C11-C12-C13-C15
21	A	844	PQN	C21-C22-C23-C25
22	6	619	LHG	O6-C4-C5-O7
20	Z	608	CLA	C13-C15-C16-C17
20	1	611	CLA	C2A-CAA-CBA-CGA
20	4	609	CLA	C2A-CAA-CBA-CGA
27	4	607	CHL	C2A-CAA-CBA-CGA
22	5	623	LHG	C4-C5-C6-O8
27	Z	601	CHL	C1C-C2C-CMC-OMC
27	4	606	CHL	C1C-C2C-CMC-OMC
27	6	618	CHL	C1C-C2C-CMC-OMC
22	5	623	LHG	O7-C5-C6-O8
26	J	3001	LMG	O1-C7-C8-O7
20	B	802	CLA	C8-C10-C11-C12
20	B	841	CLA	O1D-CGD-O2D-CED
20	B	827	CLA	CAA-CBA-CGA-O2A
20	B	824	CLA	C4-C3-C5-C6
20	A	813	CLA	C6-C7-C8-C9
20	A	812	CLA	C11-C10-C8-C9
20	A	816	CLA	C14-C13-C15-C16
20	A	833	CLA	C11-C10-C8-C9
20	A	843	CLA	C6-C7-C8-C9
20	B	826	CLA	C11-C12-C13-C14
20	B	827	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
20	B	839	CLA	C14-C13-C15-C16
20	L	203	CLA	C11-C12-C13-C14
20	8	601	CLA	C6-C7-C8-C9
21	A	844	PQN	C21-C22-C23-C24
20	1	612	CLA	O1A-CGA-O2A-C1
20	A	827	CLA	C3-C5-C6-C7
20	8	610	CLA	O1A-CGA-O2A-C1
20	B	832	CLA	CAA-CBA-CGA-O2A
28	5	624	LUT	C29-C30-C31-C32
25	B	850	DGD	CEA-CFA-CGA-CHA
20	B	828	CLA	C2-C3-C5-C6
20	7	601	CLA	O1D-CGD-O2D-CED
20	A	828	CLA	C10-C11-C12-C13
20	Z	610	CLA	C8-C10-C11-C12
20	7	616	CLA	CBA-CGA-O2A-C1
20	A	823	CLA	C1-C2-C3-C4
22	A	846	LHG	C16-C17-C18-C19
20	F	303	CLA	C2A-CAA-CBA-CGA
20	3	610	CLA	C2A-CAA-CBA-CGA
20	3	613	CLA	C2A-CAA-CBA-CGA
20	7	610	CLA	C2A-CAA-CBA-CGA
25	B	850	DGD	O1B-C1B-O2G-C2G
20	4	610	CLA	O1A-CGA-O2A-C1
20	A	807	CLA	C2-C1-O2A-CGA
20	A	831	CLA	C2-C1-O2A-CGA
20	A	834	CLA	C2-C1-O2A-CGA
20	A	854	CLA	C2-C1-O2A-CGA
20	B	827	CLA	C2-C1-O2A-CGA
20	7	613	CLA	C2-C1-O2A-CGA
20	5	613	CLA	C2-C1-O2A-CGA
27	4	607	CHL	C2-C1-O2A-CGA
20	B	816	CLA	C3-C5-C6-C7
20	1	602	CLA	C3-C5-C6-C7
22	7	625	LHG	C11-C10-C9-C8
20	A	845	CLA	O1D-CGD-O2D-CED
20	B	821	CLA	O1D-CGD-O2D-CED
22	4	622	LHG	C24-C23-O8-C6
20	4	612	CLA	O1A-CGA-O2A-C1
20	B	827	CLA	C4-C3-C5-C6
23	A	848	BCR	C23-C24-C25-C30
23	B	843	BCR	C23-C24-C25-C26
23	B	843	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
23	B	844	BCR	C23-C24-C25-C26
23	F	305	BCR	C1-C6-C7-C8
23	3	717	BCR	C5-C6-C7-C8
23	3	718	BCR	C23-C24-C25-C30
23	4	621	BCR	C1-C6-C7-C8
28	1	618	LUT	C1-C6-C7-C8
28	5	624	LUT	C1-C6-C7-C8
22	Z	620	LHG	C11-C12-C13-C14
20	A	843	CLA	C16-C17-C18-C19
20	L	203	CLA	C3-C5-C6-C7
20	1	609	CLA	C2A-CAA-CBA-CGA
20	4	603	CLA	CBA-CGA-O2A-C1
20	A	840	CLA	CBD-CGD-O2D-CED
22	A	846	LHG	C3-O3-P-O6
22	A	846	LHG	C4-O6-P-O3
22	A	855	LHG	C3-O3-P-O6
22	1	620	LHG	C3-O3-P-O6
22	1	620	LHG	C4-O6-P-O3
22	7	625	LHG	C3-O3-P-O6
22	Z	620	LHG	C3-O3-P-O6
22	Z	620	LHG	C4-O6-P-O3
20	A	843	CLA	C8-C10-C11-C12
20	A	828	CLA	C11-C12-C13-C15
20	B	817	CLA	C2-C3-C5-C6
20	B	827	CLA	C11-C10-C8-C7
20	7	601	CLA	C11-C12-C13-C15
20	A	814	CLA	C11-C12-C13-C14
20	A	835	CLA	C6-C7-C8-C9
20	A	835	CLA	C11-C12-C13-C14
20	A	854	CLA	C14-C13-C15-C16
20	B	812	CLA	C6-C7-C8-C9
20	8	601	CLA	C11-C12-C13-C14
23	4	621	BCR	C13-C14-C15-C16
20	7	610	CLA	CBA-CGA-O2A-C1
20	A	813	CLA	C2A-CAA-CBA-CGA
20	5	614	CLA	C2A-CAA-CBA-CGA
20	4	601	CLA	O1A-CGA-O2A-C1
20	Z	603	CLA	CBD-CGD-O2D-CED
20	A	828	CLA	CBA-CGA-O2A-C1
22	A	847	LHG	O1-C1-C2-C3
20	A	826	CLA	C15-C16-C17-C18
28	7	621	LUT	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
20	Z	612	CLA	CBA-CGA-O2A-C1
20	4	601	CLA	CBA-CGA-O2A-C1
20	4	612	CLA	CBA-CGA-O2A-C1
20	3	617	CLA	O1D-CGD-O2D-CED
20	Z	616	CLA	CBA-CGA-O2A-C1
20	3	604	CLA	C10-C11-C12-C13
20	7	610	CLA	C10-C11-C12-C13
20	Z	612	CLA	O1A-CGA-O2A-C1
20	B	821	CLA	O1A-CGA-O2A-C1
23	B	843	BCR	C13-C14-C15-C16
23	B	847	BCR	C13-C14-C15-C16
20	A	828	CLA	O1A-CGA-O2A-C1
20	A	813	CLA	C4-C3-C5-C6
20	8	602	CLA	C4-C3-C5-C6
21	B	842	PQN	C15-C16-C17-C18
20	B	817	CLA	CAA-CBA-CGA-O2A
19	A	801	CL0	C2-C1-O2A-CGA
20	A	830	CLA	C2-C1-O2A-CGA
20	A	842	CLA	C2-C1-O2A-CGA
20	B	819	CLA	C2-C1-O2A-CGA
20	B	829	CLA	C2-C1-O2A-CGA
20	1	604	CLA	C2-C1-O2A-CGA
20	1	609	CLA	C2-C1-O2A-CGA
20	Z	612	CLA	C2-C1-O2A-CGA
20	5	602	CLA	C2-C1-O2A-CGA
20	6	613	CLA	C2-C1-O2A-CGA
27	4	606	CHL	C2-C1-O2A-CGA
20	A	828	CLA	C5-C6-C7-C8
20	5	611	CLA	C6-C7-C8-C9
20	A	805	CLA	C2A-CAA-CBA-CGA
20	A	823	CLA	C2A-CAA-CBA-CGA
20	A	843	CLA	C2A-CAA-CBA-CGA
20	B	820	CLA	C2A-CAA-CBA-CGA
20	4	610	CLA	C2A-CAA-CBA-CGA
22	4	623	LHG	O7-C5-C6-O8
20	A	815	CLA	C3A-C2A-CAA-CBA
20	B	841	CLA	C3A-C2A-CAA-CBA
27	5	607	CHL	C3A-C2A-CAA-CBA
20	A	820	CLA	C16-C17-C18-C19
20	A	828	CLA	C16-C17-C18-C19
20	3	603	CLA	C4-C3-C5-C6
20	8	604	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	B	824	CLA	C2-C3-C5-C6
20	3	603	CLA	C2-C3-C5-C6
20	Z	609	CLA	C3-C5-C6-C7
20	5	602	CLA	C8-C10-C11-C12
20	A	806	CLA	C11-C10-C8-C9
20	A	807	CLA	C14-C13-C15-C16
20	A	814	CLA	C6-C7-C8-C9
20	A	826	CLA	C6-C7-C8-C9
20	B	805	CLA	C11-C12-C13-C14
20	B	852	CLA	C6-C7-C8-C9
20	5	601	CLA	C11-C10-C8-C9
20	A	812	CLA	C10-C11-C12-C13
20	A	843	CLA	C10-C11-C12-C13
22	A	855	LHG	C4-C5-C6-O8
23	A	852	BCR	C11-C10-C9-C34
23	A	852	BCR	C16-C17-C18-C36
23	B	845	BCR	C11-C10-C9-C34
23	B	845	BCR	C20-C21-C22-C37
23	F	305	BCR	C35-C13-C14-C15
23	L	201	BCR	C11-C10-C9-C34
20	1	614	CLA	C2A-CAA-CBA-CGA
20	3	604	CLA	C2A-CAA-CBA-CGA
20	7	609	CLA	C2A-CAA-CBA-CGA
22	4	622	LHG	O10-C23-O8-C6
20	A	806	CLA	O2A-C1-C2-C3
20	Z	603	CLA	O2A-C1-C2-C3
20	3	617	CLA	CBA-CGA-O2A-C1
23	A	852	BCR	C37-C22-C23-C24
28	Z	617	LUT	C7-C8-C9-C19
28	Z	618	LUT	C7-C8-C9-C19
20	A	806	CLA	C4-C3-C5-C6
20	A	840	CLA	C4-C3-C5-C6
27	1	601	CHL	C4-C3-C5-C6
20	A	803	CLA	C1A-C2A-CAA-CBA
20	A	837	CLA	C1A-C2A-CAA-CBA
20	B	827	CLA	C1A-C2A-CAA-CBA
20	7	608	CLA	C1A-C2A-CAA-CBA
20	Z	602	CLA	C1A-C2A-CAA-CBA
20	Z	614	CLA	C1A-C2A-CAA-CBA
20	4	614	CLA	C1A-C2A-CAA-CBA
27	4	606	CHL	C1A-C2A-CAA-CBA
27	5	618	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	A	806	CLA	C11-C12-C13-C15
20	A	814	CLA	C12-C13-C15-C16
20	B	832	CLA	C11-C10-C8-C7
20	1	611	CLA	C12-C13-C15-C16
20	Z	611	CLA	C12-C13-C15-C16
23	6	625	BCR	C13-C14-C15-C16
20	Z	606	CLA	O1D-CGD-O2D-CED
20	1	609	CLA	C13-C15-C16-C17
20	4	613	CLA	C5-C6-C7-C8
20	A	840	CLA	O1D-CGD-O2D-CED
22	A	846	LHG	C9-C10-C11-C12
20	B	802	CLA	C4-C3-C5-C6
20	K	4003	CLA	O1A-CGA-O2A-C1
20	7	601	CLA	C5-C6-C7-C8
20	5	613	CLA	C5-C6-C7-C8
22	4	623	LHG	O9-C7-O7-C5
27	5	618	CHL	O1D-CGD-O2D-CED
23	A	852	BCR	C11-C10-C9-C8
23	A	852	BCR	C16-C17-C18-C19
23	B	845	BCR	C11-C10-C9-C8
23	B	845	BCR	C20-C21-C22-C23
23	F	305	BCR	C12-C13-C14-C15
23	L	201	BCR	C11-C10-C9-C8
25	B	850	DGD	O2G-C2G-C3G-O3G
27	5	607	CHL	CAA-CBA-CGA-O2A
23	L	205	BCR	C13-C14-C15-C16
23	3	717	BCR	C19-C20-C21-C22
20	A	828	CLA	C16-C17-C18-C20
22	A	846	LHG	C24-C25-C26-C27
22	4	623	LHG	C1-C2-C3-O3
20	A	826	CLA	C8-C10-C11-C12
20	A	830	CLA	C4-C3-C5-C6
20	B	814	CLA	C4-C3-C5-C6
20	3	610	CLA	C4-C3-C5-C6
20	7	602	CLA	C4-C3-C5-C6
21	B	842	PQN	C14-C13-C15-C16
22	8	620	LHG	C24-C25-C26-C27
20	7	612	CLA	C2-C1-O2A-CGA
20	5	609	CLA	C2-C1-O2A-CGA
27	3	608	CHL	C2-C1-O2A-CGA
27	6	607	CHL	C2-C1-O2A-CGA
20	A	806	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
20	4	610	CLA	C8-C10-C11-C12
20	A	807	CLA	C11-C10-C8-C9
20	A	826	CLA	C14-C13-C15-C16
20	B	813	CLA	C8-C10-C11-C12
20	4	602	CLA	C10-C11-C12-C13
20	A	841	CLA	C2A-CAA-CBA-CGA
20	B	810	CLA	C2A-CAA-CBA-CGA
22	5	623	LHG	C24-C23-O8-C6
23	A	849	BCR	C1-C6-C7-C8
23	A	849	BCR	C23-C24-C25-C30
23	B	845	BCR	C23-C24-C25-C26
23	B	845	BCR	C23-C24-C25-C30
23	B	848	BCR	C23-C24-C25-C30
23	G	205	BCR	C23-C24-C25-C30
23	L	205	BCR	C1-C6-C7-C8
23	3	718	BCR	C23-C24-C25-C26
23	3	719	BCR	C23-C24-C25-C30
28	1	618	LUT	C5-C6-C7-C8
28	7	622	LUT	C1-C6-C7-C8
28	7	622	LUT	C5-C6-C7-C8
28	Z	618	LUT	C1-C6-C7-C8
20	A	829	CLA	CAA-CBA-CGA-O2A
20	1	609	CLA	CAA-CBA-CGA-O2A
22	4	623	LHG	C4-C5-C6-O8
23	3	717	BCR	C15-C16-C17-C18
23	6	623	BCR	C13-C14-C15-C16
20	B	822	CLA	C4-C3-C5-C6
20	8	613	CLA	C4-C3-C5-C6
20	A	854	CLA	C13-C15-C16-C17
20	A	820	CLA	C2-C3-C5-C6
20	A	840	CLA	C2-C3-C5-C6
20	B	827	CLA	C2-C3-C5-C6
20	7	601	CLA	C3-C5-C6-C7
20	B	807	CLA	O1A-CGA-O2A-C1
20	1	603	CLA	O1A-CGA-O2A-C1
20	A	818	CLA	C13-C15-C16-C17
20	B	852	CLA	C5-C6-C7-C8
20	B	835	CLA	CAA-CBA-CGA-O2A
20	3	614	CLA	CAA-CBA-CGA-O2A
20	3	609	CLA	C2A-CAA-CBA-CGA
20	3	617	CLA	C2A-CAA-CBA-CGA
20	1	603	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	B	820	CLA	C5-C6-C7-C8
22	7	625	LHG	O6-C4-C5-C6
20	3	602	CLA	C4-C3-C5-C6
20	A	814	CLA	C6-C7-C8-C10
20	A	828	CLA	C2-C3-C5-C6
23	7	623	BCR	C15-C16-C17-C18
28	7	621	LUT	C29-C30-C31-C32
19	A	801	CL0	CAA-CBA-CGA-O2A
20	B	816	CLA	C6-C7-C8-C10
20	A	802	CLA	C15-C16-C17-C18
20	B	807	CLA	CBA-CGA-O2A-C1
20	3	609	CLA	O1A-CGA-O2A-C1
20	4	613	CLA	CAA-CBA-CGA-O2A
20	A	807	CLA	C4-C3-C5-C6
20	A	809	CLA	C4-C3-C5-C6
20	B	813	CLA	C4-C3-C5-C6
20	F	301	CLA	C4-C3-C5-C6
20	L	203	CLA	C4-C3-C5-C6
20	B	834	CLA	C8-C10-C11-C12
20	4	601	CLA	C8-C10-C11-C12
20	8	603	CLA	CAA-CBA-CGA-O2A
20	B	822	CLA	C2-C3-C5-C6
20	8	602	CLA	C2-C3-C5-C6
21	B	842	PQN	C12-C13-C15-C16
20	B	812	CLA	C15-C16-C17-C18
20	5	609	CLA	CAA-CBA-CGA-O2A
20	A	804	CLA	C6-C7-C8-C9
20	A	810	CLA	C14-C13-C15-C16
20	B	802	CLA	C6-C7-C8-C9
20	B	803	CLA	C11-C12-C13-C14
20	B	809	CLA	C11-C12-C13-C14
20	B	819	CLA	C14-C13-C15-C16
20	1	608	CLA	C6-C7-C8-C9
20	1	611	CLA	C14-C13-C15-C16
20	Z	611	CLA	C14-C13-C15-C16
20	4	601	CLA	C11-C12-C13-C14
20	3	607	CLA	C3A-C2A-CAA-CBA
27	4	606	CHL	C3A-C2A-CAA-CBA
27	4	607	CHL	C3A-C2A-CAA-CBA
20	B	817	CLA	O1A-CGA-O2A-C1
22	5	623	LHG	O10-C23-O8-C6
20	B	805	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
20	B	812	CLA	CAA-CBA-CGA-O2A
20	Z	612	CLA	CAA-CBA-CGA-O2A
20	A	837	CLA	CAA-CBA-CGA-O2A
20	A	807	CLA	CAD-CBD-CGD-O2D
20	A	827	CLA	CAD-CBD-CGD-O2D
20	A	838	CLA	CAD-CBD-CGD-O2D
20	B	825	CLA	CAD-CBD-CGD-O2D
20	B	826	CLA	CAD-CBD-CGD-O2D
20	B	830	CLA	CAD-CBD-CGD-O2D
20	B	838	CLA	CAD-CBD-CGD-O2D
20	G	204	CLA	CAD-CBD-CGD-O2D
20	1	608	CLA	CAD-CBD-CGD-O2D
20	3	609	CLA	CAD-CBD-CGD-O2D
20	3	610	CLA	CAD-CBD-CGD-O2D
20	7	608	CLA	CAD-CBD-CGD-O2D
20	7	614	CLA	CAD-CBD-CGD-O2D
20	Z	602	CLA	CAD-CBD-CGD-O2D
20	Z	603	CLA	CAD-CBD-CGD-O2D
20	Z	608	CLA	CAD-CBD-CGD-O2D
20	4	602	CLA	CAD-CBD-CGD-O2D
20	5	610	CLA	CAD-CBD-CGD-O2D
20	6	603	CLA	CAD-CBD-CGD-O2D
22	7	625	LHG	O9-C7-O7-C5
25	B	850	DGD	C2B-C3B-C4B-C5B
20	1	613	CLA	CAA-CBA-CGA-O2A
20	8	616	CLA	CAA-CBA-CGA-O2A
20	Z	616	CLA	CAA-CBA-CGA-O2A
20	6	613	CLA	CAA-CBA-CGA-O2A
20	5	602	CLA	O1D-CGD-O2D-CED
20	A	803	CLA	C4-C3-C5-C6
20	A	811	CLA	C4-C3-C5-C6
20	B	810	CLA	C4-C3-C5-C6
20	1	609	CLA	C4-C3-C5-C6
20	3	614	CLA	CAA-CBA-CGA-O1A
20	A	807	CLA	C2-C3-C5-C6
20	A	830	CLA	C2-C3-C5-C6
20	B	802	CLA	C2-C3-C5-C6
20	B	810	CLA	C2-C3-C5-C6
20	B	814	CLA	C2-C3-C5-C6
20	L	203	CLA	C2-C3-C5-C6
20	B	816	CLA	CAA-CBA-CGA-O2A
20	B	824	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
20	1	616	CLA	CAA-CBA-CGA-O2A
20	8	613	CLA	CAA-CBA-CGA-O2A
20	Z	603	CLA	CAA-CBA-CGA-O2A
20	5	613	CLA	CAA-CBA-CGA-O2A
20	5	616	CLA	CAA-CBA-CGA-O2A
22	8	620	LHG	O7-C7-C8-C9
22	4	622	LHG	O7-C7-C8-C9
23	A	852	BCR	C7-C8-C9-C10
23	K	4001	BCR	C11-C12-C13-C14
23	3	717	BCR	C7-C8-C9-C10
23	7	624	BCR	C7-C8-C9-C10
23	8	619	BCR	C11-C12-C13-C14
28	Z	618	LUT	C7-C8-C9-C10
25	B	850	DGD	CBB-CCB-CDB-CEB
20	B	835	CLA	CAA-CBA-CGA-O1A
20	K	4002	CLA	CAA-CBA-CGA-O2A
20	A	806	CLA	CAA-CBA-CGA-O2A
20	B	807	CLA	CAA-CBA-CGA-O2A
20	B	813	CLA	CAA-CBA-CGA-O2A
20	1	603	CLA	CAA-CBA-CGA-O2A
20	3	607	CLA	CAA-CBA-CGA-O2A
20	7	613	CLA	CAA-CBA-CGA-O2A
20	Z	613	CLA	CAA-CBA-CGA-O2A
27	8	607	CHL	CAA-CBA-CGA-O2A
20	4	603	CLA	O1A-CGA-O2A-C1
20	A	826	CLA	C16-C17-C18-C19
26	J	3001	LMG	C31-C32-C33-C34
20	B	830	CLA	CAA-CBA-CGA-O1A
20	7	610	CLA	C8-C10-C11-C12
27	Z	601	CHL	O2A-C1-C2-C3
27	4	608	CHL	O2A-C1-C2-C3
20	Z	610	CLA	CBA-CGA-O2A-C1
20	A	804	CLA	C2A-CAA-CBA-CGA
20	B	807	CLA	C2A-CAA-CBA-CGA
20	3	612	CLA	CAA-CBA-CGA-O2A
27	Z	607	CHL	CAA-CBA-CGA-O2A
20	6	622	CLA	CAA-CBA-CGA-O2A
20	A	812	CLA	C16-C17-C18-C20
20	5	611	CLA	C6-C7-C8-C10
19	A	801	CL0	CHA-CBD-CGD-O1D
19	A	801	CL0	CHA-CBD-CGD-O2D
20	A	802	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
20	A	816	CLA	CHA-CBD-CGD-O1D
20	A	820	CLA	CHA-CBD-CGD-O1D
20	A	820	CLA	CHA-CBD-CGD-O2D
20	A	822	CLA	CHA-CBD-CGD-O1D
20	A	822	CLA	CHA-CBD-CGD-O2D
20	A	824	CLA	CHA-CBD-CGD-O1D
20	A	824	CLA	CHA-CBD-CGD-O2D
20	A	829	CLA	CHA-CBD-CGD-O1D
20	A	829	CLA	CHA-CBD-CGD-O2D
20	A	839	CLA	CHA-CBD-CGD-O1D
20	A	841	CLA	CHA-CBD-CGD-O1D
20	A	841	CLA	CHA-CBD-CGD-O2D
20	B	804	CLA	CHA-CBD-CGD-O1D
20	B	804	CLA	CHA-CBD-CGD-O2D
20	B	821	CLA	CHA-CBD-CGD-O1D
20	B	822	CLA	CHA-CBD-CGD-O2D
20	B	824	CLA	CHA-CBD-CGD-O2D
20	B	830	CLA	CHA-CBD-CGD-O2D
20	L	203	CLA	CHA-CBD-CGD-O2D
20	1	602	CLA	CHA-CBD-CGD-O2D
20	3	602	CLA	CHA-CBD-CGD-O2D
20	7	620	CLA	CHA-CBD-CGD-O1D
20	7	620	CLA	CHA-CBD-CGD-O2D
20	8	601	CLA	CHA-CBD-CGD-O2D
20	8	602	CLA	CHA-CBD-CGD-O1D
20	8	606	CLA	CHA-CBD-CGD-O1D
20	8	606	CLA	CHA-CBD-CGD-O2D
20	8	613	CLA	CHA-CBD-CGD-O1D
20	8	613	CLA	CHA-CBD-CGD-O2D
20	Z	610	CLA	CHA-CBD-CGD-O2D
20	4	601	CLA	CHA-CBD-CGD-O2D
20	5	603	CLA	CHA-CBD-CGD-O2D
20	5	616	CLA	CHA-CBD-CGD-O1D
20	5	616	CLA	CHA-CBD-CGD-O2D
20	6	616	CLA	CHA-CBD-CGD-O1D
27	6	618	CHL	CHA-CBD-CGD-O1D
27	6	618	CHL	CHA-CBD-CGD-O2D
20	A	837	CLA	CAA-CBA-CGA-O1A
20	K	4002	CLA	CAA-CBA-CGA-O1A
20	B	806	CLA	CAA-CBA-CGA-O2A
20	4	609	CLA	CAA-CBA-CGA-O2A
20	A	829	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
20	B	802	CLA	CAA-CBA-CGA-O2A
20	3	613	CLA	CAA-CBA-CGA-O2A
26	J	3001	LMG	O8-C28-C29-C30
27	1	607	CHL	CAA-CBA-CGA-O2A
20	3	609	CLA	CBA-CGA-O2A-C1
20	A	828	CLA	CAA-CBA-CGA-O2A
20	A	843	CLA	CAA-CBA-CGA-O2A
20	B	838	CLA	CAA-CBA-CGA-O2A
20	3	620	CLA	CAA-CBA-CGA-O2A
20	5	603	CLA	C2A-CAA-CBA-CGA
20	B	817	CLA	CBA-CGA-O2A-C1
20	B	832	CLA	C3-C5-C6-C7
22	4	623	LHG	C8-C7-O7-C5
22	Z	620	LHG	O7-C7-C8-C9
22	5	623	LHG	O7-C7-C8-C9
27	3	608	CHL	CAA-CBA-CGA-O2A
20	7	616	CLA	O1A-CGA-O2A-C1
20	8	616	CLA	CAA-CBA-CGA-O1A
20	A	807	CLA	C11-C10-C8-C7
20	A	811	CLA	C2-C3-C5-C6
27	1	601	CHL	C2-C3-C5-C6
20	B	816	CLA	C6-C7-C8-C9
20	A	813	CLA	CAA-CBA-CGA-O2A
20	B	826	CLA	C3-C5-C6-C7
20	A	814	CLA	C14-C13-C15-C16
20	A	842	CLA	C11-C10-C8-C9
20	B	832	CLA	C11-C10-C8-C9
20	Z	608	CLA	C11-C12-C13-C14
20	B	806	CLA	C5-C6-C7-C8
27	6	608	CHL	O1A-CGA-O2A-C1
20	6	601	CLA	CAA-CBA-CGA-O2A
22	8	620	LHG	O9-C7-C8-C9
22	1	620	LHG	C25-C26-C27-C28
20	8	603	CLA	CAA-CBA-CGA-O1A
20	A	823	CLA	CAA-CBA-CGA-O2A
23	7	624	BCR	C7-C8-C9-C34
20	Z	603	CLA	CAA-CBA-CGA-O1A
20	A	805	CLA	C6-C7-C8-C9
20	A	812	CLA	C16-C17-C18-C19
20	A	820	CLA	C16-C17-C18-C20
20	B	852	CLA	C4-C3-C5-C6
20	1	613	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
20	F	301	CLA	C2-C3-C5-C6
20	A	823	CLA	CAA-CBA-CGA-O1A
20	B	807	CLA	CAA-CBA-CGA-O1A
20	B	812	CLA	CAA-CBA-CGA-O1A
26	J	3001	LMG	O10-C28-C29-C30
20	8	601	CLA	C10-C11-C12-C13
20	A	817	CLA	C1A-C2A-CAA-CBA
20	B	841	CLA	C1A-C2A-CAA-CBA
20	F	301	CLA	C1A-C2A-CAA-CBA
20	8	602	CLA	C1A-C2A-CAA-CBA
20	4	613	CLA	C1A-C2A-CAA-CBA
20	6	609	CLA	C1A-C2A-CAA-CBA
27	4	607	CHL	C1A-C2A-CAA-CBA
27	6	608	CHL	C1A-C2A-CAA-CBA
20	Z	612	CLA	CAA-CBA-CGA-O1A
20	5	609	CLA	CAA-CBA-CGA-O1A
20	A	823	CLA	C2-C1-O2A-CGA
20	6	602	CLA	C2-C1-O2A-CGA
20	A	842	CLA	C13-C15-C16-C17
20	8	613	CLA	C8-C10-C11-C12
27	6	608	CHL	CBA-CGA-O2A-C1
20	Z	616	CLA	CAA-CBA-CGA-O1A
20	4	613	CLA	CAA-CBA-CGA-O1A
20	5	613	CLA	CAA-CBA-CGA-O1A
20	6	613	CLA	CAA-CBA-CGA-O1A
27	8	607	CHL	CAA-CBA-CGA-O1A
20	B	811	CLA	CAA-CBA-CGA-O2A
20	4	603	CLA	CAA-CBA-CGA-O2A
20	A	842	CLA	C2A-CAA-CBA-CGA
20	B	812	CLA	C2A-CAA-CBA-CGA
20	B	816	CLA	C2A-CAA-CBA-CGA
20	1	610	CLA	C2A-CAA-CBA-CGA
20	Z	610	CLA	C2A-CAA-CBA-CGA
27	3	608	CHL	C2A-CAA-CBA-CGA
20	Z	613	CLA	CAA-CBA-CGA-O1A
20	7	602	CLA	C8-C10-C11-C12
20	B	806	CLA	CAA-CBA-CGA-O1A
20	1	603	CLA	CAA-CBA-CGA-O1A
20	3	620	CLA	CAA-CBA-CGA-O1A
20	6	622	CLA	CAA-CBA-CGA-O1A
20	1	610	CLA	C5-C6-C7-C8
20	8	610	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	A	846	LHG	C3-O3-P-O5
22	A	846	LHG	C4-O6-P-O5
22	A	855	LHG	C3-O3-P-O5
22	Z	620	LHG	C3-O3-P-O5
22	Z	620	LHG	C4-O6-P-O5
22	6	619	LHG	C4-O6-P-O4
20	8	610	CLA	C11-C12-C13-C15
20	A	806	CLA	CAA-CBA-CGA-O1A
20	1	613	CLA	CAA-CBA-CGA-O1A
20	3	613	CLA	CAA-CBA-CGA-O1A
20	4	609	CLA	CAA-CBA-CGA-O1A
22	4	622	LHG	O9-C7-C8-C9
27	Z	607	CHL	CAA-CBA-CGA-O1A
20	A	826	CLA	CAA-CBA-CGA-O2A
23	B	848	BCR	C23-C24-C25-C26
23	G	205	BCR	C23-C24-C25-C26
23	L	205	BCR	C5-C6-C7-C8
23	3	719	BCR	C23-C24-C25-C26
28	Z	618	LUT	C5-C6-C7-C8
20	A	828	CLA	CAA-CBA-CGA-O1A
20	B	816	CLA	CAA-CBA-CGA-O1A
20	B	824	CLA	CAA-CBA-CGA-O1A
20	1	616	CLA	CAA-CBA-CGA-O1A
20	3	612	CLA	CAA-CBA-CGA-O1A
20	8	613	CLA	CAA-CBA-CGA-O1A
22	Z	620	LHG	O9-C7-C8-C9
27	1	607	CHL	CAA-CBA-CGA-O1A
22	A	846	LHG	C12-C13-C14-C15
20	3	610	CLA	O1A-CGA-O2A-C1
20	L	203	CLA	C16-C17-C18-C20
20	B	803	CLA	CAA-CBA-CGA-O2A
20	B	841	CLA	CAA-CBA-CGA-O2A
20	3	602	CLA	O1D-CGD-O2D-CED
20	A	843	CLA	CAA-CBA-CGA-O1A
20	7	613	CLA	CAA-CBA-CGA-O1A
27	4	607	CHL	CAA-CBA-CGA-O1A
20	A	828	CLA	C4-C3-C5-C6
20	B	820	CLA	C4-C3-C5-C6
20	8	613	CLA	C2-C3-C5-C6
20	A	814	CLA	CAD-CBD-CGD-O1D
20	A	820	CLA	CAD-CBD-CGD-O1D
20	A	826	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
20	A	829	CLA	CAD-CBD-CGD-O1D
20	A	831	CLA	CAD-CBD-CGD-O1D
20	A	839	CLA	CAD-CBD-CGD-O1D
20	B	805	CLA	CAD-CBD-CGD-O1D
20	B	813	CLA	CAD-CBD-CGD-O1D
20	B	833	CLA	CAD-CBD-CGD-O1D
20	B	836	CLA	CAD-CBD-CGD-O1D
20	L	203	CLA	CAD-CBD-CGD-O1D
20	6	622	CLA	CAD-CBD-CGD-O1D
20	A	838	CLA	CBD-CGD-O2D-CED
20	L	204	CLA	O1A-CGA-O2A-C1
20	B	813	CLA	CAA-CBA-CGA-O1A
20	B	838	CLA	CAA-CBA-CGA-O1A
22	Z	620	LHG	C25-C26-C27-C28
20	3	617	CLA	CAA-CBA-CGA-O2A
20	7	609	CLA	CAA-CBA-CGA-O2A
20	B	806	CLA	C14-C13-C15-C16
20	B	826	CLA	C6-C7-C8-C9
20	A	813	CLA	CAA-CBA-CGA-O1A
20	4	603	CLA	CAA-CBA-CGA-O1A
22	5	623	LHG	O9-C7-C8-C9
20	L	204	CLA	CBA-CGA-O2A-C1
20	A	820	CLA	C3-C5-C6-C7
20	A	802	CLA	CAA-CBA-CGA-O2A
20	A	804	CLA	CAA-CBA-CGA-O2A
20	B	809	CLA	CAA-CBA-CGA-O2A
22	Z	620	LHG	O8-C23-C24-C25
20	A	812	CLA	C8-C10-C11-C12
20	B	828	CLA	CAA-CBA-CGA-O2A
20	K	4003	CLA	CAA-CBA-CGA-O2A
20	1	613	CLA	C13-C15-C16-C17
20	8	613	CLA	C13-C15-C16-C17
23	A	849	BCR	C7-C8-C9-C34
26	J	3001	LMG	C11-C12-C13-C14
20	A	843	CLA	C12-C13-C15-C16
20	A	854	CLA	C3A-C2A-CAA-CBA
20	B	806	CLA	C12-C13-C15-C16
20	B	826	CLA	C6-C7-C8-C10
20	B	827	CLA	C6-C7-C8-C10
20	F	301	CLA	C3A-C2A-CAA-CBA
20	1	609	CLA	C11-C10-C8-C7
20	3	610	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
20	Z	608	CLA	C11-C12-C13-C15
20	6	602	CLA	C11-C12-C13-C15
20	B	809	CLA	CAA-CBA-CGA-O1A
20	3	617	CLA	CAA-CBA-CGA-O1A
20	4	601	CLA	CAA-CBA-CGA-O1A
20	5	614	CLA	CAA-CBA-CGA-O2A
20	3	617	CLA	O1A-CGA-O2A-C1
20	A	810	CLA	CAA-CBA-CGA-O2A
20	A	841	CLA	CAA-CBA-CGA-O2A
20	G	204	CLA	CAA-CBA-CGA-O2A
20	4	601	CLA	CAA-CBA-CGA-O2A
22	1	620	LHG	O7-C7-C8-C9
20	1	608	CLA	C15-C16-C17-C18
23	B	801	BCR	C21-C22-C23-C24
28	8	618	LUT	C11-C12-C13-C14
28	Z	617	LUT	C7-C8-C9-C10
20	A	802	CLA	CAA-CBA-CGA-O1A
20	A	810	CLA	CAA-CBA-CGA-O1A
20	B	811	CLA	CAA-CBA-CGA-O1A
20	6	601	CLA	CAA-CBA-CGA-O1A
22	Z	620	LHG	O10-C23-C24-C25
23	K	4001	BCR	C15-C16-C17-C18
23	5	625	BCR	C9-C10-C11-C12
28	8	617	LUT	C29-C30-C31-C32
28	Z	618	LUT	C29-C30-C31-C32
20	7	603	CLA	CAA-CBA-CGA-O2A
22	A	846	LHG	O8-C23-C24-C25
22	A	855	LHG	O8-C23-C24-C25
20	A	820	CLA	C8-C10-C11-C12
27	3	608	CHL	CAA-CBA-CGA-O1A
20	6	604	CLA	C15-C16-C17-C18
20	5	610	CLA	CAA-CBA-CGA-O2A
22	6	619	LHG	C29-C30-C31-C32
20	A	819	CLA	C10-C11-C12-C13
20	7	609	CLA	CAA-CBA-CGA-O1A
20	8	604	CLA	O1A-CGA-O2A-C1
20	7	613	CLA	C13-C15-C16-C17
20	A	828	CLA	C3-C5-C6-C7
20	G	204	CLA	CAA-CBA-CGA-O1A
22	1	620	LHG	O9-C7-C8-C9
20	A	830	CLA	CAA-CBA-CGA-O2A
20	6	603	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

247 monomers are involved in 554 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	8	619	BCR	5	0
20	B	811	CLA	1	0
20	F	304	CLA	2	0
20	K	4003	CLA	2	0
20	B	837	CLA	5	0
20	1	608	CLA	3	0
20	3	620	CLA	1	0
20	Z	613	CLA	2	0
20	A	829	CLA	11	0
20	A	806	CLA	8	0
20	5	603	CLA	1	0
20	5	604	CLA	2	0
21	A	844	PQN	1	0
20	B	813	CLA	5	0
20	5	602	CLA	5	0
20	B	802	CLA	3	0
23	B	801	BCR	4	0
27	5	607	CHL	2	0
20	B	841	CLA	5	0
20	7	606	CLA	1	0
28	6	621	LUT	7	0
20	6	616	CLA	3	0
23	A	851	BCR	4	0
20	7	612	CLA	1	0
27	3	608	CHL	5	0
20	8	610	CLA	2	0
20	4	613	CLA	3	0
20	B	814	CLA	1	0
20	6	604	CLA	2	0
20	B	839	CLA	4	0
28	3	622	LUT	3	0
20	A	810	CLA	3	0
20	Z	610	CLA	3	0
20	A	805	CLA	4	0
20	4	614	CLA	2	0
23	K	4001	BCR	2	0
20	B	817	CLA	5	0
20	8	604	CLA	1	0
20	4	612	CLA	3	0
20	5	611	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	846	BCR	4	0
23	B	843	BCR	6	0
20	B	834	CLA	2	0
23	I	172	BCR	2	0
28	7	622	LUT	3	0
20	8	608	CLA	2	0
20	B	832	CLA	5	0
20	B	807	CLA	3	0
23	J	3003	BCR	3	0
23	F	305	BCR	6	0
20	7	610	CLA	3	0
20	A	838	CLA	1	0
20	L	203	CLA	1	0
23	B	847	BCR	2	0
20	A	814	CLA	5	0
20	A	831	CLA	7	0
20	7	614	CLA	1	0
20	8	601	CLA	3	0
22	6	619	LHG	3	0
20	1	604	CLA	1	0
20	A	821	CLA	1	0
22	B	851	LHG	2	0
20	6	602	CLA	1	0
23	3	717	BCR	3	0
28	Z	618	LUT	3	0
23	L	201	BCR	3	0
23	5	625	BCR	6	0
20	3	614	CLA	1	0
28	4	619	LUT	7	0
27	8	607	CHL	1	0
20	5	601	CLA	3	0
20	5	617	CLA	2	0
20	3	607	CLA	3	0
20	5	614	CLA	1	0
23	A	856	BCR	3	0
20	A	842	CLA	3	0
20	B	821	CLA	1	0
20	A	815	CLA	3	0
20	B	835	CLA	2	0
20	3	606	CLA	2	0
20	4	611	CLA	4	0
20	A	840	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	6	618	CHL	2	0
20	3	617	CLA	2	0
27	Z	601	CHL	5	0
27	1	607	CHL	1	0
20	A	826	CLA	3	0
23	7	623	BCR	5	0
20	7	604	CLA	2	0
20	B	820	CLA	2	0
20	8	613	CLA	5	0
20	F	301	CLA	4	0
20	A	833	CLA	3	0
20	5	621	CLA	1	0
23	K	4004	BCR	1	0
20	5	609	CLA	7	0
20	A	845	CLA	1	0
20	B	831	CLA	1	0
28	7	621	LUT	6	0
28	5	620	LUT	4	0
20	F	303	CLA	2	0
20	3	610	CLA	2	0
20	7	608	CLA	2	0
21	B	842	PQN	1	0
22	4	623	LHG	1	0
27	6	606	CHL	3	0
28	3	621	LUT	3	0
20	A	822	CLA	3	0
20	A	827	CLA	2	0
20	Z	616	CLA	1	0
27	6	608	CHL	1	0
20	A	818	CLA	3	0
20	B	805	CLA	8	0
23	L	205	BCR	1	0
20	B	816	CLA	1	0
28	Z	617	LUT	5	0
20	7	613	CLA	3	0
28	Z	619	LUT	3	0
20	5	610	CLA	1	0
22	5	623	LHG	1	0
20	3	612	CLA	2	0
27	6	607	CHL	2	0
27	5	618	CHL	1	0
20	A	837	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	823	CLA	2	0
20	B	836	CLA	3	0
20	A	843	CLA	6	0
28	8	618	LUT	5	0
20	4	609	CLA	2	0
28	1	619	LUT	3	0
20	A	813	CLA	1	0
20	Z	608	CLA	5	0
20	Z	603	CLA	2	0
20	4	601	CLA	4	0
23	3	719	BCR	6	0
20	1	613	CLA	1	0
28	1	618	LUT	5	0
20	6	611	CLA	2	0
20	6	614	CLA	2	0
20	A	811	CLA	3	0
20	1	602	CLA	6	0
22	4	622	LHG	5	0
20	A	828	CLA	3	0
20	6	610	CLA	5	0
23	B	844	BCR	3	0
23	5	622	BCR	4	0
20	1	609	CLA	2	0
23	3	718	BCR	6	0
20	B	833	CLA	4	0
23	7	624	BCR	1	0
27	5	608	CHL	3	0
20	A	854	CLA	5	0
20	B	818	CLA	5	0
20	5	613	CLA	3	0
20	4	610	CLA	1	0
20	A	836	CLA	2	0
20	Z	611	CLA	1	0
20	A	817	CLA	4	0
20	B	803	CLA	1	0
20	K	4002	CLA	1	0
20	3	609	CLA	3	0
28	4	620	LUT	2	0
20	A	804	CLA	2	0
23	4	621	BCR	2	0
20	A	834	CLA	3	0
20	B	829	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	807	CLA	4	0
20	1	612	CLA	1	0
20	7	601	CLA	6	0
20	A	830	CLA	4	0
20	3	613	CLA	1	0
20	A	808	CLA	2	0
20	1	610	CLA	1	0
20	A	825	CLA	2	0
20	1	611	CLA	1	0
23	A	848	BCR	3	0
23	6	625	BCR	4	0
20	8	614	CLA	4	0
20	1	614	CLA	3	0
20	1	603	CLA	1	0
20	6	601	CLA	1	0
20	A	819	CLA	2	0
20	7	609	CLA	3	0
20	8	602	CLA	3	0
23	A	850	BCR	4	0
27	4	608	CHL	1	0
20	4	603	CLA	1	0
20	3	603	CLA	2	0
22	A	847	LHG	3	0
20	B	838	CLA	4	0
25	B	850	DGD	2	0
20	1	606	CLA	5	0
28	5	624	LUT	5	0
23	A	852	BCR	3	0
20	A	824	CLA	1	0
22	Z	620	LHG	3	0
28	8	617	LUT	10	0
28	6	624	LUT	4	0
20	A	802	CLA	5	0
20	B	823	CLA	5	0
20	A	841	CLA	8	0
20	B	815	CLA	2	0
27	1	601	CHL	2	0
20	A	839	CLA	2	0
20	4	602	CLA	4	0
20	B	840	CLA	5	0
20	8	616	CLA	1	0
20	5	606	CLA	3	0

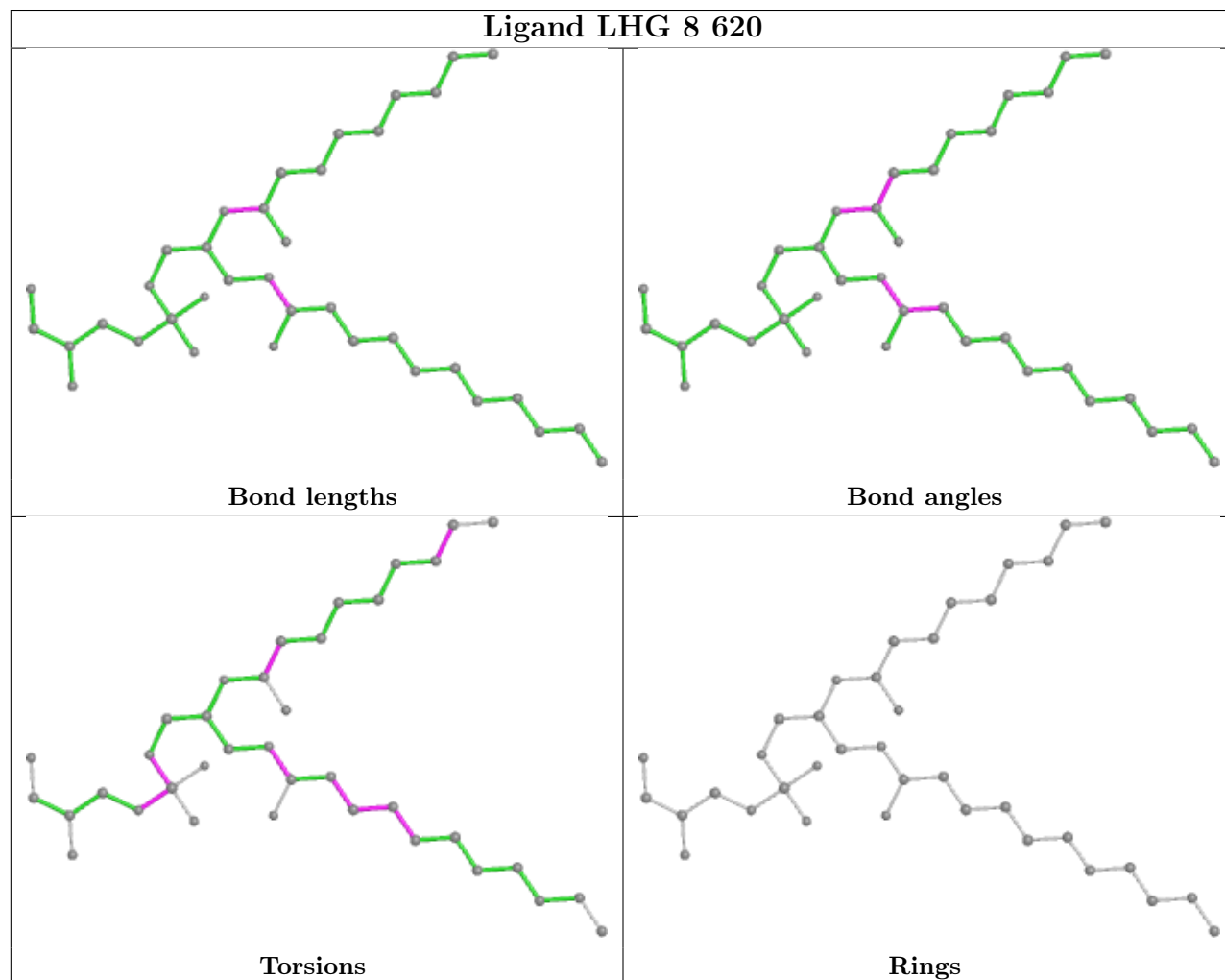
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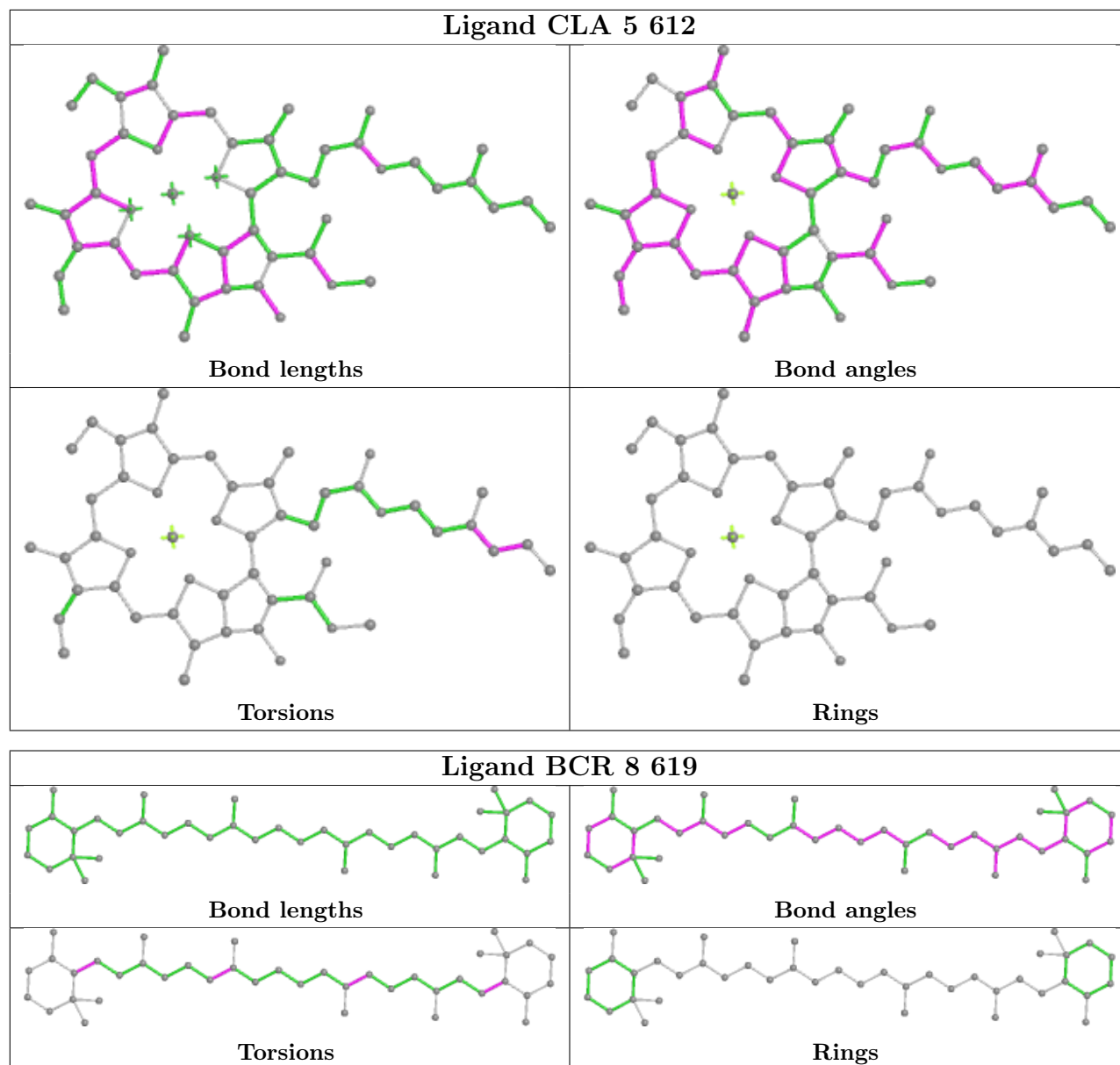
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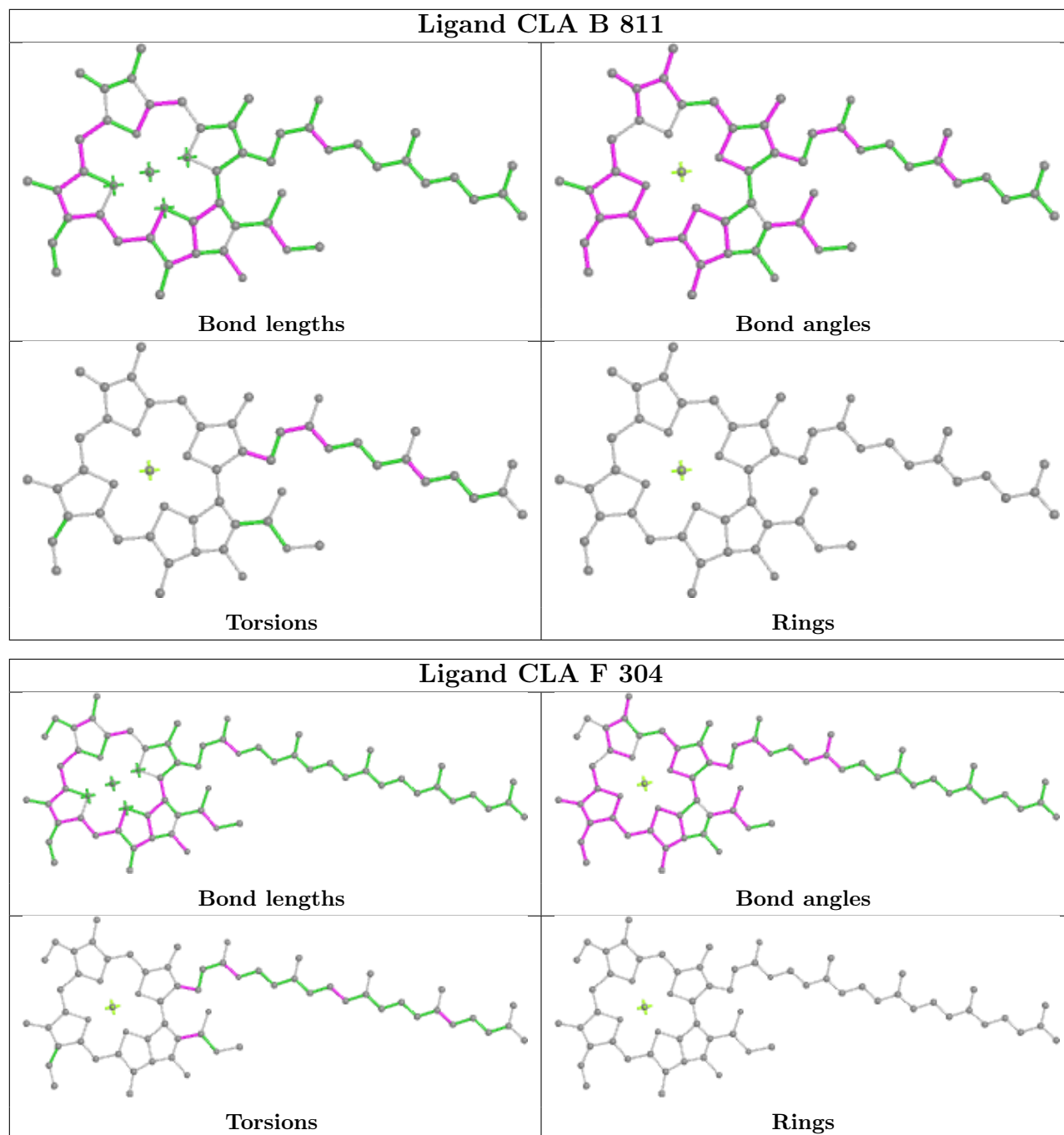
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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20	B	806	CLA	4	0
20	B	809	CLA	2	0
20	6	613	CLA	2	0
20	B	826	CLA	3	0
20	Z	602	CLA	4	0
20	Z	609	CLA	1	0
23	B	848	BCR	3	0
23	6	623	BCR	5	0
20	7	620	CLA	1	0
20	6	609	CLA	1	0
22	7	625	LHG	1	0
23	A	849	BCR	4	0
20	A	835	CLA	1	0
20	7	616	CLA	2	0
20	Z	604	CLA	1	0
20	B	828	CLA	3	0
20	B	819	CLA	2	0
20	A	816	CLA	5	0
28	1	617	LUT	7	0
20	A	820	CLA	3	0
20	B	830	CLA	3	0
20	3	602	CLA	1	0
20	A	803	CLA	2	0
20	B	827	CLA	2	0
20	B	825	CLA	5	0
20	3	604	CLA	2	0
20	B	822	CLA	1	0
20	7	602	CLA	1	0
20	8	606	CLA	2	0
20	A	809	CLA	4	0
20	6	622	CLA	2	0
20	B	824	CLA	4	0
20	Z	612	CLA	2	0
20	B	812	CLA	3	0
22	A	846	LHG	3	0
23	G	205	BCR	4	0
19	A	801	CL0	1	0
20	A	812	CLA	7	0

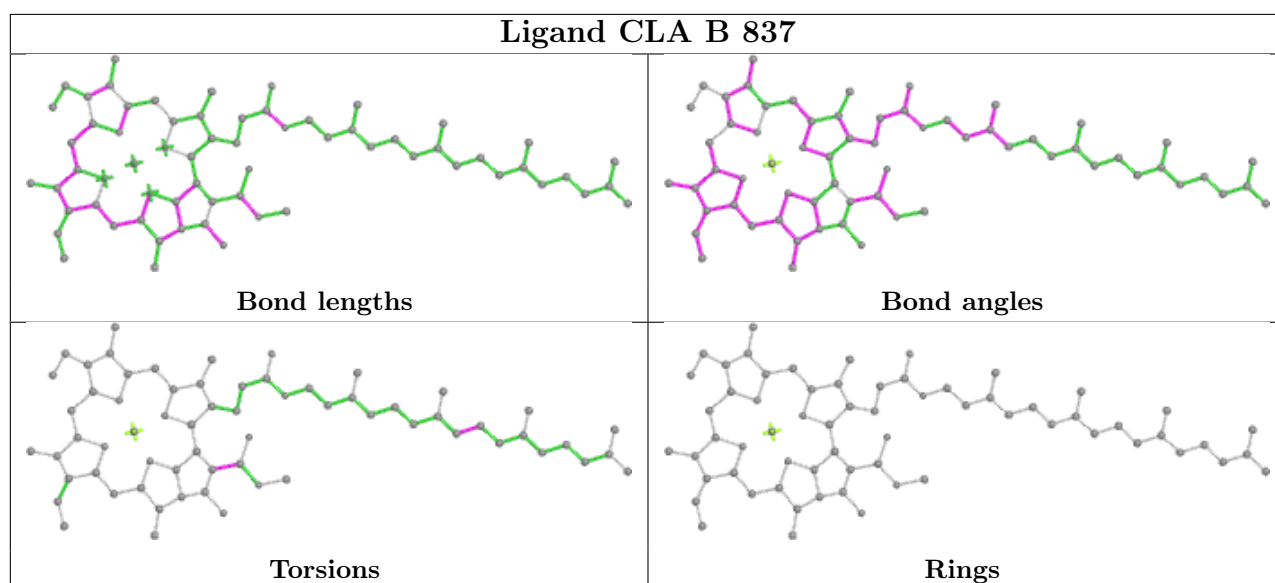
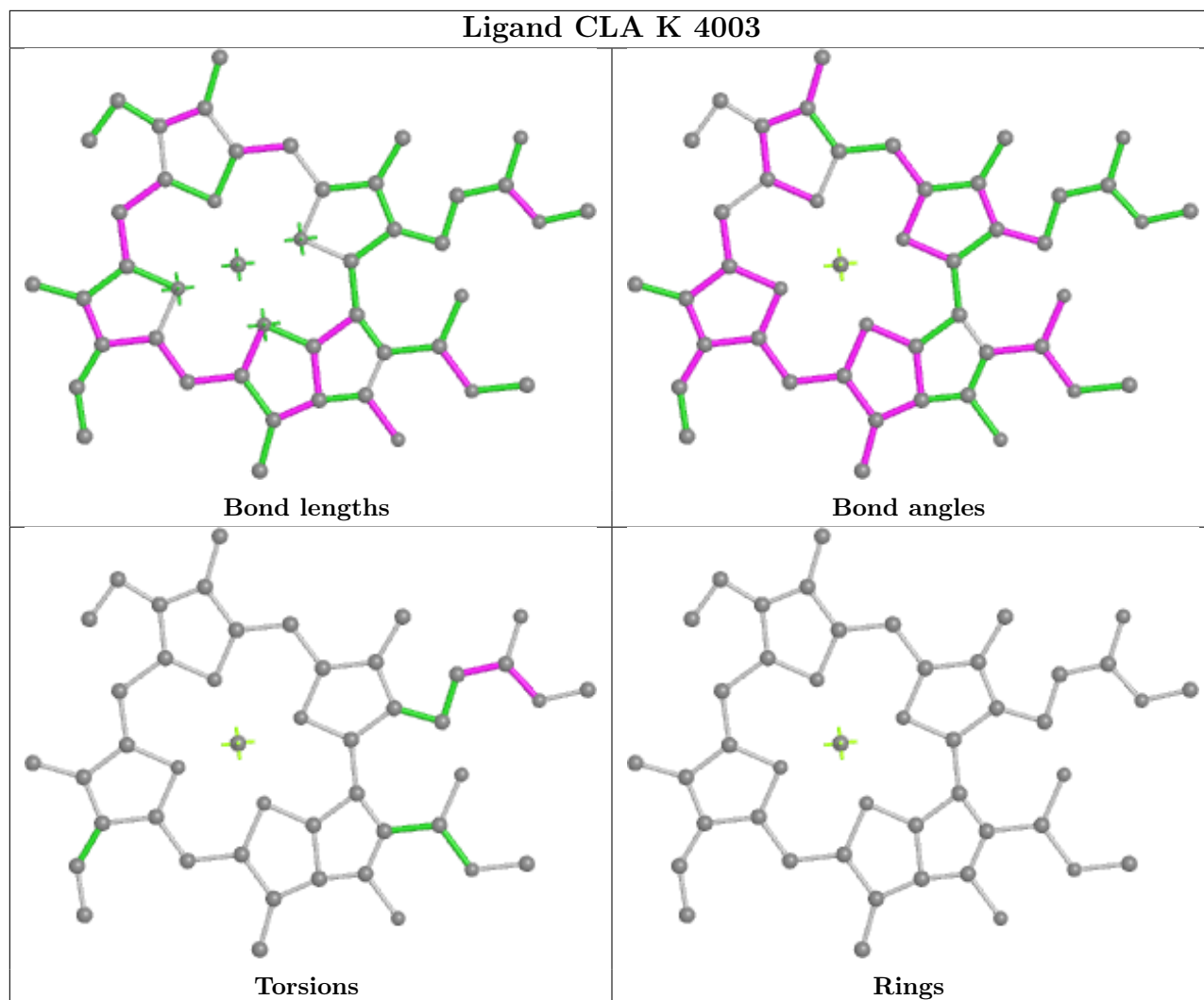
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

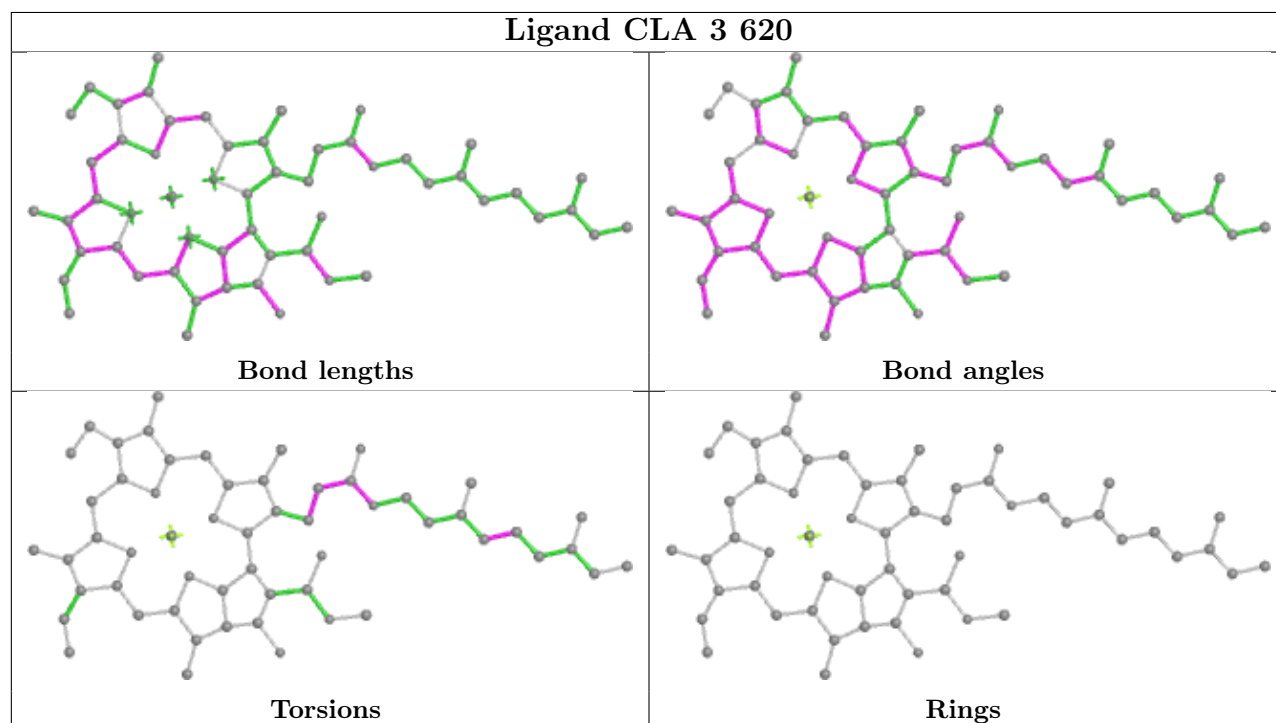
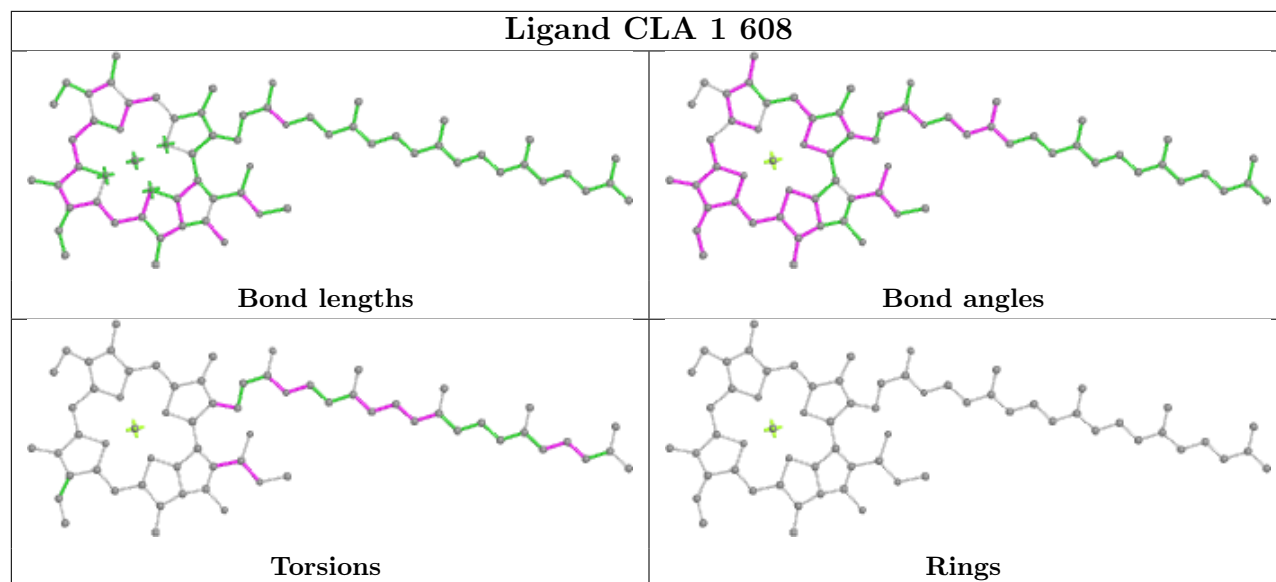
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

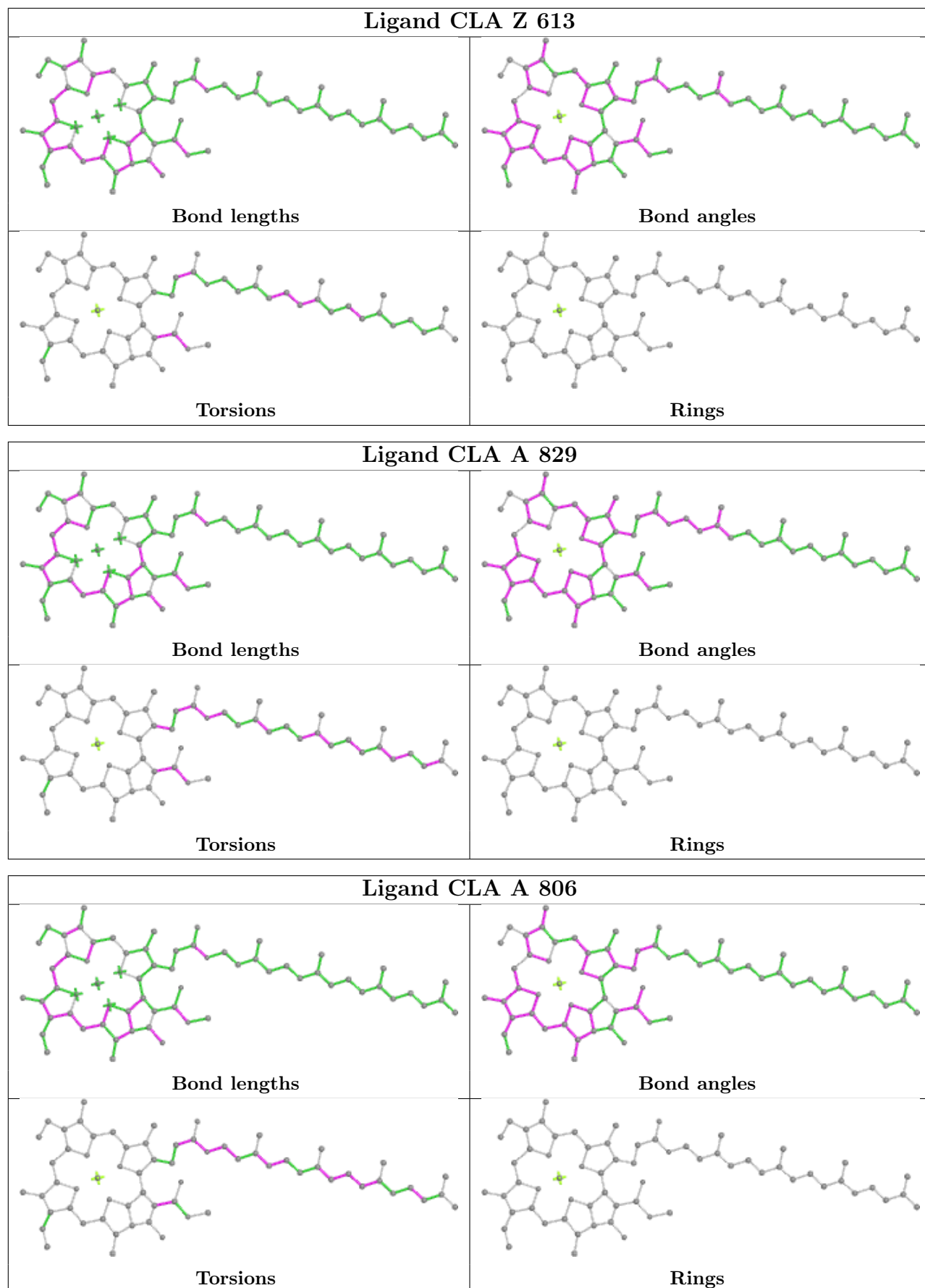


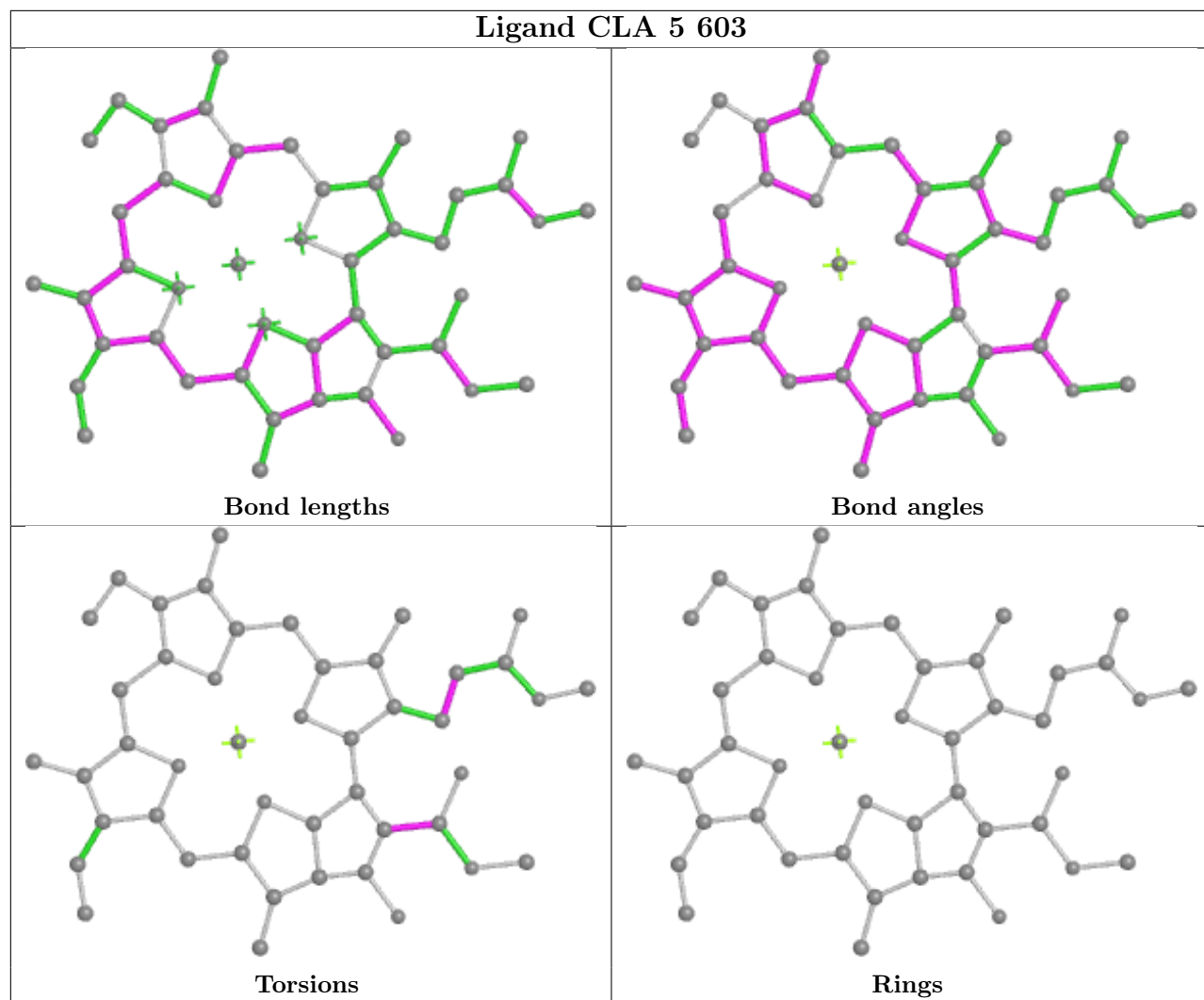


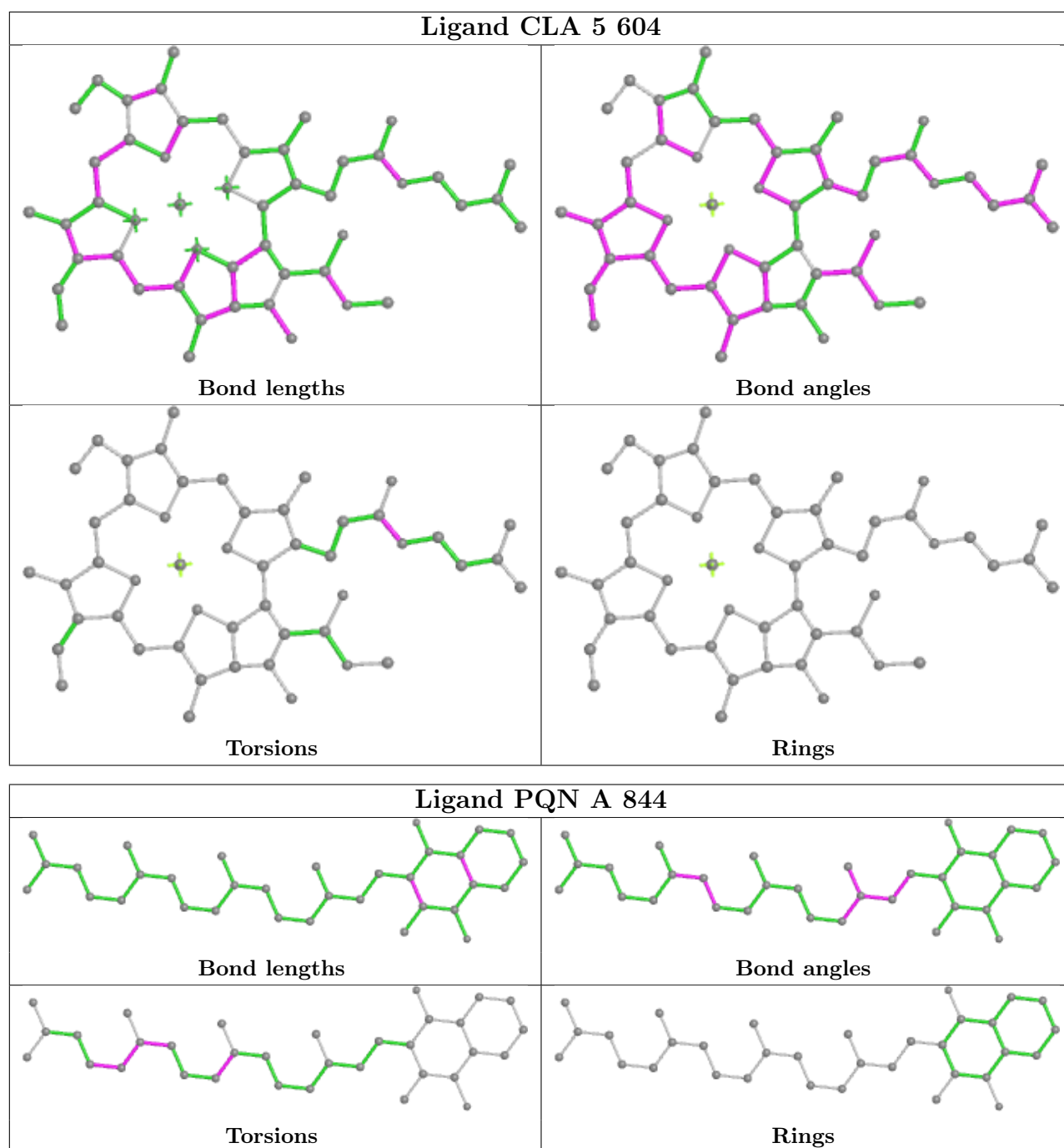


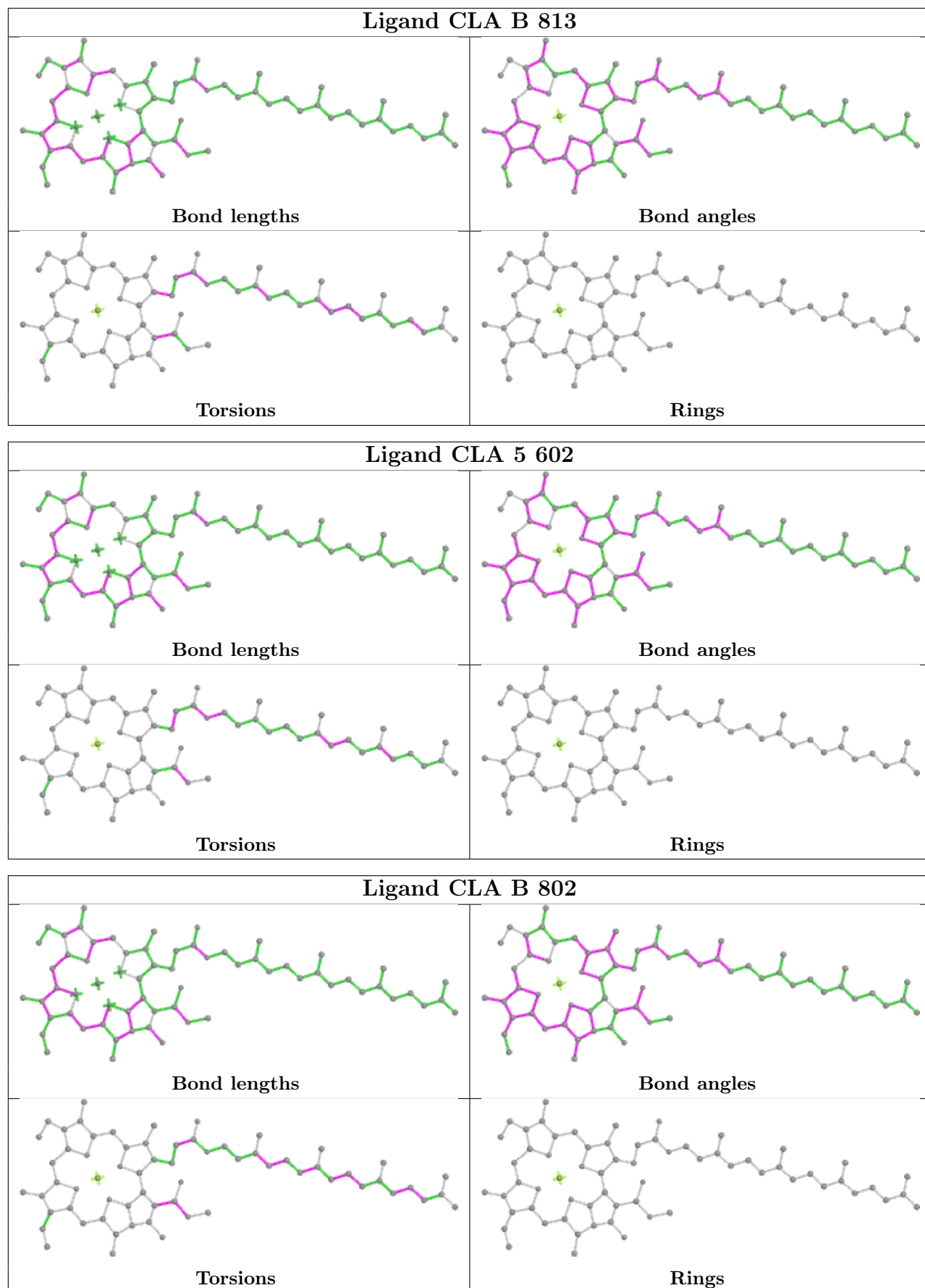


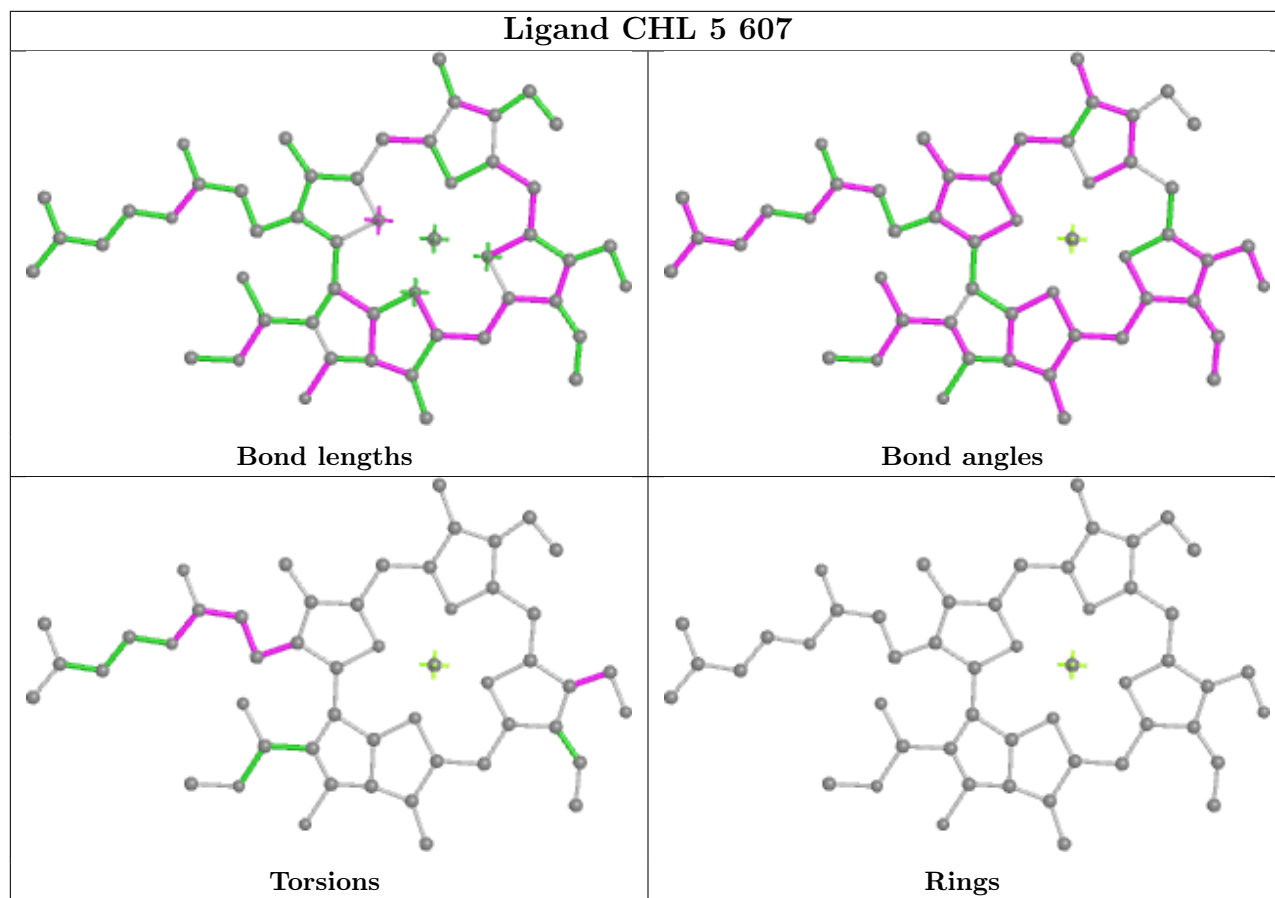
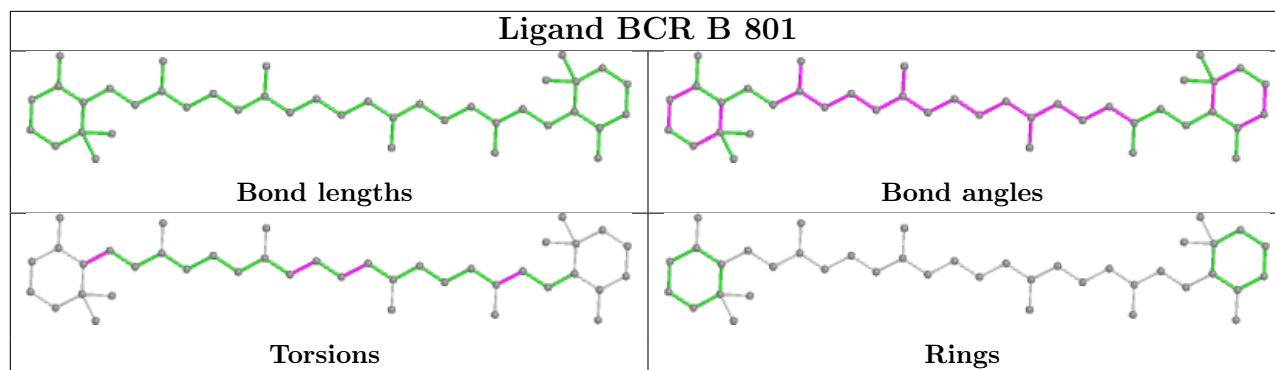


