



## Full wwPDB EM Validation Report ⓘ

Dec 19, 2022 – 03:23 am GMT

PDB ID : 7BGI  
EMDB ID : EMD-12180  
Title : Photosystem I of a temperature sensitive mutant *Chlamydomonas reinhardtii*  
Authors : Caspy, I.; Nelson, N.  
Deposited on : 2021-01-07  
Resolution : 2.54 Å (reported)  
Based on initial model : 6JO5

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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 : 1.8.4, 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) : 2.31.3

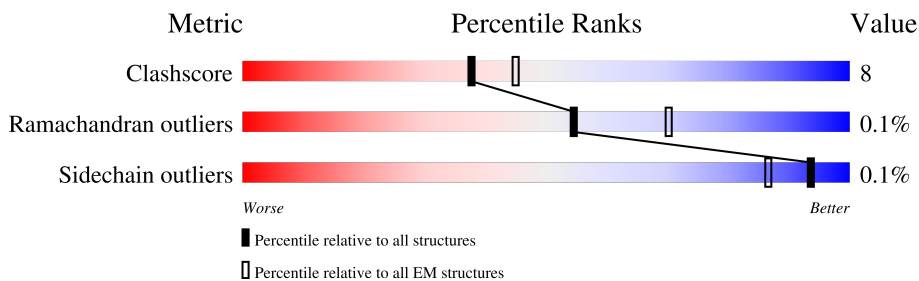
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.54 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  $\geq 3$ , 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	741	
2	B	733	
3	C	80	
4	D	144	
5	E	63	
6	F	165	
7	G	91	
8	I	37	

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Mol	Chain	Length	Quality of chain
9	J	39	 90% 10%
10	K	84	 85% 15%
11	L	138	 85% 7% 9%
12	1	194	 88% 12%
12	Z	194	 92% 8%
13	3	219	 91% 9%
14	7	213	 90% 10%
15	8	217	 88% 12%
16	4	210	 85% 15%
17	5	227	 89% 11%
18	6	229	 90% 10%
19	2	198	 81% 19%
20	9	183	 87% 13%

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
21	CL0	A	1011	X	-	-	-
22	CLA	1	601	X	-	-	-
22	CLA	1	602	X	-	-	-
22	CLA	1	603	X	-	-	-
22	CLA	1	604	X	-	-	-
22	CLA	1	605	X	-	-	-
22	CLA	1	606	X	-	-	-
22	CLA	1	607	X	-	-	-
22	CLA	1	608	X	-	-	-
22	CLA	1	611	X	-	-	-
22	CLA	1	612	X	-	-	-
22	CLA	1	613	X	-	-	-
22	CLA	1	615	X	-	-	-
22	CLA	2	601	X	-	-	-
22	CLA	2	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	2	603	X	-	-	-
22	CLA	2	604	X	-	-	-
22	CLA	2	605	X	-	-	-
22	CLA	2	606	X	-	-	-
22	CLA	2	607	X	-	-	-
22	CLA	2	608	X	-	-	-
22	CLA	2	612	X	-	-	-
22	CLA	2	615	X	-	-	-
22	CLA	3	601	X	-	-	-
22	CLA	3	602	X	-	-	-
22	CLA	3	603	X	-	-	-
22	CLA	3	604	X	-	-	-
22	CLA	3	605	X	-	-	-
22	CLA	3	606	X	-	-	-
22	CLA	3	607	X	-	-	-
22	CLA	3	608	X	-	-	-
22	CLA	3	610	X	-	-	-
22	CLA	3	612	X	-	-	-
22	CLA	3	613	X	-	-	-
22	CLA	3	616	X	-	-	-
22	CLA	3	618	X	-	-	-
22	CLA	4	601	X	-	-	-
22	CLA	4	602	X	-	-	-
22	CLA	4	603	X	-	-	-
22	CLA	4	604	X	-	-	-
22	CLA	4	605	X	-	-	-
22	CLA	4	606	X	-	-	-
22	CLA	4	607	X	-	-	-
22	CLA	4	608	X	-	-	-
22	CLA	4	609	X	-	-	-
22	CLA	4	612	X	-	-	-
22	CLA	4	615	X	-	-	-
22	CLA	5	601	X	-	-	-
22	CLA	5	602	X	-	-	-
22	CLA	5	603	X	-	-	-
22	CLA	5	604	X	-	-	-
22	CLA	5	605	X	-	-	-
22	CLA	5	606	X	-	-	-
22	CLA	5	607	X	-	-	-
22	CLA	5	608	X	-	-	-
22	CLA	5	609	X	-	-	-
22	CLA	5	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	5	613	X	-	-	-
22	CLA	5	615	X	-	-	-
22	CLA	5	618	X	-	-	-
22	CLA	5	622	X	-	-	-
22	CLA	6	601	X	-	-	-
22	CLA	6	602	X	-	-	-
22	CLA	6	603	X	-	-	-
22	CLA	6	604	X	-	-	-
22	CLA	6	605	X	-	-	-
22	CLA	6	606	X	-	-	-
22	CLA	6	607	X	-	-	-
22	CLA	6	608	X	-	-	-
22	CLA	6	609	X	-	-	-
22	CLA	6	612	X	-	-	-
22	CLA	6	615	X	-	-	-
22	CLA	6	618	X	-	-	-
22	CLA	6	619	X	-	-	-
22	CLA	7	601	X	-	-	-
22	CLA	7	602	X	-	-	-
22	CLA	7	603	X	-	-	-
22	CLA	7	604	X	-	-	-
22	CLA	7	605	X	-	-	-
22	CLA	7	606	X	-	-	-
22	CLA	7	607	X	-	-	-
22	CLA	7	608	X	-	-	-
22	CLA	7	609	X	-	-	-
22	CLA	7	611	X	-	-	-
22	CLA	7	612	X	-	-	-
22	CLA	7	613	X	-	-	-
22	CLA	7	615	X	-	-	-
22	CLA	7	616	X	-	-	-
22	CLA	8	601	X	-	-	-
22	CLA	8	602	X	-	-	-
22	CLA	8	603	X	-	-	-
22	CLA	8	604	X	-	-	-
22	CLA	8	605	X	-	-	-
22	CLA	8	606	X	-	-	-
22	CLA	8	607	X	-	-	-
22	CLA	8	608	X	-	-	-
22	CLA	8	609	X	-	-	-
22	CLA	8	611	X	-	-	-
22	CLA	8	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	8	615	X	-	-	-
22	CLA	9	601	X	-	-	-
22	CLA	9	602	X	-	-	-
22	CLA	9	603	X	-	-	-
22	CLA	9	604	X	-	-	-
22	CLA	9	606	X	-	-	-
22	CLA	9	607	X	-	-	-
22	CLA	9	608	X	-	-	-
22	CLA	9	609	X	-	-	-
22	CLA	9	612	X	-	-	-
22	CLA	A	1012	X	-	-	-
22	CLA	A	1013	X	-	-	-
22	CLA	A	1101	X	-	-	-
22	CLA	A	1102	X	-	-	-
22	CLA	A	1103	X	-	-	-
22	CLA	A	1104	X	-	-	-
22	CLA	A	1105	X	-	-	-
22	CLA	A	1106	X	-	-	-
22	CLA	A	1107	X	-	-	-
22	CLA	A	1108	X	-	-	-
22	CLA	A	1109	X	-	-	-
22	CLA	A	1110	X	-	-	-
22	CLA	A	1111	X	-	-	-
22	CLA	A	1112	X	-	-	-
22	CLA	A	1113	X	-	-	-
22	CLA	A	1114	X	-	-	-
22	CLA	A	1115	X	-	-	-
22	CLA	A	1116	X	-	-	-
22	CLA	A	1117	X	-	-	-
22	CLA	A	1118	X	-	-	-
22	CLA	A	1119	X	-	-	-
22	CLA	A	1120	X	-	-	-
22	CLA	A	1121	X	-	-	-
22	CLA	A	1122	X	-	-	-
22	CLA	A	1123	X	-	-	-
22	CLA	A	1124	X	-	-	-
22	CLA	A	1125	X	-	-	-
22	CLA	A	1126	X	-	-	-
22	CLA	A	1127	X	-	-	-
22	CLA	A	1128	X	-	-	-
22	CLA	A	1129	X	-	-	-
22	CLA	A	1130	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	1131	X	-	-	-
22	CLA	A	1132	X	-	-	-
22	CLA	A	1133	X	-	-	-
22	CLA	A	1134	X	-	-	-
22	CLA	A	1135	X	-	-	-
22	CLA	A	1136	X	-	-	-
22	CLA	A	1137	X	-	-	-
22	CLA	A	1138	X	-	-	-
22	CLA	A	1139	X	-	-	-
22	CLA	A	1140	X	-	-	-
22	CLA	A	1141	X	-	-	-
22	CLA	B	1021	X	-	-	-
22	CLA	B	1022	X	-	-	-
22	CLA	B	1023	X	-	-	-
22	CLA	B	1201	X	-	-	-
22	CLA	B	1202	X	-	-	-
22	CLA	B	1203	X	-	-	-
22	CLA	B	1204	X	-	-	-
22	CLA	B	1205	X	-	-	-
22	CLA	B	1206	X	-	-	-
22	CLA	B	1207	X	-	-	-
22	CLA	B	1208	X	-	-	-
22	CLA	B	1209	X	-	-	-
22	CLA	B	1210	X	-	-	-
22	CLA	B	1211	X	-	-	-
22	CLA	B	1212	X	-	-	-
22	CLA	B	1213	X	-	-	-
22	CLA	B	1214	X	-	-	-
22	CLA	B	1215	X	-	-	-
22	CLA	B	1216	X	-	-	-
22	CLA	B	1217	X	-	-	-
22	CLA	B	1218	X	-	-	-
22	CLA	B	1219	X	-	-	-
22	CLA	B	1220	X	-	-	-
22	CLA	B	1221	X	-	-	-
22	CLA	B	1222	X	-	-	-
22	CLA	B	1223	X	-	-	-
22	CLA	B	1224	X	-	-	-
22	CLA	B	1225	X	-	-	-
22	CLA	B	1226	X	-	-	-
22	CLA	B	1227	X	-	-	-
22	CLA	B	1228	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	1229	X	-	-	-
22	CLA	B	1230	X	-	-	-
22	CLA	B	1231	X	-	-	-
22	CLA	B	1232	X	-	-	-
22	CLA	B	1234	X	-	-	-
22	CLA	B	1235	X	-	-	-
22	CLA	B	1236	X	-	-	-
22	CLA	B	1237	X	-	-	-
22	CLA	B	1238	X	-	-	-
22	CLA	B	1239	X	-	-	-
22	CLA	B	1240	X	-	-	-
22	CLA	B	1241	X	-	-	-
22	CLA	F	1301	X	-	-	-
22	CLA	F	1302	X	-	-	-
22	CLA	G	1601	X	-	-	-
22	CLA	G	1602	X	-	-	-
22	CLA	J	1901	X	-	-	-
22	CLA	K	1401	X	-	-	-
22	CLA	K	1402	X	-	-	-
22	CLA	K	1403	X	-	-	-
22	CLA	K	1404	X	-	-	-
22	CLA	L	1502	X	-	-	-
22	CLA	L	1503	X	-	-	-
22	CLA	Z	601	X	-	-	-
22	CLA	Z	602	X	-	-	-
22	CLA	Z	603	X	-	-	-
22	CLA	Z	604	X	-	-	-
22	CLA	Z	605	X	-	-	-
22	CLA	Z	606	X	-	-	-
22	CLA	Z	607	X	-	-	-
22	CLA	Z	608	X	-	-	-
22	CLA	Z	611	X	-	-	-
22	CLA	Z	612	X	-	-	-
22	CLA	Z	615	X	-	-	-
36	RRX	F	4001	X	-	-	-
37	C7Z	1	503	X	-	-	-
37	C7Z	5	505	X	-	-	-
37	C7Z	J	4002	X	-	-	-
39	LUT	2	501	X	-	-	-
39	LUT	2	503	X	-	-	-
40	CHL	1	609	X	-	-	-
40	CHL	1	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
40	CHL	2	609	X	-	-	-
40	CHL	2	610	X	-	-	-
40	CHL	2	613	X	-	-	-
40	CHL	3	611	X	-	-	-
40	CHL	4	610	X	-	-	-
40	CHL	4	611	X	-	-	-
40	CHL	4	613	X	-	-	-
40	CHL	4	617	X	-	-	-
40	CHL	5	610	X	-	-	-
40	CHL	5	611	X	-	-	-
40	CHL	5	617	X	-	-	-
40	CHL	6	610	X	-	-	-
40	CHL	6	611	X	-	-	-
40	CHL	6	613	X	-	-	-
40	CHL	6	617	X	-	-	-
40	CHL	7	610	X	-	-	-
40	CHL	8	610	X	-	-	-
40	CHL	8	613	X	-	-	-
40	CHL	9	610	X	-	-	-
40	CHL	9	613	X	-	-	-
40	CHL	Z	609	X	-	-	-
40	CHL	Z	610	X	-	-	-
40	CHL	Z	613	X	-	-	-
42	QTB	Z	504	X	-	-	-

## 2 Entry composition [i](#)

There are 46 unique types of molecules in this entry. The entry contains 52213 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	741	5820	3805	993	1000	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	733	5825	3825	977	1005	18	0	0

- 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	601	369	103	117	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	1135	725	201	202	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	63	497	316	87	94	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	165	1266	817	213	233	3	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	74	Total	C	N	O	0	0
			550	354	94	102		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	37	Total	C	N	O	S	0	0
			282	195	39	47	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	39	Total	C	N	O	S	0	0
			321	219	45	56	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	84	Total	C	N	O	S	0	0
			571	362	98	109	2		

- Molecule 11 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	126	Total	C	N	O	S	0	0
			914	595	148	168	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
			1445	941	240	261	3		
12	Z	194	Total	C	N	O	S	0	0
			1445	941	240	261	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	3	219	Total	C	N	O	S	0	0
			1674	1092	270	304	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	7	213	1650	1072	274	298	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	8	217	1650	1073	280	293	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	4	210	1628	1068	262	293	5	0	0

- 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	227	1775	1154	297	316	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	1766	1164	292	304	6	0	0

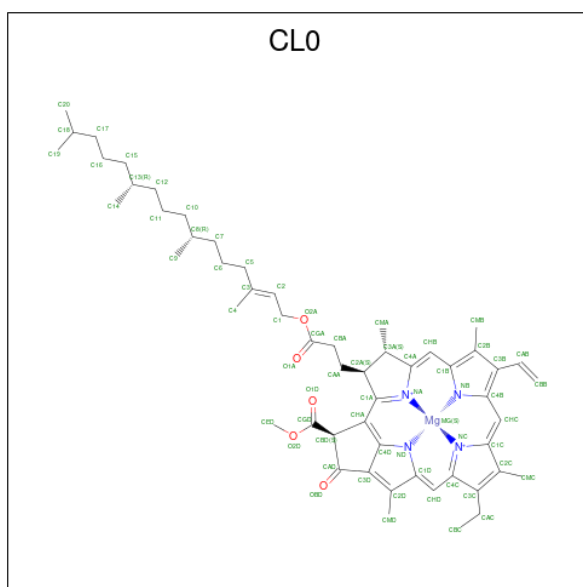
- Molecule 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	2	198	1518	983	249	276	10	0	0

- Molecule 20 is a protein called Chlorophyll a-b binding protein, chloroplastic.

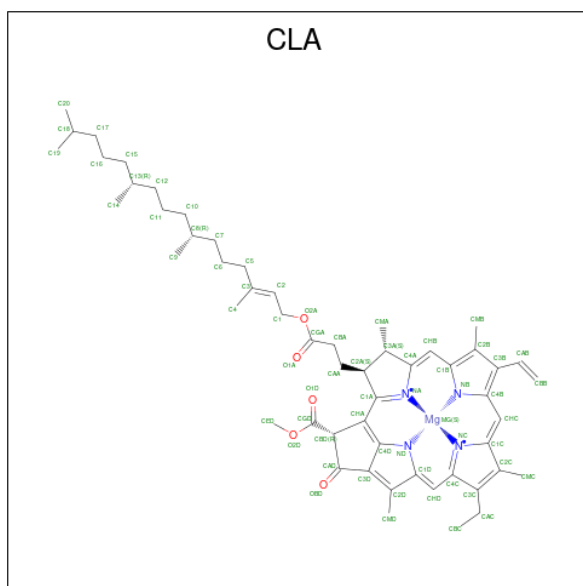
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	9	183	1406	910	235	254	7	0	0

- Molecule 21 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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

- Molecule 22 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
22	A	1	2699	2269	43	172	215	0
22	A	1	2699	2269	43	172	215	0
22	A	1	2699	2269	43	172	215	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	A	1	2699	2269	43	172	215	0
22	A	1	2699	2269	43	172	215	0
22	A	1	2699	2269	43	172	215	0
22	A	1	2699	2269	43	172	215	0
22	A	1	2699	2269	43	172	215	0
22	A	1	2699	2269	43	172	215	0
22	A	1	2699	2269	43	172	215	0
22	A	1	2699	2269	43	172	215	0
22	A	1	2699	2269	43	172	215	0
22	A	1	2699	2269	43	172	215	0
22	A	1	2699	2269	43	172	215	0
22	A	1	2699	2269	43	172	215	0
22	A	1	2699	2269	43	172	215	0
22	A	1	2699	2269	43	172	215	0
22	A	1	2699	2269	43	172	215	0
22	A	1	2699	2269	43	172	215	0
22	A	1	2699	2269	43	172	215	0
22	A	1	2699	2269	43	172	215	0
22	A	1	2699	2269	43	172	215	0
22	A	1	2699	2269	43	172	215	0
22	A	1	2699	2269	43	172	215	0
22	A	1	2699	2269	43	172	215	0
22	A	1	2699	2269	43	172	215	0
22	A	1	2699	2269	43	172	215	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	A	1	Total 2699	C 2269	Mg 43	N 172	O 215	0
22	A	1	Total 2699	C 2269	Mg 43	N 172	O 215	0
22	A	1	Total 2699	C 2269	Mg 43	N 172	O 215	0
22	A	1	Total 2699	C 2269	Mg 43	N 172	O 215	0
22	A	1	Total 2699	C 2269	Mg 43	N 172	O 215	0
22	A	1	Total 2699	C 2269	Mg 43	N 172	O 215	0
22	A	1	Total 2699	C 2269	Mg 43	N 172	O 215	0
22	A	1	Total 2699	C 2269	Mg 43	N 172	O 215	0
22	A	1	Total 2699	C 2269	Mg 43	N 172	O 215	0
22	A	1	Total 2699	C 2269	Mg 43	N 172	O 215	0
22	A	1	Total 2699	C 2269	Mg 43	N 172	O 215	0
22	A	1	Total 2699	C 2269	Mg 43	N 172	O 215	0
22	A	1	Total 2699	C 2269	Mg 43	N 172	O 215	0
22	A	1	Total 2699	C 2269	Mg 43	N 172	O 215	0
22	A	1	Total 2699	C 2269	Mg 43	N 172	O 215	0
22	A	1	Total 2699	C 2269	Mg 43	N 172	O 215	0
22	A	1	Total 2699	C 2269	Mg 43	N 172	O 215	0
22	A	1	Total 2699	C 2269	Mg 43	N 172	O 215	0
22	A	1	Total 2699	C 2269	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	B	1	Total 2680	C 2250	Mg 43	N 172	O 215	0
22	F	1	Total 110	C 90	Mg 2	N 8	O 10	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	F	1	Total 110	C 90	Mg 2	N 8	O 10	0
22	G	1	Total 96	C 76	Mg 2	N 8	O 10	0
22	G	1	Total 96	C 76	Mg 2	N 8	O 10	0
22	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	K	1	Total 205	C 165	Mg 4	N 16	O 20	0
22	K	1	Total 205	C 165	Mg 4	N 16	O 20	0
22	K	1	Total 205	C 165	Mg 4	N 16	O 20	0
22	K	1	Total 205	C 165	Mg 4	N 16	O 20	0
22	L	1	Total 115	C 95	Mg 2	N 8	O 10	0
22	L	1	Total 115	C 95	Mg 2	N 8	O 10	0
22	1	1	Total 712	C 592	Mg 12	N 48	O 60	0
22	1	1	Total 712	C 592	Mg 12	N 48	O 60	0
22	1	1	Total 712	C 592	Mg 12	N 48	O 60	0
22	1	1	Total 712	C 592	Mg 12	N 48	O 60	0
22	1	1	Total 712	C 592	Mg 12	N 48	O 60	0
22	1	1	Total 712	C 592	Mg 12	N 48	O 60	0
22	1	1	Total 712	C 592	Mg 12	N 48	O 60	0
22	1	1	Total 712	C 592	Mg 12	N 48	O 60	0
22	1	1	Total 712	C 592	Mg 12	N 48	O 60	0
22	1	1	Total 712	C 592	Mg 12	N 48	O 60	0
22	1	1	Total 712	C 592	Mg 12	N 48	O 60	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	1	1	Total 712	C 592	Mg 12	N 48	O 60	0
22	Z	1	Total 622	C 512	Mg 11	N 44	O 55	0
22	Z	1	Total 622	C 512	Mg 11	N 44	O 55	0
22	Z	1	Total 622	C 512	Mg 11	N 44	O 55	0
22	Z	1	Total 622	C 512	Mg 11	N 44	O 55	0
22	Z	1	Total 622	C 512	Mg 11	N 44	O 55	0
22	Z	1	Total 622	C 512	Mg 11	N 44	O 55	0
22	Z	1	Total 622	C 512	Mg 11	N 44	O 55	0
22	Z	1	Total 622	C 512	Mg 11	N 44	O 55	0
22	Z	1	Total 622	C 512	Mg 11	N 44	O 55	0
22	Z	1	Total 622	C 512	Mg 11	N 44	O 55	0
22	Z	1	Total 622	C 512	Mg 11	N 44	O 55	0
22	Z	1	Total 622	C 512	Mg 11	N 44	O 55	0
22	Z	1	Total 622	C 512	Mg 11	N 44	O 55	0
22	3	1	Total 748	C 618	Mg 13	N 52	O 65	0
22	3	1	Total 748	C 618	Mg 13	N 52	O 65	0
22	3	1	Total 748	C 618	Mg 13	N 52	O 65	0
22	3	1	Total 748	C 618	Mg 13	N 52	O 65	0
22	3	1	Total 748	C 618	Mg 13	N 52	O 65	0
22	3	1	Total 748	C 618	Mg 13	N 52	O 65	0
22	3	1	Total 748	C 618	Mg 13	N 52	O 65	0
22	3	1	Total 748	C 618	Mg 13	N 52	O 65	0
22	3	1	Total 748	C 618	Mg 13	N 52	O 65	0
22	3	1	Total 748	C 618	Mg 13	N 52	O 65	0

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Mol	Chain	Residues	Atoms					AltConf
22	3	1	Total	C	Mg	N	O	0
			748	618	13	52	65	
22	3	1	Total	C	Mg	N	O	0
			748	618	13	52	65	
22	3	1	Total	C	Mg	N	O	0
			748	618	13	52	65	
22	3	1	Total	C	Mg	N	O	0
			748	618	13	52	65	
22	7	1	Total	C	Mg	N	O	0
			790	654	14	56	66	
22	7	1	Total	C	Mg	N	O	0
			790	654	14	56	66	
22	7	1	Total	C	Mg	N	O	0
			790	654	14	56	66	
22	7	1	Total	C	Mg	N	O	0
			790	654	14	56	66	
22	7	1	Total	C	Mg	N	O	0
			790	654	14	56	66	
22	7	1	Total	C	Mg	N	O	0
			790	654	14	56	66	
22	7	1	Total	C	Mg	N	O	0
			790	654	14	56	66	
22	7	1	Total	C	Mg	N	O	0
			790	654	14	56	66	
22	7	1	Total	C	Mg	N	O	0
			790	654	14	56	66	
22	7	1	Total	C	Mg	N	O	0
			790	654	14	56	66	
22	7	1	Total	C	Mg	N	O	0
			790	654	14	56	66	
22	7	1	Total	C	Mg	N	O	0
			790	654	14	56	66	
22	7	1	Total	C	Mg	N	O	0
			790	654	14	56	66	
22	7	1	Total	C	Mg	N	O	0
			790	654	14	56	66	
22	8	1	Total	C	Mg	N	O	0
			694	574	12	48	60	
22	8	1	Total	C	Mg	N	O	0
			694	574	12	48	60	
22	8	1	Total	C	Mg	N	O	0
			694	574	12	48	60	

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Mol	Chain	Residues	Atoms					AltConf
22	8	1	Total	C	Mg	N	O	0
			694	574	12	48	60	
22	8	1	Total	C	Mg	N	O	0
			694	574	12	48	60	
22	8	1	Total	C	Mg	N	O	0
			694	574	12	48	60	
22	8	1	Total	C	Mg	N	O	0
			694	574	12	48	60	
22	8	1	Total	C	Mg	N	O	0
			694	574	12	48	60	
22	8	1	Total	C	Mg	N	O	0
			694	574	12	48	60	
22	8	1	Total	C	Mg	N	O	0
			694	574	12	48	60	
22	8	1	Total	C	Mg	N	O	0
			694	574	12	48	60	
22	8	1	Total	C	Mg	N	O	0
			694	574	12	48	60	
22	4	1	Total	C	Mg	N	O	0
			613	505	11	44	53	
22	4	1	Total	C	Mg	N	O	0
			613	505	11	44	53	
22	4	1	Total	C	Mg	N	O	0
			613	505	11	44	53	
22	4	1	Total	C	Mg	N	O	0
			613	505	11	44	53	
22	4	1	Total	C	Mg	N	O	0
			613	505	11	44	53	
22	4	1	Total	C	Mg	N	O	0
			613	505	11	44	53	
22	4	1	Total	C	Mg	N	O	0
			613	505	11	44	53	
22	4	1	Total	C	Mg	N	O	0
			613	505	11	44	53	
22	4	1	Total	C	Mg	N	O	0
			613	505	11	44	53	
22	4	1	Total	C	Mg	N	O	0
			613	505	11	44	53	
22	5	1	Total	C	Mg	N	O	0
			799	659	14	56	70	