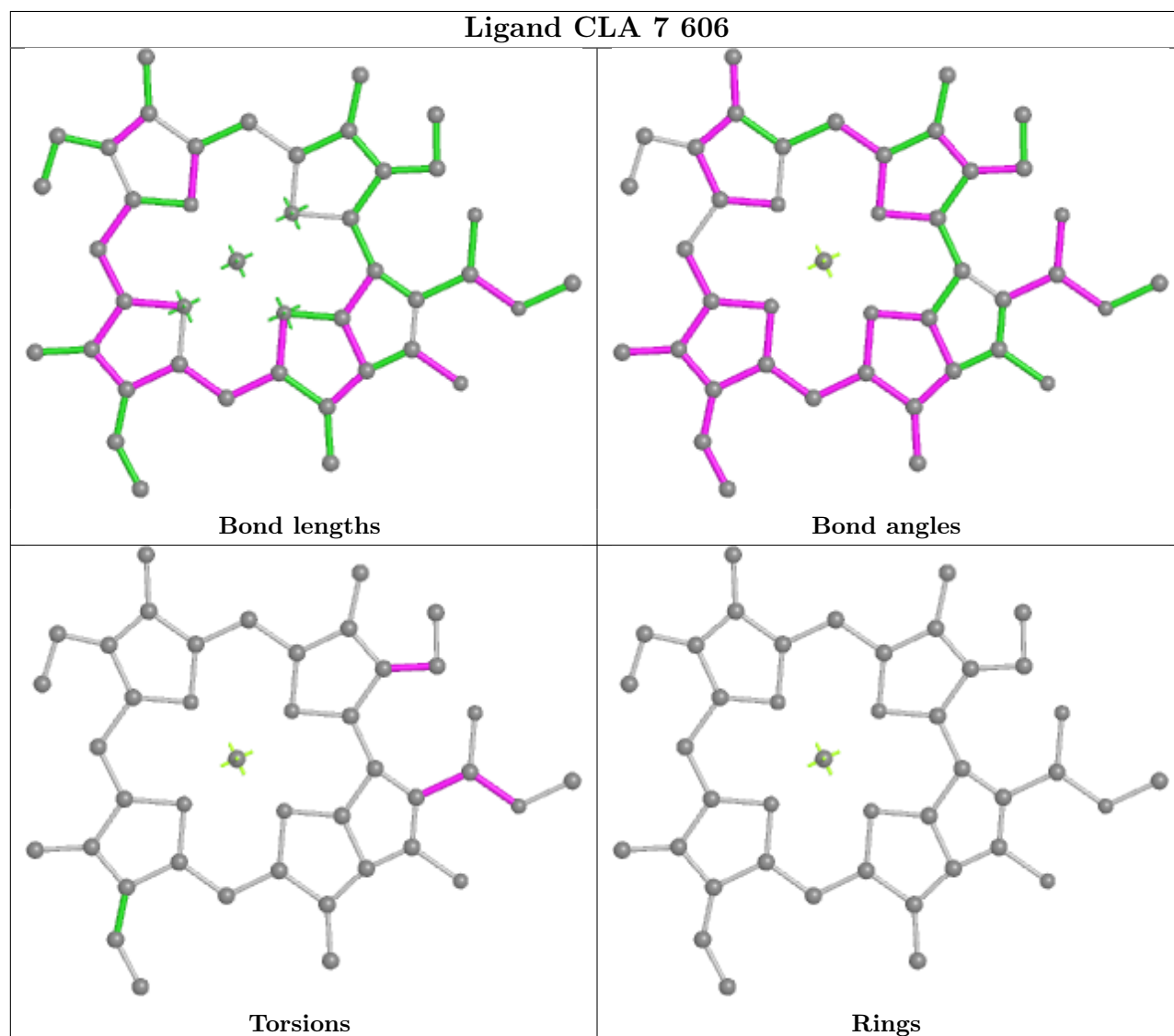
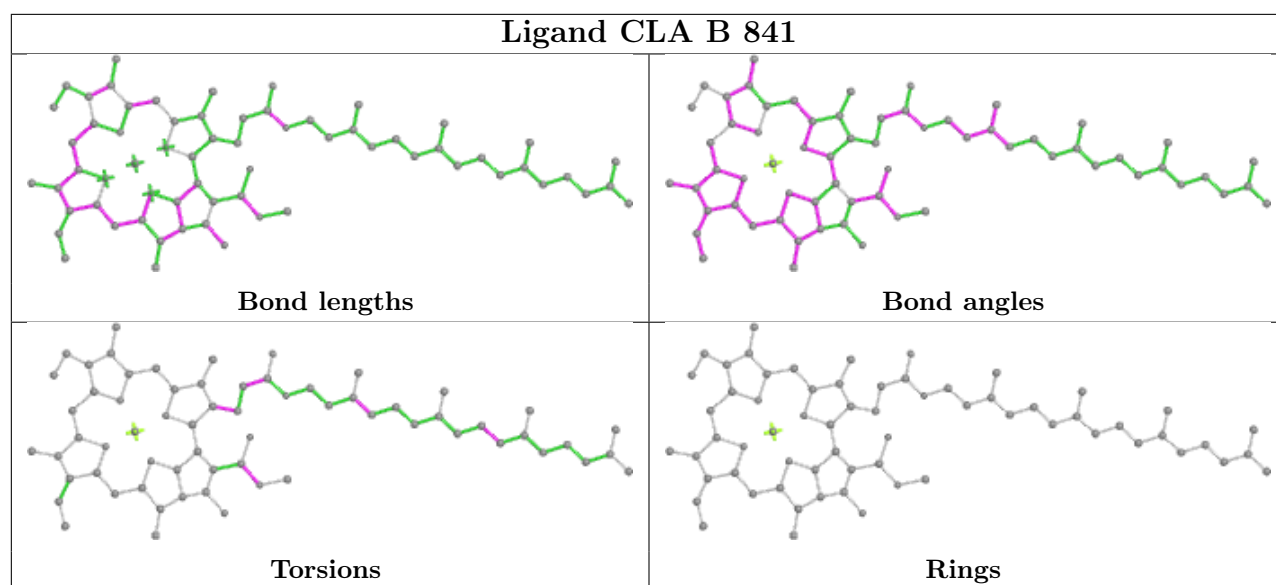


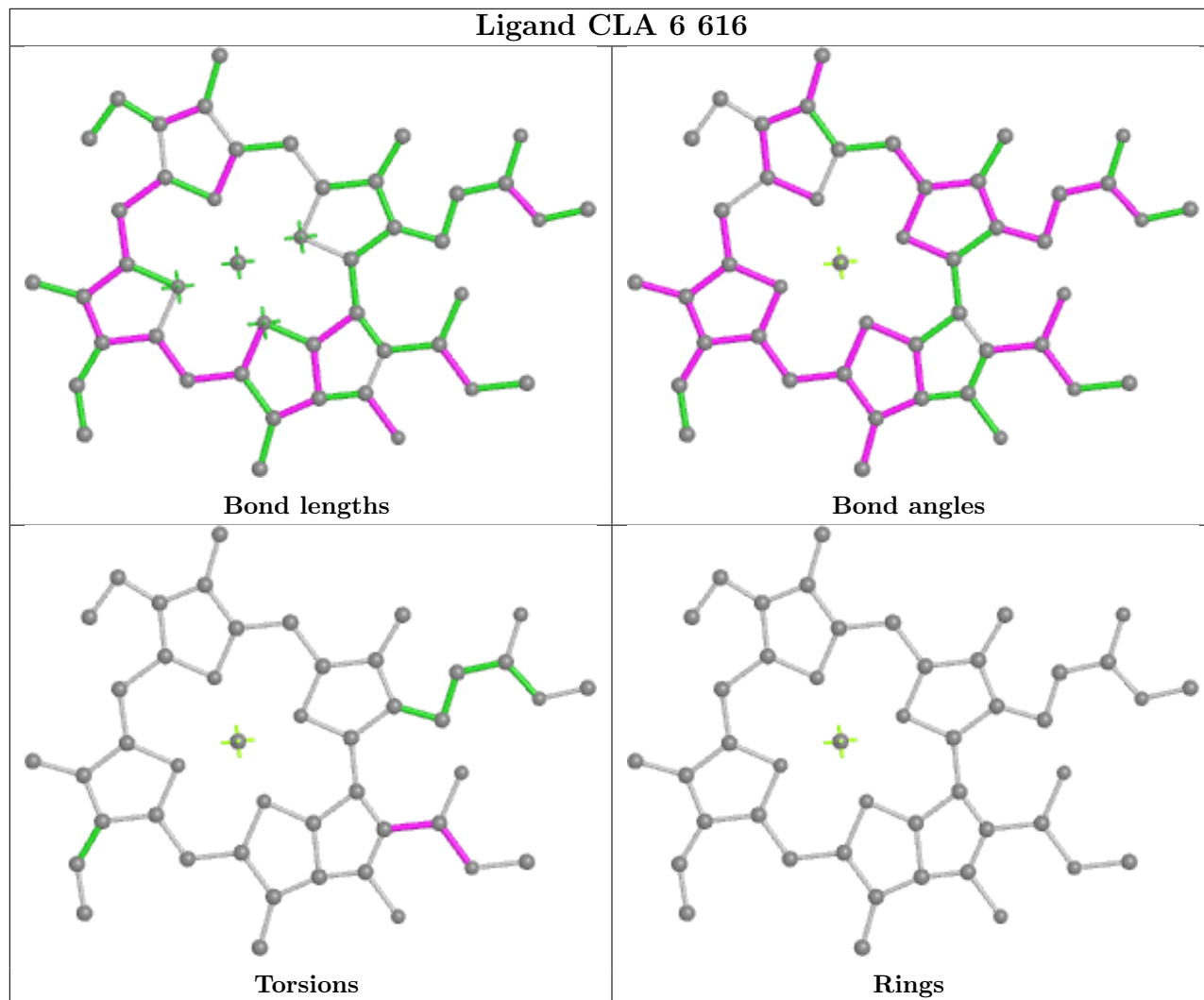
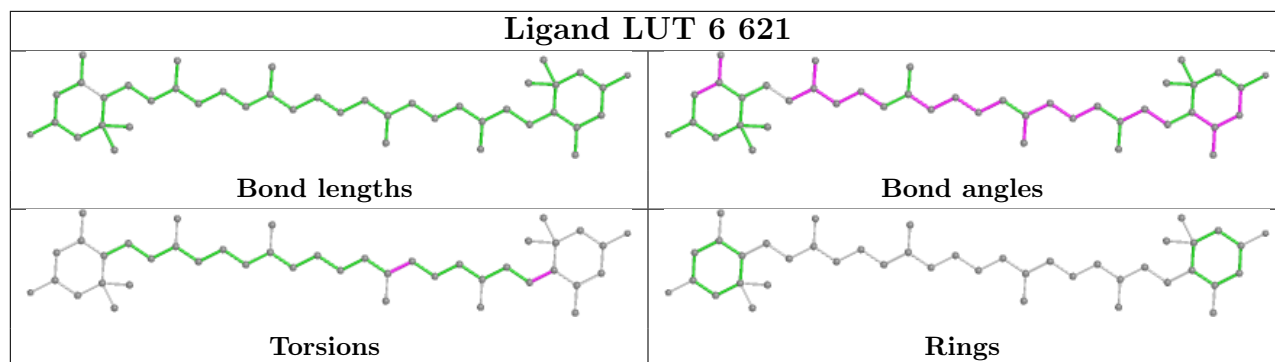


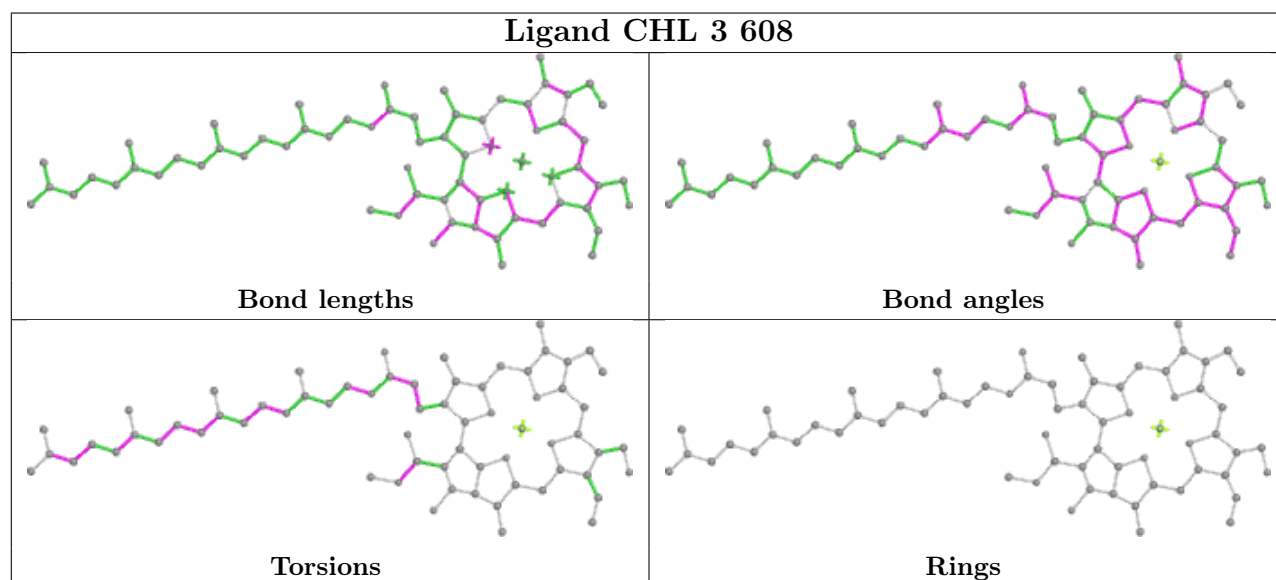
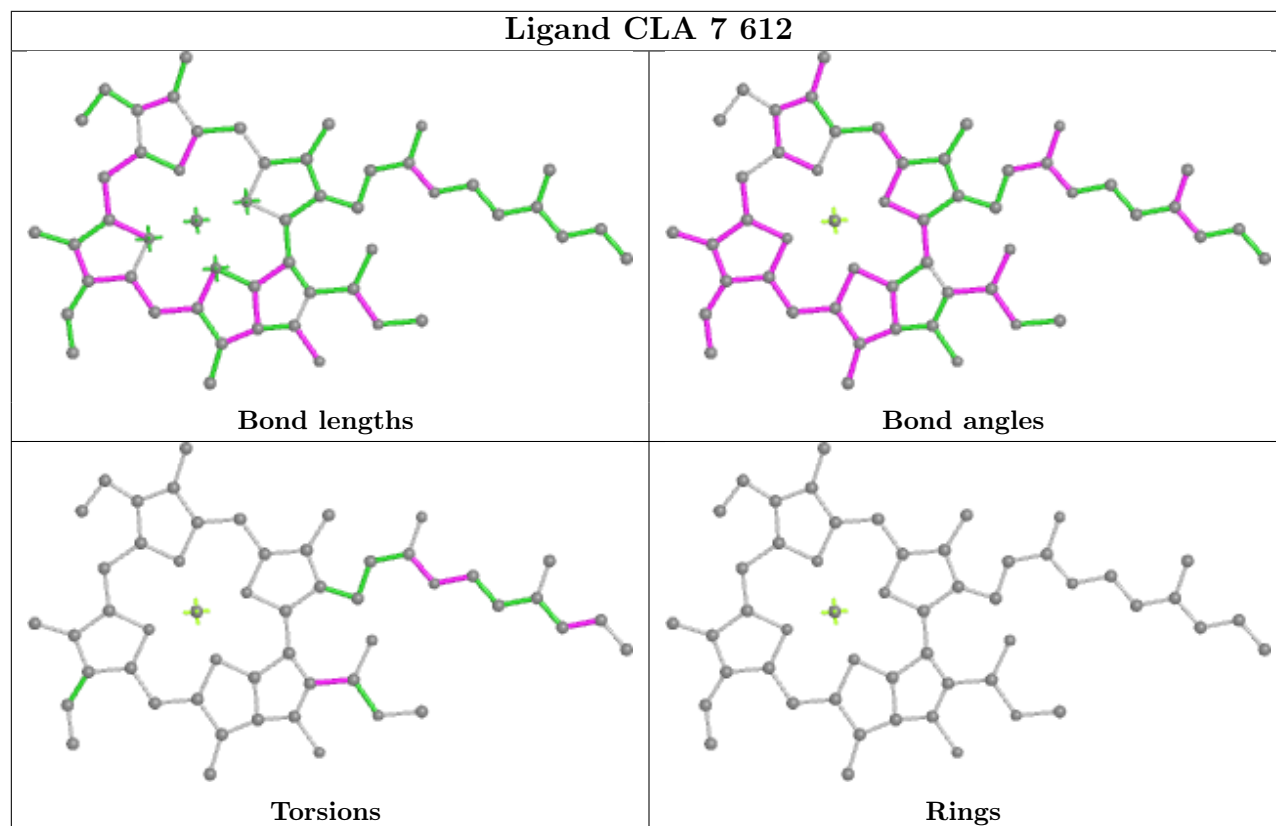
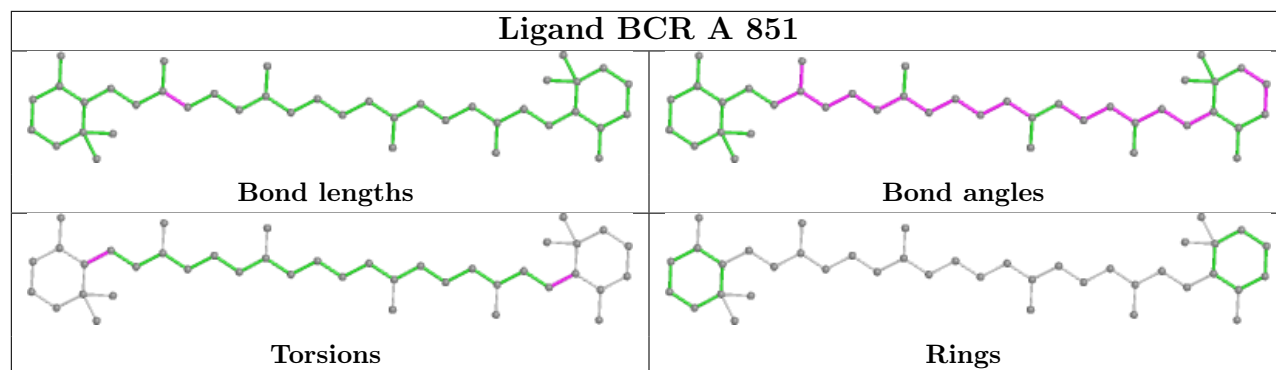


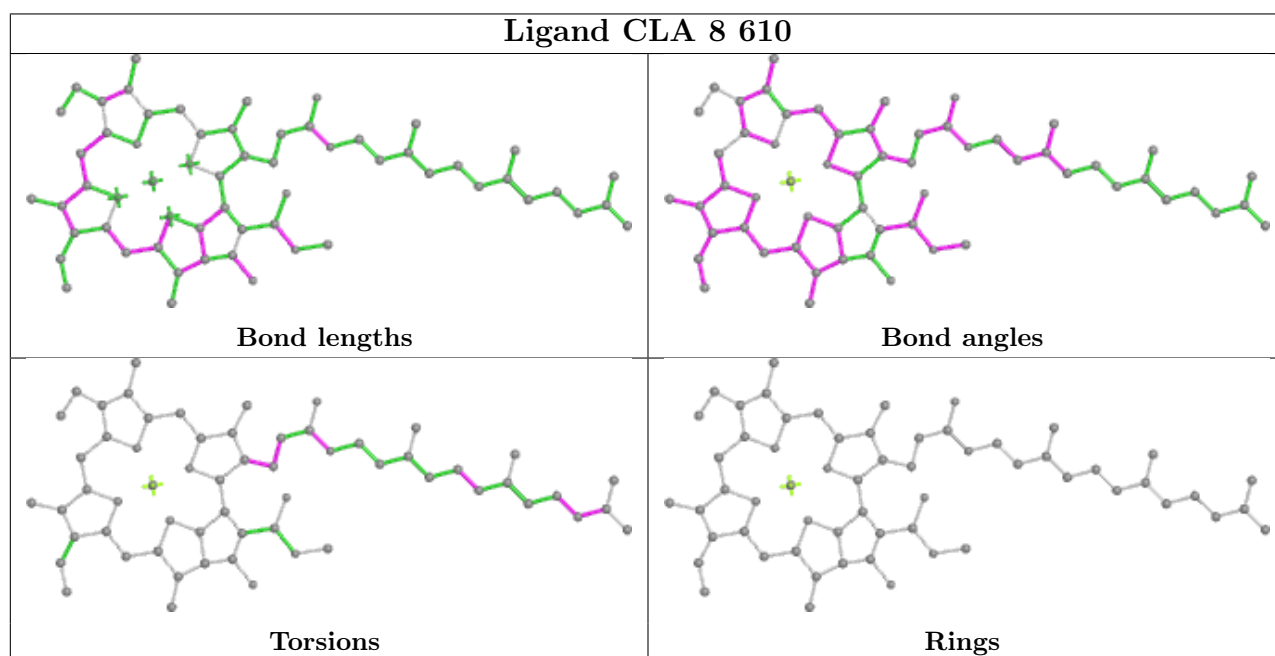
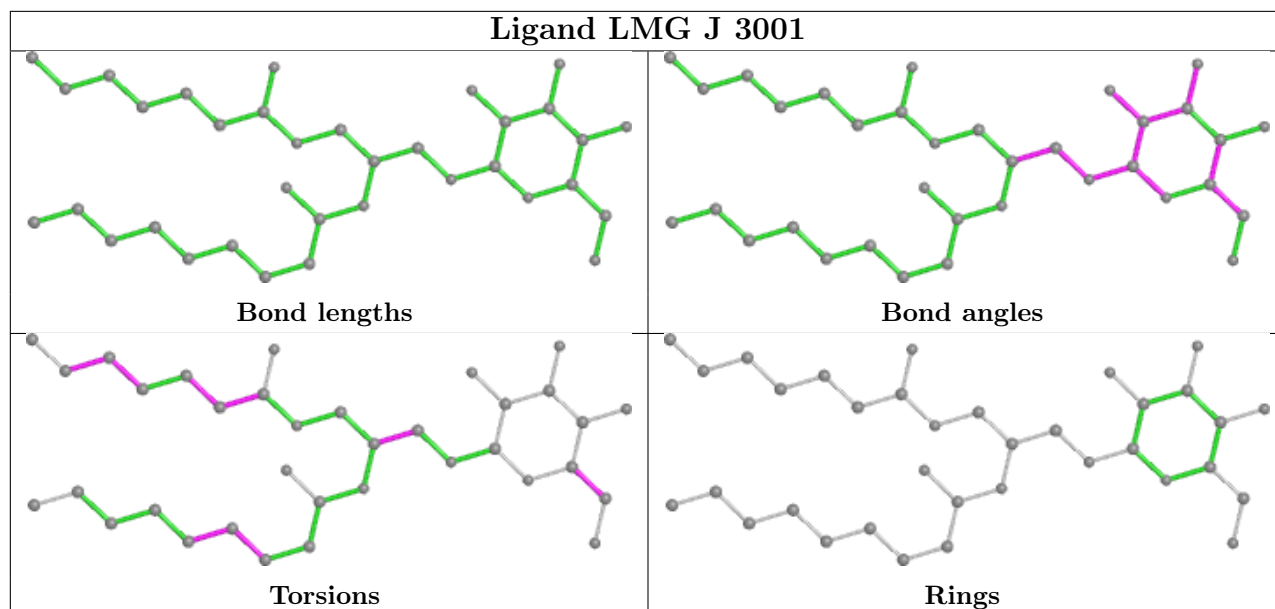




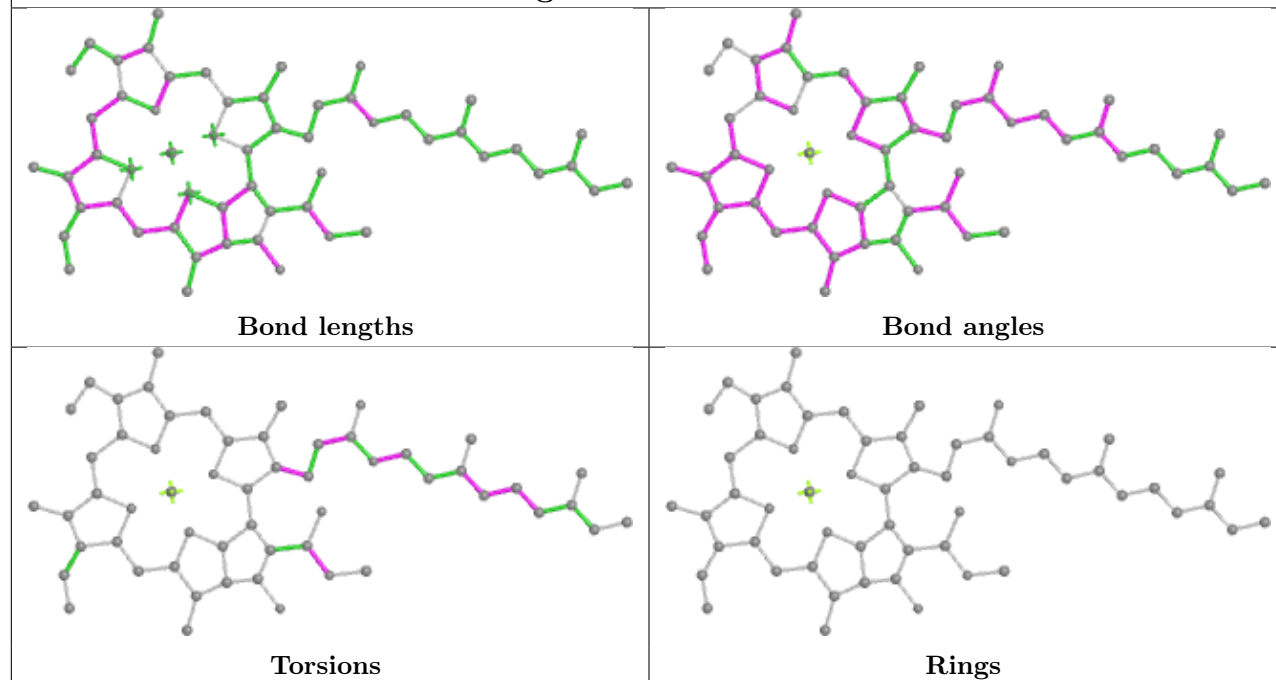




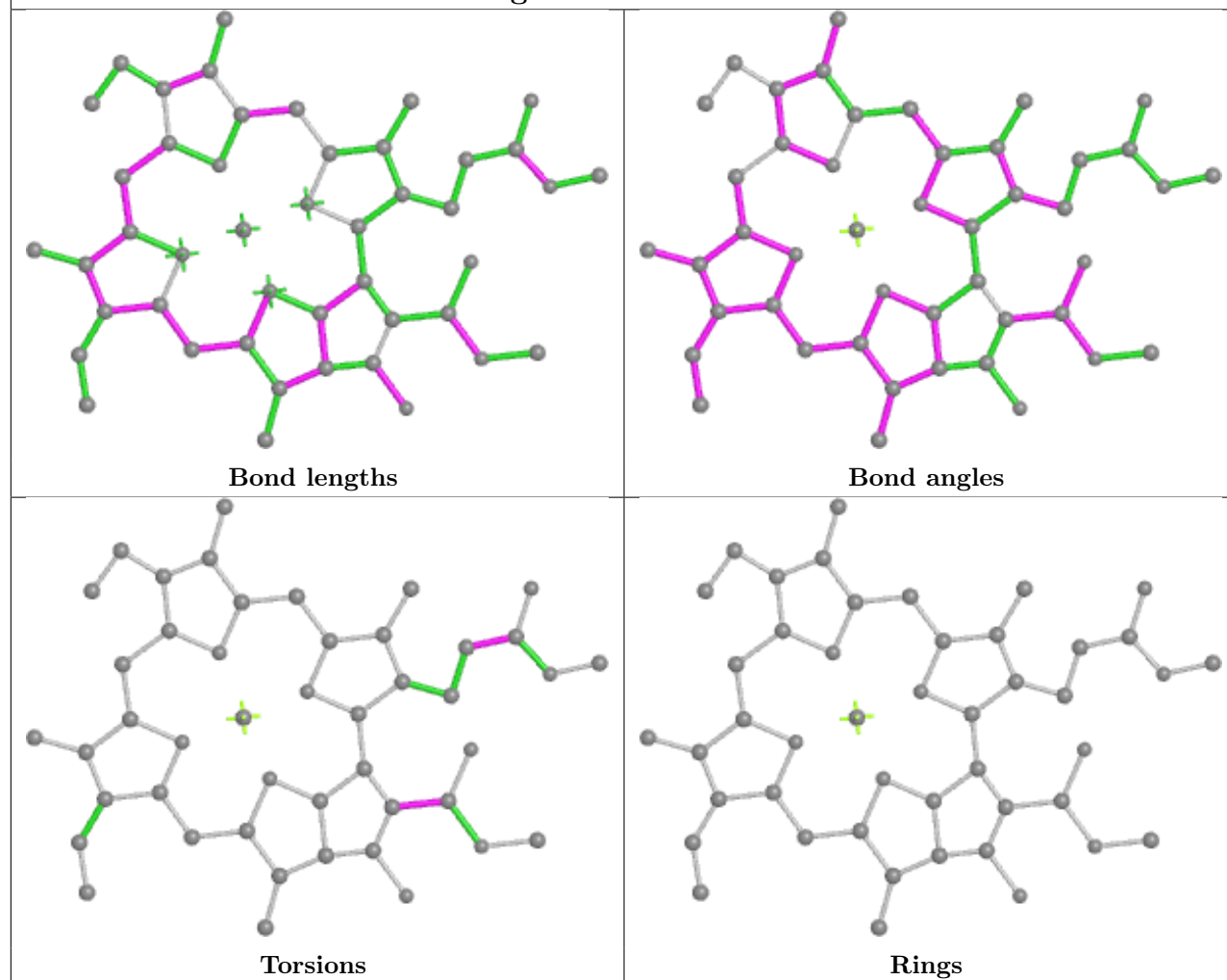


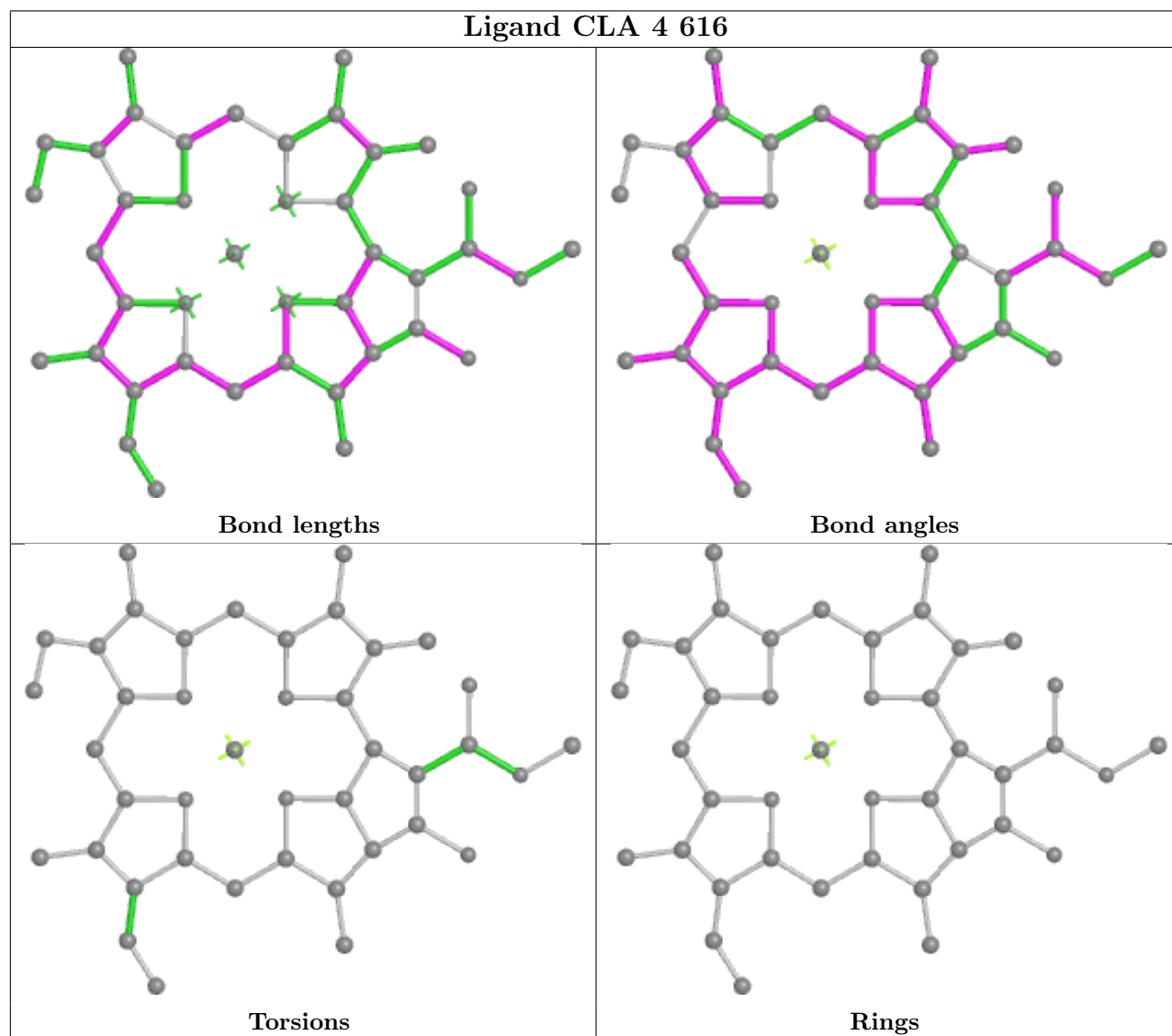
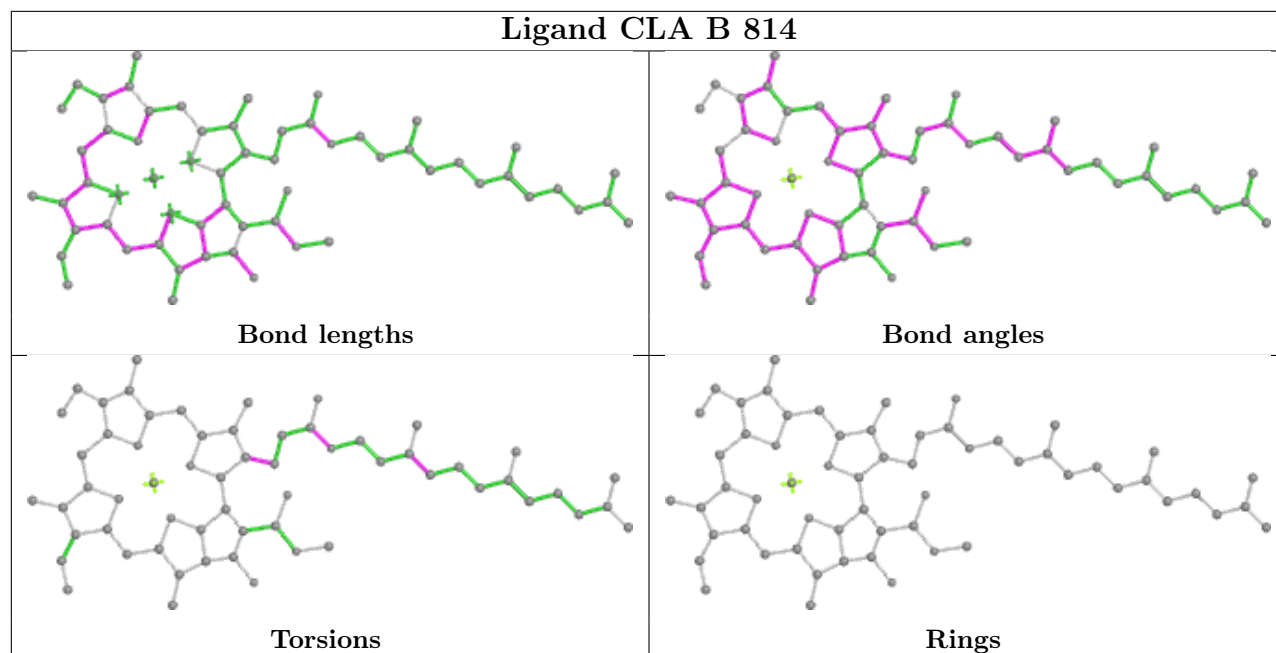


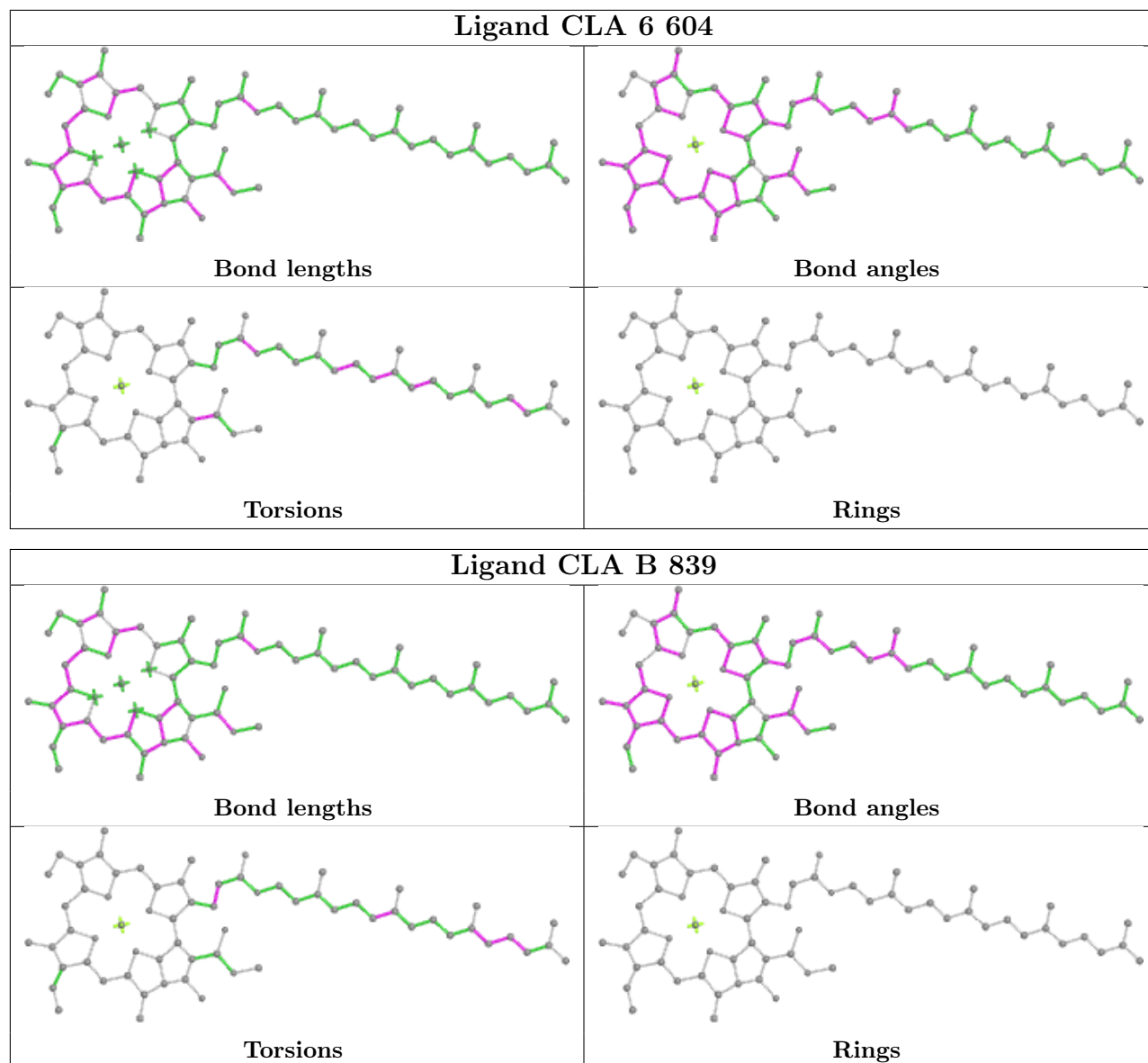
Ligand CLA 4 613

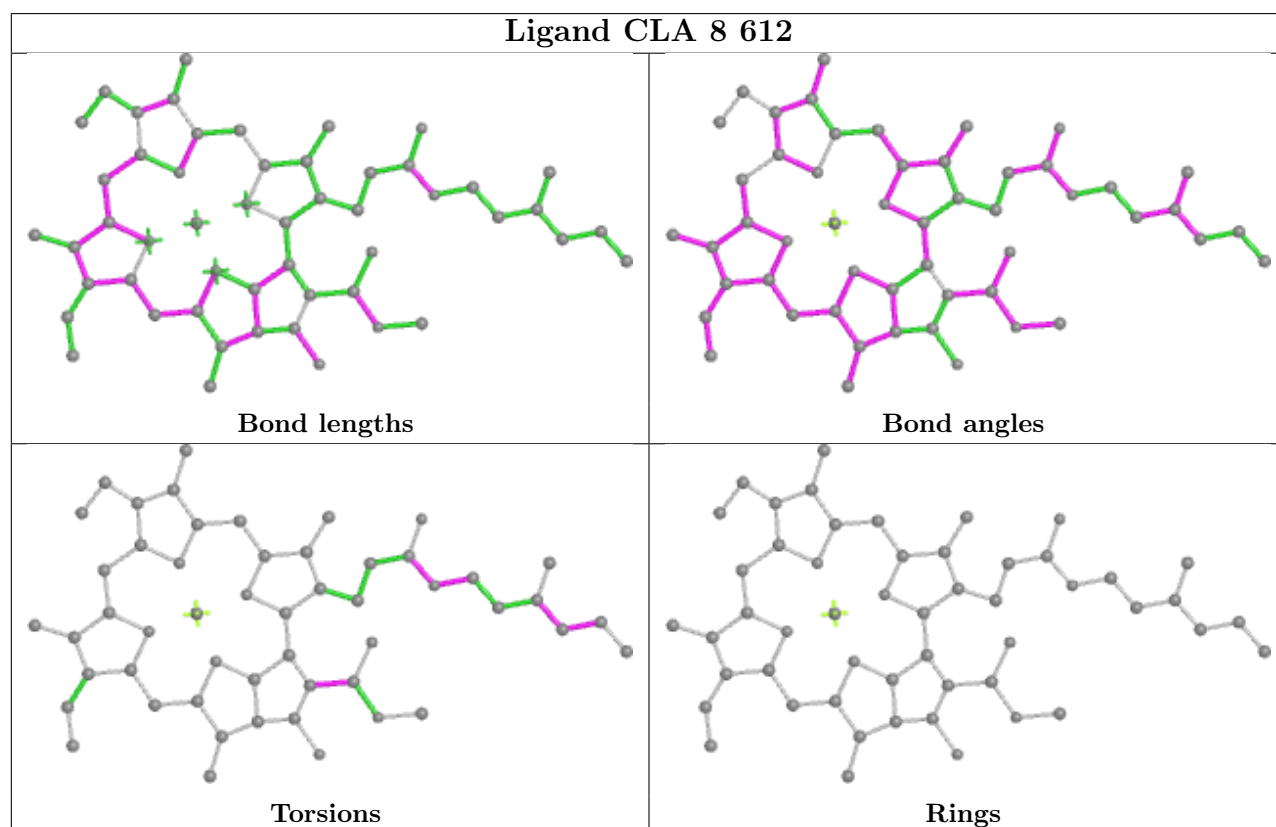
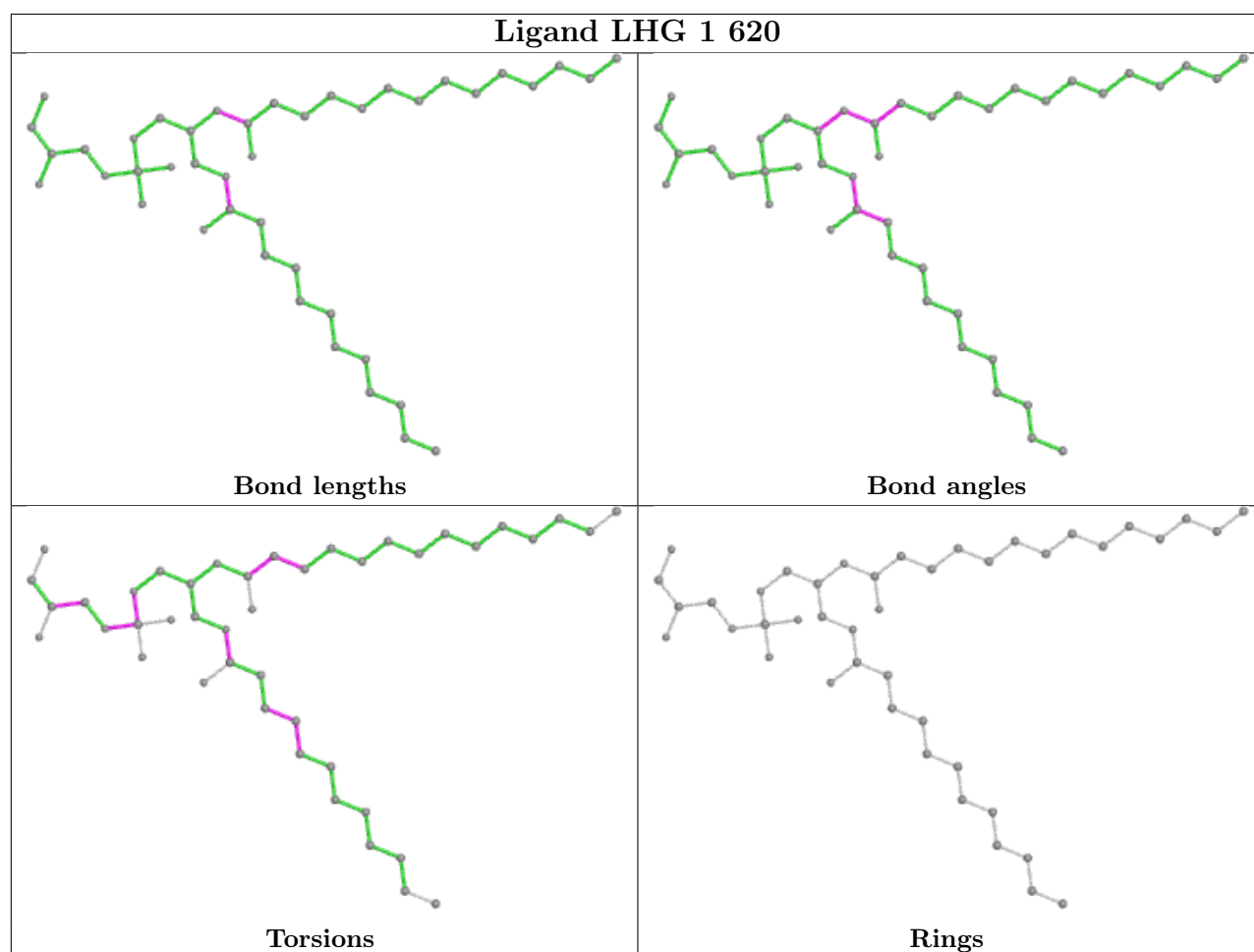


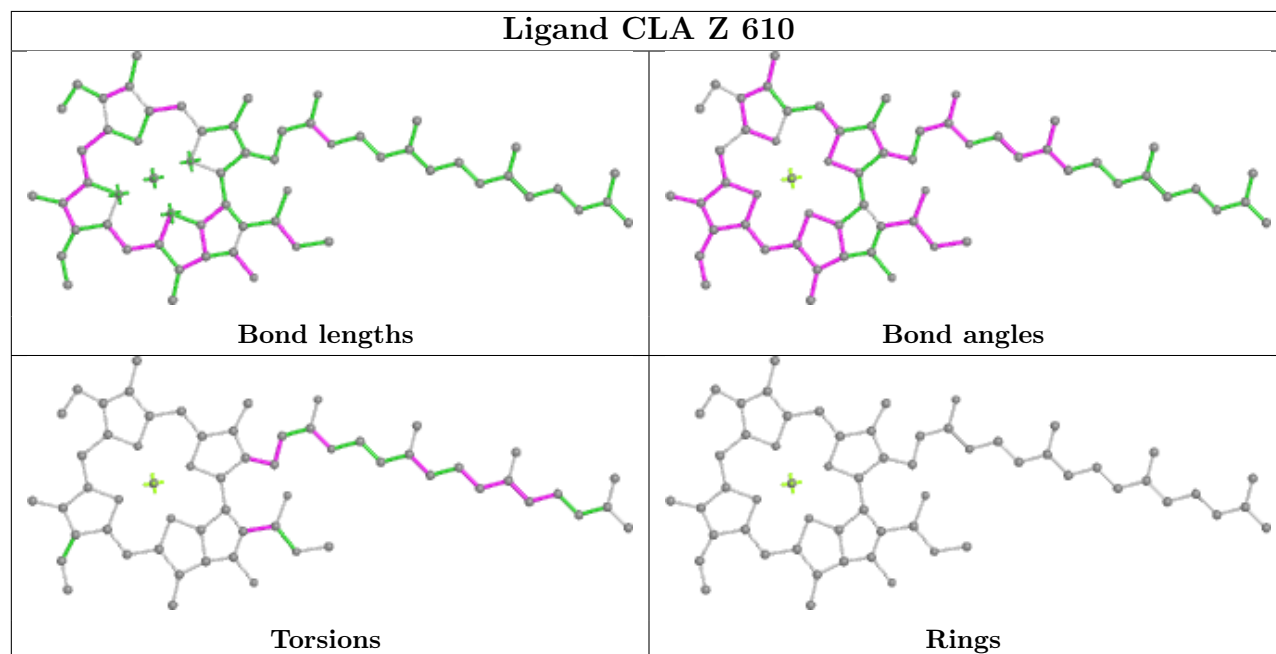
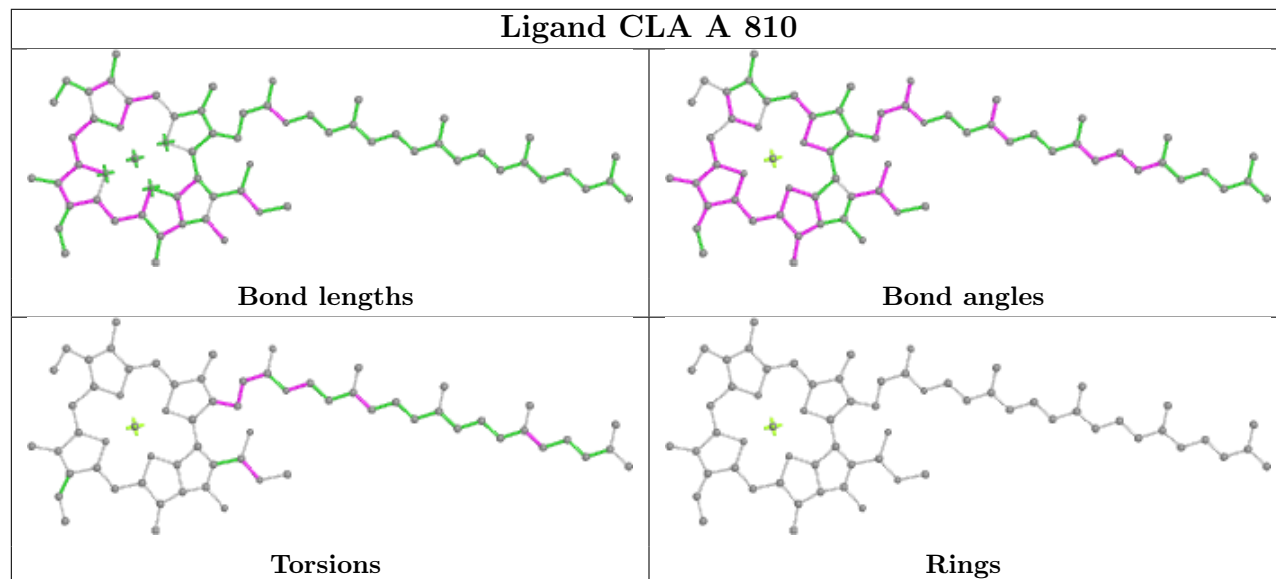
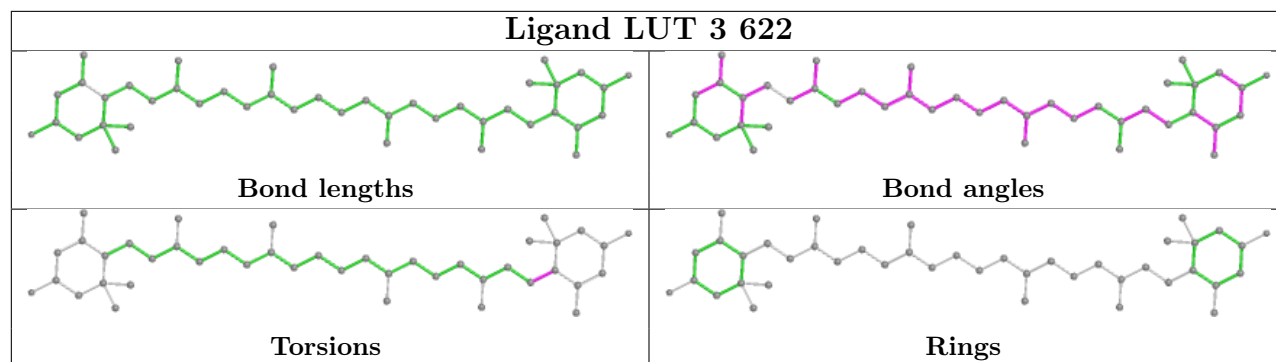
Ligand CLA G 204

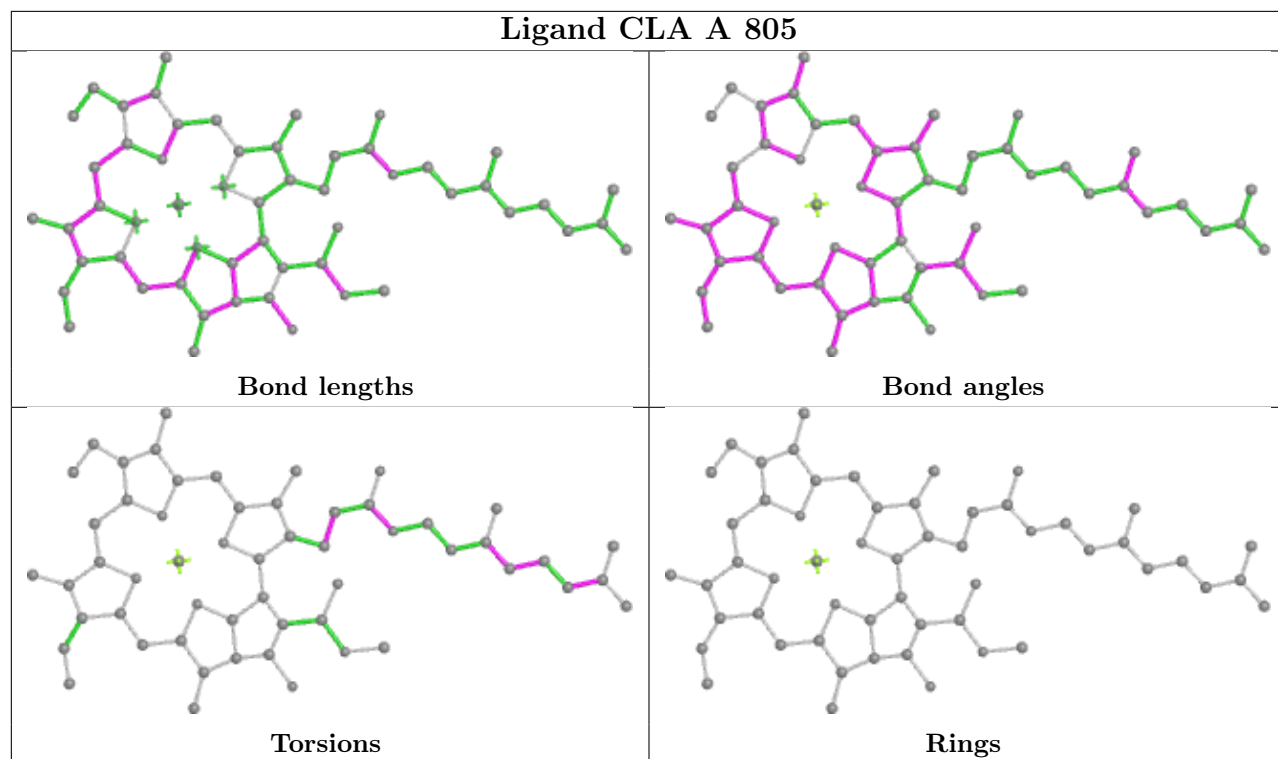


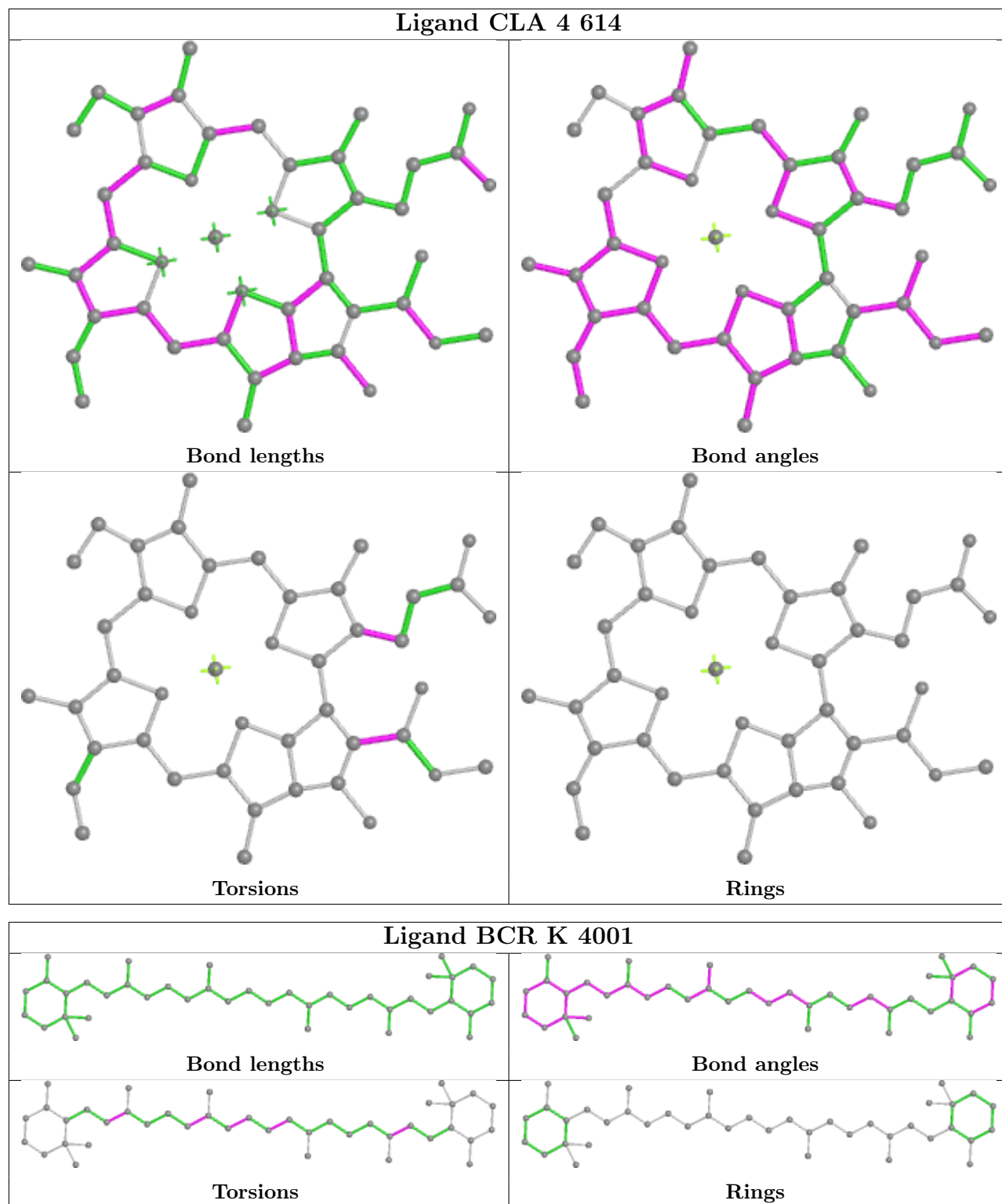


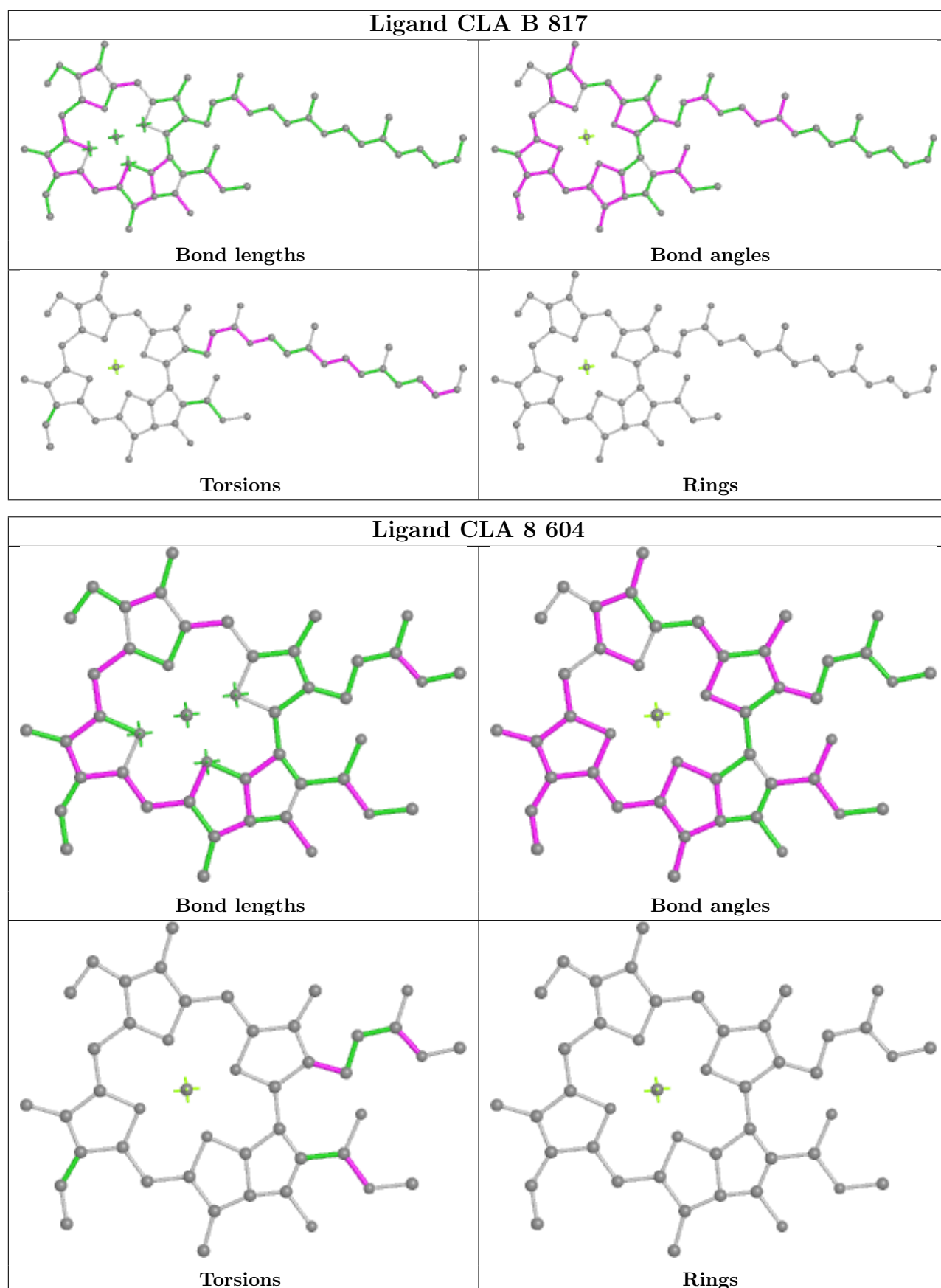


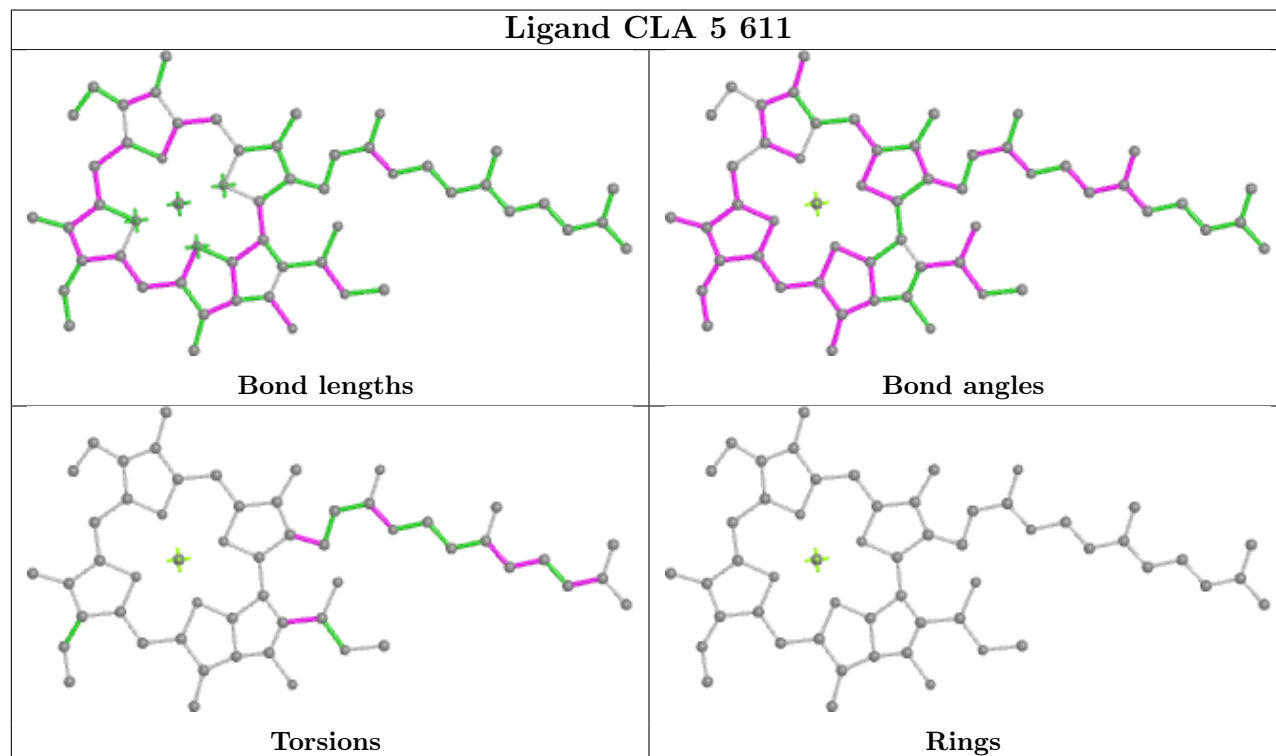
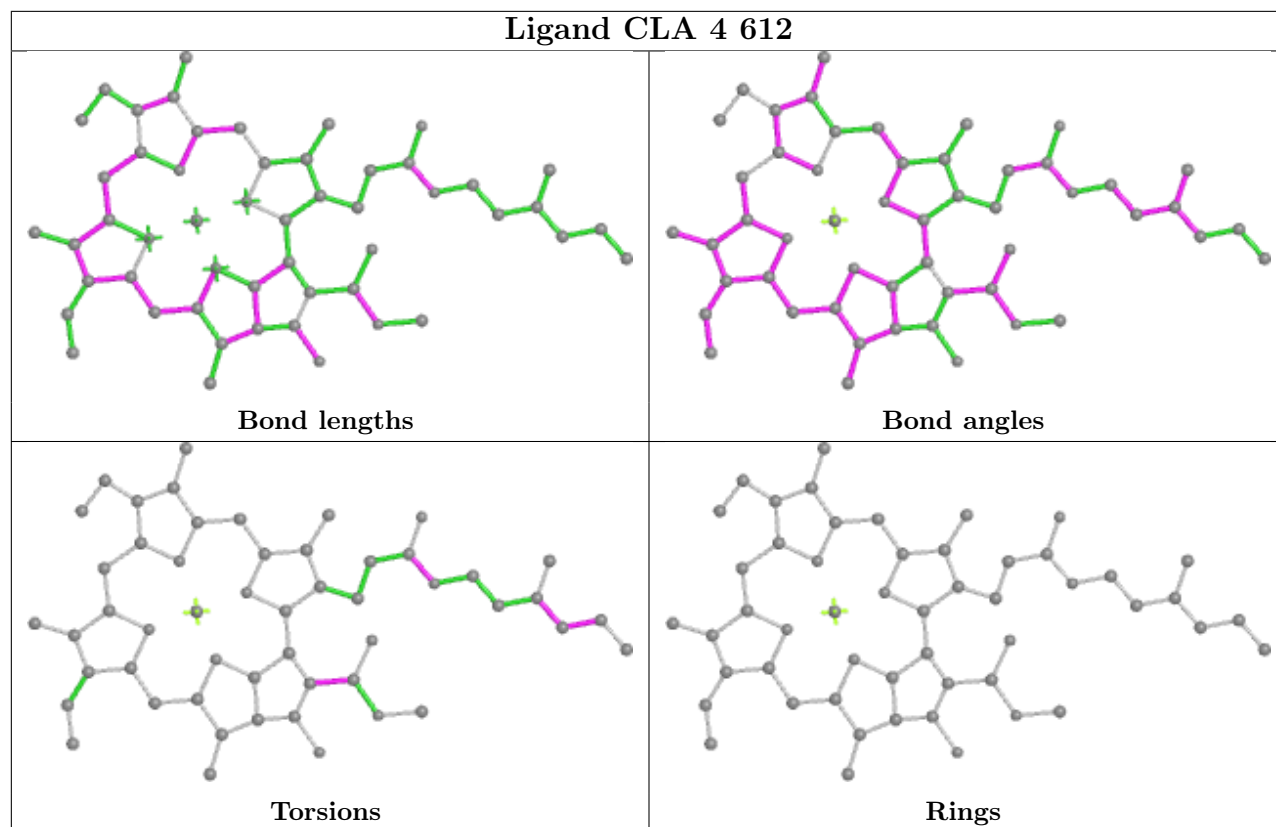


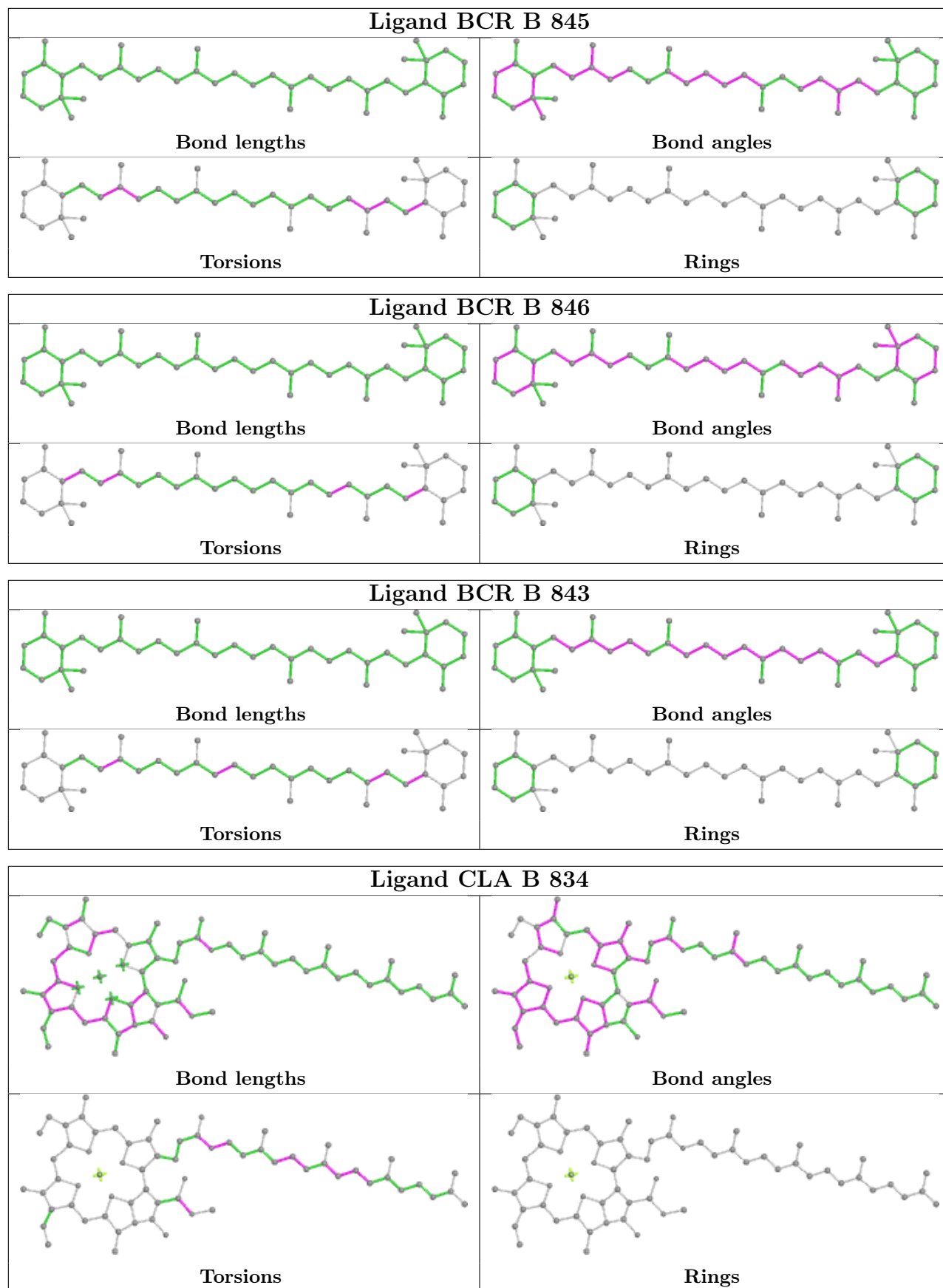


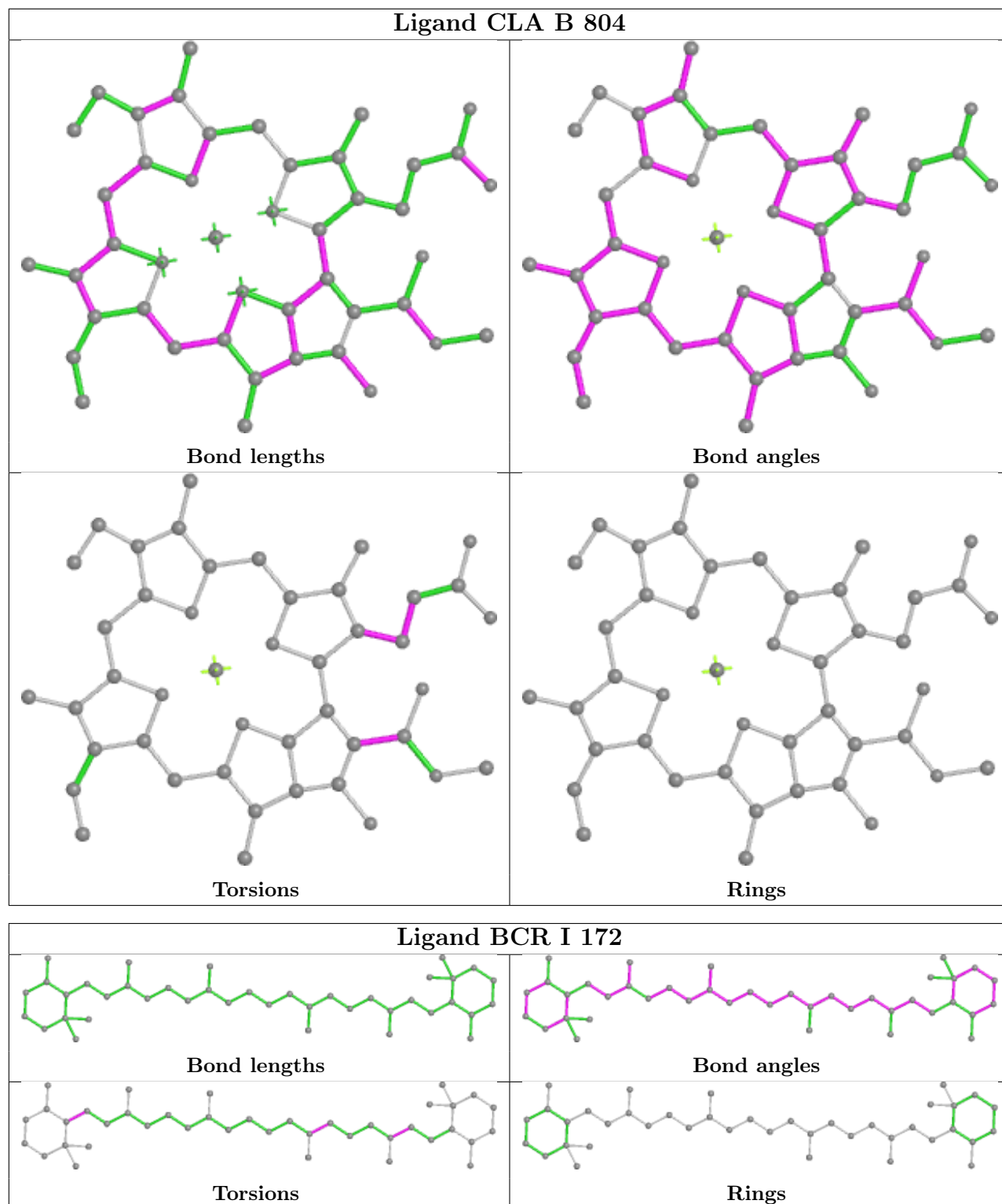


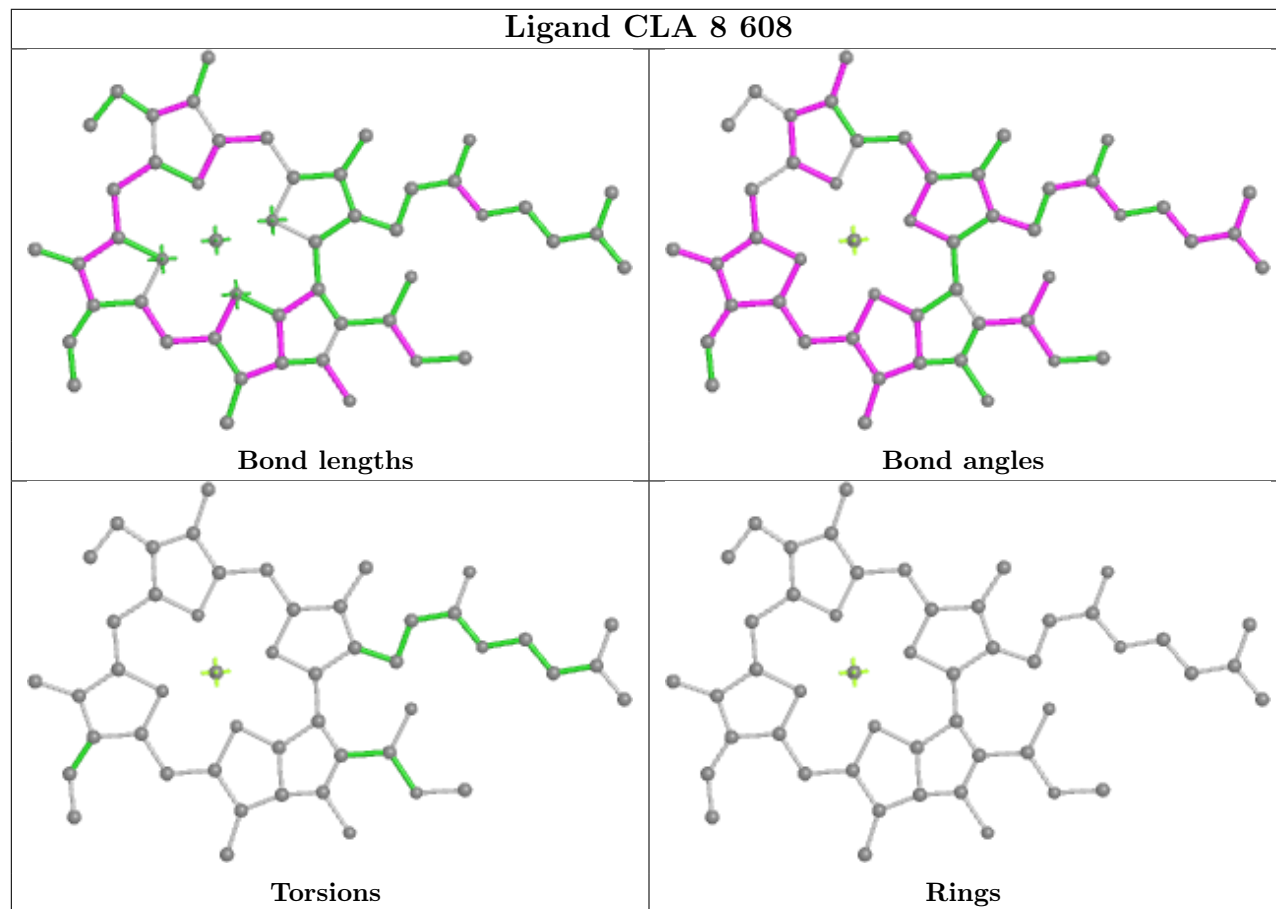
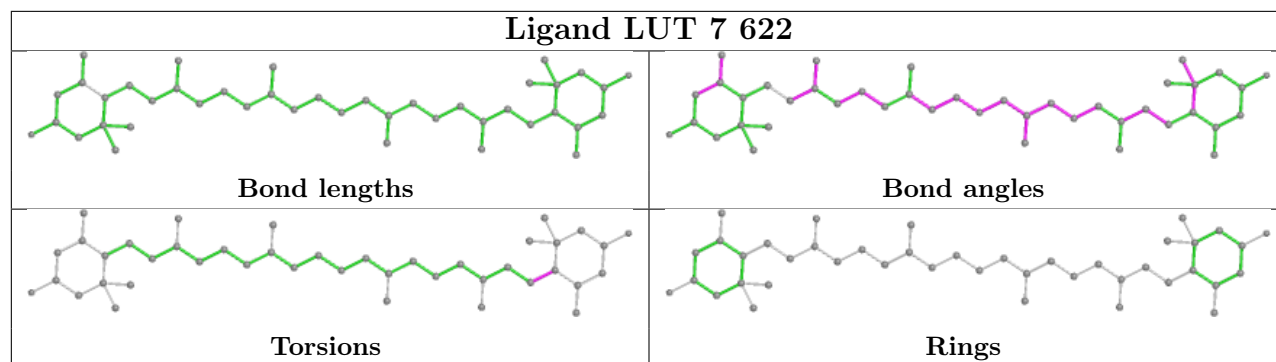


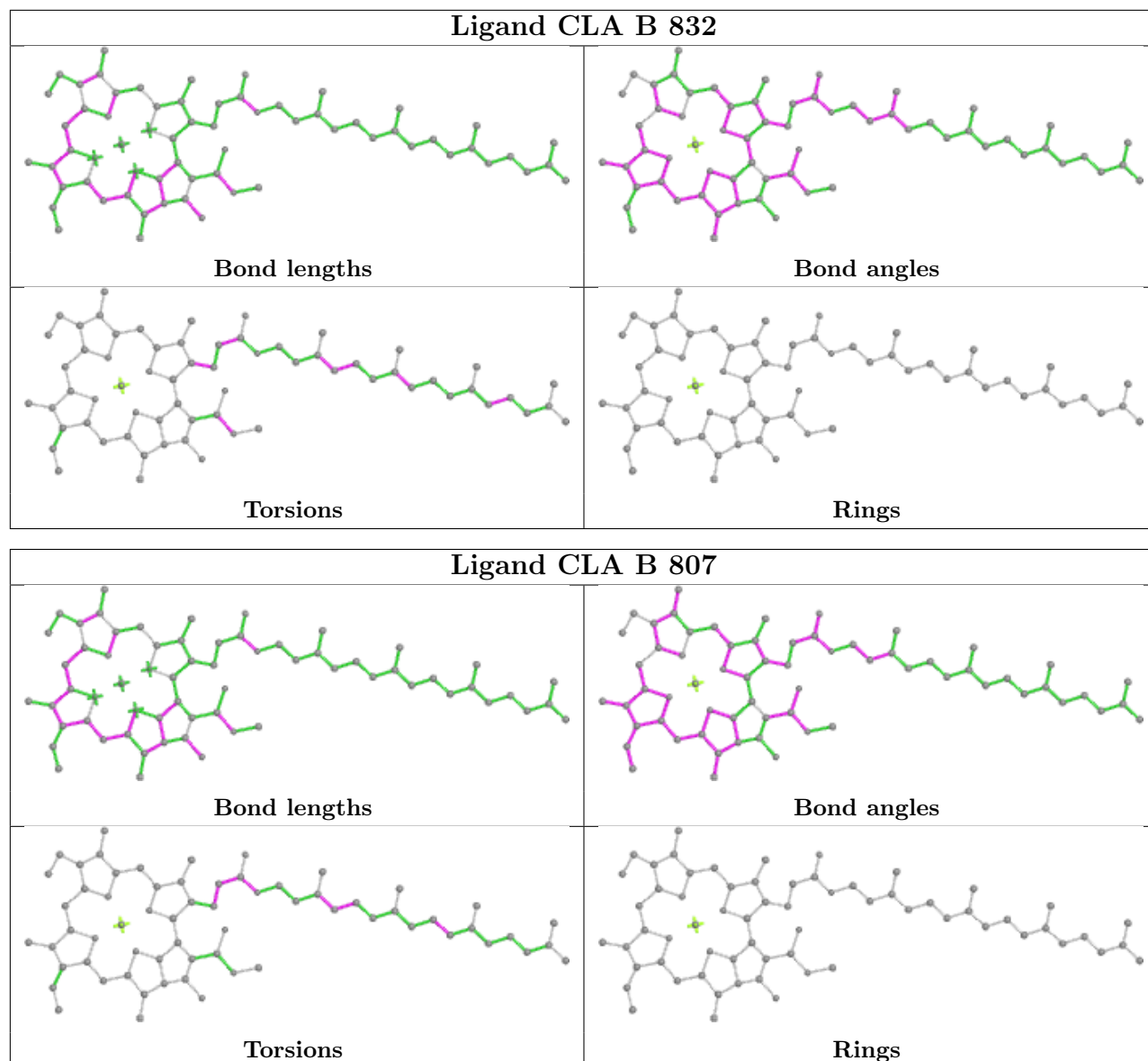


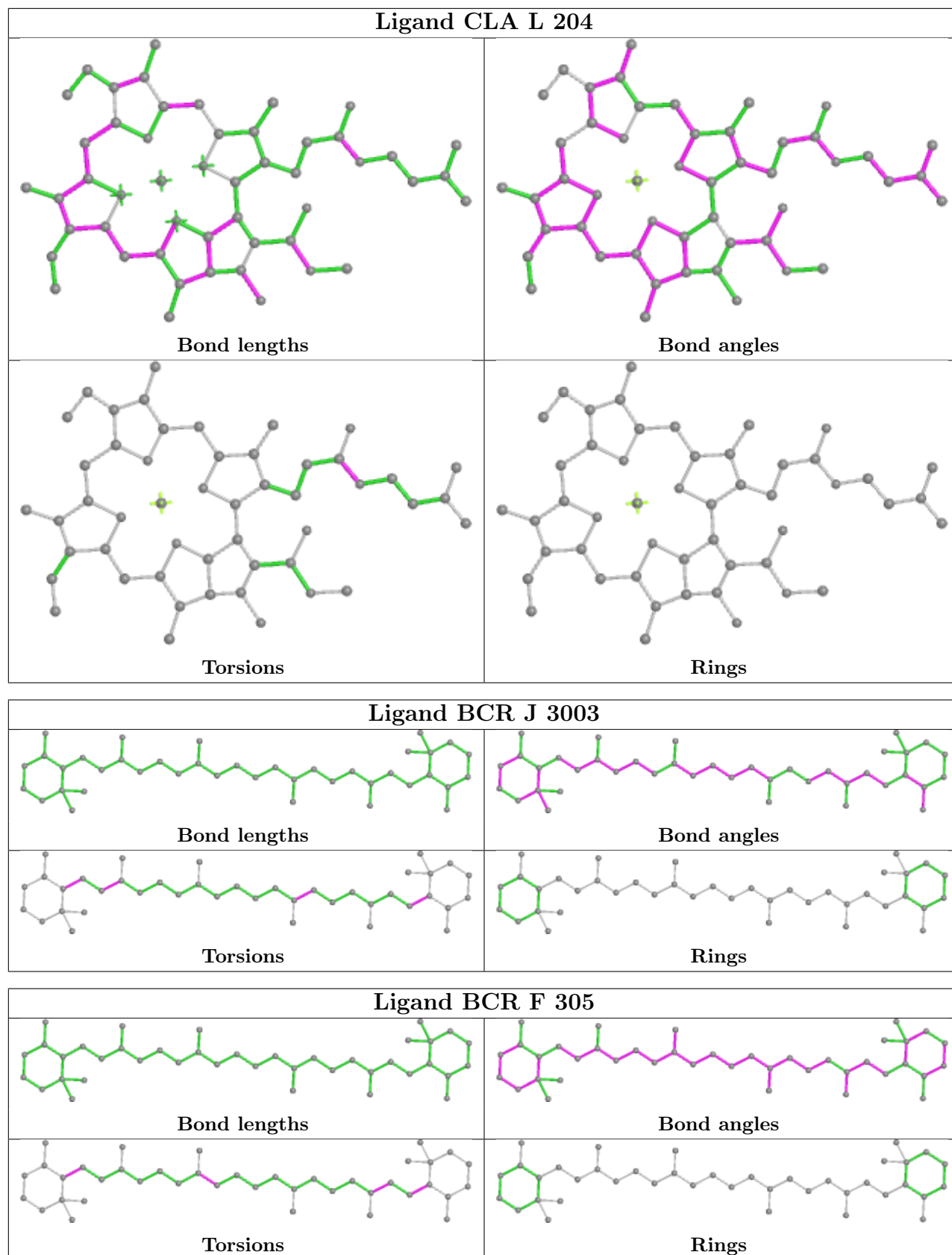


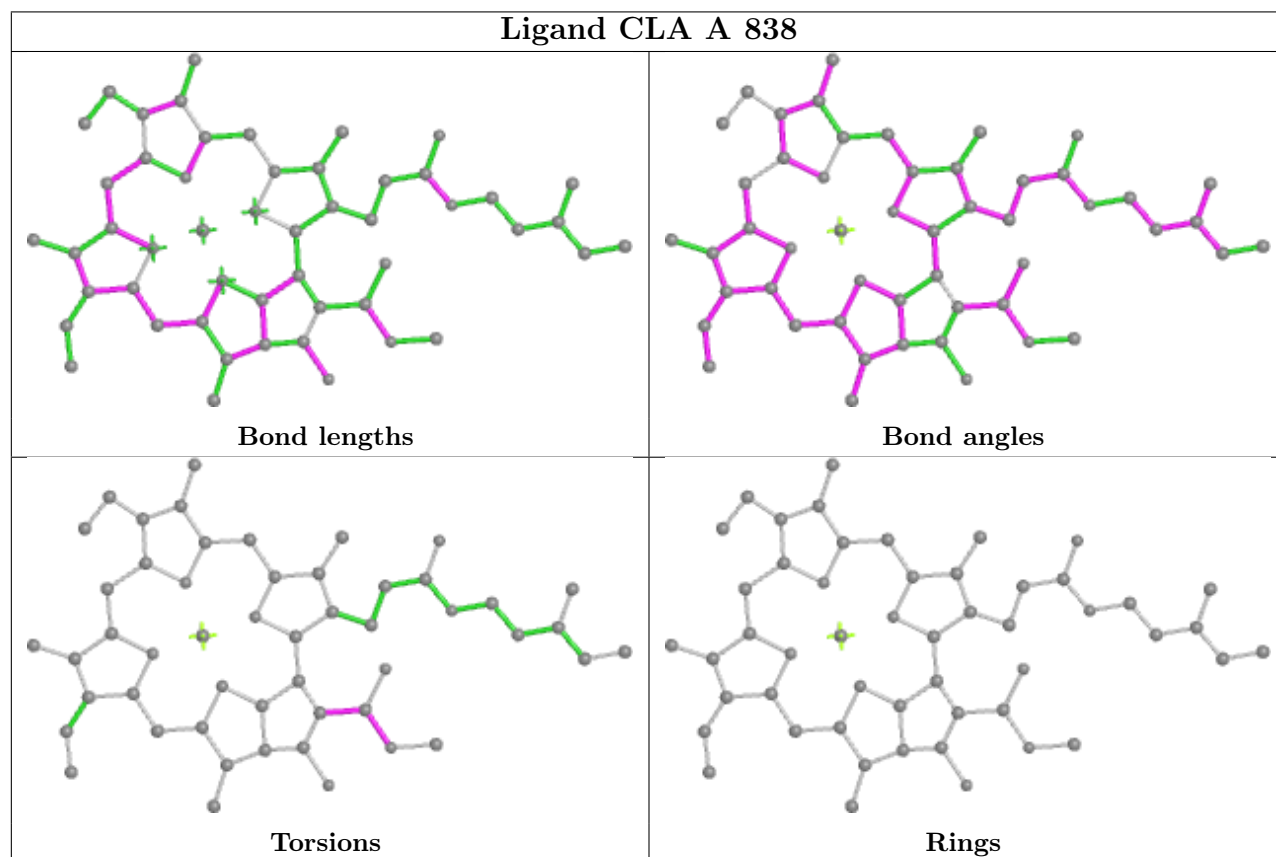
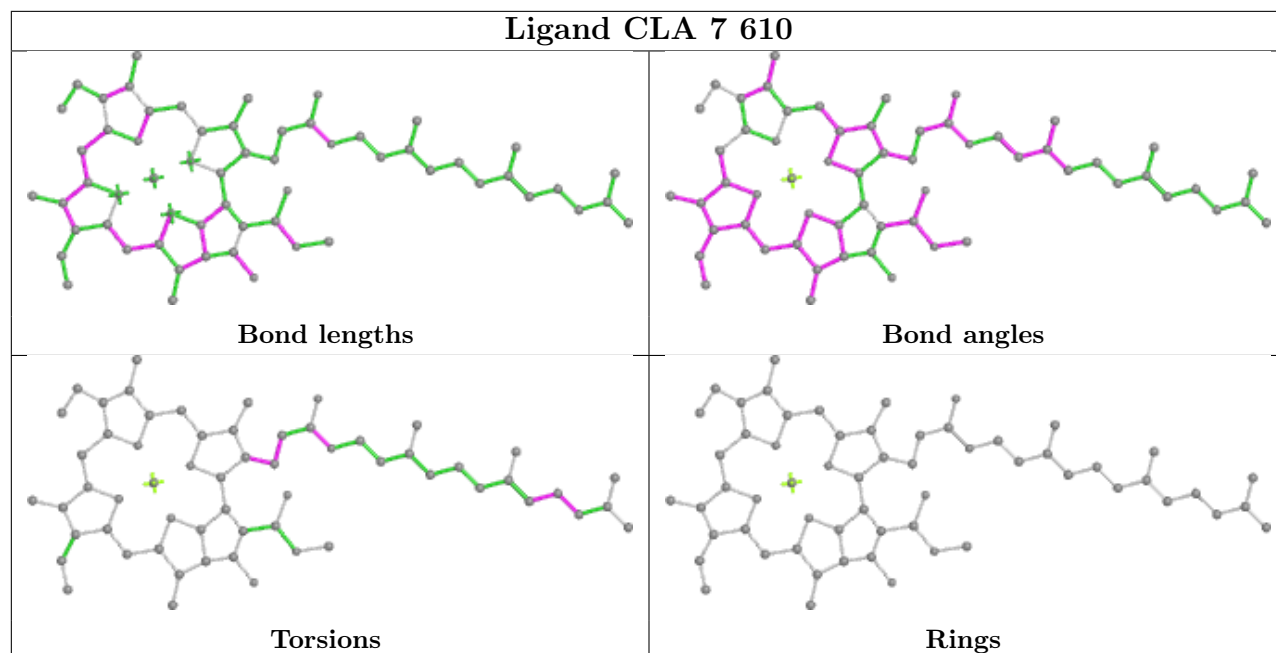


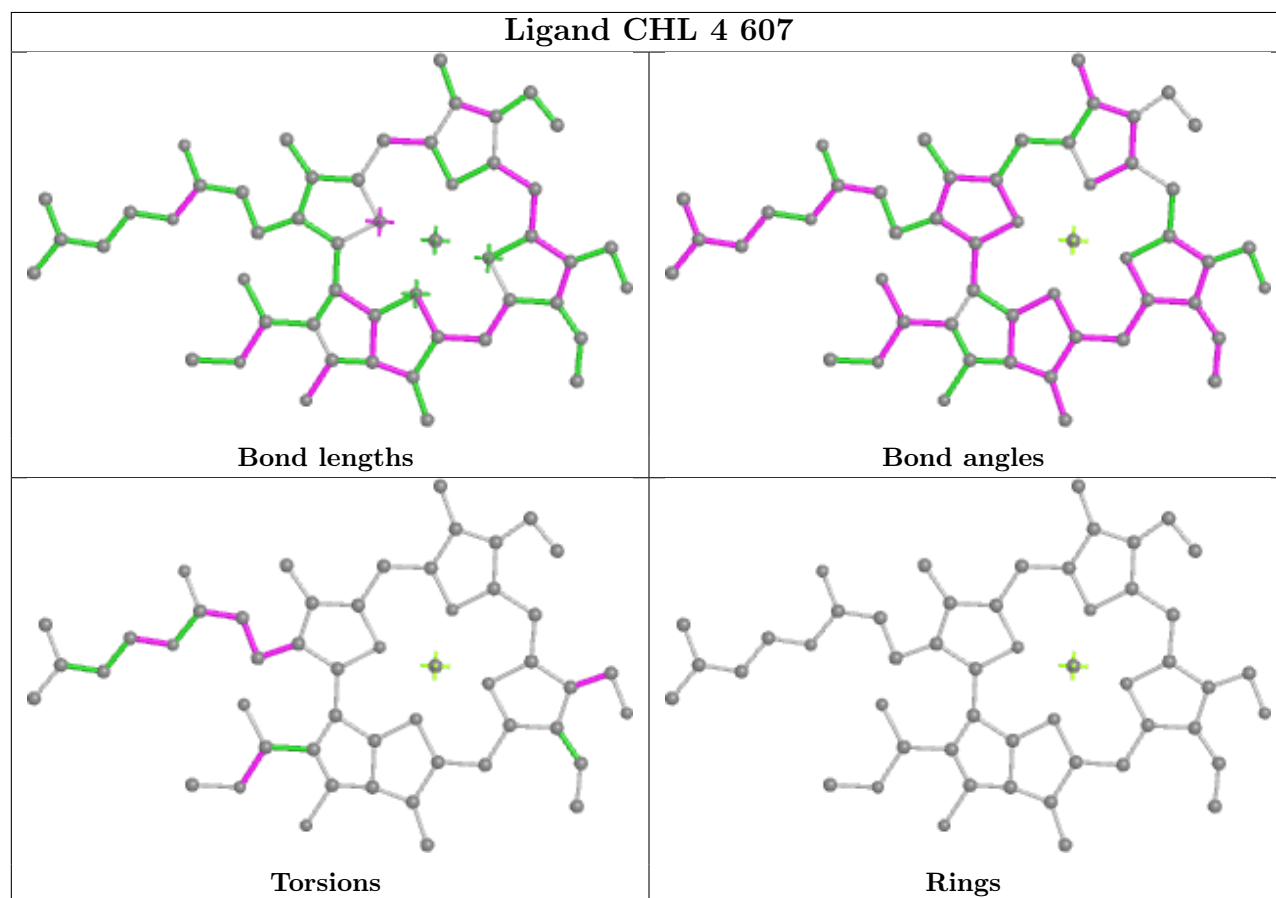
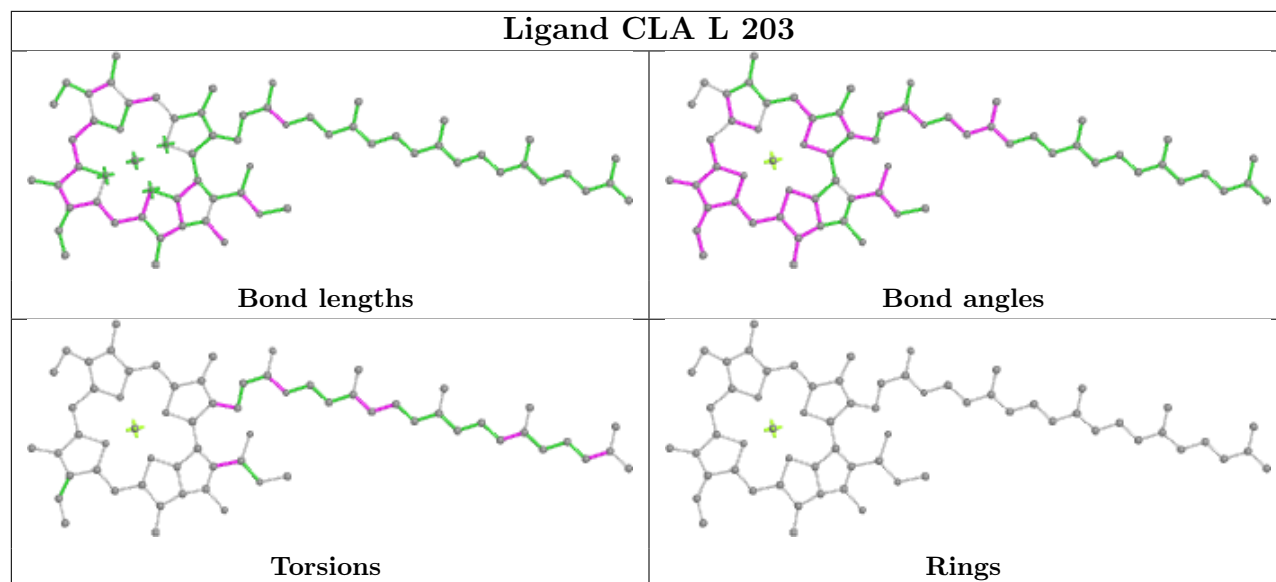


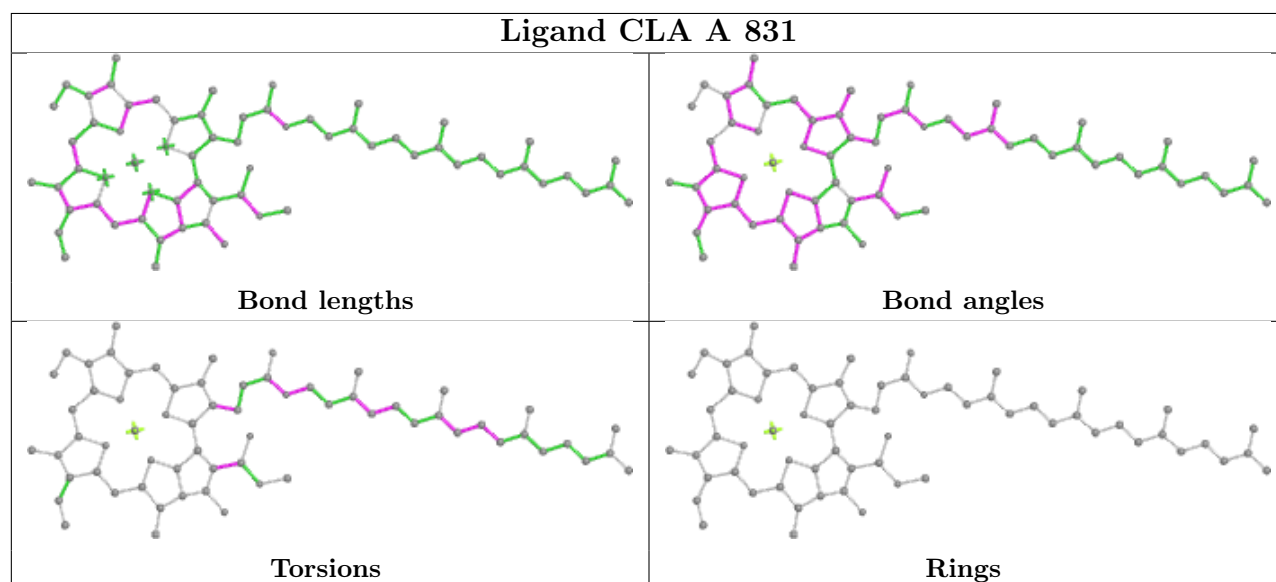
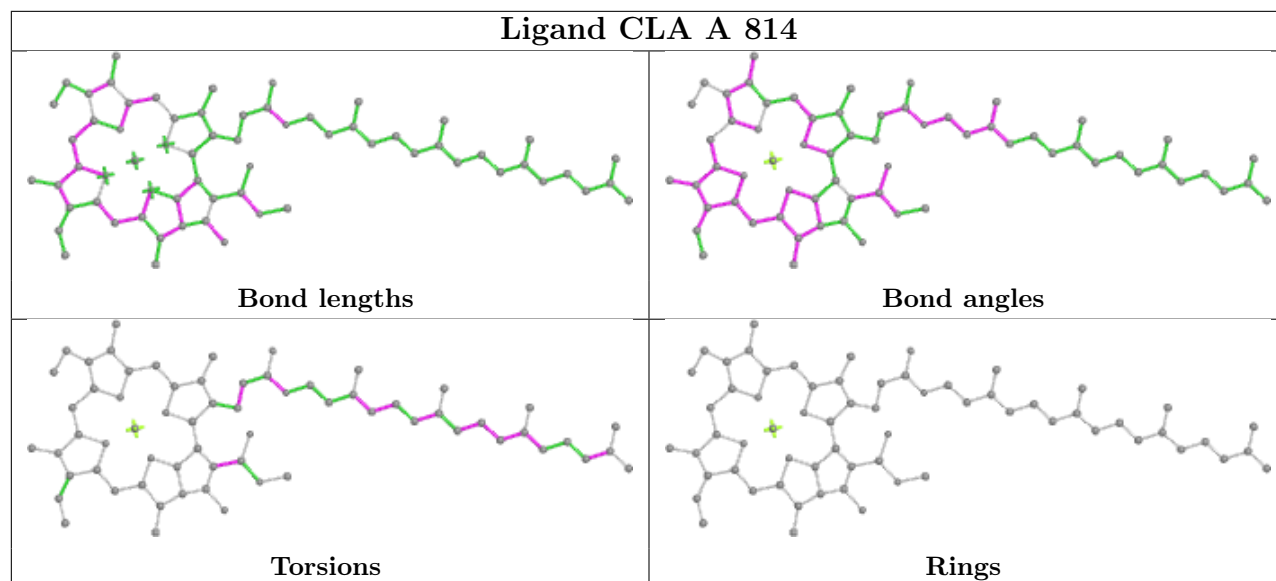
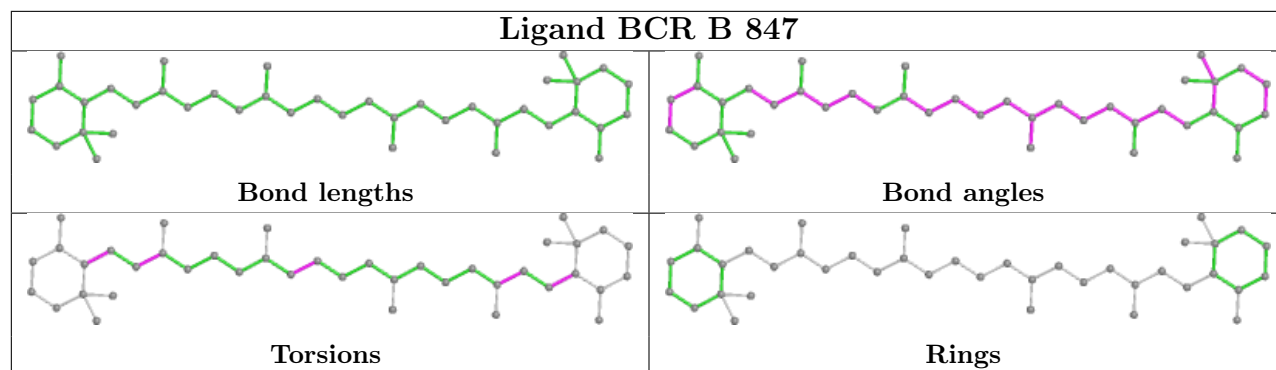


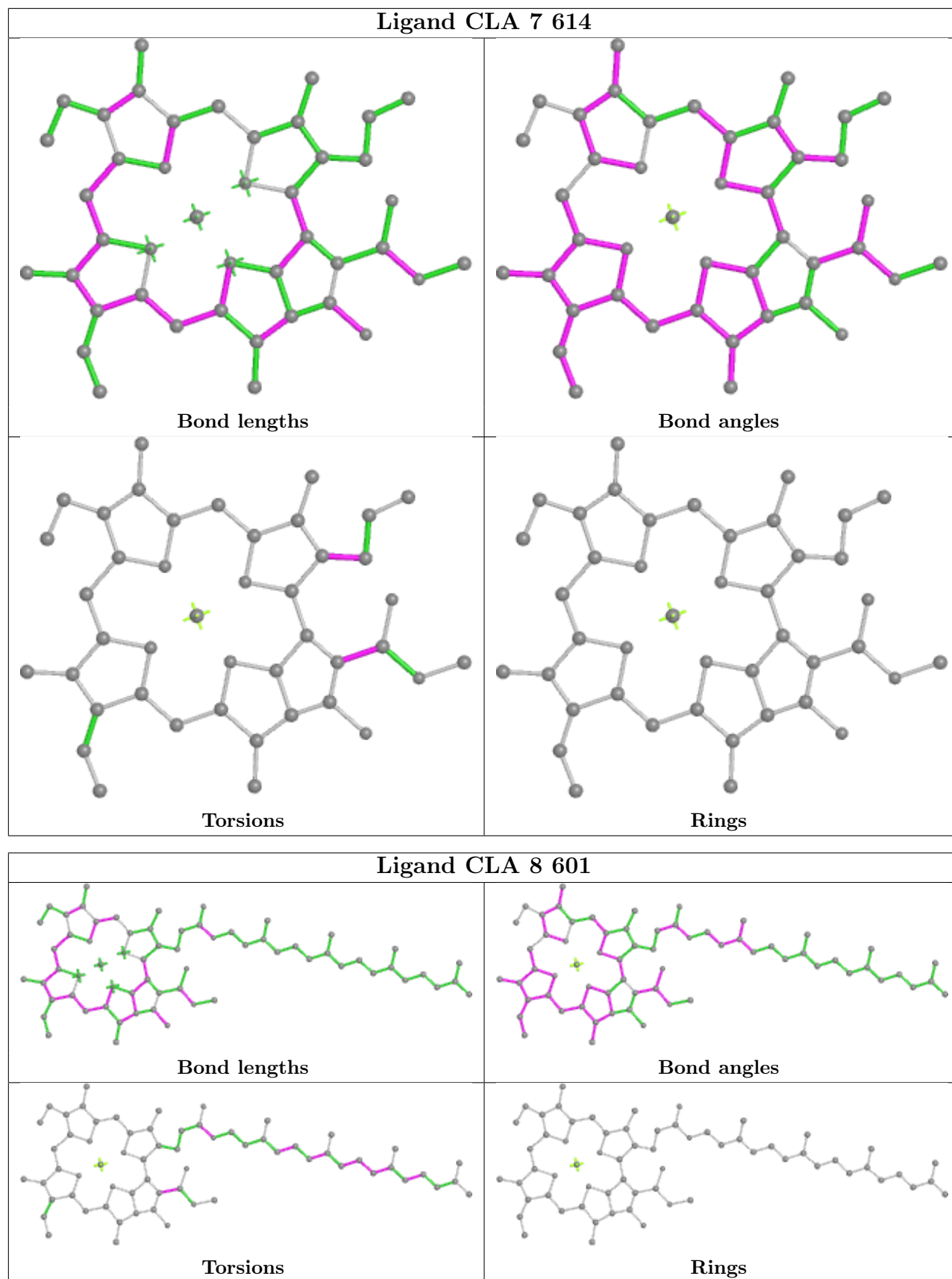


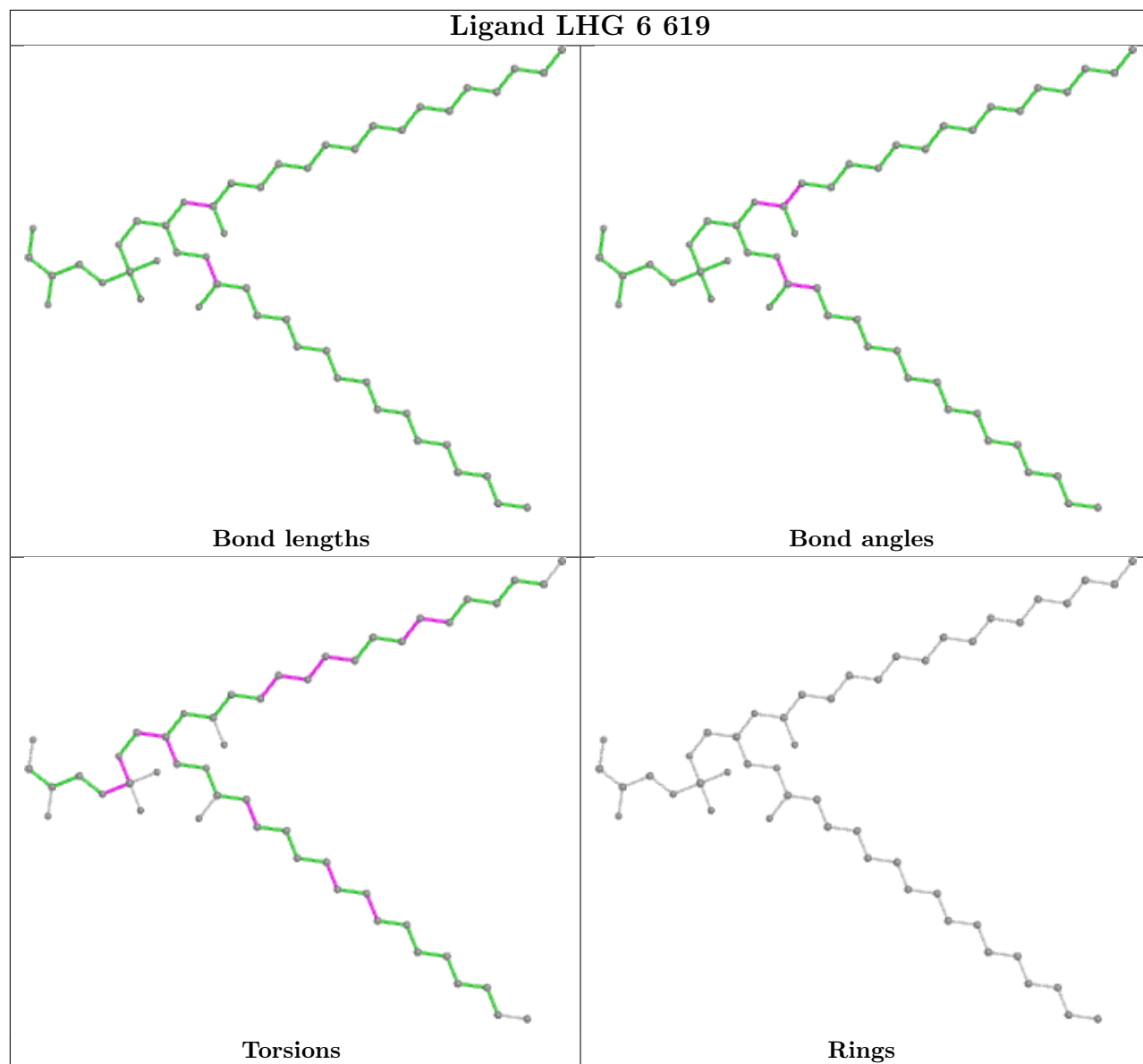


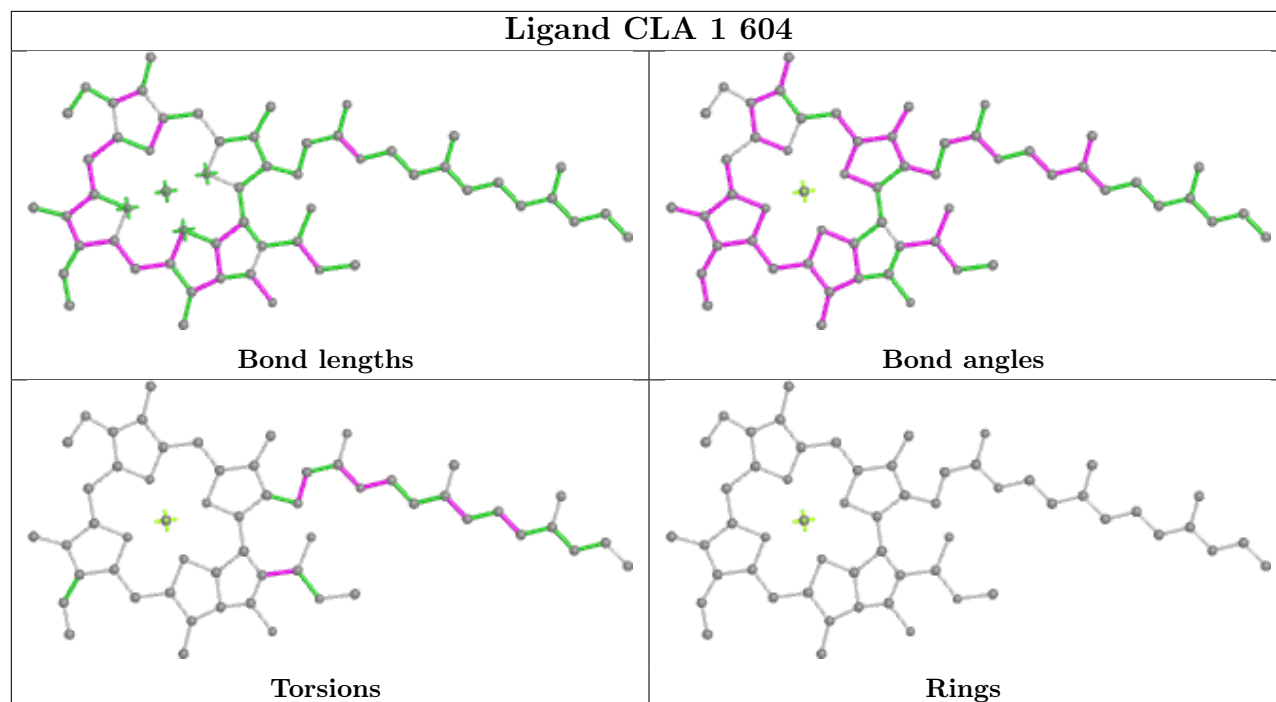


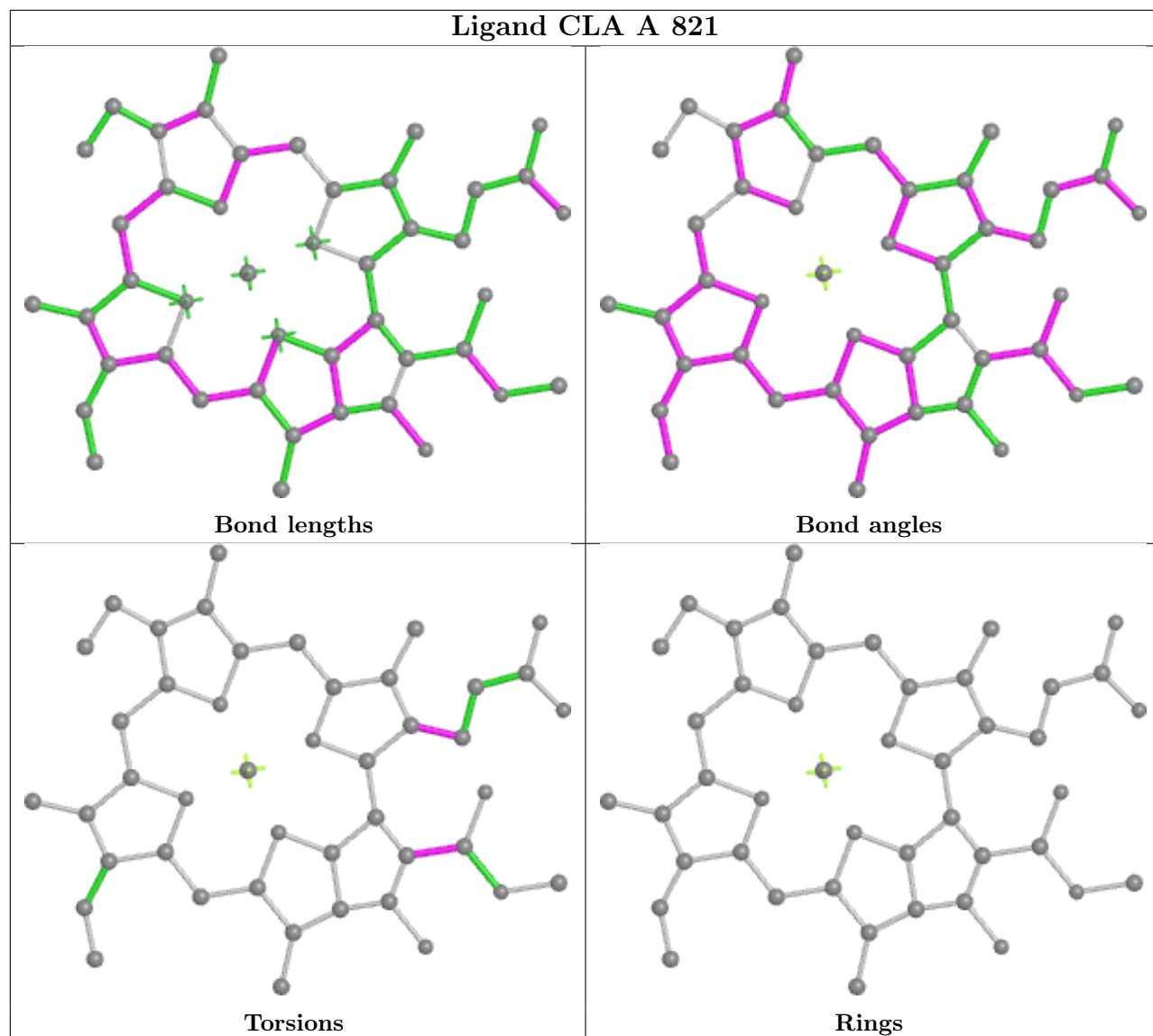


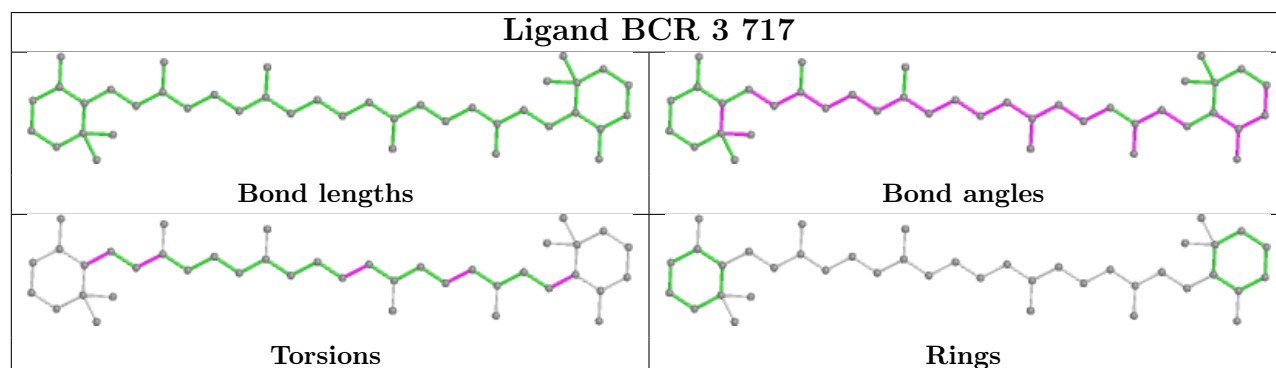
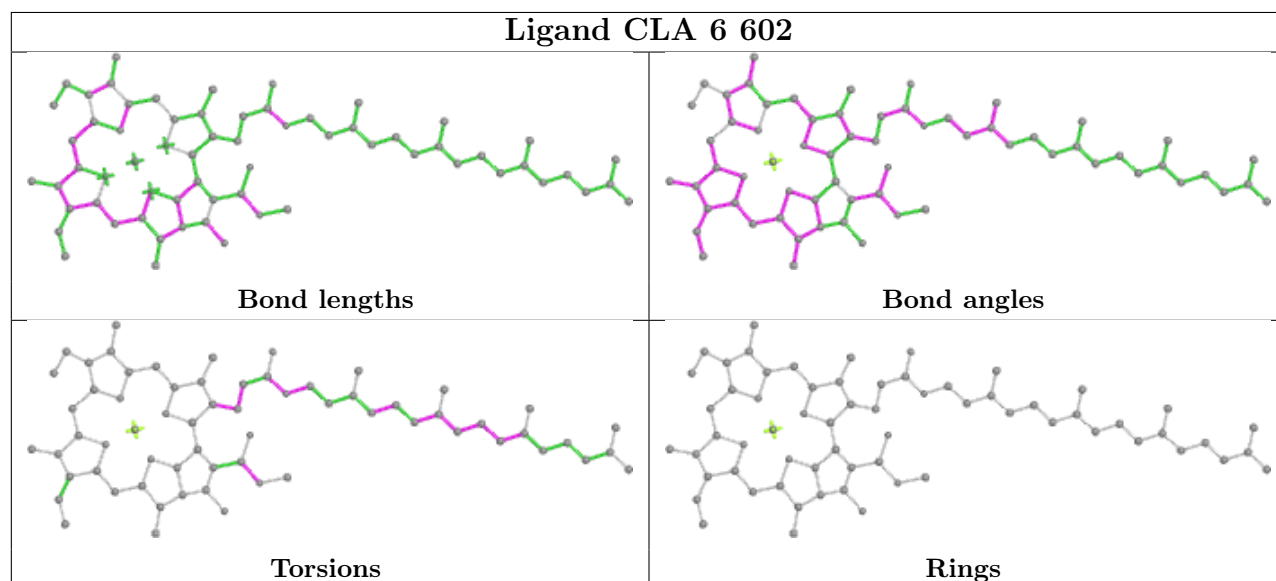
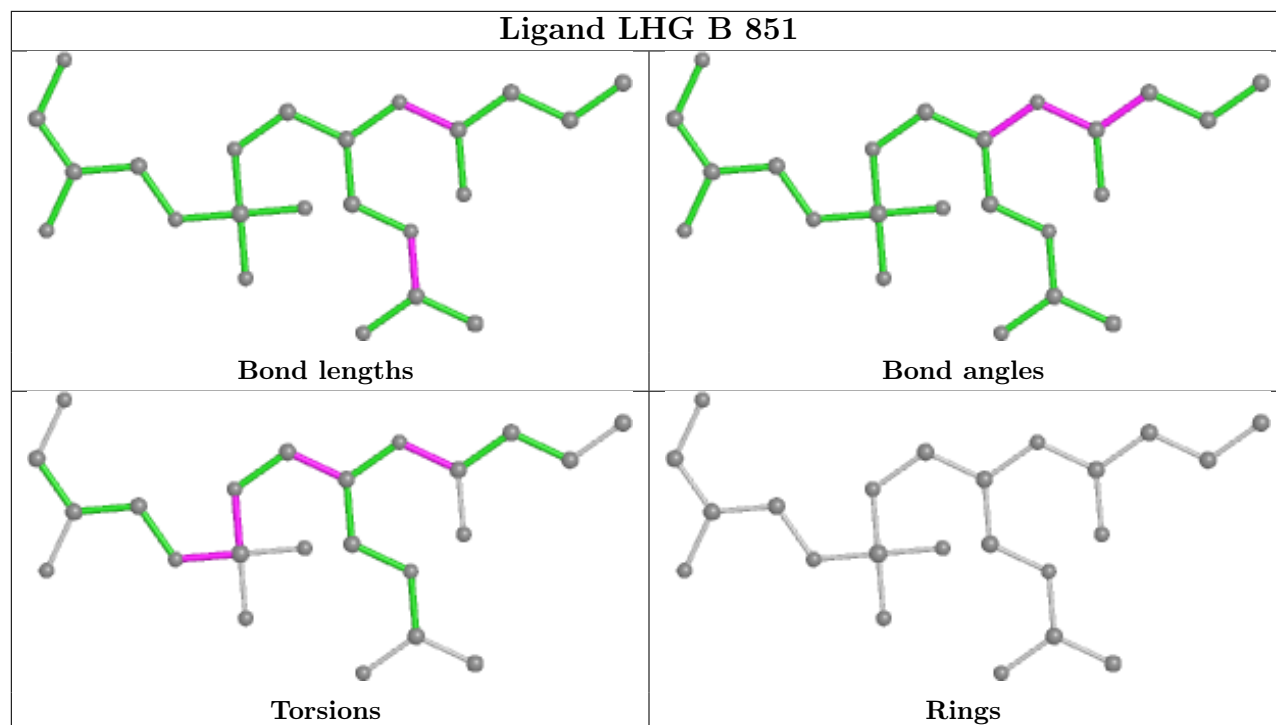


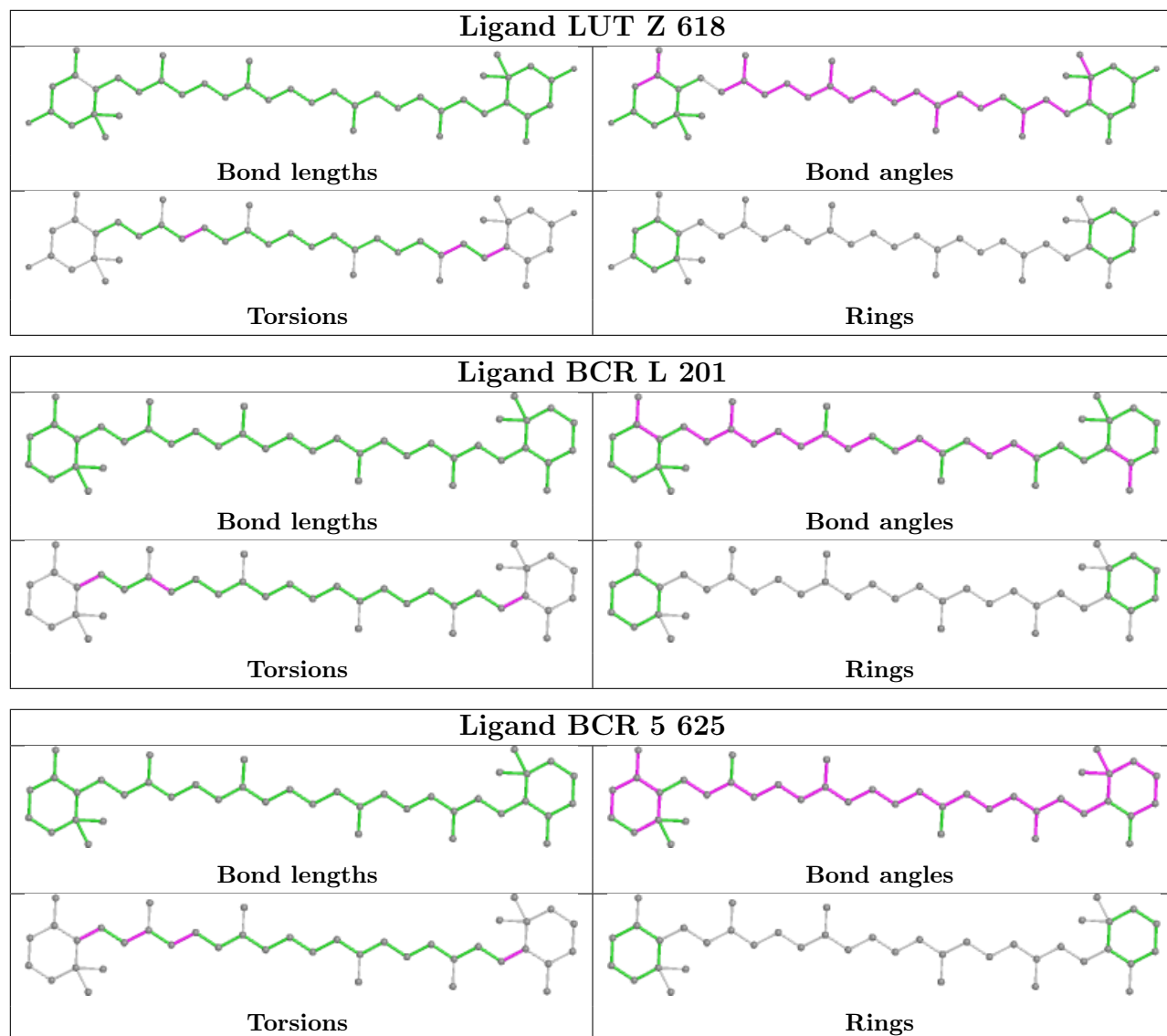


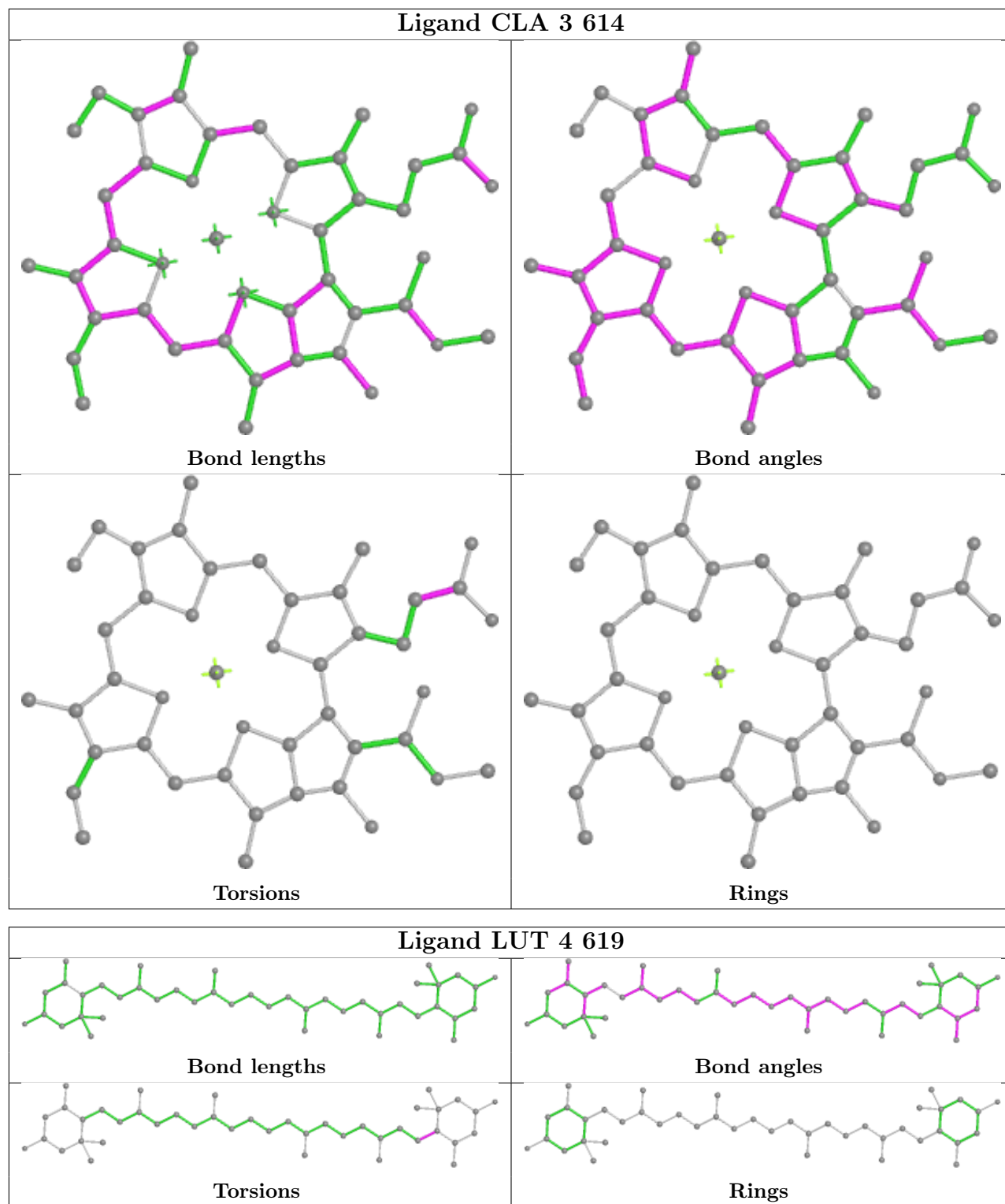


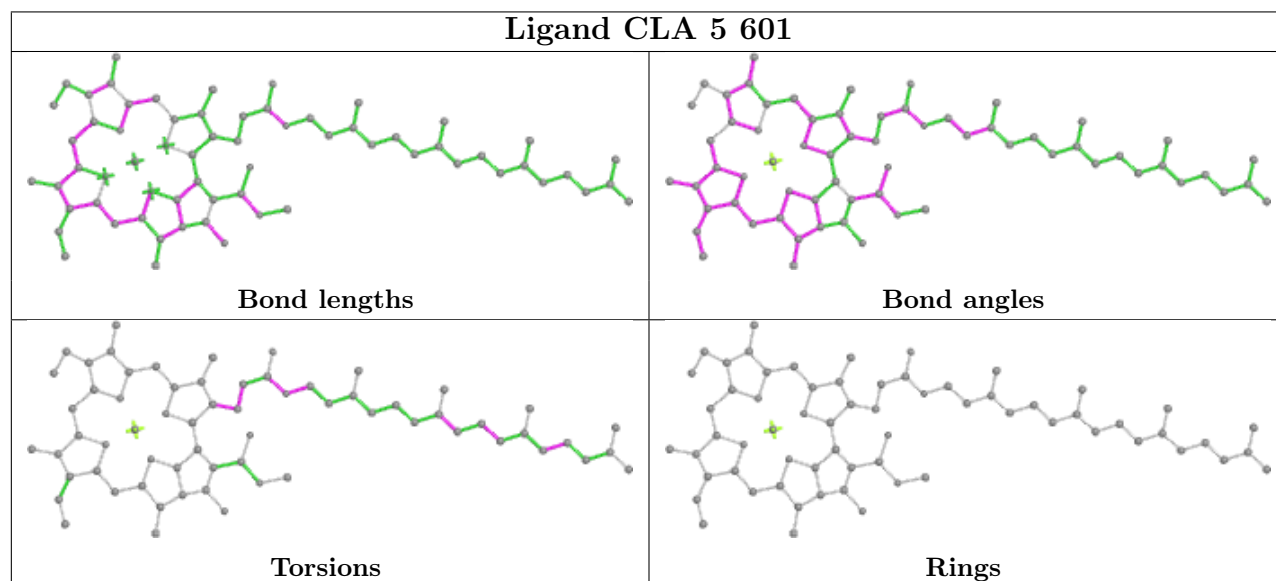
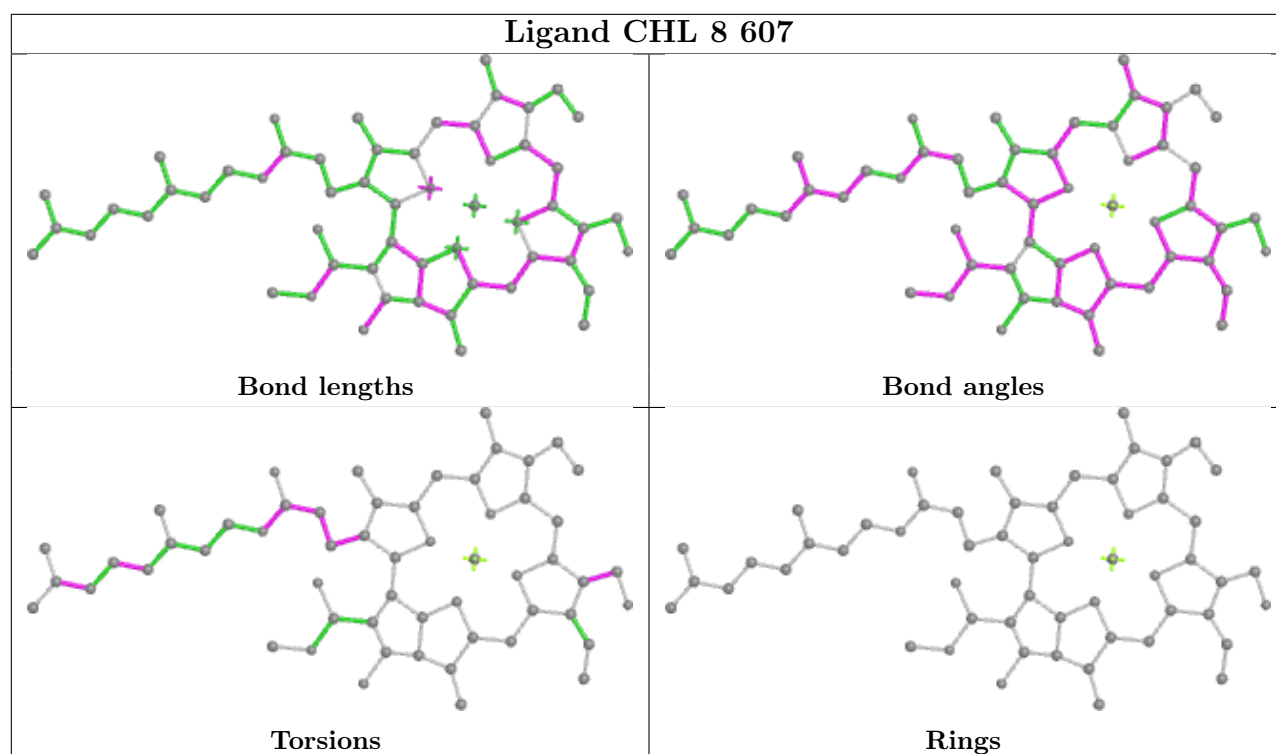


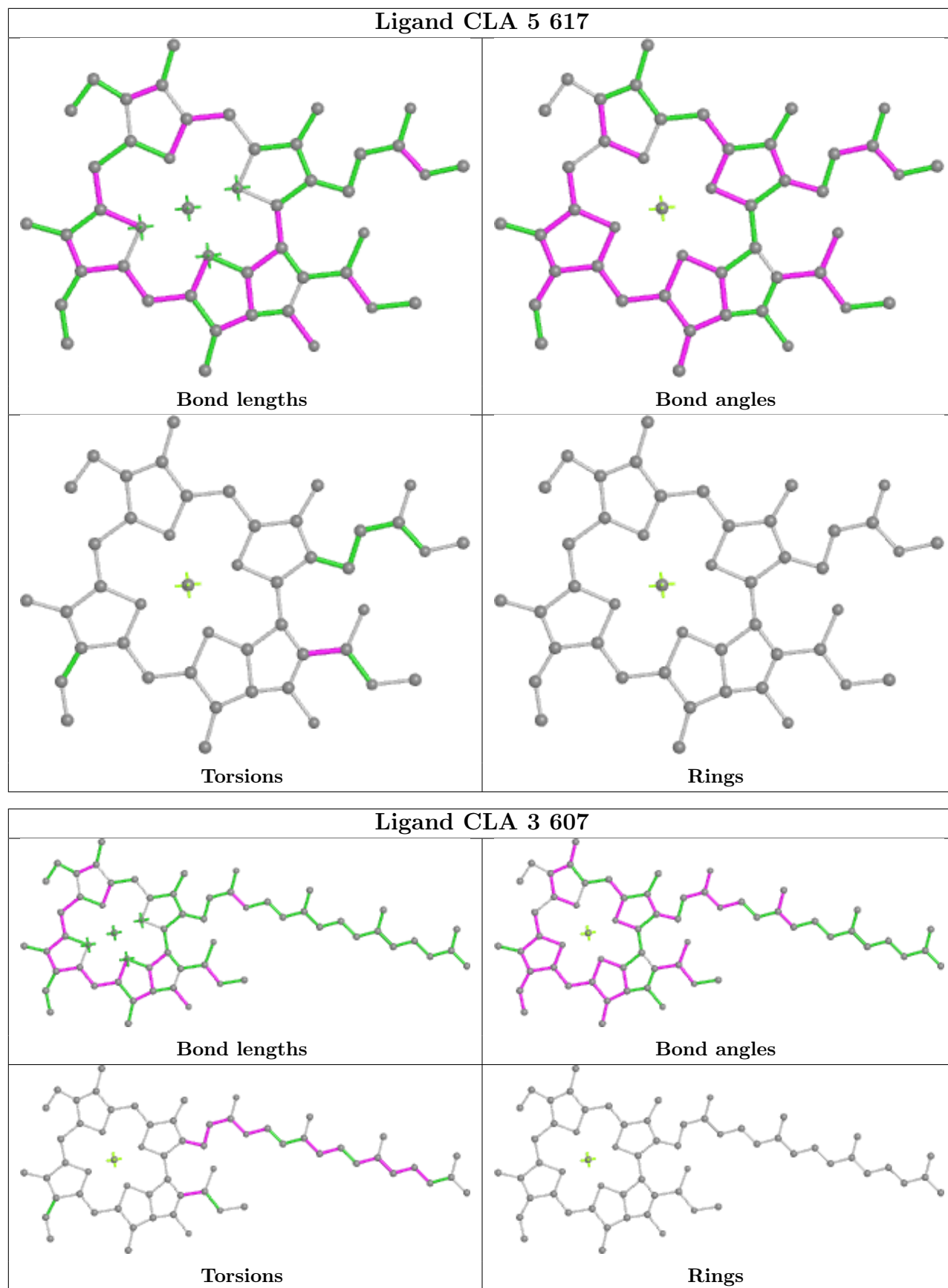


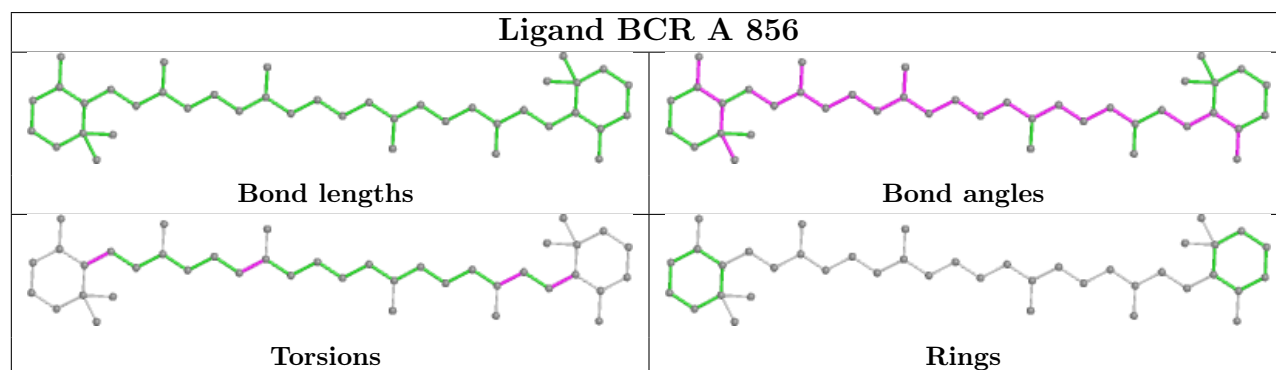
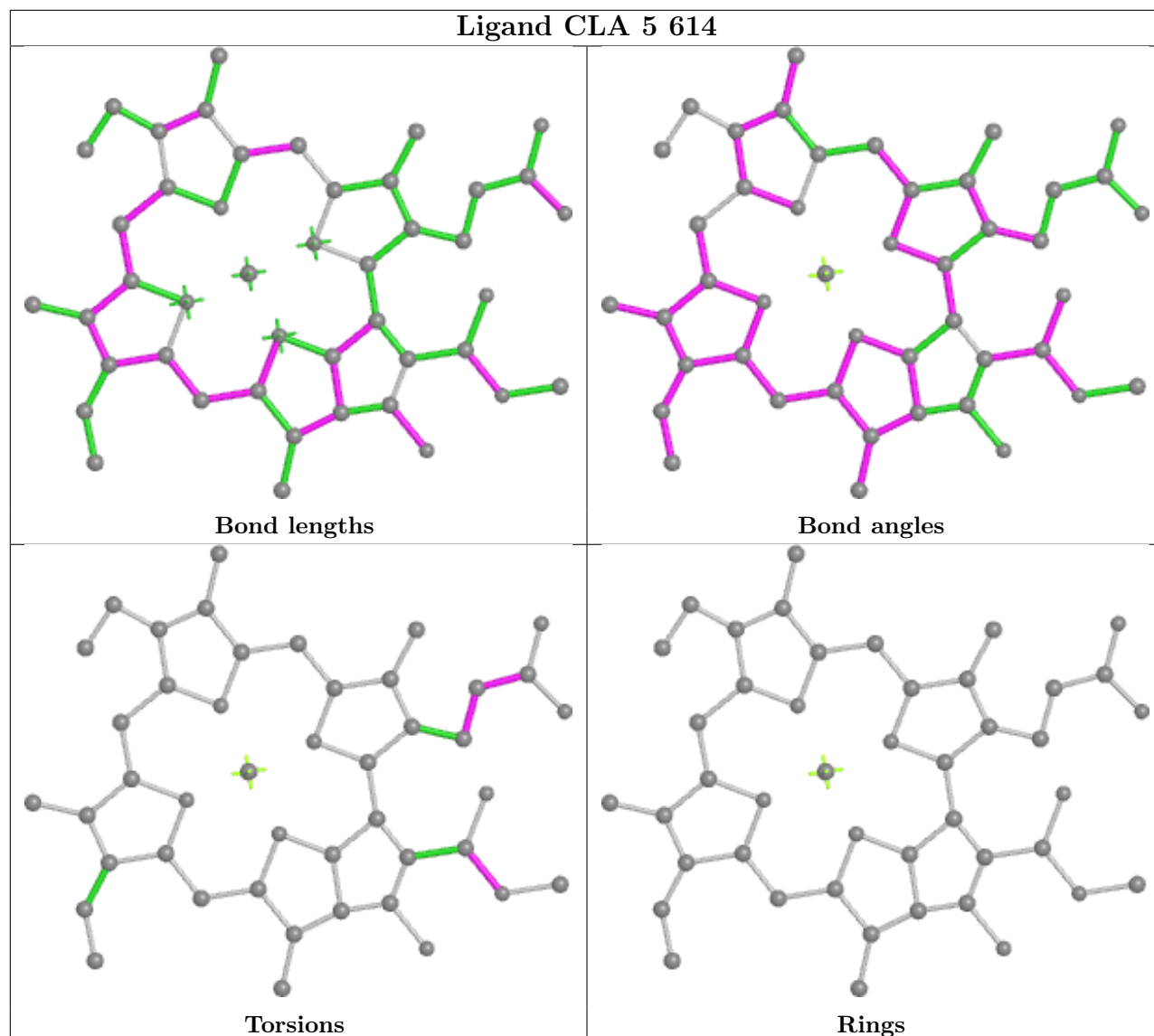


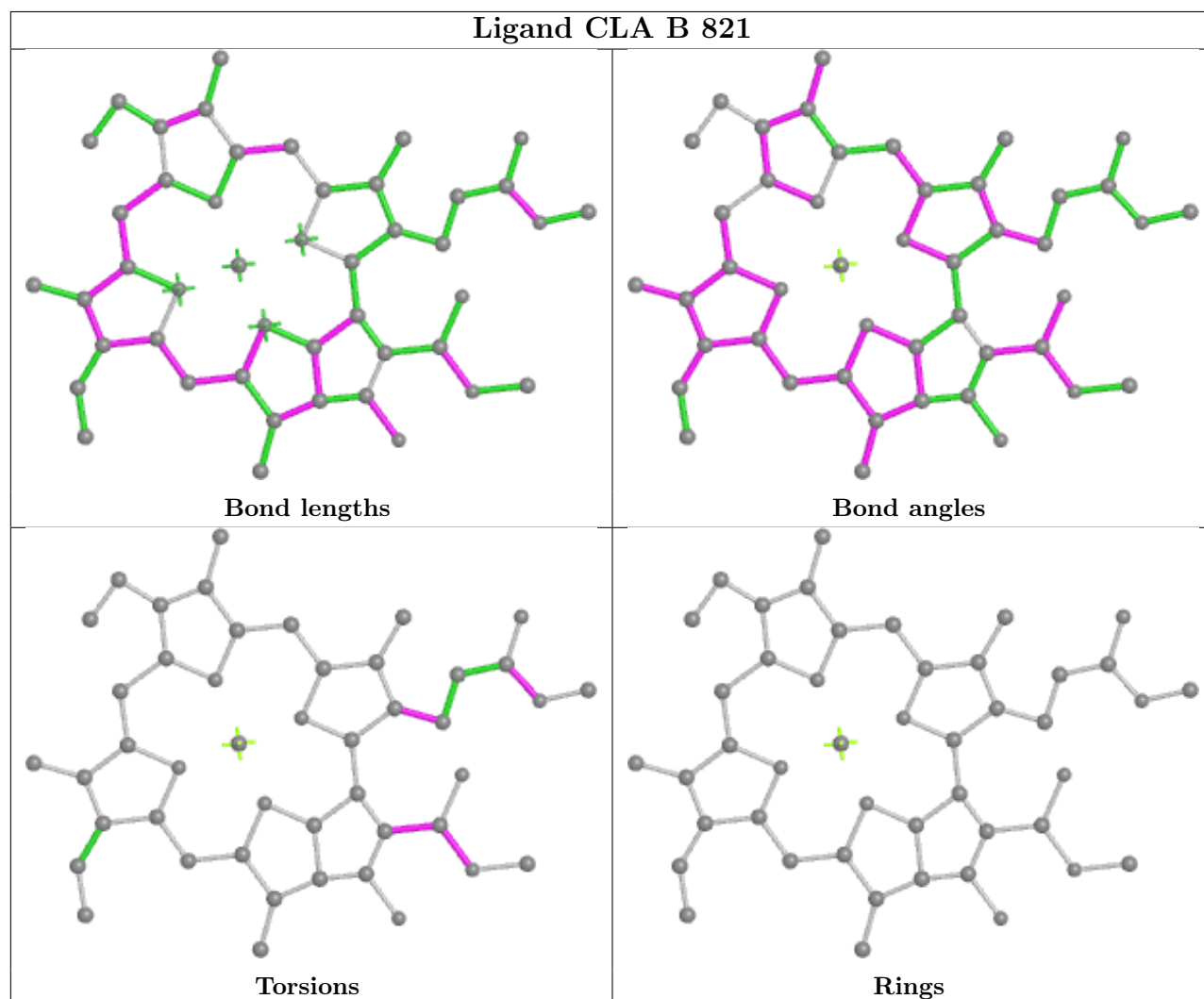
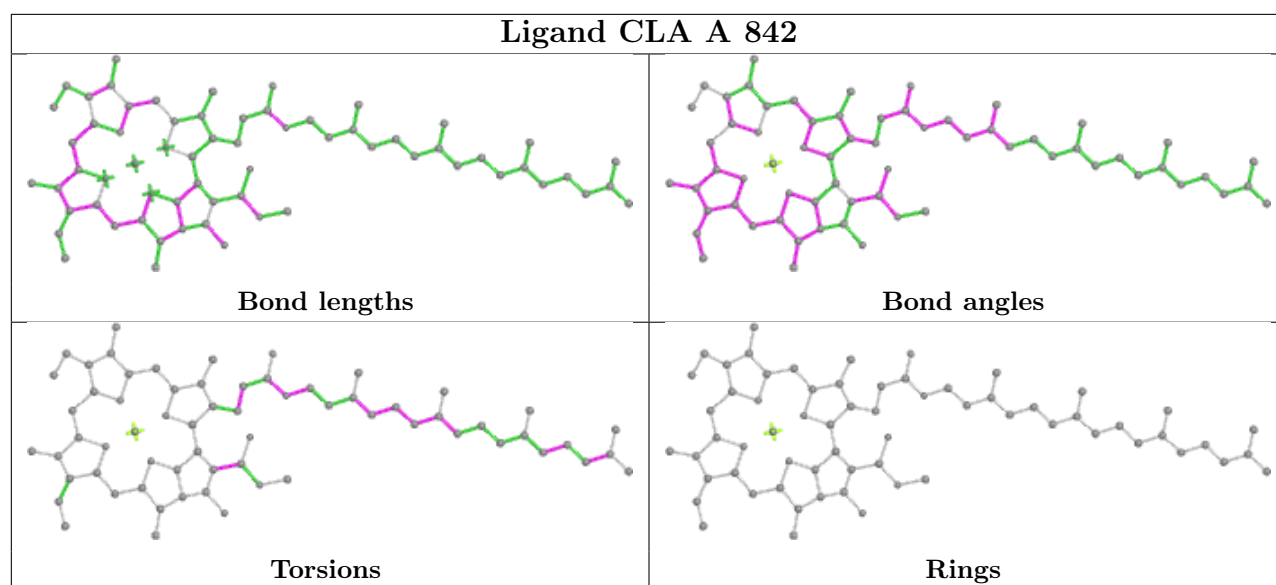


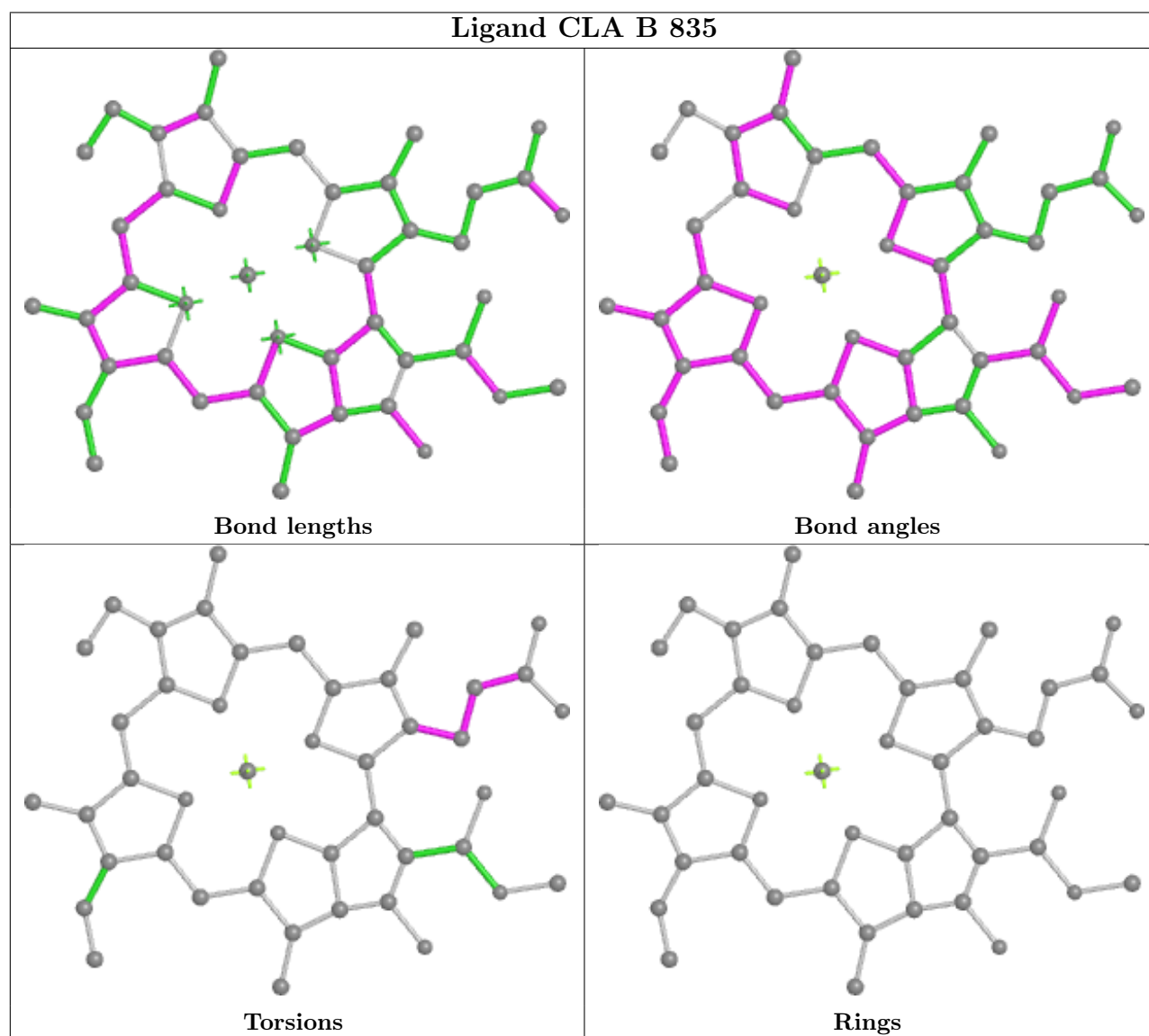
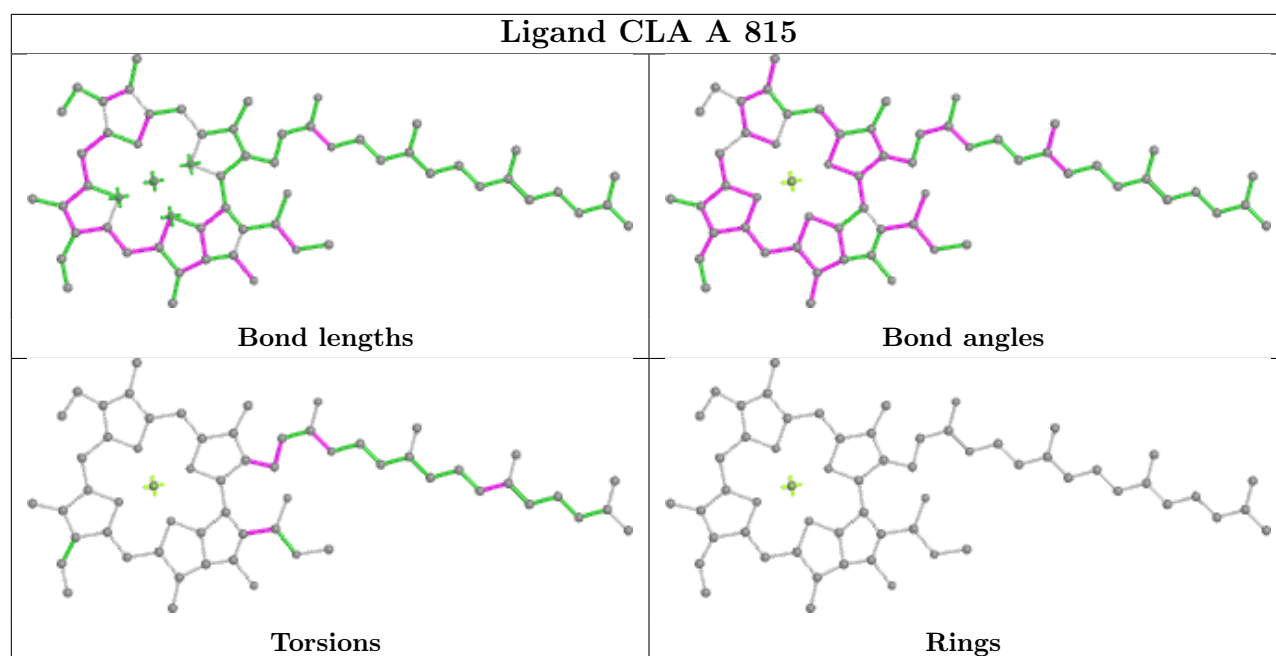


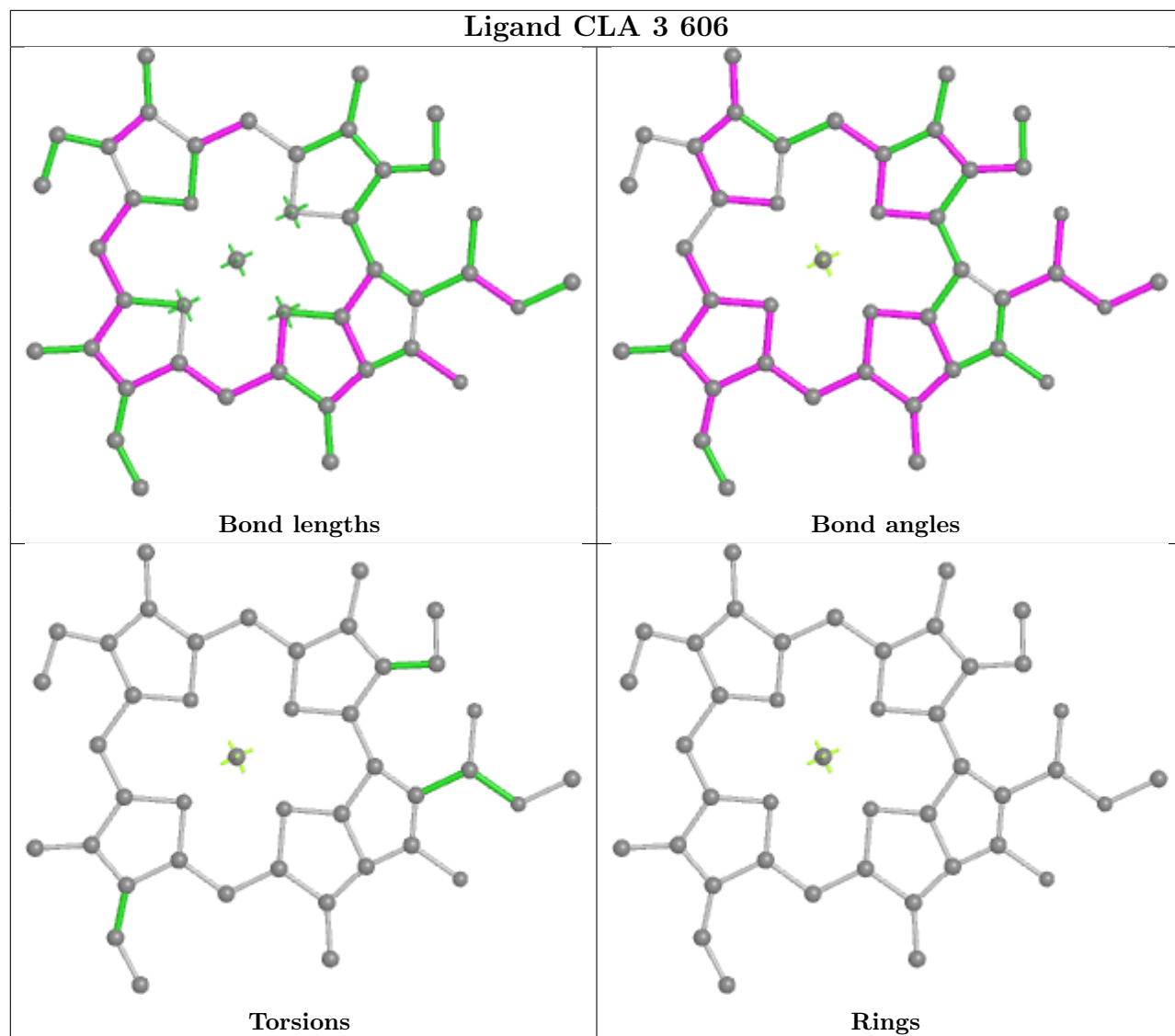


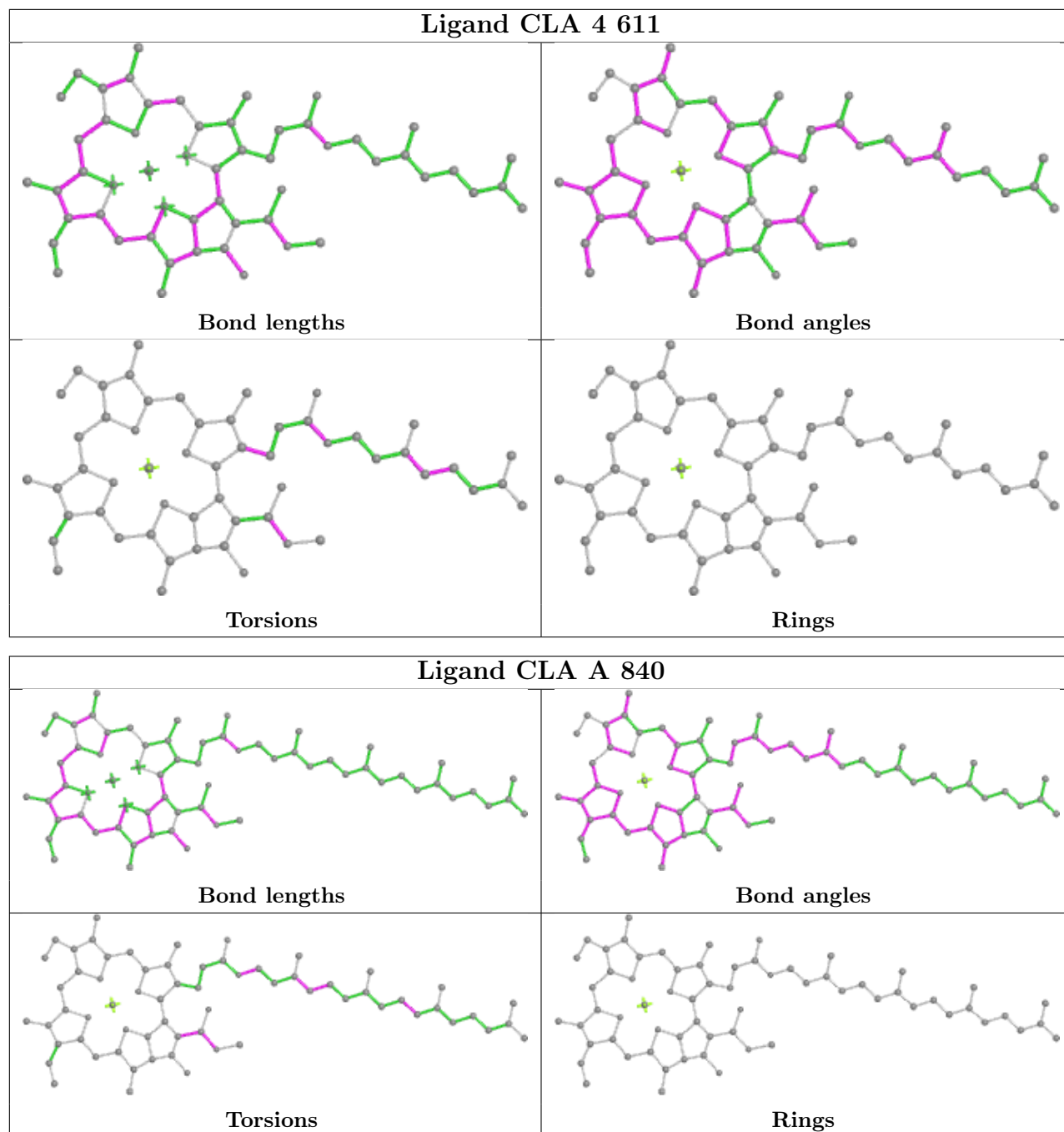


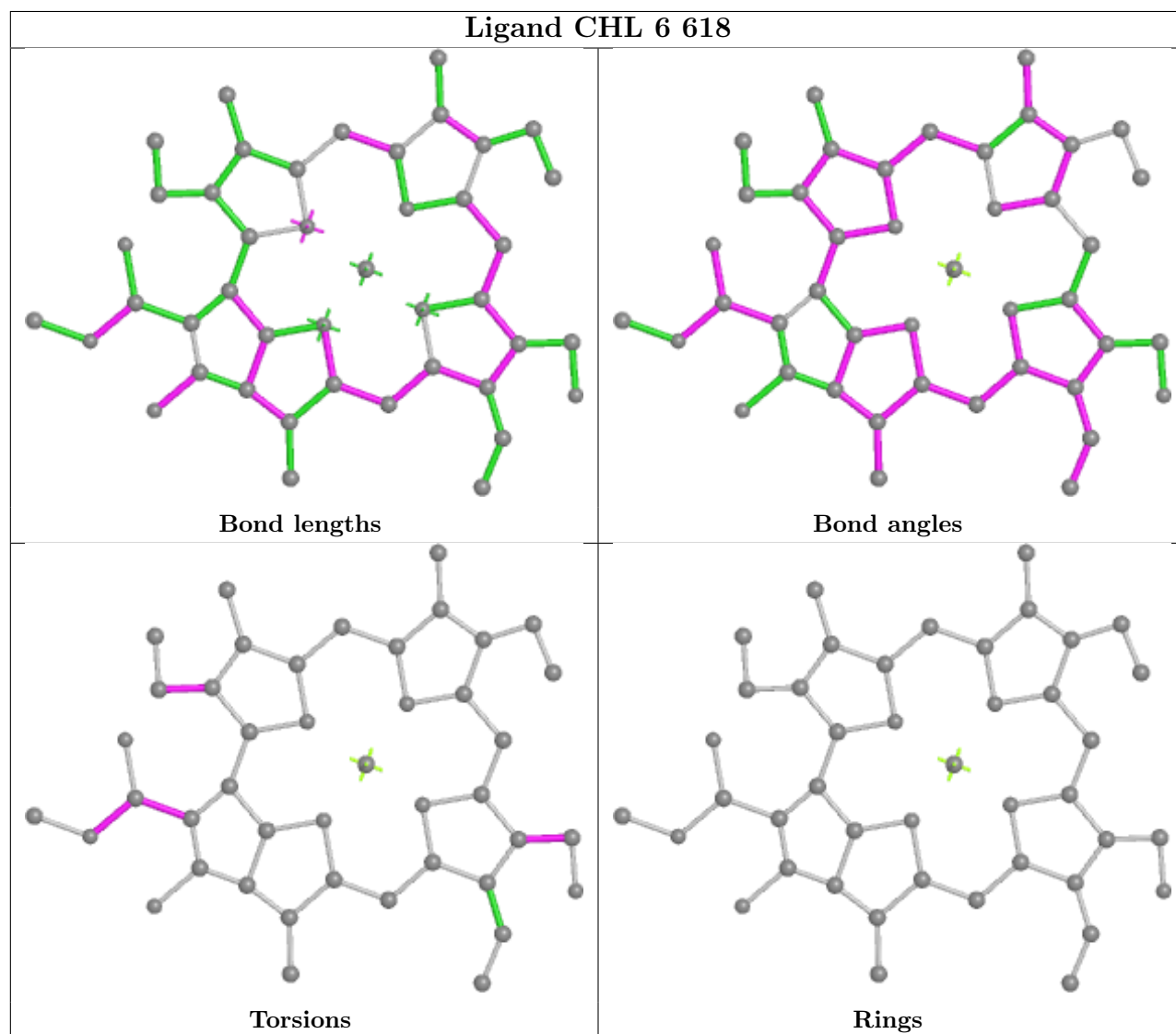
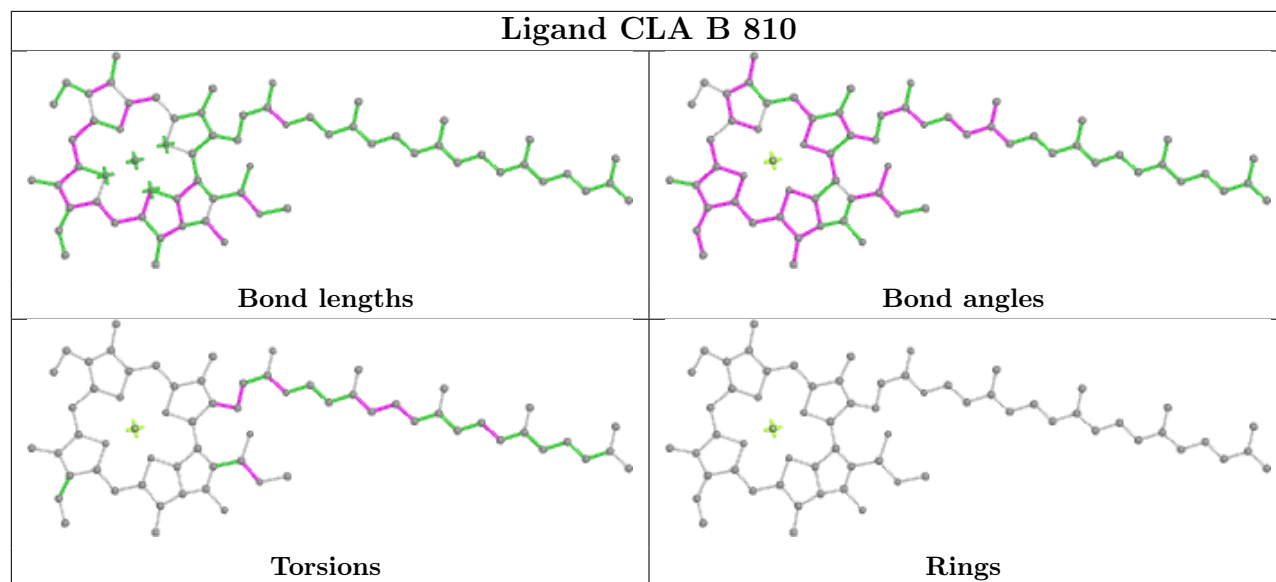