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Mol	Chain	Residues	Atoms					AltConf
22	5	1	Total	C	Mg	N	O	0
			799	659	14	56	70	
22	5	1	Total	C	Mg	N	O	0
			799	659	14	56	70	
22	5	1	Total	C	Mg	N	O	0
			799	659	14	56	70	
22	5	1	Total	C	Mg	N	O	0
			799	659	14	56	70	
22	5	1	Total	C	Mg	N	O	0
			799	659	14	56	70	
22	5	1	Total	C	Mg	N	O	0
			799	659	14	56	70	
22	5	1	Total	C	Mg	N	O	0
			799	659	14	56	70	
22	5	1	Total	C	Mg	N	O	0
			799	659	14	56	70	
22	5	1	Total	C	Mg	N	O	0
			799	659	14	56	70	
22	5	1	Total	C	Mg	N	O	0
			799	659	14	56	70	
22	5	1	Total	C	Mg	N	O	0
			799	659	14	56	70	
22	5	1	Total	C	Mg	N	O	0
			799	659	14	56	70	
22	6	1	Total	C	Mg	N	O	0
			759	629	13	52	65	
22	6	1	Total	C	Mg	N	O	0
			759	629	13	52	65	
22	6	1	Total	C	Mg	N	O	0
			759	629	13	52	65	
22	6	1	Total	C	Mg	N	O	0
			759	629	13	52	65	
22	6	1	Total	C	Mg	N	O	0
			759	629	13	52	65	
22	6	1	Total	C	Mg	N	O	0
			759	629	13	52	65	
22	6	1	Total	C	Mg	N	O	0
			759	629	13	52	65	
22	6	1	Total	C	Mg	N	O	0
			759	629	13	52	65	

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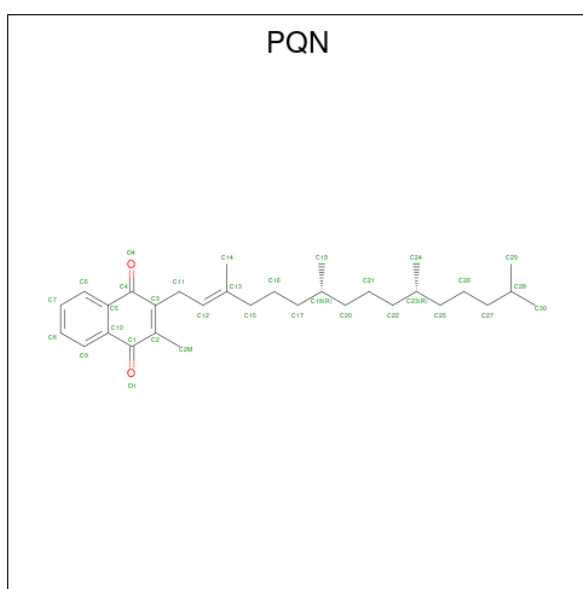
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	6	1	759	629	13	52	65	0
22	6	1	759	629	13	52	65	0
22	6	1	759	629	13	52	65	0
22	6	1	759	629	13	52	65	0
22	6	1	759	629	13	52	65	0
22	2	1	500	400	10	40	50	0
22	2	1	500	400	10	40	50	0
22	2	1	500	400	10	40	50	0
22	2	1	500	400	10	40	50	0
22	2	1	500	400	10	40	50	0
22	2	1	500	400	10	40	50	0
22	2	1	500	400	10	40	50	0
22	2	1	500	400	10	40	50	0
22	2	1	500	400	10	40	50	0
22	2	1	500	400	10	40	50	0
22	2	1	500	400	10	40	50	0
22	2	1	500	400	10	40	50	0
22	9	1	531	431	10	40	50	0
22	9	1	531	431	10	40	50	0
22	9	1	531	431	10	40	50	0
22	9	1	531	431	10	40	50	0
22	9	1	531	431	10	40	50	0
22	9	1	531	431	10	40	50	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	9	1	Total 531	C 431	Mg 10	N 40	O 50	0
22	9	1	Total 531	C 431	Mg 10	N 40	O 50	0
22	9	1	Total 531	C 431	Mg 10	N 40	O 50	0
22	9	1	Total 531	C 431	Mg 10	N 40	O 50	0

- Molecule 23 is PHYLLOQUINONE (three-letter code: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>).



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

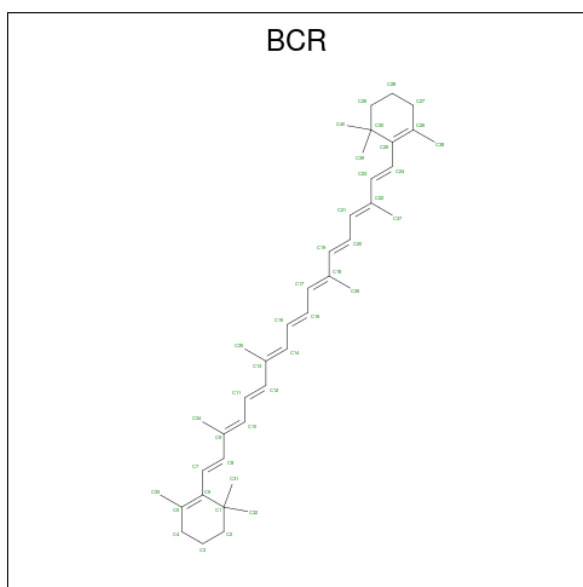
- Molecule 24 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).





Mol	Chain	Residues	Atoms	AltConf
24	A	1	Total Fe S 8 4 4	0
24	C	1	Total Fe S 16 8 8	0
24	C	1	Total Fe S 16 8 8	0

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).



Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C 200 200	0

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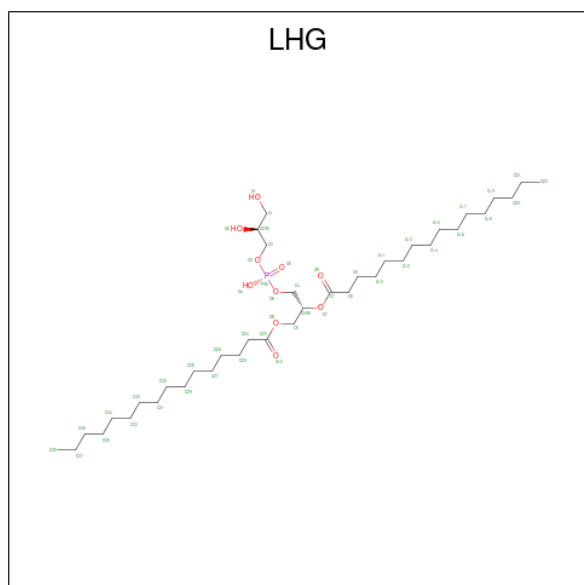
Mol	Chain	Residues	Atoms		AltConf
25	A	1	Total 200	C 200	0
25	A	1	Total 200	C 200	0
25	A	1	Total 200	C 200	0
25	A	1	Total 200	C 200	0
25	B	1	Total 280	C 280	0
25	B	1	Total 280	C 280	0
25	B	1	Total 280	C 280	0
25	B	1	Total 280	C 280	0
25	B	1	Total 280	C 280	0
25	B	1	Total 280	C 280	0
25	B	1	Total 280	C 280	0
25	B	1	Total 280	C 280	0
25	G	1	Total 40	C 40	0
25	I	1	Total 40	C 40	0
25	J	1	Total 40	C 40	0
25	K	1	Total 80	C 80	0
25	K	1	Total 80	C 80	0
25	L	1	Total 80	C 80	0
25	L	1	Total 80	C 80	0
25	3	1	Total 160	C 160	0
25	3	1	Total 160	C 160	0
25	3	1	Total 160	C 160	0

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Mol	Chain	Residues	Atoms		AltConf
25	3	1	Total	C	0
			160	160	
25	7	1	Total	C	0
			80	80	
25	7	1	Total	C	0
			80	80	
25	8	1	Total	C	0
			40	40	
25	4	1	Total	C	0
			40	40	
25	5	1	Total	C	0
			80	80	
25	5	1	Total	C	0
			80	80	
25	6	1	Total	C	0
			80	80	
25	6	1	Total	C	0
			80	80	

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



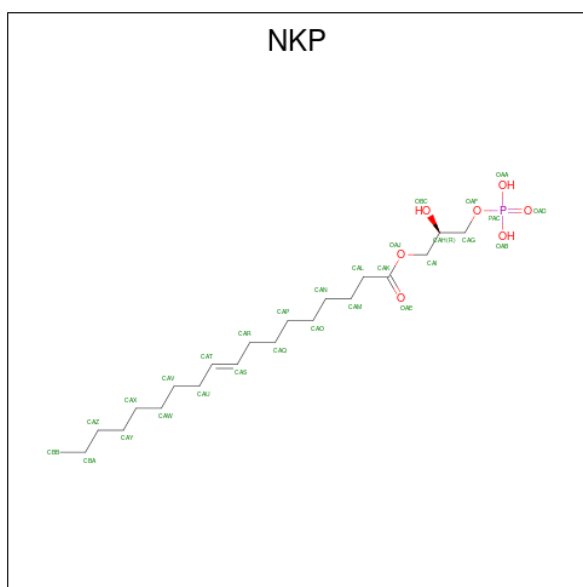
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	O	P	0
			84	62	20	2	
26	A	1	Total	C	O	P	0
			84	62	20	2	

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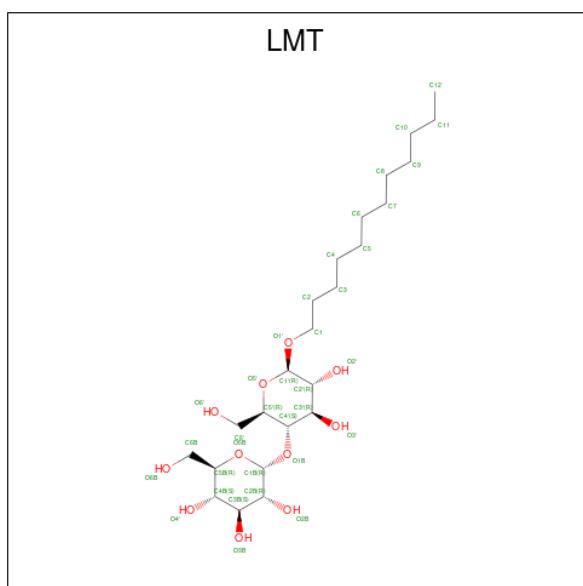
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
26	B	1	76	43	30	3	0
26	B	1	76	43	30	3	0
26	B	1	76	43	30	3	0
26	1	1	43	32	10	1	0
26	Z	1	43	32	10	1	0
26	3	1	20	9	10	1	0
26	7	1	37	26	10	1	0
26	8	1	38	27	10	1	0
26	4	1	81	59	20	2	0
26	4	1	81	59	20	2	0
26	5	1	37	26	10	1	0
26	6	1	49	38	10	1	0
26	2	1	34	23	10	1	0
26	9	1	33	22	10	1	0

- Molecule 27 is (2R)-2-hydroxy-3-(phosphonoxy)propyl (9E)-octadec-9-enoate (three-letter code: NKP) (formula: C<sub>21</sub>H<sub>41</sub>O<sub>7</sub>P).



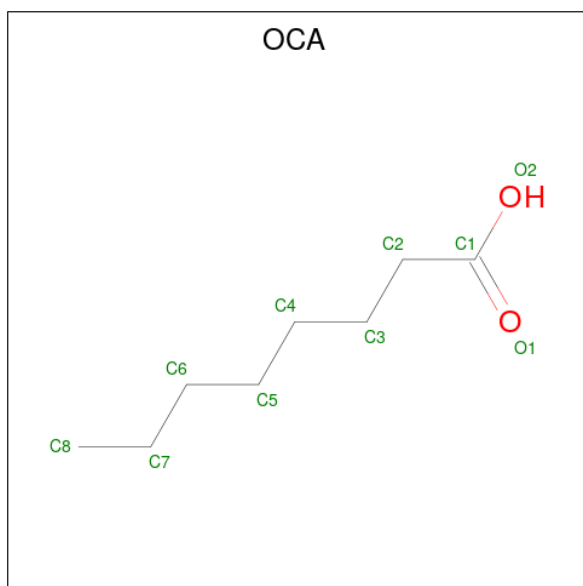
Mol	Chain	Residues	Atoms				AltConf
27	A	1	Total	C	O	P	0
			29	21	7	1	
27	3	1	Total	C	O	P	0
			16	8	7	1	
27	8	1	Total	C	O	P	0
			29	21	7	1	

- Molecule 28 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



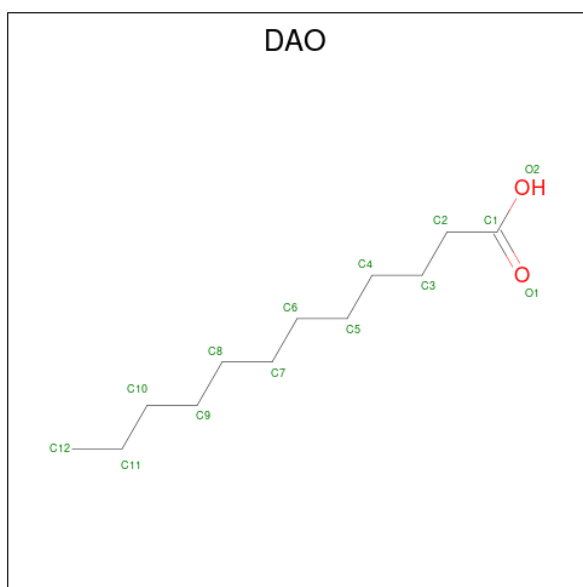
Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			35	24	11	
28	B	1	Total	C	O	0
			70	48	22	
28	B	1	Total	C	O	0
			70	48	22	
28	F	1	Total	C	O	0
			35	24	11	
28	1	1	Total	C	O	0
			35	24	11	
28	8	1	Total	C	O	0
			35	24	11	
28	4	1	Total	C	O	0
			35	24	11	
28	9	1	Total	C	O	0
			35	24	11	

- Molecule 29 is OCTANOIC ACID (CAPRYLIC ACID) (three-letter code: OCA) (formula:  $C_8H_{16}O_2$ ).



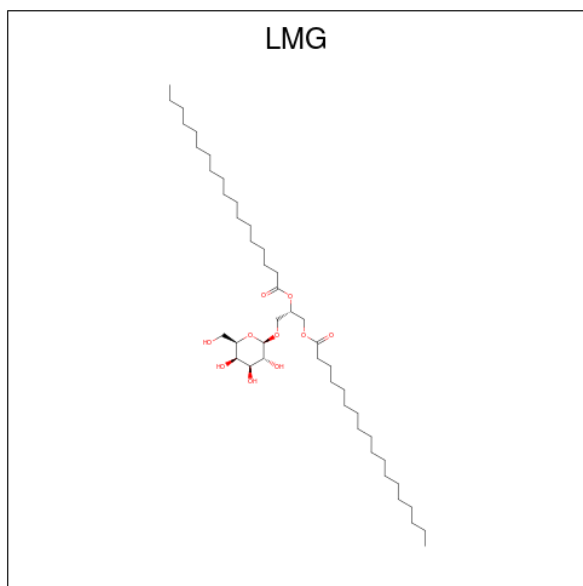
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			10	8	2	

- Molecule 30 is LAURIC ACID (three-letter code: DAO) (formula:  $C_{12}H_{24}O_2$ ).



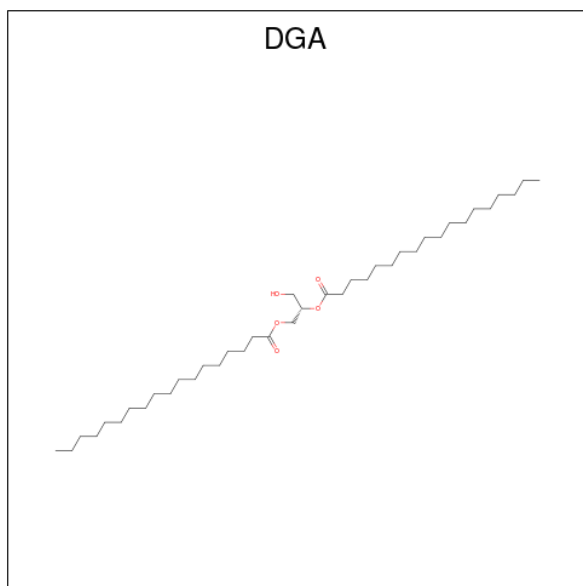
Mol	Chain	Residues	Atoms			AltConf
30	A	1	Total	C	O	0
			14	12	2	

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



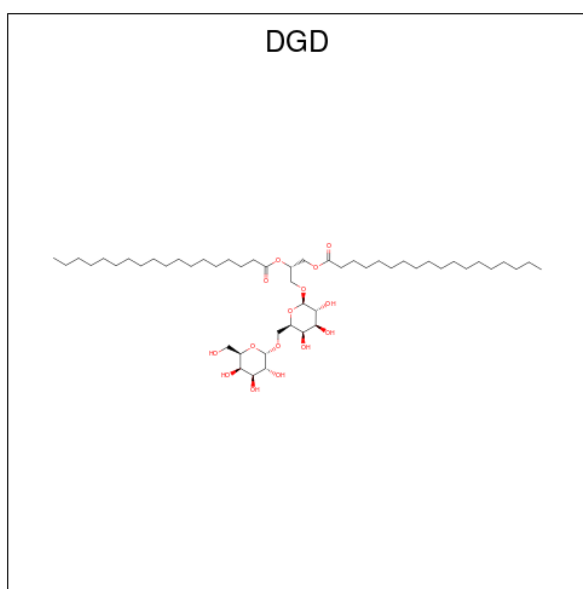
Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			29	19	10	
31	J	1	Total	C	O	0
			35	25	10	

- Molecule 32 is DIACYL GLYCEROL (three-letter code: DGA) (formula:  $C_{39}H_{76}O_5$ ).



Mol	Chain	Residues	Atoms			AltConf
32	A	1	Total	C	O	0
			44	39	5	
32	9	1	Total	C	O	0
			39	34	5	

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



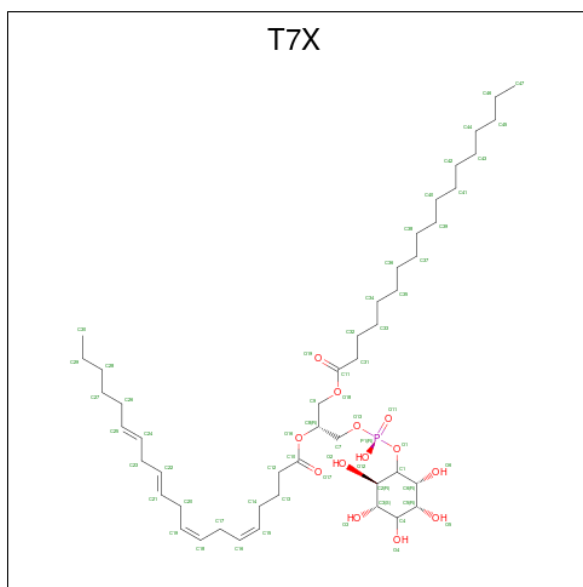


Mol	Chain	Residues	Atoms			AltConf
33	B	1	Total	C	O	0
			66	51	15	

- Molecule 34 is CALCIUM ION (three-letter code: CA) (formula: Ca).

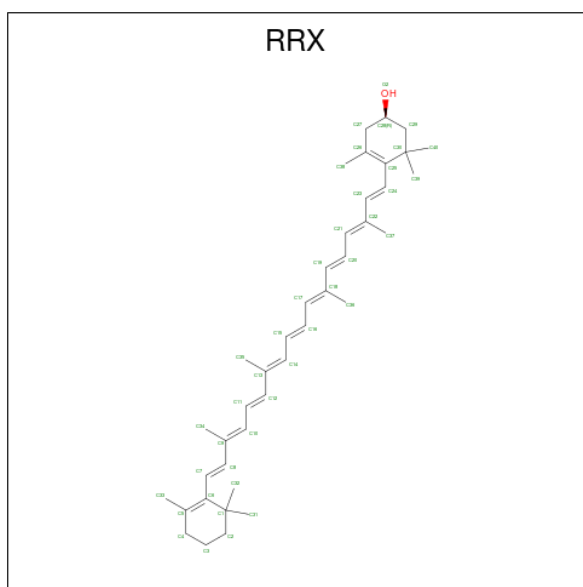
Mol	Chain	Residues	Atoms		AltConf
34	B	1	Total	Ca	0
			1	1	

- Molecule 35 is Phosphatidylinositol (three-letter code: T7X) (formula: C<sub>47</sub>H<sub>83</sub>O<sub>13</sub>P).



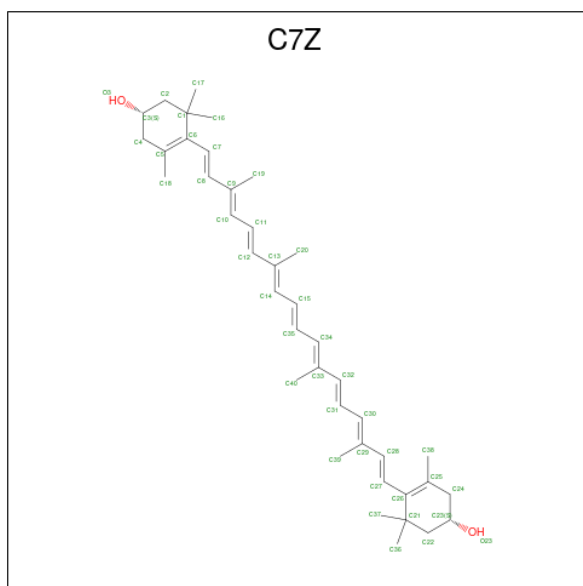
Mol	Chain	Residues	Atoms				AltConf
35	B	1	Total	C	O	P	0
			49	35	13	1	

- Molecule 36 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: C<sub>40</sub>H<sub>56</sub>O).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
36	F	1	41	40	1	0

- Molecule 37 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (three-letter code: C7Z) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



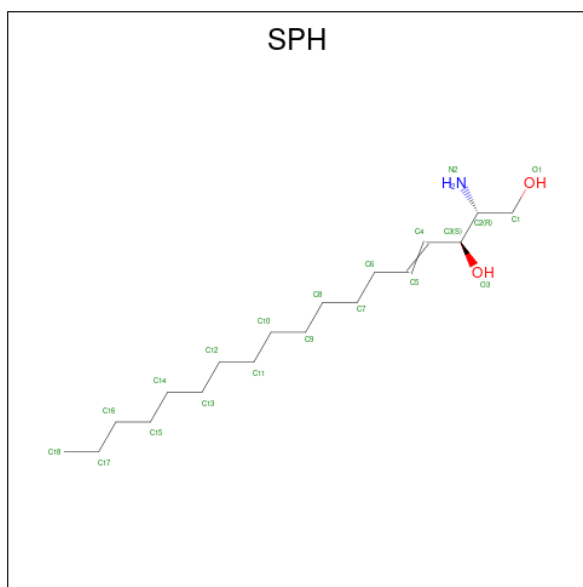
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
37	J	1	42	40	2	0

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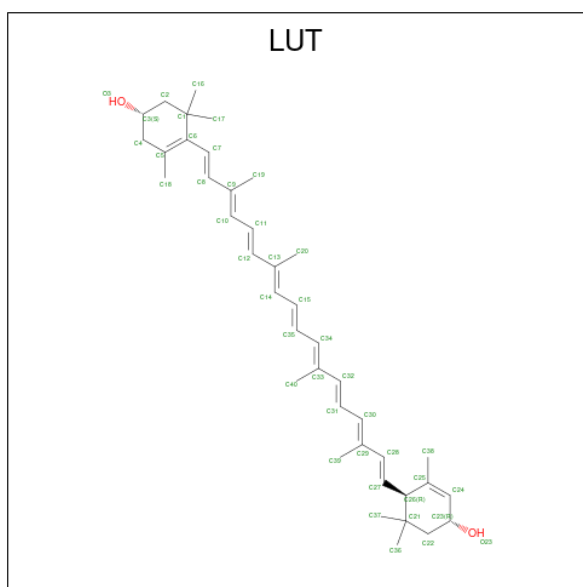
Mol	Chain	Residues	Atoms			AltConf
37	1	1	Total	C	O	0
			42	40	2	
37	5	1	Total	C	O	0
			42	40	2	

- Molecule 38 is SPHINGOSINE (three-letter code: SPH) (formula:  $C_{18}H_{37}NO_2$ ).



Mol	Chain	Residues	Atoms				AltConf
38	K	1	Total	C	N	O	0
			21	18	1	2	
38	7	1	Total	C	N	O	0
			42	36	2	4	
38	7	1	Total	C	N	O	0
			42	36	2	4	

- Molecule 39 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula:  $C_{40}H_{56}O_2$ ).