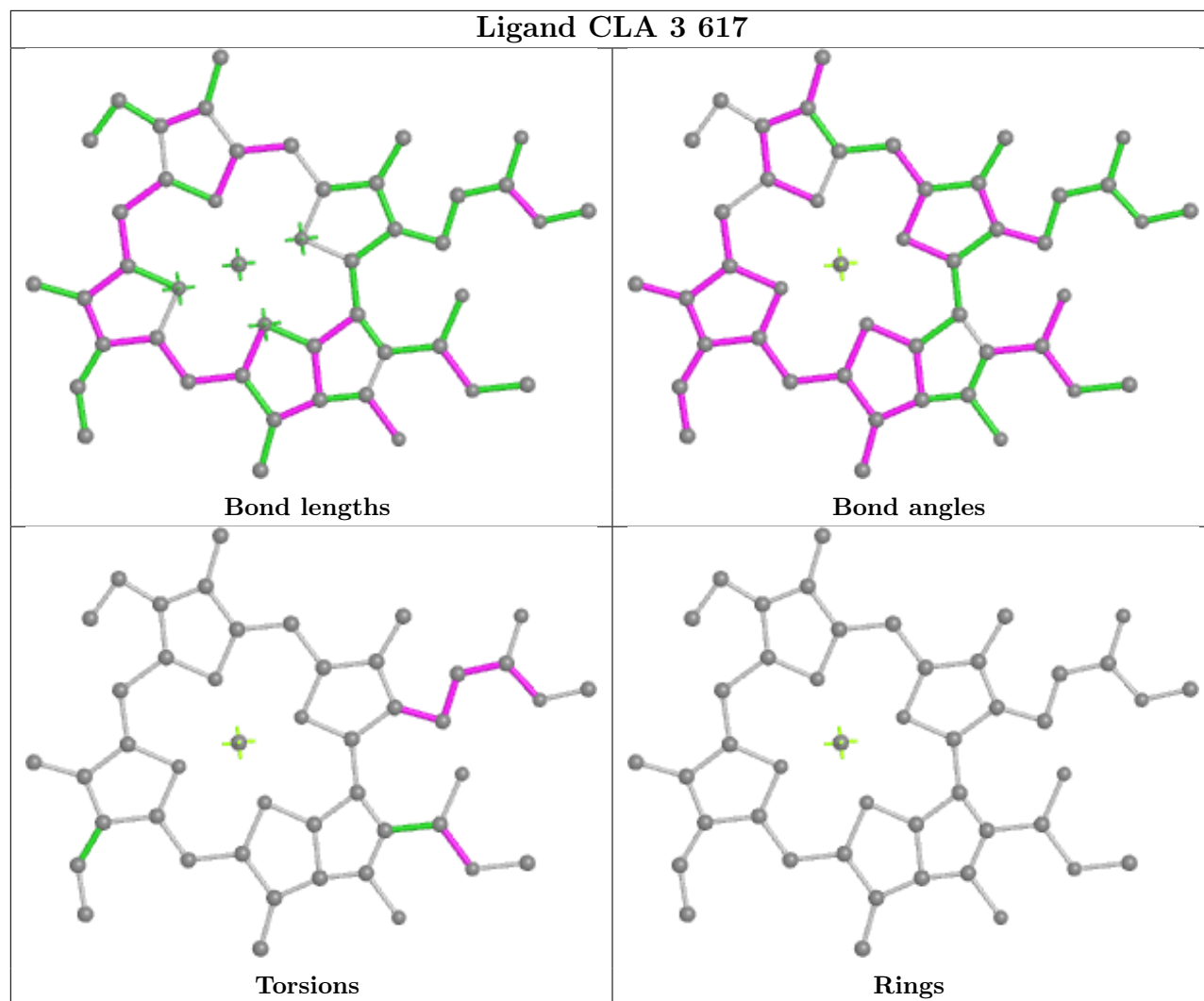


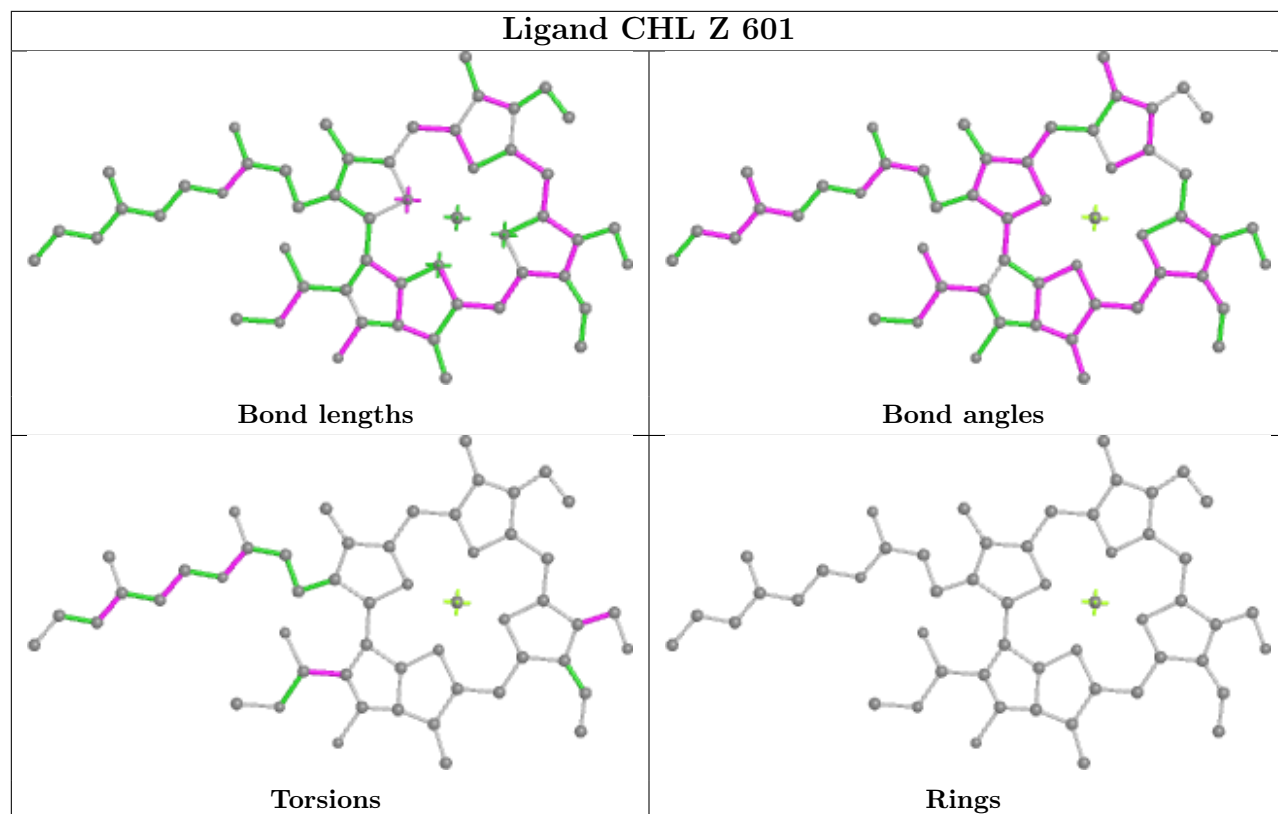


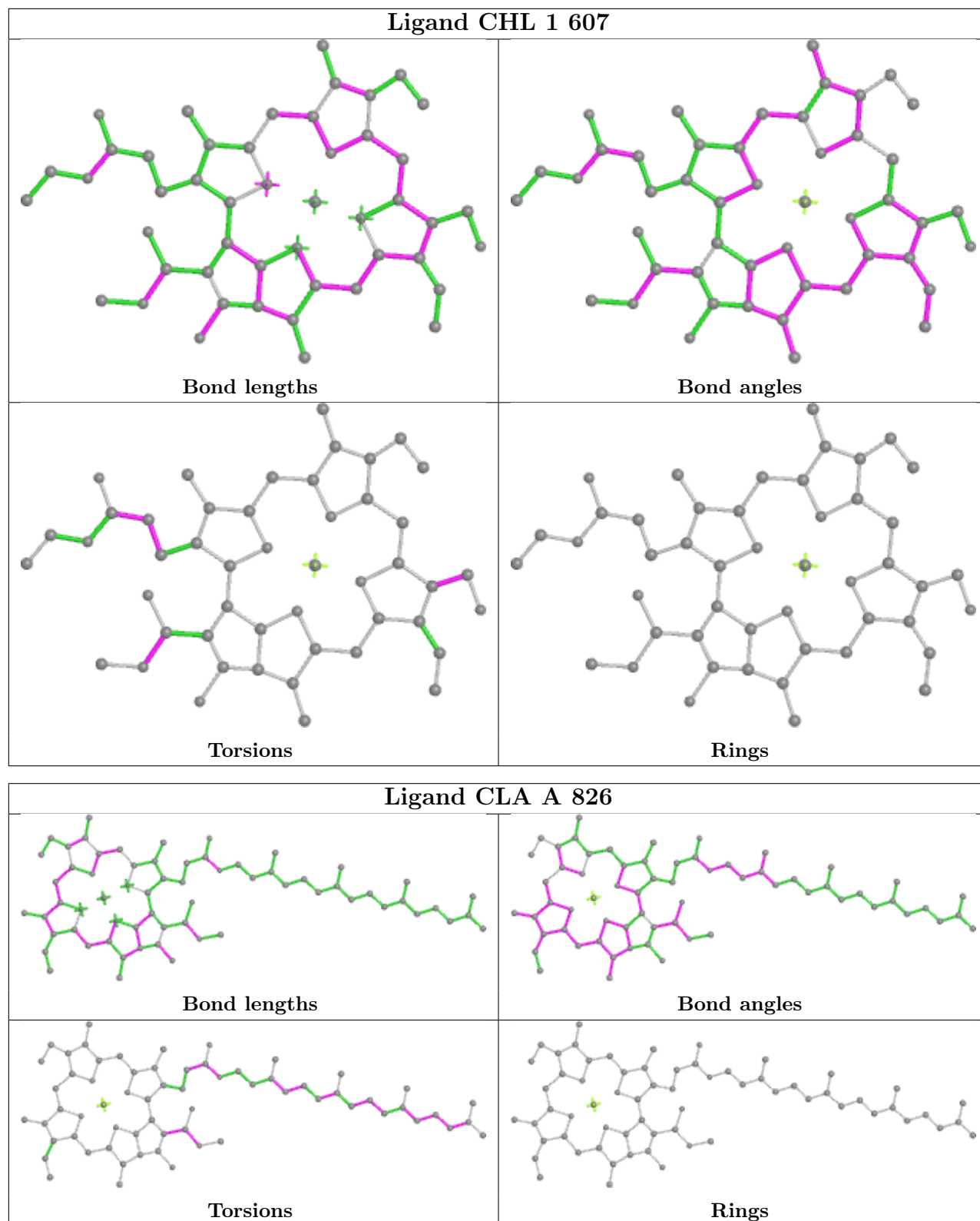


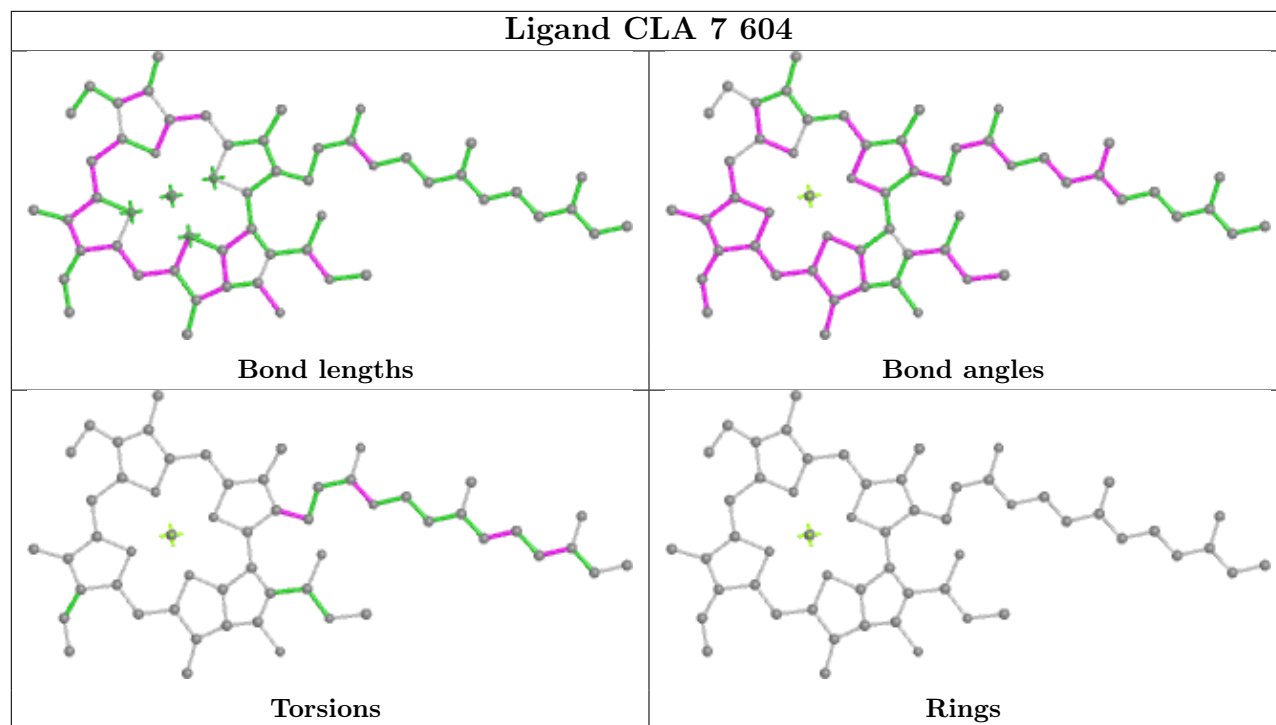
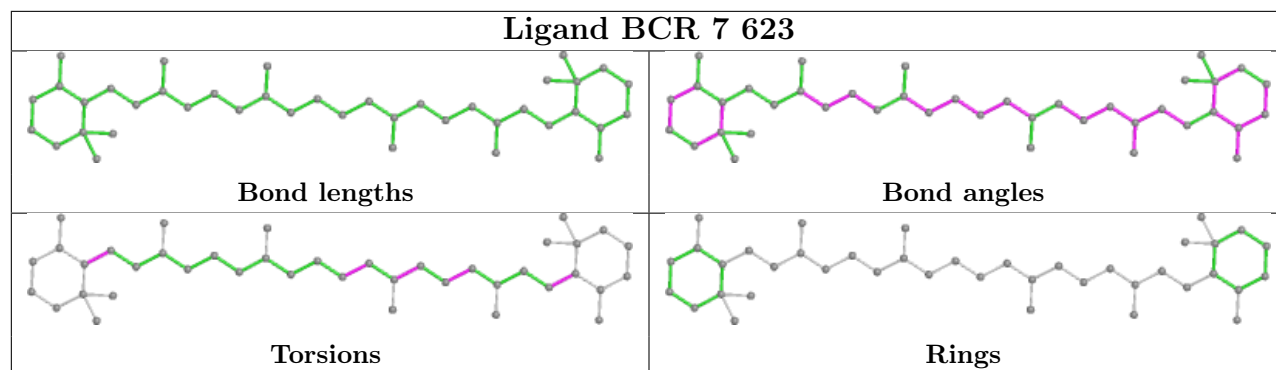


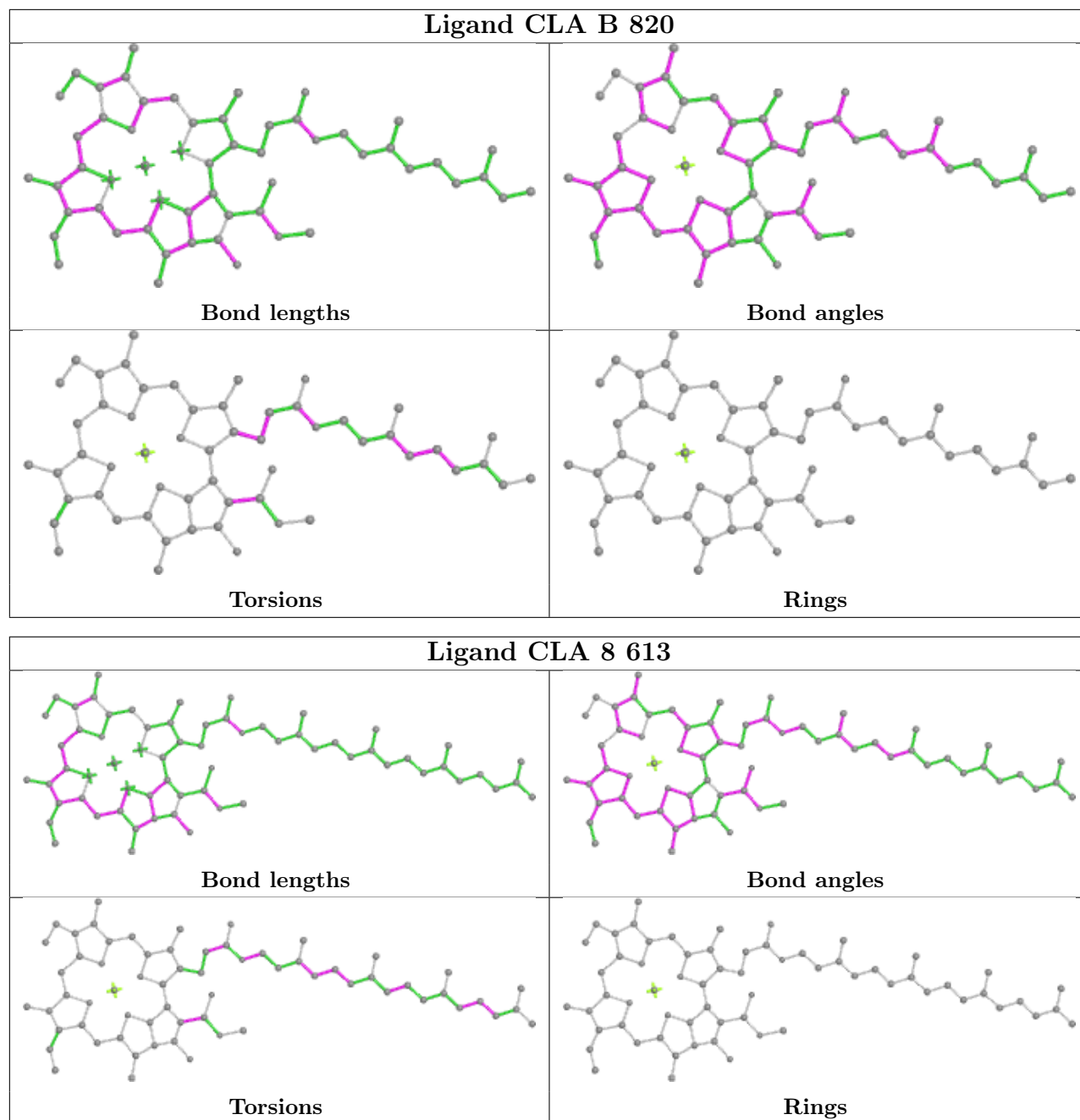


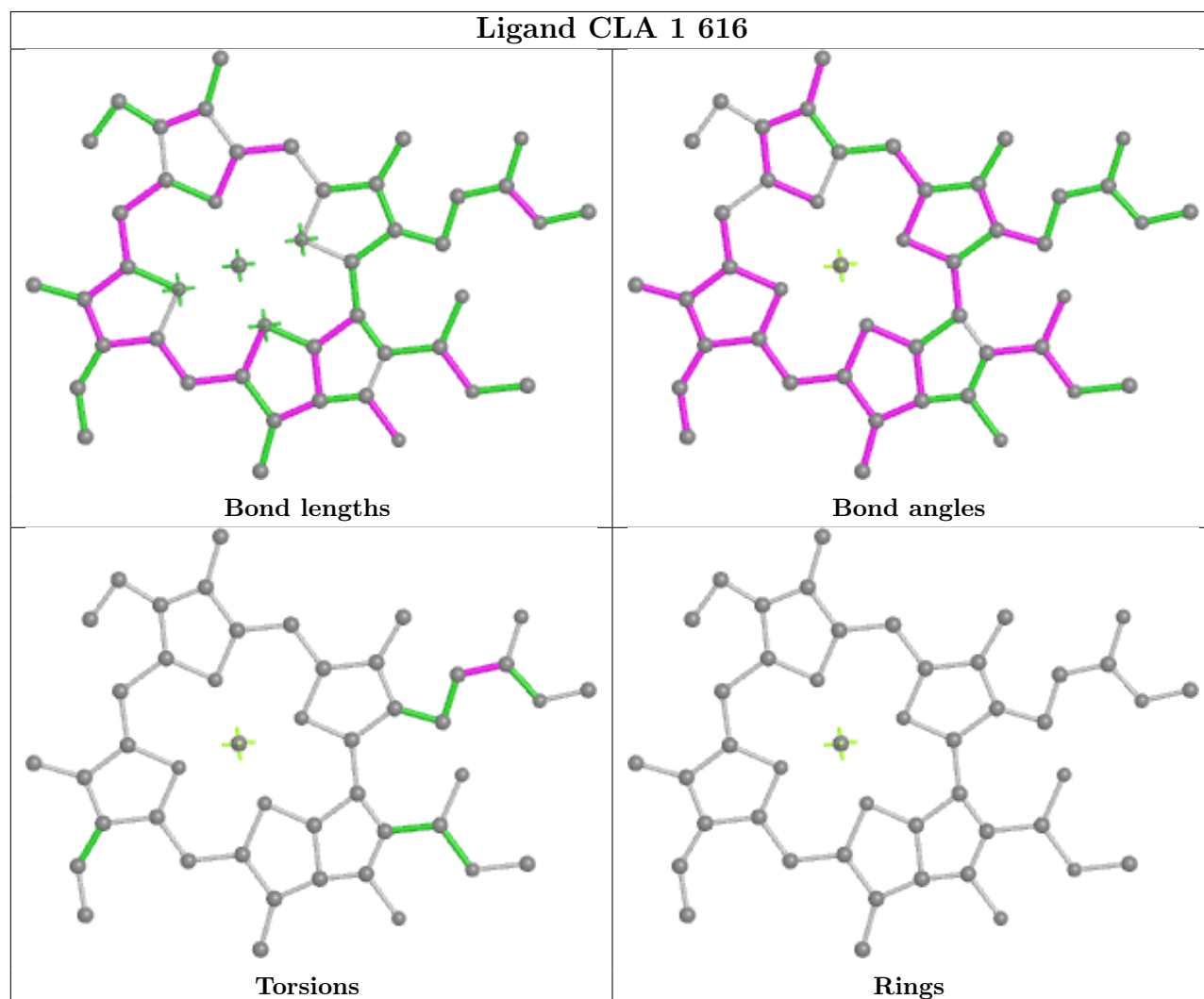
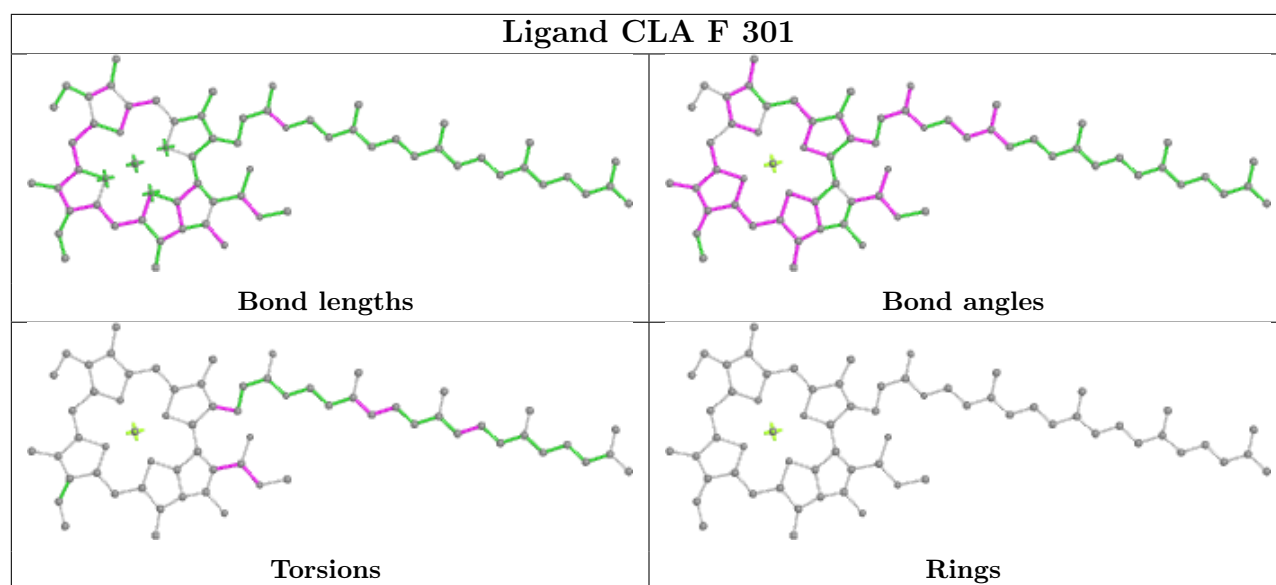


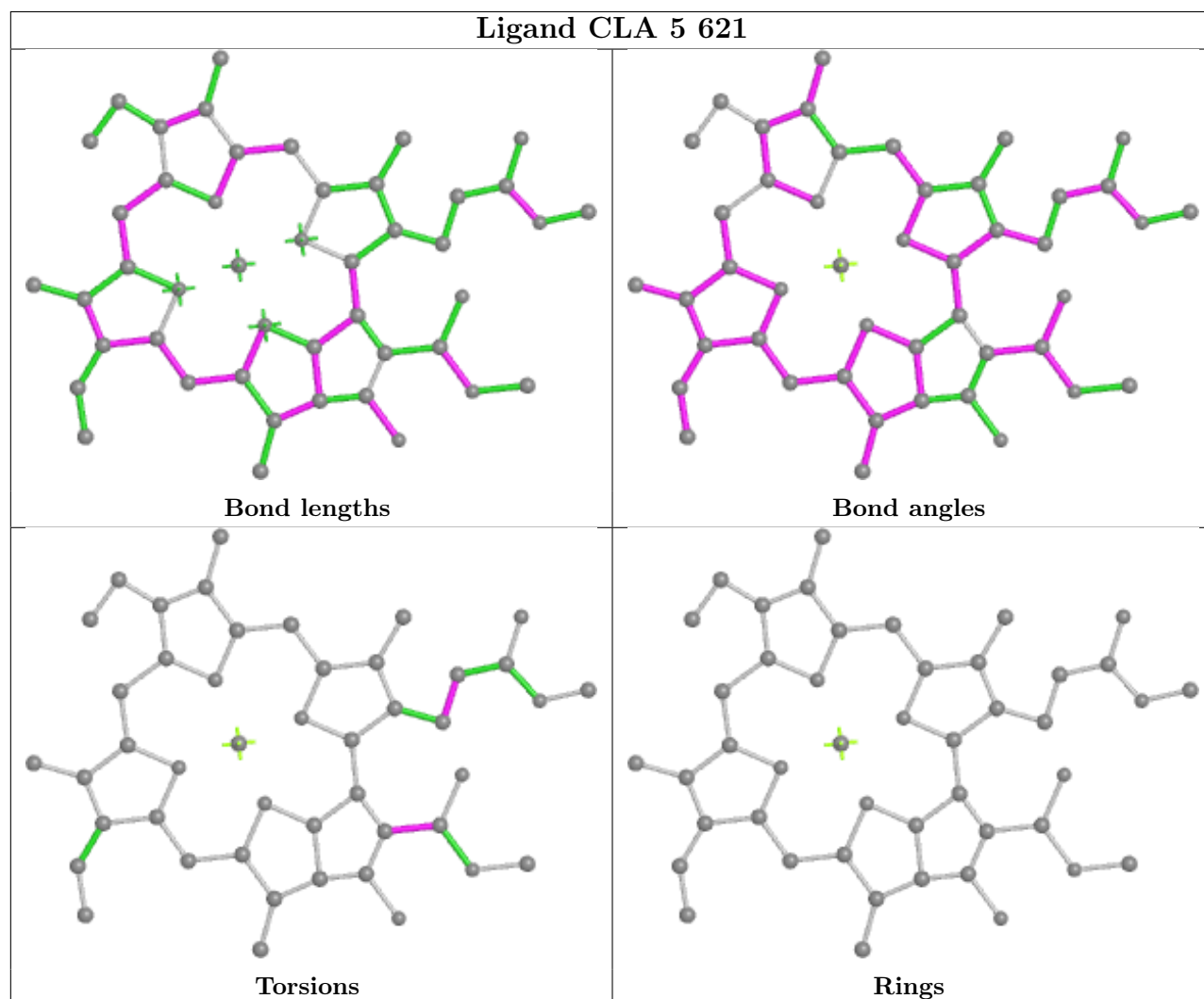
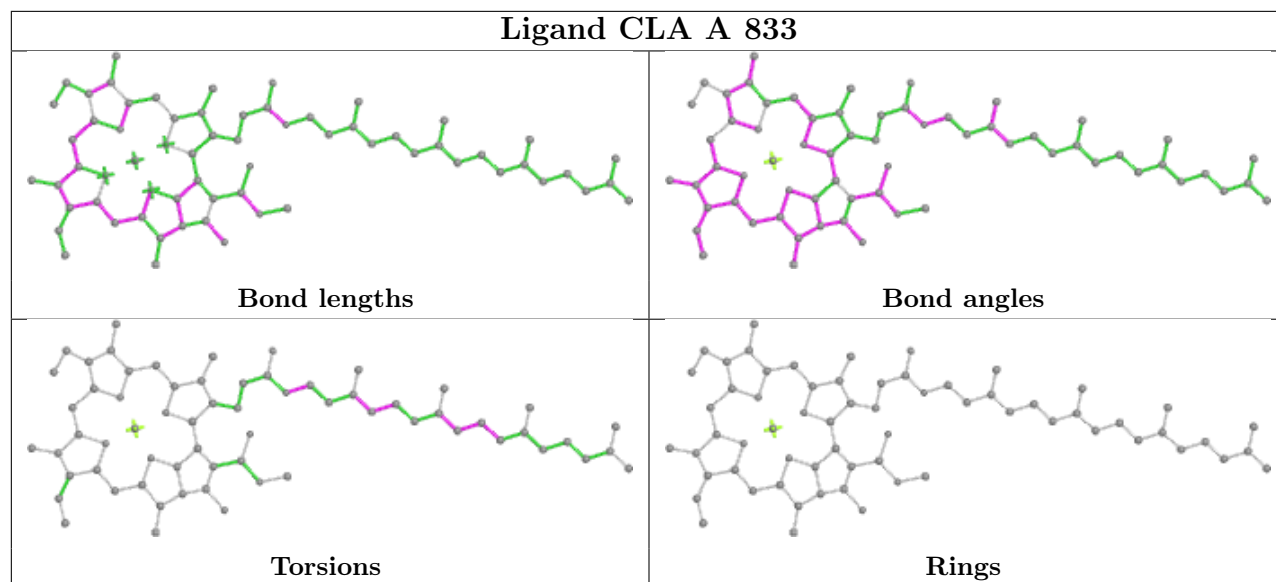


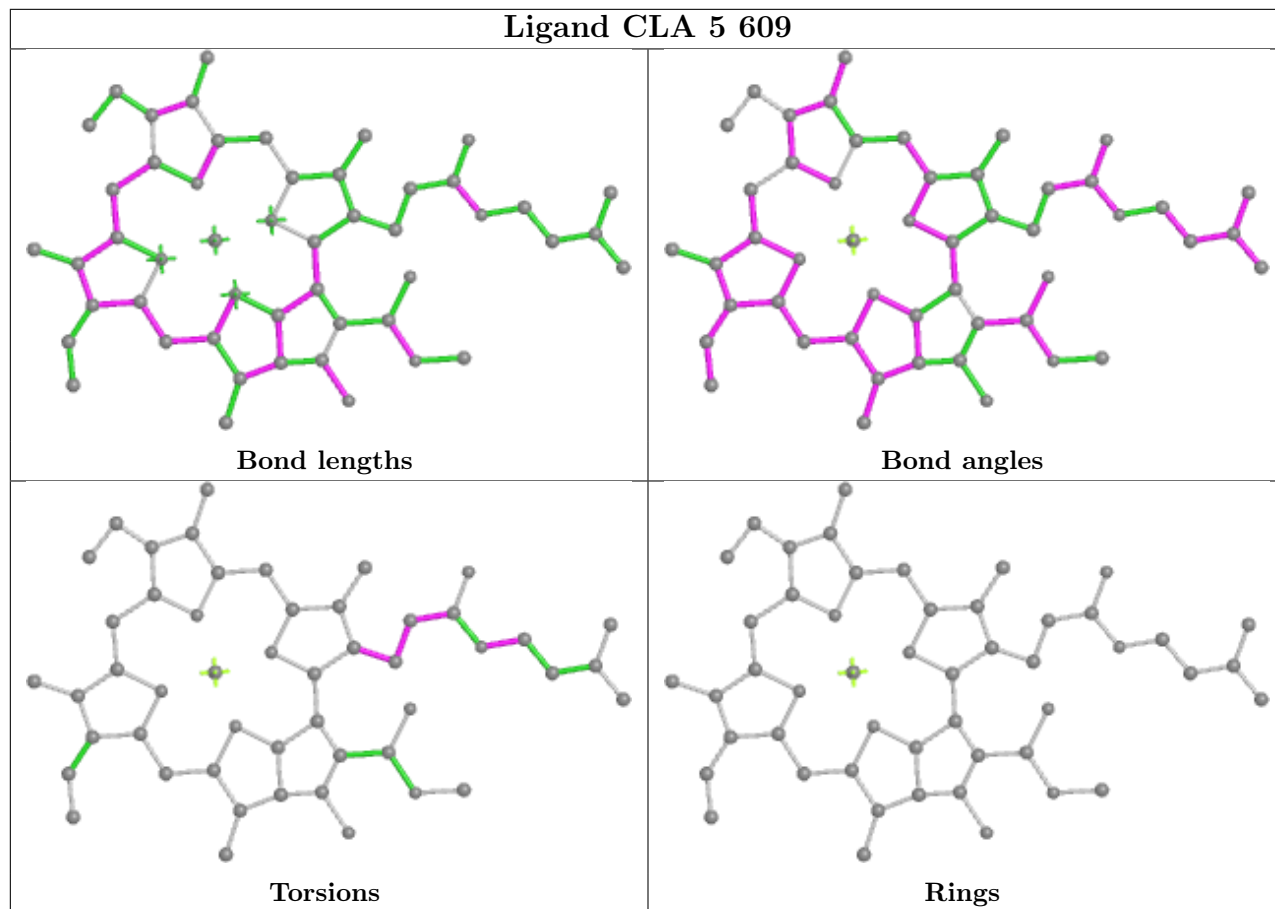
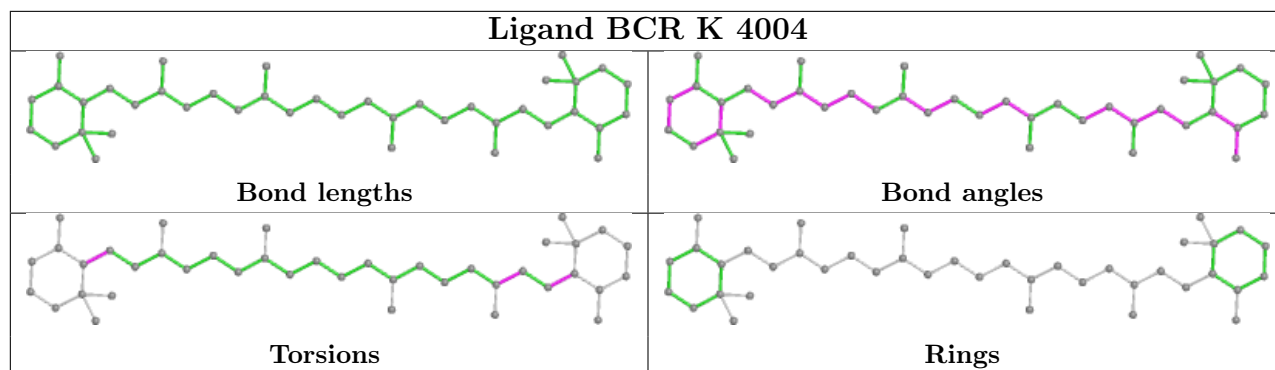


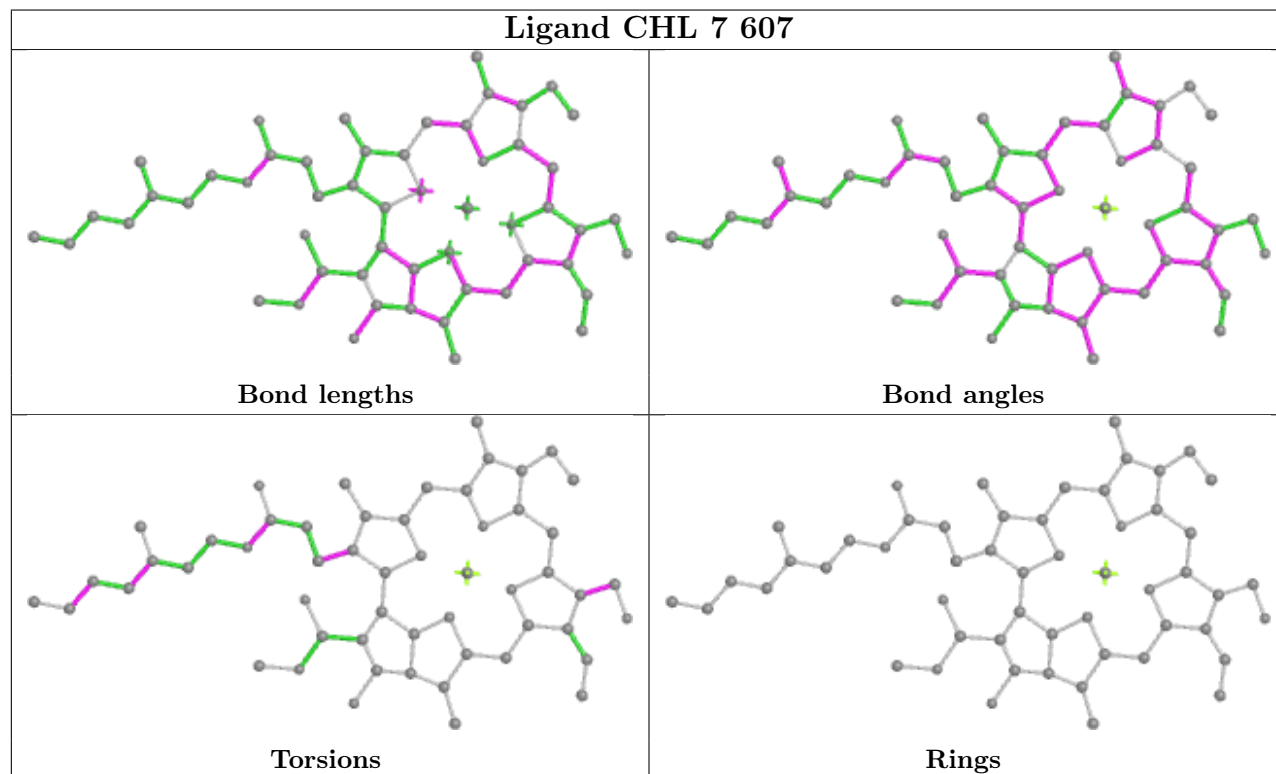
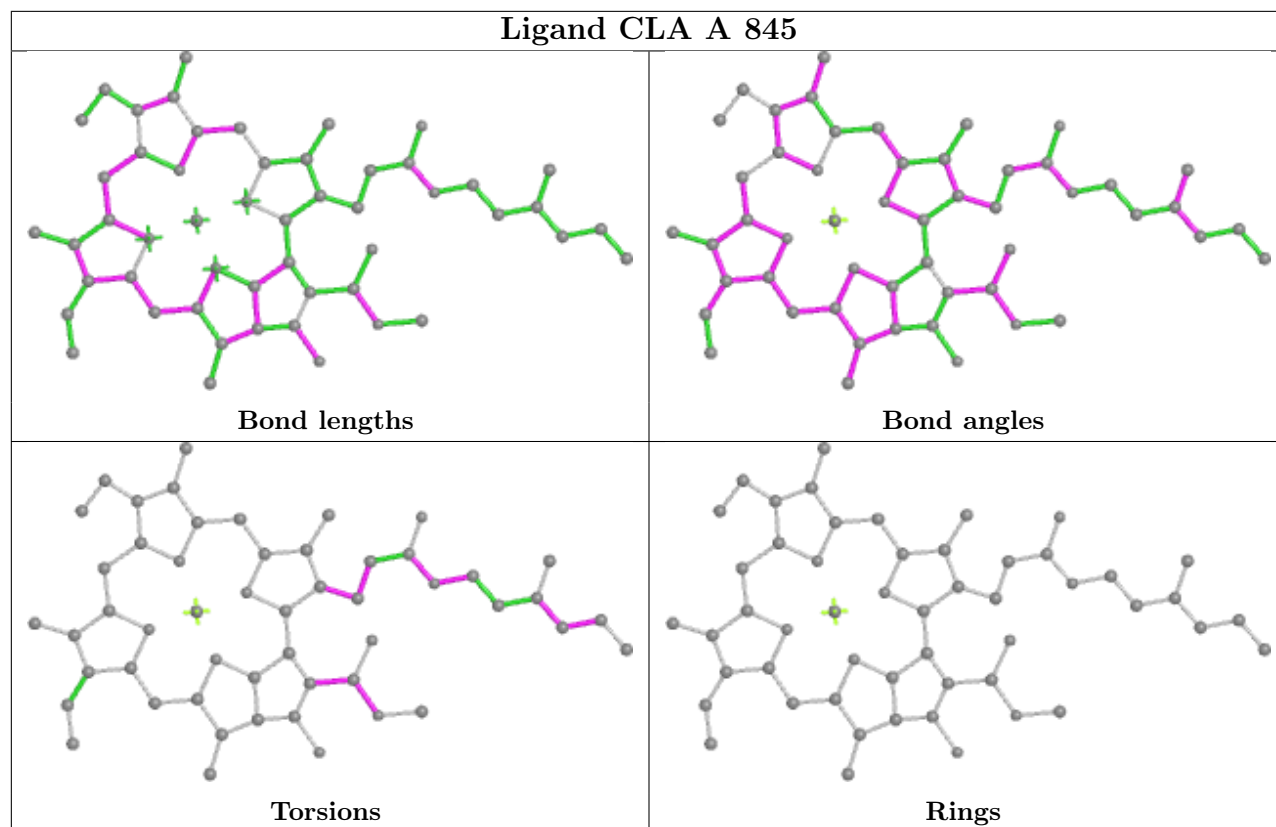


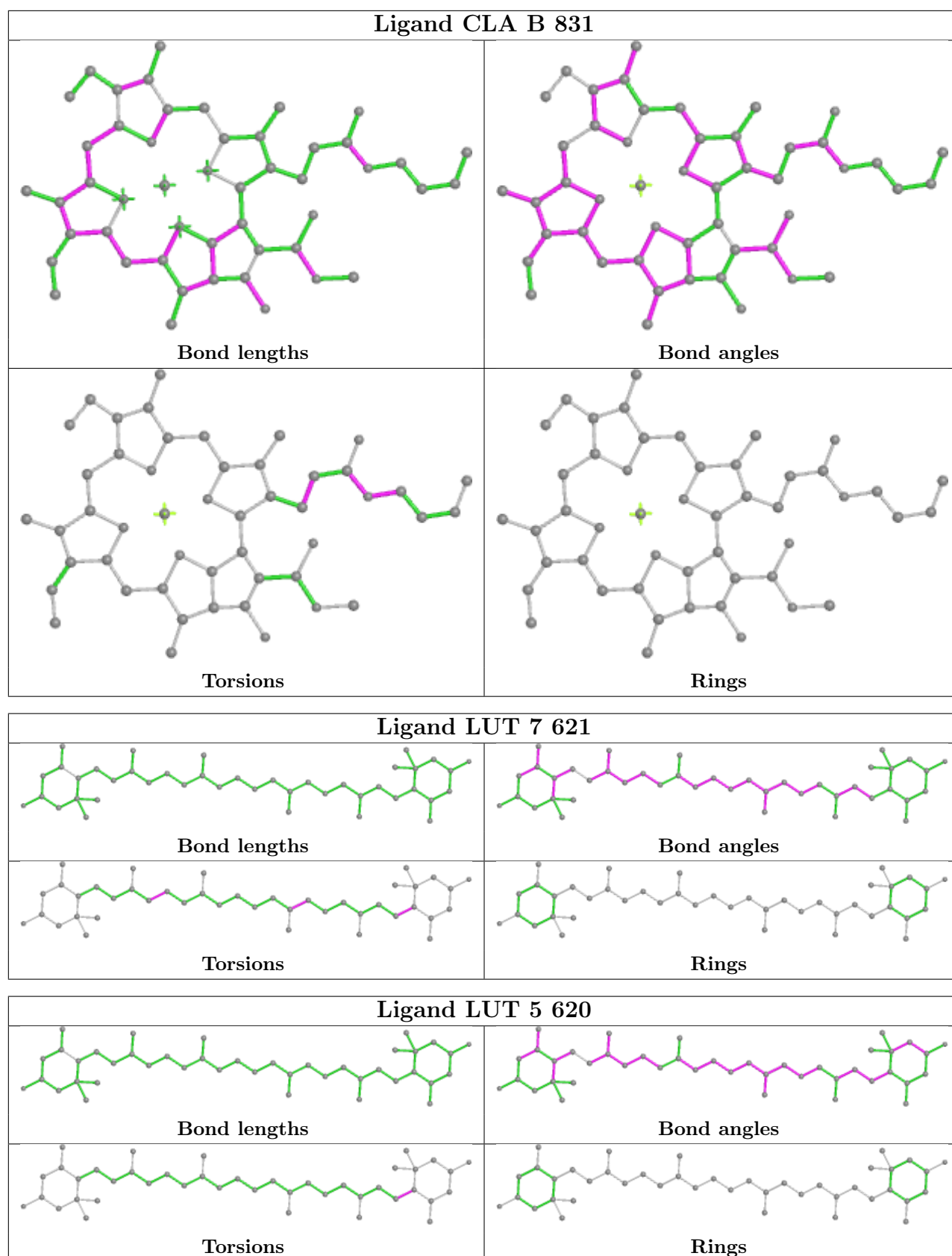


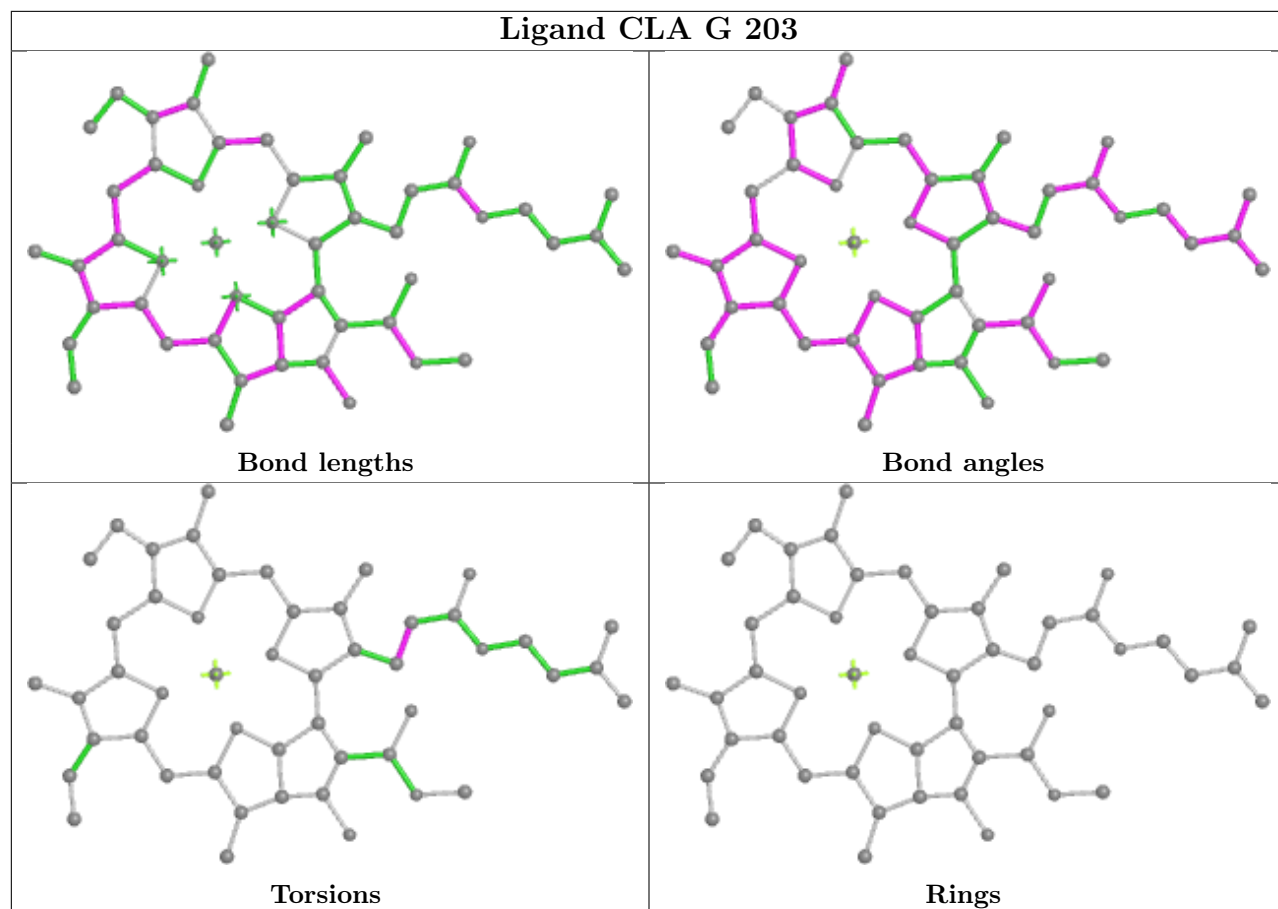


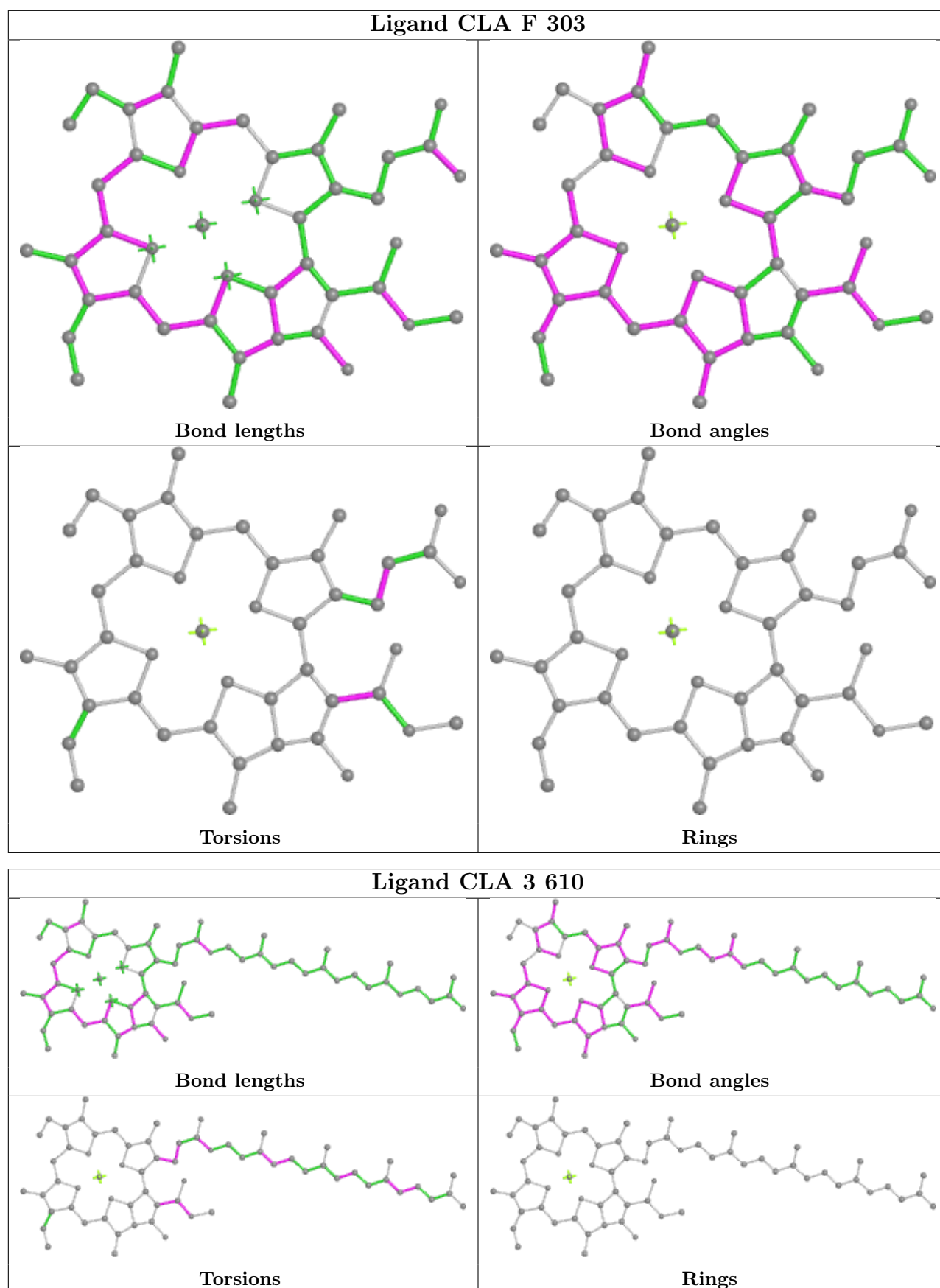


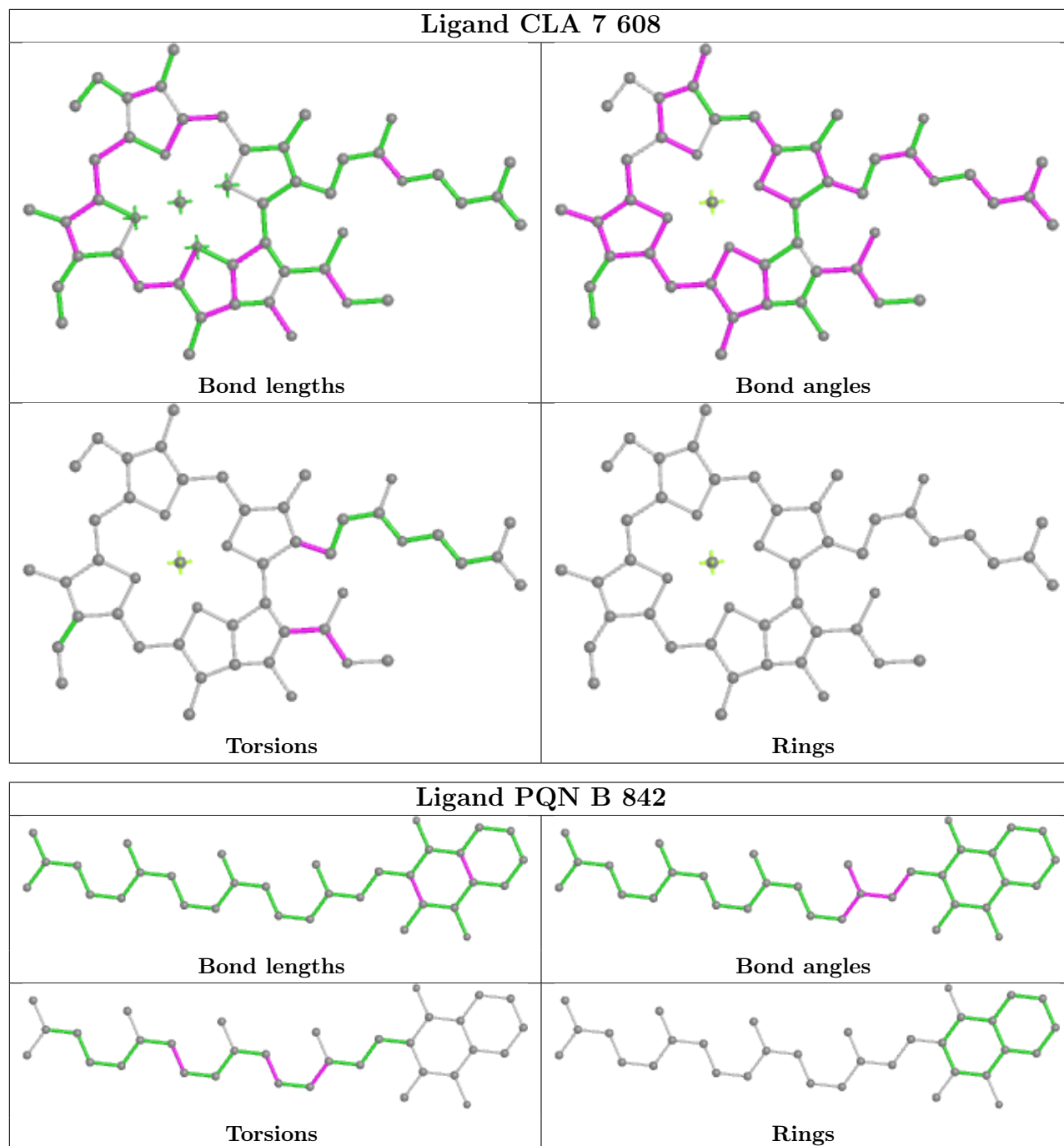


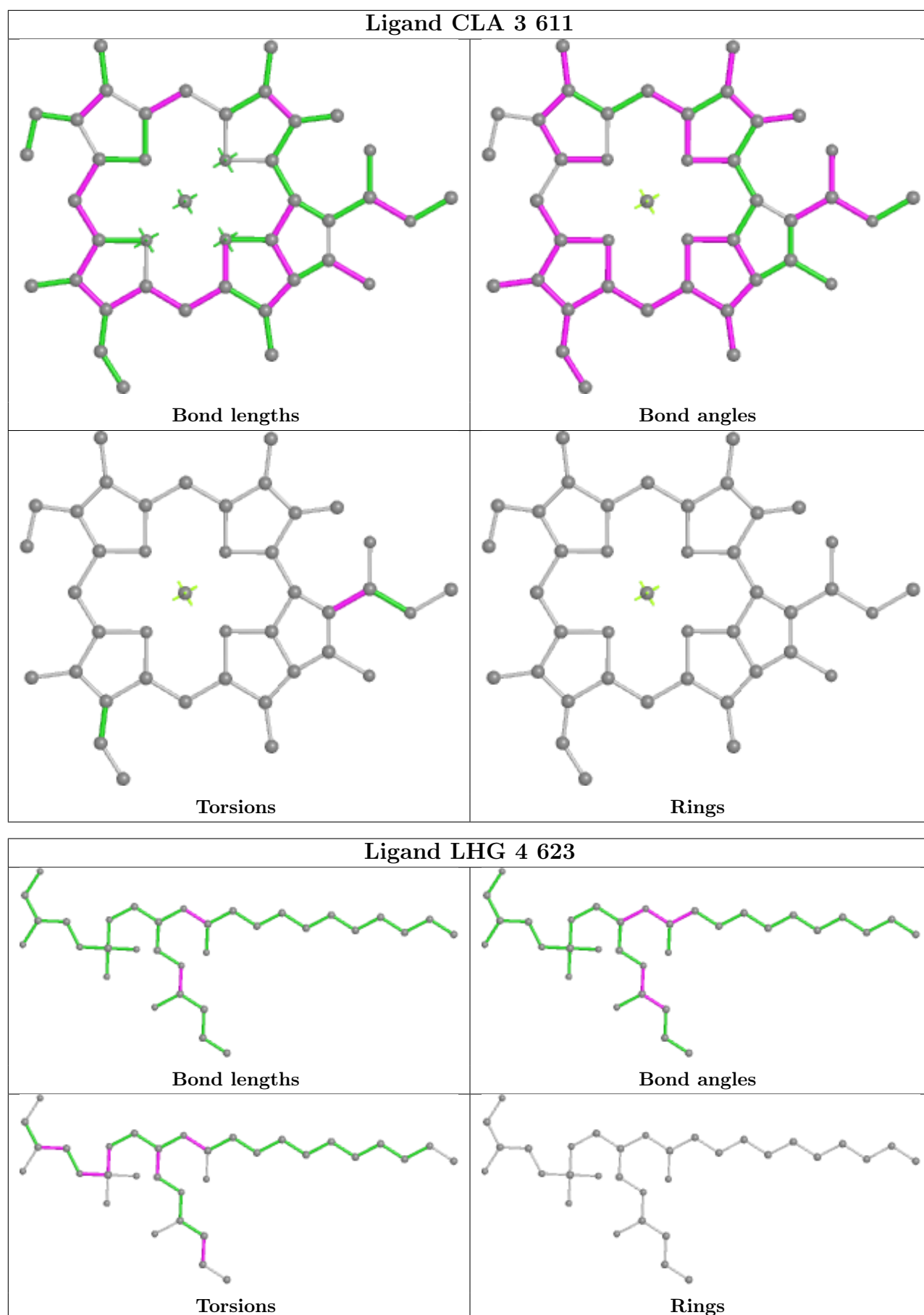


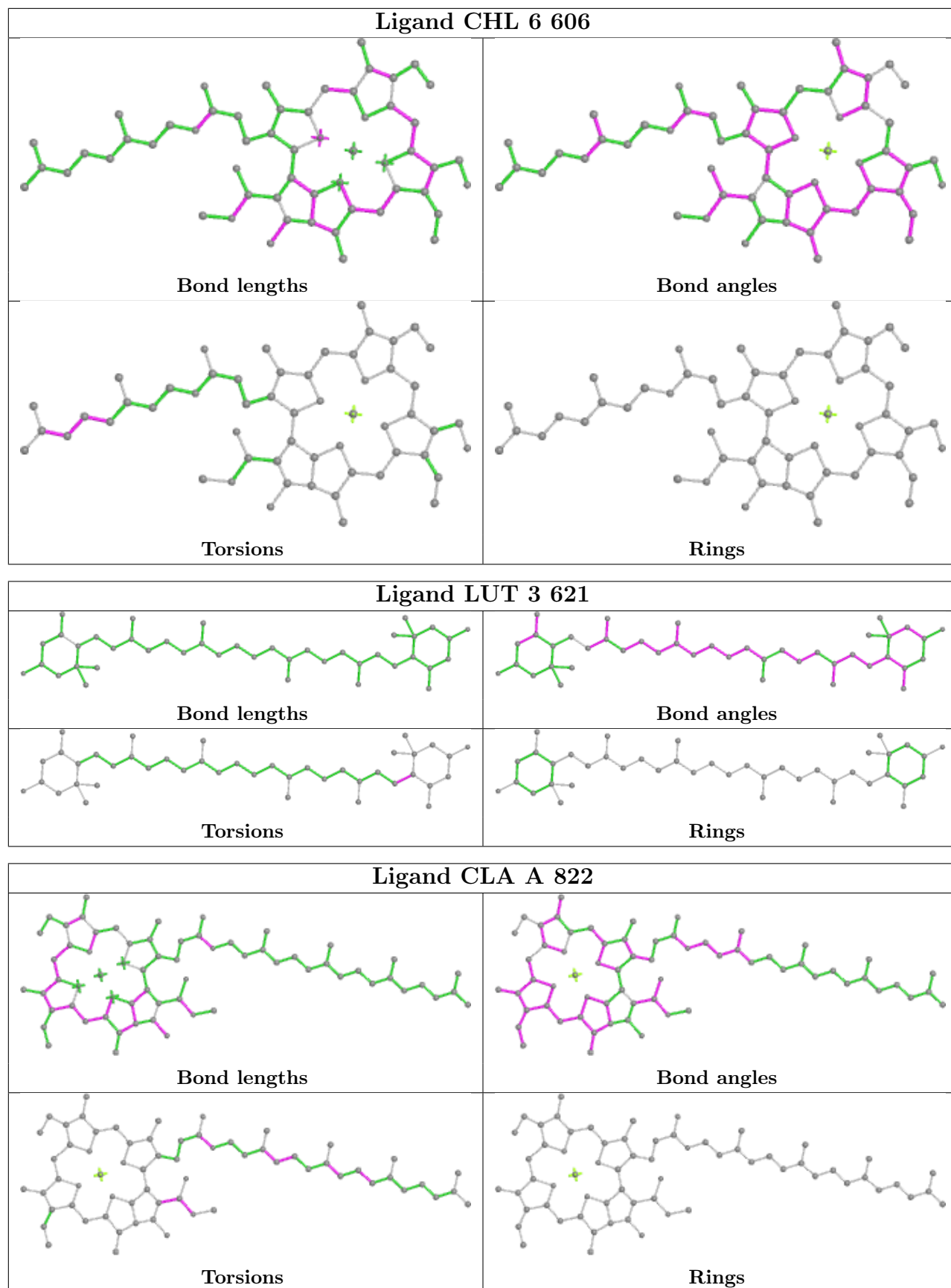


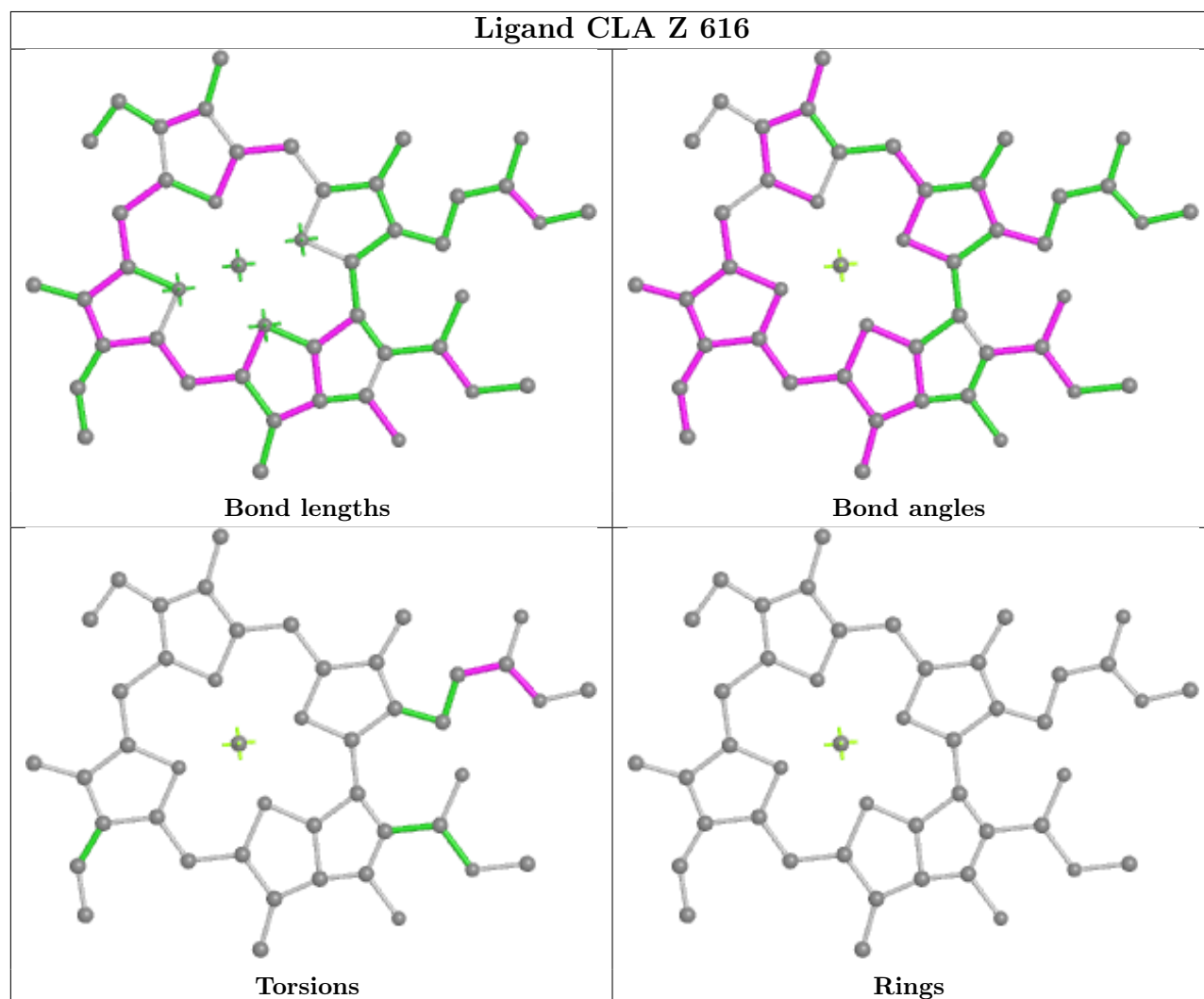
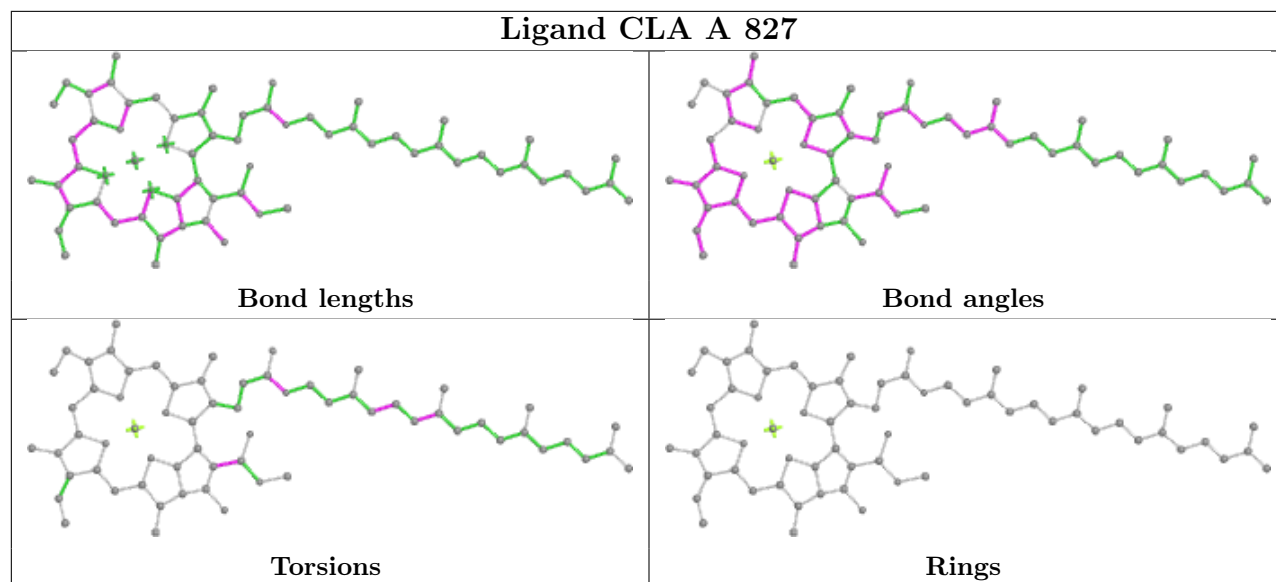


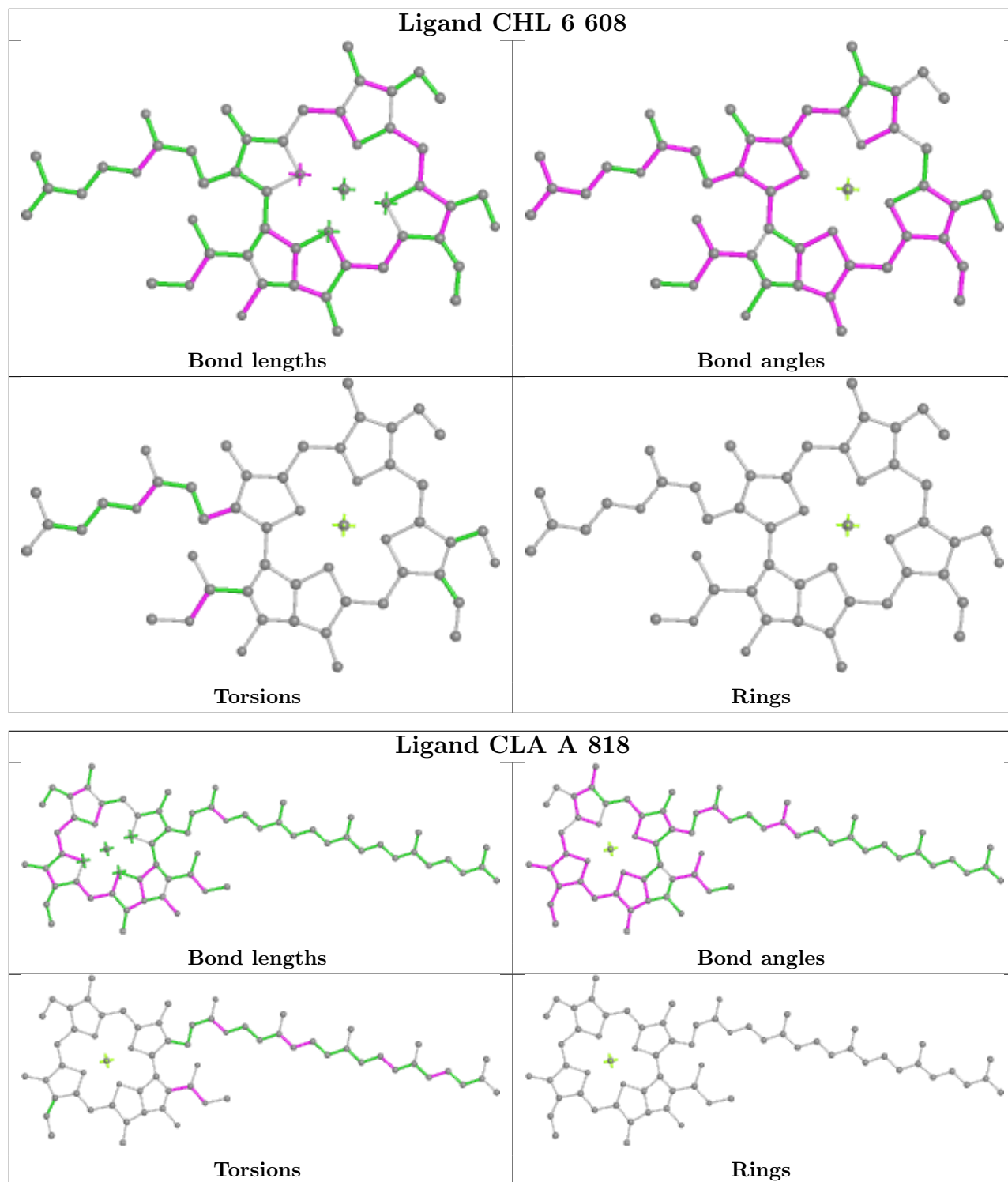


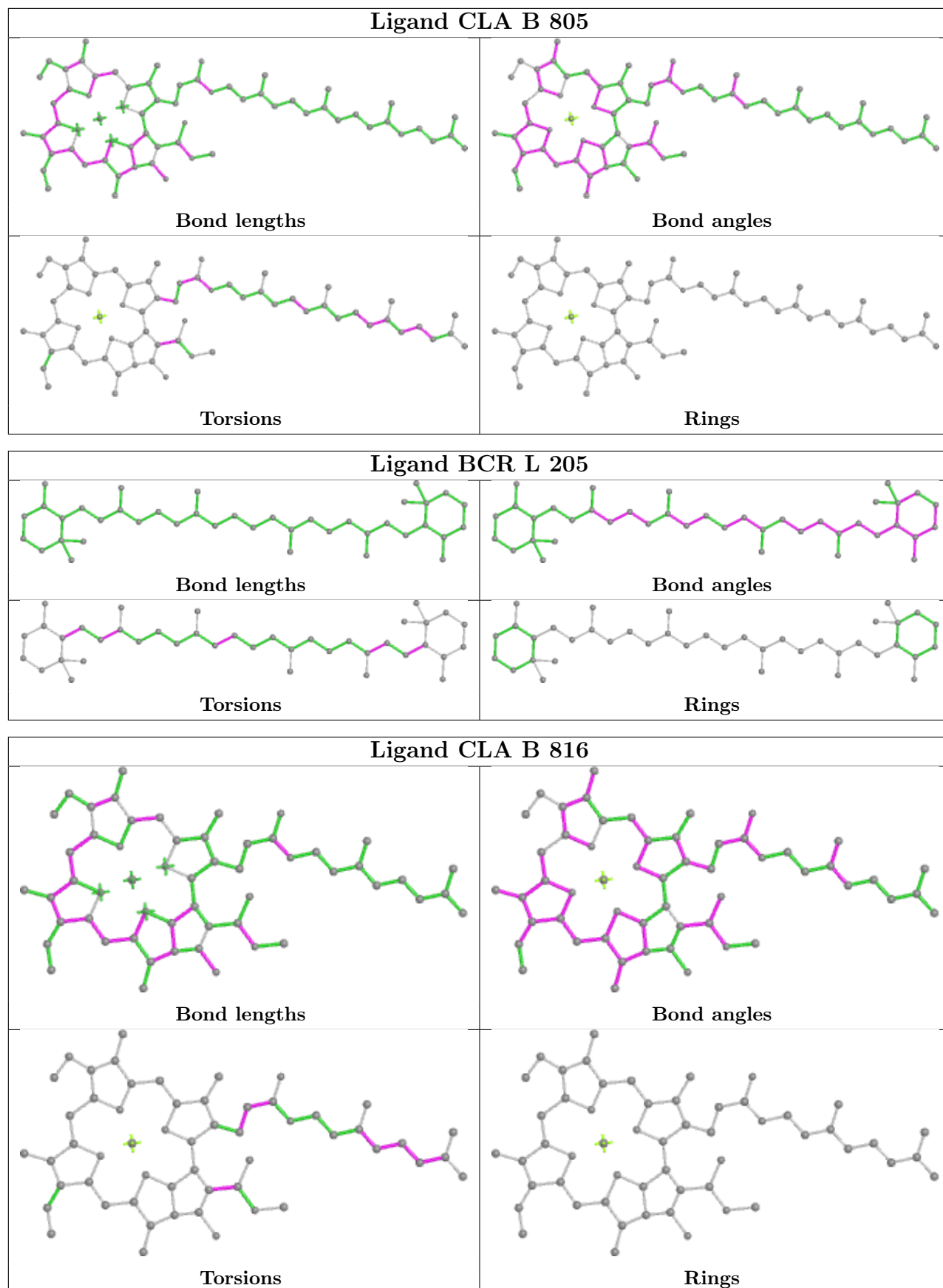


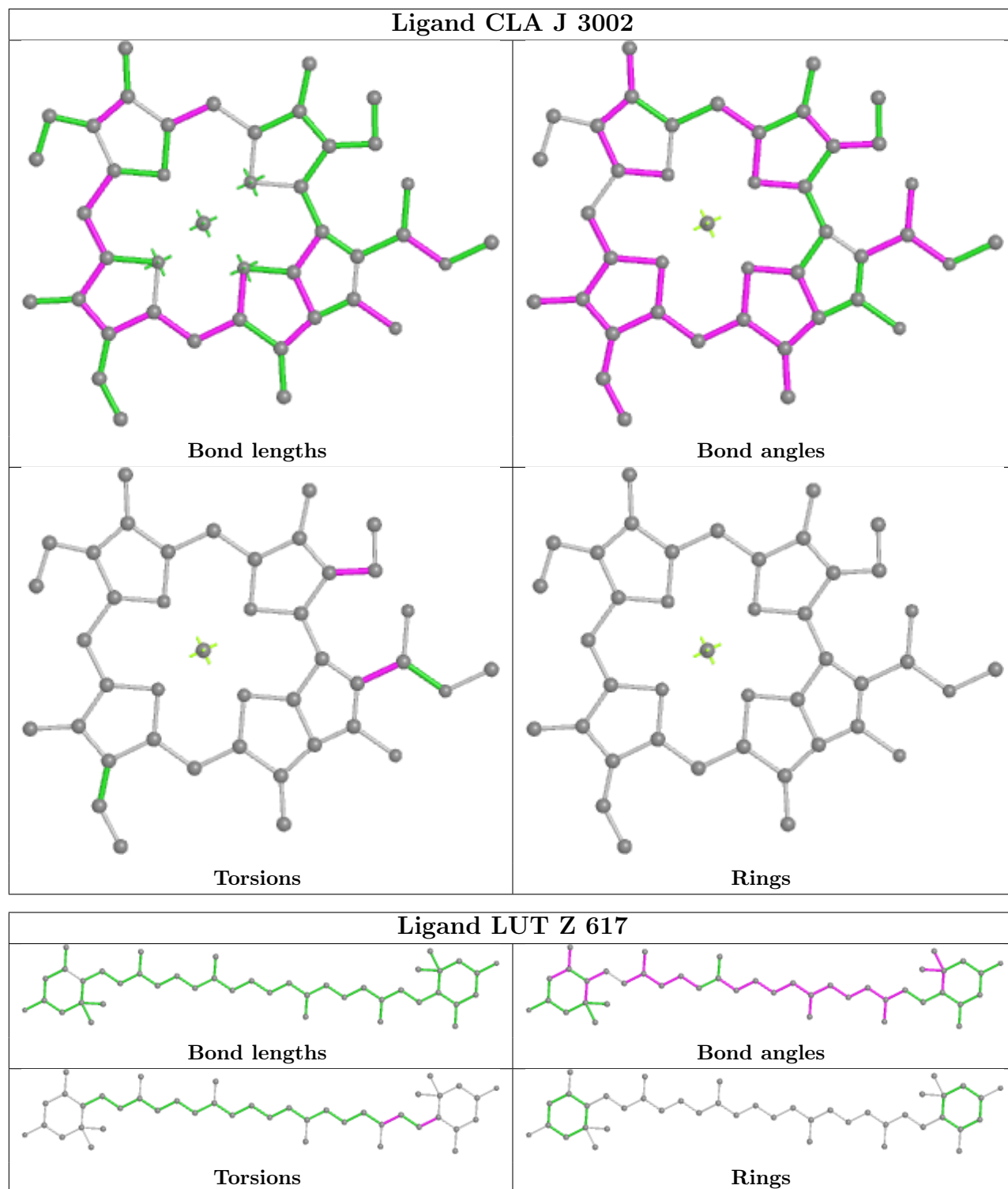


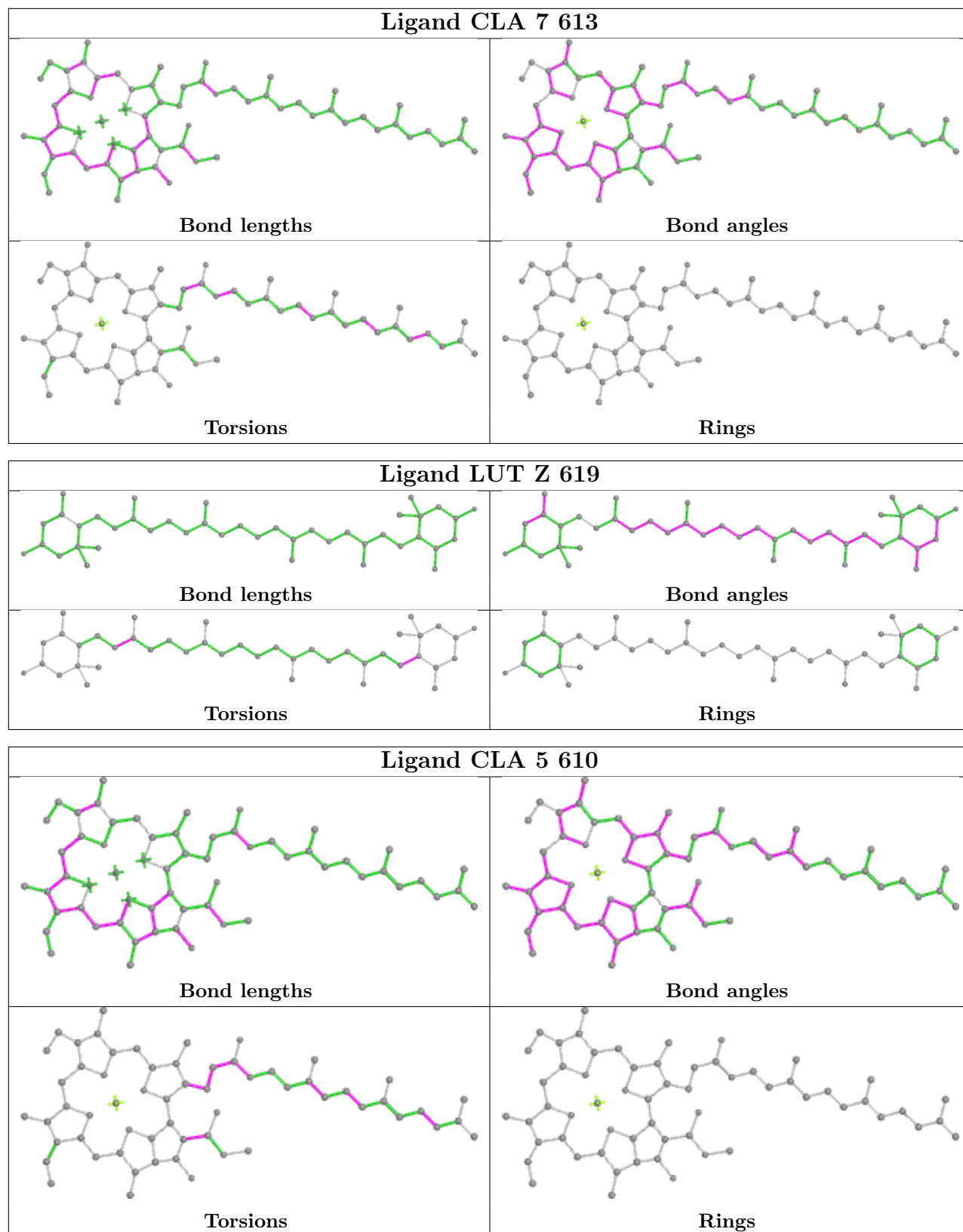


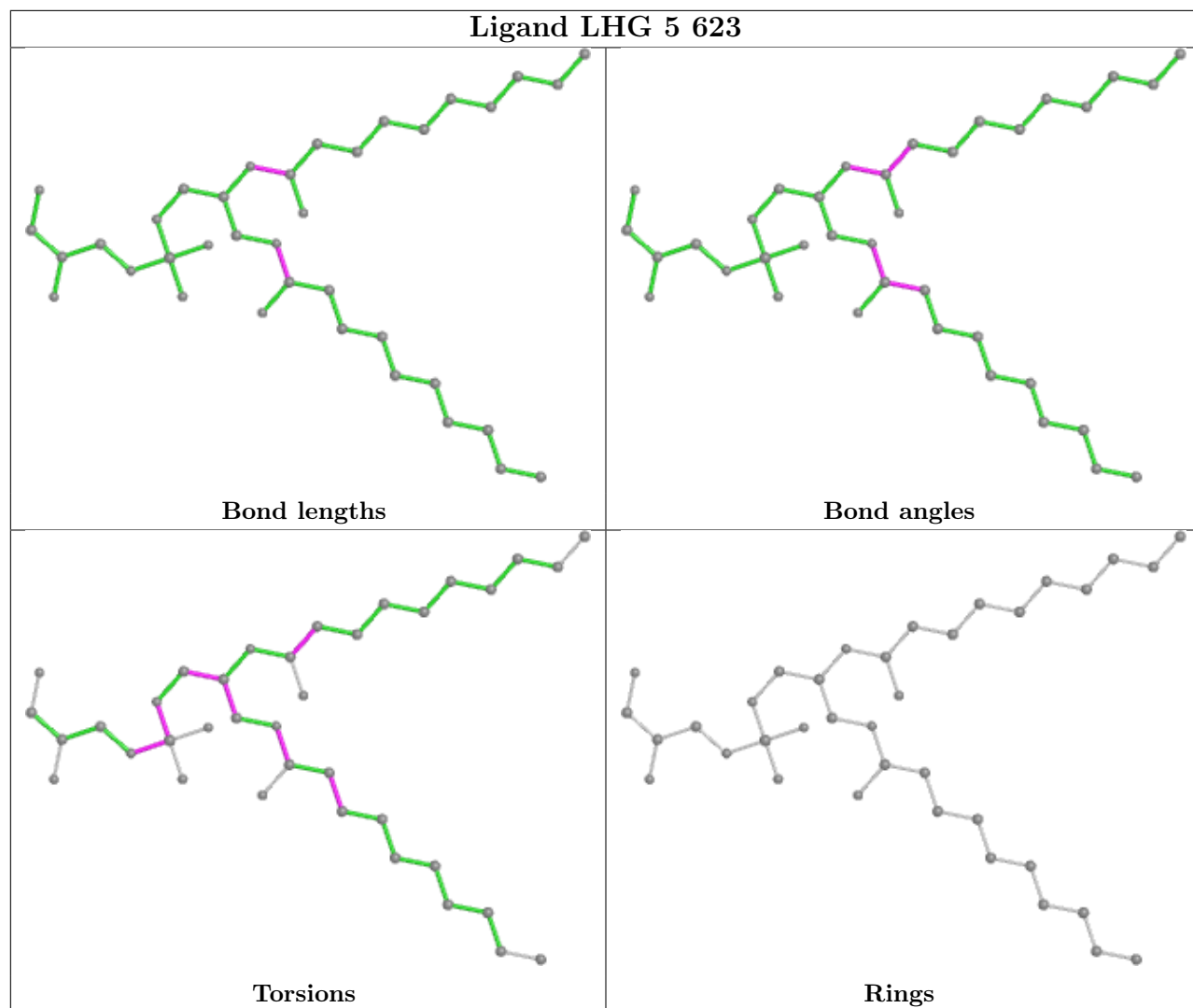


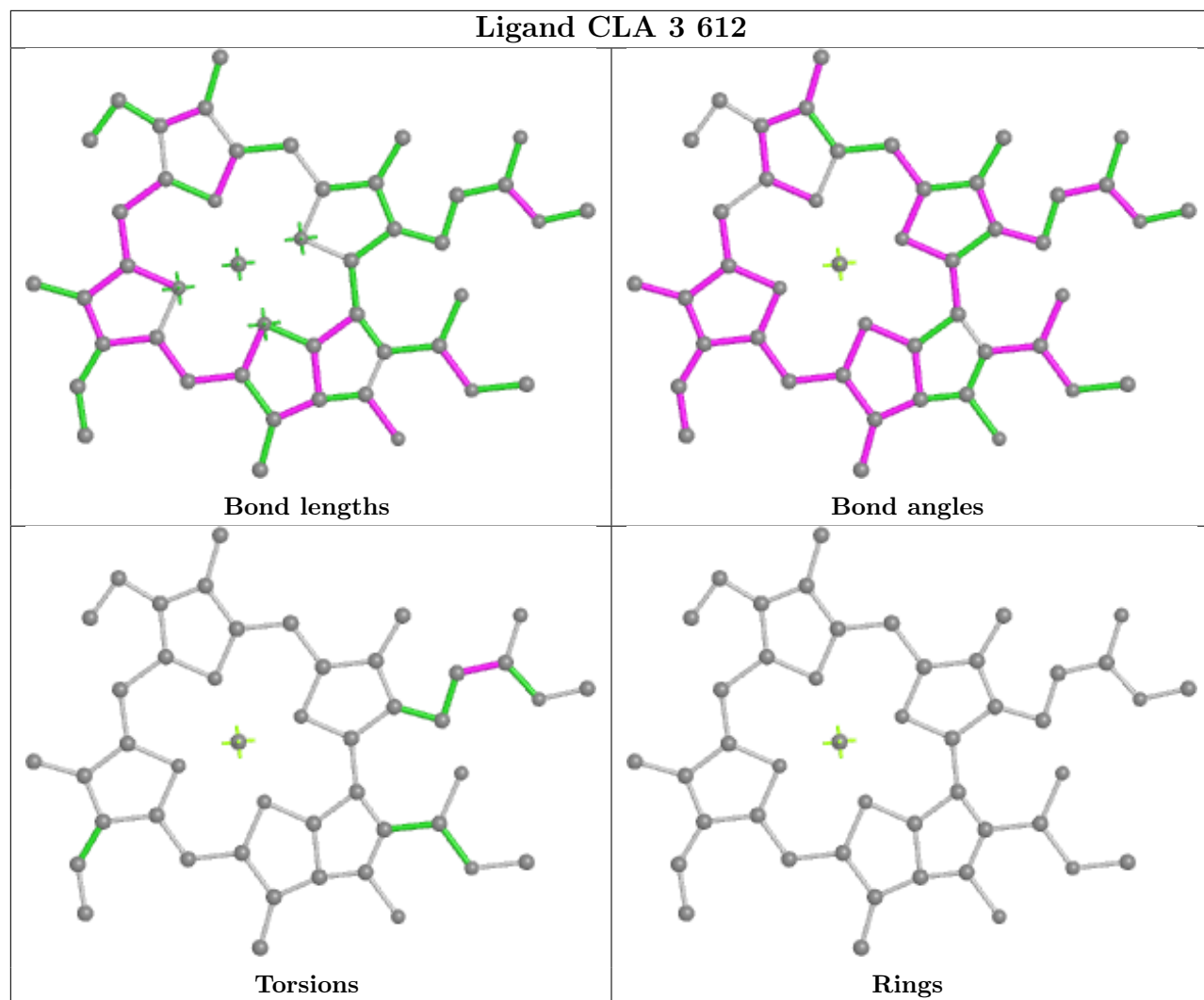


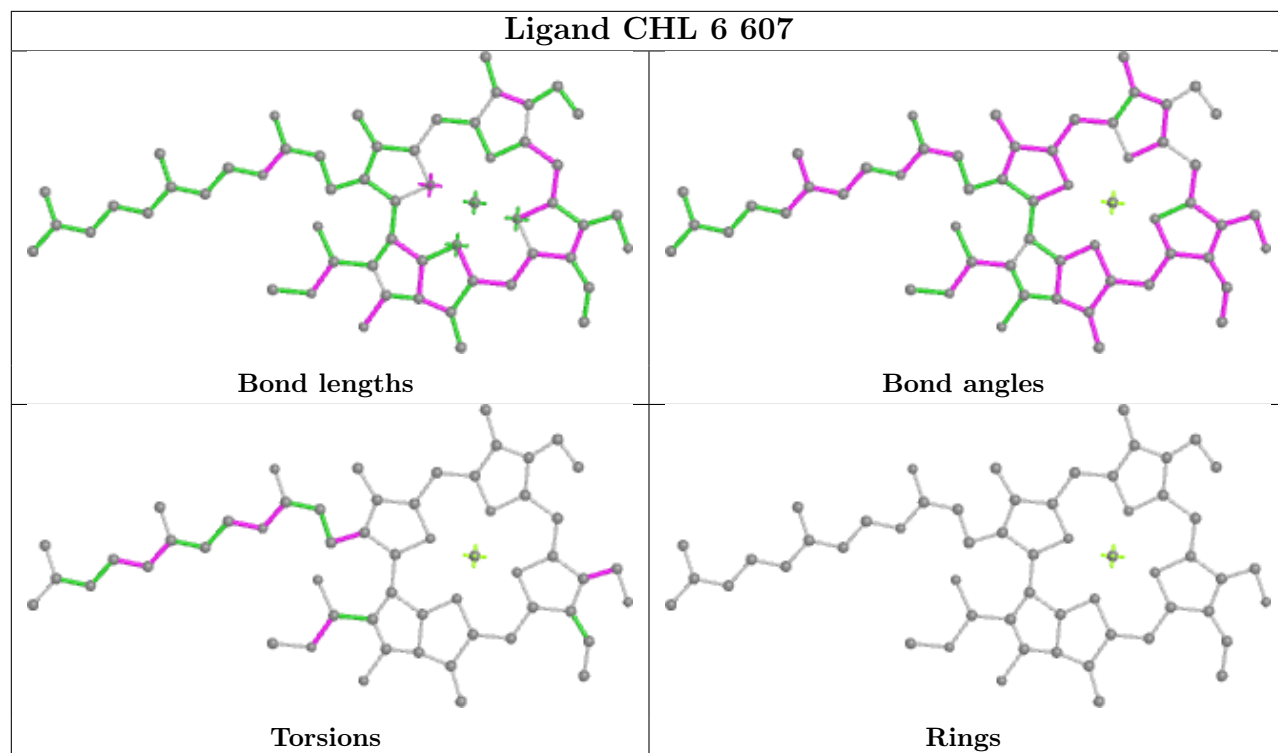


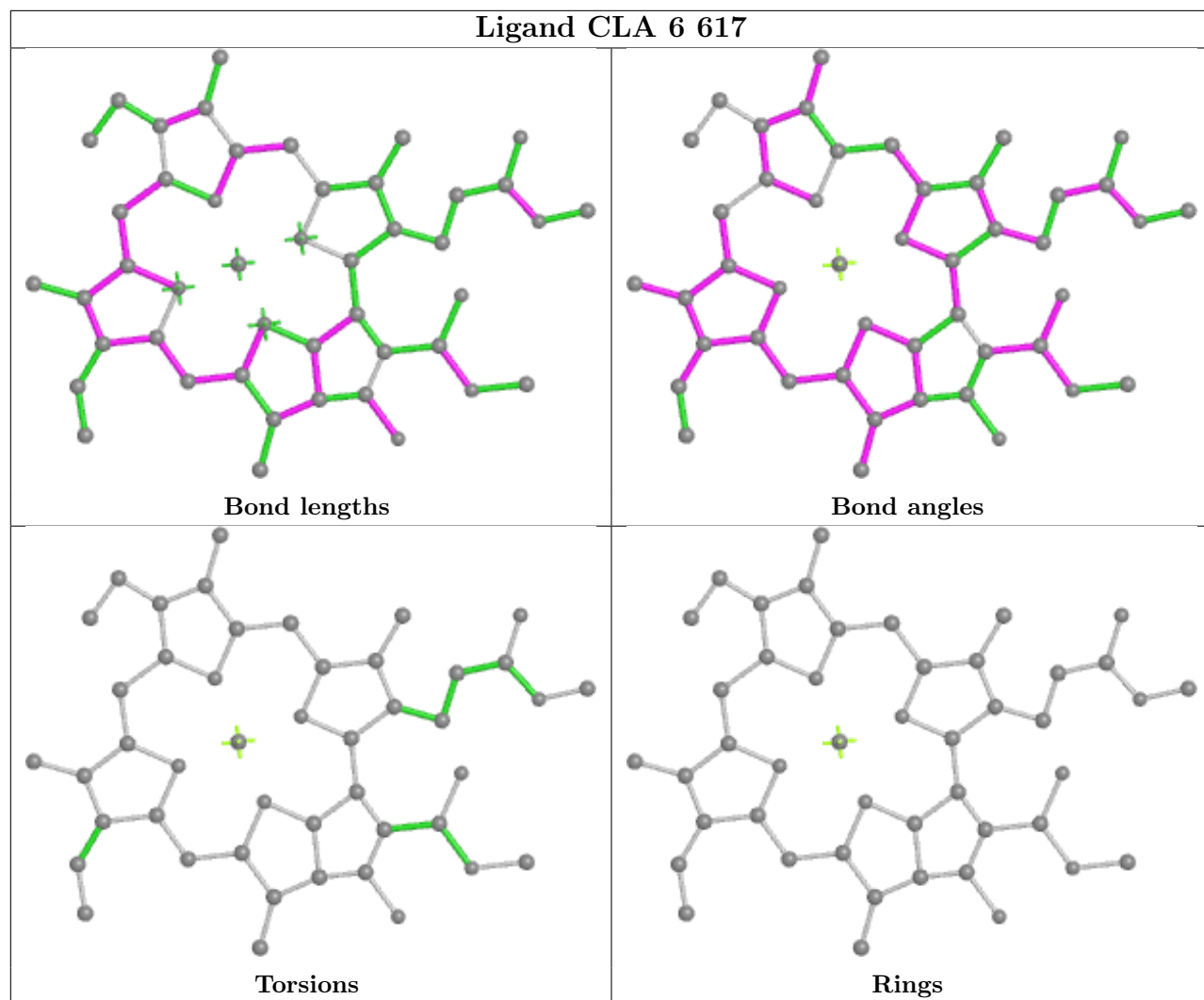


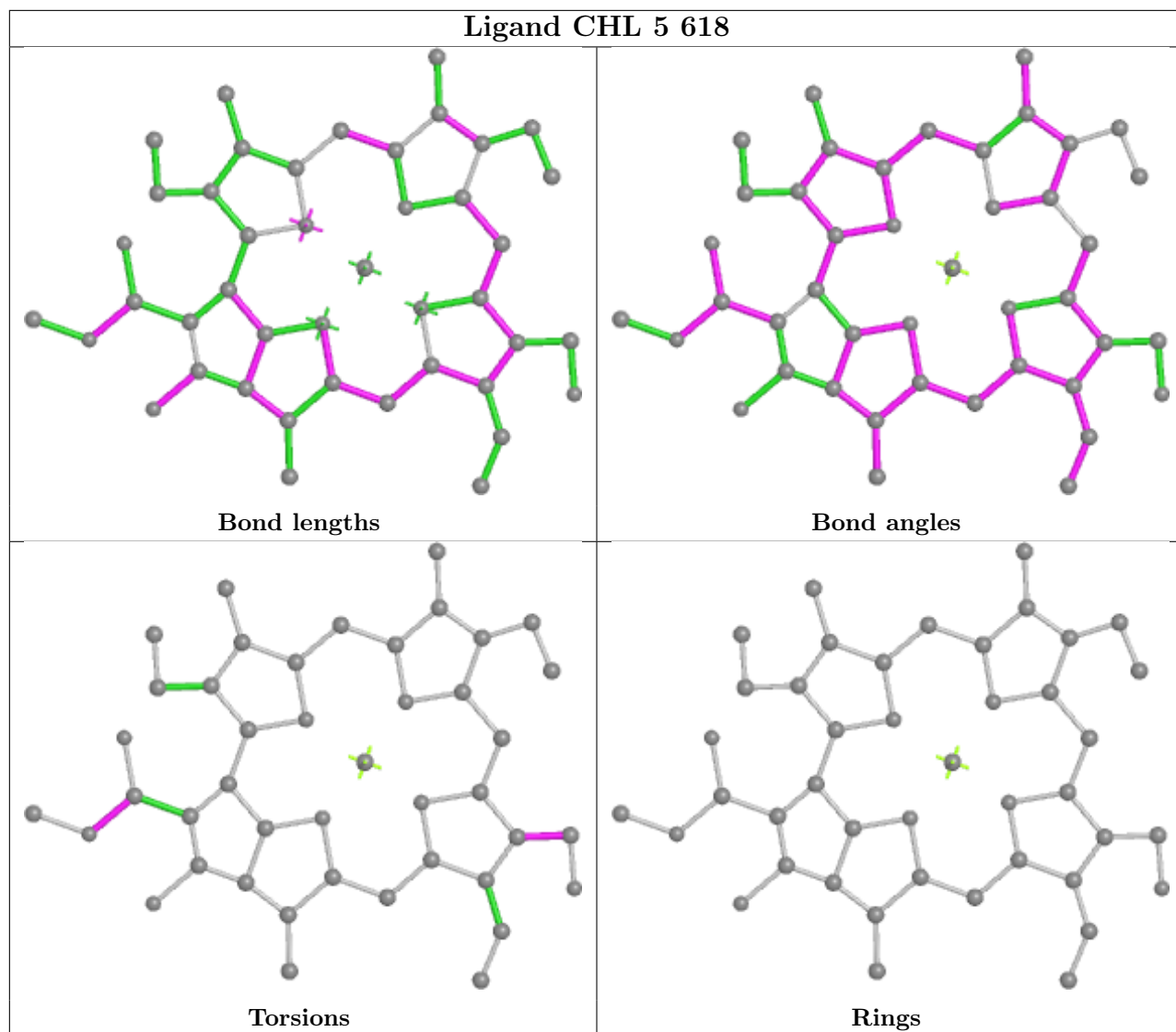


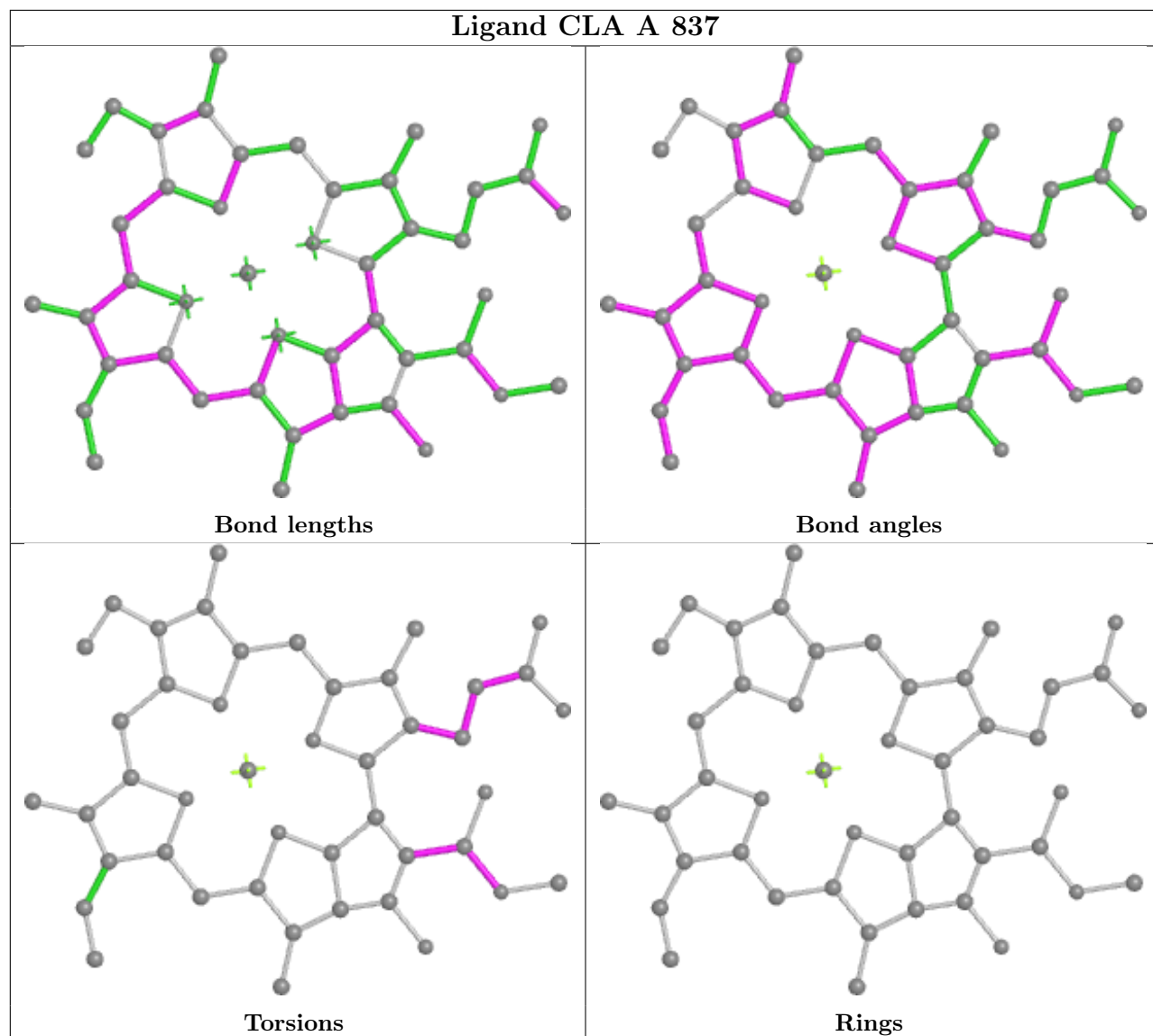


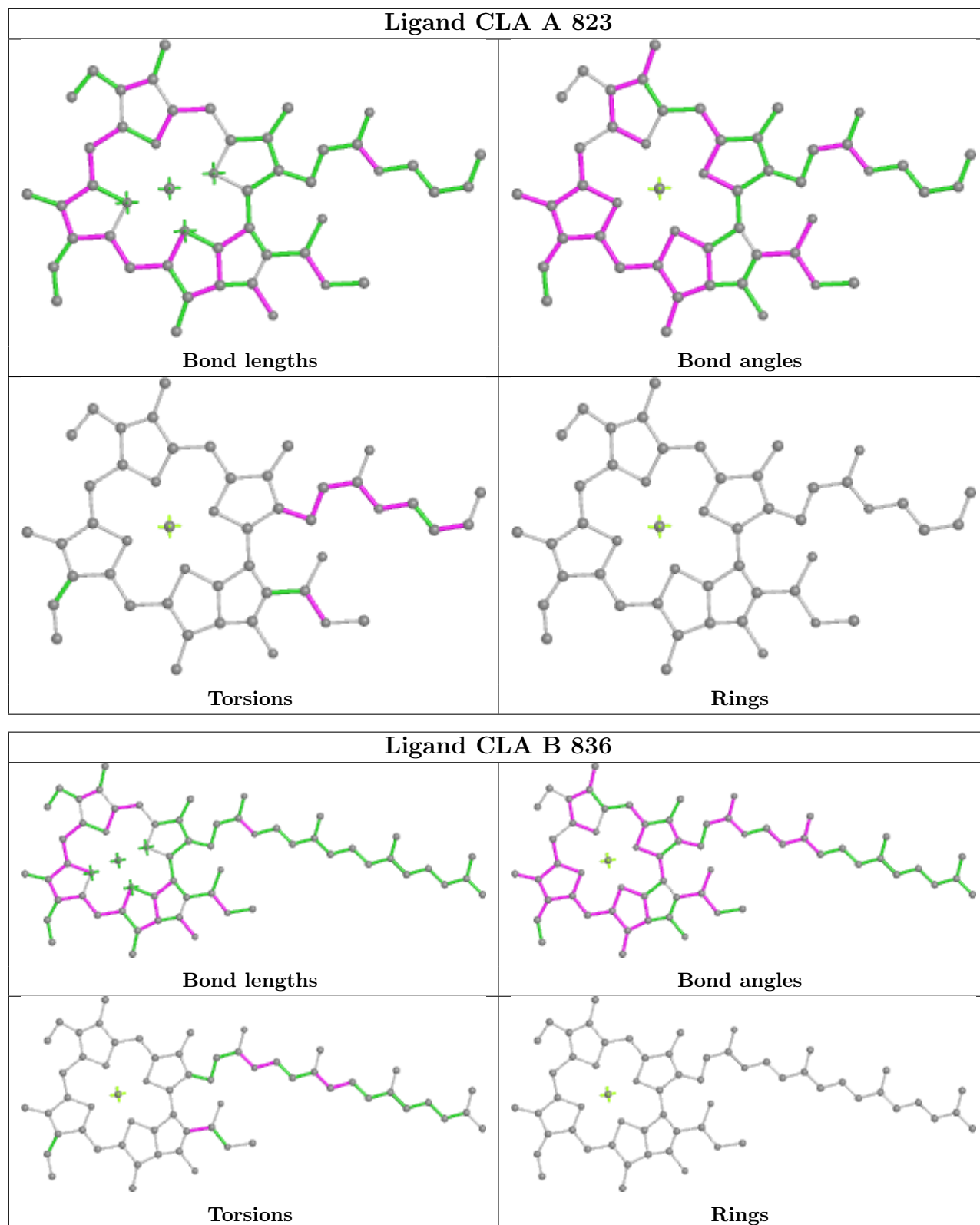


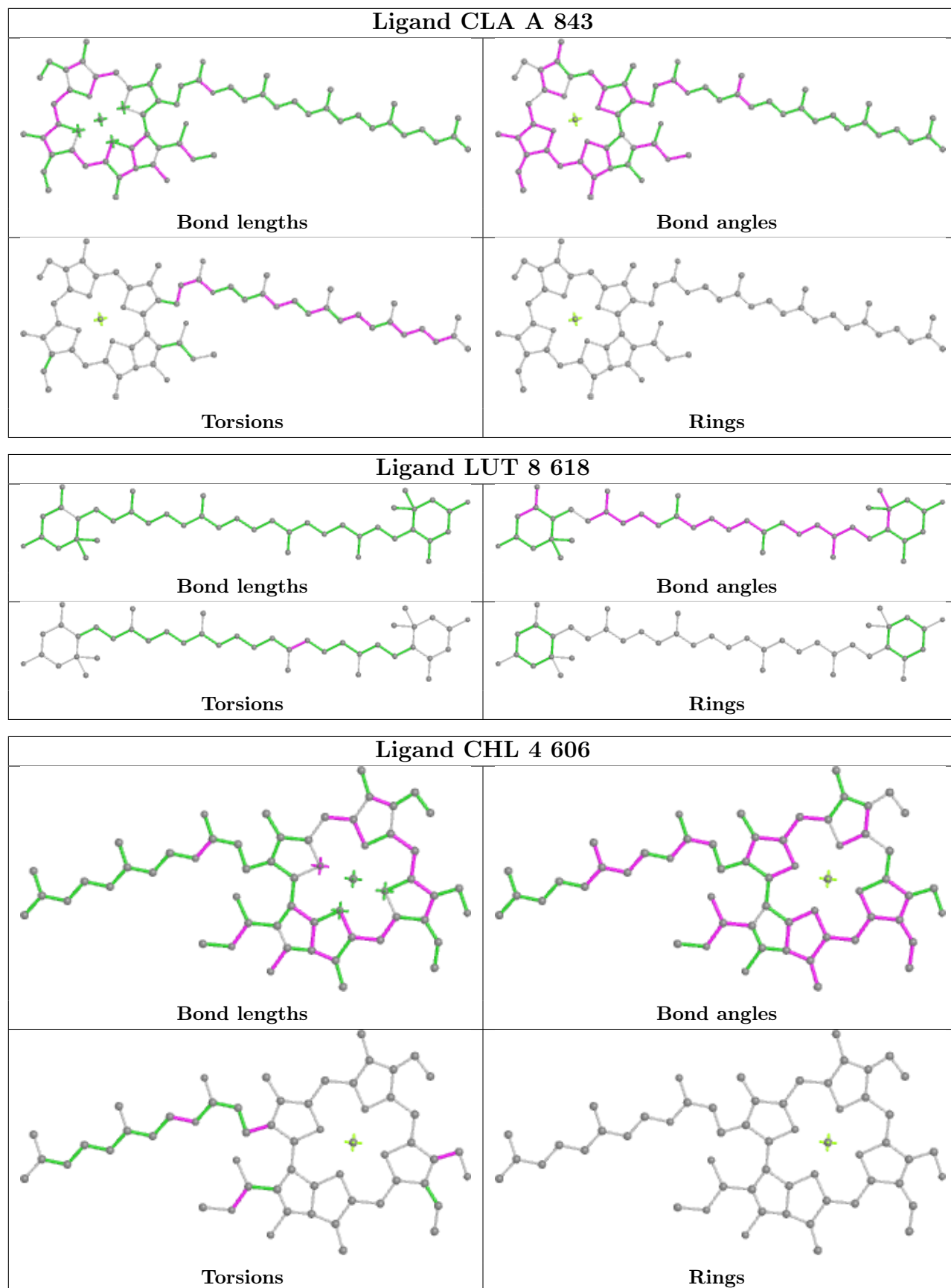


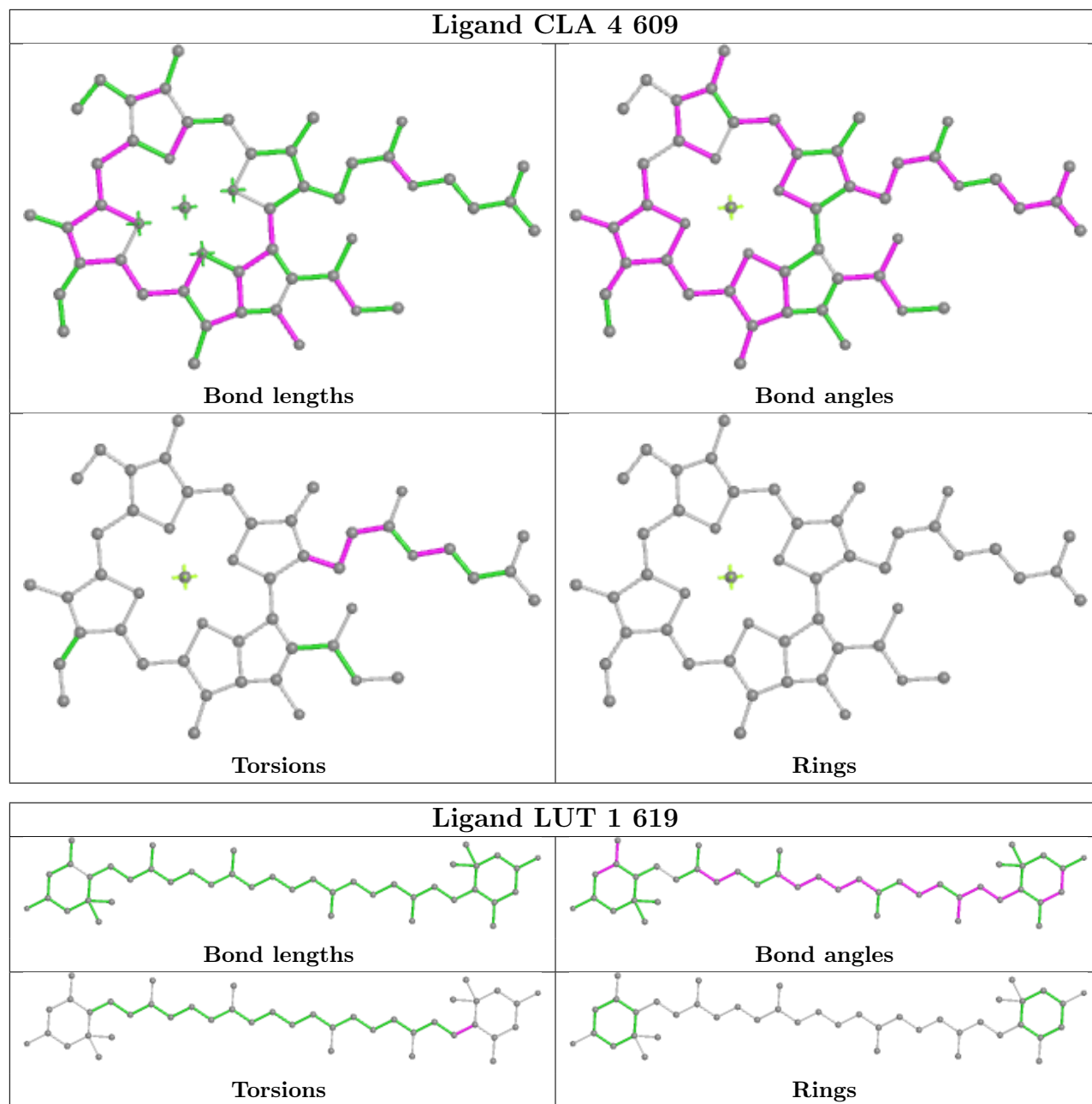


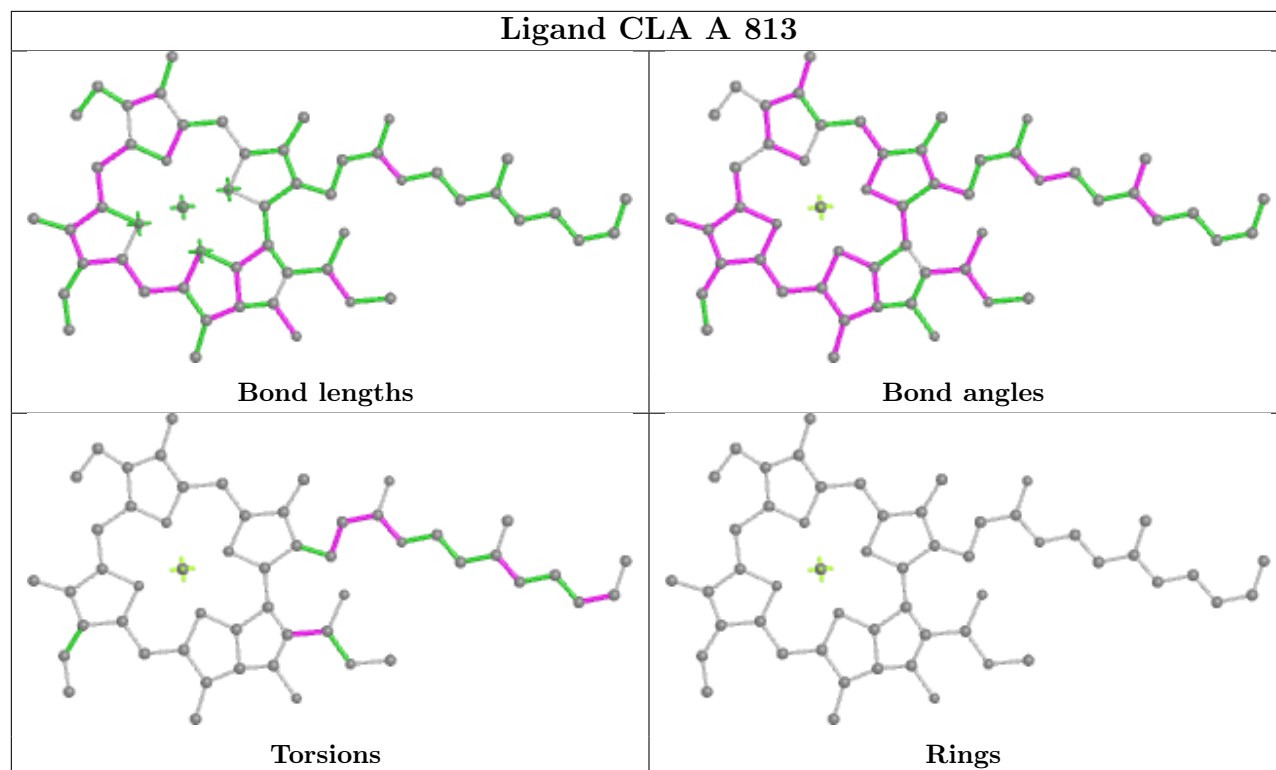


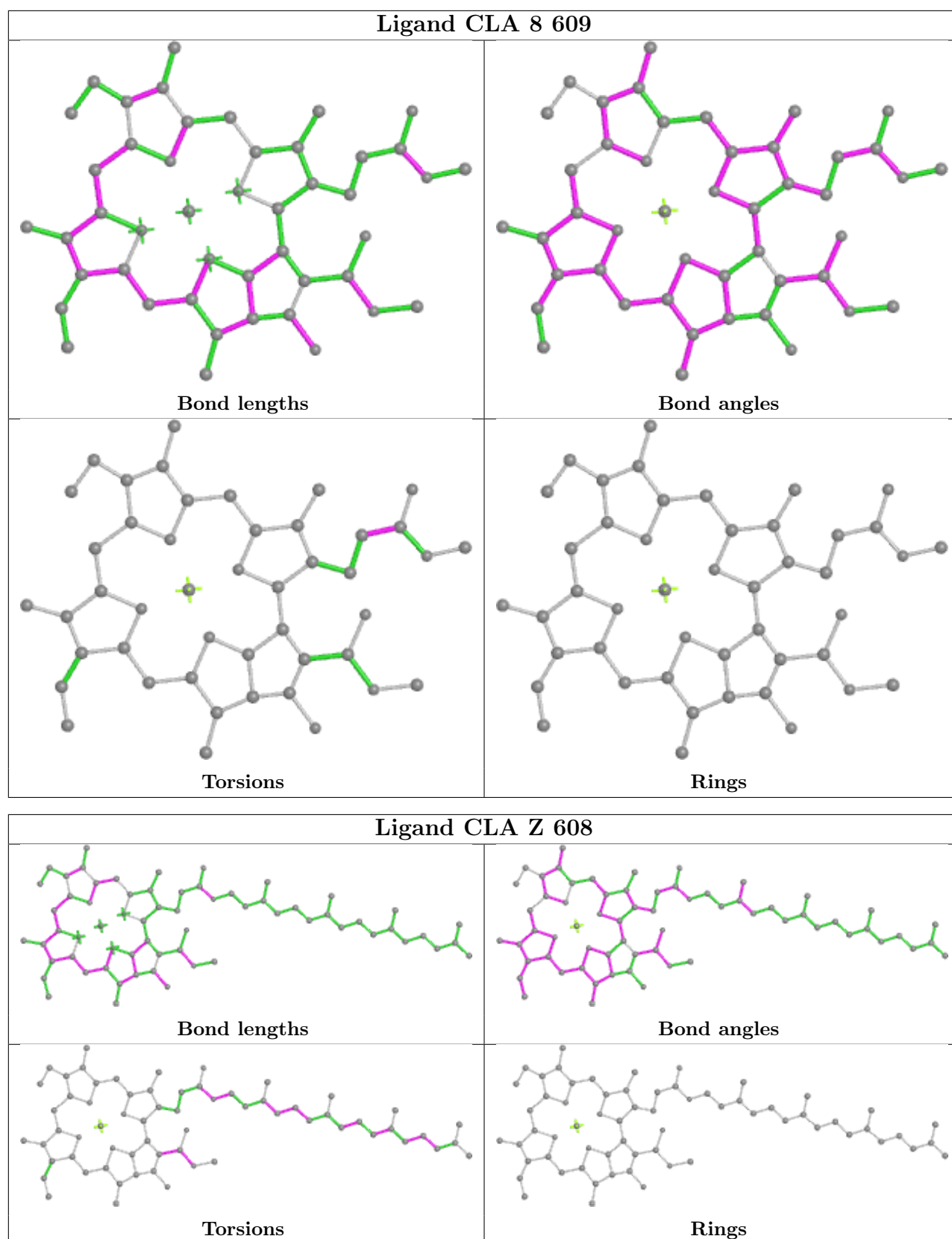


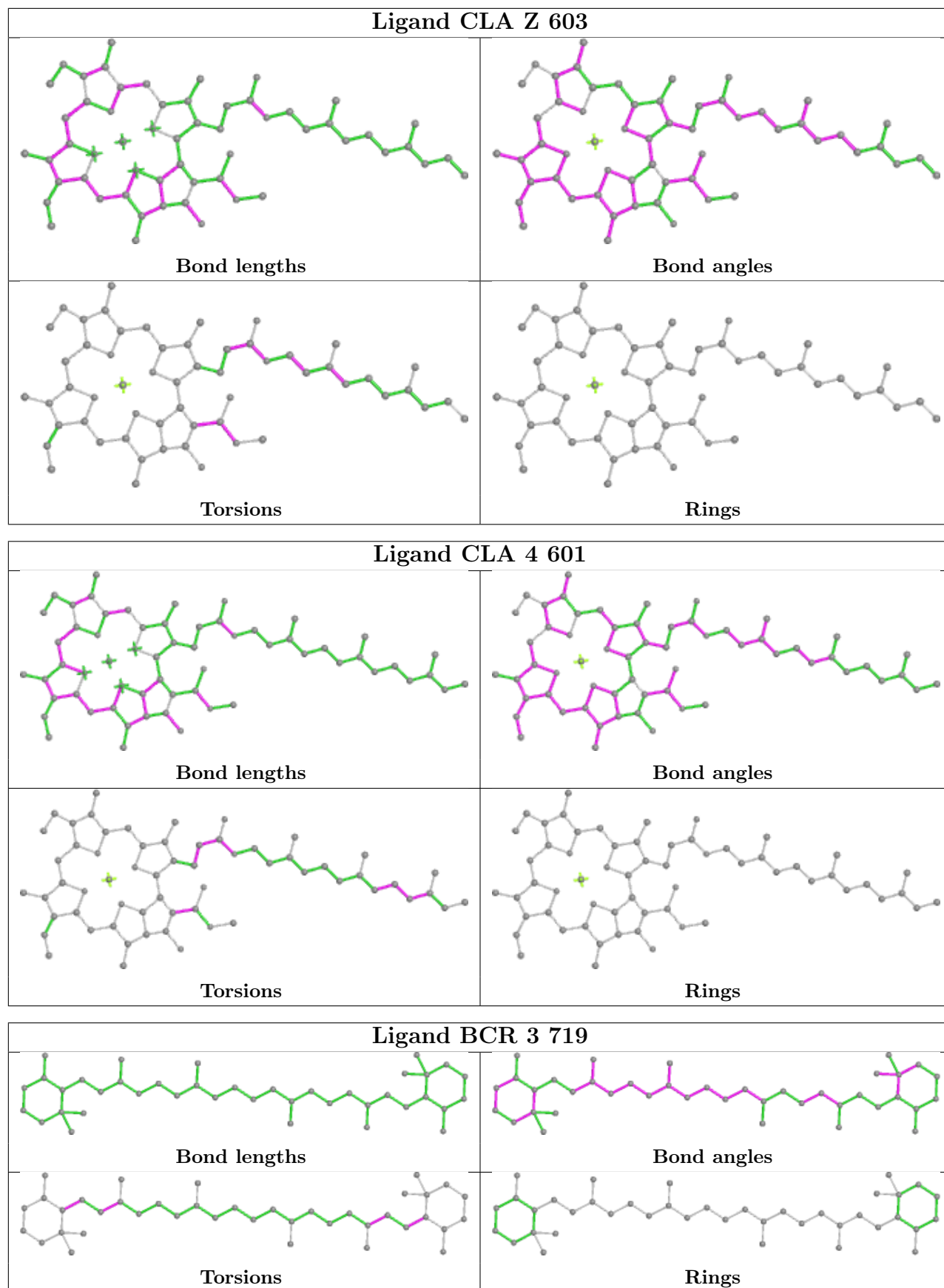


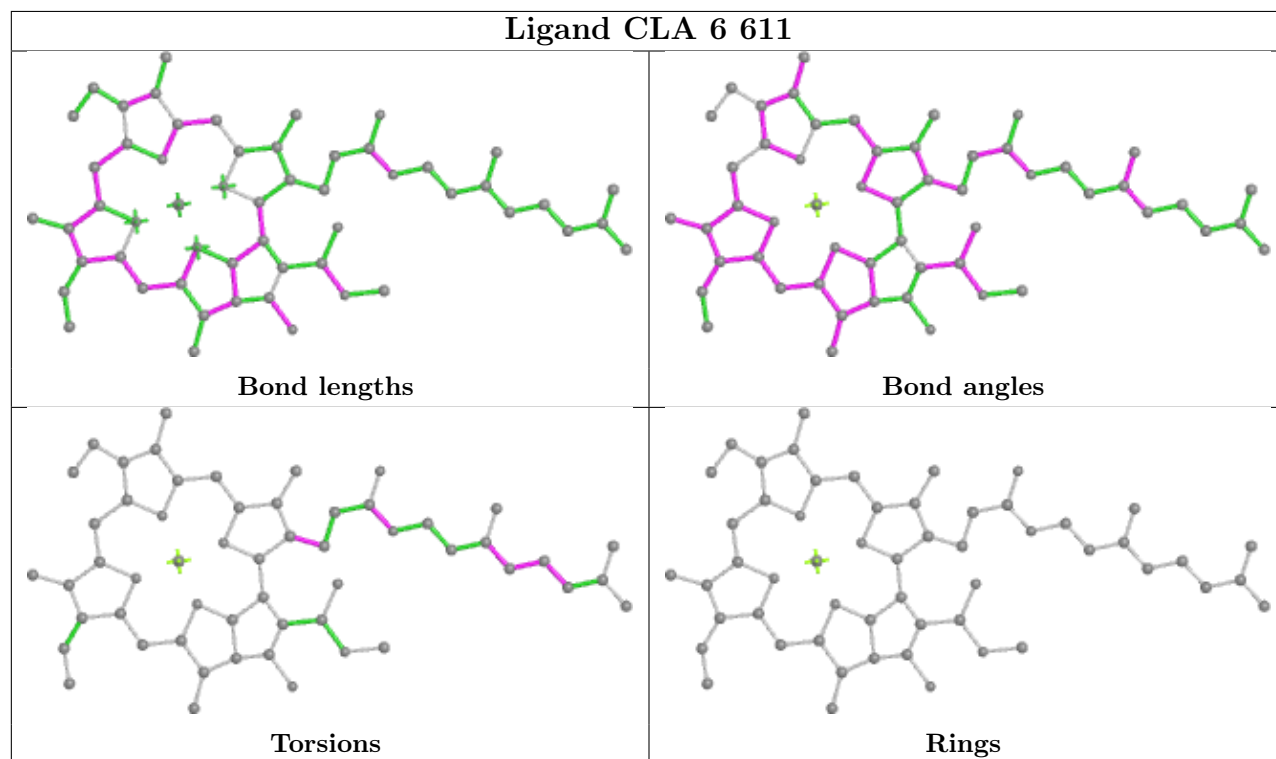
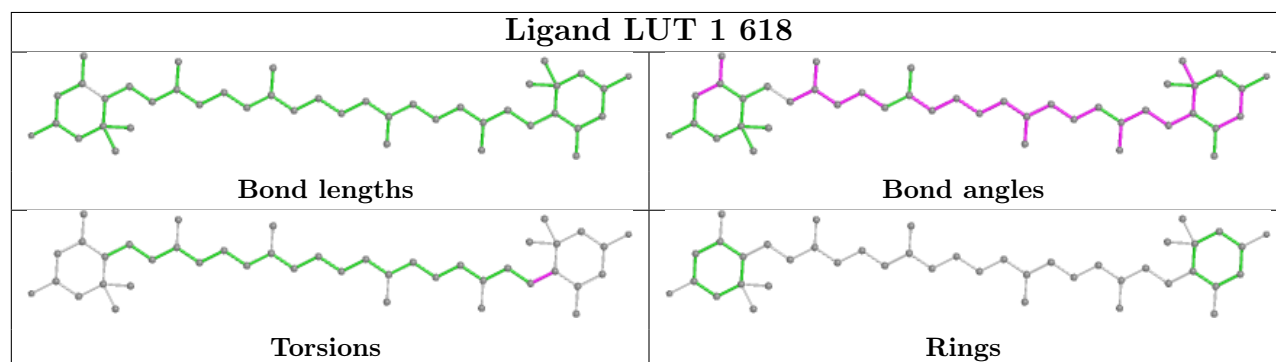
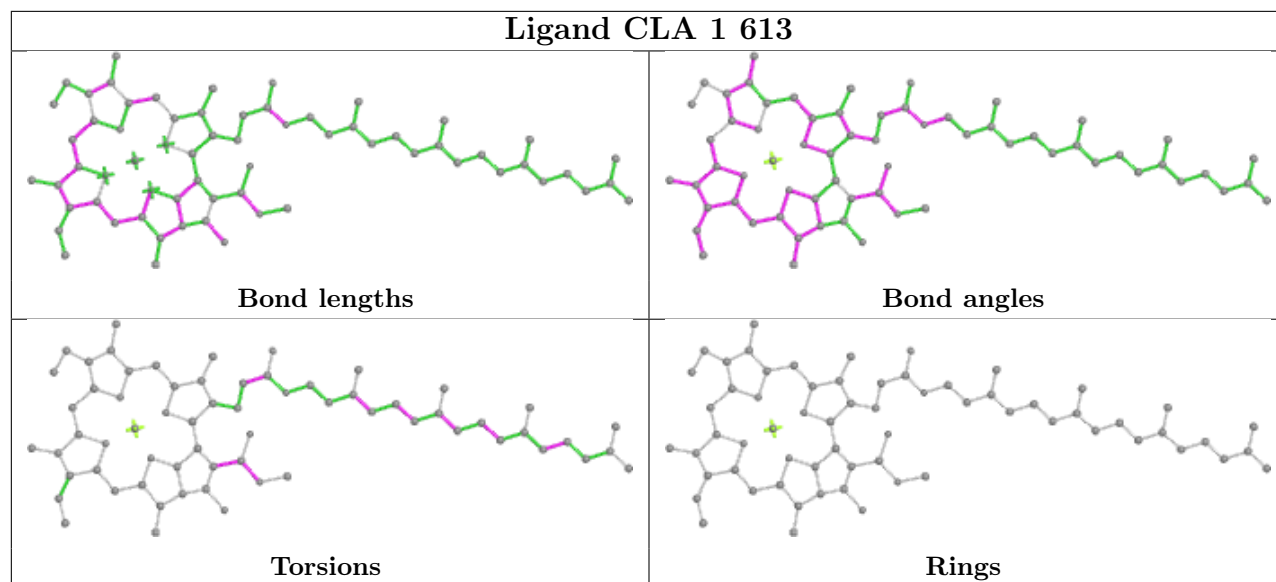


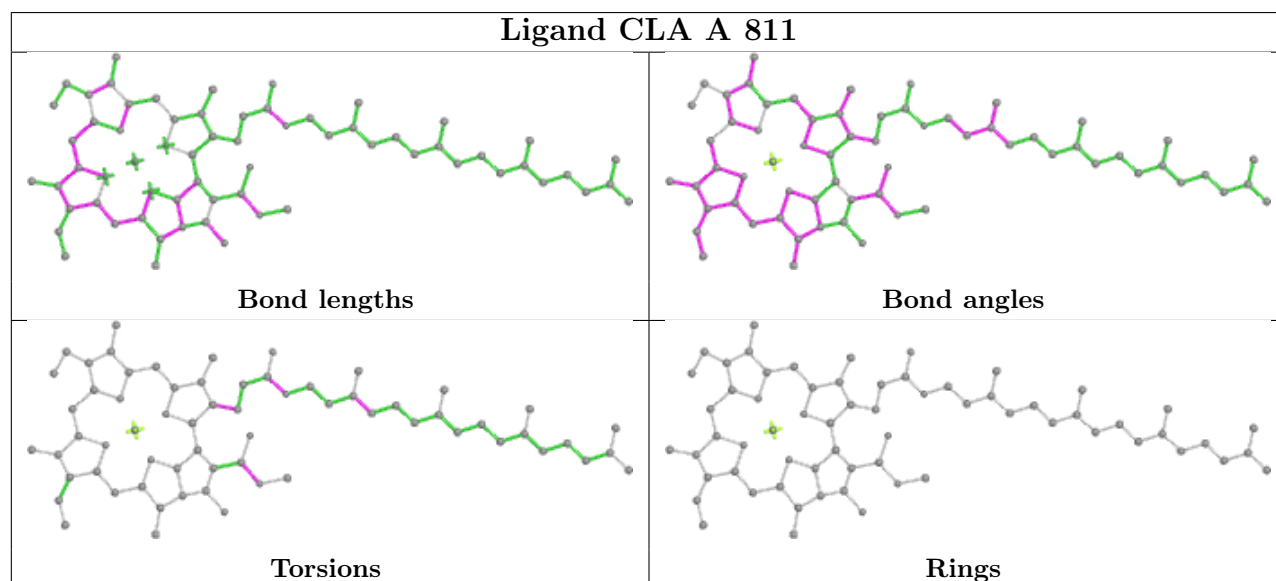
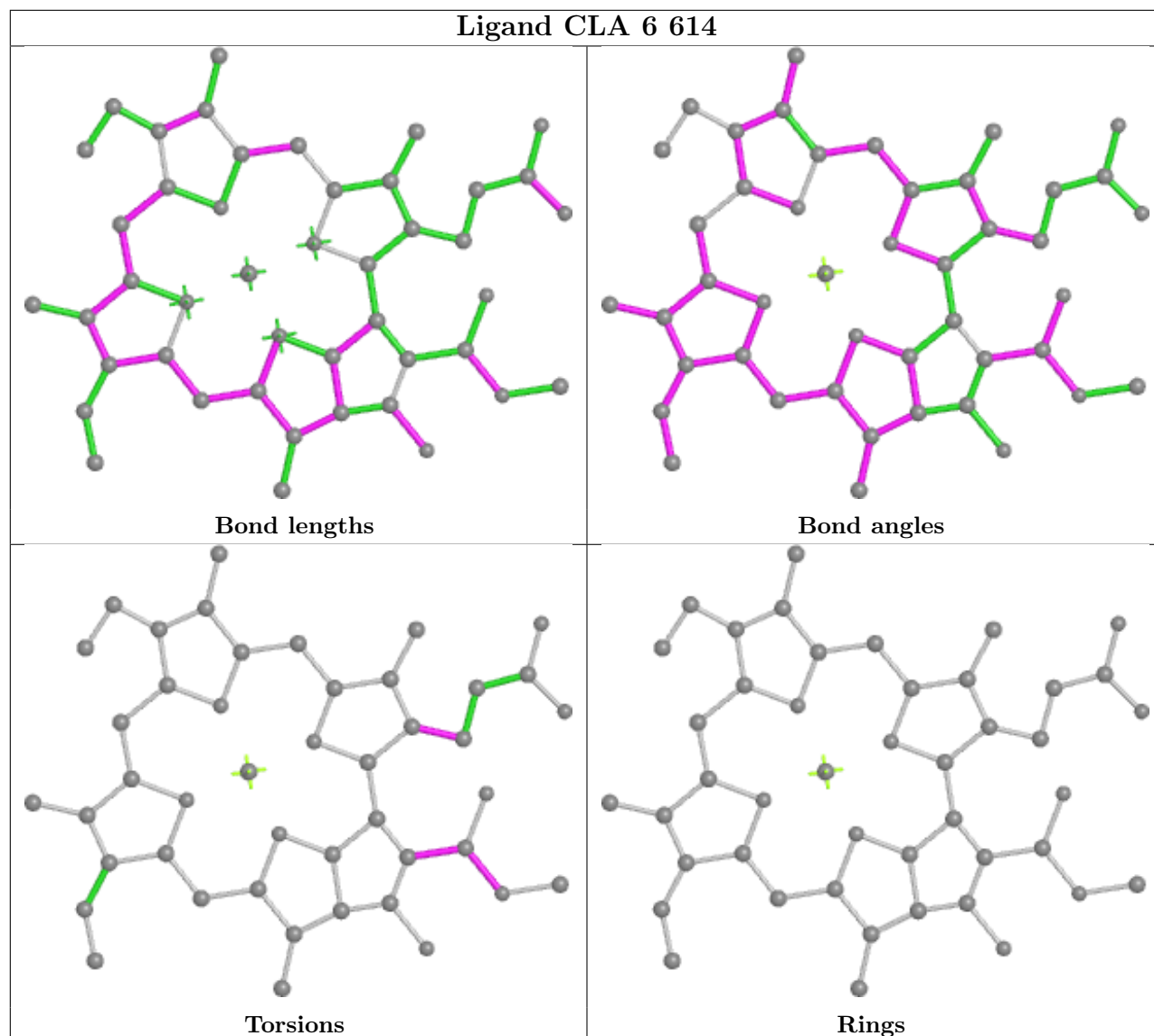


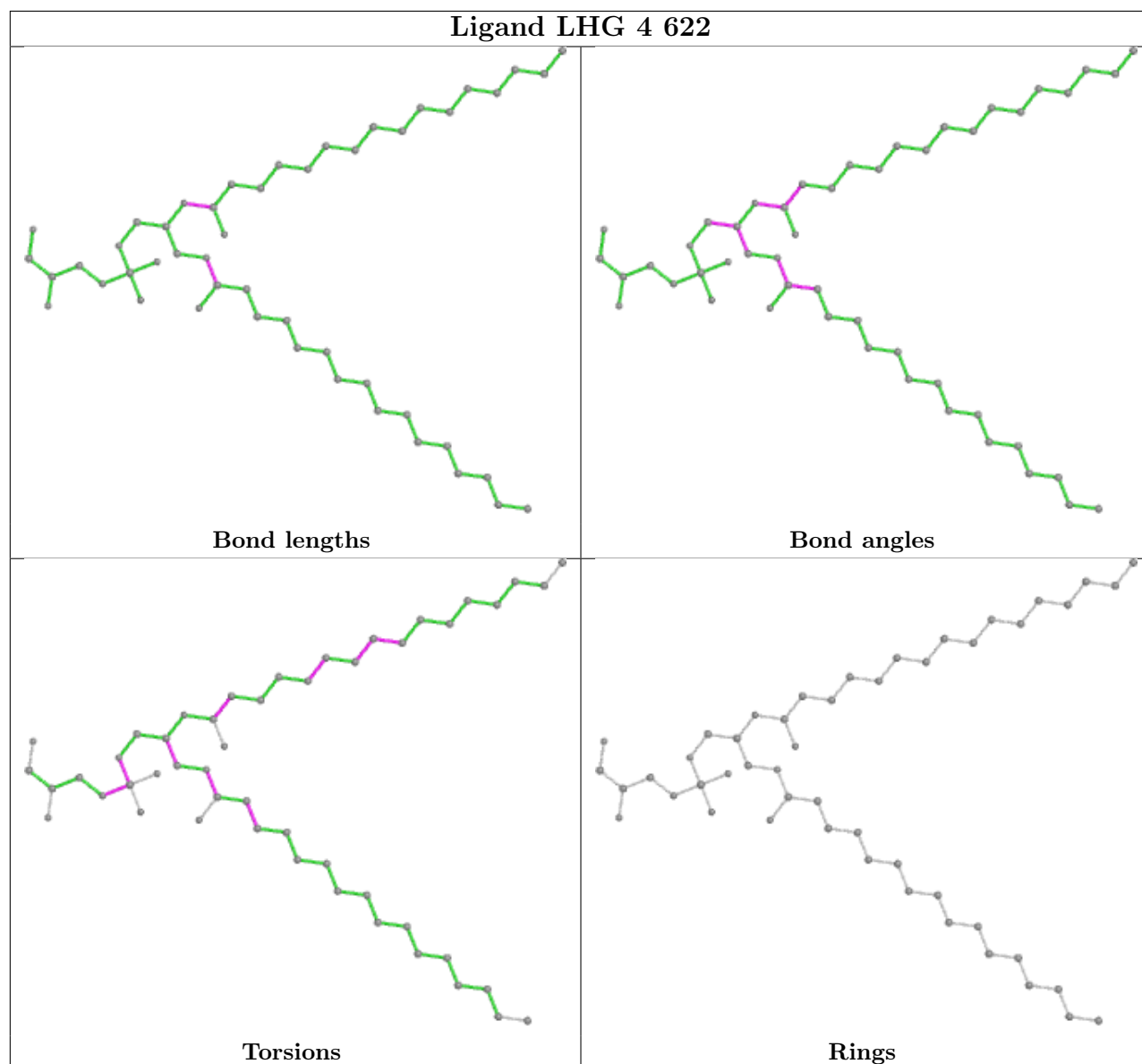
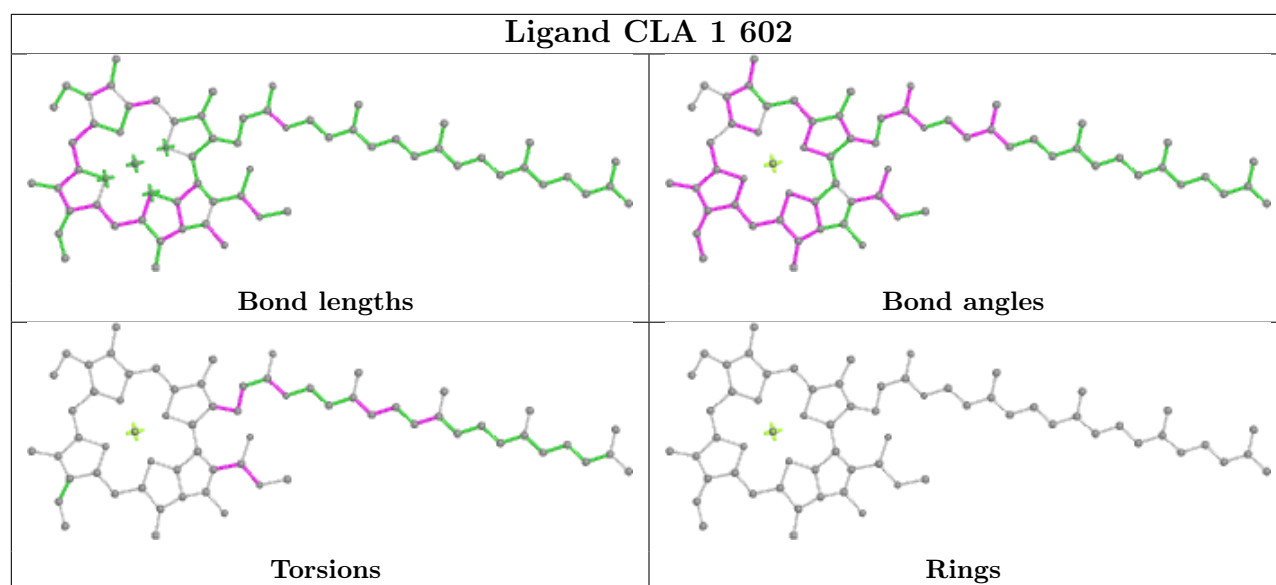


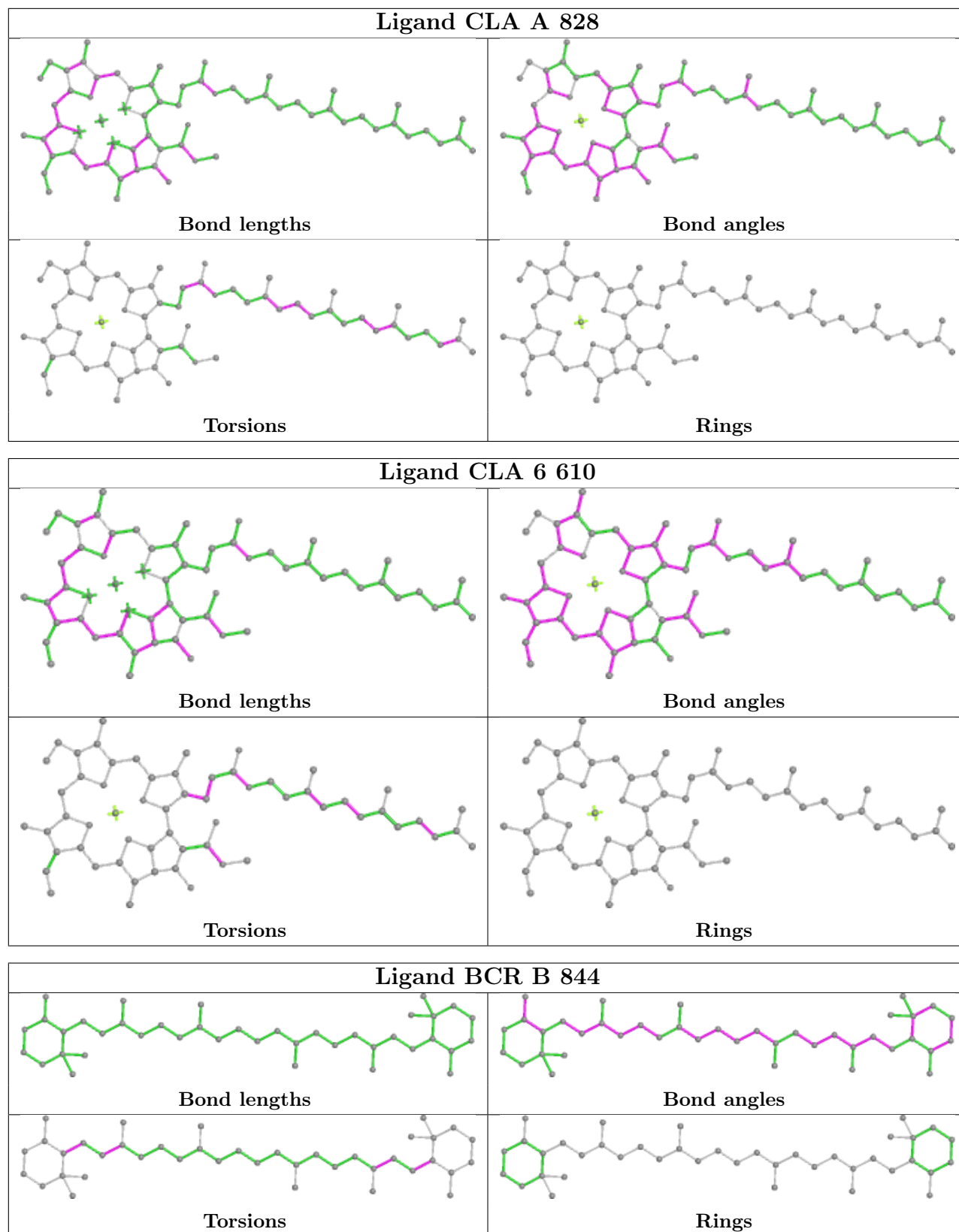


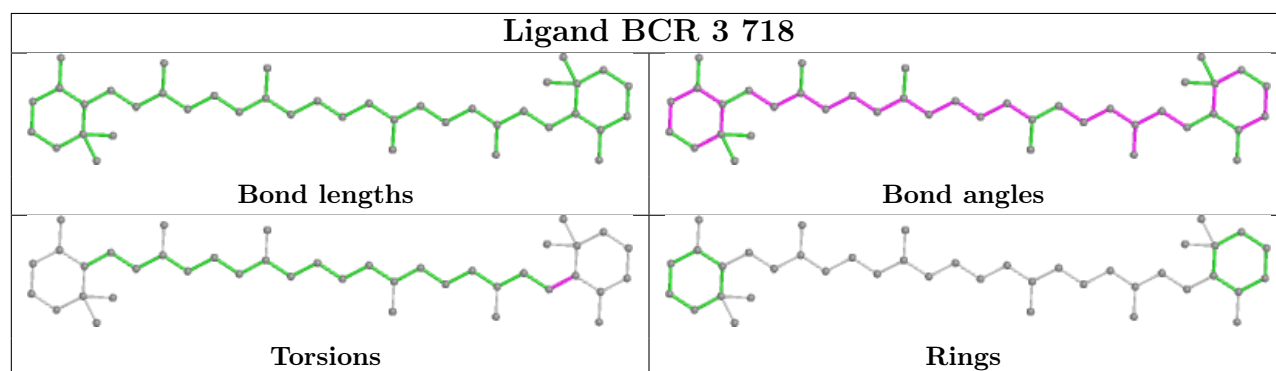
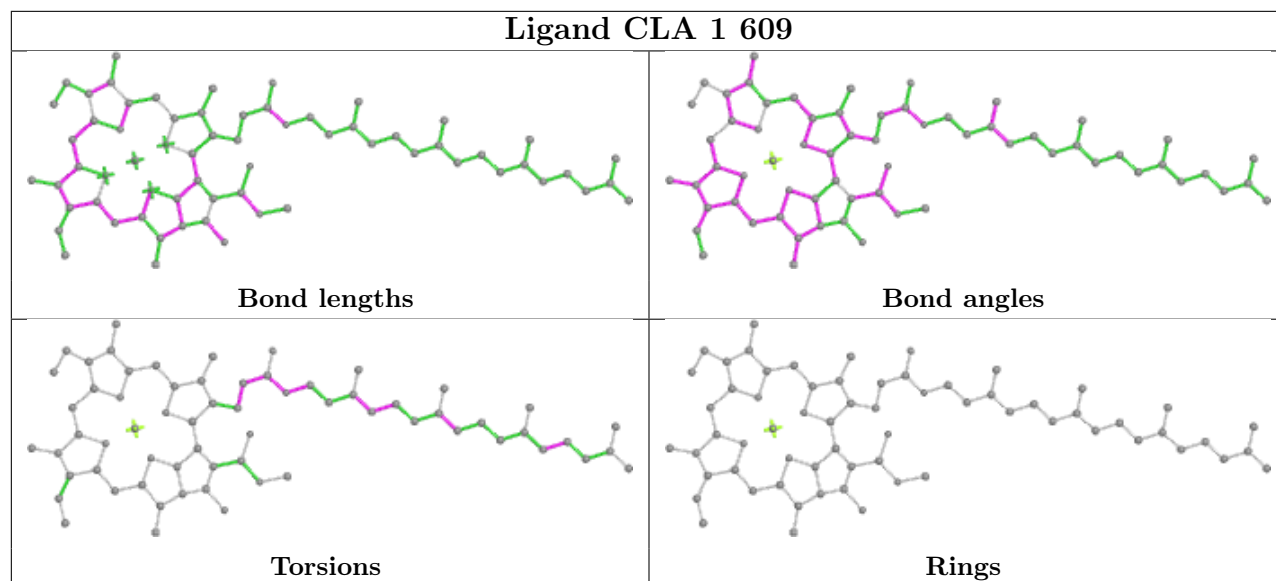
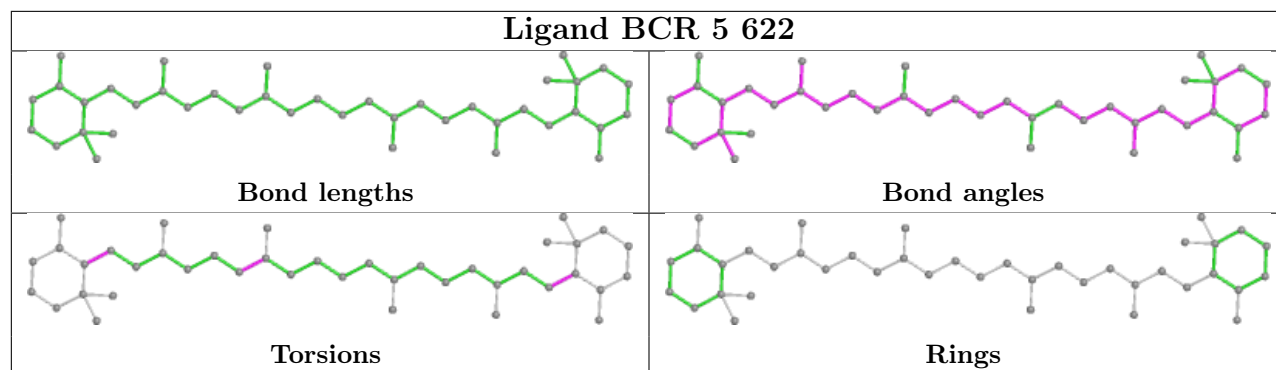


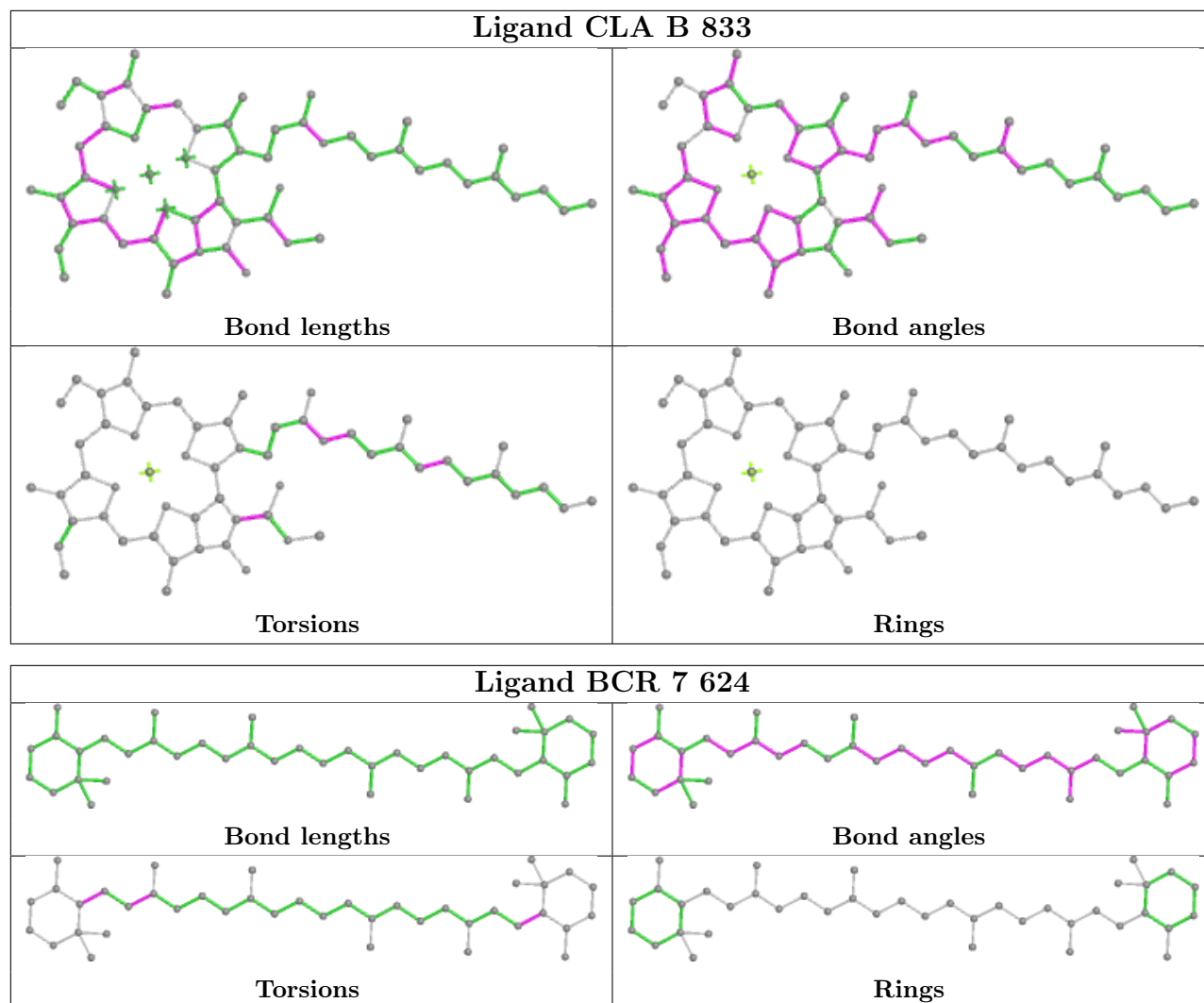


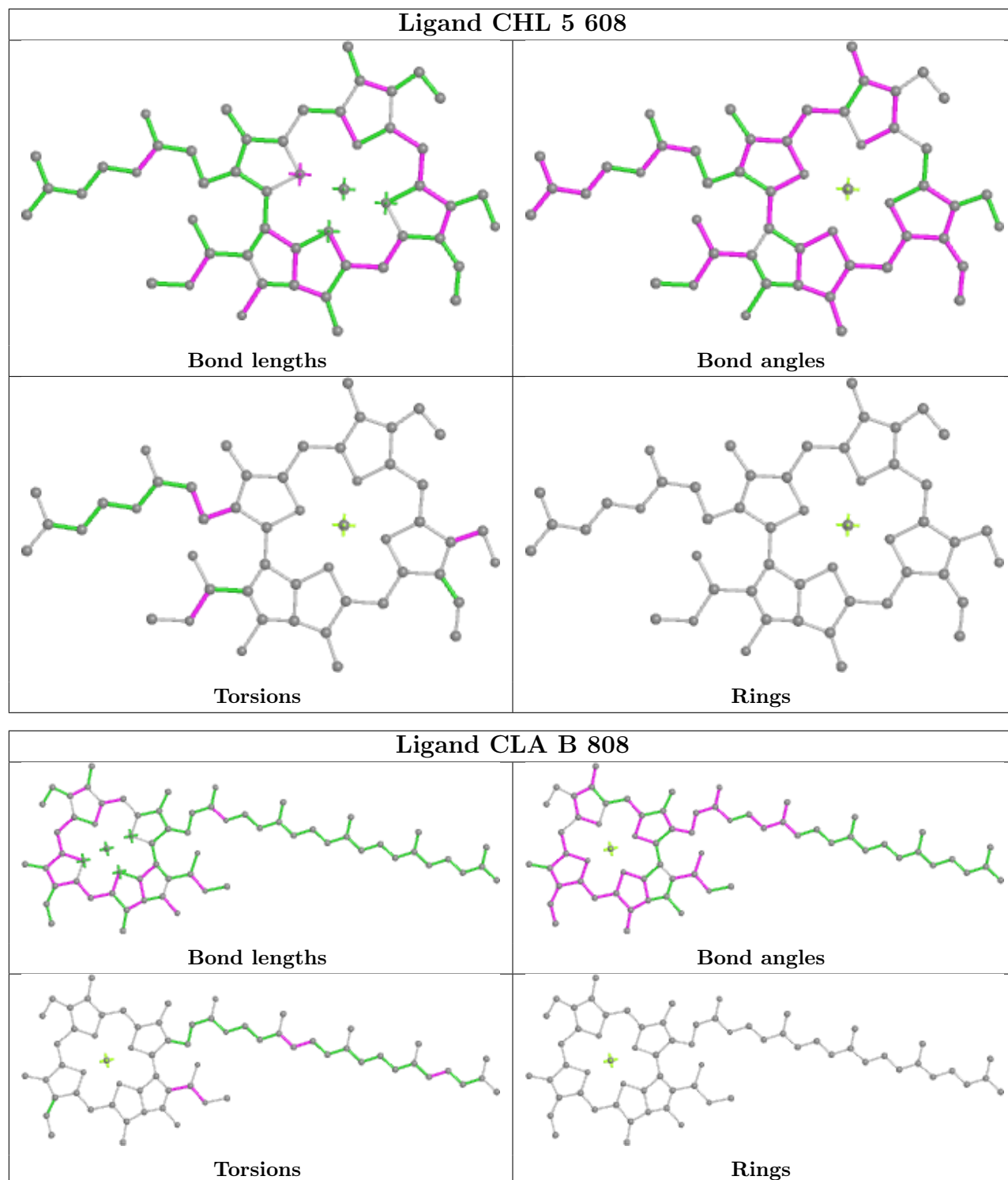


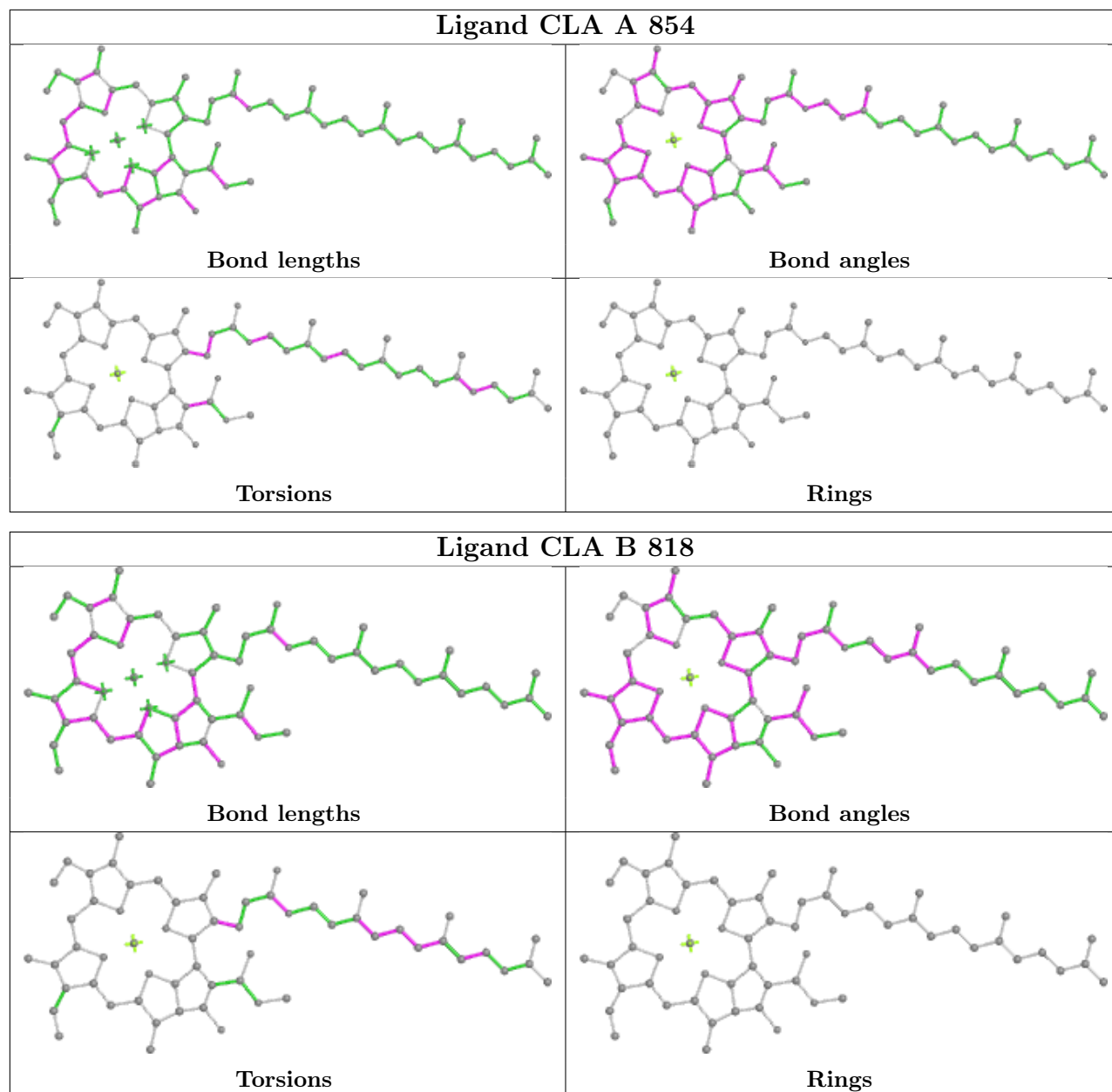


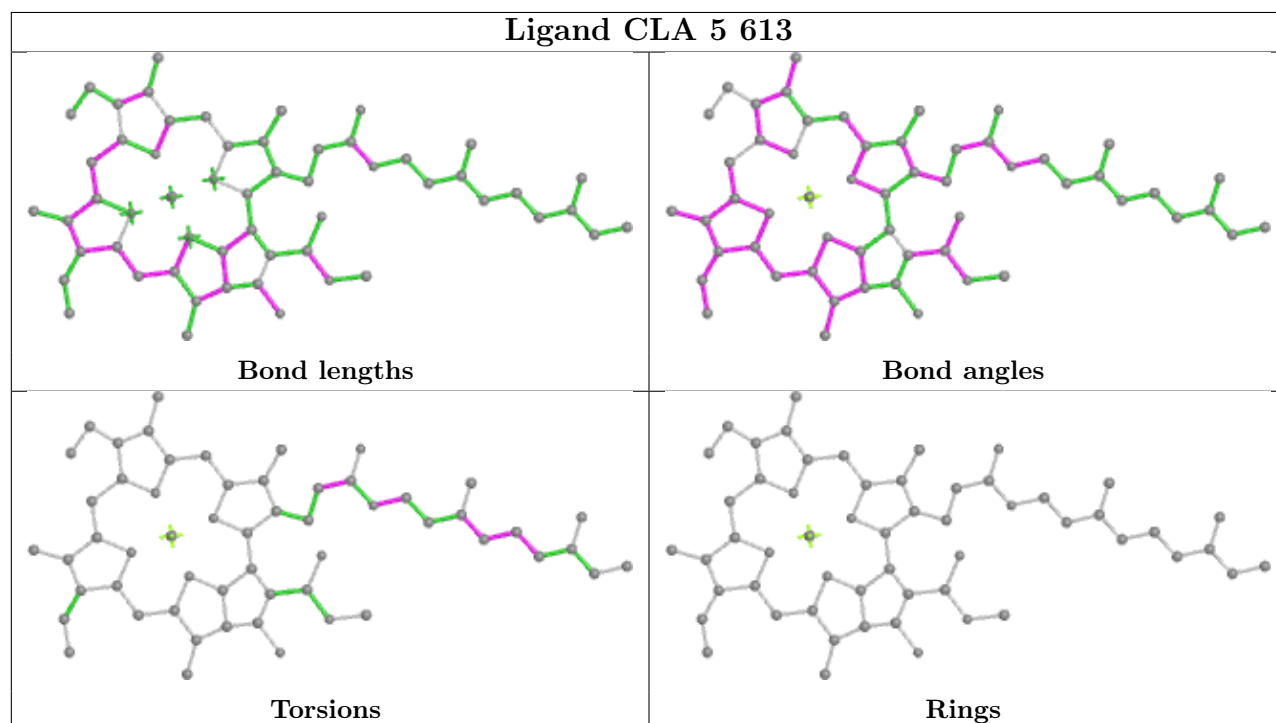
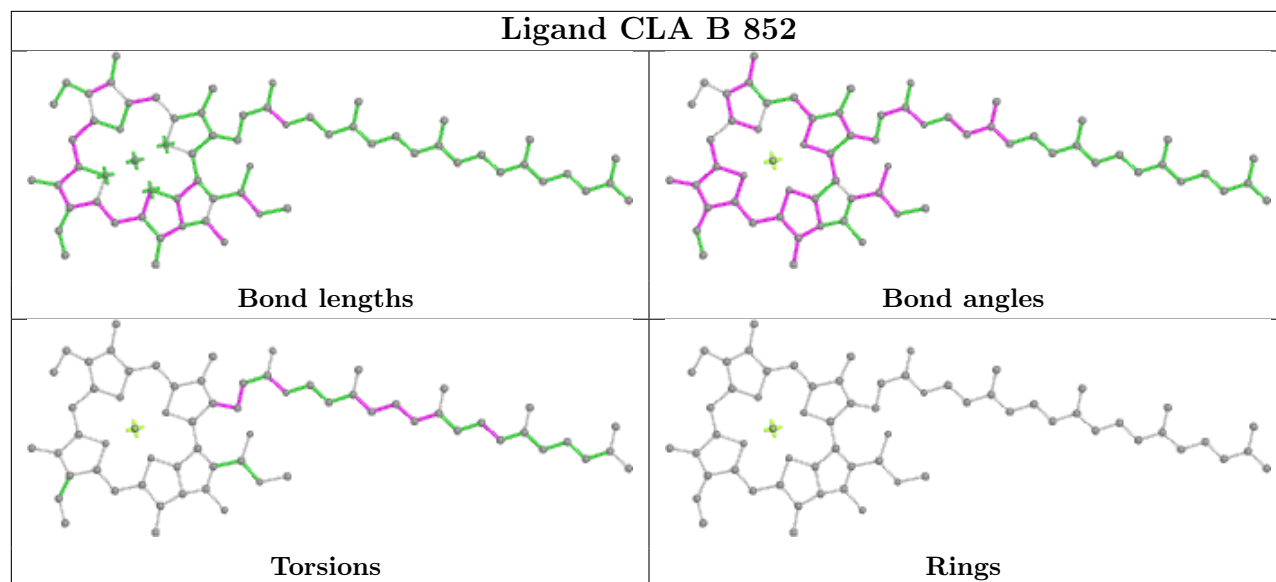


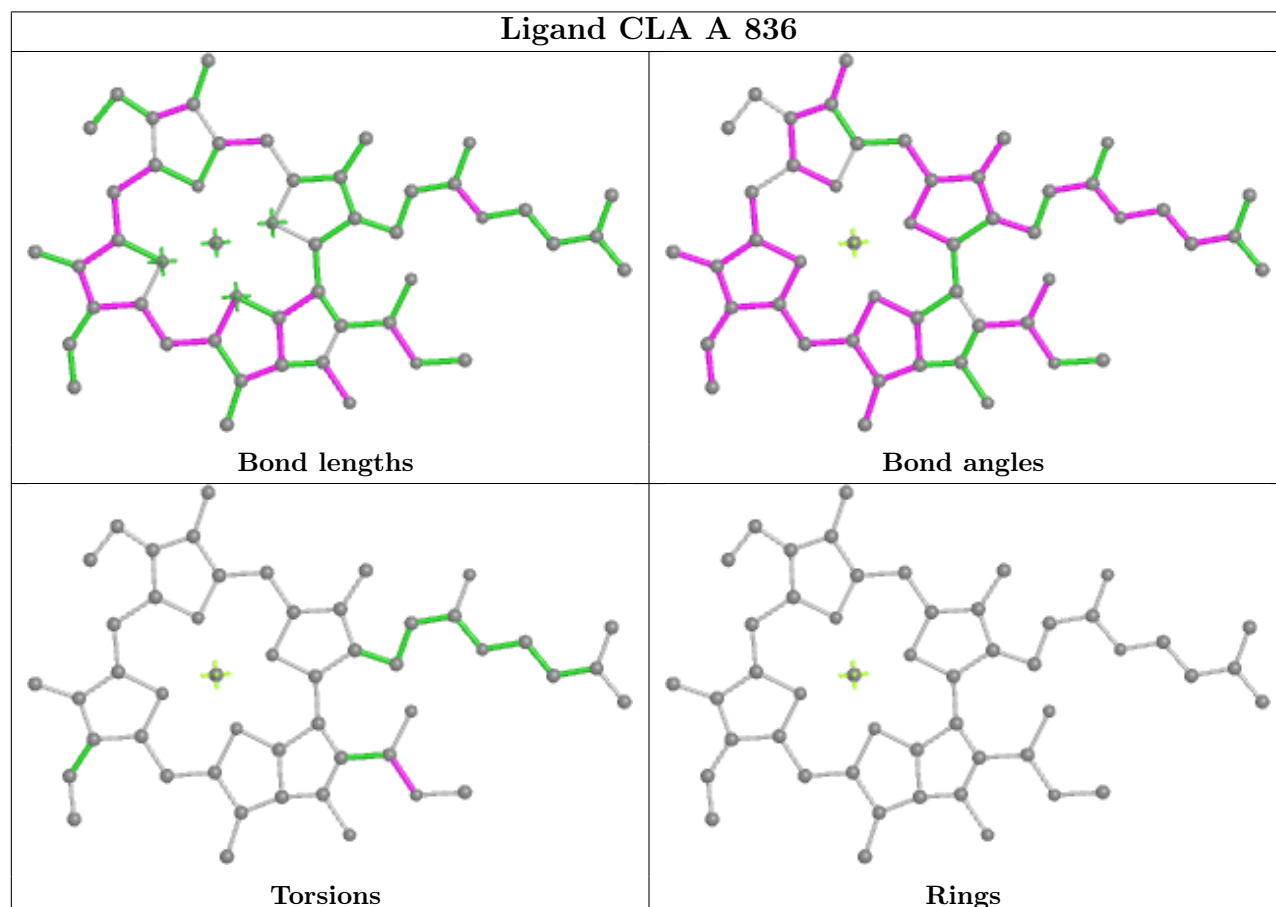
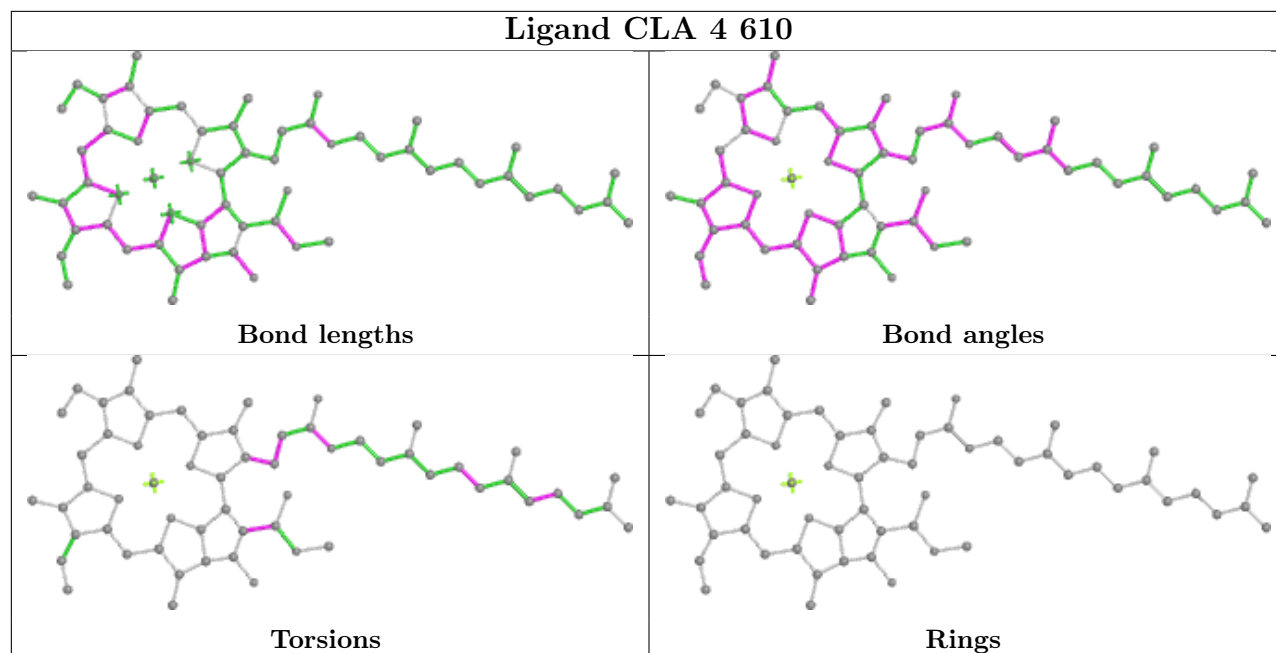