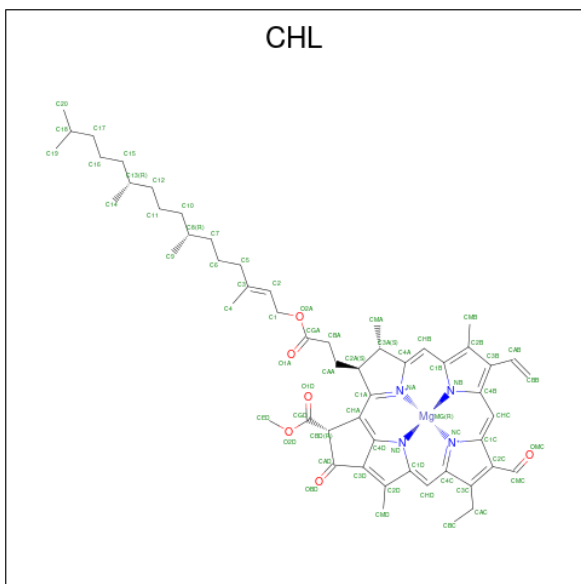
Mol	Chain	Residues	Atoms			AltConf
39	1	1	Total	C	O	0
			84	80	4	
39	1	1	Total	C	O	0
			84	80	4	
39	Z	1	Total	C	O	0
			126	120	6	
39	Z	1	Total	C	O	0
			126	120	6	
39	Z	1	Total	C	O	0
			126	120	6	
39	3	1	Total	C	O	0
			84	80	4	
39	3	1	Total	C	O	0
			84	80	4	
39	7	1	Total	C	O	0
			84	80	4	
39	7	1	Total	C	O	0
			84	80	4	
39	8	1	Total	C	O	0
			84	80	4	
39	8	1	Total	C	O	0
			84	80	4	
39	4	1	Total	C	O	0
			84	80	4	
39	4	1	Total	C	O	0
			84	80	4	
39	5	1	Total	C	O	0
			84	80	4	

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
39	5	1	84	80	4	0
39	6	1	84	80	4	0
39	6	1	84	80	4	0
39	2	1	126	120	6	0
39	2	1	126	120	6	0
39	2	1	126	120	6	0
39	9	1	84	80	4	0
39	9	1	84	80	4	0

- Molecule 40 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	
40	1	1	106	84	2	8	12	0
40	1	1	106	84	2	8	12	0
40	Z	1	178	145	3	12	18	0

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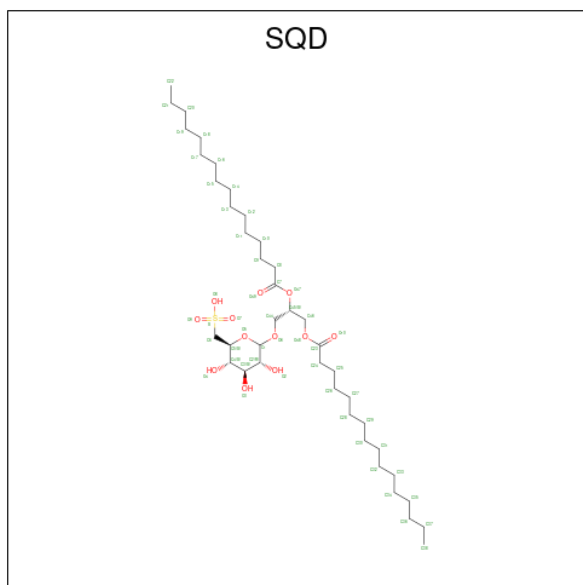
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
40	Z	1	Total 178	C 145	Mg 3	N 12	O 18	0
40	Z	1	Total 178	C 145	Mg 3	N 12	O 18	0
40	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
40	7	1	Total 54	C 43	Mg 1	N 4	O 6	0
40	8	1	Total 122	C 100	Mg 2	N 8	O 12	0
40	8	1	Total 122	C 100	Mg 2	N 8	O 12	0
40	4	1	Total 201	C 159	Mg 4	N 16	O 22	0
40	4	1	Total 201	C 159	Mg 4	N 16	O 22	0
40	4	1	Total 201	C 159	Mg 4	N 16	O 22	0
40	4	1	Total 201	C 159	Mg 4	N 16	O 22	0
40	5	1	Total 160	C 129	Mg 3	N 12	O 16	0
40	5	1	Total 160	C 129	Mg 3	N 12	O 16	0
40	5	1	Total 160	C 129	Mg 3	N 12	O 16	0
40	6	1	Total 206	C 164	Mg 4	N 16	O 22	0
40	6	1	Total 206	C 164	Mg 4	N 16	O 22	0
40	6	1	Total 206	C 164	Mg 4	N 16	O 22	0
40	6	1	Total 206	C 164	Mg 4	N 16	O 22	0
40	2	1	Total 150	C 117	Mg 3	N 12	O 18	0
40	2	1	Total 150	C 117	Mg 3	N 12	O 18	0
40	2	1	Total 150	C 117	Mg 3	N 12	O 18	0
40	9	1	Total 108	C 88	Mg 2	N 8	O 10	0

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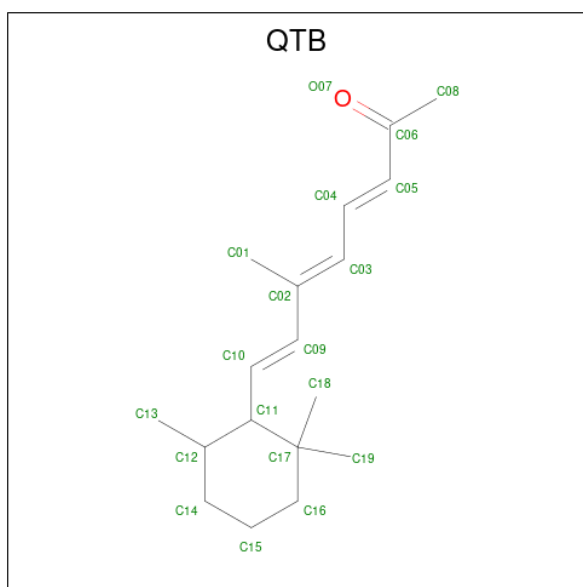
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
40	9	1	108	88	2	8	10	0

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



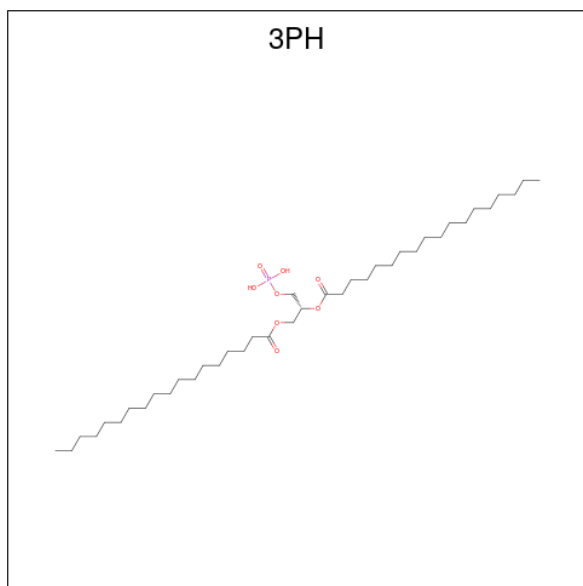
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
41	1	1	48	35	12	1	0
41	2	1	43	30	12	1	0

- Molecule 42 is (3 {E},5 {E},7 {E})-6-methyl-8-[(6 {R})-2,2,6-trimethylcyclohexyl]octa-3,5,7-trien-2-one (three-letter code: QTB) (formula:  $C_{18}H_{28}O$ ).



Mol	Chain	Residues	Atoms			AltConf
42	Z	1	Total	C	O	0
			19	18	1	

- Molecule 43 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula:  $C_{39}H_{77}O_8P$ ).



Mol	Chain	Residues	Atoms				AltConf
43	7	1	Total	C	O	P	0
			39	30	8	1	
43	8	1	Total	C	O	P	0
			30	21	8	1	

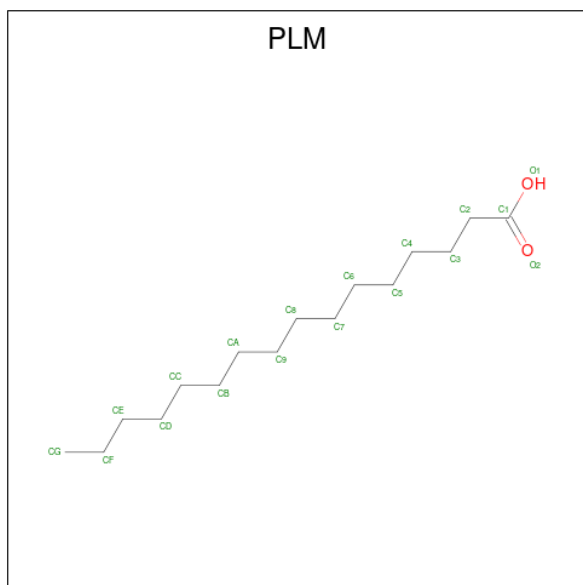
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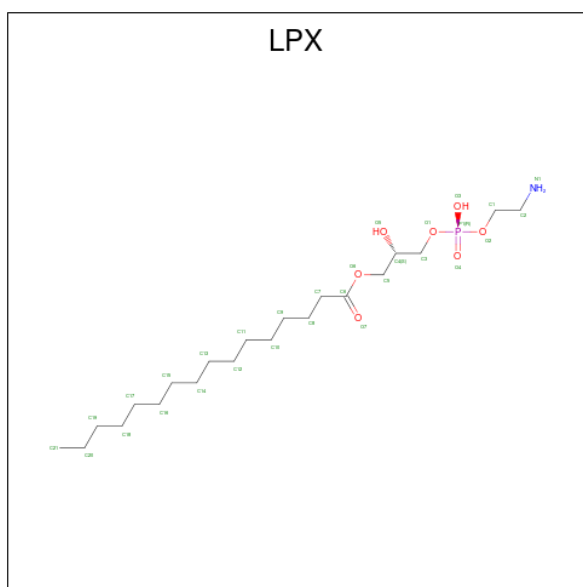
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
43	5	1	23	14	8	1	0
43	6	1	29	20	8	1	0
43	2	1	27	18	8	1	0

- Molecule 44 is PALMITIC ACID (three-letter code: PLM) (formula:  $C_{16}H_{32}O_2$ ).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
44	7	1	18	16	2	0

- Molecule 45 is (2S)-3-[[[R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy]-2-hydroxypropyl hexadecanoate (three-letter code: LPX) (formula:  $C_{21}H_{44}NO_7P$ ).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
45	8	1	30	21	1	7	1	0

- Molecule 46 is water.

Mol	Chain	Residues	Atoms		AltConf
46	A	2	Total	O	0
			91	91	
46	A	15	Total	O	0
			91	91	
46	A	2	Total	O	0
			91	91	
46	A	6	Total	O	0
			91	91	
46	A	9	Total	O	0
			91	91	
46	A	2	Total	O	0
			91	91	
46	A	7	Total	O	0
			91	91	
46	A	18	Total	O	0
			91	91	
46	A	8	Total	O	0
			91	91	
46	A	14	Total	O	0
			91	91	
46	A	1	Total	O	0
			91	91	

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Mol	Chain	Residues	Atoms	AltConf
46	A	1	Total O 91 91	0
46	A	1	Total O 91 91	0
46	A	1	Total O 91 91	0
46	A	1	Total O 91 91	0
46	A	1	Total O 91 91	0
46	A	1	Total O 91 91	0
46	A	1	Total O 91 91	0
46	B	1	Total O 79 79	0
46	B	1	Total O 79 79	0
46	B	1	Total O 79 79	0
46	B	1	Total O 79 79	0
46	B	1	Total O 79 79	0
46	B	2	Total O 79 79	0
46	B	12	Total O 79 79	0
46	B	10	Total O 79 79	0
46	B	16	Total O 79 79	0
46	B	2	Total O 79 79	0
46	B	2	Total O 79 79	0
46	B	1	Total O 79 79	0
46	B	28	Total O 79 79	0
46	B	1	Total O 79 79	0

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Mol	Chain	Residues	Atoms		AltConf
46	C	1	Total 19	O 19	0
46	C	1	Total 19	O 19	0
46	C	1	Total 19	O 19	0
46	C	1	Total 19	O 19	0
46	C	1	Total 19	O 19	0
46	C	12	Total 19	O 19	0
46	C	1	Total 19	O 19	0
46	C	1	Total 19	O 19	0
46	D	1	Total 12	O 12	0
46	D	1	Total 12	O 12	0
46	D	1	Total 12	O 12	0
46	D	2	Total 12	O 12	0
46	D	1	Total 12	O 12	0
46	D	2	Total 12	O 12	0
46	D	1	Total 12	O 12	0
46	D	2	Total 12	O 12	0
46	D	1	Total 12	O 12	0
46	E	1	Total 7	O 7	0
46	E	4	Total 7	O 7	0
46	E	1	Total 7	O 7	0
46	E	1	Total 7	O 7	0

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Mol	Chain	Residues	Atoms		AltConf
46	F	1	Total 14	O 14	0
46	F	1	Total 14	O 14	0
46	F	2	Total 14	O 14	0
46	F	8	Total 14	O 14	0
46	F	1	Total 14	O 14	0
46	F	1	Total 14	O 14	0
46	J	2	Total 3	O 3	0
46	J	1	Total 3	O 3	0
46	K	2	Total 2	O 2	0
46	L	1	Total 5	O 5	0
46	L	1	Total 5	O 5	0
46	L	1	Total 5	O 5	0
46	L	2	Total 5	O 5	0
46	1	16	Total 16	O 16	0
46	Z	1	Total 8	O 8	0
46	Z	7	Total 8	O 8	0
46	3	17	Total 17	O 17	0
46	7	18	Total 18	O 18	0
46	8	1	Total 16	O 16	0
46	8	15	Total 16	O 16	0
46	4	7	Total 7	O 7	0

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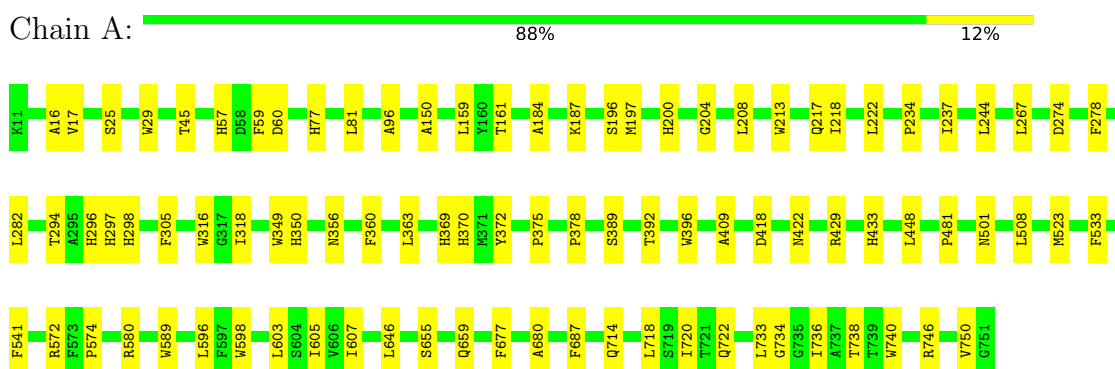
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Mol	Chain	Residues	Atoms	AltConf
46	5	9	Total O 9 9	0
46	6	8	Total O 8 8	0
46	2	4	Total O 4 4	0
46	9	2	Total O 2 2	0

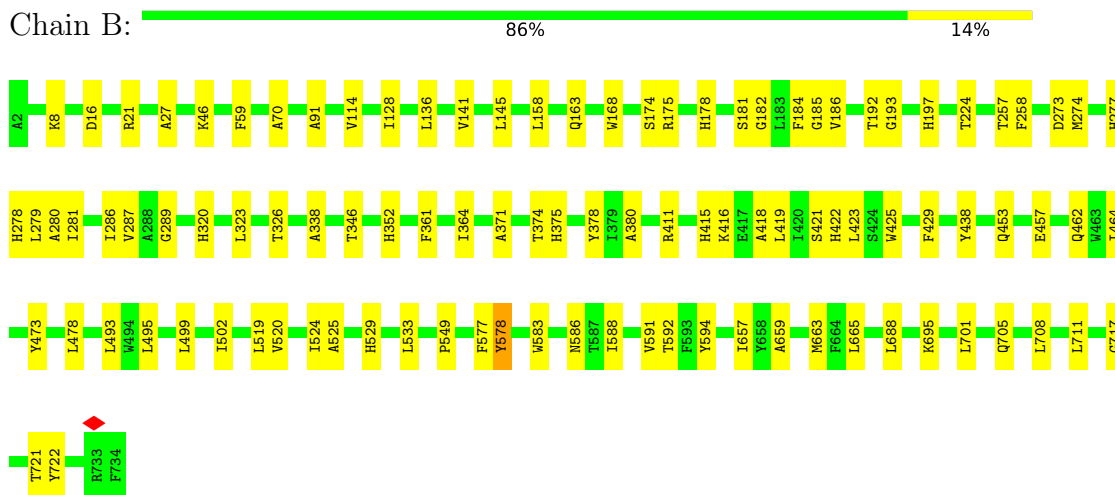
### 3 Residue-property plots

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

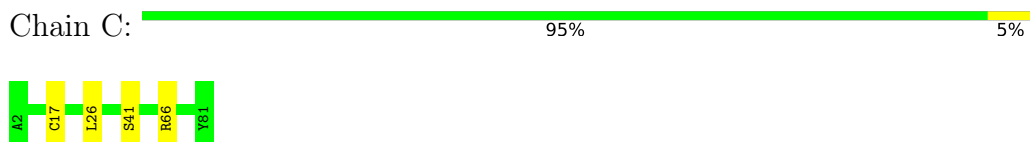
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



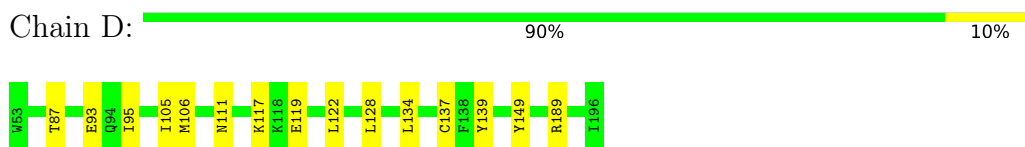
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



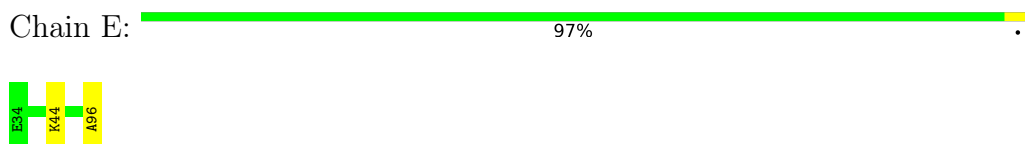
- Molecule 3: Photosystem I iron-sulfur center



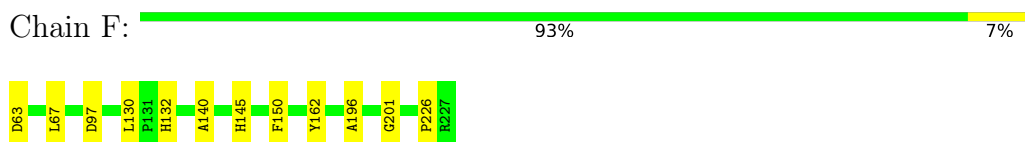
- Molecule 4: Photosystem I reaction center subunit II, chloroplastic



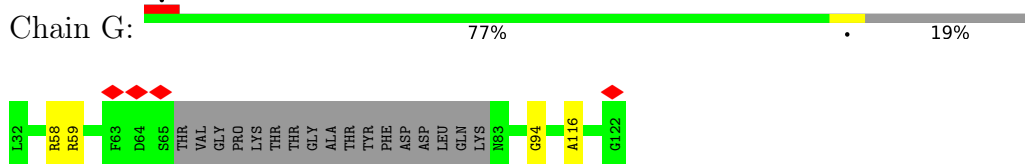
- Molecule 5: Photosystem I reaction center subunit IV, chloroplastic



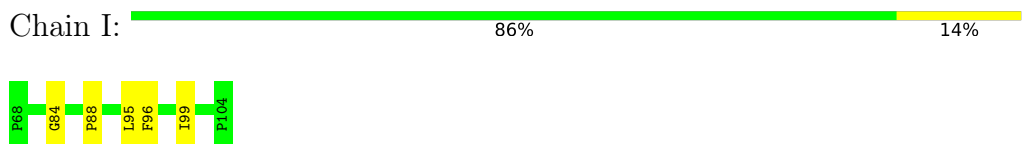
- Molecule 6: Photosystem I reaction center subunit III, chloroplastic



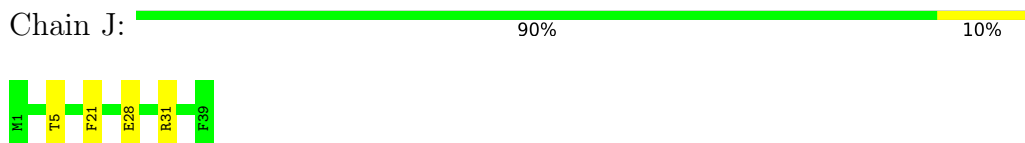
- Molecule 7: Photosystem I reaction center subunit V, chloroplastic



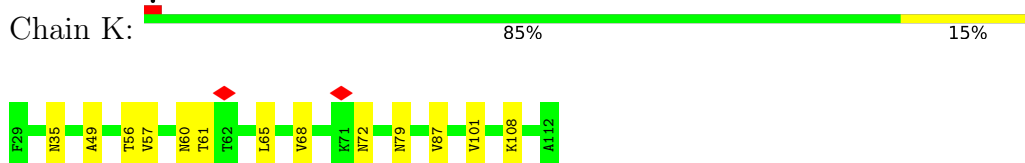
- Molecule 8: Photosystem I reaction center subunit VIII



- Molecule 9: Photosystem I reaction center subunit IX

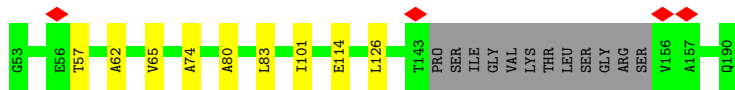
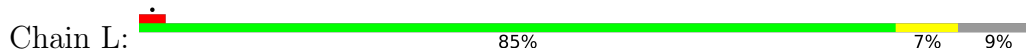


- Molecule 10: Photosystem I reaction center subunit psaK, chloroplastic

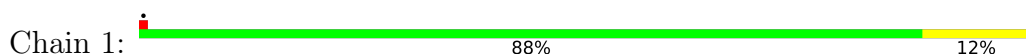




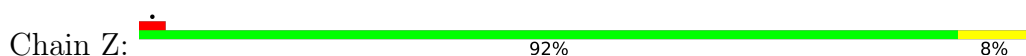
• Molecule 11: PSI subunit V



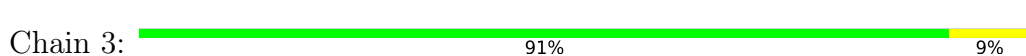
• Molecule 12: Chlorophyll a-b binding protein, chloroplastic



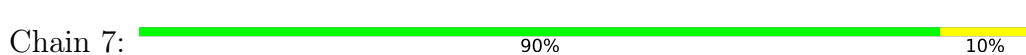
• Molecule 12: Chlorophyll a-b binding protein, chloroplastic



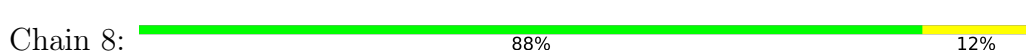
• Molecule 13: Chlorophyll a-b binding protein, chloroplastic



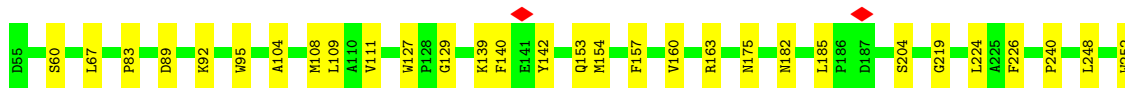
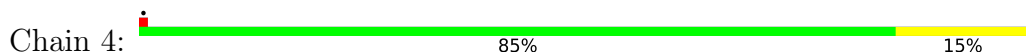
• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

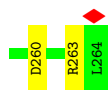


• Molecule 15: Chlorophyll a-b binding protein, chloroplastic

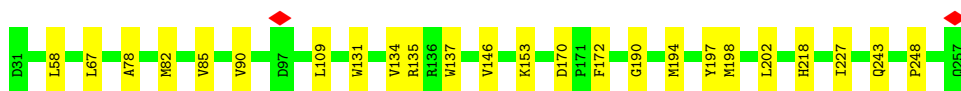
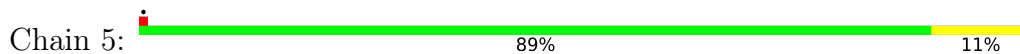


• Molecule 16: Chlorophyll a-b binding protein, chloroplastic





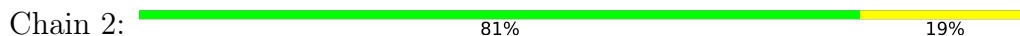
- Molecule 17: Chlorophyll a-b binding protein, chloroplastic



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



- Molecule 19: Chlorophyll a-b binding protein, chloroplastic



- Molecule 20: 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	103082	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	46.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	165000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.125	Depositor
Minimum map value	-0.058	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.01	Depositor
Map size ( $\text{\AA}$ )	264.64, 264.64, 264.64	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.827, 0.827, 0.827	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: RRX, DAO, PLM, QTB, CL0, 3PH, BCR, LUT, CLA, SQD, LPX, LMG, CA, NKP, DGA, CHL, SPH, T7X, C7Z, PQN, SF4, SNC, OCA, LHG, LMT, DGD

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	0.31	0/6016	0.51	0/8201
2	B	0.33	1/6037 (0.0%)	0.53	0/8242
3	C	0.26	0/611	0.56	0/826
4	D	0.28	0/1154	0.56	0/1556
5	E	0.28	0/507	0.50	0/689
6	F	0.29	0/1292	0.51	0/1747
7	G	0.28	0/561	0.47	0/760
8	I	0.32	0/294	0.55	0/406
9	J	0.29	0/332	0.46	0/454
10	K	0.26	0/576	0.46	0/779
11	L	0.29	0/935	0.50	0/1277
12	1	0.28	0/1491	0.45	0/2028
12	Z	0.27	0/1491	0.44	0/2028
13	3	0.31	0/1722	0.51	0/2336
14	7	0.29	0/1702	0.49	0/2310
15	8	0.28	0/1701	0.45	0/2315
16	4	0.28	0/1683	0.47	0/2296
17	5	0.28	0/1830	0.47	0/2492
18	6	0.27	0/1828	0.48	0/2497
19	2	0.28	0/1556	0.52	0/2109
20	9	0.30	0/1447	0.54	0/1967
All	All	0.30	1/34766 (0.0%)	0.50	0/47315

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	578	TYR	CD1-CE1	-5.13	1.31	1.39