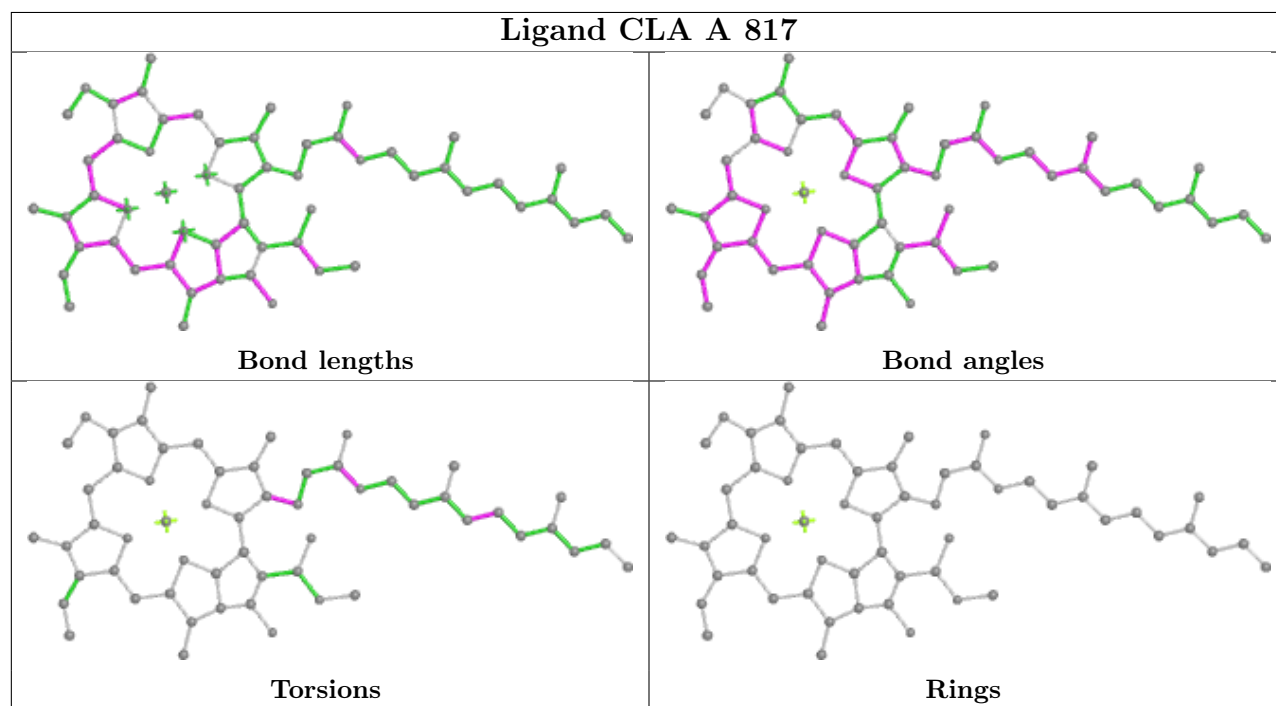
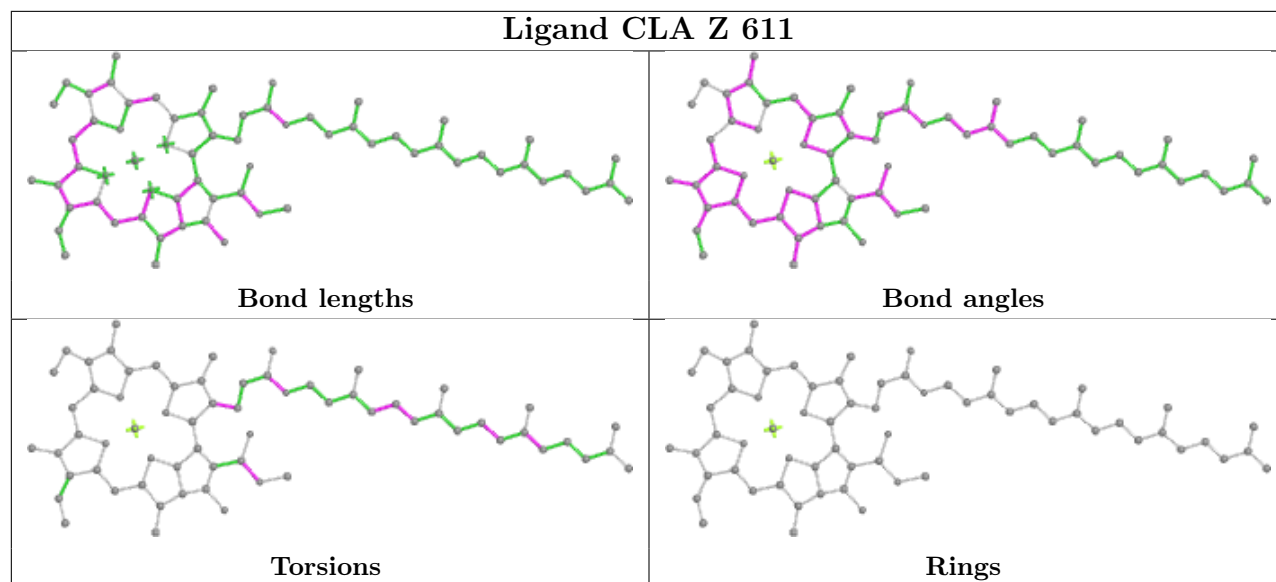


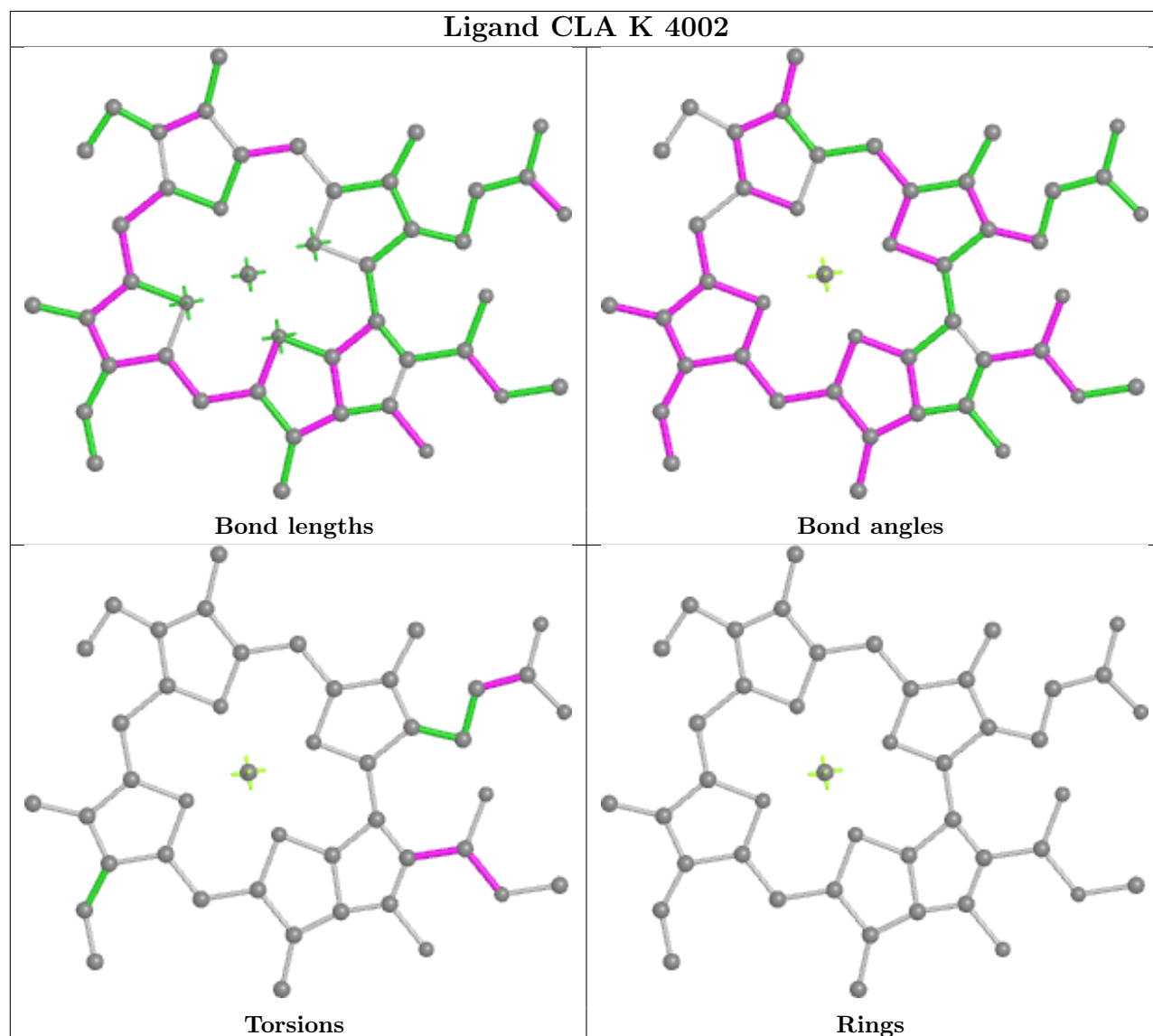
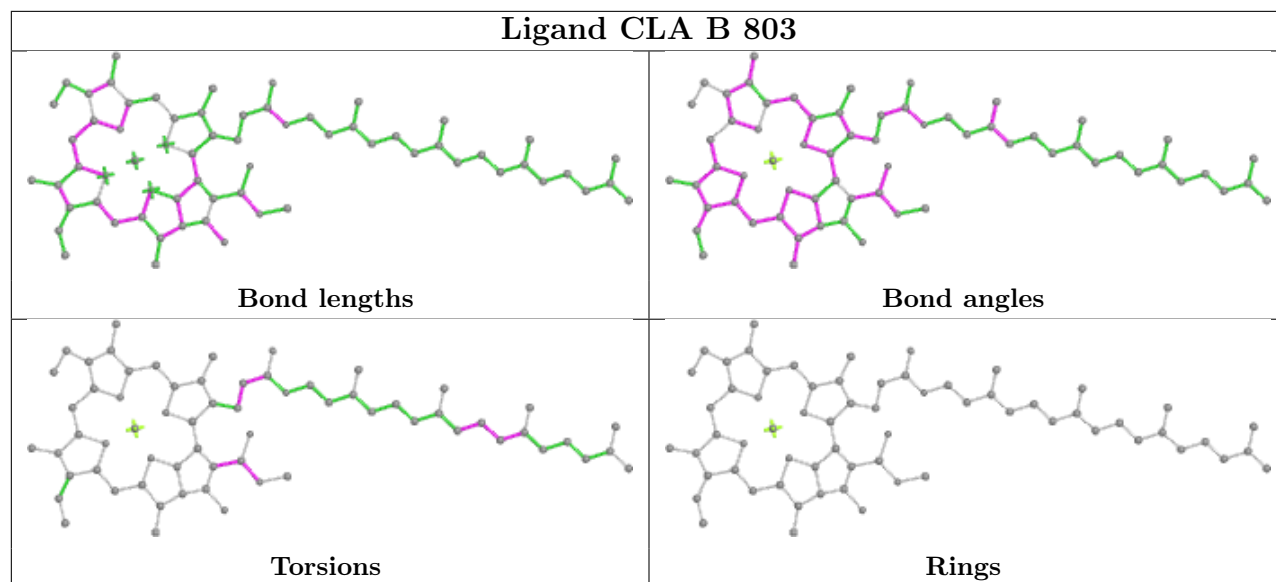


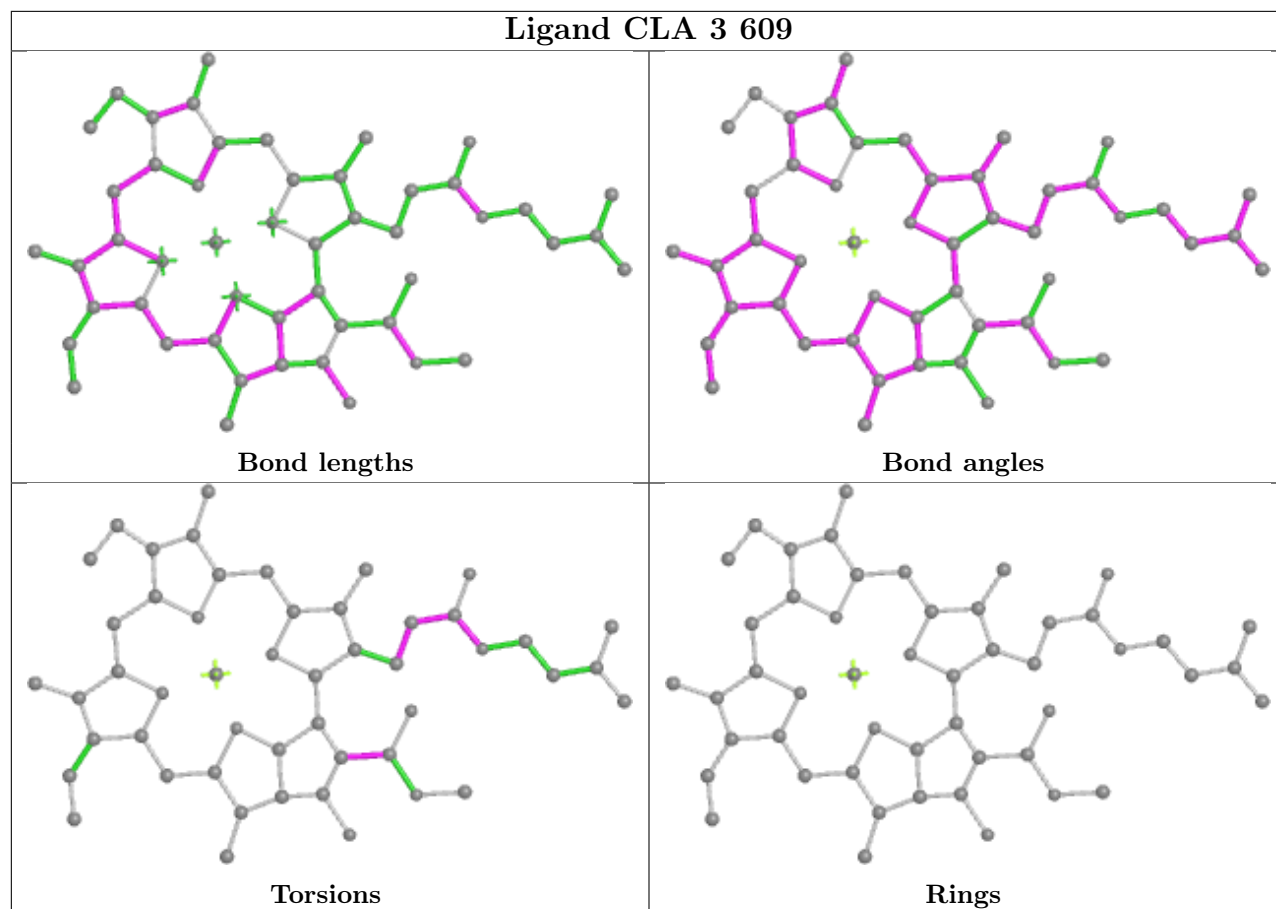


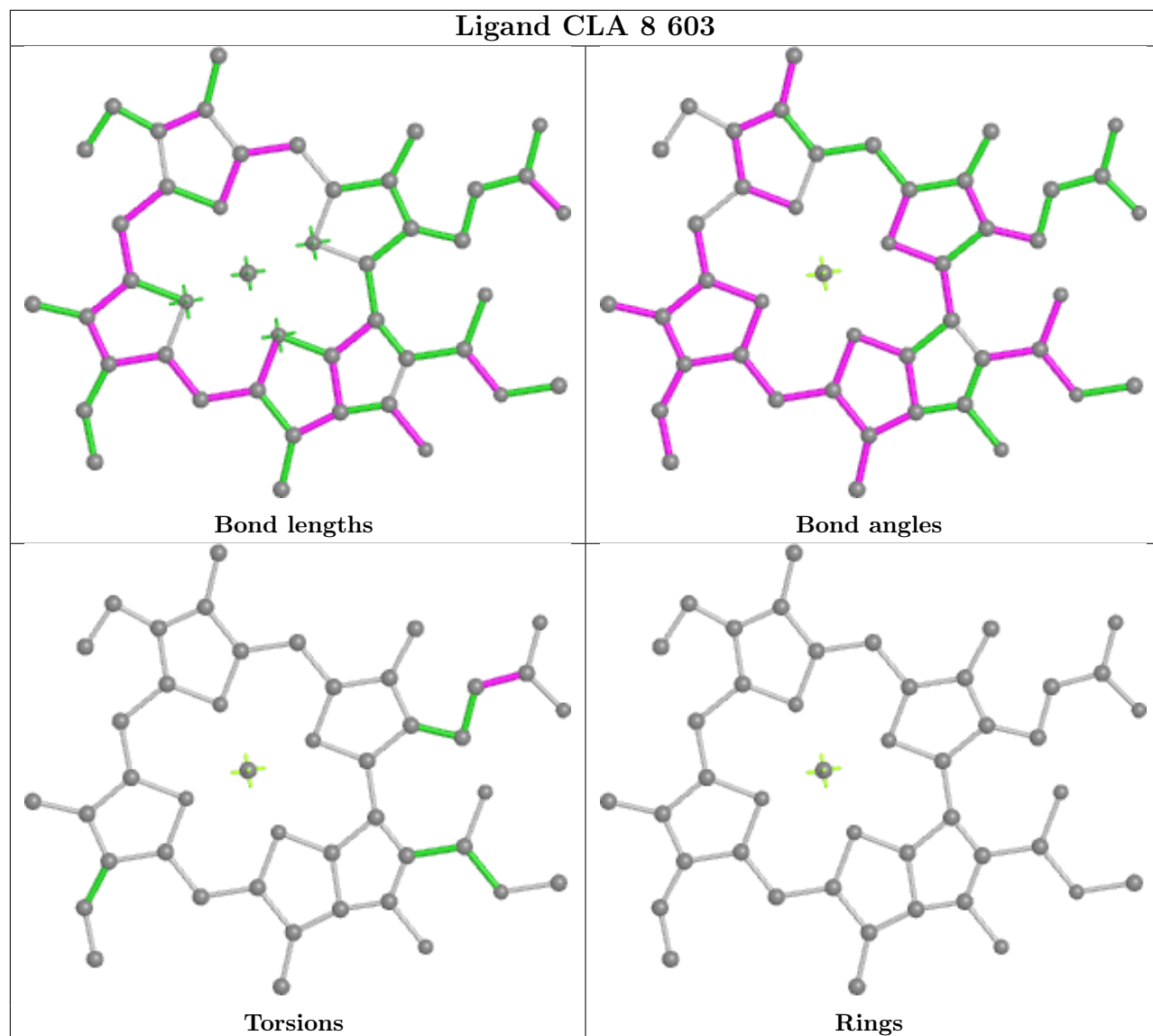


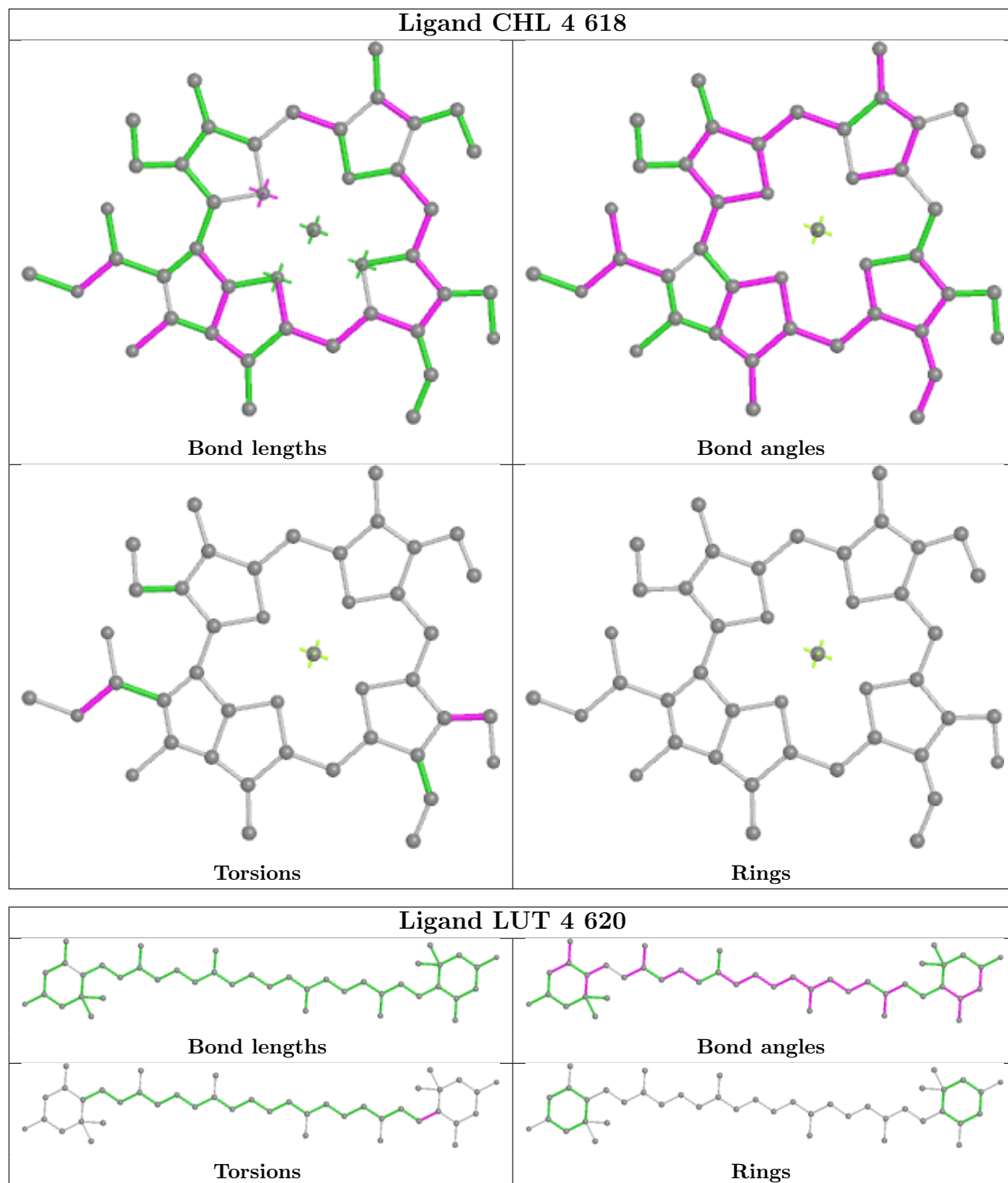


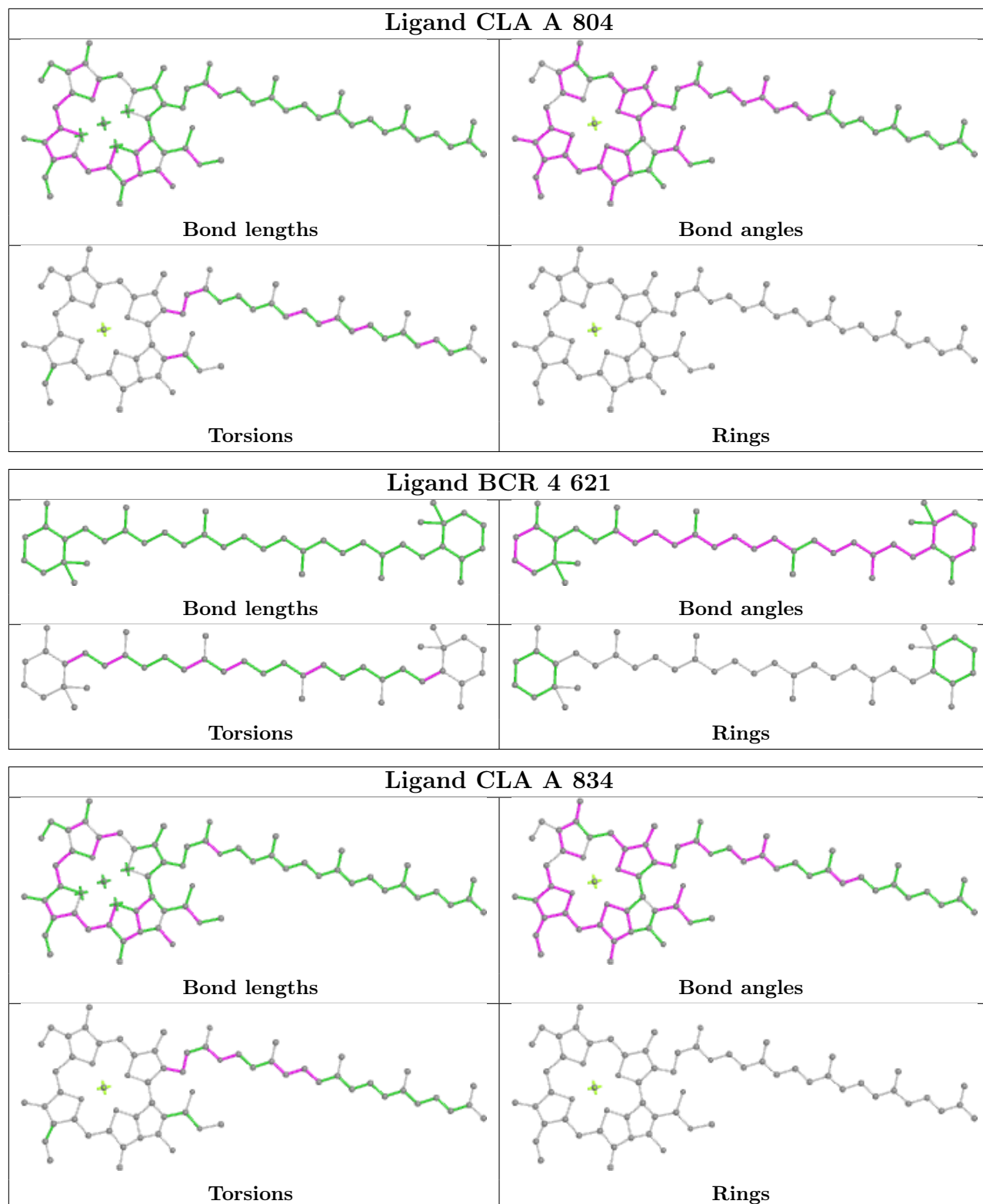


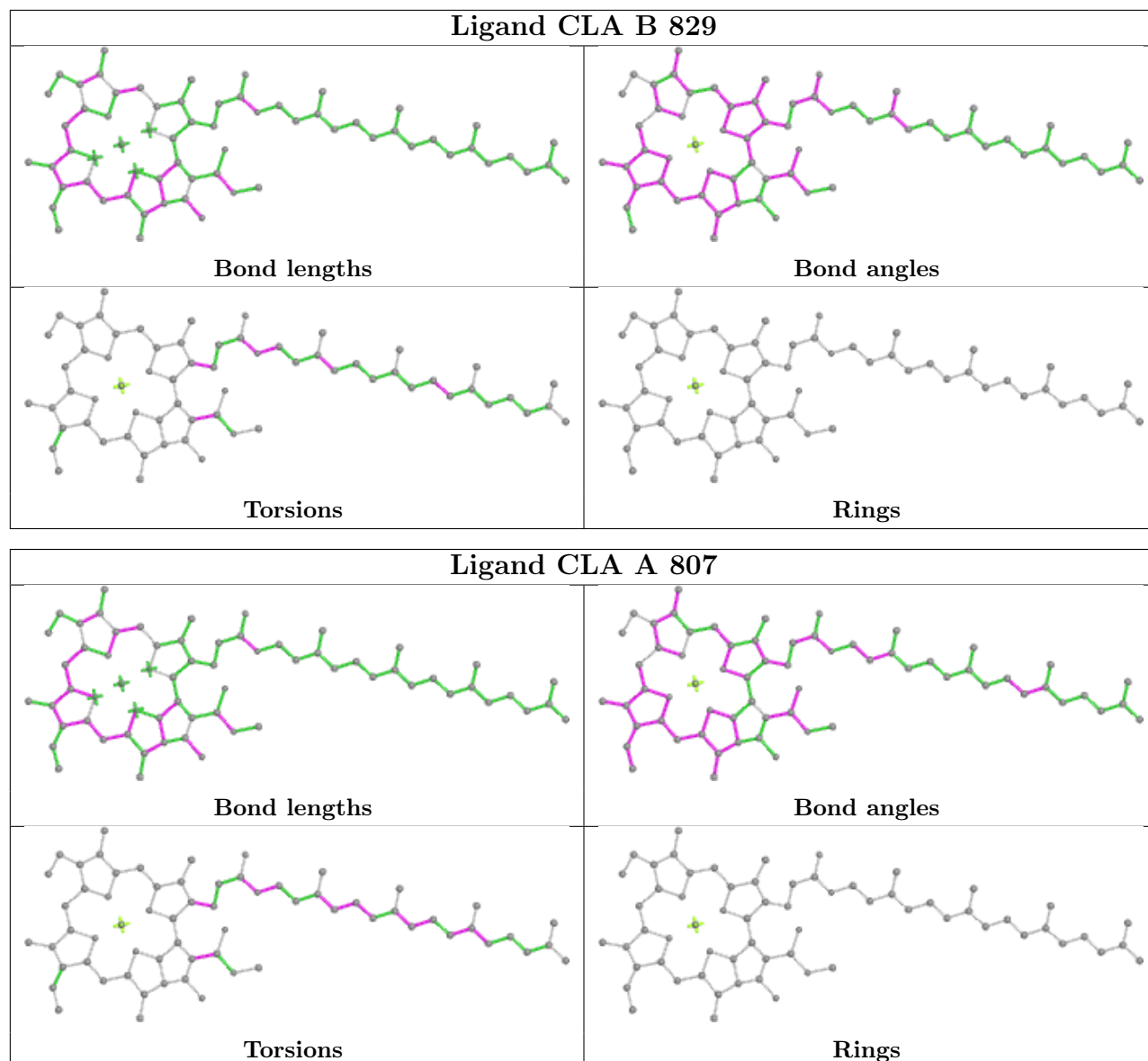


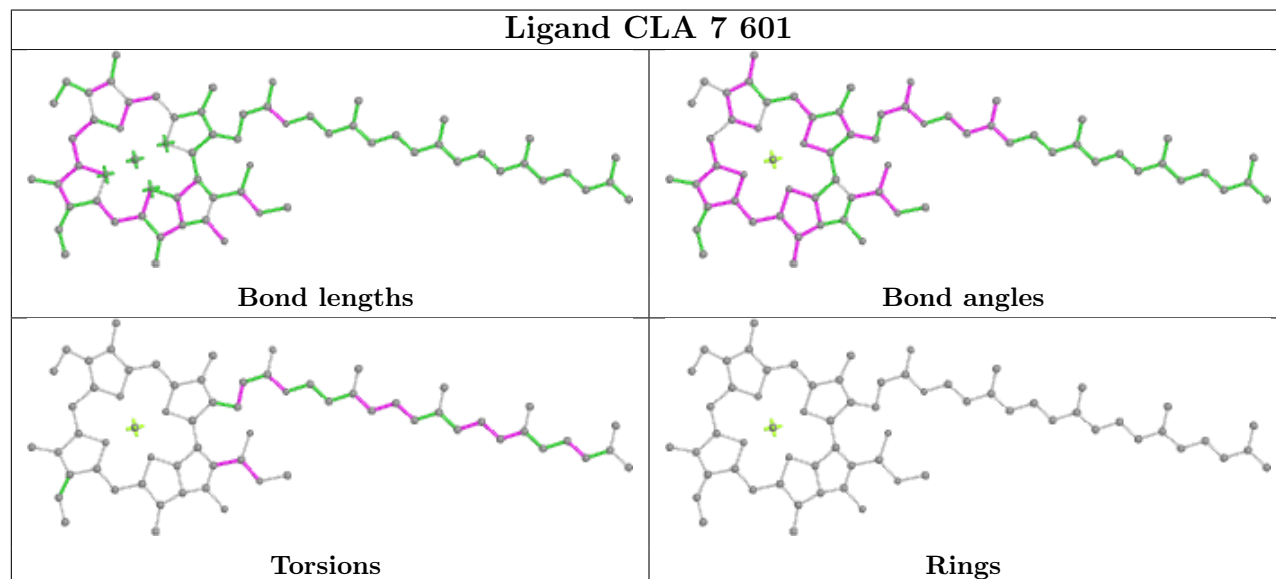
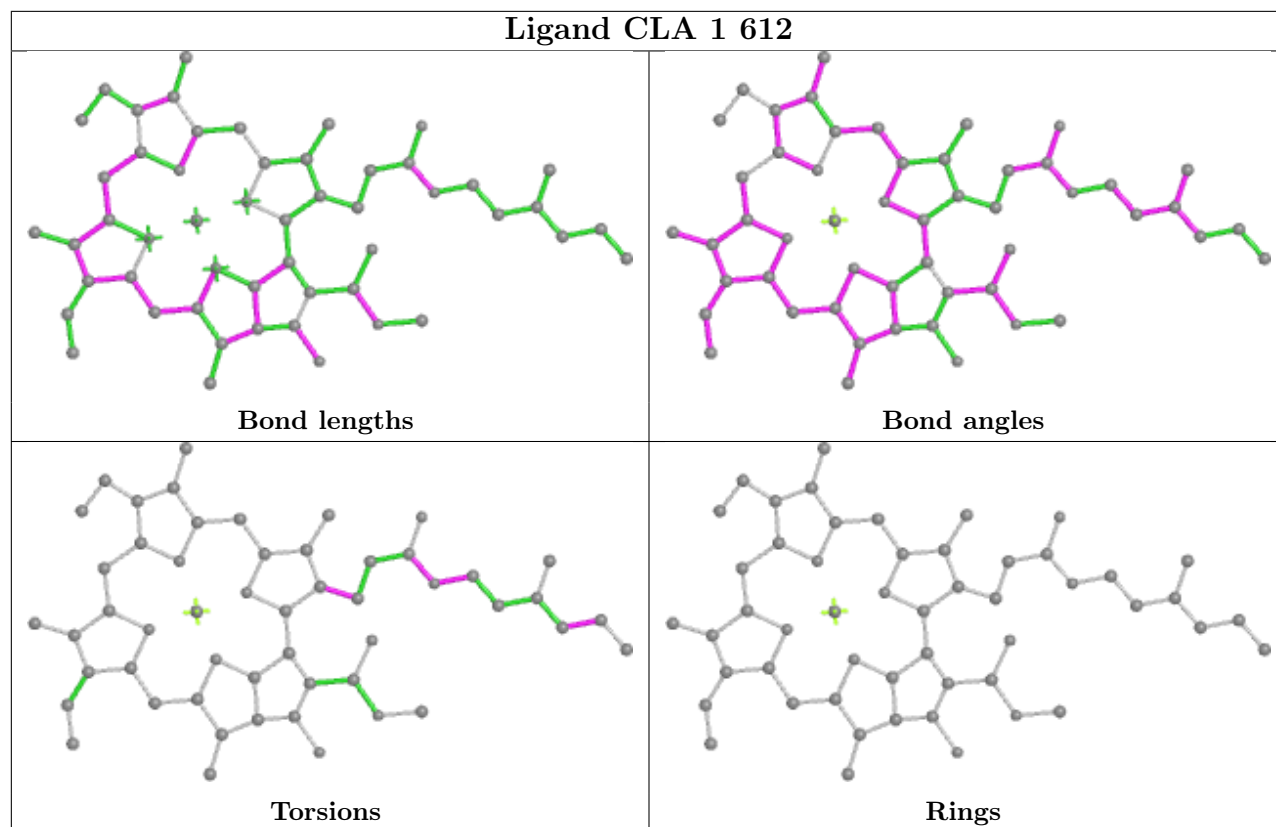


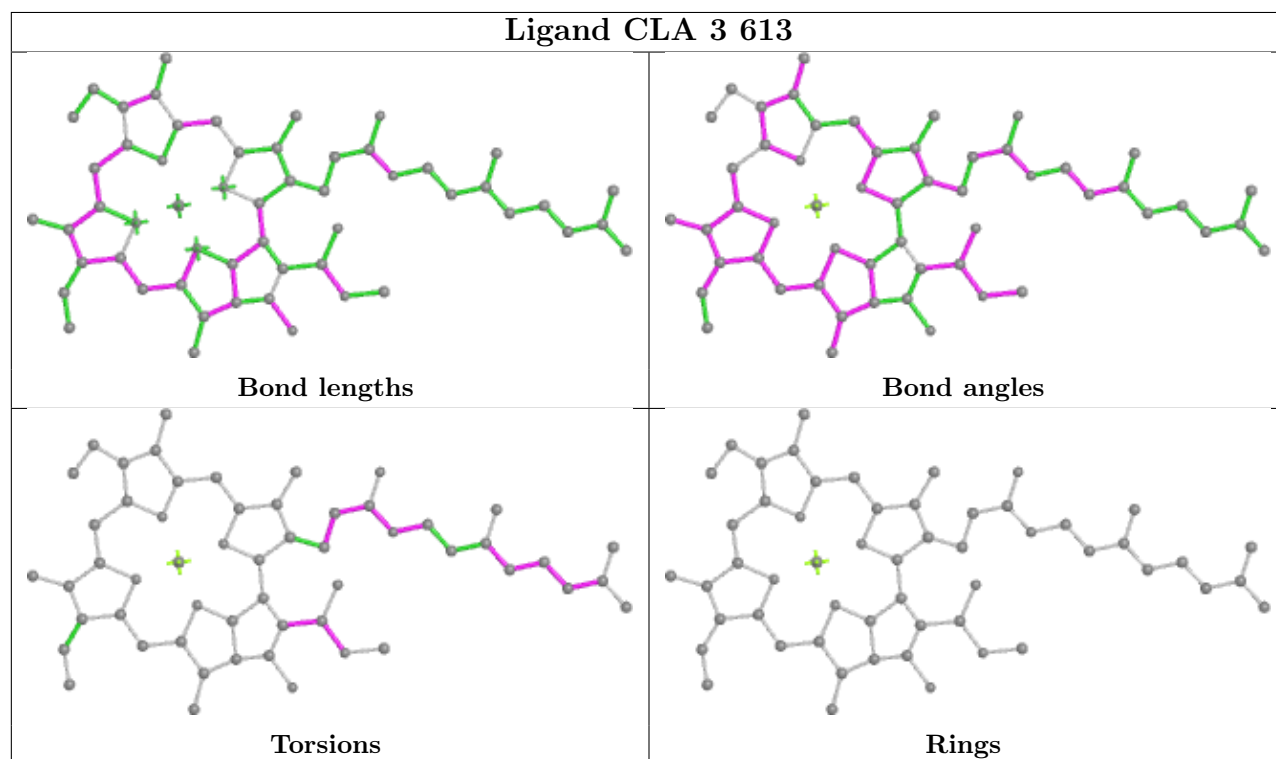
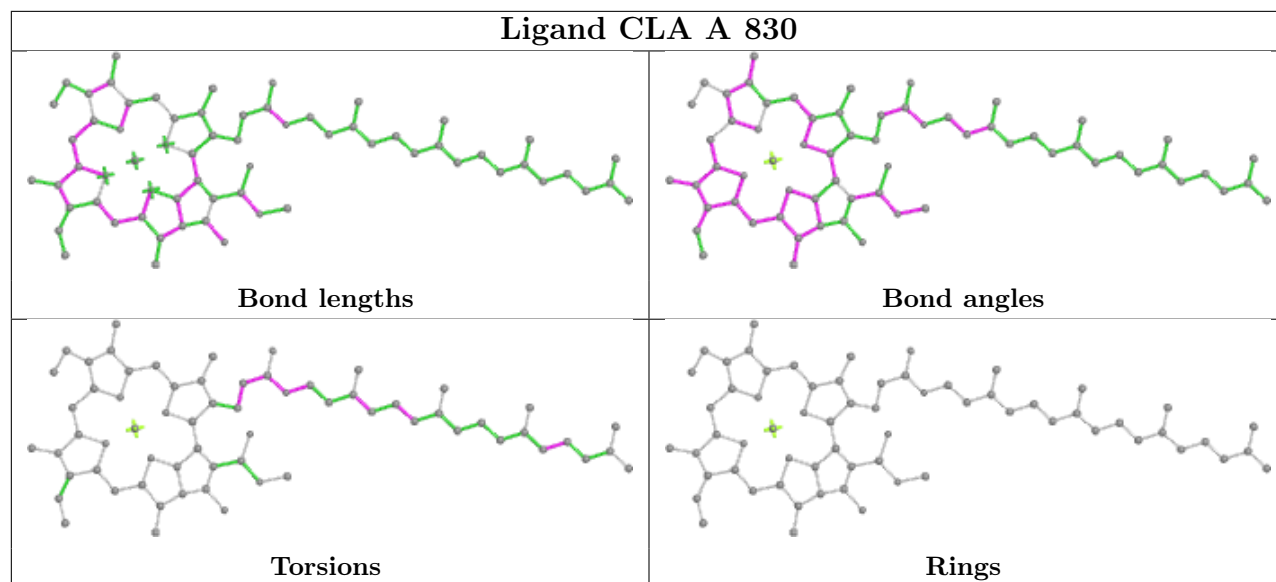


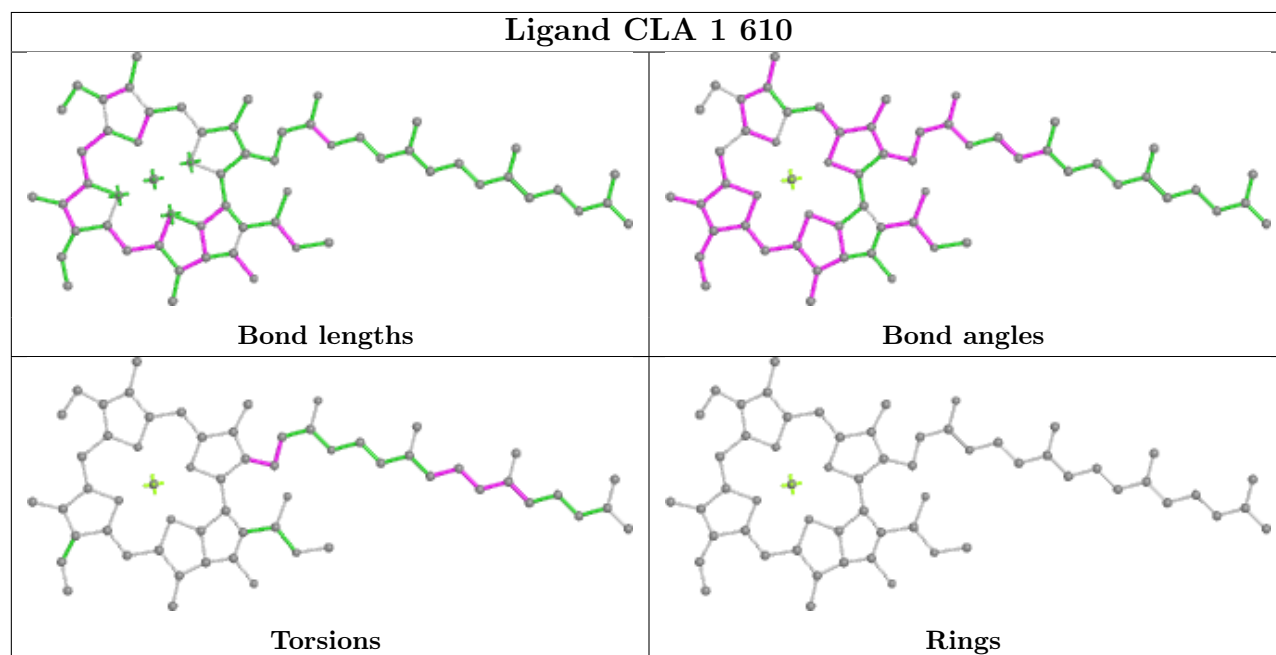
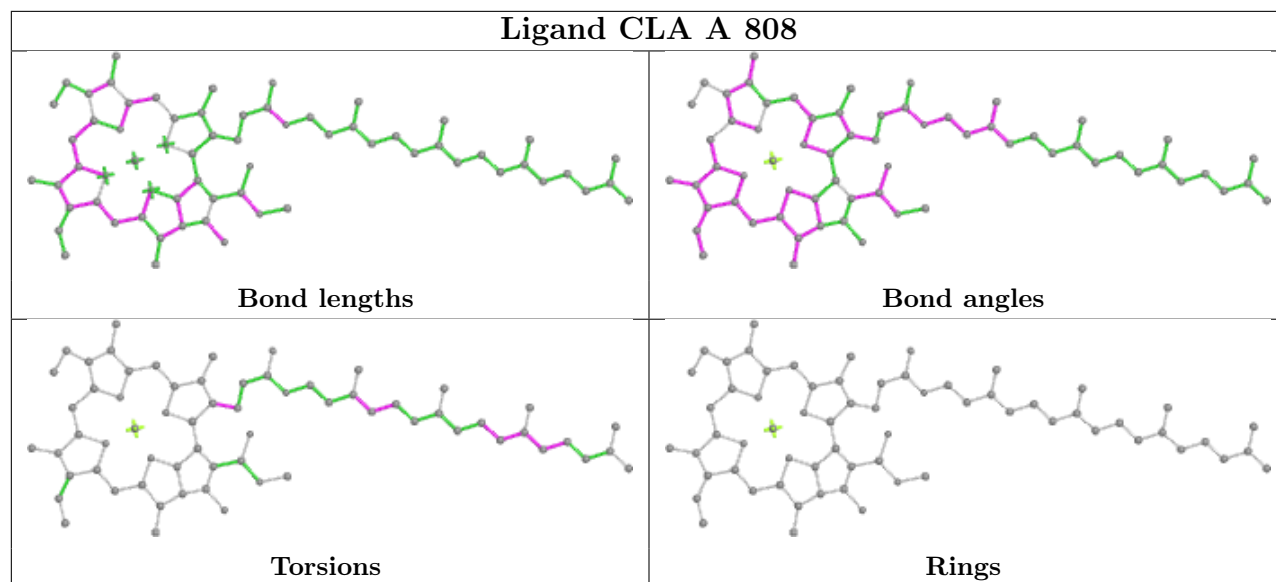


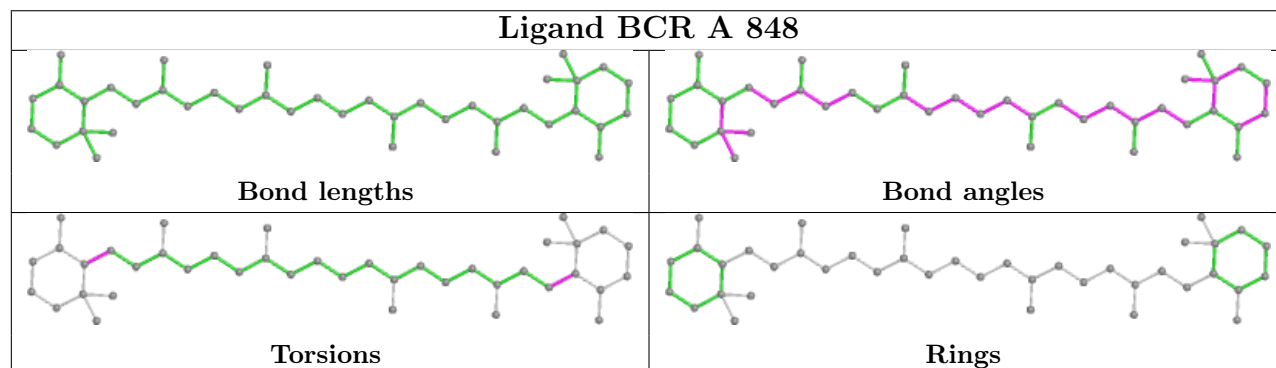
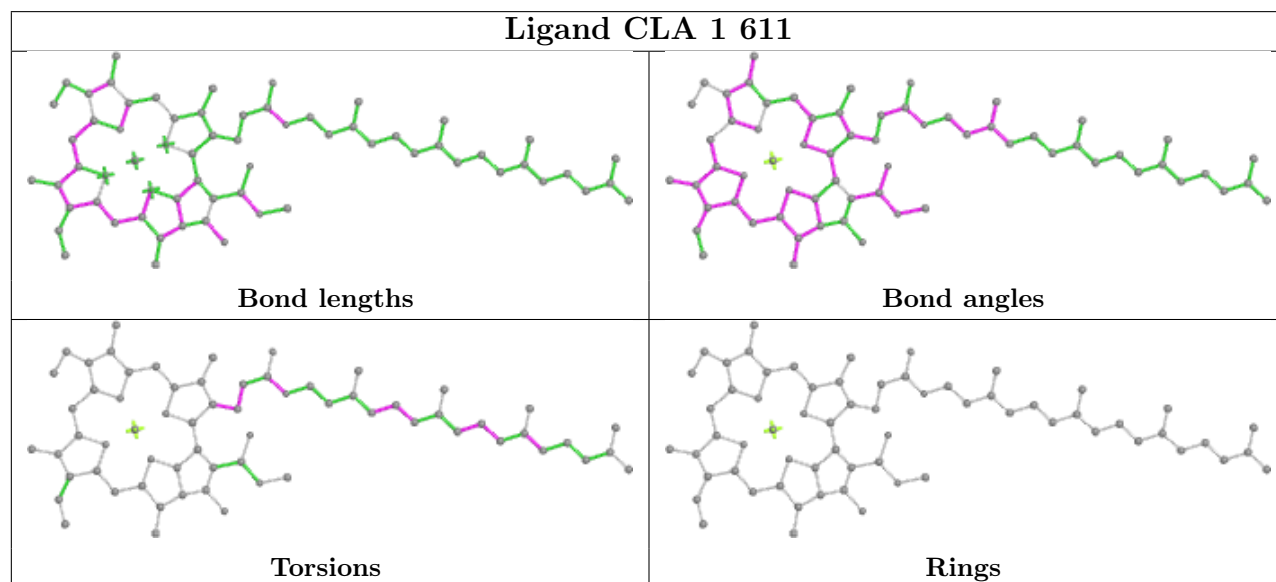
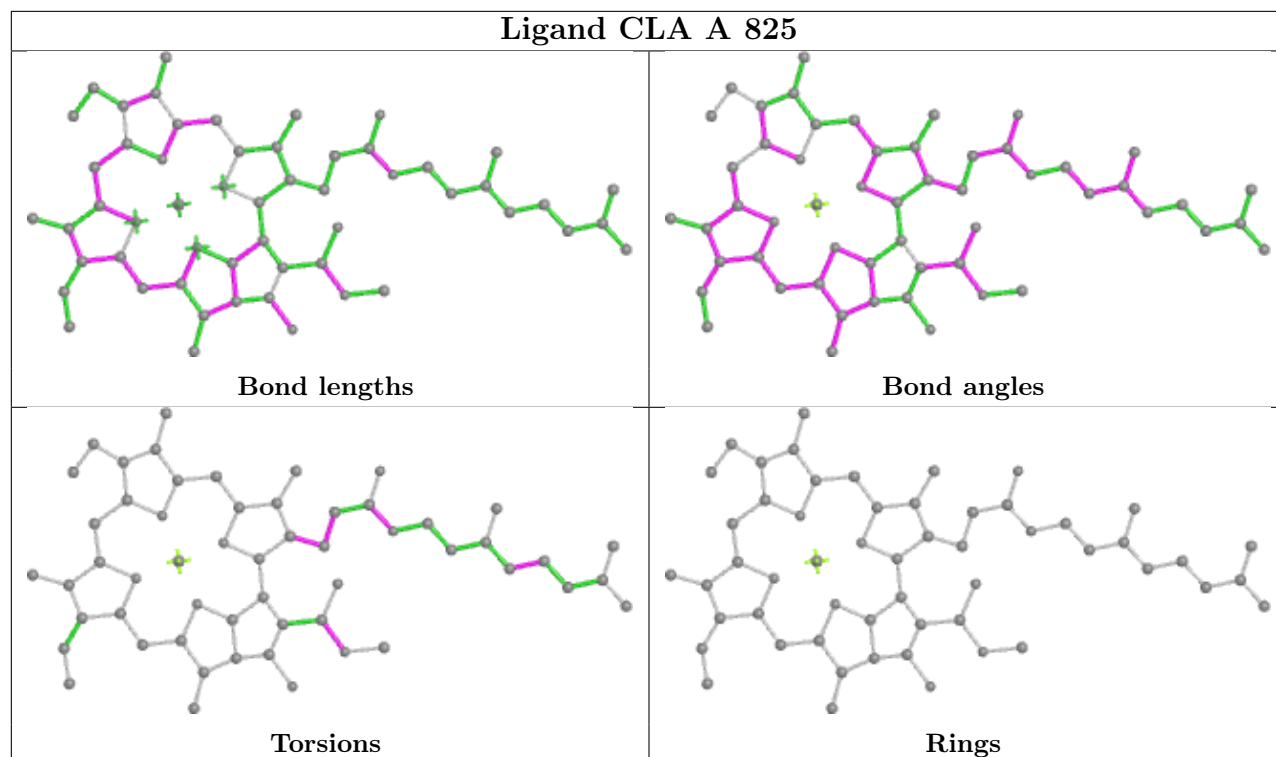


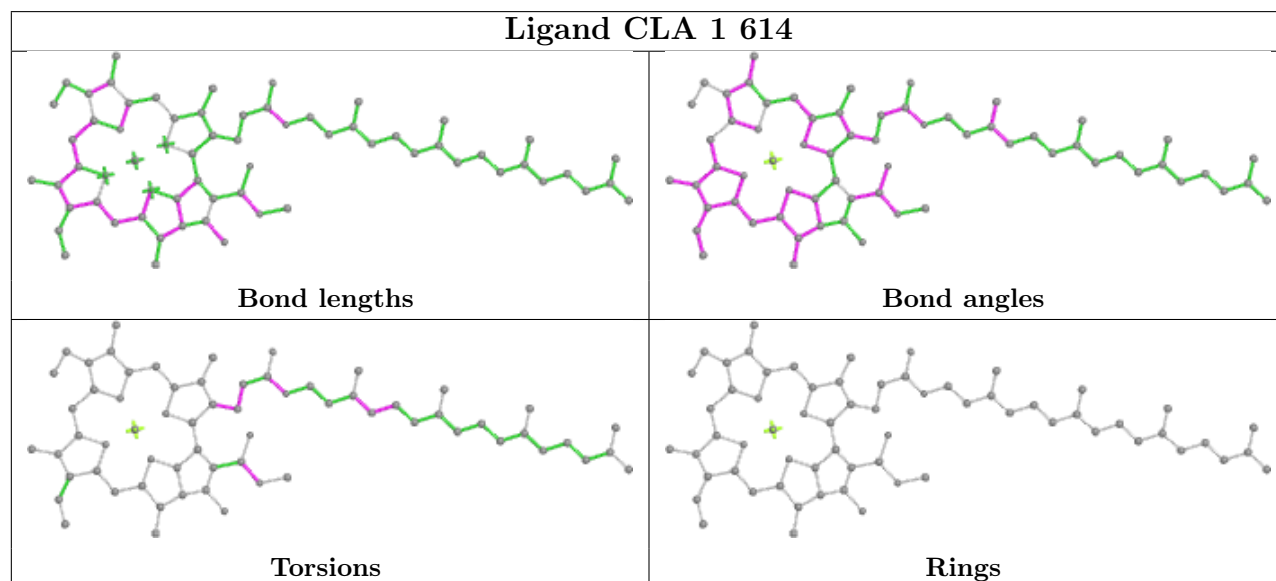
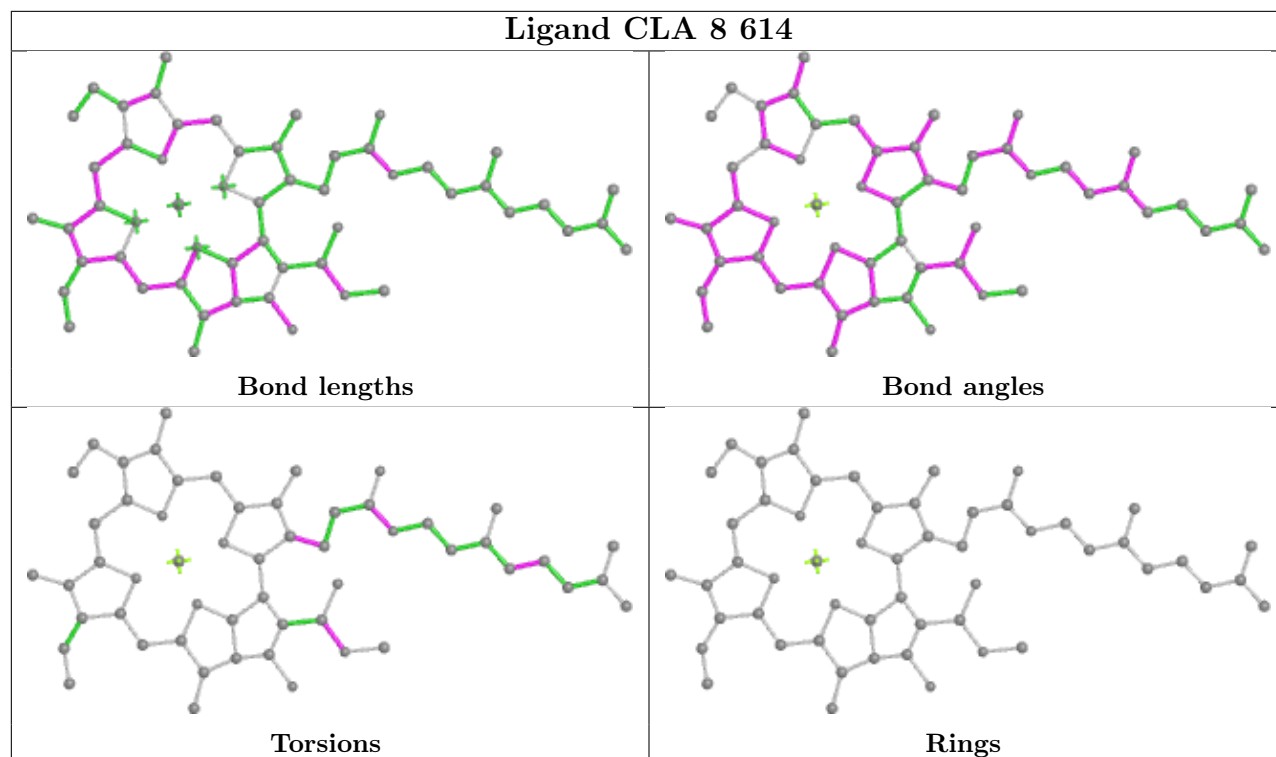
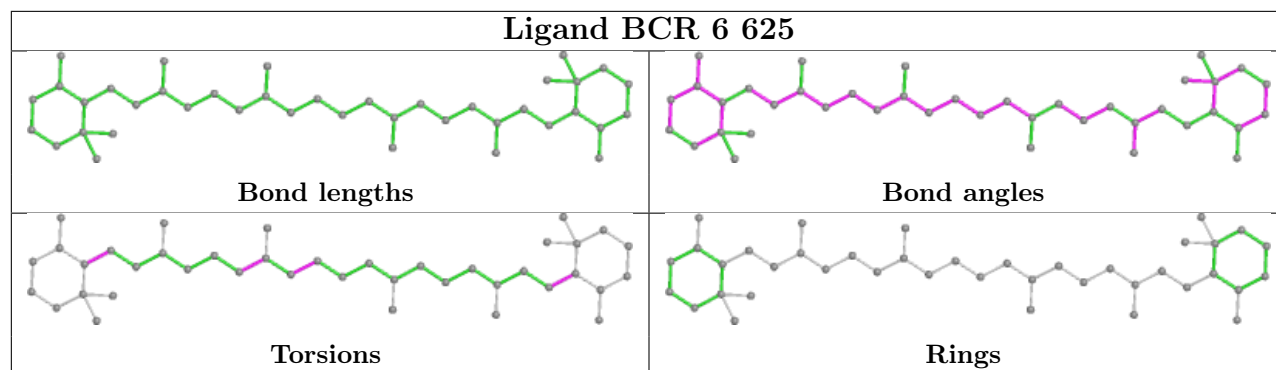


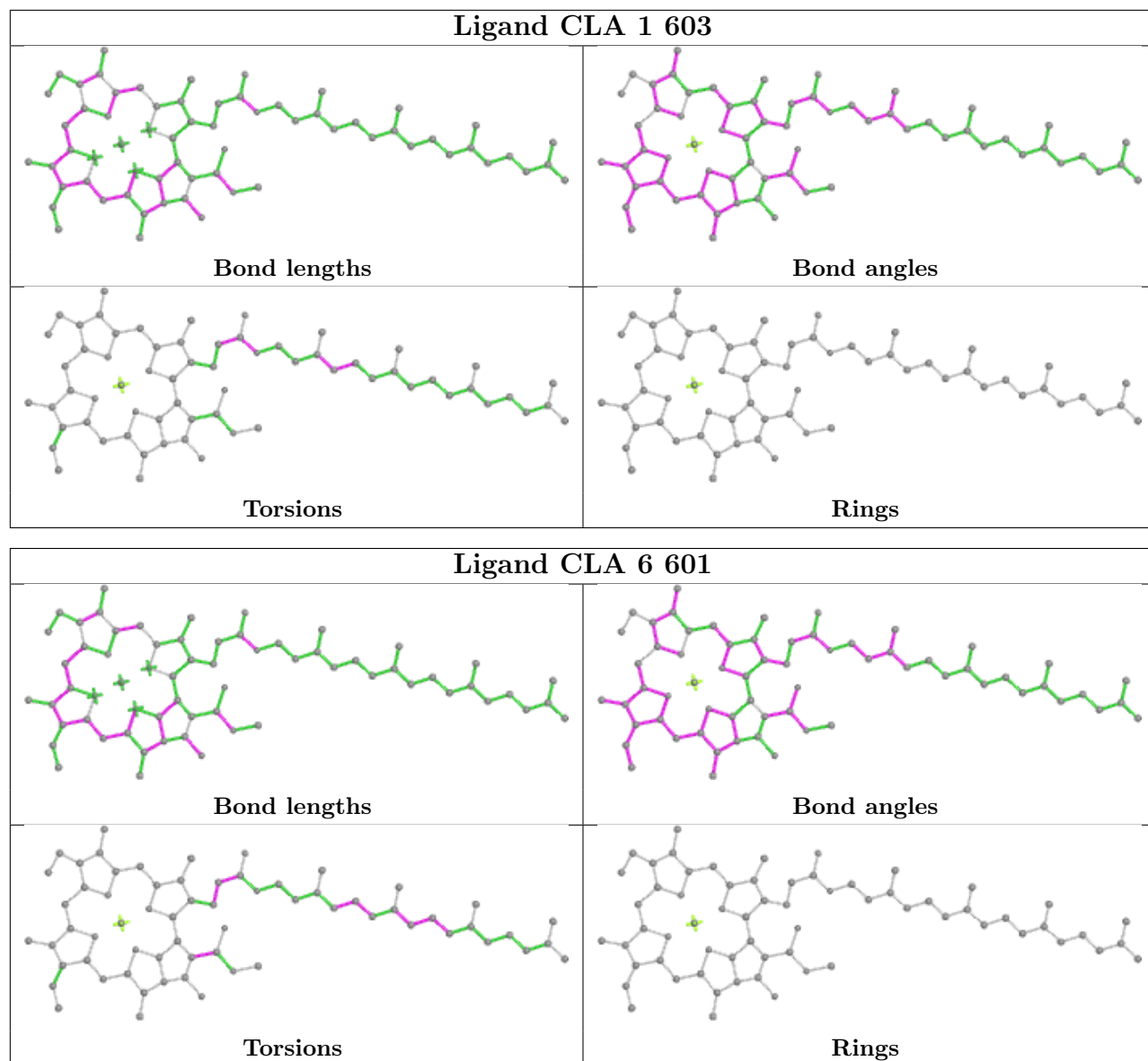


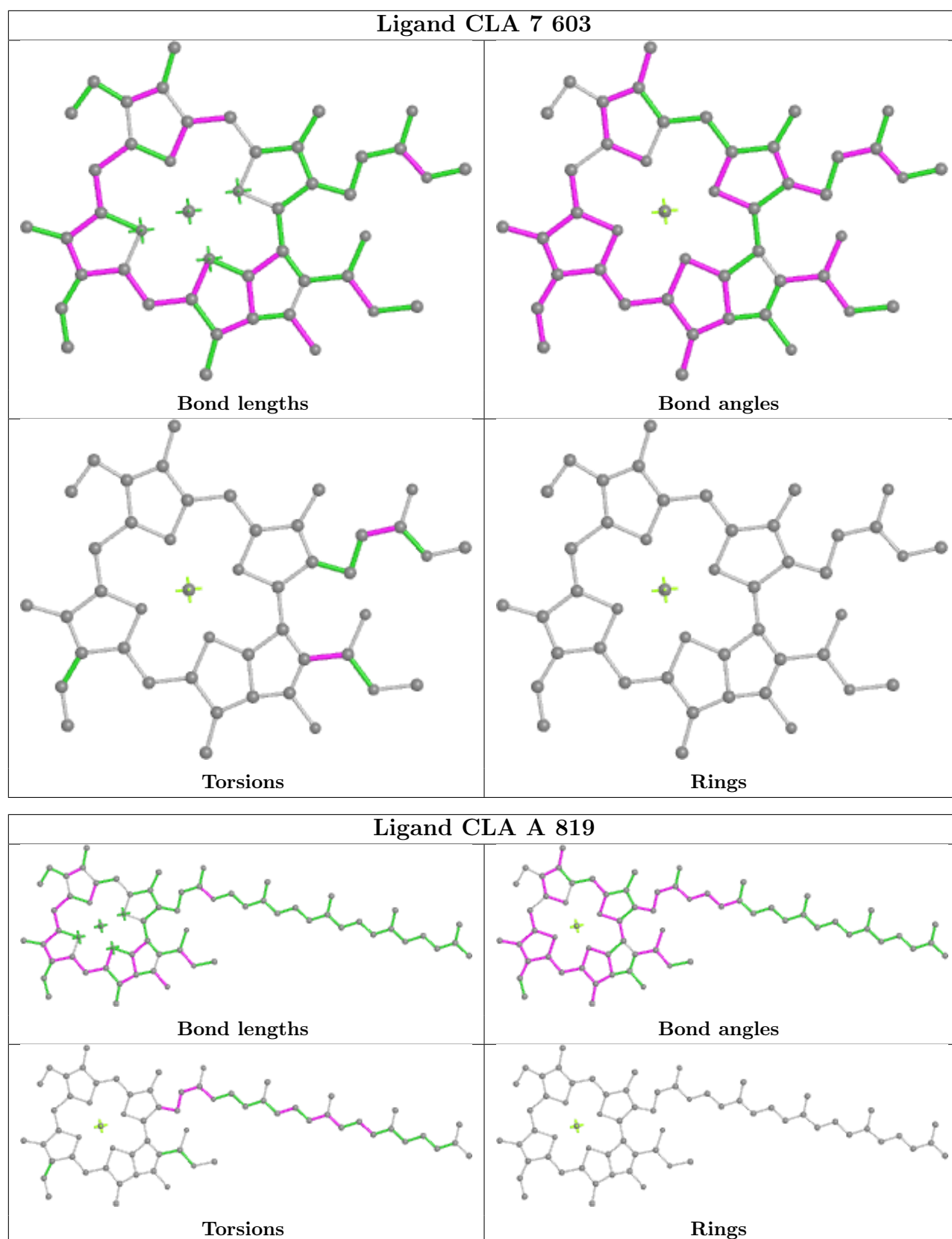


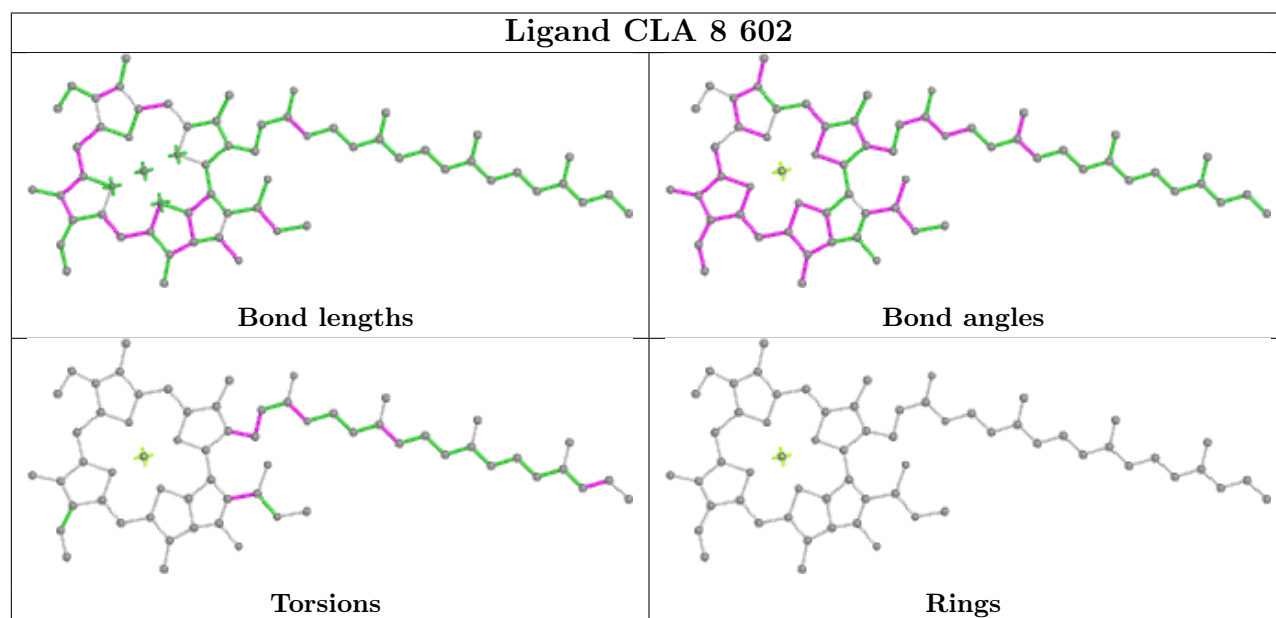
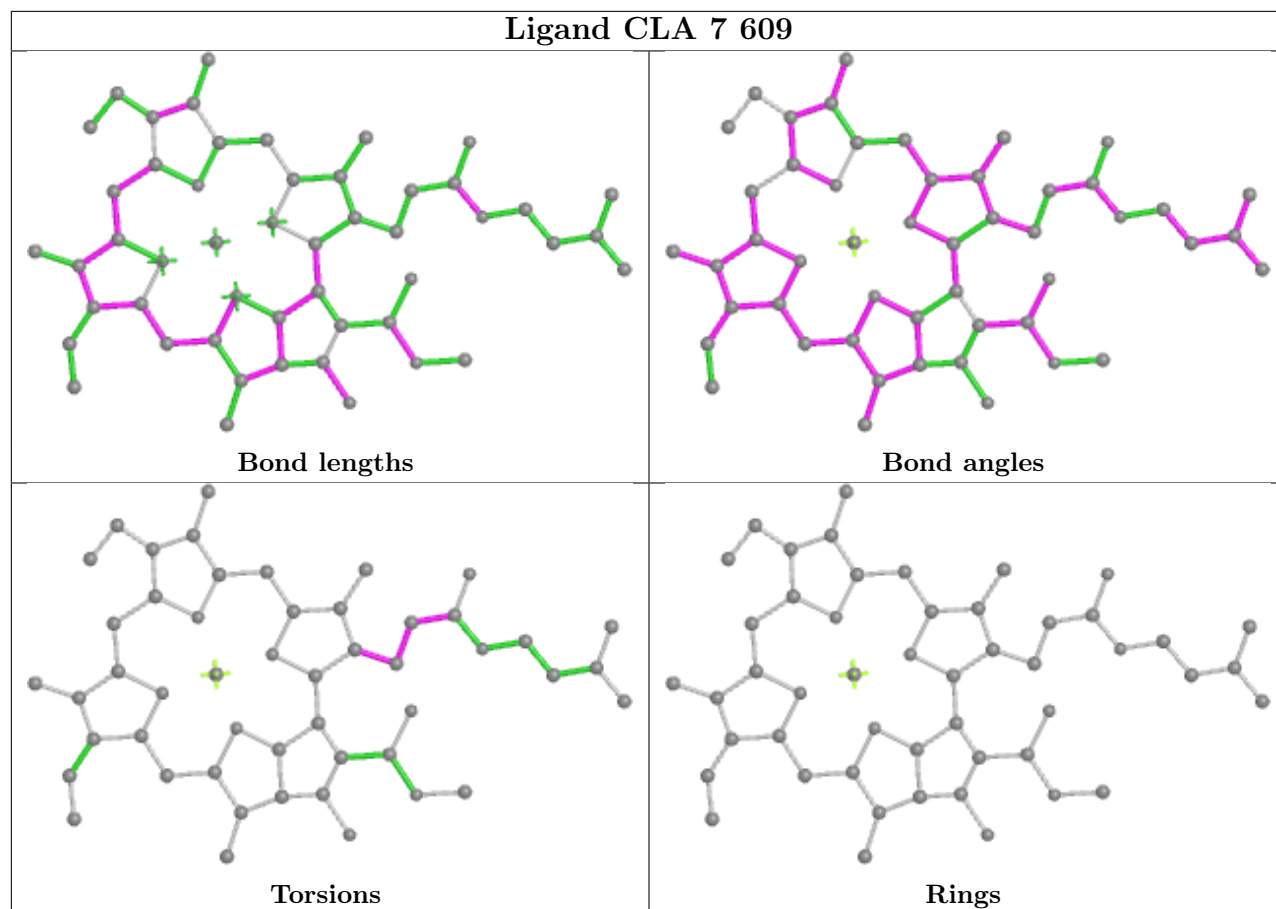


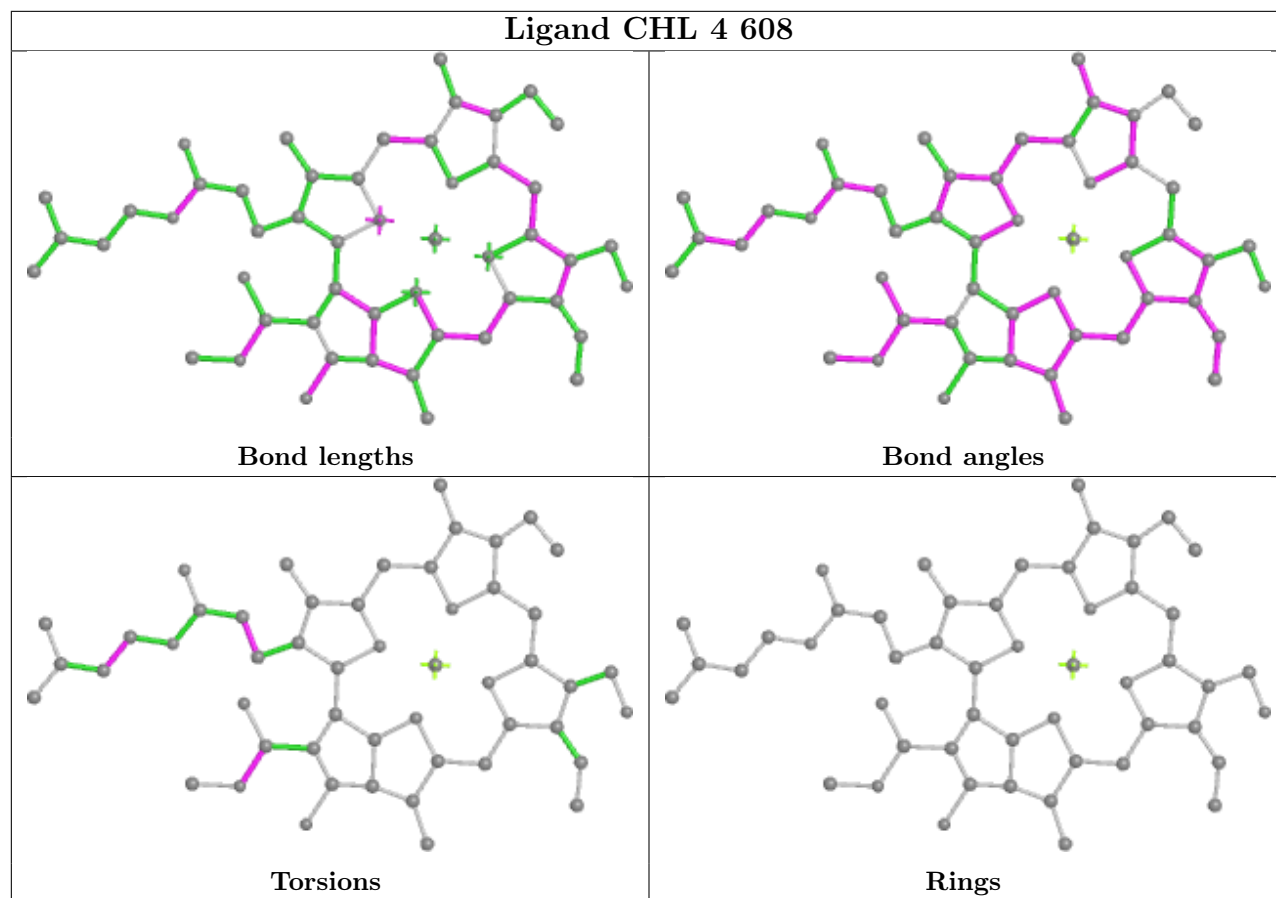
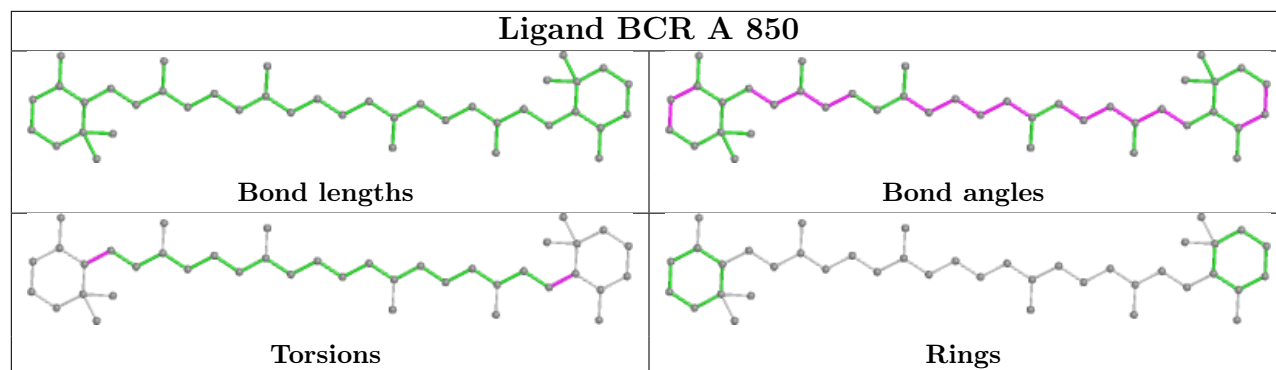


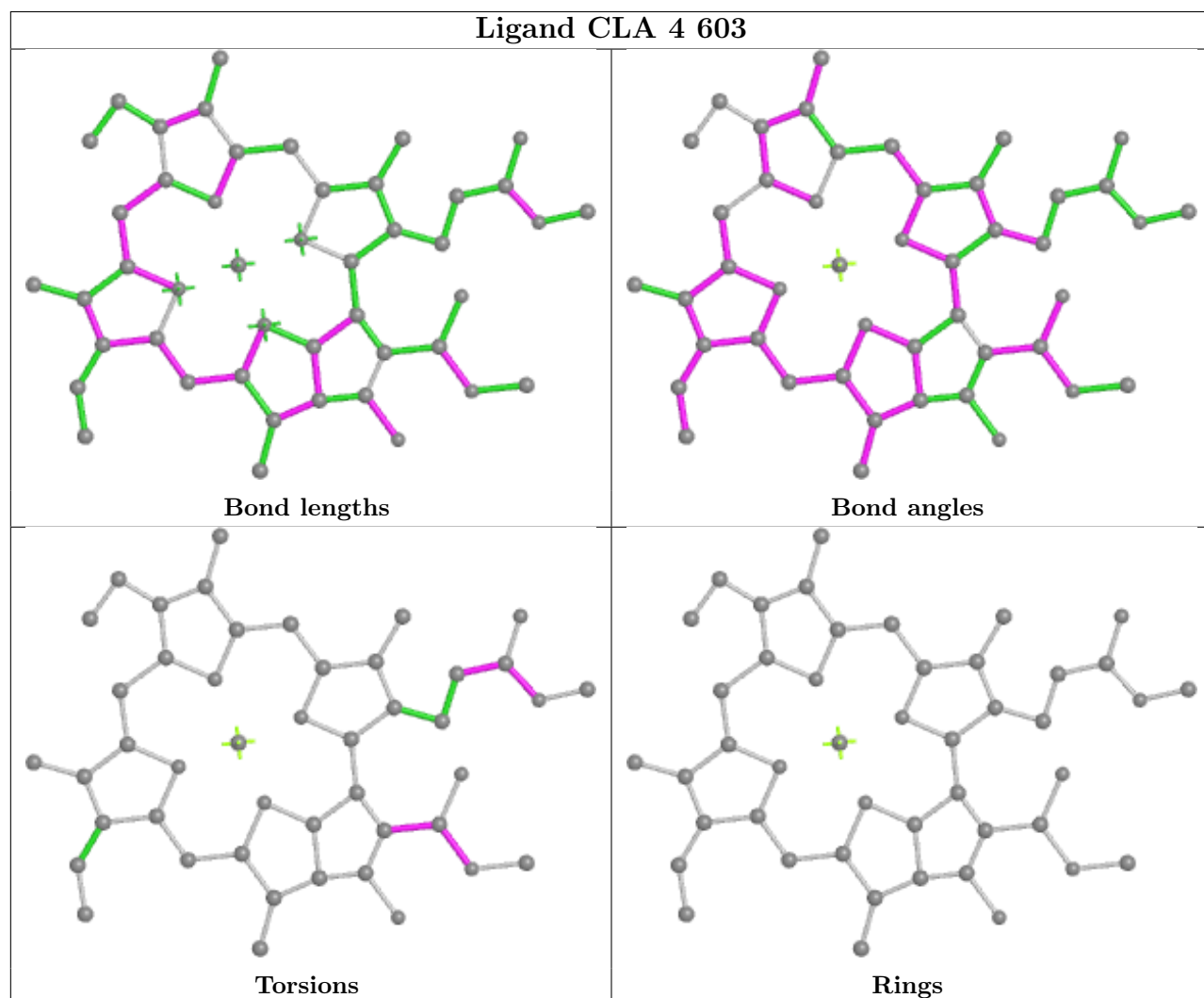
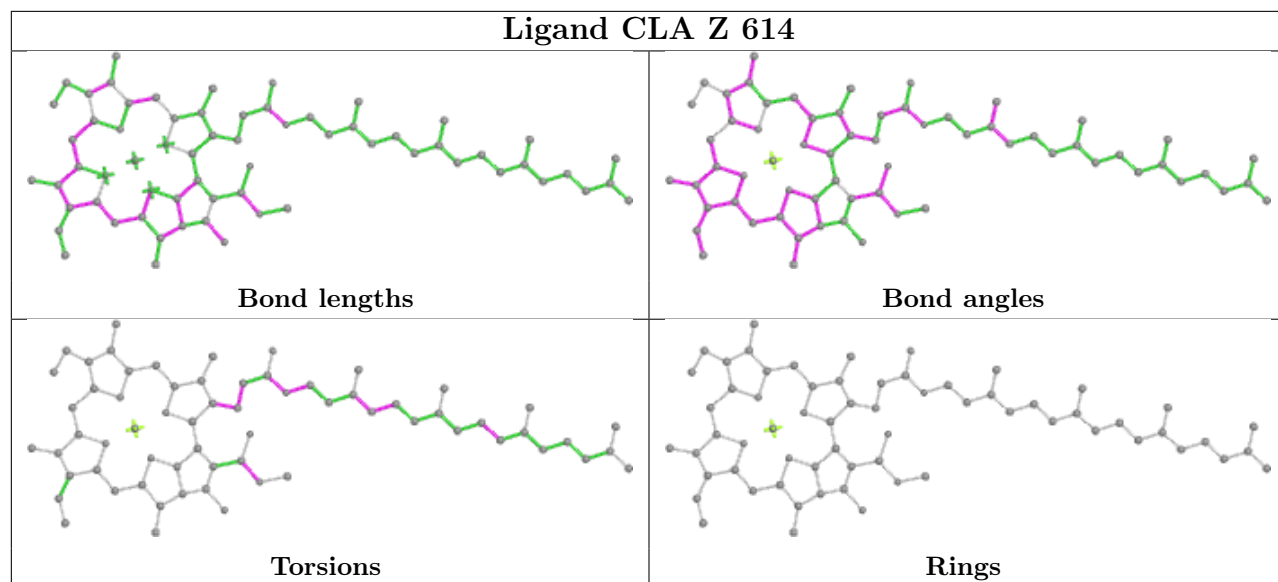