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 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	5820	0	5670	75	0
2	B	5825	0	5579	84	0
3	C	601	0	581	3	0
4	D	1135	0	1148	7	0
5	E	497	0	491	1	0
6	F	1266	0	1301	9	0
7	G	550	0	532	3	0
8	I	282	0	292	4	0
9	J	321	0	322	4	0
10	K	571	0	606	11	0
11	L	914	0	921	6	0
12	1	1445	0	1396	19	0
12	Z	1445	0	1396	16	0
13	3	1674	0	1633	18	0
14	7	1650	0	1589	18	0
15	8	1650	0	1629	19	0
16	4	1628	0	1576	25	0
17	5	1775	0	1746	24	0
18	6	1766	0	1765	20	0
19	2	1518	0	1512	32	0
20	9	1406	0	1386	20	0
21	A	65	0	72	5	0
22	1	712	0	712	30	0
22	2	500	0	398	12	0
22	3	748	0	720	32	0
22	4	613	0	567	22	0
22	5	799	0	758	35	0
22	6	759	0	741	31	0
22	7	790	0	752	26	0
22	8	694	0	671	25	0
22	9	531	0	464	17	0
22	A	2699	0	2865	138	0
22	B	2680	0	2837	127	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	F	110	0	105	6	0
22	G	96	0	72	0	0
22	J	42	0	31	3	0
22	K	205	0	168	8	0
22	L	115	0	110	2	0
22	Z	622	0	584	23	0
23	A	33	0	46	1	0
23	B	33	0	46	0	0
24	A	8	0	0	0	0
24	C	16	0	0	1	0
25	3	160	0	211	10	0
25	4	40	0	53	2	0
25	5	80	0	105	7	0
25	6	80	0	106	4	0
25	7	80	0	106	4	0
25	8	40	0	53	1	0
25	A	200	0	264	15	0
25	B	280	0	370	18	0
25	G	40	0	53	1	0
25	I	40	0	52	3	0
25	J	40	0	53	4	0
25	K	80	0	106	6	0
25	L	80	0	106	3	0
26	1	43	0	56	1	0
26	2	34	0	38	2	0
26	3	20	0	12	0	0
26	4	81	0	108	1	0
26	5	37	0	44	0	0
26	6	49	0	74	4	0
26	7	37	0	44	2	0
26	8	38	0	46	0	0
26	9	33	0	36	0	0
26	A	84	0	114	8	0
26	B	76	0	64	3	0
26	Z	43	0	56	1	0
27	3	16	0	12	0	0
27	8	29	0	39	0	0
27	A	29	0	39	0	0
28	1	35	0	45	3	0
28	4	35	0	44	1	0
28	8	35	0	46	0	0
28	9	35	0	45	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	A	35	0	46	1	0
28	B	70	0	90	5	0
28	F	35	0	45	0	0
29	A	10	0	15	0	0
30	A	14	0	23	0	0
31	A	29	0	28	1	0
31	J	35	0	40	1	0
32	9	39	0	63	4	0
32	A	44	0	76	4	0
33	B	66	0	96	4	0
34	B	1	0	0	0	0
35	B	49	0	0	0	0
36	F	41	0	56	1	0
37	1	42	0	0	0	0
37	5	42	0	0	0	0
37	J	42	0	0	0	0
38	7	42	0	74	2	0
38	K	21	0	37	1	0
39	1	84	0	110	6	0
39	2	126	0	165	7	0
39	3	84	0	110	7	0
39	4	84	0	110	11	0
39	5	84	0	110	9	0
39	6	84	0	110	4	0
39	7	84	0	110	3	0
39	8	84	0	110	6	0
39	9	84	0	110	6	0
39	Z	126	0	165	8	0
40	1	106	0	82	3	0
40	2	150	0	105	7	0
40	3	66	0	69	4	0
40	4	201	0	146	8	0
40	5	160	0	134	10	0
40	6	206	0	156	6	0
40	7	54	0	42	3	0
40	8	122	0	115	4	0
40	9	108	0	97	2	0
40	Z	178	0	168	12	0
41	1	48	0	62	1	0
41	2	43	0	49	2	0
42	Z	19	0	0	0	0
43	2	27	0	27	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	5	23	0	19	0	0
43	6	29	0	31	0	0
43	7	39	0	51	1	0
43	8	30	0	33	0	0
44	7	18	0	31	0	0
45	8	30	0	43	1	0
46	1	16	0	0	0	0
46	2	4	0	0	0	0
46	3	17	0	0	0	0
46	4	7	0	0	0	0
46	5	9	0	0	0	0
46	6	8	0	0	0	0
46	7	18	0	0	0	0
46	8	16	0	0	0	0
46	9	2	0	0	0	0
46	A	91	0	0	1	0
46	B	79	0	0	1	0
46	C	19	0	0	0	0
46	D	12	0	0	0	0
46	E	7	0	0	0	0
46	F	14	0	0	0	0
46	J	3	0	0	0	0
46	K	2	0	0	0	0
46	L	5	0	0	0	0
46	Z	8	0	0	0	0
All	All	52213	0	51749	839	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 (839) 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)
19:2:117:VAL:O	19:2:121:LEU:HD13	1.73	0.88
22:B:1220:CLA:HAB	22:B:1227:CLA:HMD2	1.59	0.84
1:A:396:TRP:CD1	22:A:1126:CLA:HAB	2.15	0.82
22:A:1138:CLA:H121	22:A:1138:CLA:HAB	1.64	0.79
22:B:1240:CLA:HBB1	22:1:605:CLA:H12	1.68	0.74
22:F:1301:CLA:HBB1	36:F:4001:RRX:H11	1.67	0.74
22:B:1218:CLA:HMD2	25:B:4001:BCR:HC7	1.70	0.73
22:B:1238:CLA:H2	22:B:1239:CLA:H142	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:1012:CLA:H2	25:A:4005:BCR:H362	1.72	0.70
1:A:204:GLY:O	1:A:208:LEU:HB2	1.91	0.70
22:A:1120:CLA:HMD2	25:K:4001:BCR:H24C	1.72	0.70
22:B:1203:CLA:H151	22:B:1225:CLA:HBB2	1.73	0.70
22:B:1234:CLA:HMB2	22:B:1236:CLA:HED1	1.73	0.69
2:B:141:VAL:O	2:B:145:LEU:HD23	1.93	0.68
16:4:153:GLN:NE2	40:4:610:CHL:OMC	2.26	0.68
39:2:501:LUT:H361	39:2:501:LUT:H393	1.74	0.68
22:A:1127:CLA:H2	25:A:4002:BCR:HC7	1.76	0.68
2:B:352:HIS:ND1	22:B:1214:CLA:OBD	2.27	0.68
22:A:1124:CLA:H61	22:A:1133:CLA:HAB	1.75	0.67
22:B:1237:CLA:HMC2	22:B:1238:CLA:H11	1.75	0.67
22:A:1110:CLA:H161	22:A:1118:CLA:HBB1	1.76	0.67
39:6:501:LUT:H30	22:6:601:CLA:H72	1.77	0.66
1:A:370:HIS:ND1	22:A:1116:CLA:OBD	2.29	0.66
19:2:117:VAL:O	19:2:121:LEU:CD1	2.42	0.66
22:2:604:CLA:HHD	40:2:609:CHL:HBB2	1.78	0.65
22:A:1104:CLA:H151	22:A:1127:CLA:HBB2	1.77	0.65
25:3:504:BCR:HC21	22:5:609:CLA:H112	1.78	0.65
22:A:1012:CLA:HAB	2:B:583:TRP:CH2	2.31	0.65
1:A:305:PHE:HE1	22:A:1119:CLA:HAB	1.60	0.65
22:A:1126:CLA:H191	25:J:4001:BCR:H19C	1.79	0.65
22:B:1023:CLA:H152	25:B:4007:BCR:H16C	1.79	0.64
15:8:181:GLU:OE1	15:8:184:LYS:NZ	2.30	0.64
22:1:603:CLA:H111	22:1:603:CLA:HAB	1.77	0.64
25:A:4005:BCR:H24C	22:B:1230:CLA:HMC2	1.80	0.63
2:B:27:ALA:HA	22:B:1226:CLA:H42	1.80	0.62
14:7:109:VAL:HG21	22:7:606:CLA:HAA2	1.80	0.62
12:1:82:MET:SD	22:1:601:CLA:HAB	2.39	0.62
17:5:82:MET:SD	22:5:601:CLA:HAB	2.40	0.62
13:3:65:ALA:HB1	13:3:191:GLY:HA3	1.82	0.62
22:B:1227:CLA:HBB2	22:B:1236:CLA:HMC2	1.82	0.61
22:A:1121:CLA:H192	25:K:4001:BCR:H21C	1.82	0.61
22:A:1107:CLA:H42	25:J:4001:BCR:H10C	1.83	0.61
17:5:85:VAL:HG11	39:5:501:LUT:H12	1.83	0.61
22:B:1201:CLA:HMA2	22:B:1241:CLA:HMD2	1.83	0.60
15:8:81:MET:SD	22:8:601:CLA:HAB	2.41	0.60
18:6:79:MET:SD	22:6:601:CLA:HAB	2.41	0.60
2:B:722:TYR:HB2	22:B:1021:CLA:HED3	1.83	0.60
39:9:502:LUT:H32	22:9:604:CLA:HBB1	1.83	0.60
40:2:609:CHL:HBC3	26:2:801:LHG:HC62	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:1133:CLA:HMD2	22:A:1134:CLA:HAB	1.84	0.60
1:A:196:SER:O	1:A:200:HIS:ND1	2.25	0.59
2:B:46:LYS:HD3	22:B:1241:CLA:HMD1	1.84	0.59
22:B:1209:CLA:HBB2	22:B:1217:CLA:H72	1.84	0.59
25:B:4004:BCR:HC41	28:B:5005:LMT:H112	1.82	0.59
22:6:609:CLA:H2	26:6:801:LHG:H141	1.85	0.59
20:9:157:LYS:HD3	22:9:602:CLA:HBD	1.83	0.59
6:F:63:ASP:N	6:F:67:LEU:O	2.35	0.59
17:5:78:ALA:HB1	17:5:190:GLY:HA3	1.83	0.59
16:4:104:ALA:HB1	16:4:219:GLY:HA3	1.84	0.59
25:5:503:BCR:H10C	22:6:608:CLA:H52	1.85	0.59
22:A:1102:CLA:HMA2	22:A:1109:CLA:HMD2	1.85	0.58
22:A:1106:CLA:H71	25:J:4001:BCR:H343	1.85	0.58
2:B:429:PHE:CE2	22:B:1235:CLA:HAB	2.38	0.58
20:9:119:MET:HG3	22:9:612:CLA:HMC3	1.85	0.58
12:Z:149:TYR:HB3	22:Z:601:CLA:HED3	1.86	0.57
22:A:1112:CLA:H122	32:A:5005:DGA:HBW1	1.84	0.57
25:B:4004:BCR:H24C	25:B:4005:BCR:H24C	1.86	0.57
1:A:448:LEU:HB3	1:A:541:PHE:HB2	1.86	0.57
13:3:69:MET:SD	22:3:601:CLA:HAB	2.44	0.57
39:9:501:LUT:H30	22:9:601:CLA:H72	1.85	0.57
22:B:1240:CLA:HBC1	28:B:5005:LMT:H6E	1.87	0.57
12:Z:82:MET:SD	22:Z:601:CLA:HAB	2.44	0.57
22:7:609:CLA:H162	22:7:603:CLA:HBC1	1.85	0.57
2:B:464:ILE:HD11	22:B:1234:CLA:H2	1.87	0.57
14:7:165:PRO:HB3	22:7:611:CLA:HBC2	1.87	0.57
22:5:605:CLA:H52	22:5:622:CLA:HAB	1.85	0.57
25:4:503:BCR:H19C	40:4:613:CHL:H11	1.87	0.57
18:6:82:VAL:HG11	39:6:501:LUT:H12	1.87	0.56
19:2:213:VAL:HG22	32:9:802:DGA:HBS2	1.86	0.56
1:A:508:LEU:HB2	1:A:523:MET:HG3	1.87	0.56
22:A:1139:CLA:HBA2	26:A:5002:LHG:H161	1.87	0.56
2:B:70:ALA:HB2	2:B:136:LEU:HB2	1.86	0.56
18:6:91:VAL:HG12	18:6:92:ARG:HG2	1.86	0.56
13:3:100:VAL:HG21	39:3:502:LUT:H22	1.87	0.56
39:1:502:LUT:H382	22:1:604:CLA:H2	1.86	0.56
22:7:602:CLA:HBB1	22:7:607:CLA:H143	1.88	0.56
1:A:45:THR:HG22	1:A:714:GLN:HB2	1.87	0.56
22:A:1117:CLA:HAB	22:A:1117:CLA:H8	1.87	0.56
2:B:184:PHE:HZ	22:B:1221:CLA:H12	1.71	0.56
2:B:525:ALA:O	2:B:529:HIS:ND1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:7:189:LYS:HG3	22:7:607:CLA:HED2	1.87	0.56
22:A:1129:CLA:HMA2	11:L:57:THR:HG21	1.87	0.56
4:D:95:ILE:HG12	4:D:105:ILE:HG12	1.87	0.56
22:8:605:CLA:H122	22:8:604:CLA:H91	1.88	0.56
22:A:1012:CLA:HMA1	22:B:1021:CLA:H202	1.87	0.56
22:Z:605:CLA:H192	40:8:613:CHL:H11	1.86	0.55
12:1:140:GLN:HB3	22:1:611:CLA:HMC3	1.88	0.55
22:A:1119:CLA:H122	22:A:1122:CLA:H93	1.87	0.55
22:A:1120:CLA:HMB2	22:A:1121:CLA:H52	1.87	0.55
3:C:17:CYS:HB3	24:C:3003:SF4:S4	2.47	0.55
40:Z:609:CHL:HHC	40:Z:609:CHL:HBB1	1.88	0.55
16:4:127:TRP:NE1	16:4:129:GLY:O	2.39	0.55
2:B:274:MET:O	2:B:278:HIS:ND1	2.40	0.55
22:A:1104:CLA:H2	22:A:1104:CLA:HED2	1.89	0.55
2:B:174:SER:O	2:B:178:HIS:ND1	2.26	0.55
22:5:612:CLA:H43	22:6:619:CLA:H92	1.89	0.55
22:A:1125:CLA:HMA1	22:A:1133:CLA:H51	1.89	0.55
22:B:1234:CLA:H142	22:B:1236:CLA:H62	1.89	0.55
12:1:46:PRO:HG2	12:1:49:LEU:HB2	1.89	0.55
22:8:609:CLA:H41	22:8:608:CLA:H42	1.88	0.55
17:5:109:LEU:HD21	22:5:613:CLA:HAC1	1.89	0.55
20:9:28:ARG:NH1	20:9:48:ASP:OD1	2.40	0.55
16:4:108:MET:SD	22:4:601:CLA:HAB	2.46	0.54
17:5:202:LEU:HD12	22:5:603:CLA:HAC2	1.88	0.54
1:A:197:MET:HB2	22:A:1111:CLA:HBC2	1.89	0.54
1:A:429:ARG:O	1:A:433:HIS:ND1	2.41	0.54
1:A:596:LEU:HD21	22:A:1128:CLA:HBC1	1.88	0.54
13:3:147:PHE:CE2	40:3:611:CHL:HBB2	2.42	0.54
25:3:504:BCR:H10C	40:3:611:CHL:HBA1	1.89	0.54
22:3:616:CLA:H8	22:3:616:CLA:HBB1	1.88	0.54
18:6:205:LEU:HD12	39:6:501:LUT:H163	1.89	0.54
19:2:209:VAL:HG13	32:9:802:DGA:HBT2	1.90	0.54
20:9:126:ARG:HA	20:9:142:PHE:HZ	1.71	0.54
8:I:96:PHE:HB2	25:L:4001:BCR:H14C	1.90	0.54
22:B:1205:CLA:HAB	22:B:1206:CLA:HAA1	1.90	0.54
1:A:396:TRP:HD1	22:A:1126:CLA:HAB	1.70	0.54
22:A:1115:CLA:H91	22:K:1402:CLA:HBC3	1.90	0.54
14:7:123:ILE:HG12	22:8:608:CLA:HAA2	1.89	0.54
1:A:305:PHE:CE1	22:A:1119:CLA:HAB	2.40	0.54
2:B:258:PHE:CD1	22:B:1214:CLA:HMB2	2.43	0.54
25:5:504:BCR:H361	40:5:610:CHL:HBA2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:201:GLY:HA3	15:8:59:LEU:HD21	1.89	0.54
26:Z:801:LHG:HC82	25:4:503:BCR:HC22	1.89	0.54
22:5:602:CLA:H141	22:5:607:CLA:H13	1.90	0.54
26:B:5001:LHG:O3	26:B:5001:LHG:O1	2.26	0.53
12:1:193:ALA:HB2	22:1:615:CLA:HED3	1.90	0.53
2:B:8:LYS:HE2	22:B:1241:CLA:HAA1	1.90	0.53
1:A:646:LEU:HD12	22:B:1021:CLA:HMC3	1.91	0.53
2:B:192:THR:HG21	2:B:279:LEU:HB2	1.89	0.53
22:K:1401:CLA:HBB1	25:K:4002:BCR:H10C	1.89	0.53
17:5:172:PHE:HD2	39:5:501:LUT:H222	1.73	0.53
18:6:255:LEU:HD13	22:6:615:CLA:HMB3	1.91	0.53
14:7:97:LEU:HD12	22:7:616:CLA:HMA2	1.89	0.53
16:4:260:ASP:OD1	16:4:263:ARG:NH2	2.40	0.53
2:B:182:GLY:HA3	22:B:1210:CLA:HBB1	1.91	0.53
18:6:121:MET:HG3	22:6:612:CLA:HMC3	1.90	0.53
32:9:802:DGA:HBN2	28:9:803:LMT:H101	1.90	0.53
1:A:572:ARG:NH1	26:A:5002:LHG:O10	2.42	0.53
2:B:549:PRO:HB3	6:F:226:PRO:HG2	1.90	0.53
14:7:195:ARG:NH2	22:7:604:CLA:O1D	2.41	0.53
12:1:119:VAL:HG11	22:1:613:CLA:HMD1	1.90	0.53
13:3:62:VAL:HG11	13:3:161:ALA:HB1	1.91	0.52
25:5:503:BCR:H19C	22:5:613:CLA:H2	1.92	0.52
39:4:501:LUT:H30	22:4:601:CLA:H52	1.91	0.52
22:A:1105:CLA:H12	22:J:1901:CLA:HBC1	1.92	0.52
13:3:40:LEU:HD22	39:3:502:LUT:H222	1.92	0.52
16:4:60:SER:HB2	16:4:67:LEU:HD11	1.91	0.52
39:4:502:LUT:H30	22:4:604:CLA:H72	1.90	0.52
18:6:251:PHE:HB2	25:6:504:BCR:H282	1.91	0.52
2:B:371:ALA:HB1	22:B:1224:CLA:HMA1	1.92	0.52
1:A:296:HIS:HD2	22:A:1116:CLA:HMB1	1.75	0.52
14:7:80:MET:SD	22:7:601:CLA:HAB	2.49	0.52
20:9:78:MET:SD	22:9:601:CLA:HAB	2.49	0.52
1:A:501:ASN:HB3	22:A:1115:CLA:HED2	1.91	0.52
12:Z:79:ARG:NH1	22:Z:611:CLA:OBD	2.43	0.52
19:2:198:ILE:HG21	22:2:603:CLA:H42	1.91	0.52
2:B:423:LEU:HD13	2:B:533:LEU:HA	1.92	0.52
1:A:77:HIS:ND1	22:A:1111:CLA:OBD	2.42	0.51
1:A:274:ASP:N	1:A:274:ASP:OD1	2.41	0.51
1:A:481:PRO:HG3	1:A:533:PHE:HB2	1.92	0.51
22:A:1104:CLA:H8	26:A:5002:LHG:H351	1.91	0.51
2:B:361:PHE:HB3	2:B:364:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:1216:CLA:HMB2	22:B:1221:CLA:HMA3	1.92	0.51
15:8:191:LYS:HD3	22:8:602:CLA:HBA2	1.92	0.51
19:2:33:PRO:O	20:9:128:GLN:NE2	2.41	0.51
19:2:78:MET:SD	22:2:601:CLA:HAB	2.49	0.51
2:B:418:ALA:O	2:B:422:HIS:ND1	2.33	0.51
22:A:1137:CLA:H143	25:A:4004:BCR:H371	1.92	0.51
14:7:147:ASP:OD1	14:7:147:ASP:N	2.43	0.51
13:3:42:LEU:HD13	22:3:604:CLA:H42	1.92	0.51
22:K:1401:CLA:HBB1	25:K:4002:BCR:C11	2.41	0.51
22:7:616:CLA:H13	22:7:616:CLA:HMC2	1.93	0.51
17:5:198:MET:HG3	22:5:605:CLA:HBB2	1.93	0.51
25:5:503:BCR:HC42	26:6:801:LHG:H111	1.92	0.51
22:A:1121:CLA:H11	10:K:65:LEU:HD11	1.92	0.51
22:A:1126:CLA:H92	22:A:1126:CLA:H41	1.92	0.51
22:5:602:CLA:HHC	22:5:602:CLA:HBB1	1.93	0.51
1:A:580:ARG:NH1	46:A:6042:HOH:O	2.43	0.51
2:B:273:ASP:HB3	22:B:1214:CLA:HMA1	1.92	0.51
17:5:131:TRP:HB2	22:6:609:CLA:H11	1.91	0.51
19:2:117:VAL:HG12	19:2:121:LEU:HD13	1.93	0.51
1:A:244:LEU:O	28:A:5006:LMT:O2'	2.29	0.51
22:B:1212:CLA:H43	25:B:4003:BCR:H313	1.92	0.51
1:A:733:LEU:HD22	22:A:1139:CLA:HMA1	1.92	0.50
22:B:1220:CLA:H171	22:B:1240:CLA:H51	1.93	0.50
14:7:223:LEU:HD22	18:6:225:PRO:HB3	1.92	0.50
13:3:216:LEU:HB2	39:3:501:LUT:H22	1.93	0.50
39:5:502:LUT:H371	22:5:604:CLA:H142	1.92	0.50
2:B:588:ILE:HA	2:B:591:VAL:HG22	1.93	0.50
22:3:605:CLA:H101	22:3:612:CLA:H42	1.92	0.50
22:3:613:CLA:H8	22:5:615:CLA:H42	1.92	0.50
19:2:75:ARG:NE	19:2:157:GLU:OE2	2.38	0.50
22:A:1012:CLA:HBC2	2:B:586:ASN:HB2	1.92	0.50
22:A:1116:CLA:HAC1	22:A:1133:CLA:H42	1.92	0.50
22:B:1222:CLA:H61	22:B:1240:CLA:H201	1.94	0.50
39:8:501:LUT:H30	22:8:601:CLA:H72	1.93	0.50
19:2:220:ILE:HD11	28:9:803:LMT:H81	1.93	0.50
25:3:505:BCR:H343	22:3:603:CLA:HBC1	1.92	0.50
22:4:609:CLA:HMB2	22:6:618:CLA:HED2	1.92	0.50
17:5:90:VAL:HG11	22:5:606:CLA:HAC2	1.93	0.50
22:7:616:CLA:H11	18:6:251:PHE:HA	1.94	0.50
39:4:502:LUT:H32	22:4:604:CLA:HAB	1.94	0.50
1:A:218:ILE:HA	1:A:222:LEU:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:HIS:HB2	22:A:1116:CLA:C1B	2.42	0.50
2:B:416:LYS:HA	2:B:419:LEU:HD12	1.94	0.50
15:8:240:LEU:HD13	15:8:243:LEU:HD12	1.94	0.50
22:6:609:CLA:HBB2	22:6:604:CLA:HHD	1.93	0.50
22:B:1225:CLA:H8	25:B:4002:BCR:H21C	1.93	0.50
17:5:135:ARG:NH2	17:5:146:VAL:O	2.45	0.50
40:6:610:CHL:HMB1	40:6:610:CHL:HBB1	1.94	0.50
12:1:72:GLU:HB3	12:1:148:VAL:HG22	1.93	0.49
1:A:598:TRP:CH2	22:B:1022:CLA:HAB	2.48	0.49
22:B:1216:CLA:H12	22:B:1221:CLA:HBB1	1.94	0.49
28:1:803:LMT:H21	22:1:612:CLA:HMB2	1.95	0.49
22:Z:604:CLA:H71	22:Z:605:CLA:HMA1	1.94	0.49
22:A:1110:CLA:HHC	22:A:1110:CLA:HBB1	1.94	0.49
2:B:185:GLY:HA3	2:B:286:ILE:HG13	1.94	0.49
12:Z:46:PRO:HG2	12:Z:49:LEU:HB2	1.93	0.49
22:A:1109:CLA:H72	22:A:1101:CLA:HBB2	1.94	0.49
22:A:1120:CLA:HED1	10:K:61:THR:H	1.76	0.49
2:B:438:TYR:CD2	22:B:1021:CLA:H203	2.47	0.49
26:7:801:LHG:H101	26:7:801:LHG:H292	1.94	0.49
12:1:106:ALA:HB1	12:1:123:LEU:HD22	1.94	0.49
1:A:409:ALA:HB1	25:A:4003:BCR:H271	1.95	0.49
22:F:1301:CLA:H93	22:1:615:CLA:HBB	1.94	0.49
22:1:608:CLA:H11	40:Z:610:CHL:H203	1.94	0.49
40:4:617:CHL:HHC	40:4:617:CHL:HBB1	1.95	0.49
19:2:168:PHE:CZ	39:2:502:LUT:H30	2.48	0.49
22:A:1138:CLA:H172	22:A:1140:CLA:H52	1.94	0.49
2:B:224:THR:OG1	20:9:204:THR:O	2.31	0.49
40:2:609:CHL:HHC	40:2:609:CHL:HBB1	1.95	0.49
40:9:613:CHL:HHC	40:9:613:CHL:HBB1	1.95	0.48
22:B:1224:CLA:HBA2	22:B:1224:CLA:H3A	1.59	0.48
6:F:140:ALA:HA	6:F:145:HIS:HB2	1.94	0.48
19:2:46:LEU:O	19:2:67:ARG:NH2	2.42	0.48
22:A:1138:CLA:HED2	2:B:425:TRP:HB2	1.95	0.48
2:B:457:GLU:OE1	6:F:132:HIS:ND1	2.41	0.48
12:1:149:TYR:HB3	22:1:601:CLA:HED3	1.95	0.48
22:3:606:CLA:H3A	22:3:606:CLA:HBA2	1.56	0.48
40:6:617:CHL:HHC	40:6:617:CHL:HBB1	1.95	0.48
5:E:44:LYS:HB2	5:E:96:ALA:HB3	1.94	0.48
25:5:504:BCR:H403	40:5:610:CHL:HMB2	1.94	0.48
20:9:81:VAL:HG11	39:9:501:LUT:H12	1.96	0.48
22:2:605:CLA:HBC1	40:2:610:CHL:HAB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:TRP:HB2	22:A:1126:CLA:HBB1	1.95	0.48
13:3:27:LEU:HD21	13:3:43:LEU:HD12	1.95	0.48
22:A:1134:CLA:HMB1	25:A:4004:BCR:H281	1.95	0.48
22:2:602:CLA:HBC1	22:2:607:CLA:HBC2	1.96	0.48
1:A:598:TRP:HE1	22:B:1023:CLA:C1D	2.27	0.48
22:A:1129:CLA:HAB	22:A:1137:CLA:HBB2	1.96	0.48
13:3:162:TYR:HB3	22:3:601:CLA:HED3	1.96	0.48
22:3:606:CLA:H2	22:3:613:CLA:CAD	2.44	0.48
22:A:1114:CLA:H2	32:A:5005:DGA:HB22	1.96	0.48
25:A:4001:BCR:H362	25:A:4002:BCR:H21C	1.96	0.48
38:7:804:SPH:H91	22:7:616:CLA:HAC2	1.95	0.48
22:A:1116:CLA:H3A	22:A:1116:CLA:HBA2	1.59	0.47
2:B:175:ARG:NH2	46:B:6051:HOH:O	2.47	0.47
22:B:1222:CLA:HMB1	22:B:1222:CLA:HBB1	1.95	0.47
19:2:28:ARG:NH2	19:2:41:LEU:O	2.41	0.47
22:A:1116:CLA:O1A	22:A:1125:CLA:HBB2	2.14	0.47
2:B:280:ALA:CB	22:B:1214:CLA:HAB	2.44	0.47
22:B:1216:CLA:HBA2	22:B:1216:CLA:H3A	1.48	0.47
12:Z:119:VAL:HG11	40:Z:613:CHL:HMD1	1.95	0.47
15:8:160:LEU:HD22	22:8:611:CLA:HMC2	1.96	0.47
22:4:605:CLA:HAC2	40:4:610:CHL:HBB2	1.96	0.47
28:B:5005:LMT:H2'	28:1:803:LMT:H6'1	1.96	0.47
38:K:5001:SPH:H72	13:3:229:LEU:HD22	1.96	0.47
12:1:53:TYR:HB2	22:1:604:CLA:HMD1	1.96	0.47
38:7:803:SPH:H142	22:8:607:CLA:H72	1.96	0.47
19:2:165:MET:SD	22:2:604:CLA:HAB	2.54	0.47
39:9:502:LUT:H32	22:9:604:CLA:CBB	2.44	0.47
22:A:1138:CLA:H3A	22:A:1138:CLA:HBA2	1.67	0.47
2:B:520:VAL:HG21	2:B:594:TYR:HB2	1.96	0.47
2:B:657:ILE:HG12	22:B:1239:CLA:HMB3	1.96	0.47
22:A:1114:CLA:C4C	22:3:610:CLA:HBB2	2.44	0.47
22:B:1209:CLA:HHC	22:B:1209:CLA:HBB1	1.97	0.47
22:B:1229:CLA:HBB2	25:B:4006:BCR:HC41	1.97	0.47
22:1:608:CLA:H8	40:Z:610:CHL:H13	1.97	0.47
22:A:1102:CLA:H43	22:A:1109:CLA:HMC2	1.97	0.47
2:B:181:SER:HB3	2:B:289:GLY:HA3	1.97	0.47
22:B:1203:CLA:H111	22:B:1203:CLA:H71	1.57	0.47
22:B:1236:CLA:H42	25:B:4005:BCR:H352	1.97	0.47
8:I:95:LEU:O	8:I:99:ILE:HG12	2.15	0.47
11:L:126:LEU:HD11	41:2:803:SQD:H312	1.96	0.47
41:1:802:SQD:O9	15:8:142:ARG:NH2	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:4:604:CLA:H3A	22:4:604:CLA:HBA2	1.62	0.47
22:B:1210:CLA:H151	22:B:1225:CLA:HMD2	1.95	0.47
22:B:1217:CLA:HBA2	22:B:1217:CLA:H3A	1.56	0.47
22:B:1235:CLA:HBA2	22:B:1235:CLA:H3A	1.62	0.47
12:1:91:VAL:HG23	12:1:96:TYR:HB2	1.96	0.47
22:1:611:CLA:H192	22:1:611:CLA:HMC2	1.97	0.47
40:Z:613:CHL:HMB1	40:Z:613:CHL:HBB1	1.96	0.47
22:3:606:CLA:H102	22:5:615:CLA:H2	1.97	0.47
22:7:607:CLA:H141	22:7:607:CLA:H161	1.80	0.47
40:7:610:CHL:HHC	40:7:610:CHL:HBB1	1.96	0.47
40:5:617:CHL:HHC	40:5:617:CHL:HBB1	1.96	0.47
22:A:1115:CLA:H93	10:K:101:VAL:HG12	1.97	0.47
2:B:287:VAL:HG22	25:B:4001:BCR:H14C	1.97	0.47
12:Z:58:LEU:HD11	15:8:175:PRO:HB3	1.96	0.47
16:4:157:PHE:HA	16:4:160:VAL:HG22	1.95	0.47
22:4:612:CLA:H12	28:4:803:LMT:H92	1.96	0.47
40:5:611:CHL:HMB2	22:5:613:CLA:H62	1.97	0.47
19:2:29:PRO:HG3	26:2:801:LHG:HC31	1.96	0.47
22:A:1130:CLA:HBB1	22:A:1136:CLA:H193	1.97	0.47
26:A:5001:LHG:H111	26:A:5001:LHG:H242	1.96	0.47
2:B:717:GLY:O	2:B:721:THR:OG1	2.25	0.47
6:F:196:ALA:HB1	22:F:1302:CLA:HED2	1.97	0.47
40:7:610:CHL:CMC	22:7:613:CLA:HAB	2.45	0.47
40:5:610:CHL:H142	22:6:619:CLA:H8	1.96	0.47
40:2:610:CHL:HHC	40:2:610:CHL:HBB1	1.97	0.47
22:B:1022:CLA:CAD	22:B:1021:CLA:HMB3	2.45	0.47
15:8:36:ILE:HD12	15:8:53:GLY:HA3	1.97	0.47
15:8:67:ARG:NH2	15:8:141:ILE:O	2.43	0.47
40:6:613:CHL:HMB1	40:6:613:CHL:HBB1	1.97	0.47
22:B:1209:CLA:H43	28:B:6101:LMT:H41	1.97	0.46
22:B:1240:CLA:H3A	22:B:1240:CLA:HBA2	1.47	0.46
4:D:87:THR:HA	4:D:111:ASN:O	2.14	0.46
7:G:58:ARG:NH2	7:G:94:GLY:O	2.47	0.46
22:5:601:CLA:H3A	22:5:601:CLA:HBA2	1.58	0.46
1:A:267:LEU:O	10:K:108:LYS:NZ	2.43	0.46
22:A:1012:CLA:H112	22:B:1230:CLA:HBC1	1.97	0.46
22:B:1222:CLA:H42	22:B:1235:CLA:HBA1	1.97	0.46
22:1:601:CLA:H71	22:1:602:CLA:HMA1	1.96	0.46
13:3:43:LEU:HD21	22:3:604:CLA:HMA2	1.96	0.46
1:A:418:ASP:O	1:A:422:ASN:ND2	2.47	0.46
22:A:1111:CLA:H93	22:A:1111:CLA:H111	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:1236:CLA:H193	22:B:1236:CLA:H102	1.97	0.46
15:8:176:LEU:HD12	39:8:501:LUT:H222	1.98	0.46
18:6:166:PRO:HD2	22:6:601:CLA:H11	1.97	0.46
2:B:178:HIS:CG	22:B:1210:CLA:HMC2	2.50	0.46
4:D:139:TYR:HD1	4:D:149:TYR:HA	1.79	0.46
17:5:170:ASP:HA	39:5:501:LUT:H24	1.97	0.46
18:6:208:HIS:CG	22:6:603:CLA:HAA2	2.51	0.46
19:2:42:ASP:N	19:2:42:ASP:OD1	2.47	0.46
2:B:352:HIS:HB3	22:B:1214:CLA:HED2	1.98	0.46
12:Z:171:LEU:HD23	22:Z:607:CLA:HED3	1.96	0.46
25:3:506:BCR:H271	22:3:604:CLA:HAC2	1.97	0.46
1:A:59:PHE:CD2	22:A:1103:CLA:HMC2	2.50	0.46
1:A:213:TRP:NE1	22:A:1117:CLA:O1D	2.41	0.46
2:B:277:HIS:HB2	22:B:1214:CLA:C1B	2.46	0.46
22:B:1215:CLA:H3A	22:B:1215:CLA:HBA2	1.66	0.46
6:F:97:ASP:OD1	6:F:97:ASP:N	2.48	0.46
22:K:1402:CLA:H11	22:K:1402:CLA:H51	1.75	0.46
12:Z:119:VAL:HG12	12:Z:121:PHE:H	1.80	0.46
22:Z:611:CLA:H51	22:Z:611:CLA:H11	1.74	0.46
13:3:153:ILE:HD13	17:5:58:LEU:HA	1.96	0.46
19:2:41:LEU:HD11	19:2:52:ASP:HB2	1.98	0.46
1:A:363:LEU:HD22	22:A:1127:CLA:HBC1	1.97	0.46
1:A:677:PHE:CG	25:A:4005:BCR:H363	2.51	0.46
22:A:1114:CLA:HMB1	22:A:1114:CLA:HBB1	1.96	0.46
2:B:524:ILE:HG12	2:B:591:VAL:HG12	1.97	0.46
17:5:194:MET:SD	22:5:604:CLA:HBB1	2.56	0.46
22:5:618:CLA:H61	22:5:618:CLA:H41	1.72	0.46
1:A:356:ASN:ND2	22:A:1103:CLA:OBD	2.38	0.46
2:B:27:ALA:HB1	33:B:5003:DGD:HB21	1.97	0.46
2:B:193:GLY:O	2:B:197:HIS:HB2	2.15	0.46
2:B:374:THR:HG23	2:B:592:THR:HG21	1.98	0.46
1:A:96:ALA:HB2	1:A:159:LEU:HB2	1.96	0.46
22:A:1111:CLA:H61	22:A:1111:CLA:H41	1.58	0.46
2:B:493:LEU:HD22	22:B:1213:CLA:HED2	1.98	0.46
22:B:1205:CLA:H3A	22:B:1205:CLA:HBA2	1.67	0.46
22:Z:615:CLA:HMC1	16:4:154:MET:HG2	1.97	0.46
22:7:612:CLA:H3A	22:7:612:CLA:HBA2	1.54	0.46
39:8:502:LUT:H35	39:8:502:LUT:H401	1.84	0.46
22:8:612:CLA:HBA2	22:8:612:CLA:H3A	1.52	0.46
22:6:607:CLA:H41	22:6:607:CLA:H62	1.75	0.46
1:A:282:LEU:HD21	1:A:375:PRO:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:ASP:HB3	2:B:21:ARG:HB2	1.98	0.46
22:1:611:CLA:H51	22:1:611:CLA:H11	1.81	0.46
40:3:611:CHL:HHC	40:3:611:CHL:HBB1	1.98	0.46
14:7:164:TYR:HB3	22:7:601:CLA:HED3	1.98	0.46
39:7:502:LUT:H35	39:7:502:LUT:H401	1.85	0.46
1:A:736:ILE:HG21	22:A:1126:CLA:HMC2	1.98	0.45
22:A:1012:CLA:HAB	2:B:583:TRP:HH2	1.78	0.45
22:A:1106:CLA:HBA2	22:A:1106:CLA:H3A	1.40	0.45
2:B:438:TYR:CE1	2:B:519:LEU:HB3	2.51	0.45
22:B:1206:CLA:HBA1	22:B:1206:CLA:H3A	1.52	0.45
14:7:42:HIS:NE2	14:7:54:ASP:OD2	2.47	0.45
40:2:613:CHL:HBB1	40:2:613:CHL:HMB1	1.98	0.45
1:A:60:ASP:OD2	1:A:350:HIS:NE2	2.45	0.45
22:A:1012:CLA:HMB3	22:B:1021:CLA:H201	1.96	0.45
22:B:1227:CLA:HAB	22:B:1236:CLA:CBB	2.45	0.45
12:Z:184:PHE:CD2	39:Z:502:LUT:H12	2.51	0.45
1:A:161:THR:HG21	22:A:1114:CLA:HBA1	1.98	0.45
1:A:680:ALA:HB3	22:A:1013:CLA:HBB2	1.98	0.45
22:A:1119:CLA:HMB2	22:A:1123:CLA:HMA3	1.97	0.45
10:K:35:ASN:HD21	22:K:1401:CLA:HED2	1.81	0.45
15:8:153:PHE:HD2	15:8:156:PHE:HB3	1.82	0.45
17:5:248:PRO:HG2	40:5:610:CHL:H43	1.99	0.45
19:2:156:LYS:HG3	22:2:607:CLA:HED2	1.99	0.45
20:9:80:ALA:HA	22:9:606:CLA:HBB1	1.99	0.45
22:9:603:CLA:HBA1	22:9:603:CLA:HBD	1.98	0.45
22:B:1220:CLA:HBB1	22:B:1220:CLA:H162	1.97	0.45
40:Z:610:CHL:HBB1	40:Z:610:CHL:HMB1	1.98	0.45
1:A:392:THR:HG23	1:A:607:ILE:HG21	1.98	0.45
22:A:1130:CLA:HBA2	22:A:1130:CLA:H3A	1.70	0.45
2:B:438:TYR:HD2	22:B:1021:CLA:H203	1.81	0.45
22:B:1022:CLA:H203	22:B:1207:CLA:HMC2	1.99	0.45
22:B:1207:CLA:HAB	8:I:84:GLY:HA3	1.98	0.45
12:Z:83:LEU:HD13	22:Z:606:CLA:HBB2	1.99	0.45
39:5:502:LUT:H162	22:5:606:CLA:HMB3	1.99	0.45
22:6:608:CLA:H62	22:6:609:CLA:H122	1.99	0.45
22:A:1128:CLA:H191	22:A:1013:CLA:H191	1.98	0.45
22:A:1136:CLA:H62	22:A:1136:CLA:H41	1.67	0.45
2:B:59:PHE:HE2	25:B:4003:BCR:H373	1.82	0.45
22:B:1214:CLA:H3A	22:B:1214:CLA:HBA2	1.45	0.45
39:7:501:LUT:H35	39:7:501:LUT:H401	1.81	0.45
22:8:609:CLA:HHC	22:8:609:CLA:HBB1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:5:501:LUT:H371	22:5:601:CLA:H52	1.98	0.45
1:A:29:TRP:HE1	22:A:1109:CLA:CHB	2.29	0.45
22:A:1124:CLA:H92	22:A:1124:CLA:H62	1.83	0.45
22:B:1203:CLA:H51	33:B:5003:DGD:HB71	1.98	0.45
22:B:1226:CLA:H41	22:B:1226:CLA:H62	1.57	0.45
17:5:227:ILE:HB	22:5:603:CLA:H11	1.98	0.45
22:5:609:CLA:H93	22:5:609:CLA:H111	1.86	0.45
22:9:604:CLA:H141	22:9:604:CLA:H161	1.78	0.45
2:B:378:TYR:CD2	22:B:1224:CLA:HAB	2.51	0.45
39:1:501:LUT:H15	39:1:501:LUT:H201	1.87	0.45
39:Z:503:LUT:H15	39:Z:503:LUT:H201	1.79	0.45
22:Z:605:CLA:H2A	22:Z:605:CLA:H2	1.98	0.45
22:3:613:CLA:HED2	22:5:615:CLA:HMD2	1.99	0.45
22:8:606:CLA:H92	22:8:606:CLA:H61	1.83	0.45
18:6:60:ASN:HB3	18:6:63:SER:HB2	1.98	0.45
1:A:389:SER:HB3	22:A:1126:CLA:HMA1	1.98	0.45
22:A:1129:CLA:CHA	26:A:5001:LHG:HC92	2.47	0.45
2:B:375:HIS:HB2	22:B:1224:CLA:C1B	2.47	0.45
22:3:618:CLA:HMA2	22:7:609:CLA:H93	1.99	0.45
40:6:611:CHL:HMB1	40:6:611:CHL:HBB1	1.99	0.45
22:6:615:CLA:HBA1	22:6:615:CLA:H3A	1.56	0.45
22:9:605:CLA:H92	22:9:605:CLA:H61	1.75	0.45
1:A:17:VAL:HG11	1:A:184:ALA:HB1	1.99	0.44
22:A:1103:CLA:H72	25:A:4002:BCR:HC8	1.98	0.44
22:B:1023:CLA:H142	25:I:4001:BCR:H393	1.99	0.44
22:B:1207:CLA:H142	22:B:1207:CLA:H111	1.76	0.44
6:F:162:TYR:CE2	22:F:1302:CLA:HBD	2.52	0.44
25:7:503:BCR:H10C	22:8:608:CLA:H41	1.99	0.44
22:8:607:CLA:H3A	22:8:607:CLA:HBA2	1.45	0.44
25:6:503:BCR:H393	22:6:606:CLA:H72	1.98	0.44
20:9:32:LEU:HD12	20:9:32:LEU:HA	1.88	0.44
3:C:26:LEU:HA	3:C:41:SER:O	2.17	0.44
13:3:223:PRO:HG2	22:3:608:CLA:HMB3	1.98	0.44
14:7:200:ALA:HA	22:7:603:CLA:HBB1	1.98	0.44
15:8:81:MET:HG3	15:8:196:GLY:HA2	1.98	0.44
40:4:613:CHL:HBB1	40:4:613:CHL:HMB1	1.99	0.44
22:5:607:CLA:H62	22:5:607:CLA:H102	1.67	0.44
1:A:294:THR:O	1:A:298:HIS:ND1	2.51	0.44
22:A:1130:CLA:HMB1	22:B:1237:CLA:HAA2	1.99	0.44
33:B:5003:DGD:HA51	33:B:5003:DGD:HA22	1.87	0.44
14:7:115:ILE:HG12	25:7:504:BCR:H281	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ALA:HB1	1:A:187:LYS:HD3	2.00	0.44
2:B:663:MET:HB2	22:B:1023:CLA:C1C	2.48	0.44
22:B:1208:CLA:H3A	22:B:1208:CLA:HBA2	1.52	0.44
22:Z:607:CLA:H93	22:Z:607:CLA:H111	1.84	0.44
18:6:127:ARG:NH2	18:6:138:VAL:O	2.50	0.44
22:6:612:CLA:HBA2	22:6:612:CLA:H3A	1.58	0.44
1:A:349:TRP:HB3	22:A:1103:CLA:HAC1	1.98	0.44
1:A:740:TRP:NE1	22:A:1126:CLA:O1A	2.49	0.44
21:A:1011:CL0:H15	22:A:1012:CLA:O1D	2.18	0.44
2:B:578:TYR:HE1	2:B:711:LEU:HB2	1.82	0.44
2:B:695:LYS:HB2	22:B:1238:CLA:HED3	2.00	0.44
22:B:1209:CLA:H141	22:B:1209:CLA:H162	1.78	0.44
22:B:1240:CLA:H91	22:B:1240:CLA:H112	1.87	0.44
25:3:506:BCR:H351	25:3:506:BCR:H15C	1.68	0.44
15:8:183:ASP:N	15:8:183:ASP:OD1	2.50	0.44
16:4:83:PRO:HD2	39:4:502:LUT:H23	2.00	0.44
21:A:1011:CL0:H8	21:A:1011:CL0:CGD	2.48	0.44
22:A:1107:CLA:HMB1	22:A:1107:CLA:HBB1	1.99	0.44
22:A:1118:CLA:HAA2	10:K:87:VAL:HG13	2.00	0.44
2:B:91:ALA:HA	2:B:114:VAL:HG12	1.99	0.44
2:B:168:TRP:HB2	28:B:6101:LMT:H6'1	1.98	0.44
22:B:1218:CLA:H2	25:B:4001:BCR:HC32	2.00	0.44
22:B:1225:CLA:H3A	22:B:1225:CLA:HBA2	1.49	0.44
22:1:604:CLA:H3A	22:1:604:CLA:HBA2	1.60	0.44
25:7:503:BCR:H15C	25:7:503:BCR:H351	1.80	0.44
22:8:606:CLA:HBA2	22:8:606:CLA:H3A	1.75	0.44
1:A:655:SER:O	1:A:659:GLN:HG2	2.18	0.44
22:A:1105:CLA:H3A	22:A:1105:CLA:HBA2	1.73	0.44
22:B:1222:CLA:HBA2	22:B:1222:CLA:H3A	1.68	0.44
22:3:607:CLA:H51	22:3:607:CLA:H11	1.75	0.44
22:7:615:CLA:H3A	22:7:615:CLA:HBA2	1.61	0.44
22:4:601:CLA:HBA2	22:4:601:CLA:H3A	1.63	0.44
22:5:605:CLA:HMD2	22:5:612:CLA:C1D	2.48	0.44
39:6:502:LUT:H15	39:6:502:LUT:H201	1.88	0.44
22:A:1128:CLA:H41	22:A:1128:CLA:H62	1.64	0.44
26:A:5002:LHG:H312	26:A:5002:LHG:H281	1.72	0.44
2:B:423:LEU:HB3	2:B:533:LEU:HB2	2.00	0.44
22:B:1216:CLA:HBC2	22:B:1221:CLA:H192	2.00	0.44
22:8:605:CLA:H111	22:8:605:CLA:H71	1.74	0.44
40:8:610:CHL:HBB1	40:8:610:CHL:HMB1	1.99	0.44
39:4:501:LUT:H35	39:4:501:LUT:H401	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:1208:CLA:H52	22:B:1208:CLA:H8	1.82	0.44
22:B:1210:CLA:H93	22:B:1210:CLA:H61	1.84	0.44
12:1:162:ASP:OD1	12:1:162:ASP:N	2.49	0.44
40:1:610:CHL:HBB1	40:1:610:CHL:HMB1	2.00	0.44
13:3:117:ILE:HD13	22:3:613:CLA:HMD3	1.99	0.44
14:7:221:ASP:HB3	14:7:229:VAL:HG11	1.99	0.44
22:8:601:CLA:H62	22:8:601:CLA:H41	1.75	0.44
22:8:601:CLA:HBA2	22:8:601:CLA:H3A	1.63	0.44
17:5:153:LYS:HA	17:5:153:LYS:HD3	1.88	0.44
19:2:28:ARG:NH1	19:2:42:ASP:O	2.51	0.44
19:2:30:MET:HB3	19:2:35:ALA:HB3	1.99	0.44
39:2:502:LUT:H15	39:2:502:LUT:H201	1.82	0.44
39:2:503:LUT:H15	39:2:503:LUT:H201	1.80	0.44
22:A:1107:CLA:H122	25:J:4001:BCR:HC41	1.99	0.43
22:A:1124:CLA:HAB	25:A:4004:BCR:C8	2.48	0.43
2:B:708:LEU:HD23	33:B:5003:DGD:HA31	1.98	0.43
22:B:1220:CLA:H3A	22:B:1220:CLA:HBA2	1.64	0.43
22:B:1238:CLA:H193	25:I:4001:BCR:H16C	2.00	0.43
25:B:4004:BCR:H351	25:B:4004:BCR:H15C	1.81	0.43
22:K:1401:CLA:HBB1	25:K:4002:BCR:C10	2.47	0.43
22:1:601:CLA:H3A	22:1:601:CLA:HBA2	1.59	0.43
22:5:618:CLA:HED1	26:6:801:LHG:H301	1.99	0.43
19:2:107:ASN:HA	19:2:110:LEU:HD12	1.99	0.43
19:2:128:ILE:HD13	19:2:136:GLY:HA3	2.00	0.43
40:9:610:CHL:HHC	40:9:610:CHL:HBB1	2.00	0.43
1:A:278:PHE:HE1	1:A:296:HIS:HD2	1.65	0.43
2:B:287:VAL:HG21	22:B:1213:CLA:H143	1.99	0.43
22:B:1210:CLA:H143	22:B:1210:CLA:H112	1.76	0.43
12:Z:105:TRP:CE2	12:Z:112:ALA:HB2	2.53	0.43
22:A:1111:CLA:H143	22:A:1111:CLA:H161	1.80	0.43
25:A:4002:BCR:H282	25:3:505:BCR:H10C	2.00	0.43
2:B:578:TYR:CE1	2:B:711:LEU:HB2	2.53	0.43
2:B:659:ALA:C	22:B:1023:CLA:HAB	2.39	0.43
22:3:612:CLA:H3A	22:3:612:CLA:HBA2	1.49	0.43
22:4:608:CLA:H42	22:4:609:CLA:H41	2.00	0.43
26:6:801:LHG:H311	22:6:603:CLA:H93	1.99	0.43
39:2:502:LUT:H11	39:2:502:LUT:H191	1.81	0.43
2:B:411:ARG:O	2:B:415:HIS:ND1	2.45	0.43
11:L:74:ALA:HB2	22:L:1502:CLA:HMD1	2.00	0.43
12:1:48:ASP:OD1	12:1:48:ASP:N	2.50	0.43
12:1:184:PHE:CD2	39:1:502:LUT:H12	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:Z:503:LUT:H401	39:Z:503:LUT:H35	1.71	0.43
22:3:618:CLA:HED2	22:7:609:CLA:HMB2	2.00	0.43
22:4:602:CLA:H11	22:4:602:CLA:H52	1.77	0.43
1:A:296:HIS:CD2	22:A:1116:CLA:HMB1	2.53	0.43
1:A:356:ASN:O	1:A:360:PHE:HB2	2.18	0.43
22:A:1114:CLA:H2	32:A:5005:DGA:HB42	2.00	0.43
22:B:1231:CLA:H91	22:B:1231:CLA:H111	1.86	0.43
13:3:77:ALA:HB2	25:3:504:BCR:H383	2.00	0.43
22:3:603:CLA:H2	22:3:608:CLA:OBD	2.19	0.43
22:3:612:CLA:HBB	22:3:618:CLA:HBC2	2.01	0.43
40:4:610:CHL:HMB1	40:4:610:CHL:HBB1	1.99	0.43
40:5:610:CHL:HHC	40:5:610:CHL:HBB1	2.00	0.43
22:A:1105:CLA:HMA1	22:A:1106:CLA:HMB3	1.98	0.43
22:B:1215:CLA:HAB	22:B:1215:CLA:H8	2.00	0.43
22:B:1216:CLA:H41	22:B:1216:CLA:H61	1.68	0.43
22:B:1230:CLA:H61	22:B:1230:CLA:H41	1.82	0.43
11:L:62:ALA:HB3	11:L:65:VAL:HG22	2.01	0.43
40:1:609:CHL:HHC	40:1:609:CHL:HBB1	2.00	0.43
39:Z:503:LUT:H7	40:Z:613:CHL:HAA1	2.00	0.43
22:Z:604:CLA:H142	22:Z:604:CLA:H112	1.79	0.43
40:4:611:CHL:HBB1	40:4:611:CHL:HMB1	1.99	0.43
40:5:611:CHL:HMB1	40:5:611:CHL:HBB1	1.99	0.43
22:A:1125:CLA:H2	22:A:1125:CLA:H61	1.80	0.43
2:B:168:TRP:CZ2	22:B:1208:CLA:HMA1	2.53	0.43
2:B:478:LEU:HD23	2:B:478:LEU:HA	1.86	0.43
22:1:608:CLA:HAA2	15:8:125:VAL:HG22	2.01	0.43
22:7:603:CLA:HBA1	22:7:603:CLA:HBD	2.01	0.43
20:9:174:VAL:HG12	22:9:603:CLA:HMD3	2.01	0.43
1:A:605:ILE:HD12	21:A:1011:CL0:H53	2.01	0.43
1:A:687:PHE:CD1	2:B:665:LEU:HB3	2.54	0.43
23:A:2001:PQN:H302	23:A:2001:PQN:H262	1.79	0.43
2:B:158:LEU:O	2:B:163:GLN:NE2	2.51	0.43
22:B:1231:CLA:H193	22:B:1232:CLA:HBC3	2.01	0.43
40:7:610:CHL:HMC	22:7:613:CLA:HAB	2.00	0.43
16:4:89:ASP:HB3	16:4:92:LYS:HB2	2.00	0.43
39:5:502:LUT:H15	39:5:502:LUT:H201	1.82	0.43
18:6:188:VAL:HG11	22:6:604:CLA:H18	2.00	0.43
22:6:609:CLA:HBA2	22:6:609:CLA:H3A	1.62	0.43
19:2:198:ILE:HG12	19:2:207:THR:HG21	2.00	0.43
39:9:501:LUT:H11	39:9:501:LUT:H191	1.94	0.43
22:A:1107:CLA:H93	22:A:1107:CLA:H61	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:1127:CLA:H102	22:A:1127:CLA:H62	1.73	0.43
22:F:1301:CLA:H143	22:F:1301:CLA:H112	1.81	0.43
22:1:603:CLA:H8	26:1:801:LHG:H321	2.00	0.43
22:1:615:CLA:H2	22:1:615:CLA:H61	1.59	0.43
20:9:62:ARG:NH2	20:9:66:TYR:OH	2.50	0.43
1:A:589:TRP:CD1	22:A:1128:CLA:HMD1	2.54	0.43
39:Z:502:LUT:H15	39:Z:502:LUT:H201	1.85	0.43
39:Z:502:LUT:H35	39:Z:502:LUT:H401	1.87	0.43
17:5:137:TRP:CG	22:5:618:CLA:HBC1	2.54	0.43
22:6:605:CLA:H2	22:6:605:CLA:H61	1.89	0.43
19:2:118:PHE:CZ	40:2:613:CHL:HAB	2.54	0.43
20:9:170:ILE:HD11	22:9:605:CLA:HAB	2.00	0.43
22:9:603:CLA:H93	22:9:603:CLA:H61	1.81	0.43
22:B:1216:CLA:HMD2	22:B:1221:CLA:H193	2.00	0.42
10:K:72:ASN:OD1	10:K:72:ASN:N	2.52	0.42
12:Z:140:GLN:HB3	22:Z:611:CLA:HMC3	2.00	0.42
22:Z:605:CLA:HMD2	22:Z:612:CLA:C1D	2.49	0.42
22:3:605:CLA:H111	22:3:605:CLA:H91	1.82	0.42
40:8:613:CHL:HHC	40:8:613:CHL:HBB1	2.01	0.42
39:9:501:LUT:H35	39:9:501:LUT:H401	1.83	0.42
1:A:234:PRO:HA	1:A:237:ILE:HD12	2.01	0.42
1:A:574:PRO:HB3	1:A:720:ILE:HB	2.02	0.42
22:A:1111:CLA:H121	22:A:1111:CLA:HMB3	2.01	0.42
22:A:1122:CLA:H141	26:A:5001:LHG:H172	2.01	0.42
22:A:1141:CLA:HMB3	26:A:5001:LHG:HC61	2.00	0.42
22:1:602:CLA:OBD	22:1:607:CLA:H2	2.19	0.42
25:3:504:BCR:C7	40:3:611:CHL:HMB2	2.50	0.42
22:4:605:CLA:HMD2	22:4:612:CLA:C1D	2.49	0.42
25:6:503:BCR:H351	25:6:503:BCR:H15C	1.74	0.42
1:A:17:VAL:HG21	22:A:1108:CLA:HED3	2.00	0.42
1:A:396:TRP:HB3	22:A:1126:CLA:HMC3	2.01	0.42
1:A:718:LEU:HB3	1:A:722:GLN:HG2	2.01	0.42
1:A:734:GLY:O	1:A:738:THR:OG1	2.28	0.42
22:A:1139:CLA:H41	22:A:1139:CLA:H61	1.66	0.42
2:B:453:GLN:HE21	6:F:130:LEU:HD13	1.84	0.42
39:1:502:LUT:H15	39:1:502:LUT:H201	1.90	0.42
22:1:605:CLA:HMD2	22:1:612:CLA:C1D	2.49	0.42
40:Z:610:CHL:HAB	40:Z:613:CHL:HBB2	1.99	0.42
22:3:606:CLA:H141	22:3:606:CLA:H161	1.84	0.42
22:7:603:CLA:H203	22:7:603:CLA:H161	1.86	0.42
16:4:111:VAL:HG11	39:4:501:LUT:H10	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:2:603:CLA:HBA1	22:2:603:CLA:HBD	2.00	0.42
21:A:1011:CL0:H13	22:A:1012:CLA:CAD	2.50	0.42
22:A:1113:CLA:H141	22:A:1113:CLA:H161	1.74	0.42
4:D:93:GLU:HA	4:D:106:MET:O	2.18	0.42
12:1:79:ARG:NH1	22:1:611:CLA:OBD	2.47	0.42
12:1:171:LEU:HD23	22:1:607:CLA:HED3	2.00	0.42
39:3:501:LUT:H30	22:3:601:CLA:H72	2.01	0.42
25:5:504:BCR:H383	40:5:610:CHL:H12	2.01	0.42
22:5:618:CLA:H112	22:5:618:CLA:H91	1.79	0.42
19:2:155:LEU:HD22	22:2:607:CLA:HED3	2.02	0.42
1:A:740:TRP:CG	25:A:4005:BCR:HC41	2.54	0.42
22:A:1126:CLA:O1D	22:A:1127:CLA:HHB	2.19	0.42
22:A:1128:CLA:H122	22:A:1139:CLA:HMA2	2.01	0.42
39:Z:501:LUT:H371	22:Z:601:CLA:H61	2.02	0.42
14:7:156:GLU:OE2	14:7:168:ARG:NH1	2.52	0.42
26:4:801:LHG:HC82	25:6:503:BCR:HC32	2.02	0.42
22:2:603:CLA:H92	22:2:603:CLA:H61	1.77	0.42
20:9:105:ASP:N	20:9:105:ASP:OD1	2.52	0.42
31:A:5003:LMG:HC2	14:7:60:GLN:HE22	1.85	0.42
2:B:338:ALA:HB1	22:B:1202:CLA:HED2	2.00	0.42
22:B:1230:CLA:HBA2	22:B:1230:CLA:H3A	1.82	0.42
25:3:503:BCR:H341	22:5:609:CLA:H172	2.01	0.42
39:8:501:LUT:H32	22:8:601:CLA:CAB	2.50	0.42
39:4:502:LUT:H32	22:4:604:CLA:CAB	2.49	0.42
22:B:1212:CLA:H2A	22:B:1212:CLA:HED2	2.02	0.42
22:B:1213:CLA:O1A	7:G:116:ALA:HB1	2.19	0.42
3:C:66:ARG:HA	3:C:66:ARG:HD2	1.91	0.42
39:3:502:LUT:H35	39:3:502:LUT:H401	1.89	0.42
22:8:606:CLA:H111	45:8:803:LPX:H8	2.02	0.42
17:5:202:LEU:HD23	17:5:202:LEU:HA	1.85	0.42
19:2:71:LEU:HD23	19:2:71:LEU:HA	1.92	0.42
22:A:1112:CLA:H91	22:A:1112:CLA:H111	1.89	0.42
2:B:495:LEU:HD23	2:B:495:LEU:HA	1.85	0.42
12:1:205:HIS:CG	22:1:603:CLA:HAA2	2.55	0.42
39:3:502:LUT:H15	39:3:502:LUT:H201	1.85	0.42
22:7:616:CLA:H93	22:7:616:CLA:H111	1.88	0.42
39:8:502:LUT:H15	39:8:502:LUT:H201	1.90	0.42
16:4:226:PHE:CZ	39:4:502:LUT:H10	2.55	0.42
17:5:134:VAL:HG11	22:6:609:CLA:H2A	2.01	0.42
19:2:96:TRP:CD1	19:2:97:THR:HG23	2.55	0.42
1:A:396:TRP:HA	1:A:603:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:1220:CLA:H142	22:B:1220:CLA:H111	1.84	0.42
22:B:1240:CLA:HMB2	26:B:5001:LHG:HC81	2.01	0.42
25:G:4001:BCR:H15C	25:G:4001:BCR:H351	1.92	0.42
22:1:608:CLA:H13	22:1:608:CLA:H102	1.86	0.42
40:Z:610:CHL:HBB2	40:Z:613:CHL:HBB2	2.02	0.42
43:7:802:3PH:H372	43:7:802:3PH:H3A1	1.66	0.42
22:4:609:CLA:H92	22:4:609:CLA:H62	1.80	0.42
17:5:197:TYR:CD2	39:5:502:LUT:H12	2.54	0.42
18:6:125:GLU:HG3	22:6:612:CLA:C4B	2.50	0.42
1:A:25:SER:O	22:A:1109:CLA:HBB	2.20	0.42
1:A:81:LEU:HD12	22:A:1111:CLA:HED1	2.02	0.42
1:A:605:ILE:HG13	21:A:1011:CL0:H66	2.02	0.42
2:B:128:ILE:HG22	22:B:1215:CLA:HED2	2.02	0.42
2:B:323:LEU:HA	2:B:326:THR:HG22	2.02	0.42
22:B:1237:CLA:H142	22:B:1237:CLA:H111	1.87	0.42
22:B:1208:CLA:H42	22:9:605:CLA:H71	2.02	0.42
39:1:502:LUT:H11	39:1:502:LUT:H191	1.94	0.42
12:Z:134:MET:HG3	22:Z:612:CLA:HMC3	2.02	0.42
16:4:240:PRO:O	39:4:501:LUT:O3	2.37	0.42
18:6:192:MET:HG3	22:6:603:CLA:HAC2	2.02	0.42
19:2:117:VAL:C	19:2:121:LEU:HD13	2.38	0.42
22:A:1124:CLA:H193	22:A:1124:CLA:H162	1.88	0.41
22:A:1133:CLA:H41	22:A:1133:CLA:H62	1.78	0.41
22:A:1137:CLA:H143	22:A:1137:CLA:H111	1.84	0.41
22:B:1204:CLA:H3A	22:B:1204:CLA:HBA2	1.74	0.41
9:J:21:PHE:CD1	22:J:1901:CLA:HBB2	2.55	0.41
9:J:28:GLU:OE1	9:J:31:ARG:NH2	2.49	0.41
13:3:195:MET:SD	22:3:604:CLA:HAB	2.60	0.41
22:8:603:CLA:HBD	22:8:603:CLA:HBA1	2.01	0.41
22:4:609:CLA:H41	22:4:609:CLA:H61	1.80	0.41
1:A:369:HIS:HA	1:A:372:TYR:CE1	2.56	0.41
2:B:688:LEU:HB3	25:L:4002:BCR:HC31	2.02	0.41
22:B:1021:CLA:H112	22:B:1021:CLA:H152	1.77	0.41
22:B:1208:CLA:H93	22:B:1210:CLA:HMB3	2.02	0.41
25:3:505:BCR:H17C	22:3:612:CLA:H142	2.01	0.41
16:4:111:VAL:HG11	39:4:501:LUT:H12	2.02	0.41
22:4:612:CLA:HBA2	22:4:612:CLA:H3A	1.49	0.41
17:5:202:LEU:HD11	22:5:615:CLA:HMB3	2.02	0.41
25:5:503:BCR:H15C	25:5:503:BCR:H351	1.86	0.41
22:6:605:CLA:HBA1	22:6:605:CLA:H3A	1.82	0.41
20:9:133:THR:HG23	20:9:135:THR:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:1117:CLA:H2	22:A:1127:CLA:H92	2.02	0.41
22:B:1237:CLA:HHD	25:B:4007:BCR:H383	2.01	0.41
10:K:49:ALA:HB1	10:K:56:THR:HG22	2.02	0.41
22:L:1502:CLA:H51	25:L:4002:BCR:HC21	2.02	0.41
16:4:175:ASN:HB3	16:4:185:LEU:HB2	2.02	0.41
20:9:63:LEU:HD12	22:9:604:CLA:HMA2	2.02	0.41
22:9:604:CLA:HBB1	22:9:604:CLA:HHC	2.02	0.41
2:B:499:LEU:HA	2:B:502:ILE:HG22	2.02	0.41
22:B:1205:CLA:H92	25:B:4007:BCR:HC7	2.01	0.41
9:J:5:THR:HB	31:J:5001:LMG:HC92	2.03	0.41
9:J:28:GLU:HG3	22:J:1901:CLA:C1B	2.50	0.41
22:K:1404:CLA:HMD2	25:K:4002:BCR:H21C	2.03	0.41
16:4:95:TRP:CZ2	22:4:612:CLA:HAA2	2.55	0.41
39:4:502:LUT:H15	39:4:502:LUT:H201	1.91	0.41
17:5:67:LEU:HD12	22:5:604:CLA:HMA2	2.02	0.41
22:A:1126:CLA:H72	22:A:1126:CLA:H111	1.81	0.41
2:B:320:HIS:HB3	2:B:323:LEU:HD12	2.02	0.41
11:L:80:ALA:HB3	11:L:83:LEU:HD23	2.03	0.41
12:1:210:TRP:HB3	15:8:117:ALA:HB2	2.03	0.41
40:Z:610:CHL:CBB	40:Z:613:CHL:HBB2	2.50	0.41
22:8:608:CLA:H62	22:8:608:CLA:H92	1.85	0.41
22:4:605:CLA:H11	22:4:605:CLA:HMA2	2.03	0.41
18:6:165:ILE:HG12	22:6:601:CLA:HBA2	2.03	0.41
40:6:610:CHL:HBB2	22:6:612:CLA:HBC1	2.02	0.41
20:9:125:LYS:HA	20:9:125:LYS:HD2	1.90	0.41
1:A:150:ALA:HB2	1:A:378:PRO:HD2	2.01	0.41
22:A:1103:CLA:HBA1	22:A:1103:CLA:H3A	1.62	0.41
32:A:5005:DGA:HA51	14:7:239:PRO:HB2	2.02	0.41
2:B:277:HIS:CE1	2:B:281:ILE:HD13	2.56	0.41
22:1:607:CLA:HMC2	22:1:608:CLA:H111	2.02	0.41
12:Z:83:LEU:HB3	22:Z:606:CLA:HAB	2.02	0.41
22:Z:604:CLA:HHD	40:Z:609:CHL:HBB2	2.03	0.41
22:Z:605:CLA:H112	22:Z:605:CLA:H151	1.84	0.41
22:3:612:CLA:H91	22:3:612:CLA:H111	1.83	0.41
25:7:503:BCR:H311	22:8:607:CLA:HAB	2.02	0.41
22:8:605:CLA:H141	22:8:605:CLA:H162	1.85	0.41
39:2:502:LUT:H27	22:2:606:CLA:HMB3	2.02	0.41
22:A:1115:CLA:H62	22:A:1115:CLA:H41	1.46	0.41
22:A:1130:CLA:H111	22:A:1130:CLA:H143	1.80	0.41
22:A:1133:CLA:H142	22:A:1133:CLA:H111	1.84	0.41
22:A:1134:CLA:H52	22:A:1134:CLA:H11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:701:LEU:HB3	2:B:705:GLN:HG2	2.03	0.41
22:B:1021:CLA:HBA2	22:B:1021:CLA:H3A	1.79	0.41
22:B:1201:CLA:HMC3	22:B:1203:CLA:HED2	2.02	0.41
39:7:501:LUT:H30	22:7:601:CLA:H72	2.03	0.41
1:A:57:HIS:HB2	22:A:1128:CLA:HBA1	2.03	0.41
22:A:1013:CLA:H161	22:A:1013:CLA:H121	1.81	0.41
2:B:186:VAL:HG11	25:B:4002:BCR:H341	2.01	0.41
22:B:1209:CLA:HBA2	22:B:1209:CLA:H3A	1.86	0.41
4:D:117:LYS:HE3	4:D:119:GLU:HB3	2.01	0.41
4:D:122:LEU:HD12	4:D:122:LEU:HA	1.84	0.41
8:I:88:PRO:HG2	25:I:4001:BCR:H14C	2.03	0.41
12:1:157:LEU:HD12	39:1:501:LUT:H222	2.03	0.41
22:3:618:CLA:HED1	26:7:801:LHG:H311	2.03	0.41
25:8:503:BCR:H382	40:8:613:CHL:H111	2.03	0.41
22:2:612:CLA:HMA2	41:2:803:SQD:H82	2.03	0.41
20:9:126:ARG:NH2	22:9:612:CLA:O1D	2.44	0.41
1:A:318:ILE:HG13	22:A:1118:CLA:HED1	2.02	0.41
22:A:1117:CLA:H3A	22:A:1117:CLA:HBA2	1.74	0.41
22:A:1126:CLA:H3A	22:A:1126:CLA:HBA2	1.72	0.41
22:A:1133:CLA:H172	22:A:1137:CLA:H112	2.03	0.41
22:A:1138:CLA:HED3	2:B:421:SER:HB3	2.03	0.41
25:A:4005:BCR:H21C	22:A:1013:CLA:H122	2.02	0.41
2:B:462:GLN:HG2	2:B:473:TYR:CZ	2.56	0.41
2:B:577:PHE:CE1	22:B:1226:CLA:HAC2	2.55	0.41
22:B:1210:CLA:H203	25:B:4002:BCR:H271	2.03	0.41
22:B:1213:CLA:H51	22:B:1213:CLA:NC	2.35	0.41
7:G:59:ARG:NH2	28:1:803:LMT:O2B	2.52	0.41
22:1:601:CLA:H41	22:1:601:CLA:H62	1.83	0.41
40:1:610:CHL:HMC	22:1:613:CLA:HAB	2.03	0.41
12:Z:53:TYR:HB2	22:Z:604:CLA:HMD1	2.02	0.41
22:Z:605:CLA:H141	22:Z:605:CLA:H161	1.89	0.41
14:7:128:MET:HG3	22:7:612:CLA:HMC3	2.02	0.41
39:8:501:LUT:H35	39:8:501:LUT:H401	1.88	0.41
16:4:139:LYS:HE3	40:4:610:CHL:HED2	2.02	0.41
16:4:204:SER:HB3	22:4:601:CLA:HAA2	2.02	0.41
17:5:197:TYR:CZ	39:5:502:LUT:H10	2.56	0.41
22:6:609:CLA:H143	22:6:609:CLA:H161	1.86	0.41
19:2:53:PRO:HD2	39:2:502:LUT:H3	2.03	0.41
19:2:225:LYS:HA	19:2:225:LYS:HD2	1.92	0.41
28:9:803:LMT:H82	28:9:803:LMT:H51	1.94	0.41
1:A:217:GLN:OE1	1:A:298:HIS:ND1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:1140:CLA:H71	22:F:1302:CLA:HMD3	2.03	0.41
22:A:1101:CLA:H62	22:A:1101:CLA:H101	1.73	0.41
26:B:5006:LHG:H241	26:B:5006:LHG:H272	1.86	0.41
40:Z:609:CHL:HED3	16:4:163:ARG:HD2	2.02	0.41
15:8:45:ALA:O	15:8:51:ASN:ND2	2.53	0.41
16:4:140:PHE:HB3	16:4:142:TYR:CE2	2.56	0.41
20:9:140:ASN:OD1	20:9:140:ASN:N	2.53	0.41
22:A:1124:CLA:H18	25:A:4003:BCR:H342	2.03	0.40
2:B:257:THR:OG1	2:B:273:ASP:OD1	2.38	0.40
22:B:1239:CLA:H203	22:B:1239:CLA:H161	1.81	0.40
10:K:79:ASN:H	22:K:1404:CLA:HED1	1.87	0.40
11:L:101:ILE:HG12	11:L:114:GLU:HA	2.03	0.40
16:4:224:LEU:HD23	16:4:224:LEU:HA	1.93	0.40
22:B:1202:CLA:HBD	22:B:1202:CLA:H122	2.03	0.40
22:B:1229:CLA:H2	22:B:1229:CLA:H62	1.81	0.40
12:Z:184:PHE:CE1	39:Z:502:LUT:H10	2.55	0.40
22:Z:604:CLA:H3A	22:Z:604:CLA:H12	2.02	0.40
13:3:228:ILE:HD12	22:3:603:CLA:H43	2.02	0.40
22:8:602:CLA:HED3	22:4:605:CLA:H2	2.02	0.40
16:4:109:LEU:HB3	22:4:606:CLA:HAB	2.02	0.40
16:4:252:TRP:HB3	18:6:109:GLY:H	1.87	0.40
17:5:218:HIS:CG	22:5:603:CLA:HAA2	2.56	0.40
18:6:257:PRO:HB2	22:6:619:CLA:CAB	2.50	0.40
40:6:610:CHL:H8	40:6:610:CHL:H51	1.96	0.40
22:A:1104:CLA:H12	22:A:1128:CLA:H2	2.02	0.40
22:A:1108:CLA:HBC1	22:3:605:CLA:H121	2.02	0.40
22:A:1125:CLA:H152	22:A:1125:CLA:H111	1.84	0.40
22:B:1240:CLA:HED1	25:B:4004:BCR:H353	2.02	0.40
16:4:182:ASN:OD1	16:4:182:ASN:N	2.53	0.40
22:5:607:CLA:H61	22:5:607:CLA:H41	1.81	0.40
22:5:618:CLA:HED2	22:6:609:CLA:HMB2	2.03	0.40
19:2:212:ALA:HB3	32:9:802:DGA:HBT1	2.02	0.40
20:9:45:LEU:HD23	20:9:45:LEU:HA	1.93	0.40
1:A:316:TRP:HB3	10:K:57:VAL:HG23	2.02	0.40
1:A:746:ARG:O	1:A:750:VAL:HG22	2.22	0.40
25:A:4003:BCR:H351	25:A:4003:BCR:H15C	1.85	0.40
2:B:346:THR:HB	2:B:380:ALA:HB2	2.04	0.40
22:B:1214:CLA:H72	22:B:1214:CLA:H111	1.91	0.40
22:B:1230:CLA:H2	25:B:4006:BCR:H333	2.03	0.40
22:B:1240:CLA:H41	22:B:1240:CLA:H62	1.76	0.40
4:D:128:LEU:HD22	4:D:134:LEU:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1:40:ASP:OD1	15:8:143:LYS:NZ	2.53	0.40
22:Z:604:CLA:H3A	22:Z:604:CLA:HBA2	1.63	0.40
39:3:502:LUT:H163	22:3:613:CLA:HMC2	2.02	0.40
15:8:228:PRO:HG2	22:8:608:CLA:HMB3	2.03	0.40
16:4:248:LEU:HD23	16:4:248:LEU:HA	1.96	0.40
22:4:609:CLA:H11	18:6:123:TRP:HB2	2.03	0.40
40:5:610:CHL:H202	22:5:618:CLA:HBB1	2.03	0.40
19:2:117:VAL:CG1	19:2:121:LEU:HD13	2.51	0.40
22:A:1131:CLA:HBB1	22:A:1132:CLA:H2	2.03	0.40
10:K:60:ASN:N	10:K:68:VAL:O	2.47	0.40
22:7:603:CLA:H51	22:7:603:CLA:NC	2.37	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	739/741 (100%)	720 (97%)	19 (3%)	0	100	100
2	B	731/733 (100%)	707 (97%)	24 (3%)	0	100	100
3	C	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
4	D	141/144 (98%)	135 (96%)	6 (4%)	0	100	100
5	E	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
6	F	163/165 (99%)	158 (97%)	4 (2%)	1 (1%)	25	34
7	G	70/91 (77%)	70 (100%)	0	0	100	100
8	I	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
9	J	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	82/84 (98%)	81 (99%)	1 (1%)	0	100	100
11	L	122/138 (88%)	119 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	1	192/194 (99%)	185 (96%)	7 (4%)	0	100	100
12	Z	192/194 (99%)	188 (98%)	4 (2%)	0	100	100
13	3	217/219 (99%)	209 (96%)	8 (4%)	0	100	100
14	7	211/213 (99%)	203 (96%)	8 (4%)	0	100	100
15	8	215/217 (99%)	210 (98%)	5 (2%)	0	100	100
16	4	208/210 (99%)	199 (96%)	9 (4%)	0	100	100
17	5	225/227 (99%)	221 (98%)	3 (1%)	1 (0%)	34	46
18	6	227/229 (99%)	223 (98%)	4 (2%)	0	100	100
19	2	196/198 (99%)	187 (95%)	8 (4%)	1 (0%)	29	40
20	9	181/183 (99%)	170 (94%)	10 (6%)	1 (1%)	25	34
All	All	4323/4399 (98%)	4187 (97%)	132 (3%)	4 (0%)	54	65