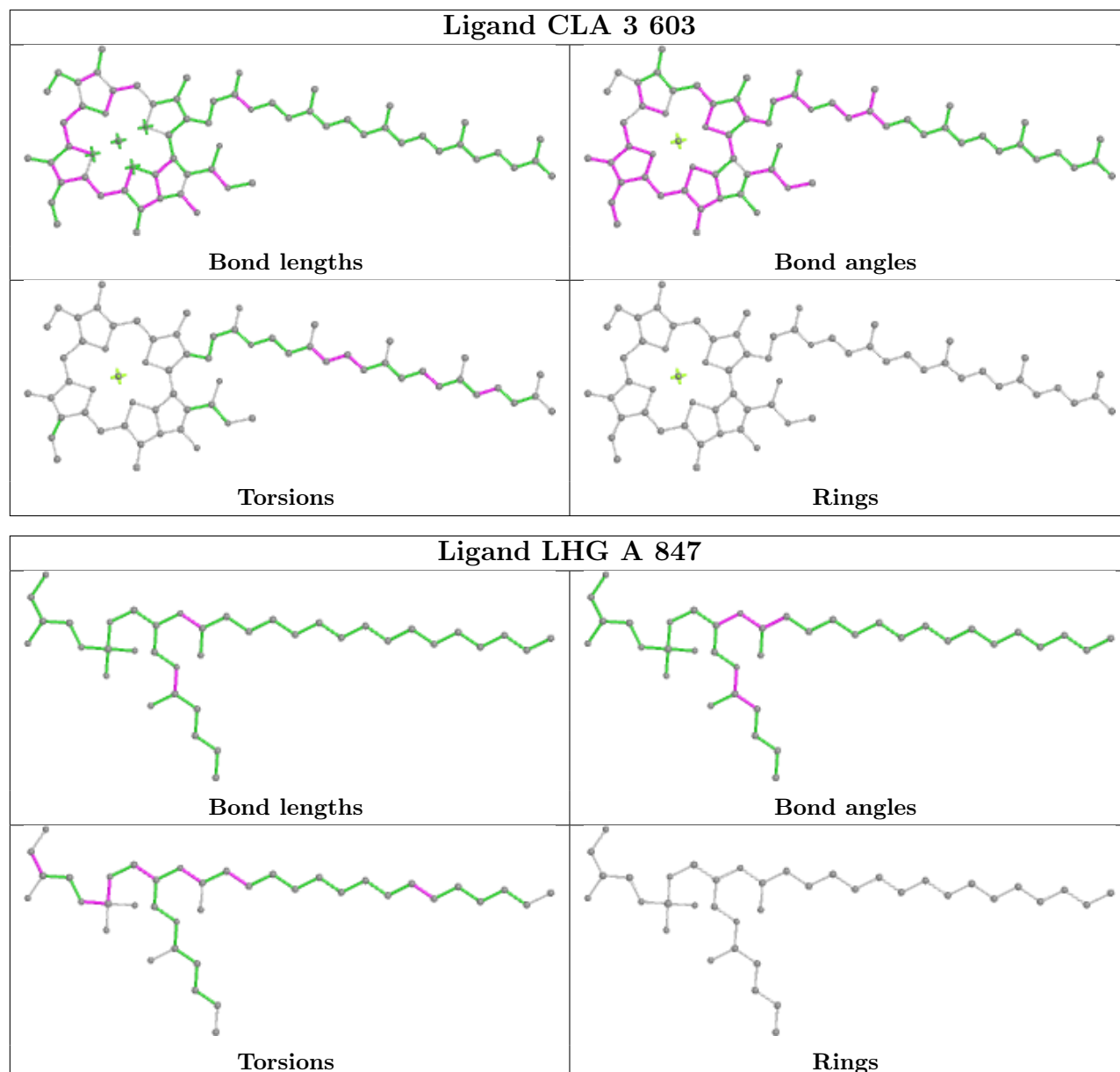


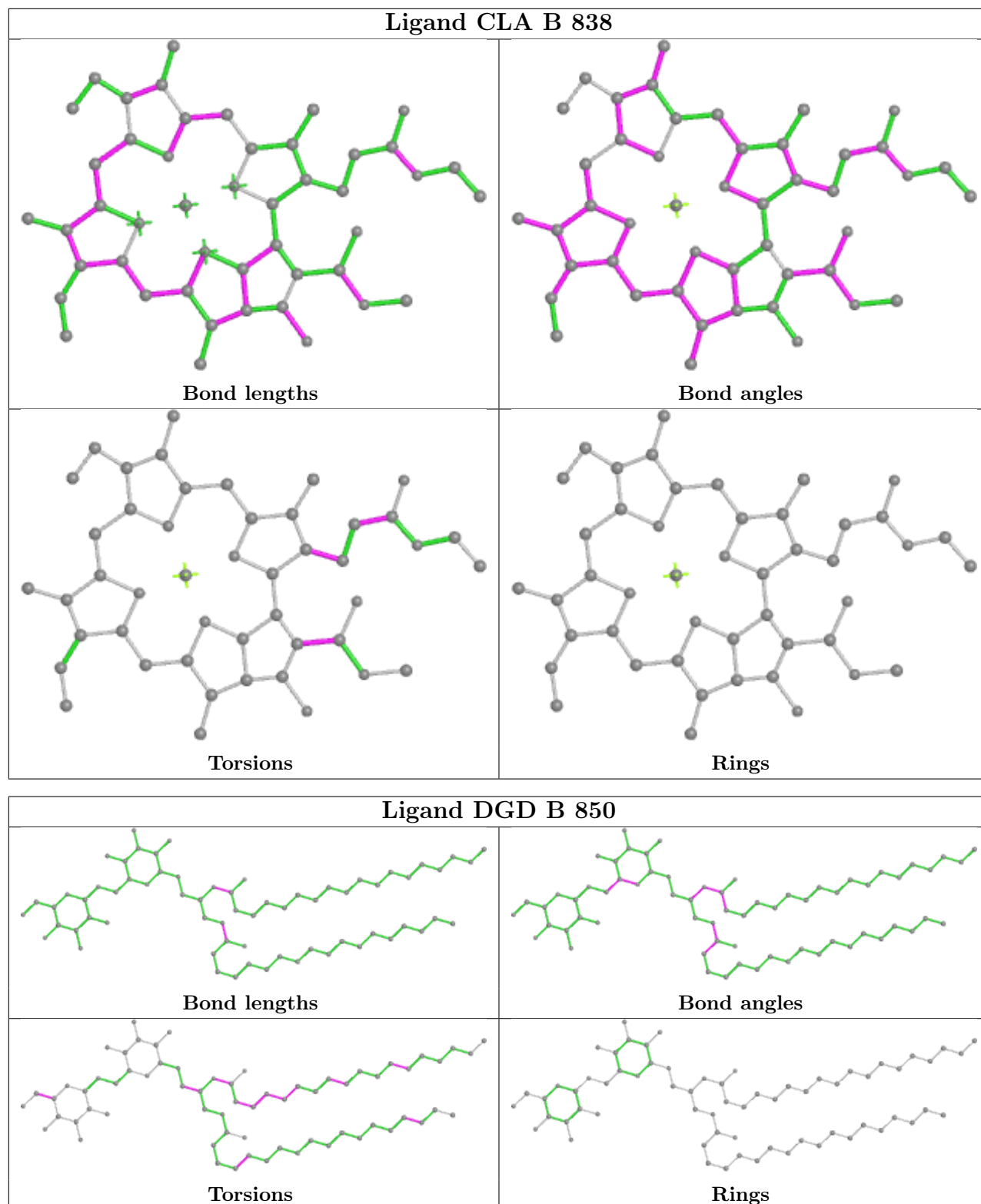


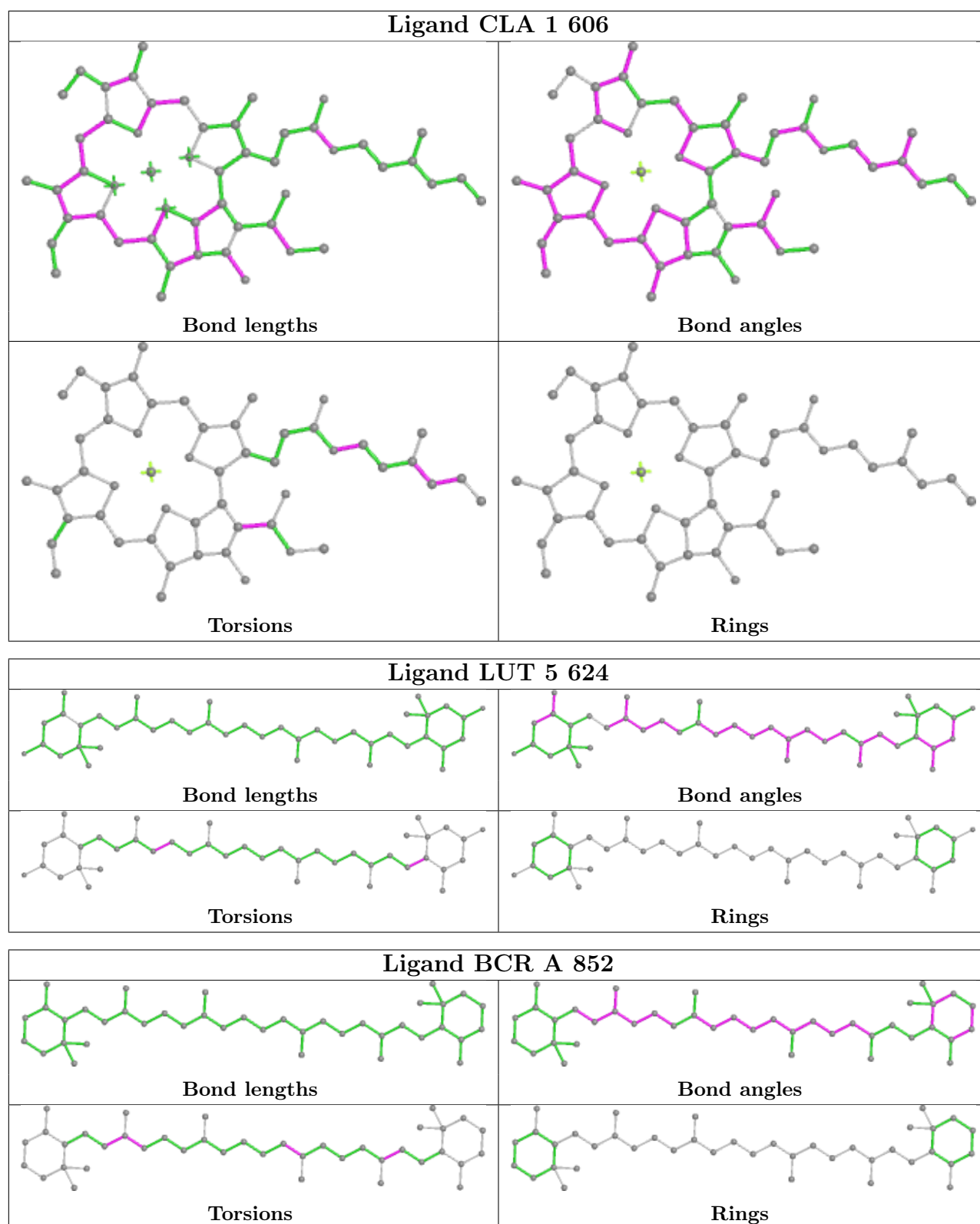


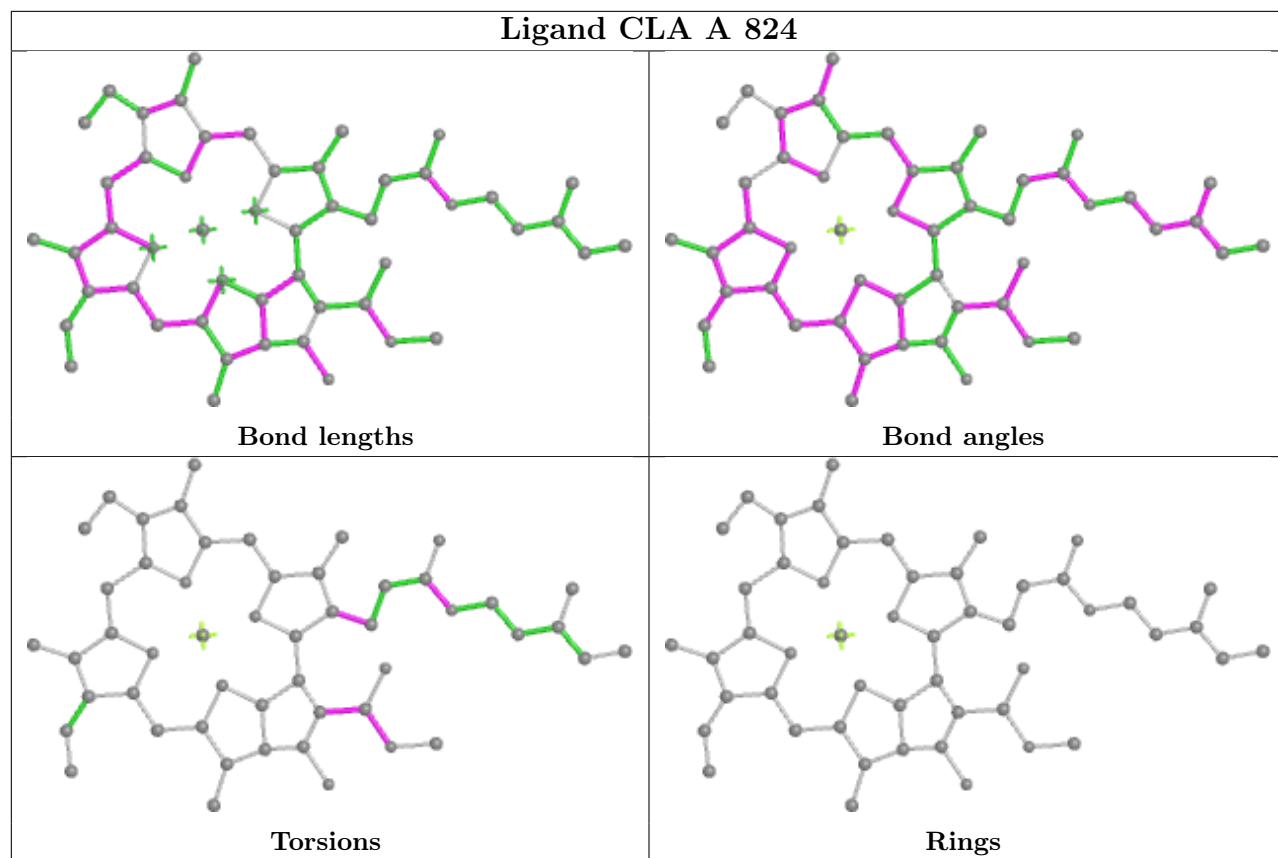


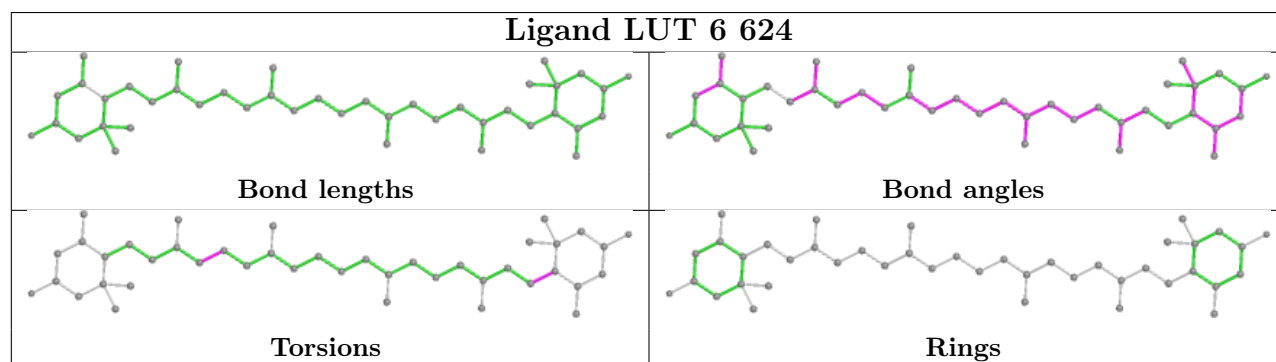
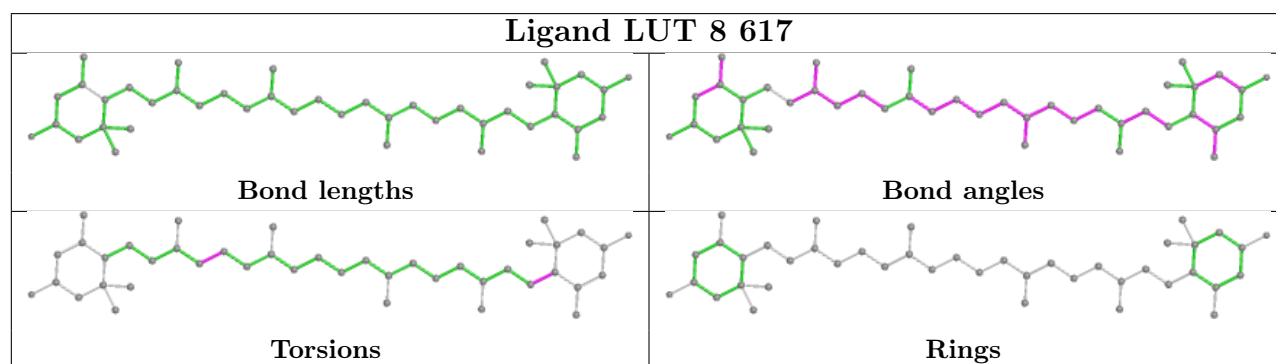
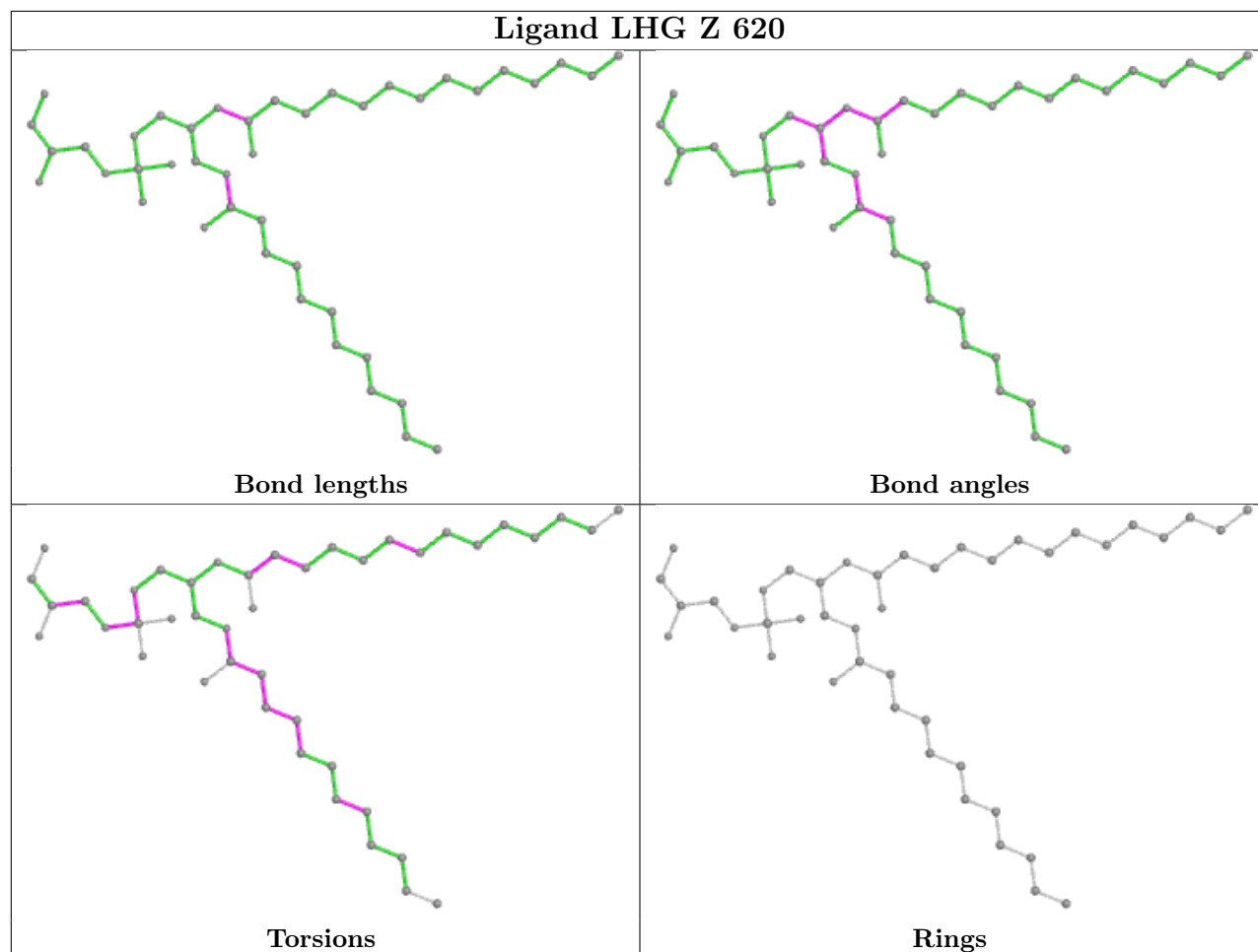


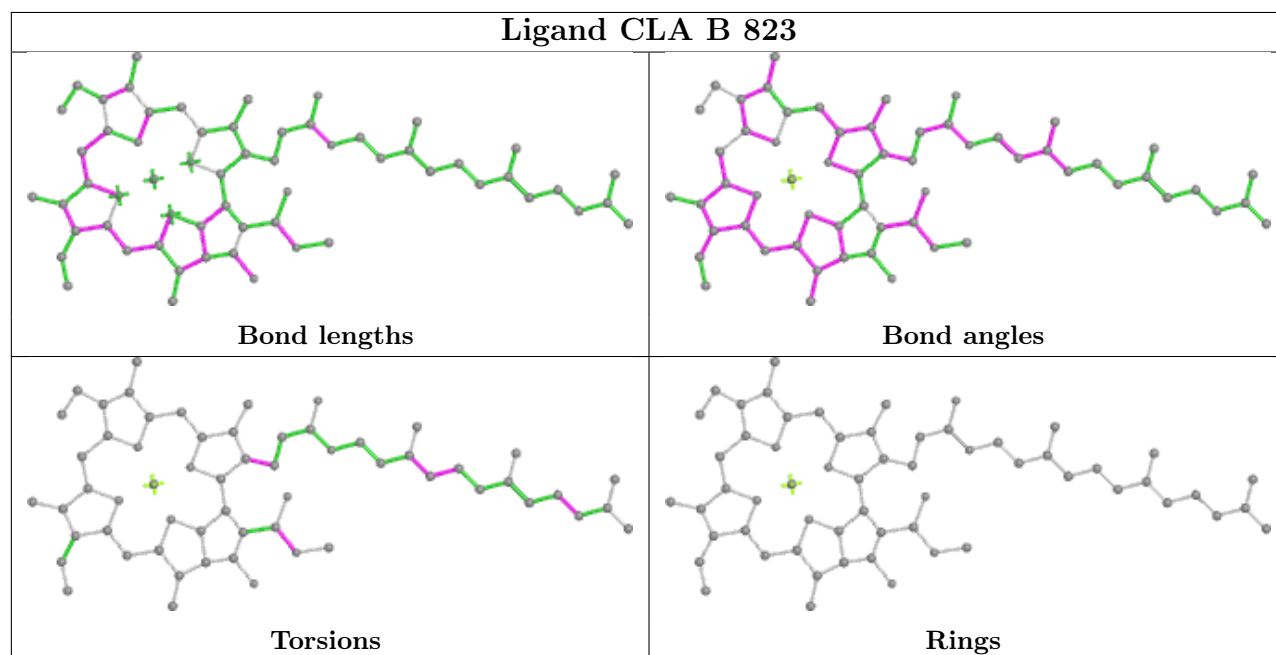
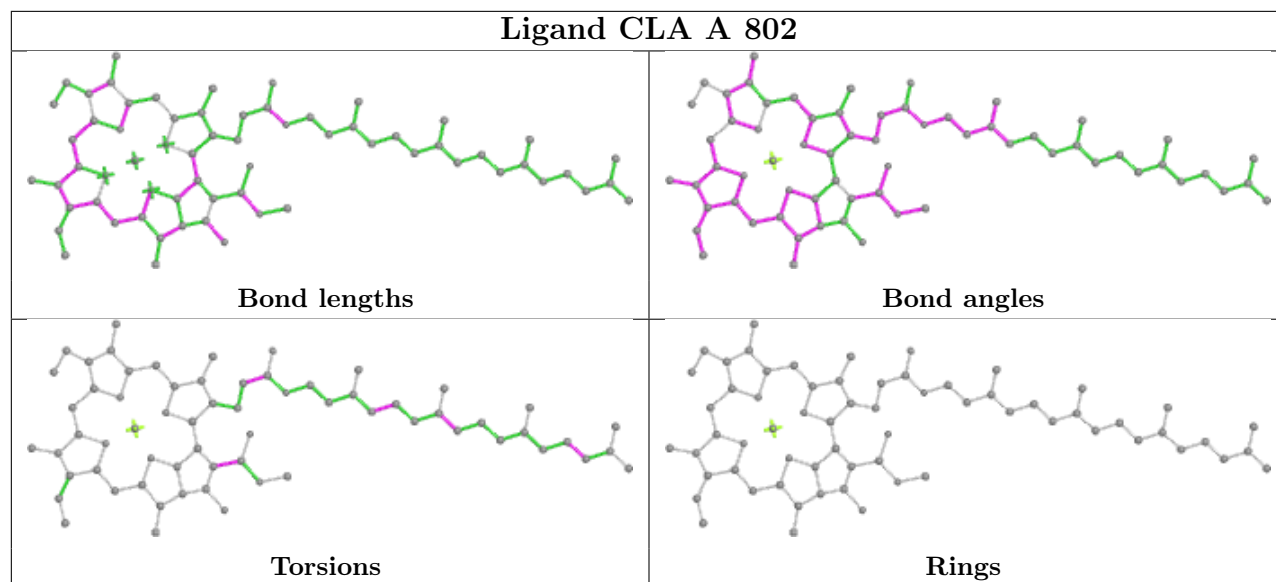


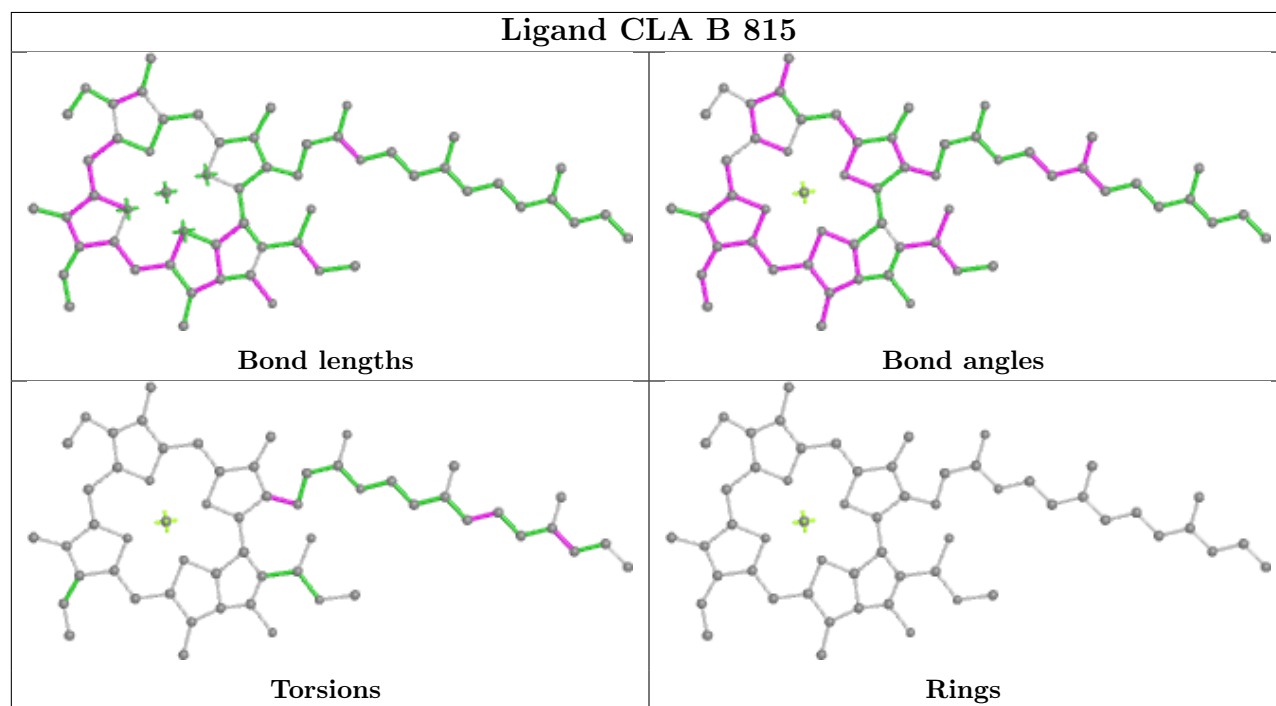
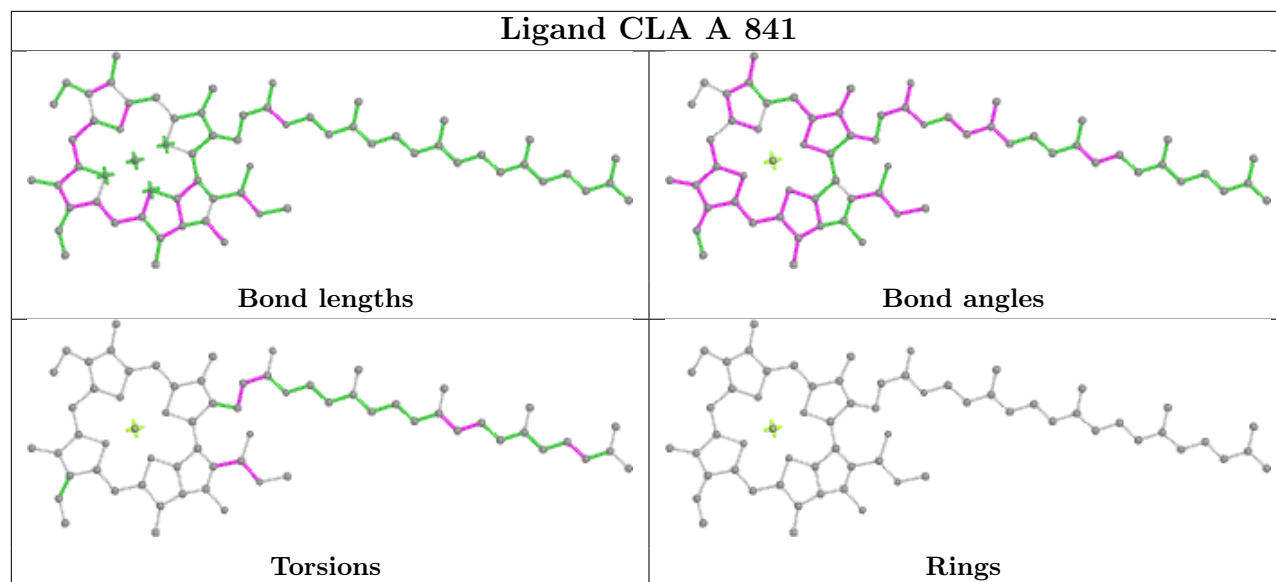


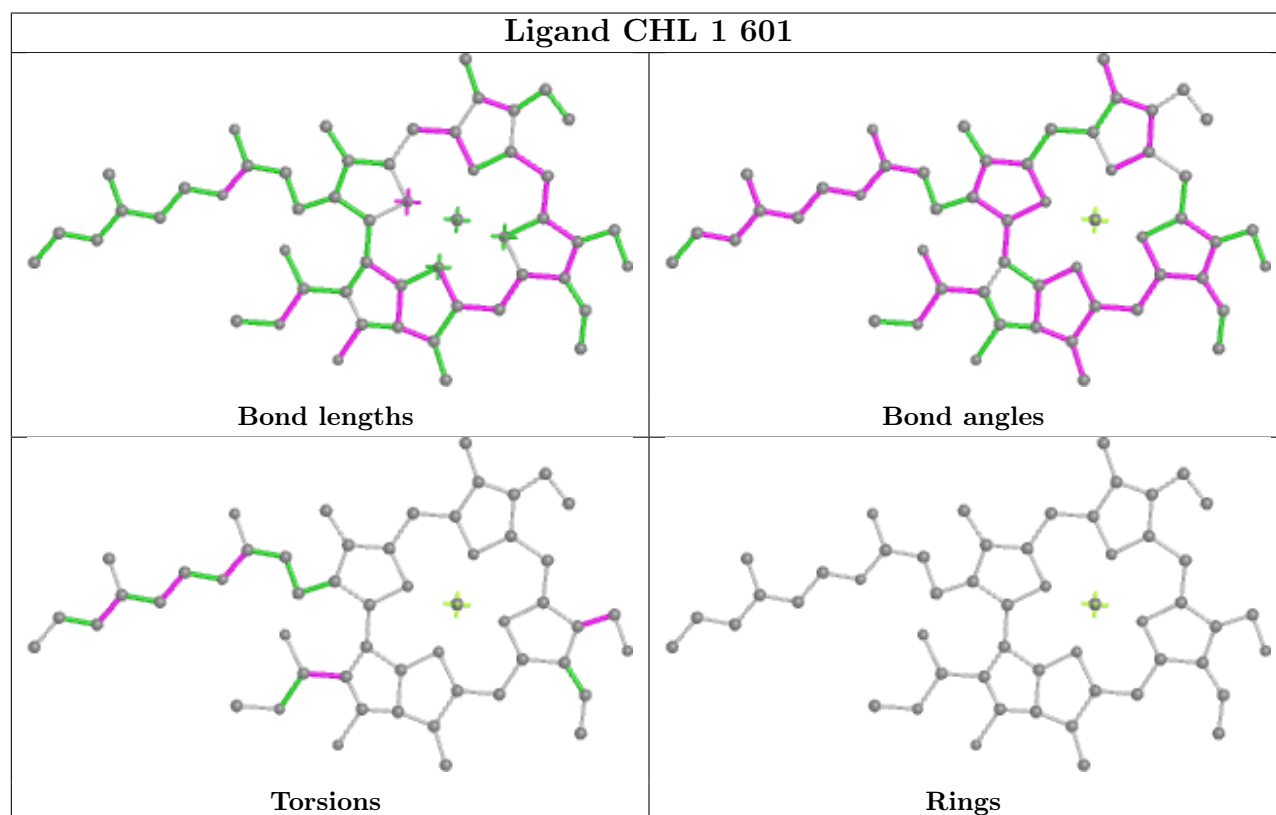
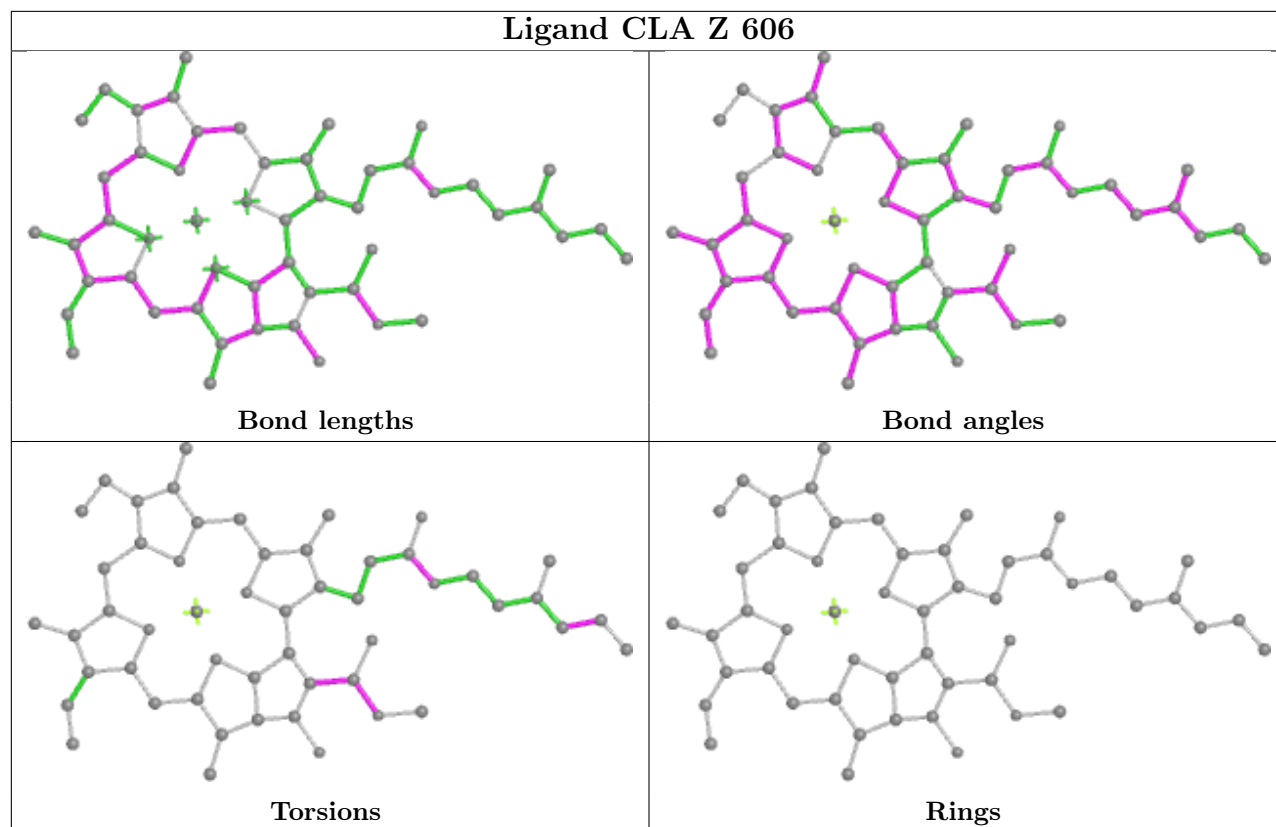


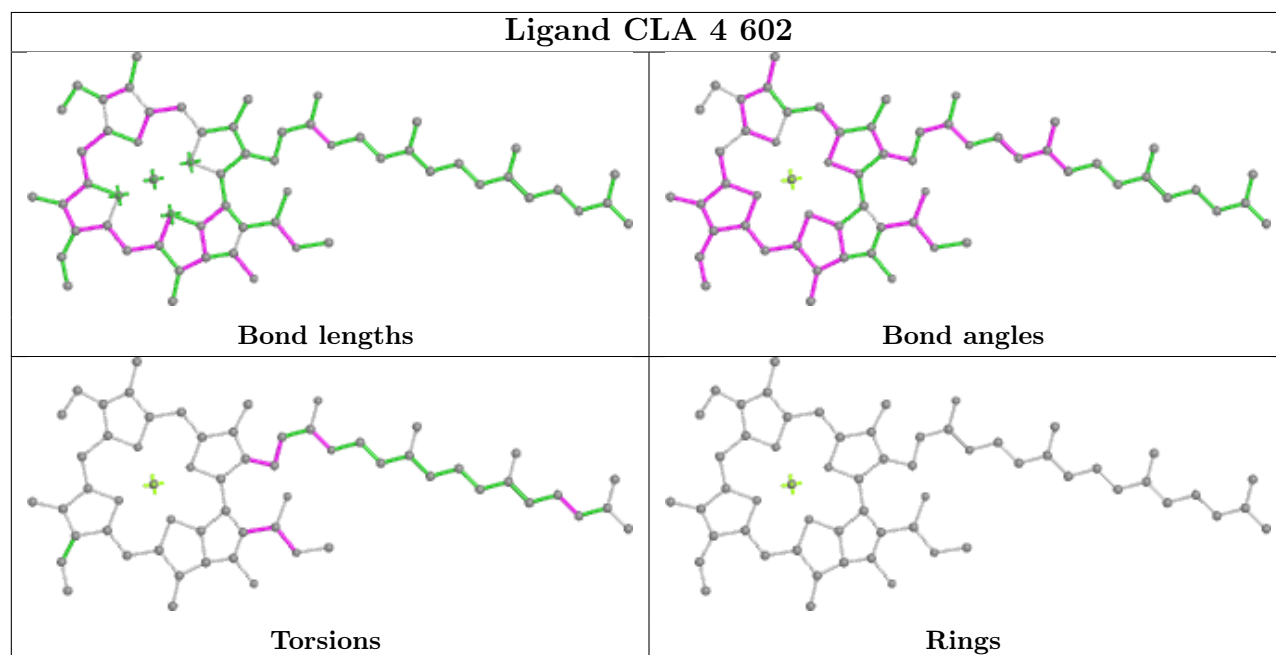
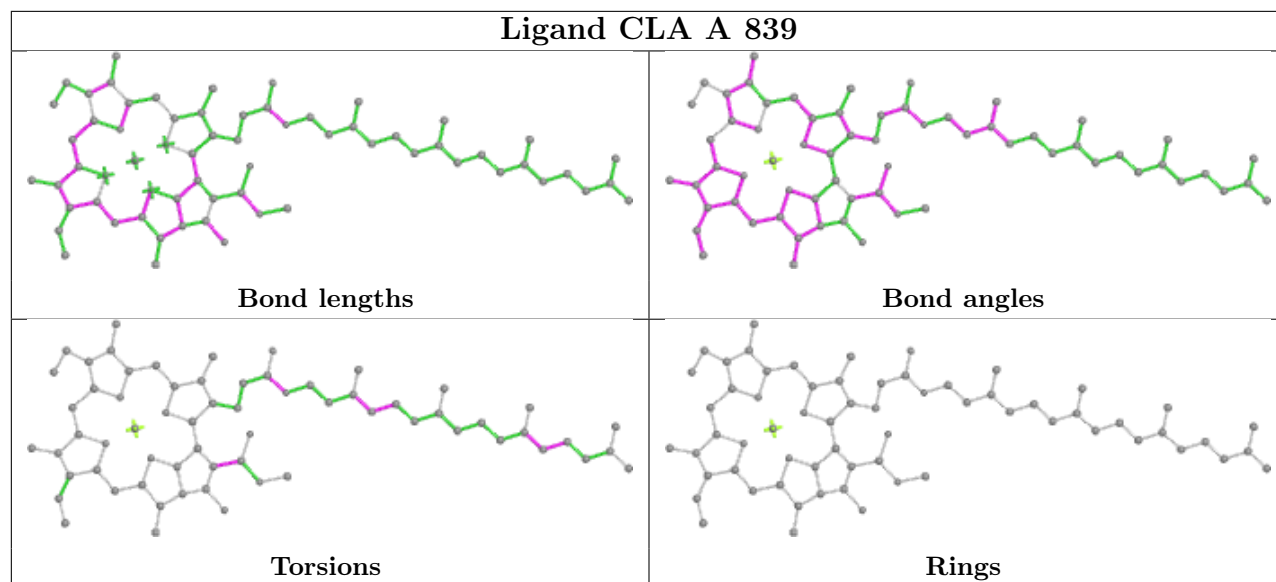


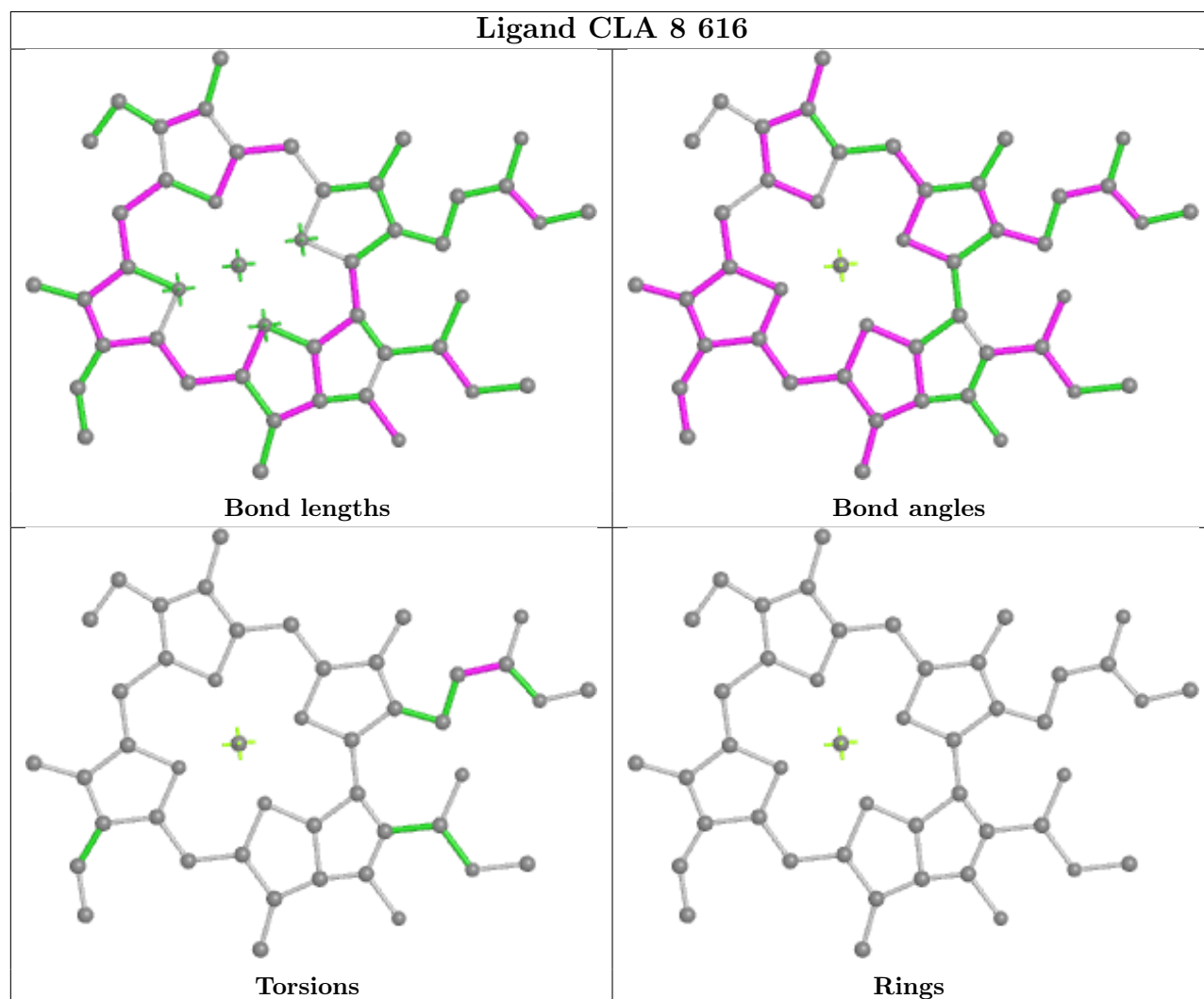
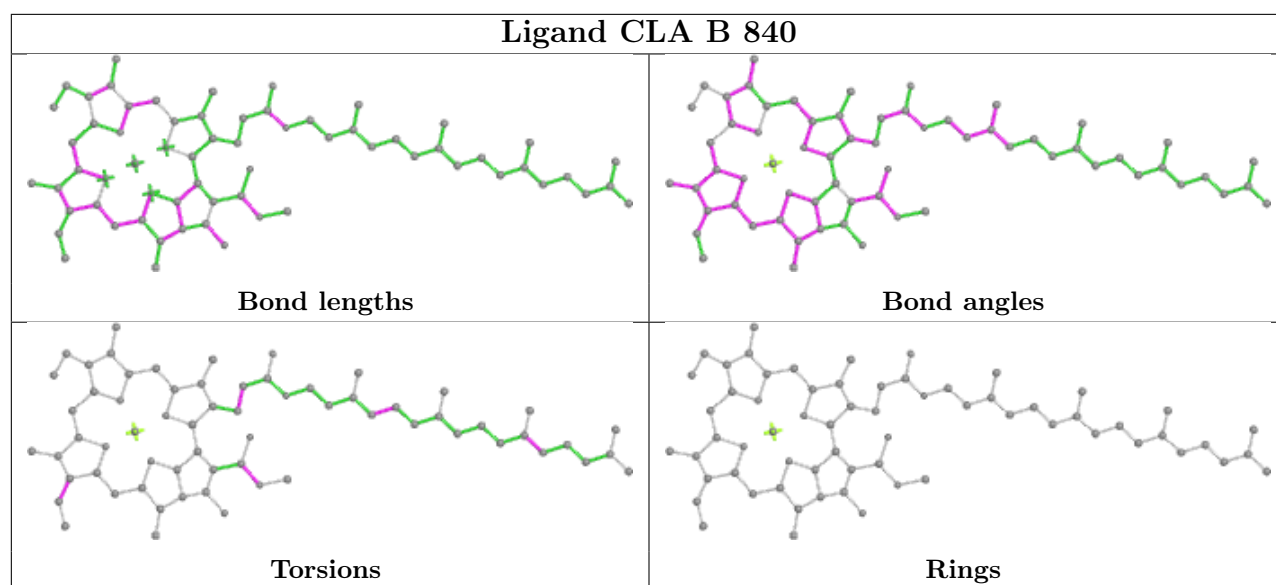




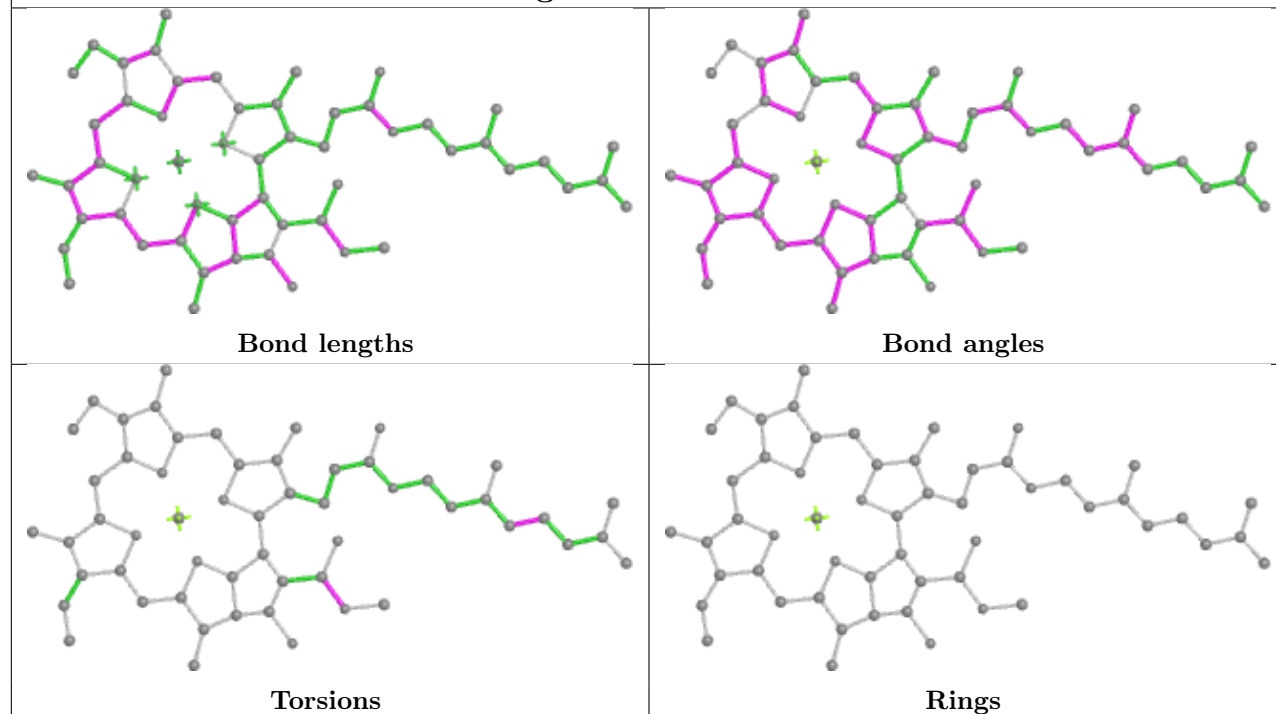




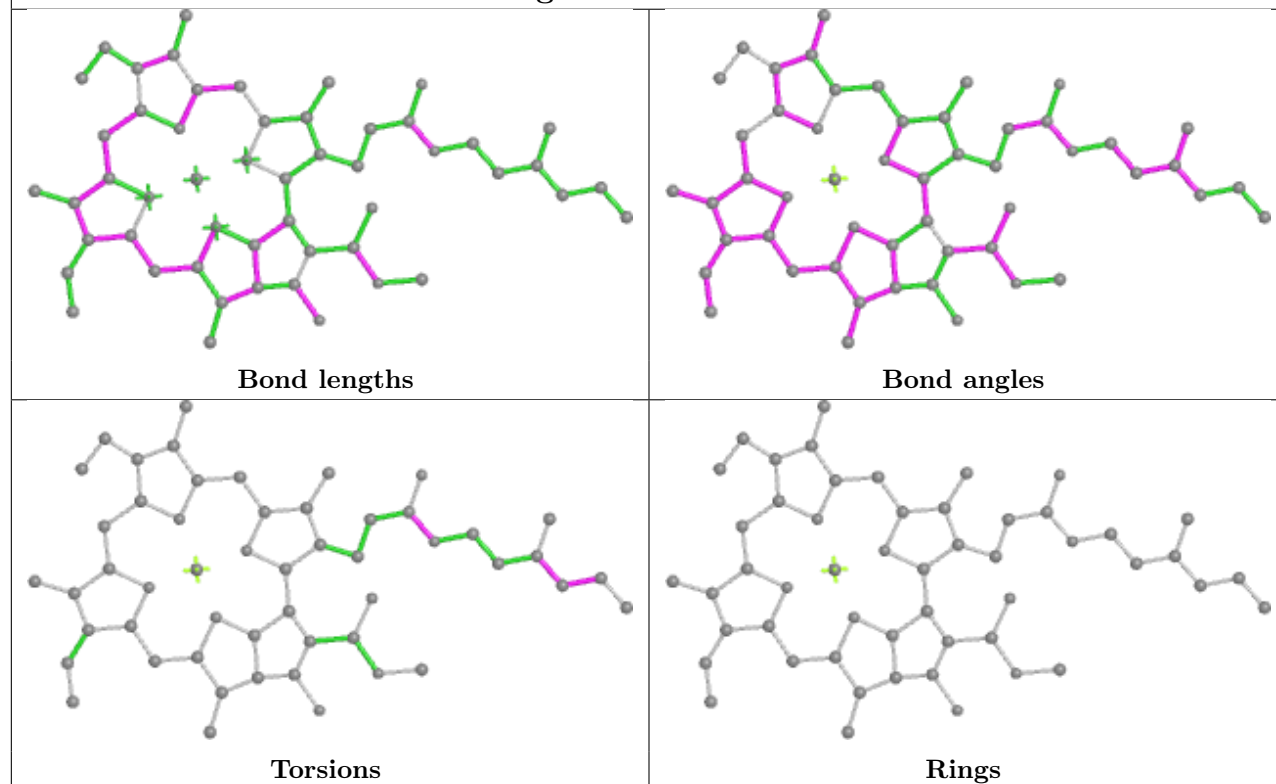


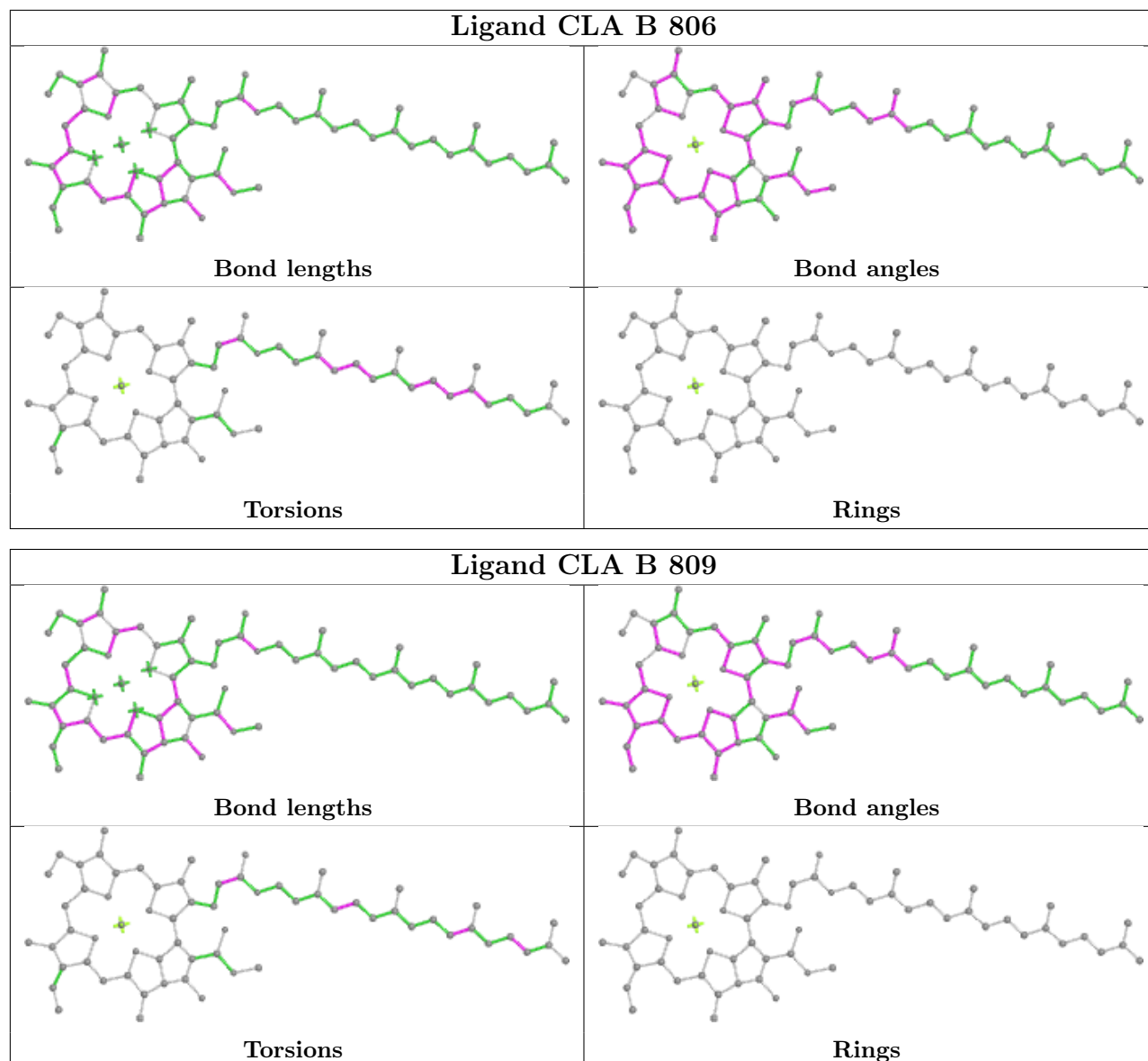


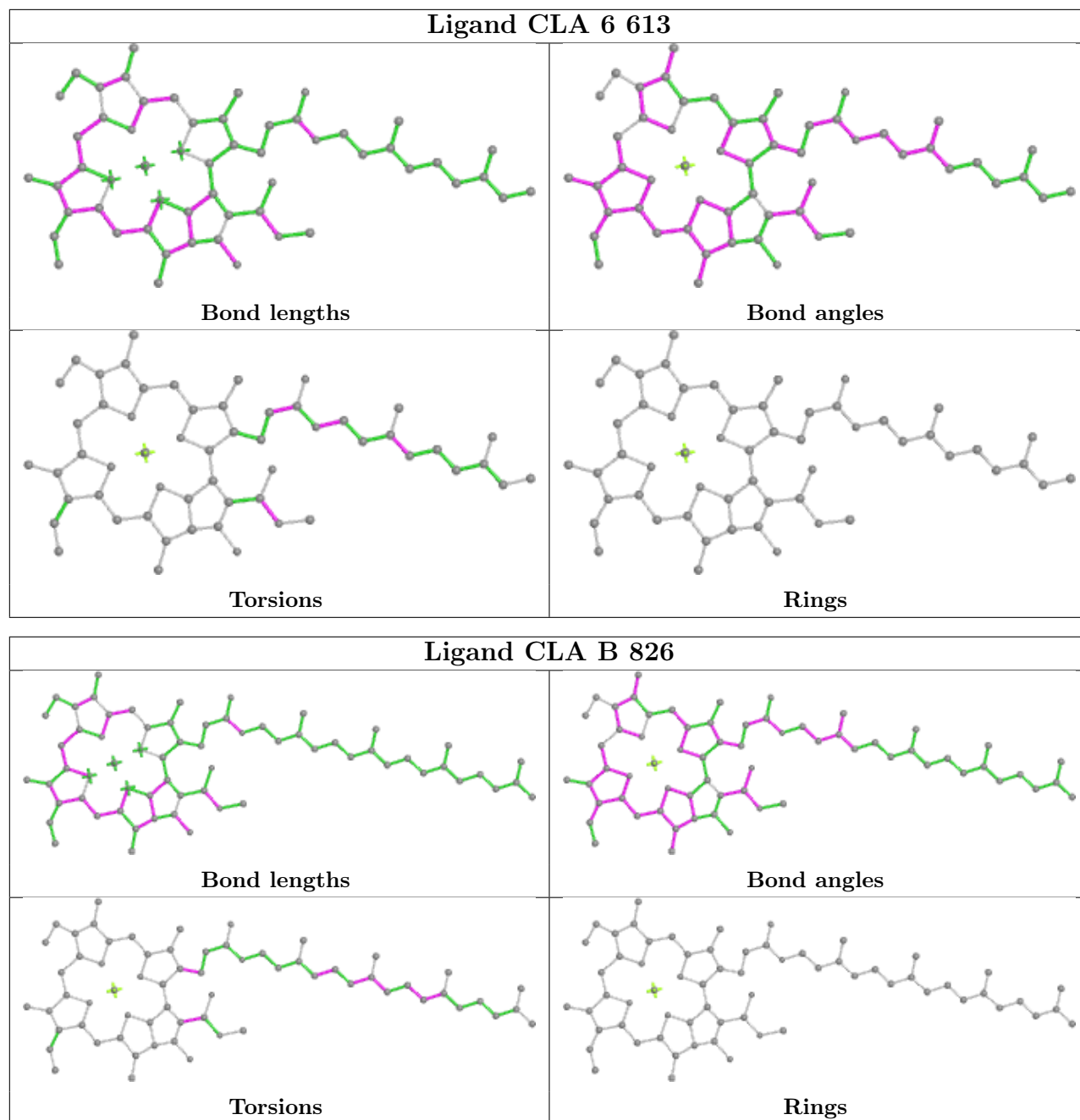
Ligand CLA 5 606

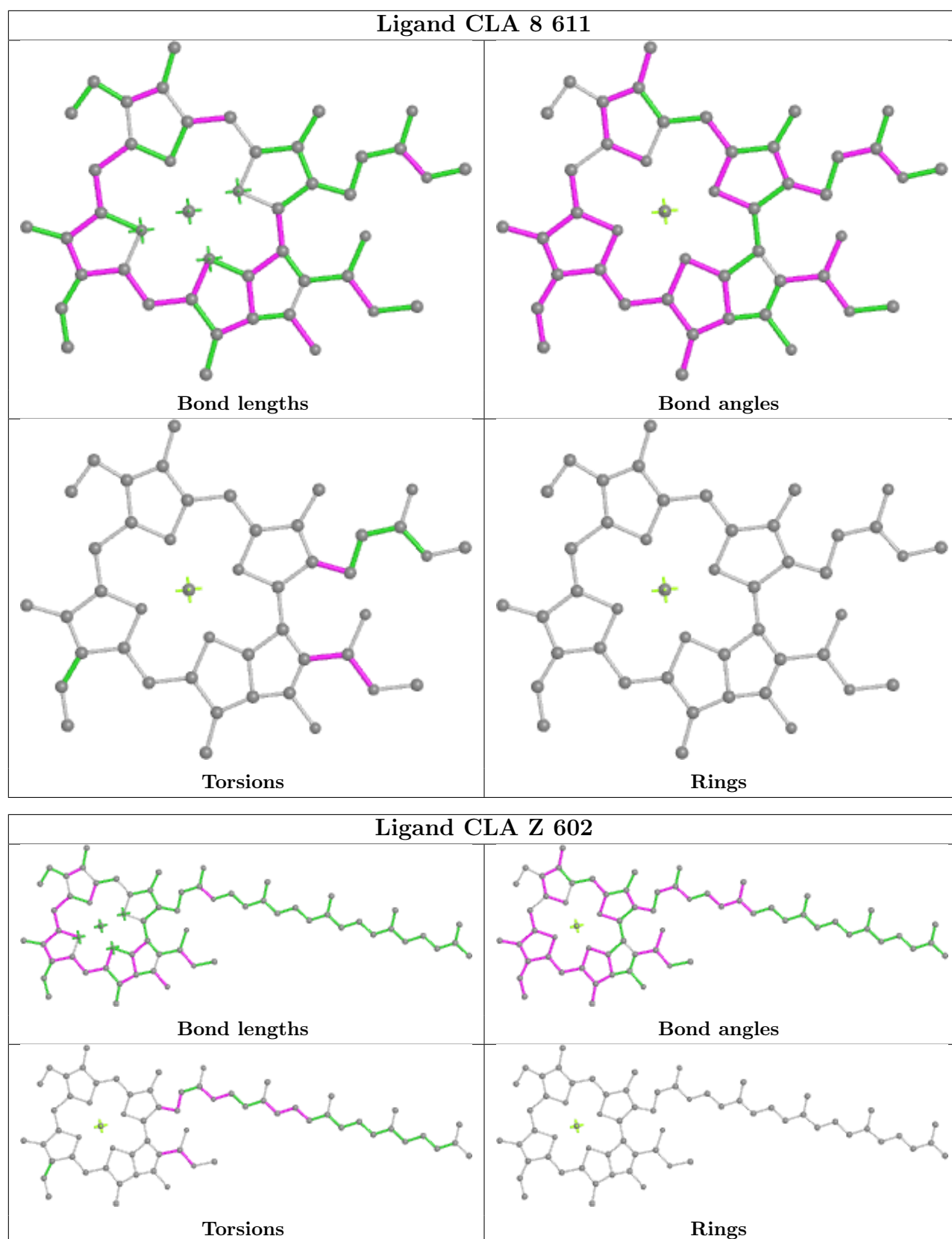


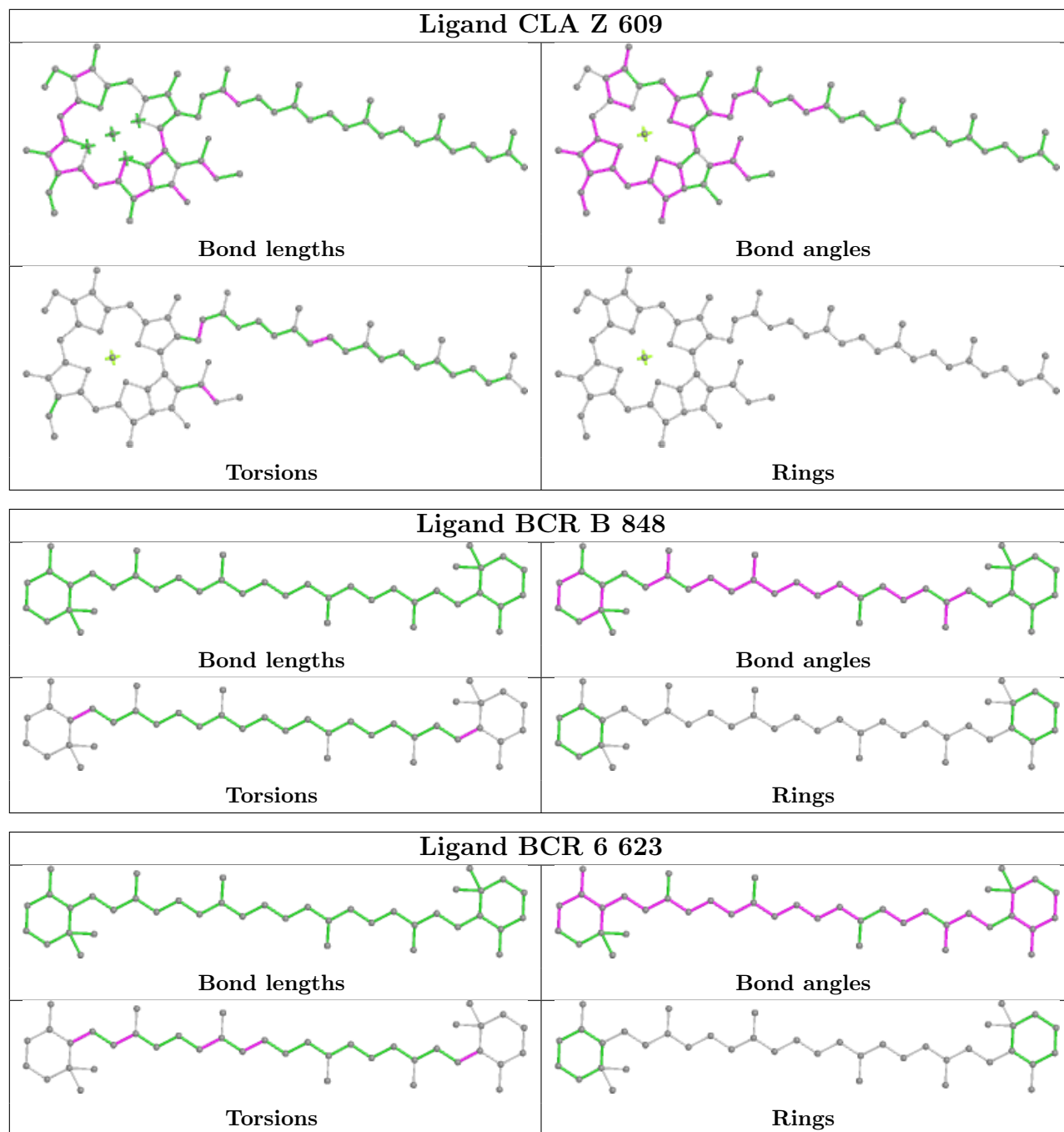
Ligand CLA 6 612

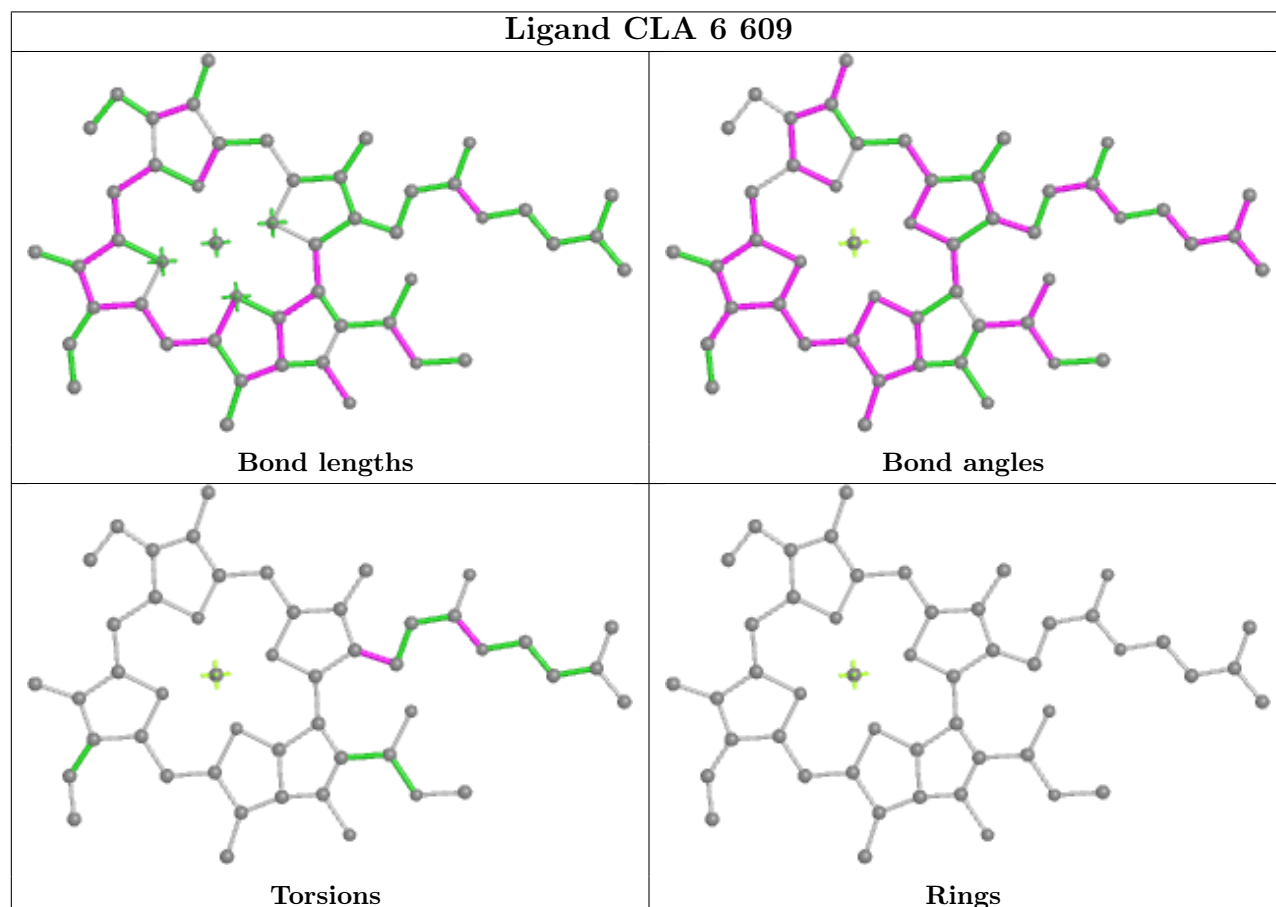
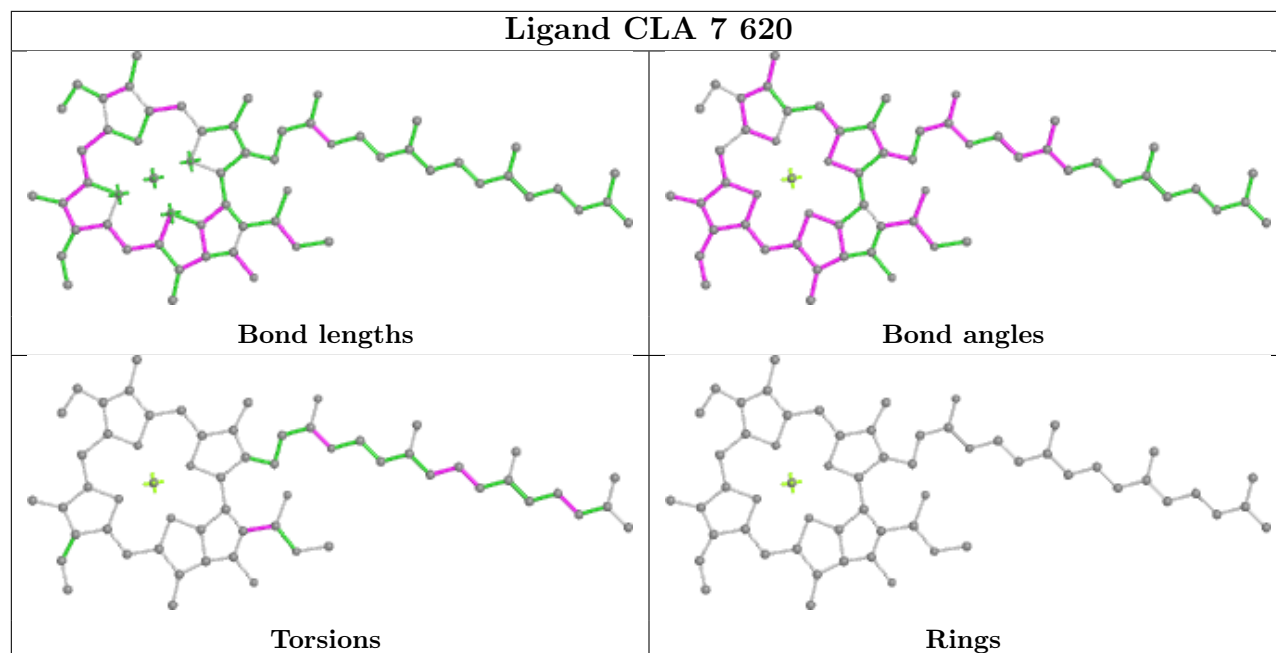


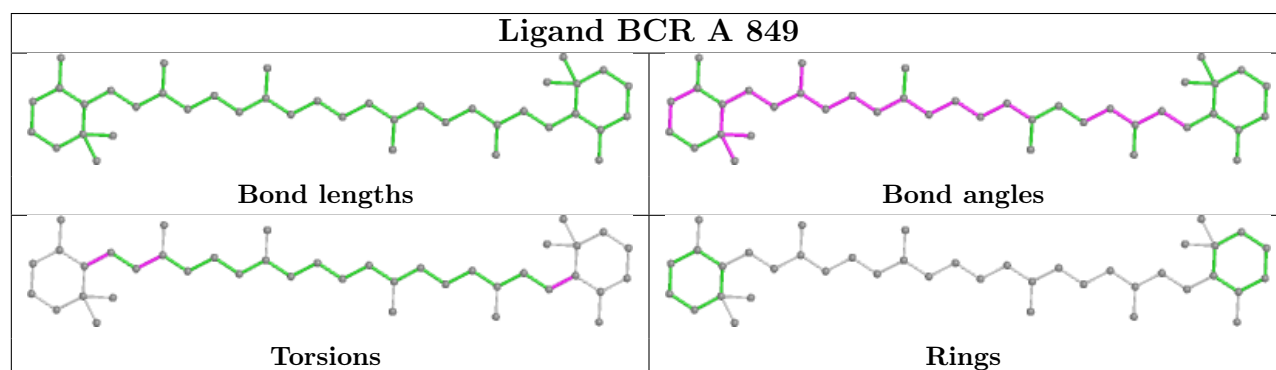
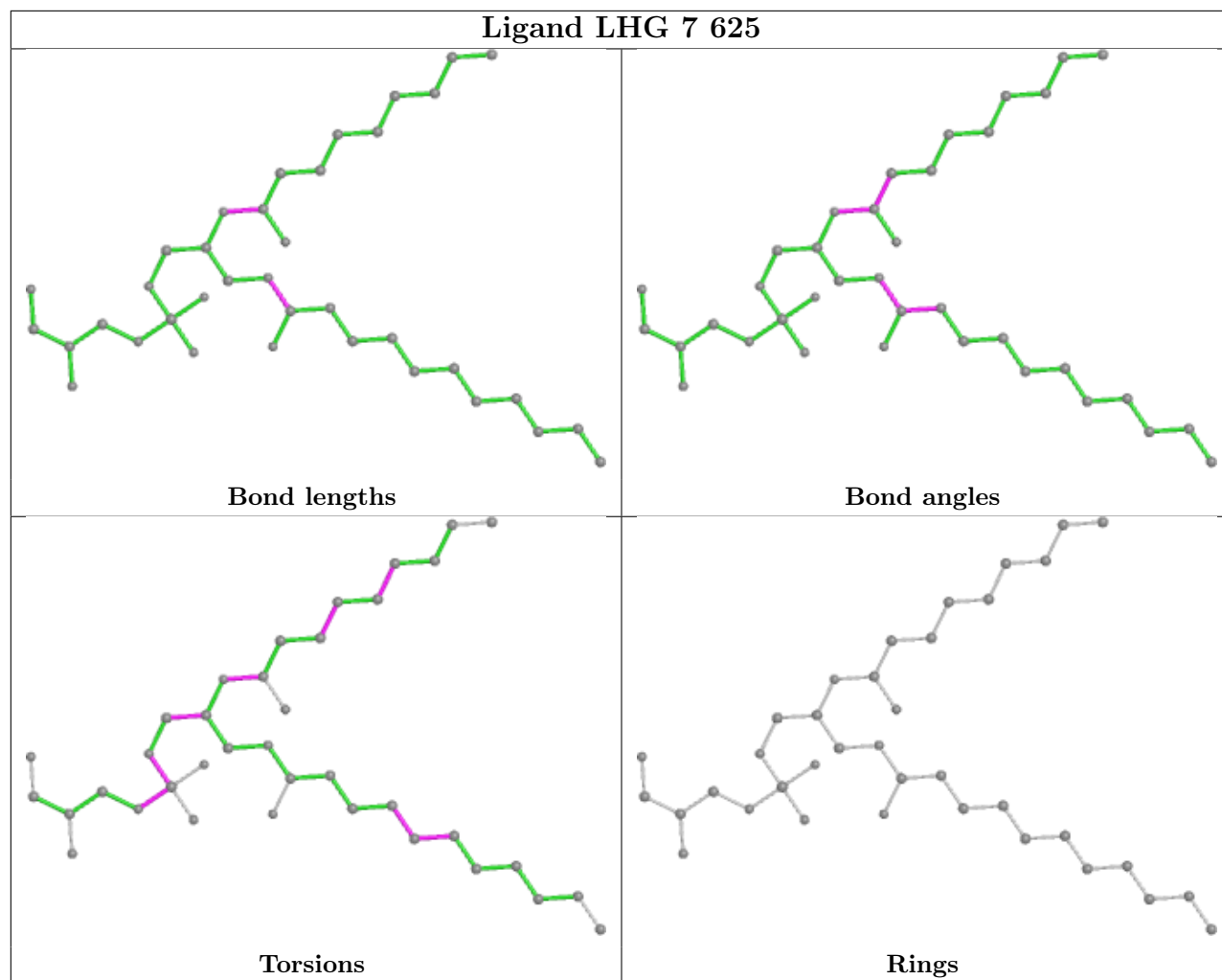


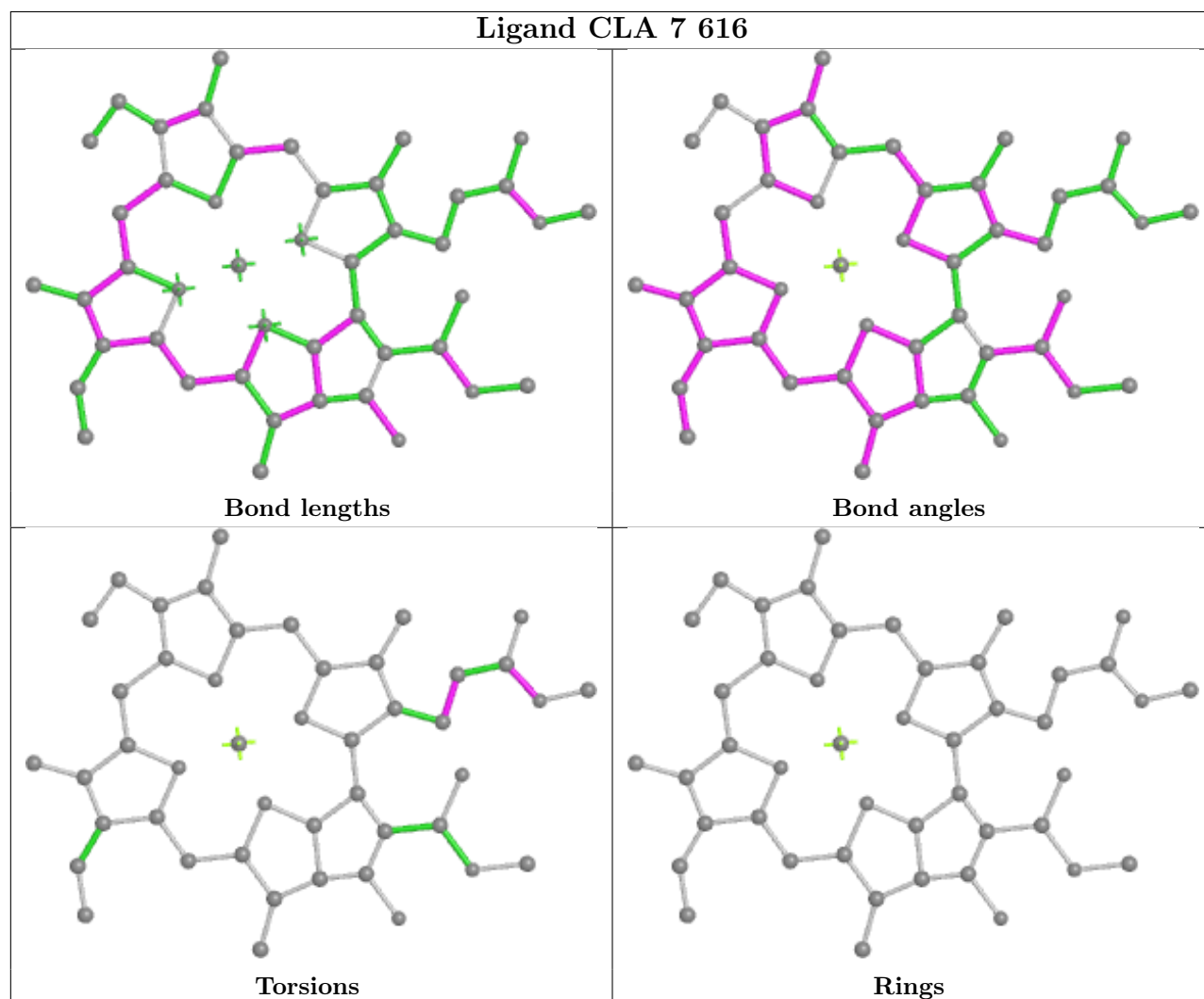
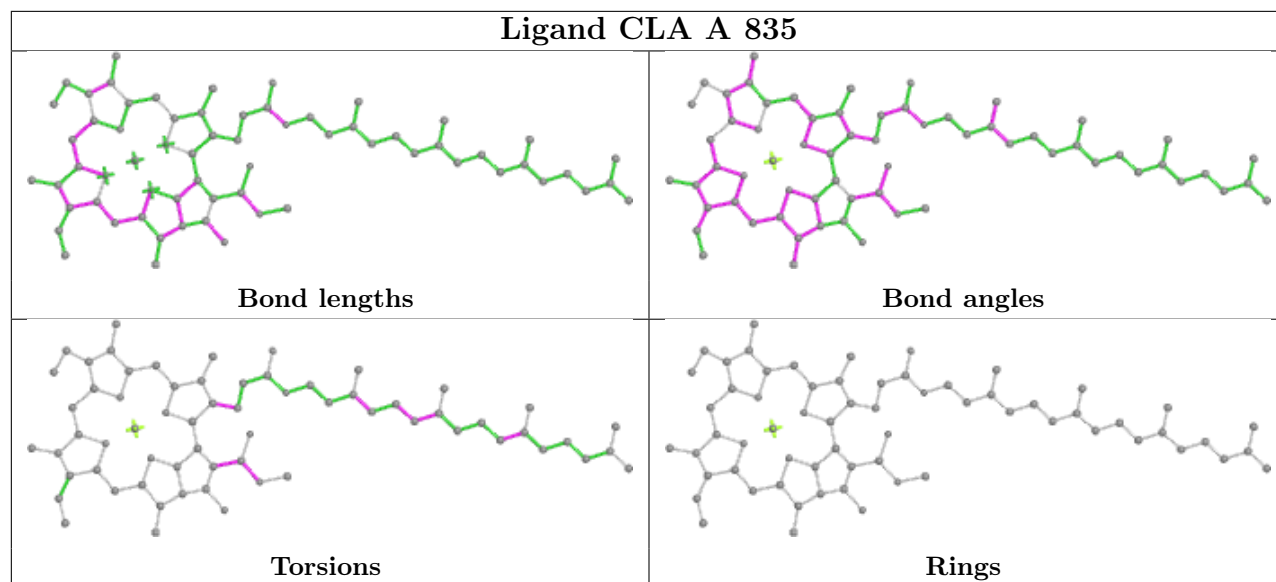


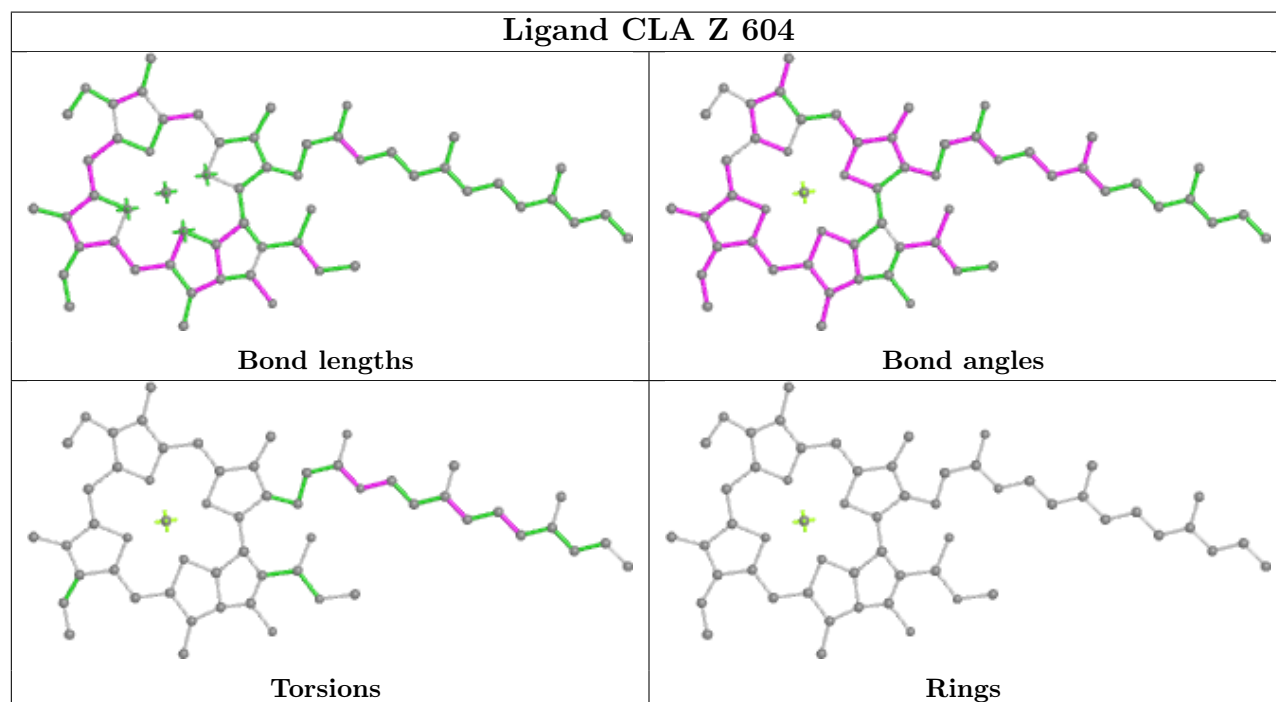
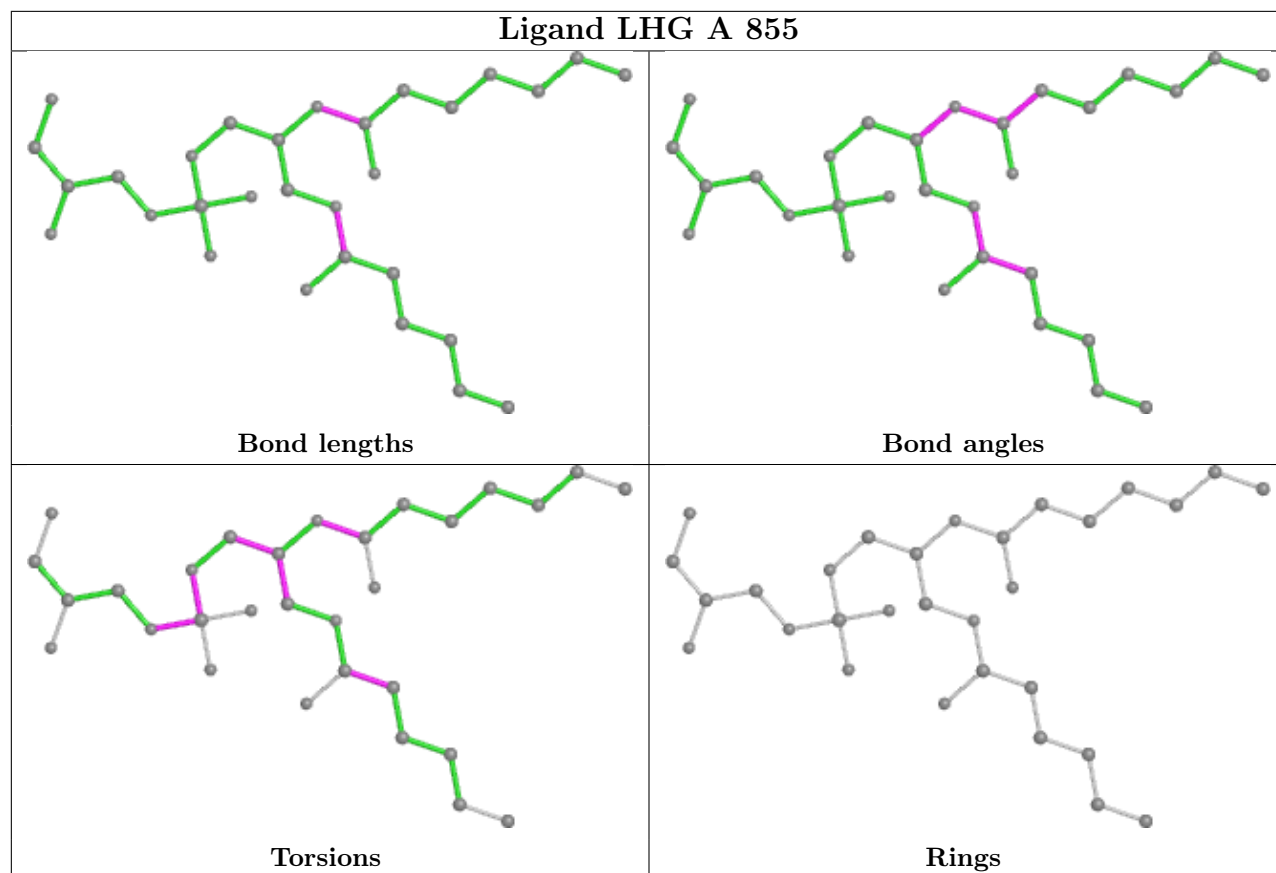