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	150	PHE
17	5	243	GLN
19	2	180	LYS
20	9	139	ILE

### 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	601/601 (100%)	601 (100%)	0	100	100
2	B	596/596 (100%)	596 (100%)	0	100	100
3	C	69/69 (100%)	69 (100%)	0	100	100
4	D	120/120 (100%)	119 (99%)	1 (1%)	81	88
5	E	54/54 (100%)	54 (100%)	0	100	100
6	F	127/127 (100%)	127 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	54/68 (79%)	54 (100%)	0	100	100
8	I	31/31 (100%)	31 (100%)	0	100	100
9	J	35/35 (100%)	35 (100%)	0	100	100
10	K	58/58 (100%)	58 (100%)	0	100	100
11	L	92/102 (90%)	92 (100%)	0	100	100
12	1	137/137 (100%)	137 (100%)	0	100	100
12	Z	137/137 (100%)	137 (100%)	0	100	100
13	3	167/167 (100%)	167 (100%)	0	100	100
14	7	164/164 (100%)	164 (100%)	0	100	100
15	8	163/163 (100%)	163 (100%)	0	100	100
16	4	164/165 (99%)	164 (100%)	0	100	100
17	5	184/184 (100%)	184 (100%)	0	100	100
18	6	183/183 (100%)	183 (100%)	0	100	100
19	2	154/156 (99%)	153 (99%)	1 (1%)	86	92
20	9	141/141 (100%)	141 (100%)	0	100	100
All	All	3431/3458 (99%)	3429 (100%)	2 (0%)	93	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	189	ARG
19	2	148	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	296	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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
4	SNC	D	137	4	4,7,8	1.06	0	1,7,9	3.60	1 (100%)

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
4	SNC	D	137	4	-	0/0/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	137	SNC	CA-CB-SG	-3.60	105.28	112.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 354 ligands modelled in this entry, 1 is monoatomic - leaving 353 for Mogul analysis.



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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
31	LMG	J	5001	-	35,35,55	0.48	0	43,43,63	1.12	2 (4%)
22	CLA	A	1122	-	65,73,73	1.36	8 (12%)	76,113,113	2.00	17 (22%)
22	CLA	5	601	-	60,68,73	1.41	8 (13%)	70,107,113	2.07	17 (24%)
22	CLA	A	1109	-	65,73,73	1.35	8 (12%)	76,113,113	2.03	16 (21%)
22	CLA	8	603	-	65,73,73	1.35	8 (12%)	76,113,113	2.19	19 (25%)
22	CLA	A	1131	-	65,73,73	1.36	7 (10%)	76,113,113	1.97	16 (21%)
22	CLA	Z	605	-	65,73,73	1.33	9 (13%)	76,113,113	2.00	18 (23%)
39	LUT	5	502	-	42,43,43	2.26	1 (2%)	51,60,60	1.77	11 (21%)
22	CLA	A	1116	-	60,68,73	1.45	10 (16%)	70,107,113	2.04	18 (25%)
22	CLA	B	1206	-	65,73,73	1.35	7 (10%)	76,113,113	2.01	15 (19%)
22	CLA	3	607	-	60,68,73	1.43	9 (15%)	70,107,113	2.16	17 (24%)
22	CLA	A	1121	-	65,73,73	1.37	8 (12%)	76,113,113	2.03	18 (23%)
28	LMT	B	5005	-	36,36,36	1.21	6 (16%)	47,47,47	1.11	3 (6%)
39	LUT	Z	503	-	42,43,43	2.35	1 (2%)	51,60,60	2.08	13 (25%)
22	CLA	2	606	-	46,54,73	1.63	8 (17%)	53,90,113	2.18	11 (20%)
26	LHG	5	801	-	36,36,48	0.43	0	39,42,54	1.17	4 (10%)
26	LHG	A	5002	-	48,48,48	0.39	0	51,54,54	0.98	2 (3%)
22	CLA	B	1226	-	65,73,73	1.41	9 (13%)	76,113,113	2.16	22 (28%)
25	BCR	K	4002	-	41,41,41	1.83	4 (9%)	56,56,56	4.24	19 (33%)
22	CLA	4	604	-	60,68,73	1.39	7 (11%)	70,107,113	2.08	20 (28%)
22	CLA	8	612	-	46,54,73	1.60	8 (17%)	53,90,113	2.12	12 (22%)
39	LUT	3	501	-	42,43,43	2.32	1 (2%)	51,60,60	1.95	12 (23%)
25	BCR	5	504	-	41,41,41	1.84	5 (12%)	56,56,56	4.50	22 (39%)
22	CLA	9	607	-	55,63,73	1.49	7 (12%)	64,101,113	2.11	16 (25%)
22	CLA	K	1401	-	46,54,73	1.61	7 (15%)	53,90,113	2.08	13 (24%)
22	CLA	2	605	-	50,58,73	1.56	9 (18%)	58,95,113	2.23	17 (29%)
40	CHL	1	609	12	58,66,74	0.93	4 (6%)	63,104,114	1.26	8 (12%)
22	CLA	1	608	-	60,68,73	1.39	8 (13%)	70,107,113	2.06	15 (21%)
39	LUT	5	501	-	42,43,43	2.44	2 (4%)	51,60,60	1.91	12 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	2	603	-	55,63,73	1.48	8 (14%)	64,101,113	2.30	20 (31%)
22	CLA	B	1204	-	65,73,73	1.36	8 (12%)	76,113,113	1.98	15 (19%)
22	CLA	1	606	-	61,69,73	1.38	8 (13%)	71,108,113	2.05	17 (23%)
45	LPX	8	803	-	29,29,29	1.00	2 (6%)	31,33,33	1.00	1 (3%)
22	CLA	G	1602	-	46,54,73	1.62	8 (17%)	53,90,113	2.11	12 (22%)
22	CLA	A	1135	-	51,59,73	1.59	10 (19%)	59,96,113	2.20	17 (28%)
22	CLA	A	1120	-	55,63,73	1.45	7 (12%)	64,101,113	2.26	21 (32%)
22	CLA	Z	607	-	57,65,73	1.45	8 (14%)	66,103,113	2.07	17 (25%)
22	CLA	7	602	-	50,58,73	1.53	6 (12%)	58,95,113	2.17	17 (29%)
22	CLA	B	1240	-	65,73,73	1.37	8 (12%)	76,113,113	1.97	20 (26%)
22	CLA	2	607	-	46,54,73	1.64	9 (19%)	53,90,113	2.14	13 (24%)
25	BCR	3	506	-	41,41,41	1.86	4 (9%)	56,56,56	4.40	15 (26%)
40	CHL	6	611	-	51,59,74	0.91	2 (3%)	55,96,114	1.41	11 (20%)
22	CLA	A	1104	1	65,73,73	1.36	9 (13%)	76,113,113	1.97	18 (23%)
25	BCR	B	4005	-	41,41,41	1.86	4 (9%)	56,56,56	4.49	16 (28%)
25	BCR	B	4007	-	41,41,41	1.84	4 (9%)	56,56,56	4.16	13 (23%)
22	CLA	5	607	-	61,69,73	1.41	8 (13%)	71,108,113	1.98	16 (22%)
22	CLA	8	605	-	65,73,73	1.36	9 (13%)	76,113,113	1.96	19 (25%)
40	CHL	7	610	-	54,62,74	0.92	3 (5%)	58,99,114	1.40	12 (20%)
22	CLA	A	1107	1	65,73,73	1.36	6 (9%)	76,113,113	1.97	16 (21%)
40	CHL	5	617	-	43,51,74	1.05	3 (6%)	45,86,114	1.33	7 (15%)
22	CLA	1	607	-	60,68,73	1.41	8 (13%)	70,107,113	2.09	18 (25%)
22	CLA	L	1503	-	50,58,73	1.53	6 (12%)	58,95,113	2.28	19 (32%)
22	CLA	8	606	-	60,68,73	1.39	7 (11%)	70,107,113	2.03	19 (27%)
22	CLA	3	602	-	46,54,73	1.60	8 (17%)	53,90,113	2.06	12 (22%)
25	BCR	B	4003	-	41,41,41	1.86	5 (12%)	56,56,56	4.26	17 (30%)
39	LUT	2	502	-	42,43,43	2.32	1 (2%)	51,60,60	1.94	13 (25%)
38	SPH	7	804	-	19,20,20	0.64	0	18,21,21	1.11	1 (5%)
22	CLA	5	602	-	61,69,73	1.41	8 (13%)	71,108,113	1.94	16 (22%)
25	BCR	B	4006	-	41,41,41	1.81	4 (9%)	56,56,56	4.14	14 (25%)
37	C7Z	1	503	-	43,43,43	5.39	27 (62%)	58,60,60	2.30	20 (34%)
25	BCR	B	4001	-	41,41,41	1.83	5 (12%)	56,56,56	4.12	15 (26%)
22	CLA	K	1402	-	55,63,73	1.48	9 (16%)	64,101,113	2.18	17 (26%)
31	LMG	A	5003	-	29,29,55	0.56	0	37,37,63	1.20	3 (8%)
40	CHL	2	609	19	51,59,74	1.07	4 (7%)	55,96,114	1.39	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
40	CHL	Z	613	-	46,54,74	0.95	2 (4%)	49,90,114	1.39	8 (16%)
22	CLA	B	1225	-	65,73,73	1.38	8 (12%)	76,113,113	1.81	12 (15%)
22	CLA	B	1239	-	65,73,73	1.37	7 (10%)	76,113,113	2.03	16 (21%)
22	CLA	A	1126	-	65,73,73	1.38	9 (13%)	76,113,113	1.99	17 (22%)
22	CLA	5	608	-	45,53,73	1.62	9 (20%)	52,89,113	2.19	14 (26%)
36	RRX	F	4001	-	42,42,42	4.83	24 (57%)	57,58,58	2.50	24 (42%)
22	CLA	B	1230	-	58,66,73	1.41	7 (12%)	67,104,113	2.15	18 (26%)
22	CLA	5	612	-	65,73,73	1.33	7 (10%)	76,113,113	1.98	17 (22%)
38	SPH	K	5001	-	19,20,20	0.61	0	18,21,21	1.12	2 (11%)
22	CLA	1	612	-	65,73,73	1.36	8 (12%)	76,113,113	1.97	17 (22%)
22	CLA	A	1127	-	65,73,73	1.39	7 (10%)	76,113,113	1.85	14 (18%)
22	CLA	6	618	-	46,54,73	1.60	8 (17%)	53,90,113	2.16	14 (26%)
29	OCA	A	5008	-	9,9,9	0.70	0	9,9,9	1.36	1 (11%)
22	CLA	5	609	17	65,73,73	1.36	8 (12%)	76,113,113	1.92	17 (22%)
37	C7Z	J	4002	-	43,43,43	5.37	27 (62%)	58,60,60	2.23	20 (34%)
22	CLA	A	1102	-	55,63,73	1.46	7 (12%)	64,101,113	2.20	20 (31%)
28	LMT	4	803	-	36,36,36	1.17	5 (13%)	47,47,47	1.01	1 (2%)
22	CLA	Z	606	-	57,65,73	1.44	8 (14%)	66,103,113	2.18	17 (25%)
22	CLA	B	1238	-	65,73,73	1.35	8 (12%)	76,113,113	2.02	15 (19%)
22	CLA	Z	603	-	50,58,73	1.54	8 (16%)	58,95,113	2.27	18 (31%)
40	CHL	1	610	-	48,56,74	0.92	2 (4%)	51,92,114	1.40	10 (19%)
39	LUT	7	501	-	42,43,43	2.36	1 (2%)	51,60,60	1.91	12 (23%)
43	3PH	6	802	-	28,28,47	1.11	4 (14%)	32,33,52	1.25	2 (6%)
22	CLA	A	1124	46	65,73,73	1.37	8 (12%)	76,113,113	1.95	17 (22%)
22	CLA	9	612	-	50,58,73	1.55	9 (18%)	58,95,113	2.23	18 (31%)
22	CLA	7	605	-	61,69,73	1.40	8 (13%)	71,108,113	2.03	19 (26%)
22	CLA	B	1203	-	65,73,73	1.35	8 (12%)	76,113,113	1.90	17 (22%)
26	LHG	2	801	-	33,33,48	0.45	0	36,39,54	1.22	3 (8%)
40	CHL	6	613	-	56,64,74	0.88	2 (3%)	61,102,114	1.22	9 (14%)
43	3PH	2	802	-	26,26,47	1.14	4 (15%)	30,31,52	1.30	2 (6%)
22	CLA	7	611	-	50,58,73	1.50	7 (14%)	58,95,113	2.33	19 (32%)
22	CLA	7	615	14	58,66,73	1.45	8 (13%)	67,104,113	2.10	18 (26%)
22	CLA	B	1229	-	65,73,73	1.35	8 (12%)	76,113,113	1.99	19 (25%)
33	DGD	B	5003	-	67,67,67	1.18	7 (10%)	81,81,81	1.02	4 (4%)
22	CLA	2	615	-	46,54,73	1.58	7 (15%)	53,90,113	2.15	14 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	B	1235	-	65,73,73	1.37	9 (13%)	76,113,113	2.03	17 (22%)
22	CLA	3	606	-	65,73,73	1.33	7 (10%)	76,113,113	2.09	16 (21%)
42	QTB	Z	504	-	19,19,19	2.46	5 (26%)	20,26,26	2.76	7 (35%)
22	CLA	A	1140	-	65,73,73	1.37	8 (12%)	76,113,113	1.93	17 (22%)
22	CLA	B	1216	-	65,73,73	1.35	8 (12%)	76,113,113	1.93	16 (21%)
22	CLA	6	601	-	60,68,73	1.41	8 (13%)	70,107,113	2.09	18 (25%)
25	BCR	G	4001	-	41,41,41	1.84	4 (9%)	56,56,56	4.20	14 (25%)
22	CLA	A	1123	-	65,73,73	1.36	7 (10%)	76,113,113	2.04	19 (25%)
22	CLA	Z	604	-	65,73,73	1.35	9 (13%)	76,113,113	2.01	19 (25%)
40	CHL	9	613	-	42,50,74	1.50	4 (9%)	44,85,114	1.36	8 (18%)
22	CLA	B	1207	-	65,73,73	1.36	7 (10%)	76,113,113	1.96	17 (22%)
22	CLA	A	1125	-	65,73,73	1.35	7 (10%)	76,113,113	2.07	20 (26%)
22	CLA	2	604	-	56,64,73	1.44	8 (14%)	65,102,113	2.29	18 (27%)
24	SF4	A	3001	2,1	0,12,12	-	-	-	-	-
43	3PH	8	806	-	29,29,47	1.08	4 (13%)	33,34,52	1.18	2 (6%)
43	3PH	7	802	-	38,38,47	0.94	3 (7%)	42,43,52	1.12	2 (4%)
22	CLA	B	1214	-	59,67,73	1.43	8 (13%)	68,105,113	2.21	20 (29%)
22	CLA	L	1502	-	65,73,73	1.35	8 (12%)	76,113,113	2.04	16 (21%)
22	CLA	A	1114	-	61,69,73	1.38	7 (11%)	71,108,113	2.09	18 (25%)
22	CLA	Z	615	12	46,54,73	1.61	9 (19%)	53,90,113	2.15	14 (26%)
22	CLA	5	604	-	65,73,73	1.37	8 (12%)	76,113,113	1.99	20 (26%)
40	CHL	4	613	-	56,64,74	0.86	2 (3%)	61,102,114	1.39	13 (21%)
25	BCR	L	4002	-	41,41,41	1.83	4 (9%)	56,56,56	4.21	15 (26%)
22	CLA	K	1404	-	55,63,73	1.48	8 (14%)	64,101,113	2.18	15 (23%)
22	CLA	1	611	-	65,73,73	1.35	8 (12%)	76,113,113	2.03	18 (23%)
26	LHG	B	5001	-	22,22,48	0.55	0	25,28,54	1.30	1 (4%)
22	CLA	B	1224	-	65,73,73	1.38	9 (13%)	76,113,113	2.03	18 (23%)
22	CLA	A	1106	-	65,73,73	1.37	9 (13%)	76,113,113	2.00	16 (21%)
22	CLA	B	1217	-	56,64,73	1.47	9 (16%)	65,102,113	2.10	18 (27%)
40	CHL	5	610	-	66,74,74	0.90	3 (4%)	73,114,114	1.17	8 (10%)
27	NKP	3	802	-	15,15,28	2.07	3 (20%)	18,19,32	1.53	2 (11%)
22	CLA	A	1117	-	65,73,73	1.35	7 (10%)	76,113,113	2.04	18 (23%)
22	CLA	7	603	14	65,73,73	1.38	8 (12%)	76,113,113	2.15	19 (25%)
27	NKP	A	5004	-	28,28,28	1.52	3 (10%)	31,32,32	1.25	3 (9%)
22	CLA	A	1118	-	60,68,73	1.41	8 (13%)	70,107,113	2.12	18 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	3	608	-	45,53,73	1.63	9 (20%)	52,89,113	2.17	12 (23%)
22	CLA	7	609	14	65,73,73	1.35	8 (12%)	76,113,113	2.01	16 (21%)
37	C7Z	5	505	-	43,43,43	5.41	25 (58%)	58,60,60	2.25	19 (32%)
39	LUT	6	502	-	42,43,43	2.32	1 (2%)	51,60,60	1.85	13 (25%)
22	CLA	9	602	-	45,53,73	1.61	7 (15%)	52,89,113	2.13	14 (26%)
22	CLA	6	605	-	55,63,73	1.46	7 (12%)	64,101,113	2.18	20 (31%)
26	LHG	4	802	-	31,31,48	0.47	0	34,37,54	1.12	2 (5%)
39	LUT	4	502	-	42,43,43	2.29	1 (2%)	51,60,60	1.81	12 (23%)
22	CLA	A	1129	-	50,58,73	1.54	9 (18%)	58,95,113	2.18	17 (29%)
25	BCR	6	503	-	41,41,41	1.83	4 (9%)	56,56,56	4.28	14 (25%)
22	CLA	B	1228	-	65,73,73	1.34	7 (10%)	76,113,113	2.00	19 (25%)
26	LHG	B	5006	-	32,32,48	0.45	0	35,38,54	1.20	3 (8%)
22	CLA	B	1021	-	65,73,73	1.37	8 (12%)	76,113,113	1.92	15 (19%)
40	CHL	9	610	-	66,74,74	0.90	4 (6%)	73,114,114	1.18	10 (13%)
40	CHL	4	617	-	43,51,74	1.05	3 (6%)	45,86,114	1.35	9 (20%)
22	CLA	7	606	-	56,64,73	1.46	8 (14%)	65,102,113	2.12	15 (23%)
22	CLA	A	1101	-	65,73,73	1.35	8 (12%)	76,113,113	2.02	19 (25%)
25	BCR	5	503	-	41,41,41	1.84	4 (9%)	56,56,56	4.25	15 (26%)
40	CHL	5	611	-	51,59,74	0.89	2 (3%)	55,96,114	1.44	11 (20%)
40	CHL	2	613	-	51,59,74	0.95	3 (5%)	55,96,114	1.39	8 (14%)
22	CLA	9	601	-	60,68,73	1.42	7 (11%)	70,107,113	2.12	16 (22%)
22	CLA	9	605	-	55,63,73	1.47	8 (14%)	64,101,113	2.14	19 (29%)
22	CLA	1	603	-	65,73,73	1.36	8 (12%)	76,113,113	2.04	18 (23%)
25	BCR	J	4001	-	41,41,41	1.82	4 (9%)	56,56,56	4.22	16 (28%)
28	LMT	B	6101	-	36,36,36	1.19	5 (13%)	47,47,47	1.08	3 (6%)
22	CLA	B	1202	-	65,73,73	1.33	7 (10%)	76,113,113	2.11	21 (27%)
39	LUT	9	502	-	42,43,43	2.24	1 (2%)	51,60,60	1.83	14 (27%)
22	CLA	3	618	-	46,54,73	1.61	9 (19%)	53,90,113	2.11	13 (24%)
22	CLA	3	613	46	55,63,73	1.46	7 (12%)	64,101,113	2.10	14 (21%)
25	BCR	I	4001	-	41,41,41	1.83	4 (9%)	56,56,56	4.25	16 (28%)
22	CLA	Z	608	-	56,64,73	1.45	9 (16%)	65,102,113	2.09	17 (26%)
22	CLA	1	613	-	46,54,73	1.61	9 (19%)	53,90,113	2.11	15 (28%)
22	CLA	5	606	-	50,58,73	1.54	7 (14%)	58,95,113	2.27	16 (27%)
22	CLA	4	606	-	50,58,73	1.53	8 (16%)	58,95,113	2.19	19 (32%)
22	CLA	6	607	-	55,63,73	1.48	8 (14%)	64,101,113	2.09	15 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	B	1236	-	65,73,73	1.38	9 (13%)	76,113,113	1.97	16 (21%)
25	BCR	4	503	-	41,41,41	1.84	4 (9%)	56,56,56	4.21	16 (28%)
22	CLA	A	1139	-	65,73,73	1.38	8 (12%)	76,113,113	2.00	17 (22%)
28	LMT	8	805	-	36,36,36	1.21	6 (16%)	47,47,47	1.15	3 (6%)
22	CLA	B	1219	-	59,67,73	1.43	8 (13%)	68,105,113	2.15	17 (25%)
22	CLA	B	1234	-	60,68,73	1.41	8 (13%)	70,107,113	2.07	19 (27%)
22	CLA	A	1137	-	65,73,73	1.34	6 (9%)	76,113,113	2.06	20 (26%)
26	LHG	7	801	-	36,36,48	0.45	0	39,42,54	1.17	3 (7%)
22	CLA	Z	602	-	46,54,73	1.58	7 (15%)	53,90,113	2.15	14 (26%)
22	CLA	4	612	-	50,58,73	1.51	8 (16%)	58,95,113	2.34	18 (31%)
22	CLA	A	1128	-	65,73,73	1.38	7 (10%)	76,113,113	2.01	16 (21%)
40	CHL	Z	610	-	66,74,74	0.77	2 (3%)	73,114,114	1.23	10 (13%)
22	CLA	B	1232	-	45,53,73	1.64	8 (17%)	52,89,113	2.07	14 (26%)
40	CHL	8	613	-	66,74,74	0.88	3 (4%)	73,114,114	1.17	10 (13%)
22	CLA	7	613	-	42,50,73	1.66	7 (16%)	48,85,113	2.26	17 (35%)
22	CLA	2	601	-	60,68,73	1.40	9 (15%)	70,107,113	2.10	17 (24%)
22	CLA	B	1211	-	60,68,73	1.38	6 (10%)	70,107,113	2.23	17 (24%)
39	LUT	8	502	-	42,43,43	2.27	1 (2%)	51,60,60	1.86	15 (29%)
39	LUT	2	501	-	42,43,43	2.37	1 (2%)	51,60,60	2.36	13 (25%)
26	LHG	B	5002	-	19,19,48	0.84	1 (5%)	20,24,54	1.36	1 (5%)
22	CLA	A	1012	-	65,73,73	1.39	8 (12%)	76,113,113	1.99	18 (23%)
22	CLA	1	604	-	60,68,73	1.40	7 (11%)	70,107,113	2.06	18 (25%)
22	CLA	4	602	-	52,60,73	1.52	8 (15%)	60,97,113	2.19	17 (28%)
39	LUT	7	502	-	42,43,43	2.31	1 (2%)	51,60,60	1.94	13 (25%)
22	CLA	5	618	-	65,73,73	1.34	7 (10%)	76,113,113	2.03	16 (21%)
22	CLA	8	611	-	50,58,73	1.53	8 (16%)	58,95,113	2.29	17 (29%)
25	BCR	3	504	-	41,41,41	1.87	5 (12%)	56,56,56	4.31	16 (28%)
22	CLA	A	1112	-	60,68,73	1.43	8 (13%)	70,107,113	2.05	16 (22%)
22	CLA	A	1136	-	65,73,73	1.35	7 (10%)	76,113,113	2.01	17 (22%)
39	LUT	9	501	-	42,43,43	2.36	1 (2%)	51,60,60	1.94	15 (29%)
22	CLA	B	1201	-	45,53,73	1.58	8 (17%)	52,89,113	2.17	15 (28%)
22	CLA	J	1901	-	42,50,73	1.66	8 (19%)	48,85,113	2.26	17 (35%)
26	LHG	Z	801	-	42,42,48	0.41	0	45,48,54	1.16	4 (8%)
22	CLA	A	1119	-	65,73,73	1.37	8 (12%)	76,113,113	1.82	16 (21%)
22	CLA	3	604	-	60,68,73	1.39	9 (15%)	70,107,113	2.16	19 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	7	616	-	60,68,73	1.43	9 (15%)	70,107,113	2.10	17 (24%)
30	DAO	A	5007	-	13,13,13	0.79	1 (7%)	13,13,13	0.97	0
22	CLA	F	1301	-	65,73,73	1.37	8 (12%)	76,113,113	1.97	20 (26%)
22	CLA	7	604	-	65,73,73	1.36	8 (12%)	76,113,113	2.06	21 (27%)
22	CLA	A	1103	-	65,73,73	1.30	6 (9%)	76,113,113	2.04	18 (23%)
22	CLA	1	605	-	55,63,73	1.45	9 (16%)	64,101,113	2.18	18 (28%)
25	BCR	L	4001	-	41,41,41	1.82	4 (9%)	56,56,56	4.23	14 (25%)
32	DGA	9	802	-	38,38,43	1.15	3 (7%)	40,40,45	1.61	3 (7%)
25	BCR	7	503	-	41,41,41	1.83	4 (9%)	56,56,56	4.31	15 (26%)
22	CLA	2	608	-	45,53,73	1.61	7 (15%)	52,89,113	2.25	16 (30%)
22	CLA	6	604	-	65,73,73	1.36	8 (12%)	76,113,113	2.04	20 (26%)
23	PQN	A	2001	-	34,34,34	0.39	0	42,45,45	1.07	2 (4%)
22	CLA	5	613	-	55,63,73	1.48	9 (16%)	64,101,113	2.03	15 (23%)
22	CLA	1	615	12	65,73,73	1.39	8 (12%)	76,113,113	1.87	14 (18%)
40	CHL	6	610	-	56,64,74	0.84	2 (3%)	61,102,114	1.40	13 (21%)
22	CLA	A	1110	-	65,73,73	1.38	8 (12%)	76,113,113	2.00	17 (22%)
22	CLA	B	1205	-	65,73,73	1.37	7 (10%)	76,113,113	2.06	17 (22%)
28	LMT	A	5006	-	36,36,36	1.20	6 (16%)	47,47,47	1.04	1 (2%)
25	BCR	6	504	-	41,41,41	1.89	4 (9%)	56,56,56	4.30	15 (26%)
22	CLA	G	1601	-	50,58,73	1.54	7 (14%)	58,95,113	2.19	17 (29%)
41	SQD	1	802	-	47,48,54	0.83	0	56,59,65	0.94	2 (3%)
22	CLA	9	609	20	46,54,73	1.65	9 (19%)	53,90,113	2.12	14 (26%)
22	CLA	8	607	-	55,63,73	1.48	7 (12%)	64,101,113	2.06	16 (25%)
22	CLA	B	1218	-	65,73,73	1.34	8 (12%)	76,113,113	2.11	19 (25%)
22	CLA	Z	612	-	65,73,73	1.36	7 (10%)	76,113,113	1.96	16 (21%)
27	NKP	8	802	-	28,28,28	1.50	2 (7%)	31,32,32	1.25	3 (9%)
22	CLA	9	608	-	45,53,73	1.63	9 (20%)	52,89,113	2.13	13 (25%)
22	CLA	K	1403	10	49,57,73	1.57	7 (14%)	55,93,113	2.22	15 (27%)
22	CLA	9	603	-	60,68,73	1.42	6 (10%)	70,107,113	2.23	19 (27%)
22	CLA	A	1132	-	65,73,73	1.37	7 (10%)	76,113,113	2.04	17 (22%)
22	CLA	6	608	-	55,63,73	1.49	10 (18%)	64,101,113	2.14	15 (23%)
22	CLA	3	603	-	65,73,73	1.37	9 (13%)	76,113,113	2.08	16 (21%)
39	LUT	Z	502	-	42,43,43	2.24	1 (2%)	51,60,60	1.91	12 (23%)
39	LUT	8	501	-	42,43,43	2.30	1 (2%)	51,60,60	1.92	13 (25%)
22	CLA	4	605	-	65,73,73	1.35	9 (13%)	76,113,113	1.95	16 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	BCR	3	503	-	41,41,41	1.82	4 (9%)	56,56,56	4.17	16 (28%)
22	CLA	Z	601	-	60,68,73	1.40	8 (13%)	70,107,113	2.07	18 (25%)
22	CLA	7	608	-	43,51,73	1.66	8 (18%)	49,86,113	2.20	13 (26%)
25	BCR	A	4005	-	41,41,41	1.83	4 (9%)	56,56,56	4.23	12 (21%)
25	BCR	A	4002	-	41,41,41	1.83	5 (12%)	56,56,56	4.18	14 (25%)
26	LHG	6	801	-	48,48,48	0.40	0	51,54,54	1.08	4 (7%)
22	CLA	6	615	-	61,69,73	1.40	8 (13%)	71,108,113	2.09	19 (26%)
28	LMT	F	5001	-	36,36,36	1.19	6 (16%)	47,47,47	0.97	1 (2%)
22	CLA	A	1115	-	60,68,73	1.41	7 (11%)	70,107,113	1.91	15 (21%)
22	CLA	4	615	-	41,49,73	1.69	8 (19%)	47,84,113	2.29	15 (31%)
26	LHG	4	801	-	48,48,48	0.39	0	51,54,54	1.11	4 (7%)
26	LHG	8	801	-	37,37,48	0.43	0	40,43,54	1.07	2 (5%)
25	BCR	8	503	-	41,41,41	1.83	4 (9%)	56,56,56	4.26	17 (30%)
35	T7X	B	5004	-	49,49,61	0.93	4 (8%)	59,61,73	1.03	3 (5%)
22	CLA	2	602	-	46,54,73	1.60	7 (15%)	53,90,113	2.18	15 (28%)
40	CHL	4	610	-	51,59,74	0.87	2 (3%)	55,96,114	1.51	13 (23%)
22	CLA	2	612	-	50,58,73	1.54	7 (14%)	58,95,113	2.25	19 (32%)
22	CLA	A	1141	26	52,60,73	1.51	8 (15%)	60,97,113	2.27	18 (30%)
22	CLA	9	606	-	50,58,73	1.57	9 (18%)	58,95,113	2.18	16 (27%)
22	CLA	B	1241	-	65,73,73	1.35	9 (13%)	76,113,113	2.11	20 (26%)
26	LHG	A	5001	22	34,34,48	0.46	0	37,40,54	1.18	4 (10%)
22	CLA	A	1013	-	65,73,73	1.35	8 (12%)	76,113,113	1.93	17 (22%)
22	CLA	A	1113	-	65,73,73	1.34	6 (9%)	76,113,113	2.01	18 (23%)
40	CHL	6	617	-	43,51,74	1.05	3 (6%)	45,86,114	1.36	9 (20%)
22	CLA	B	1237	-	65,73,73	1.36	8 (12%)	76,113,113	1.97	13 (17%)
22	CLA	1	602	-	45,53,73	1.63	9 (20%)	52,89,113	2.09	14 (26%)
22	CLA	5	605	-	55,63,73	1.47	8 (14%)	64,101,113	2.24	23 (35%)
39	LUT	Z	501	-	42,43,43	2.36	1 (2%)	51,60,60	1.87	13 (25%)
26	LHG	9	801	-	32,32,48	0.45	0	35,38,54	1.11	2 (5%)
22	CLA	9	604	-	65,73,73	1.40	8 (12%)	76,113,113	2.01	21 (27%)
22	CLA	A	1134	1	55,63,73	1.48	8 (14%)	64,101,113	2.21	19 (29%)
22	CLA	B	1212	-	57,65,73	1.44	7 (12%)	66,103,113	2.18	20 (30%)
22	CLA	B	1210	-	65,73,73	1.36	8 (12%)	76,113,113	2.14	21 (27%)
22	CLA	8	602	-	65,73,73	1.36	7 (10%)	76,113,113	1.93	15 (19%)
22	CLA	7	601	-	60,68,73	1.42	9 (15%)	70,107,113	2.14	20 (28%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	5	615	17	50,58,73	1.55	8 (16%)	58,95,113	2.27	18 (31%)
25	BCR	K	4001	-	41,41,41	1.83	4 (9%)	56,56,56	4.34	15 (26%)
22	CLA	8	609	15	65,73,73	1.38	8 (12%)	76,113,113	2.02	17 (22%)
22	CLA	6	602	-	52,60,73	1.52	8 (15%)	60,97,113	2.19	16 (26%)
25	BCR	A	4003	-	41,41,41	1.82	4 (9%)	56,56,56	4.33	19 (33%)
40	CHL	8	610	-	56,64,74	0.87	2 (3%)	61,102,114	1.41	11 (18%)
28	LMT	1	803	-	36,36,36	1.19	5 (13%)	47,47,47	0.98	2 (4%)
24	SF4	C	3002	3	0,12,12	-	-	-	-	-
22	CLA	A	1108	-	65,73,73	1.35	6 (9%)	76,113,113	2.01	19 (25%)
44	PLM	7	805	-	17,17,17	0.56	0	17,17,17	1.11	1 (5%)
22	CLA	5	622	-	46,54,73	1.62	8 (17%)	53,90,113	2.18	13 (24%)
22	CLA	3	610	13	60,68,73	1.44	8 (13%)	70,107,113	2.03	18 (25%)
40	CHL	4	611	-	51,59,74	0.90	2 (3%)	55,96,114	1.39	11 (20%)
22	CLA	4	601	-	60,68,73	1.41	8 (13%)	70,107,113	2.12	20 (28%)
39	LUT	4	501	-	42,43,43	2.37	1 (2%)	51,60,60	1.84	12 (23%)
24	SF4	C	3003	3	0,12,12	-	-	-	-	-
40	CHL	Z	609	12	66,74,74	0.87	4 (6%)	73,114,114	1.21	10 (13%)
22	CLA	Z	611	-	55,63,73	1.47	8 (14%)	64,101,113	2.16	19 (29%)
32	DGA	A	5005	-	43,43,43	1.15	3 (6%)	45,45,45	1.49	3 (6%)
22	CLA	8	601	-	60,68,73	1.41	9 (15%)	70,107,113	2.09	18 (25%)
22	CLA	6	612	-	50,58,73	1.53	8 (16%)	58,95,113	2.26	16 (27%)
28	LMT	9	803	-	36,36,36	1.18	5 (13%)	47,47,47	1.04	3 (6%)
43	3PH	5	802	-	22,22,47	1.23	3 (13%)	26,27,52	1.27	2 (7%)
22	CLA	F	1302	-	45,53,73	1.62	8 (17%)	52,89,113	2.08	13 (25%)
22	CLA	A	1130	-	65,73,73	1.36	7 (10%)	76,113,113	1.92	15 (19%)
40	CHL	3	611	-	66,74,74	1.00	3 (4%)	73,114,114	1.27	10 (13%)
22	CLA	B	1223	-	65,73,73	1.37	8 (12%)	76,113,113	1.95	18 (23%)
22	CLA	B	1227	-	50,58,73	1.56	9 (18%)	58,95,113	2.07	18 (31%)
22	CLA	A	1133	-	65,73,73	1.35	7 (10%)	76,113,113	1.93	14 (18%)
22	CLA	A	1138	-	65,73,73	1.35	7 (10%)	76,113,113	2.04	16 (21%)
39	LUT	6	501	-	42,43,43	2.38	1 (2%)	51,60,60	1.87	14 (27%)
22	CLA	B	1221	-	65,73,73	1.35	9 (13%)	76,113,113	2.18	21 (27%)
22	CLA	8	608	-	55,63,73	1.48	8 (14%)	64,101,113	2.04	16 (25%)
22	CLA	6	609	18	65,73,73	1.36	7 (10%)	76,113,113	2.01	17 (22%)
22	CLA	3	605	-	65,73,73	1.37	9 (13%)	76,113,113	1.87	17 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	6	603	-	65,73,73	1.37	8 (12%)	76,113,113	2.12	17 (22%)
22	CLA	4	608	-	55,63,73	1.48	8 (14%)	64,101,113	2.12	16 (25%)
39	LUT	1	502	-	42,43,43	2.31	1 (2%)	51,60,60	1.89	14 (27%)
21	CL0	A	1011	-	65,73,73	2.35	17 (26%)	76,113,113	2.54	21 (27%)
22	CLA	B	1209	-	65,73,73	1.39	7 (10%)	76,113,113	2.02	16 (21%)
25	BCR	3	505	-	41,41,41	1.83	4 (9%)	56,56,56	4.31	12 (21%)
26	LHG	3	801	-	19,19,48	0.92	1 (5%)	20,24,54	1.34	1 (5%)
22	CLA	B	1022	46	65,73,73	1.40	7 (10%)	76,113,113	1.90	19 (25%)
25	BCR	A	4004	-	41,41,41	1.82	5 (12%)	56,56,56	4.32	19 (33%)
26	LHG	1	801	-	42,42,48	0.44	0	45,48,54	1.18	4 (8%)
22	CLA	A	1105	-	65,73,73	1.37	9 (13%)	76,113,113	1.96	17 (22%)
38	SPH	7	803	-	19,20,20	0.67	0	18,21,21	0.96	1 (5%)
40	CHL	2	610	-	48,56,74	0.99	3 (6%)	51,92,114	1.29	7 (13%)
22	CLA	B	1215	-	60,68,73	1.40	8 (13%)	70,107,113	2.07	16 (22%)
25	BCR	B	4004	-	41,41,41	1.85	4 (9%)	56,56,56	4.23	15 (26%)
25	BCR	B	4002	-	41,41,41	1.83	4 (9%)	56,56,56	4.19	10 (17%)
22	CLA	8	604	-	62,70,73	1.39	8 (12%)	72,109,113	2.10	22 (30%)
22	CLA	B	1222	-	65,73,73	1.34	7 (10%)	76,113,113	1.99	21 (27%)
22	CLA	1	601	-	65,73,73	1.35	8 (12%)	76,113,113	2.00	21 (27%)
23	PQN	B	2002	-	34,34,34	0.40	0	42,45,45	1.04	2 (4%)
22	CLA	4	609	16	60,68,73	1.41	8 (13%)	70,107,113	2.01	16 (22%)
22	CLA	B	1231	-	65,73,73	1.37	8 (12%)	76,113,113	1.93	15 (19%)
39	LUT	1	501	-	42,43,43	2.35	1 (2%)	51,60,60	1.84	13 (25%)
41	SQD	2	803	-	42,43,54	0.88	0	51,54,65	0.97	2 (3%)
22	CLA	B	1023	-	65,73,73	1.34	7 (10%)	76,113,113	2.07	16 (21%)
39	LUT	3	502	-	42,43,43	2.38	1 (2%)	51,60,60	1.97	14 (27%)
22	CLA	5	603	-	56,64,73	1.46	7 (12%)	65,102,113	2.28	18 (27%)
39	LUT	2	503	-	42,43,43	2.40	1 (2%)	51,60,60	2.63	23 (45%)
25	BCR	7	504	-	41,41,41	1.85	4 (9%)	56,56,56	4.47	18 (32%)
22	CLA	6	606	-	65,73,73	1.35	8 (12%)	76,113,113	2.03	17 (22%)
22	CLA	3	612	-	60,68,73	1.40	9 (15%)	70,107,113	2.02	15 (21%)
22	CLA	7	612	-	50,58,73	1.54	6 (12%)	58,95,113	2.25	17 (29%)
22	CLA	4	607	-	55,63,73	1.48	9 (16%)	64,101,113	2.12	15 (23%)
22	CLA	3	616	-	56,64,73	1.47	8 (14%)	65,102,113	2.17	18 (27%)
22	CLA	4	603	-	65,73,73	1.36	8 (12%)	76,113,113	2.11	20 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	BCR	A	4001	-	41,41,41	1.82	4 (9%)	56,56,56	4.13	15 (26%)
22	CLA	B	1208	-	56,64,73	1.45	8 (14%)	65,102,113	2.16	18 (27%)
22	CLA	B	1220	-	65,73,73	1.35	7 (10%)	76,113,113	1.93	16 (21%)
22	CLA	B	1213	-	65,73,73	1.37	8 (12%)	76,113,113	2.09	20 (26%)
22	CLA	6	619	18	65,73,73	1.35	8 (12%)	76,113,113	2.06	18 (23%)
22	CLA	A	1111	-	65,73,73	1.35	7 (10%)	76,113,113	2.06	19 (25%)
22	CLA	8	615	15	46,54,73	1.61	8 (17%)	53,90,113	2.20	14 (26%)
22	CLA	3	601	-	65,73,73	1.36	8 (12%)	76,113,113	2.06	21 (27%)
22	CLA	7	607	-	65,73,73	1.35	8 (12%)	76,113,113	1.95	17 (22%)