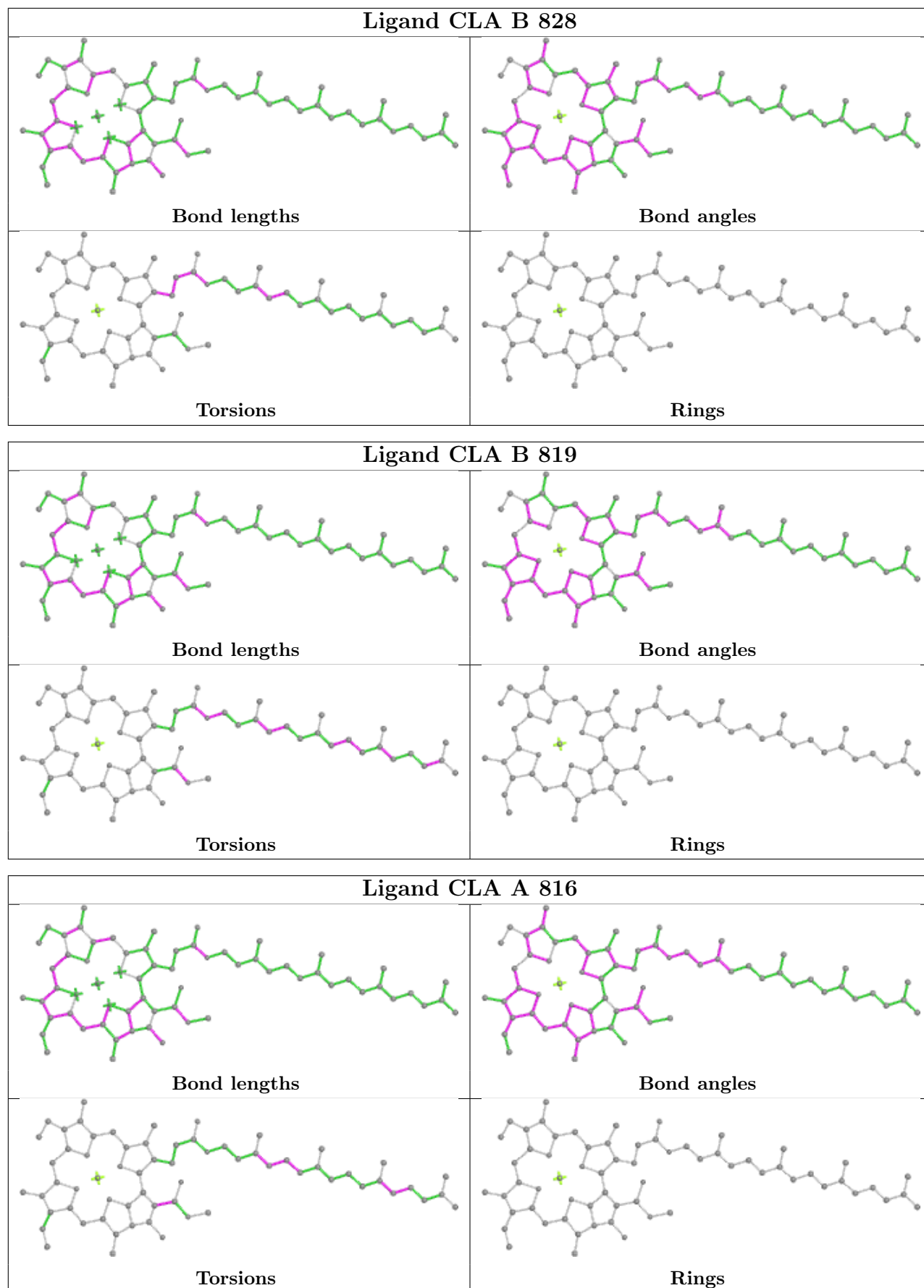


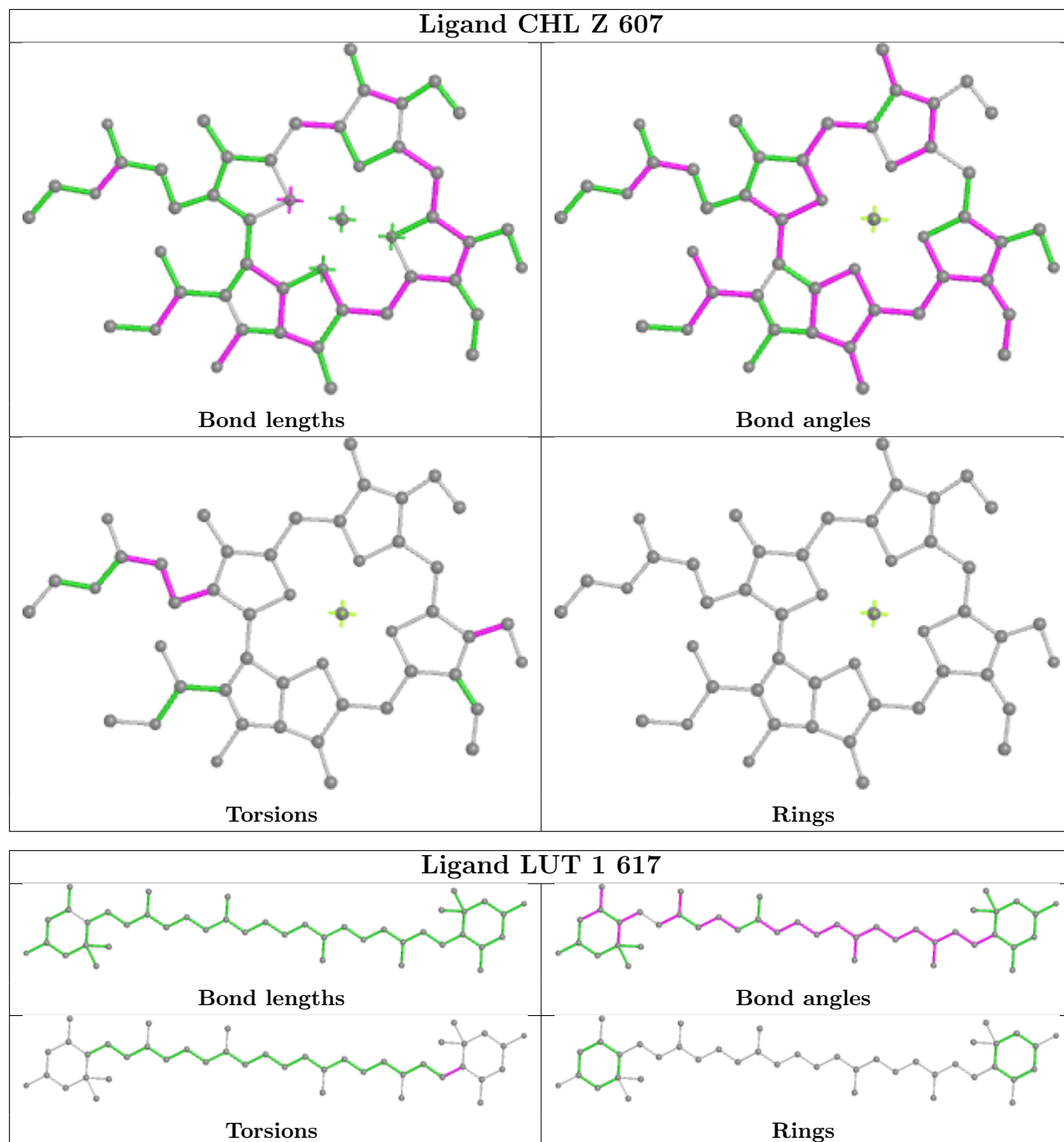


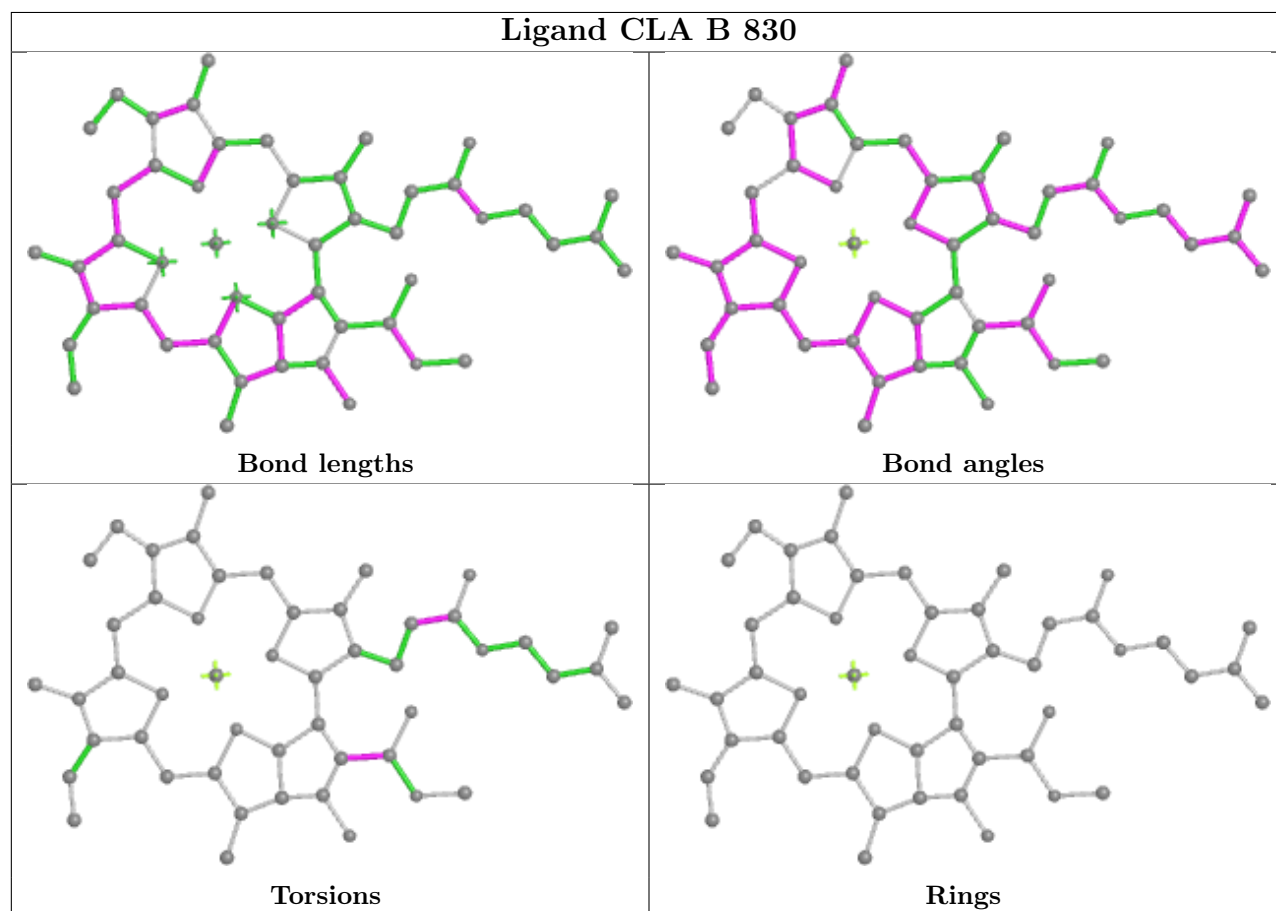
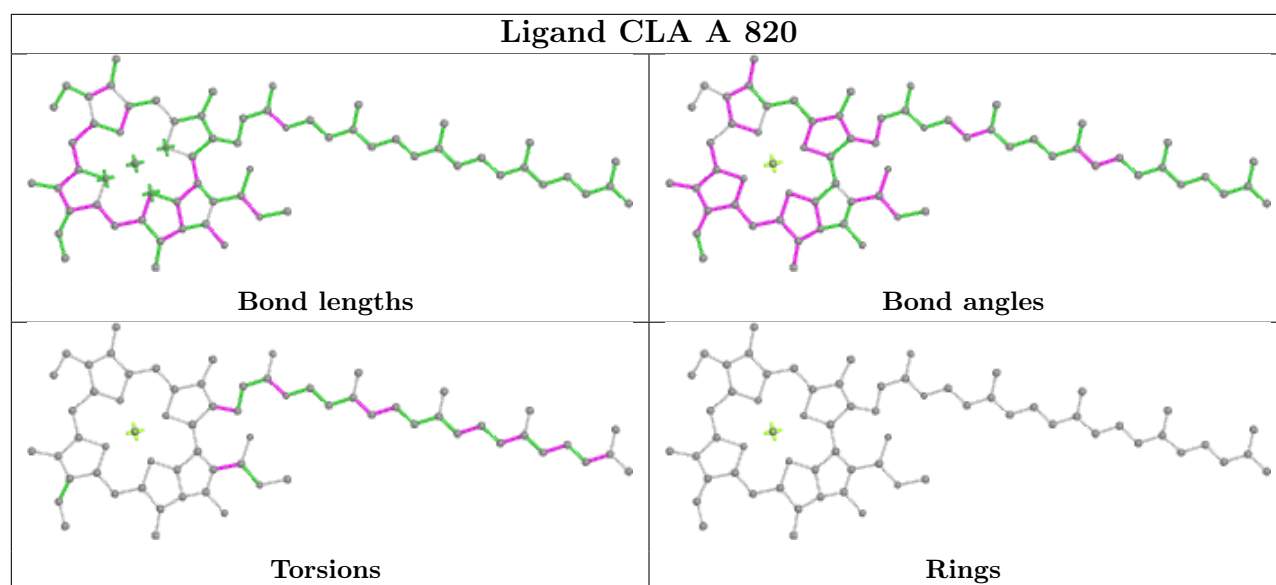


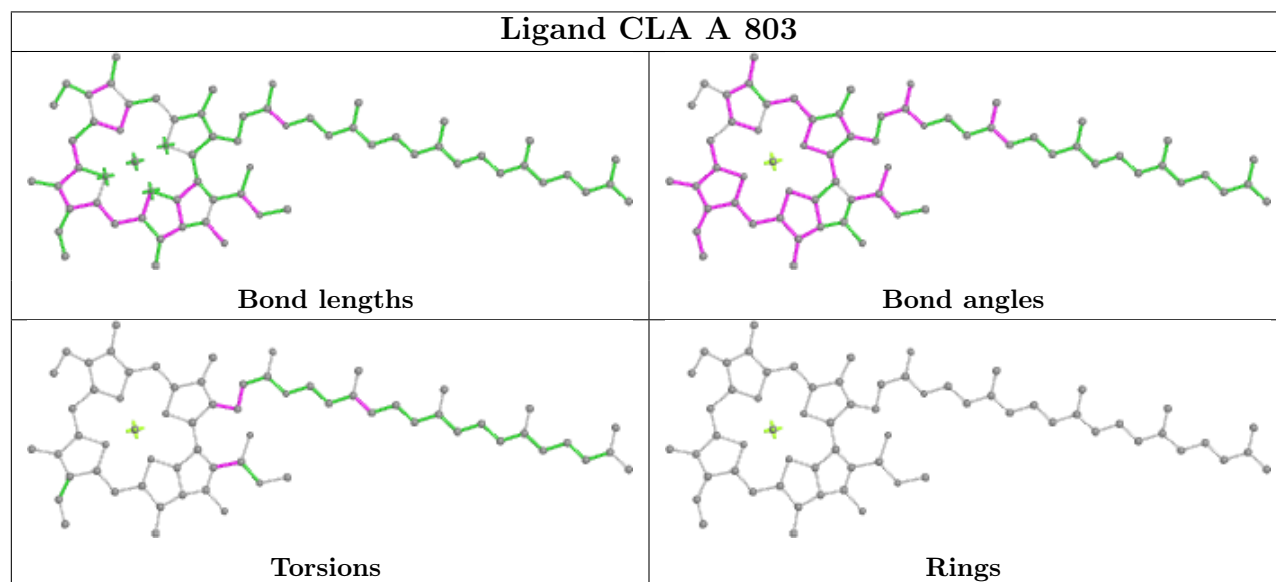
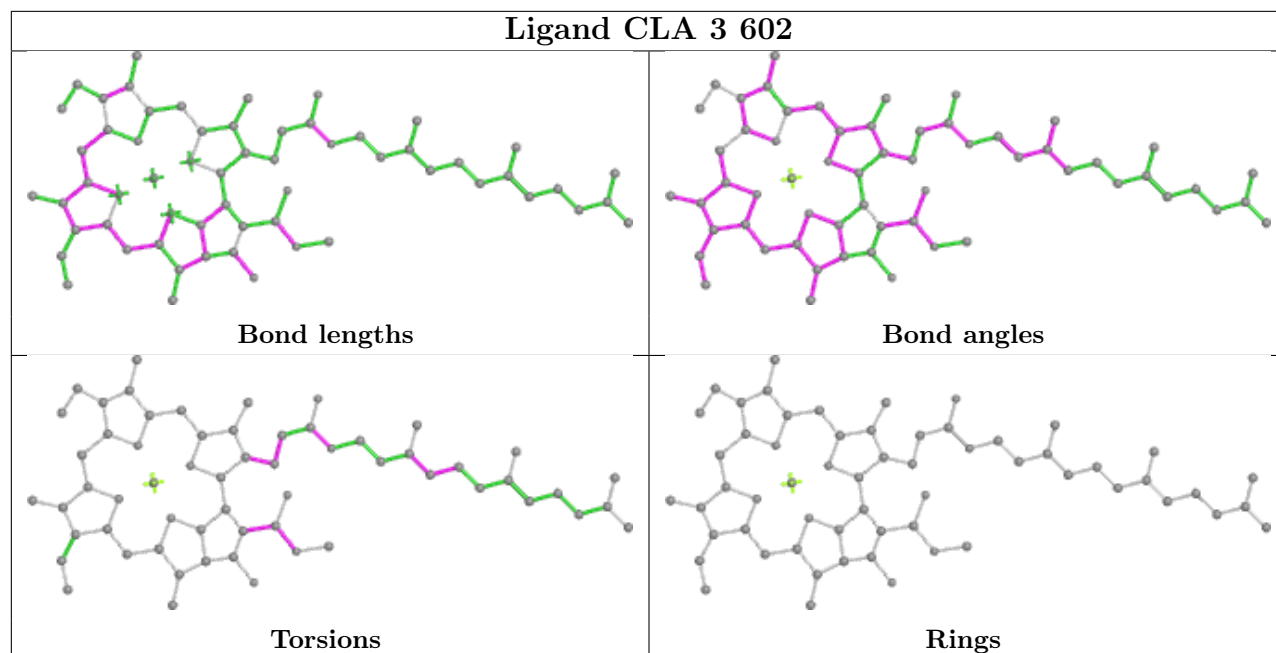


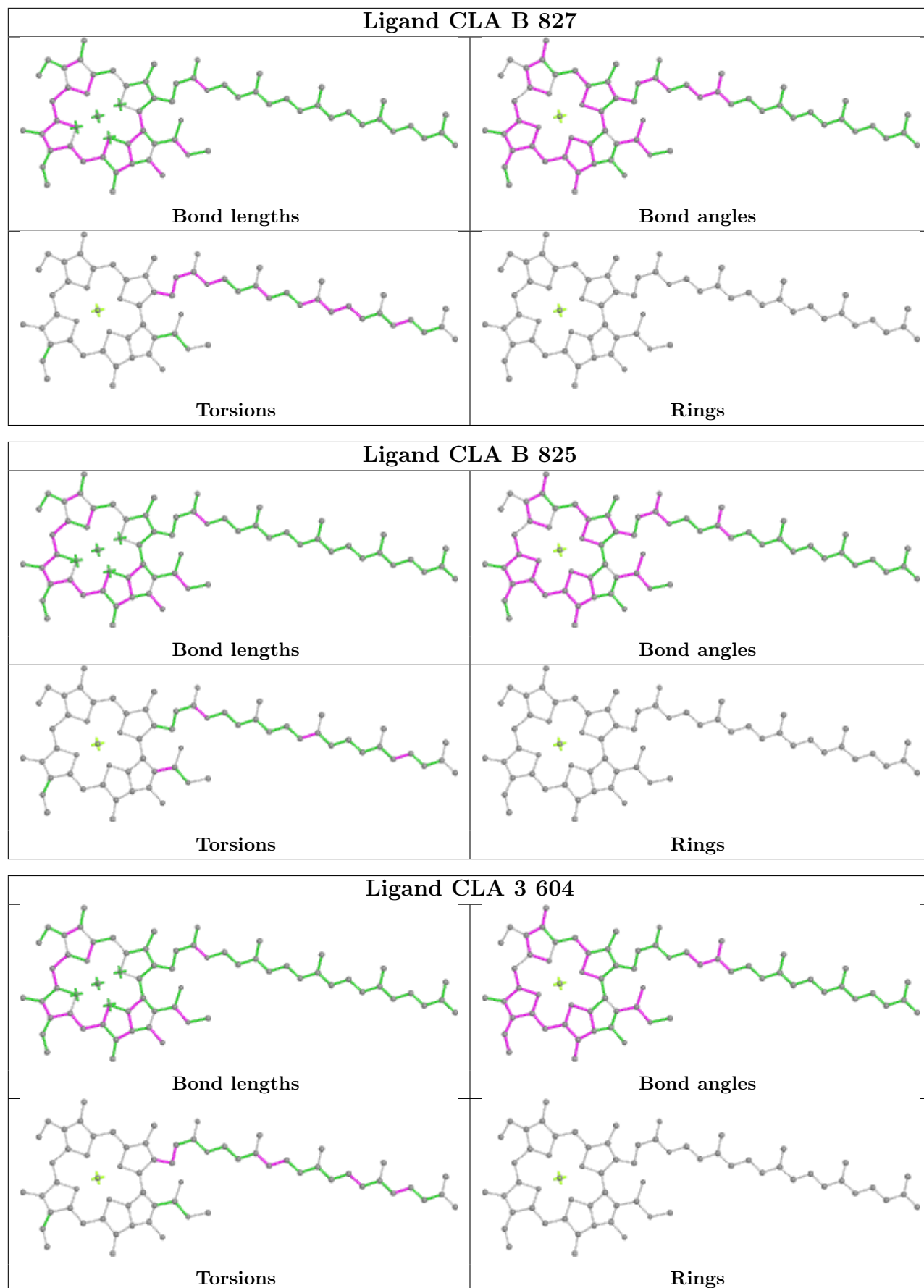


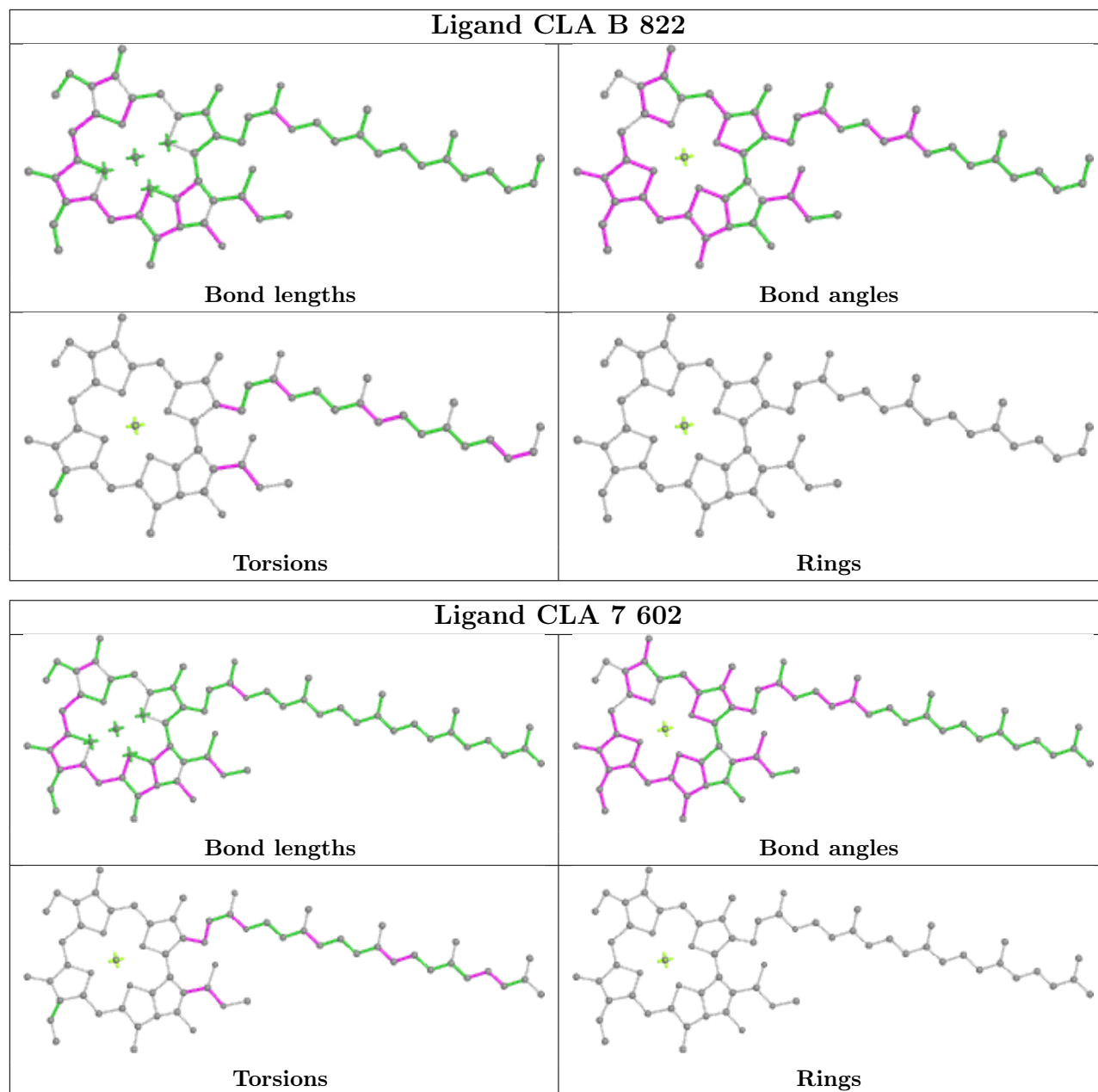


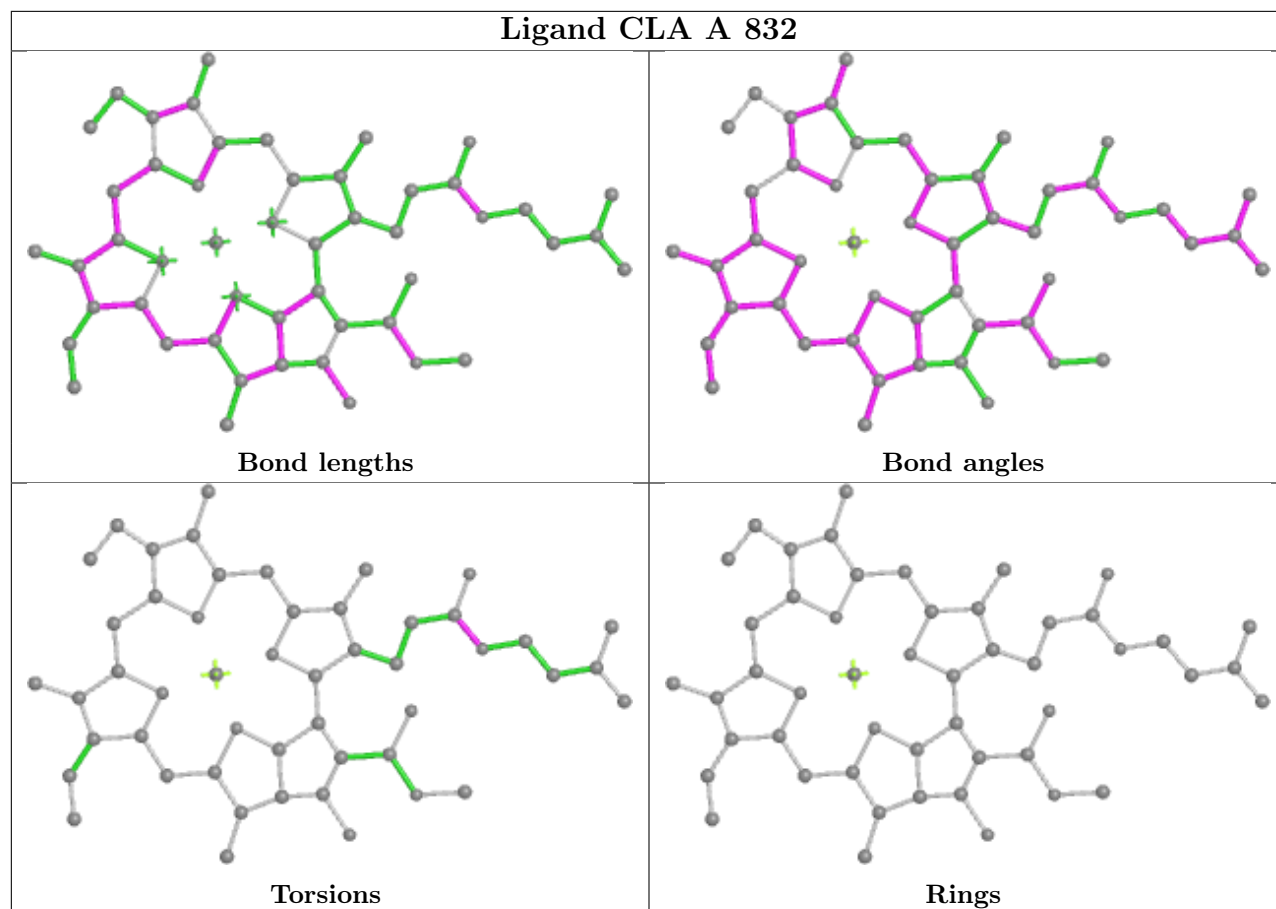


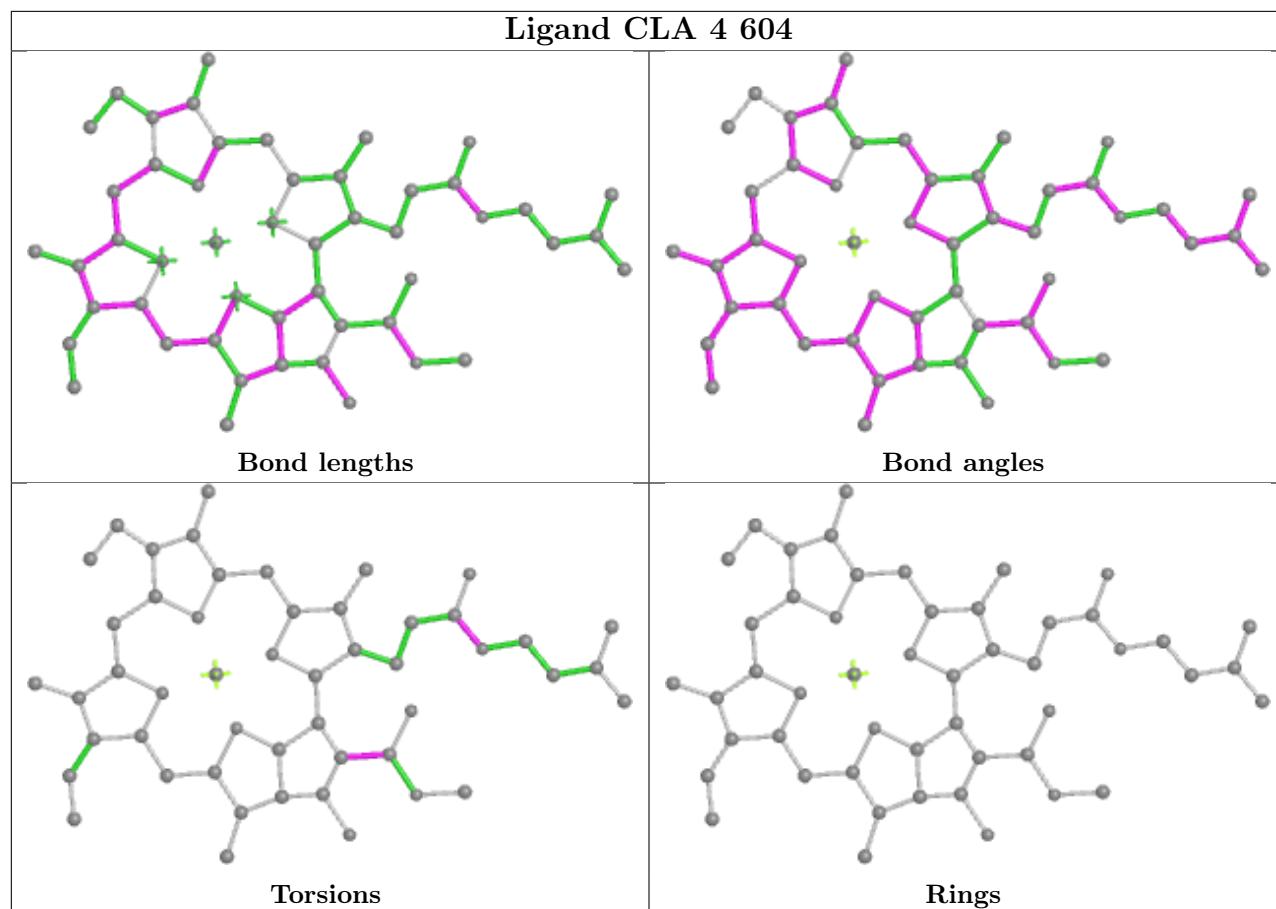


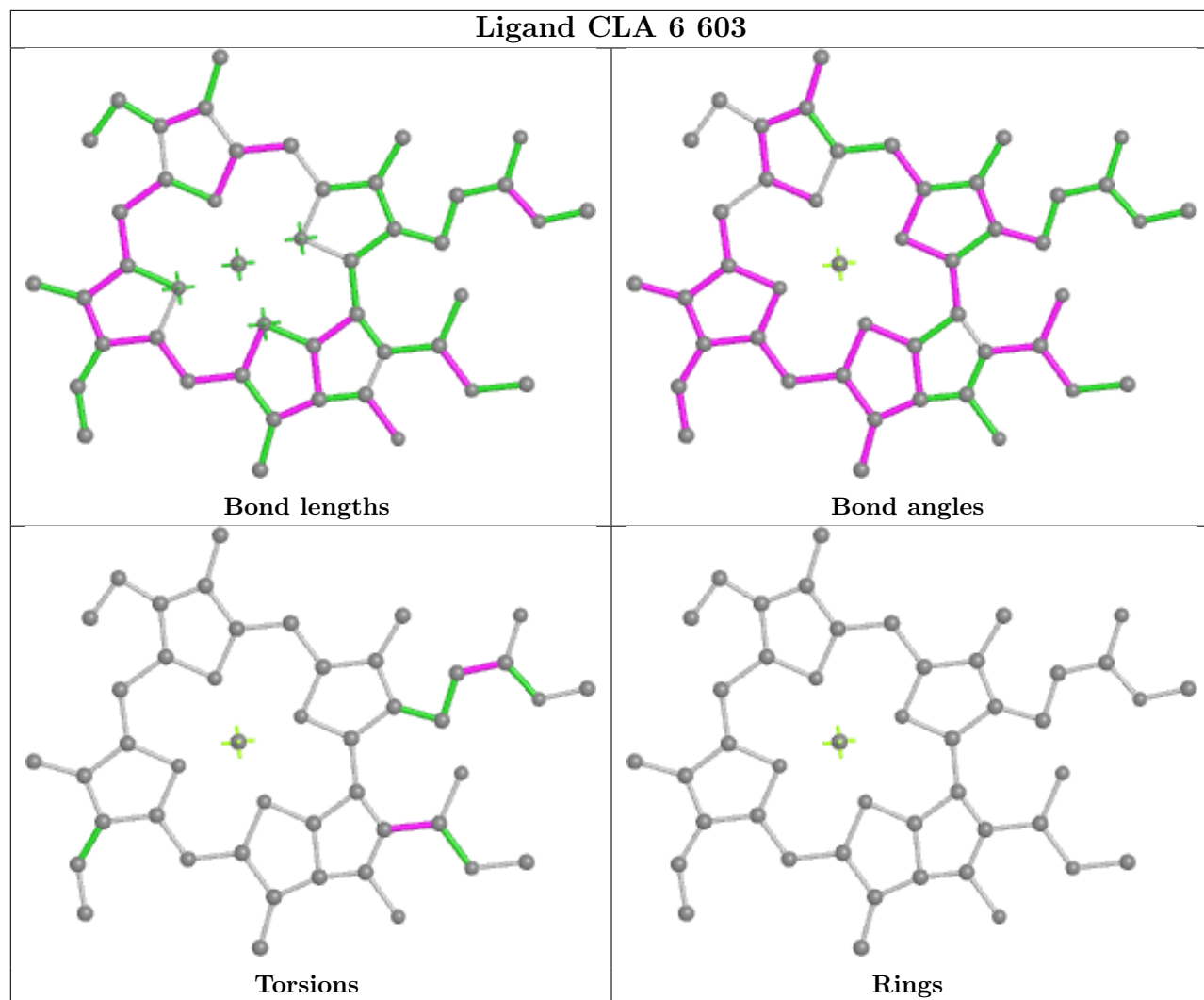


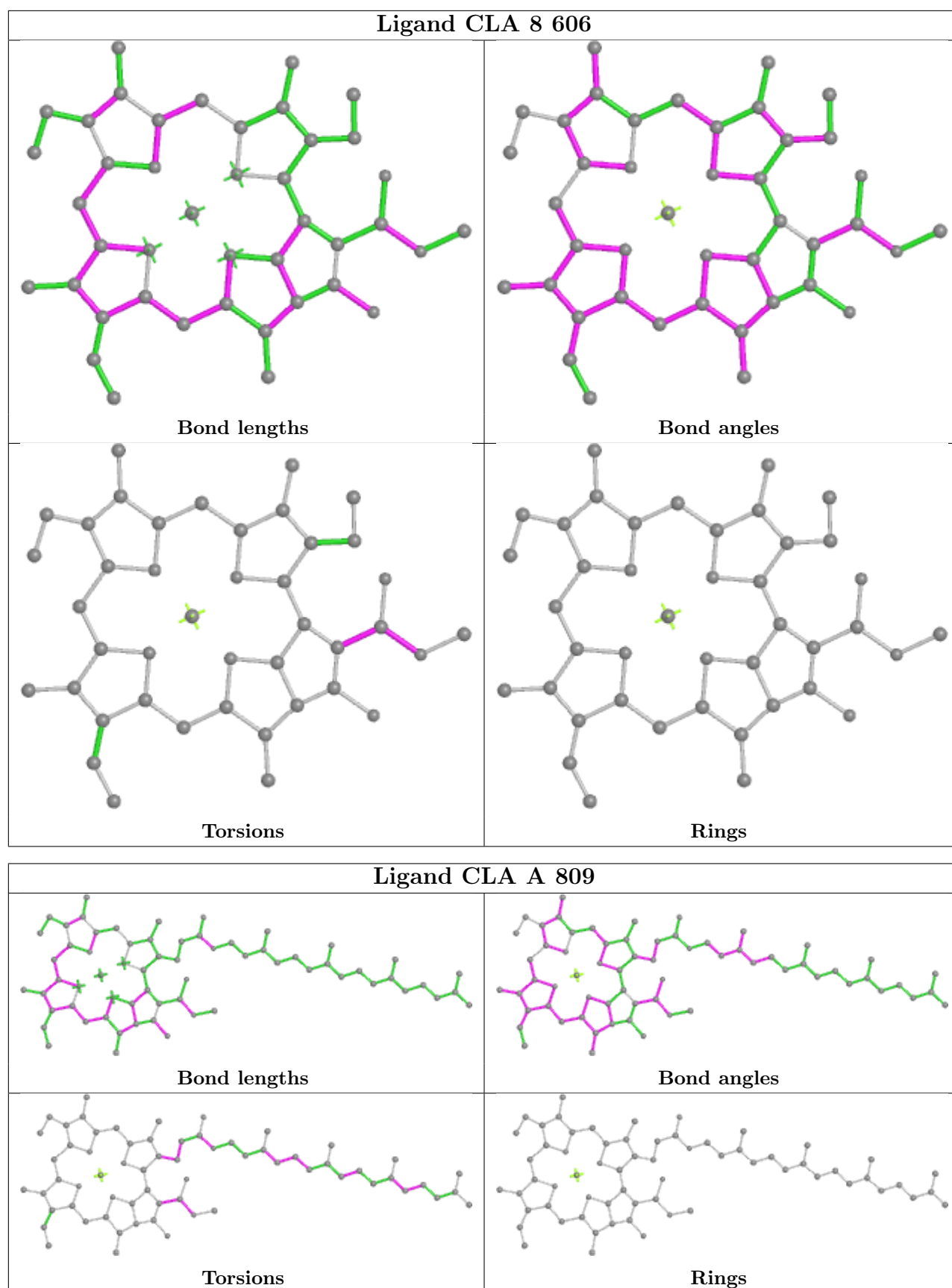


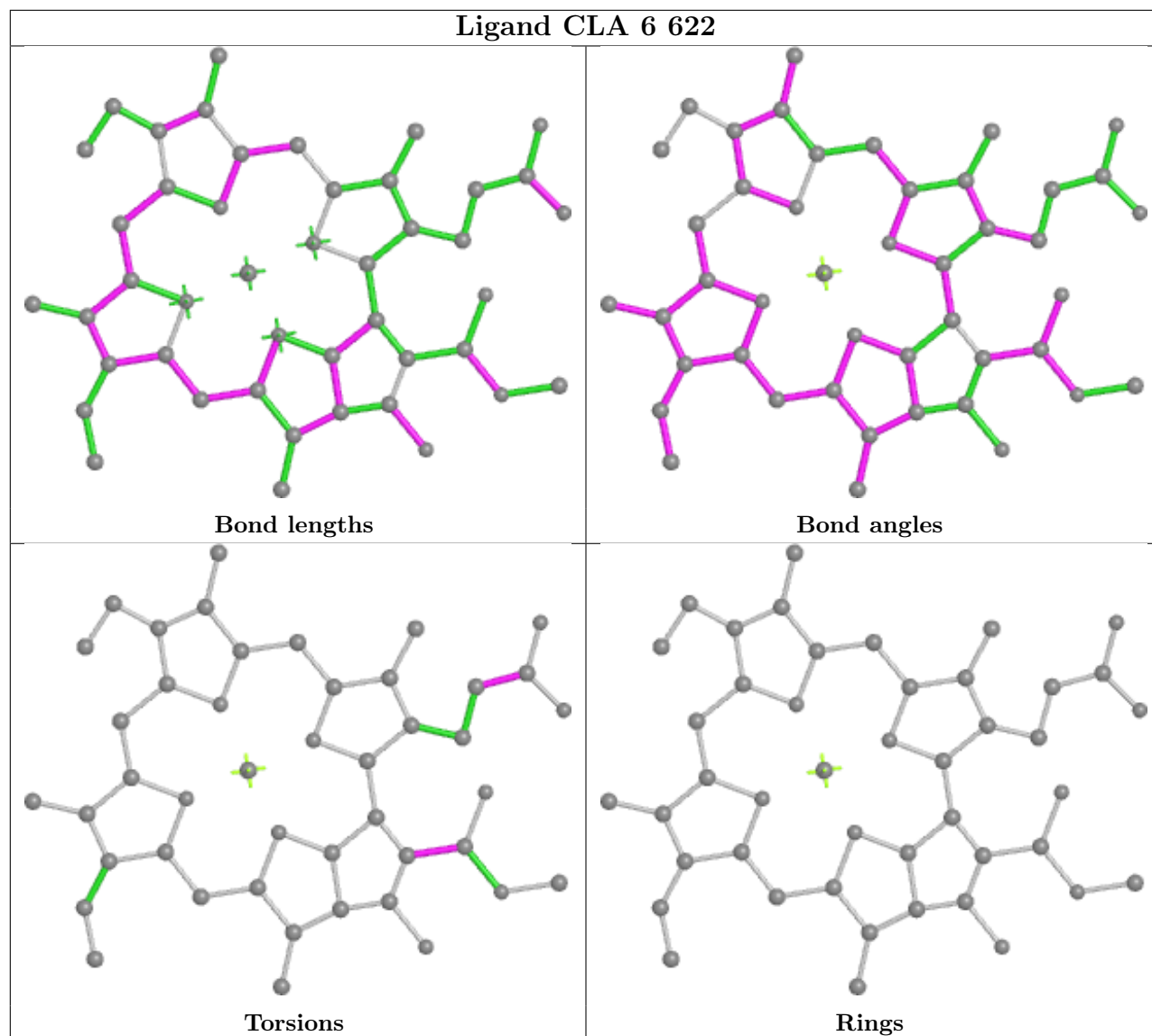


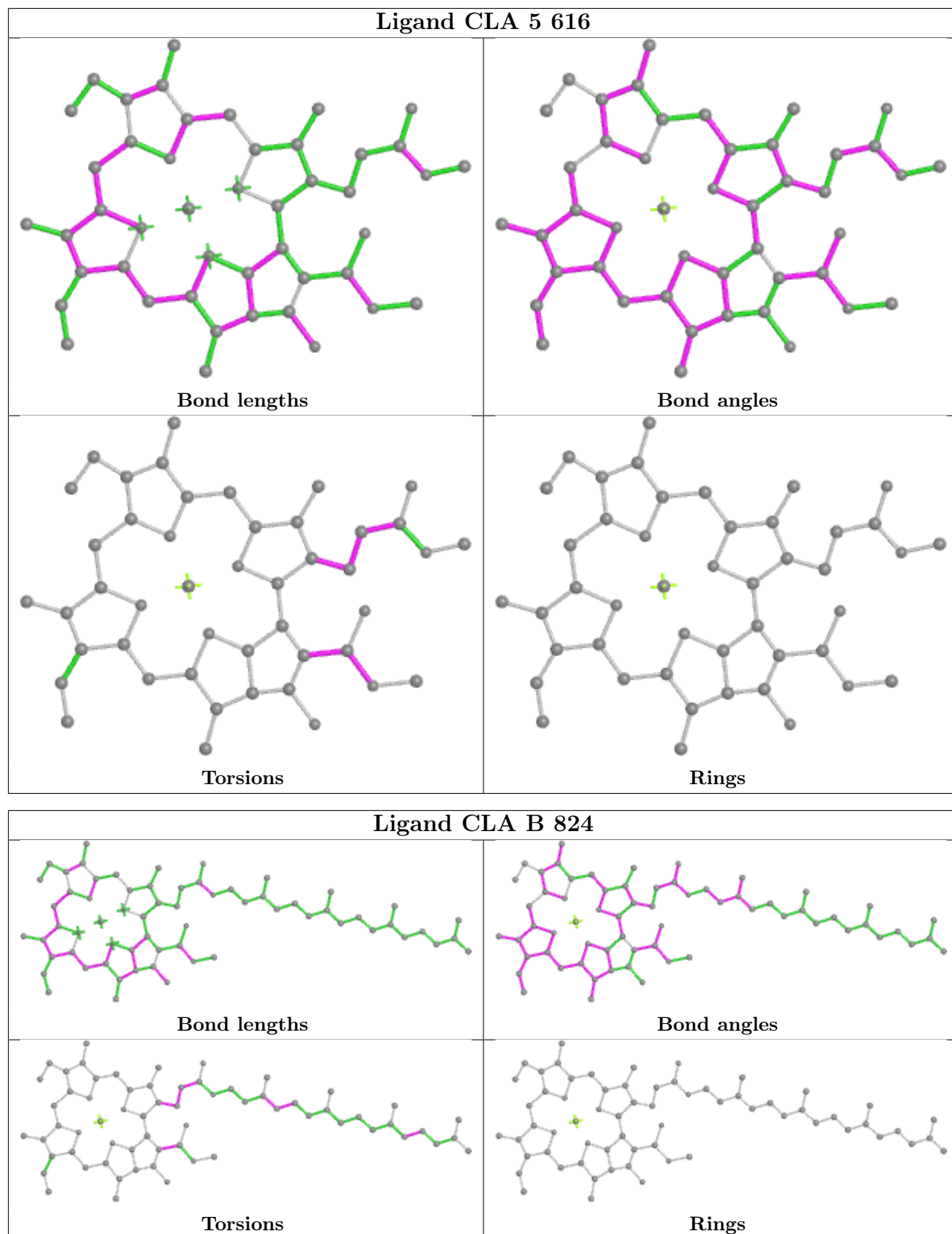


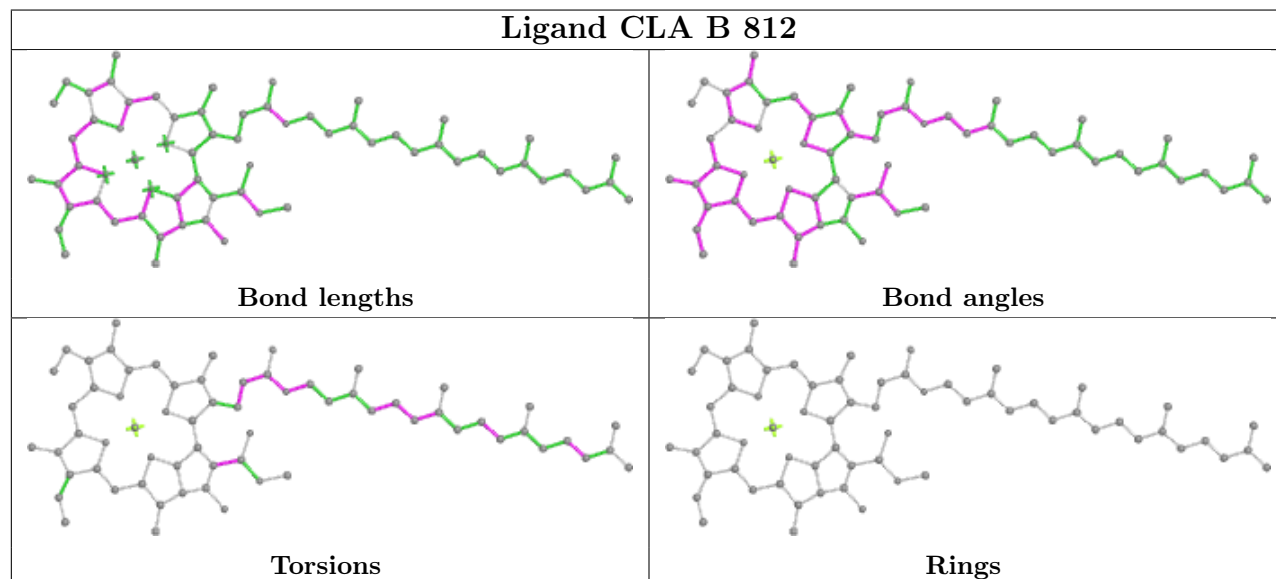
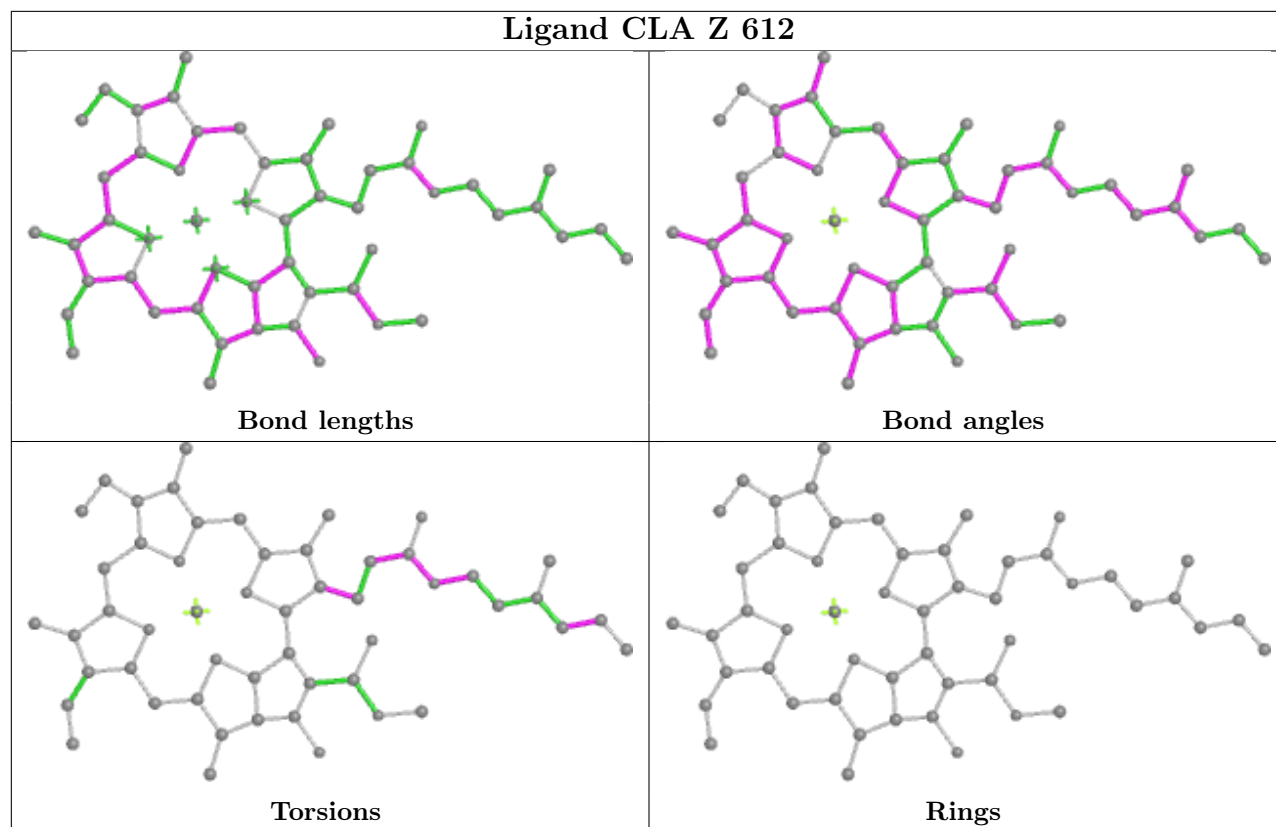


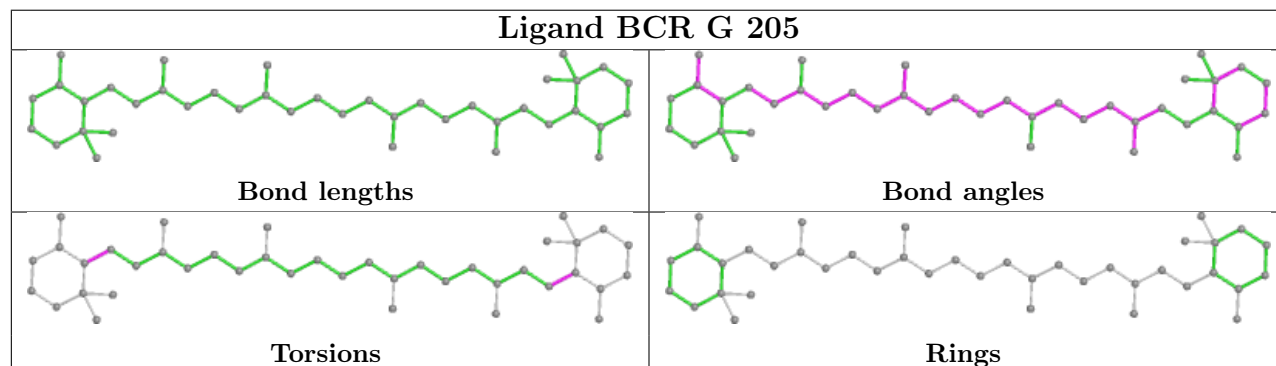
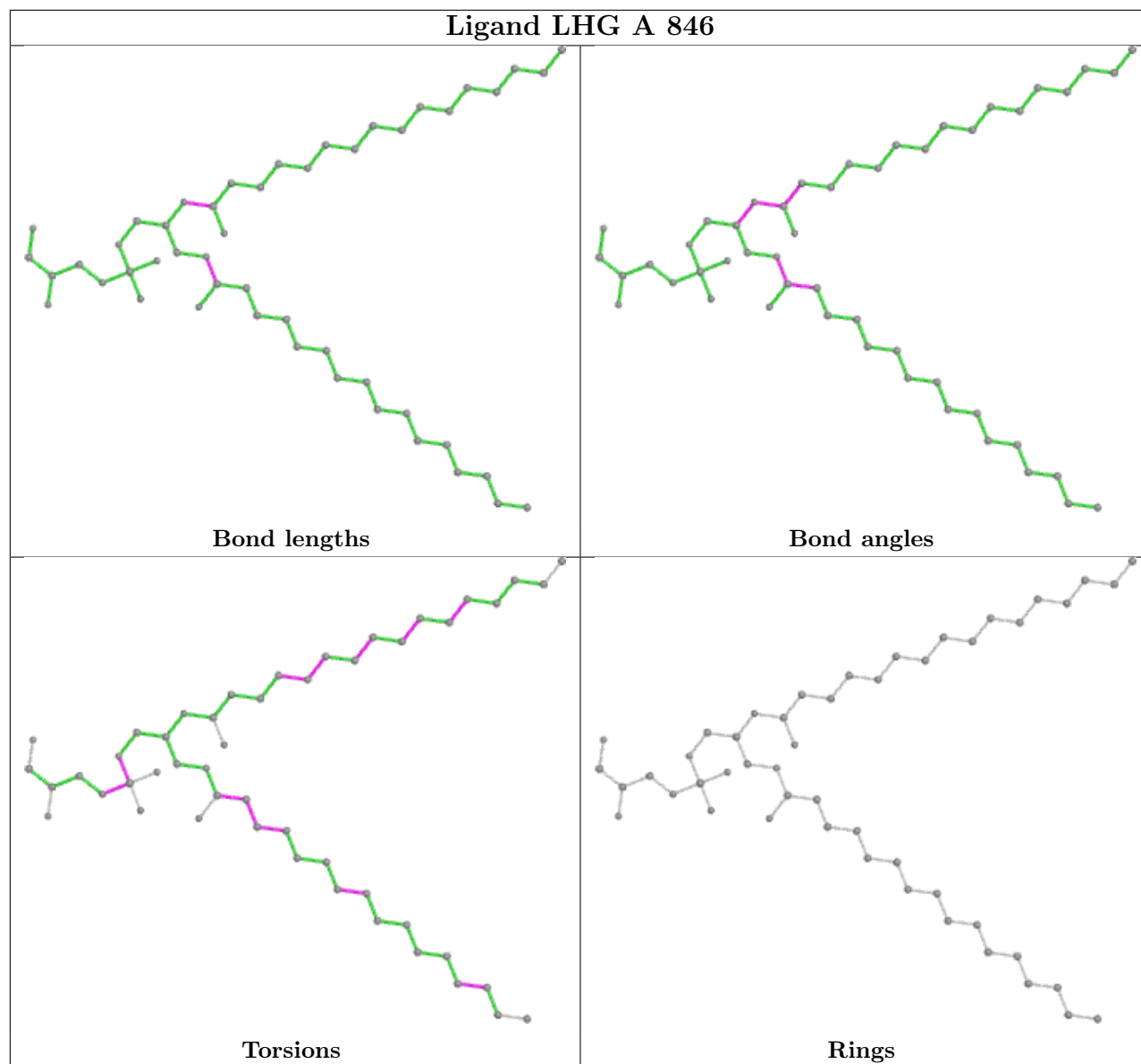


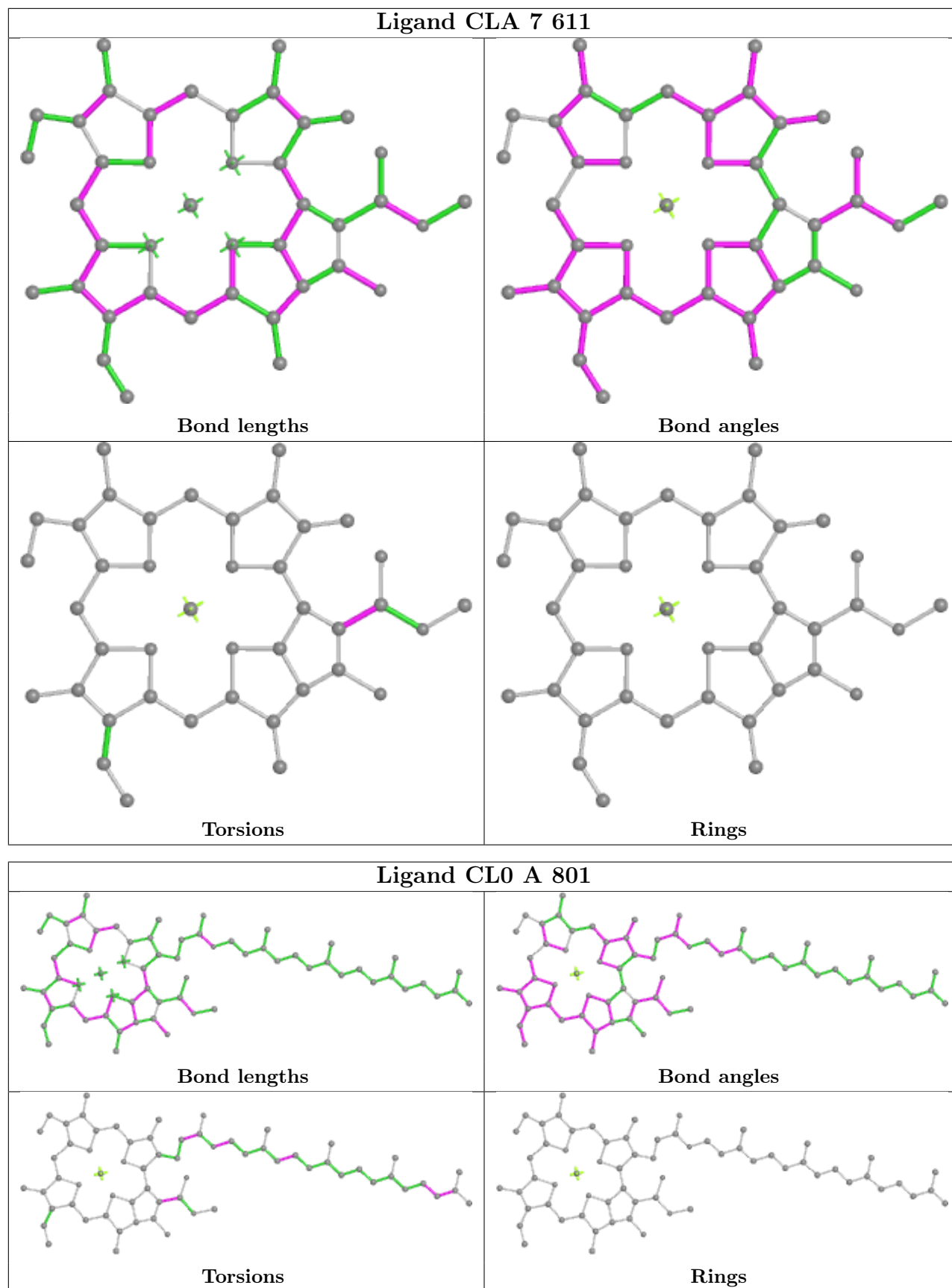


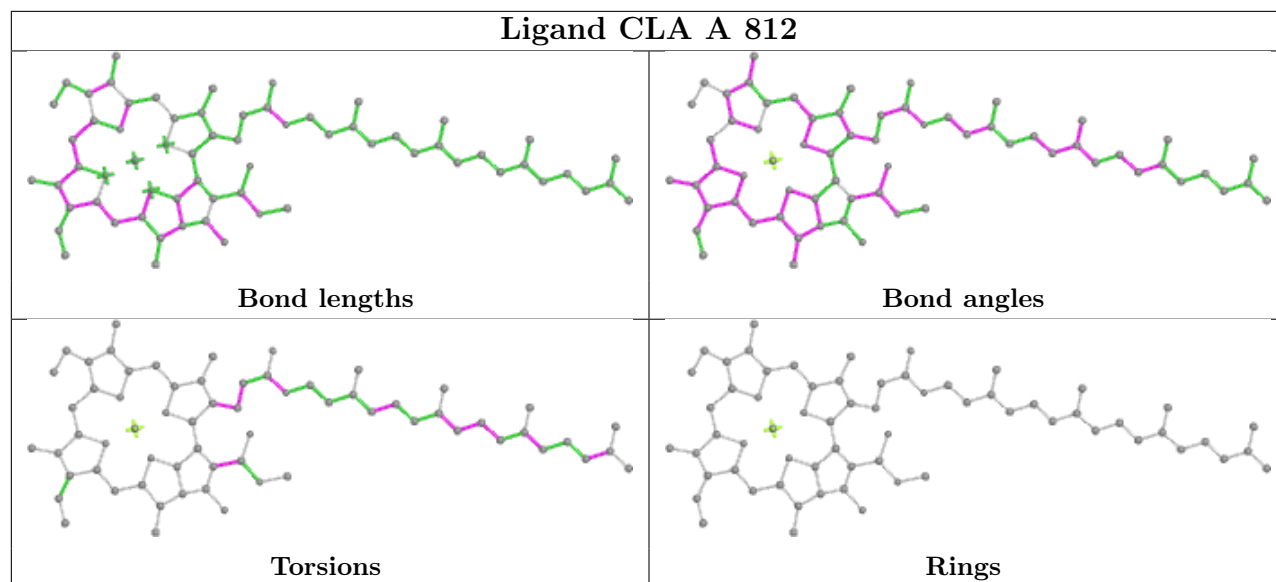












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

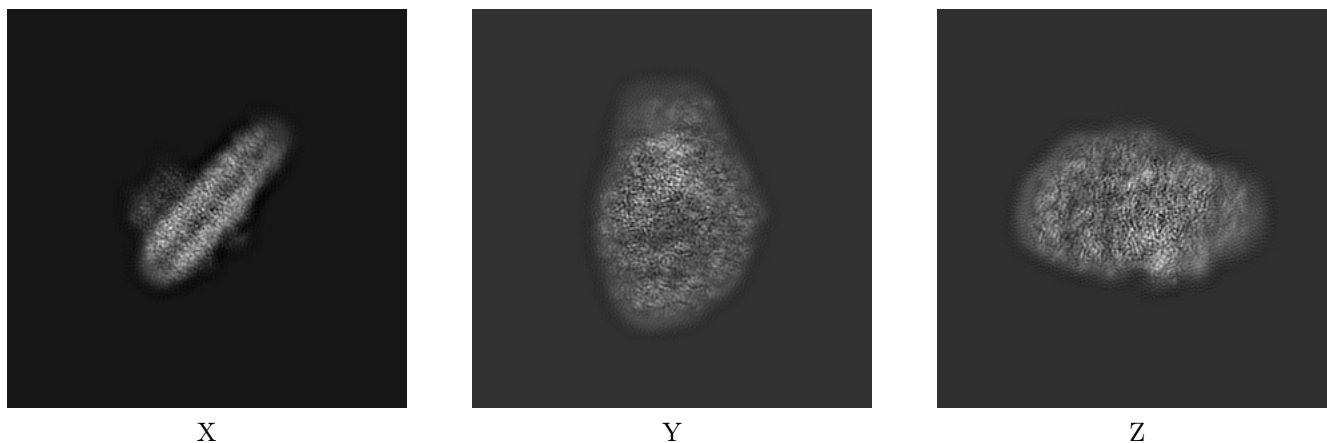
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9854. 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](#)

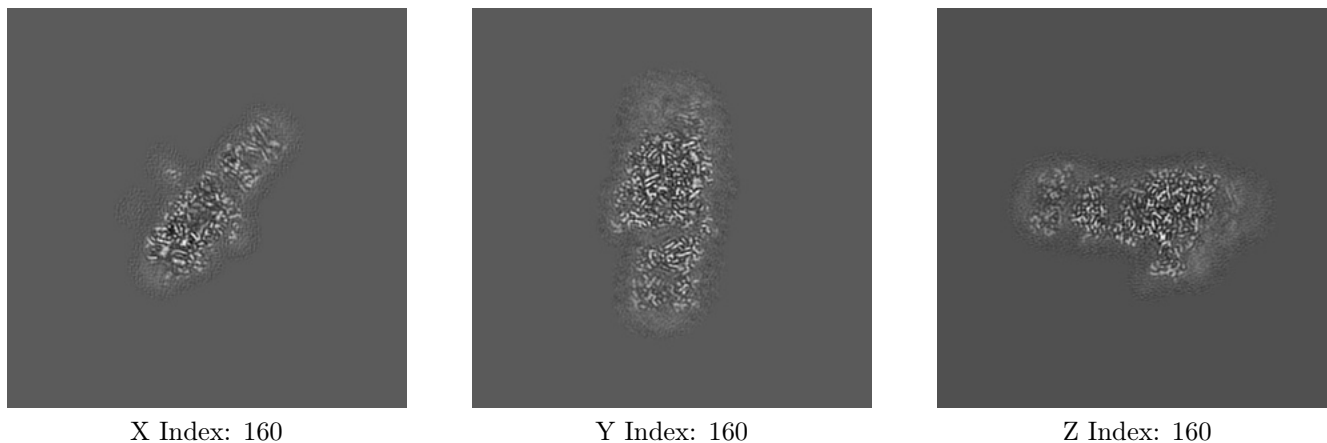
6.1.1 Primary map



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

6.2 Central slices [i](#)

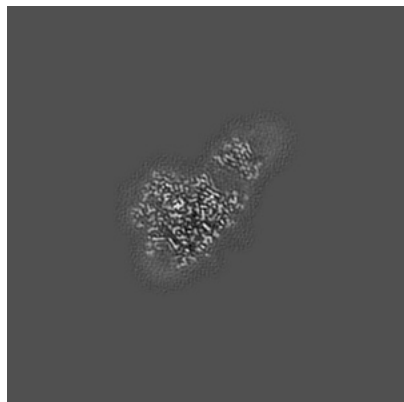
6.2.1 Primary map



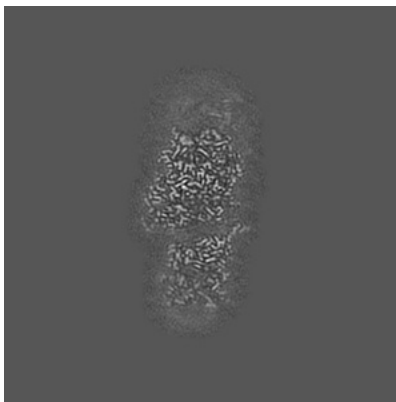
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

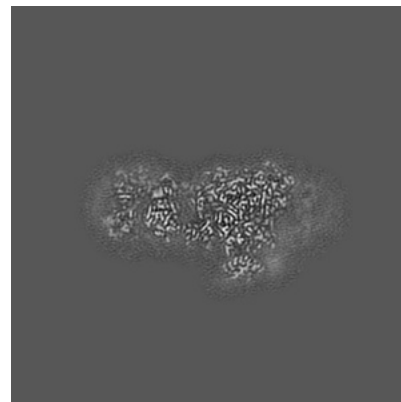
6.3.1 Primary map



X Index: 179



Y Index: 158

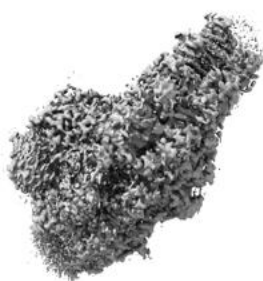


Z Index: 156

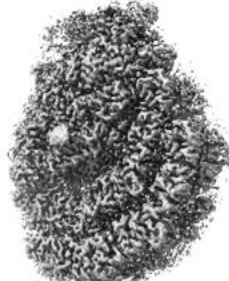
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

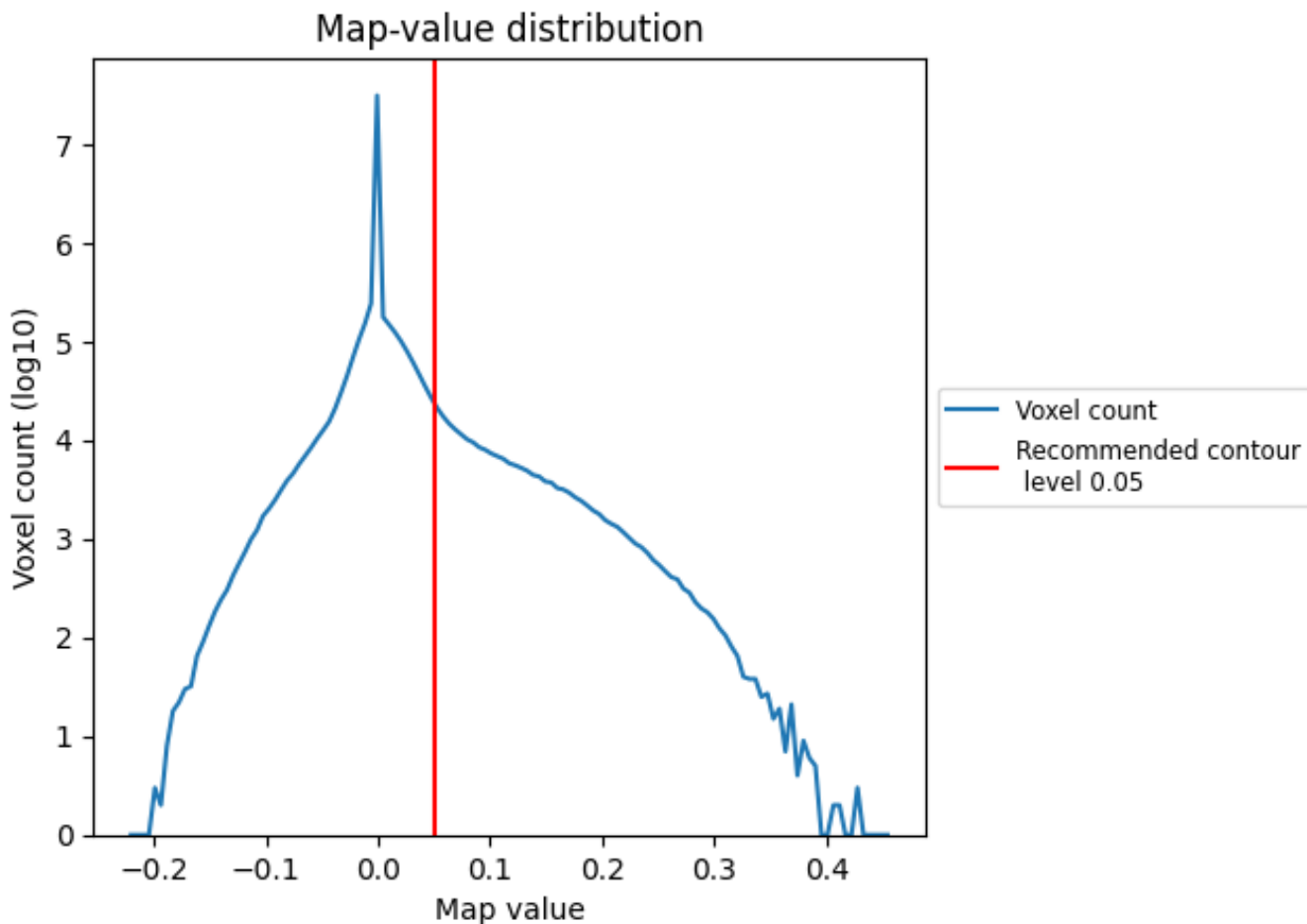
6.5 Mask visualisation

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

7 Map analysis [i](#)

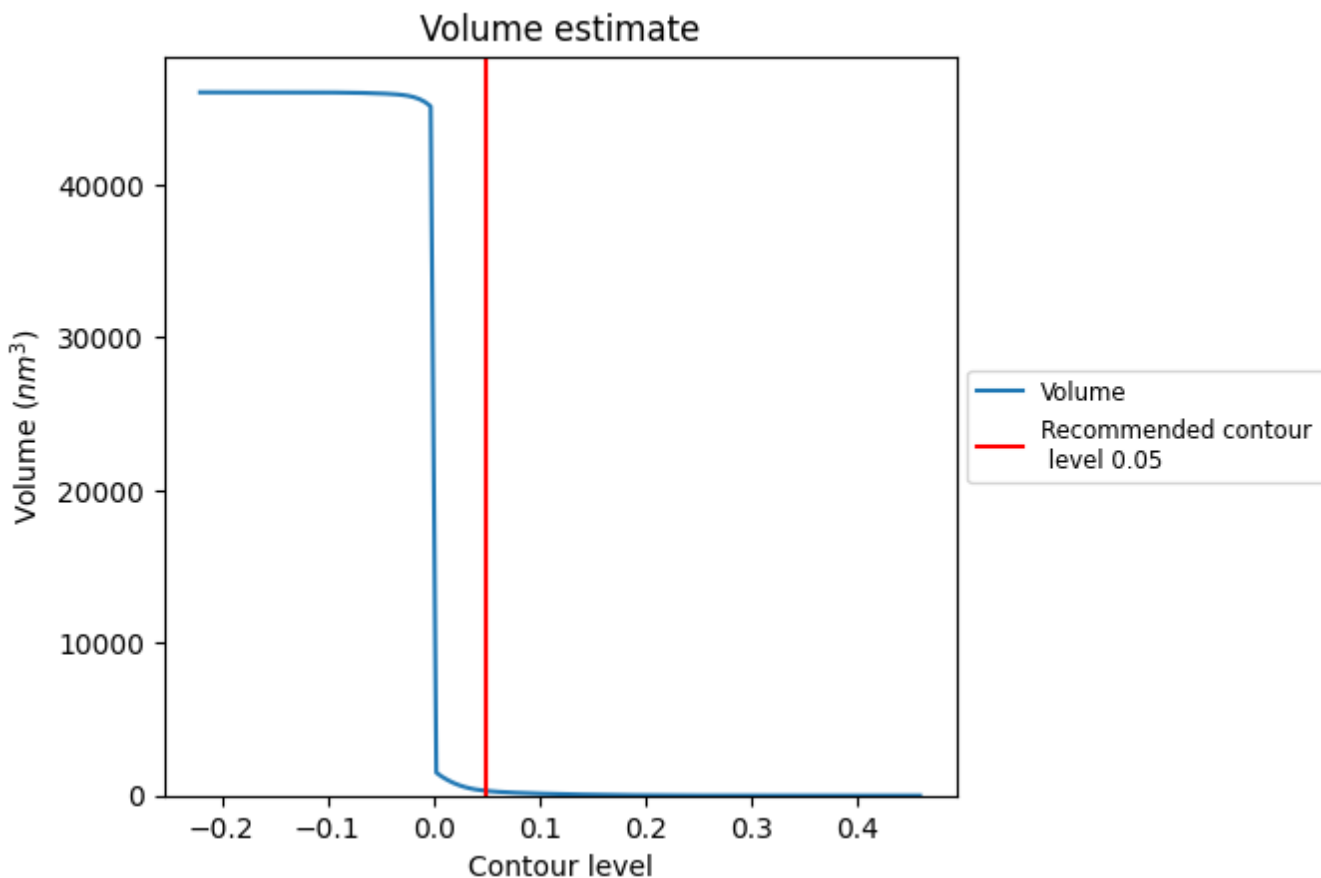
This section contains the results of statistical analysis of the map.

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.

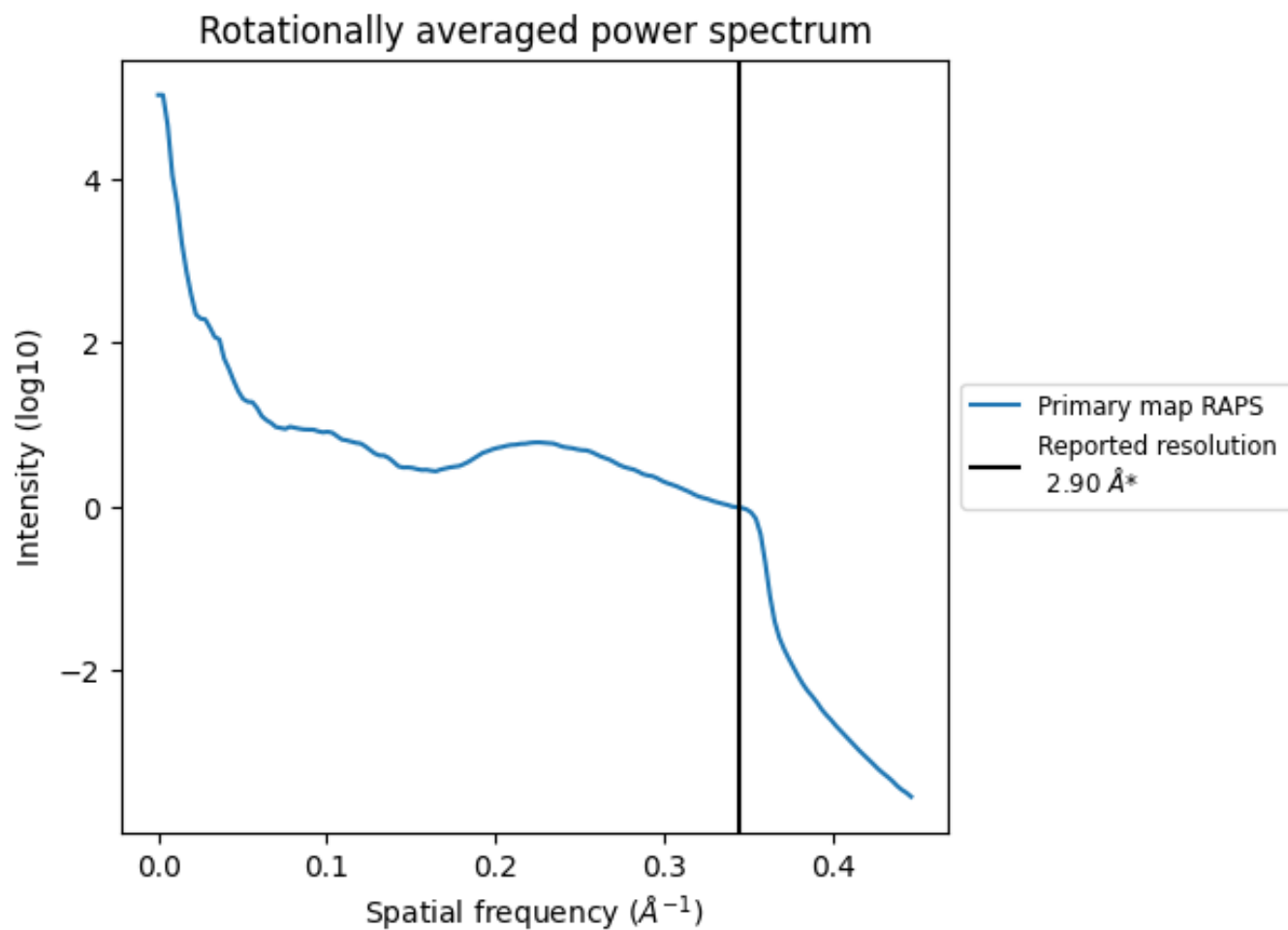
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 308 nm³; this corresponds to an approximate mass of 278 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.345\AA^{-1}

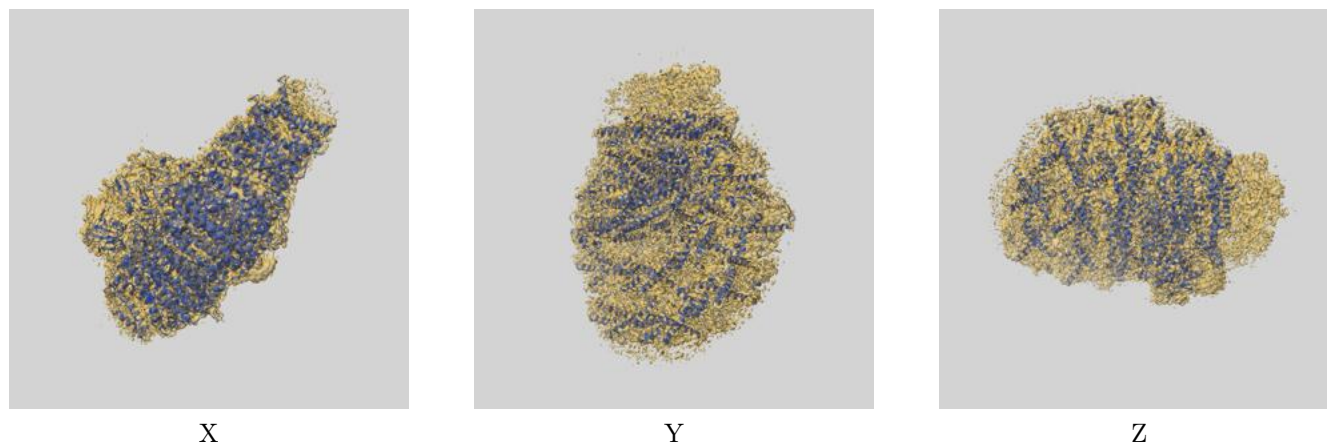
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

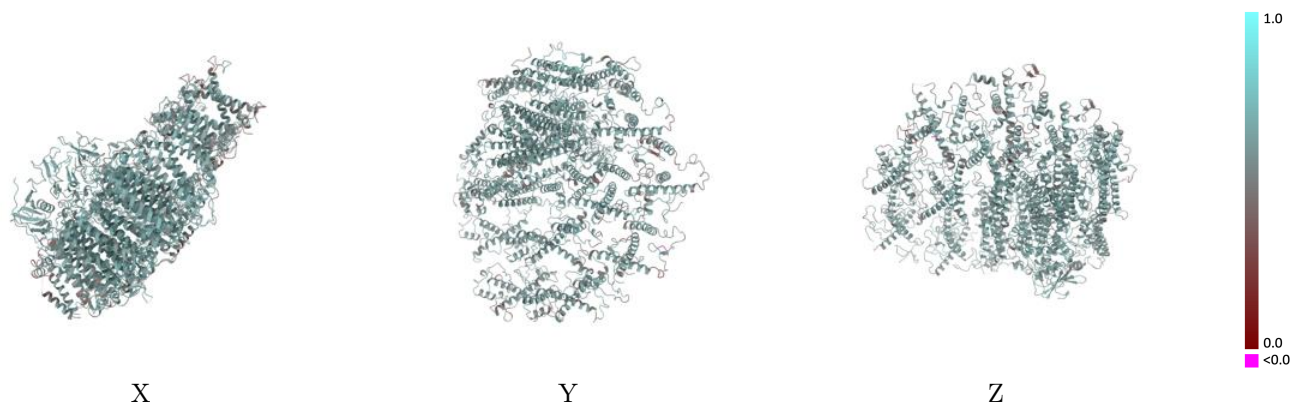
This section contains information regarding the fit between EMDB map EMD-9854 and PDB model 6JO6. Per-residue inclusion information can be found in section 3 on page 32.

9.1 Map-model overlay [i](#)



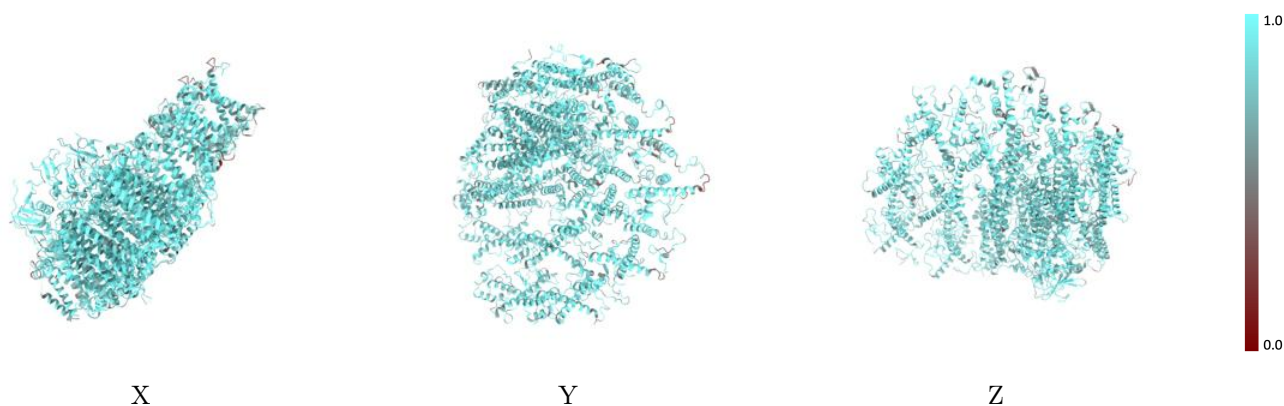
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



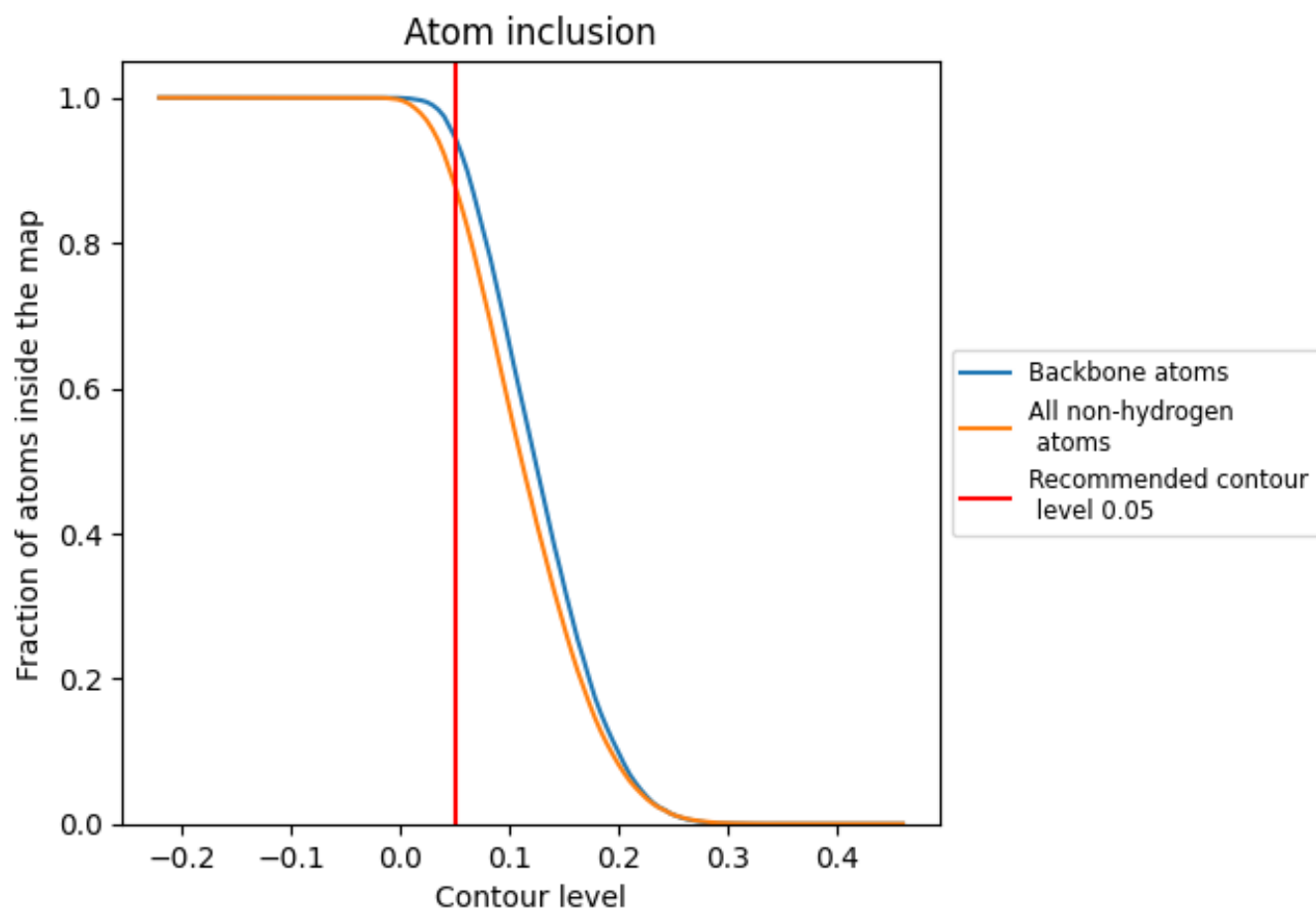
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).









































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 88% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8788	 0.5910
1	 0.8386	 0.5770
3	 0.8874	 0.5890
4	 0.8395	 0.5540
5	 0.8451	 0.5630
6	 0.8417	 0.5630
7	 0.8786	 0.5960
8	 0.8880	 0.5940
A	 0.9256	 0.6190
B	 0.9187	 0.6180
C	 0.9435	 0.6050
D	 0.9054	 0.5830
E	 0.8994	 0.5890
F	 0.8651	 0.5780
G	 0.7769	 0.5650
I	 0.8464	 0.5720
J	 0.9042	 0.6080
K	 0.7804	 0.5480
L	 0.7831	 0.5440
Z	 0.7727	 0.5450