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
31	LMG	J	5001	-	-	14/30/50/70	0/1/1/1
22	CLA	A	1122	-	1/1/15/20	21/37/115/115	-
22	CLA	5	601	-	1/1/14/20	12/31/109/115	-
22	CLA	A	1109	-	1/1/15/20	13/37/115/115	-
22	CLA	8	603	-	1/1/15/20	8/37/115/115	-
22	CLA	A	1131	-	1/1/15/20	14/37/115/115	-
22	CLA	Z	605	-	1/1/15/20	13/37/115/115	-
39	LUT	5	502	-	-	2/29/67/67	0/2/2/2
22	CLA	A	1116	-	1/1/14/20	10/31/109/115	-
22	CLA	B	1206	-	1/1/15/20	21/37/115/115	-
22	CLA	3	607	-	1/1/14/20	17/31/109/115	-
22	CLA	A	1121	-	1/1/15/20	21/37/115/115	-
28	LMT	B	5005	-	-	6/21/61/61	0/2/2/2
39	LUT	Z	503	-	-	10/29/67/67	0/2/2/2
22	CLA	2	606	-	1/1/11/20	8/15/93/115	-
26	LHG	5	801	-	-	27/41/41/53	-
26	LHG	A	5002	-	-	31/53/53/53	-
22	CLA	B	1226	-	1/1/15/20	13/37/115/115	-
25	BCR	K	4002	-	-	11/29/63/63	0/2/2/2
22	CLA	4	604	-	1/1/14/20	11/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	8	612	-	1/1/11/20	9/15/93/115	-
39	LUT	3	501	-	-	1/29/67/67	0/2/2/2
25	BCR	5	504	-	-	11/29/63/63	0/2/2/2
22	CLA	9	607	-	1/1/13/20	9/25/103/115	-
22	CLA	K	1401	-	1/1/11/20	6/15/93/115	-
22	CLA	2	605	-	1/1/12/20	9/19/97/115	-
40	CHL	1	609	12	4/4/18/26	3/30/128/137	-
22	CLA	1	608	-	1/1/14/20	11/31/109/115	-
39	LUT	5	501	-	-	3/29/67/67	0/2/2/2
22	CLA	2	603	-	1/1/13/20	8/25/103/115	-
22	CLA	B	1204	-	1/1/15/20	12/37/115/115	-
22	CLA	1	606	-	1/1/14/20	12/33/111/115	-
45	LPX	8	803	-	-	10/31/31/31	-
22	CLA	G	1602	-	1/1/11/20	5/15/93/115	-
22	CLA	A	1135	-	1/1/12/20	7/21/99/115	-
22	CLA	A	1120	-	1/1/13/20	12/25/103/115	-
22	CLA	Z	607	-	1/1/13/20	15/28/106/115	-
22	CLA	7	602	-	1/1/12/20	5/19/97/115	-
22	CLA	B	1240	-	1/1/15/20	21/37/115/115	-
22	CLA	2	607	-	1/1/11/20	9/15/93/115	-
25	BCR	3	506	-	-	15/29/63/63	0/2/2/2
40	CHL	6	611	-	3/3/17/26	5/21/119/137	-
22	CLA	A	1104	1	1/1/15/20	21/37/115/115	-
25	BCR	B	4005	-	-	15/29/63/63	0/2/2/2
25	BCR	B	4007	-	-	13/29/63/63	0/2/2/2
22	CLA	5	607	-	1/1/14/20	12/33/111/115	-
22	CLA	8	605	-	1/1/15/20	16/37/115/115	-
40	CHL	7	610	-	3/3/17/26	4/25/123/137	-
22	CLA	A	1107	1	1/1/15/20	13/37/115/115	-
40	CHL	5	617	-	3/3/15/26	0/12/110/137	-
22	CLA	1	607	-	1/1/14/20	15/31/109/115	-
22	CLA	L	1503	-	1/1/12/20	11/19/97/115	-
22	CLA	8	606	-	1/1/14/20	16/31/109/115	-
22	CLA	3	602	-	1/1/11/20	4/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	B	4003	-	-	5/29/63/63	0/2/2/2
39	LUT	2	502	-	-	5/29/67/67	0/2/2/2
38	SPH	7	804	-	-	7/21/21/21	-
22	CLA	5	602	-	1/1/14/20	13/33/111/115	-
25	BCR	B	4006	-	-	11/29/63/63	0/2/2/2
37	C7Z	1	503	-	1/1/12/26	8/29/67/67	0/2/2/2
25	BCR	B	4001	-	-	12/29/63/63	0/2/2/2
22	CLA	K	1402	-	1/1/13/20	14/25/103/115	-
31	LMG	A	5003	-	-	8/24/44/70	0/1/1/1
40	CHL	2	609	19	3/3/17/26	4/21/119/137	-
40	CHL	Z	613	-	3/3/16/26	5/15/113/137	-
22	CLA	B	1225	-	1/1/15/20	4/37/115/115	-
22	CLA	B	1239	-	1/1/15/20	13/37/115/115	-
22	CLA	A	1126	-	1/1/15/20	20/37/115/115	-
22	CLA	5	608	-	1/1/11/20	4/13/91/115	-
36	RRX	F	4001	-	1/1/11/25	9/29/65/65	0/2/2/2
22	CLA	B	1230	-	1/1/13/20	14/29/107/115	-
22	CLA	5	612	-	1/1/15/20	11/37/115/115	-
38	SPH	K	5001	-	-	12/21/21/21	-
22	CLA	1	612	-	1/1/15/20	24/37/115/115	-
22	CLA	A	1127	-	1/1/15/20	12/37/115/115	-
22	CLA	6	618	-	1/1/11/20	8/15/93/115	-
29	OCA	A	5008	-	-	0/7/7/7	-
22	CLA	5	609	17	1/1/15/20	19/37/115/115	-
37	C7Z	J	4002	-	1/1/12/26	13/29/67/67	0/2/2/2
22	CLA	A	1102	-	1/1/13/20	9/25/103/115	-
28	LMT	4	803	-	-	9/21/61/61	0/2/2/2
22	CLA	Z	606	-	1/1/13/20	11/28/106/115	-
22	CLA	B	1238	-	1/1/15/20	11/37/115/115	-
22	CLA	Z	603	-	1/1/12/20	9/19/97/115	-
40	CHL	1	610	-	3/3/16/26	7/18/116/137	-
39	LUT	7	501	-	-	3/29/67/67	0/2/2/2
43	3PH	6	802	-	-	12/30/30/49	-
22	CLA	A	1124	46	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	9	612	-	1/1/12/20	2/19/97/115	-
22	CLA	7	605	-	1/1/14/20	12/33/111/115	-
22	CLA	B	1203	-	1/1/15/20	17/37/115/115	-
26	LHG	2	801	-	-	16/38/38/53	-
40	CHL	6	613	-	4/4/18/26	4/27/125/137	-
43	3PH	2	802	-	-	8/28/28/49	-
22	CLA	7	611	-	1/1/12/20	5/19/97/115	-
22	CLA	7	615	14	1/1/13/20	12/29/107/115	-
22	CLA	B	1229	-	1/1/15/20	13/37/115/115	-
33	DGD	B	5003	-	-	16/55/95/95	0/2/2/2
22	CLA	2	615	-	1/1/11/20	6/15/93/115	-
22	CLA	B	1235	-	1/1/15/20	15/37/115/115	-
22	CLA	3	606	-	1/1/15/20	18/37/115/115	-
42	QTB	Z	504	-	1/1/5/10	7/11/28/28	0/1/1/1
22	CLA	A	1140	-	1/1/15/20	10/37/115/115	-
22	CLA	B	1216	-	1/1/15/20	26/37/115/115	-
22	CLA	6	601	-	1/1/14/20	11/31/109/115	-
25	BCR	G	4001	-	-	13/29/63/63	0/2/2/2
22	CLA	A	1123	-	1/1/15/20	12/37/115/115	-
22	CLA	Z	604	-	1/1/15/20	16/37/115/115	-
40	CHL	9	613	-	3/3/15/26	0/10/108/137	-
22	CLA	B	1207	-	1/1/15/20	18/37/115/115	-
22	CLA	A	1125	-	1/1/15/20	17/37/115/115	-
22	CLA	2	604	-	1/1/13/20	13/27/105/115	-
43	3PH	8	806	-	-	19/31/31/49	-
24	SF4	A	3001	2,1	-	-	0/6/5/5
43	3PH	7	802	-	-	19/40/40/49	-
22	CLA	B	1214	-	1/1/13/20	11/30/108/115	-
22	CLA	L	1502	-	1/1/15/20	22/37/115/115	-
22	CLA	A	1114	-	1/1/14/20	9/33/111/115	-
22	CLA	Z	615	12	1/1/11/20	7/15/93/115	-
22	CLA	5	604	-	1/1/15/20	11/37/115/115	-
40	CHL	4	613	-	4/4/18/26	2/27/125/137	-
25	BCR	L	4002	-	-	13/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	K	1404	-	1/1/13/20	12/25/103/115	-
22	CLA	1	611	-	1/1/15/20	18/37/115/115	-
26	LHG	B	5001	-	-	13/26/26/53	-
22	CLA	B	1224	-	1/1/15/20	15/37/115/115	-
22	CLA	A	1106	-	1/1/15/20	15/37/115/115	-
22	CLA	B	1217	-	1/1/13/20	10/27/105/115	-
40	CHL	5	610	-	4/4/20/26	6/39/137/137	-
27	NKP	3	802	-	-	5/15/15/28	-
22	CLA	A	1117	-	1/1/15/20	20/37/115/115	-
22	CLA	7	603	14	1/1/15/20	13/37/115/115	-
27	NKP	A	5004	-	-	12/28/28/28	-
22	CLA	A	1118	-	1/1/14/20	9/31/109/115	-
22	CLA	3	608	-	1/1/11/20	5/13/91/115	-
22	CLA	7	609	14	1/1/15/20	18/37/115/115	-
37	C7Z	5	505	-	1/1/12/26	10/29/67/67	0/2/2/2
39	LUT	6	502	-	-	4/29/67/67	0/2/2/2
22	CLA	9	602	-	1/1/11/20	4/13/91/115	-
22	CLA	6	605	-	1/1/13/20	16/25/103/115	-
26	LHG	4	802	-	-	25/36/36/53	-
39	LUT	4	502	-	-	2/29/67/67	0/2/2/2
22	CLA	A	1129	-	1/1/12/20	9/19/97/115	-
25	BCR	6	503	-	-	13/29/63/63	0/2/2/2
22	CLA	B	1228	-	1/1/15/20	20/37/115/115	-
26	LHG	B	5006	-	-	17/37/37/53	-
22	CLA	B	1021	-	1/1/15/20	9/37/115/115	-
40	CHL	9	610	-	4/4/20/26	5/39/137/137	-
40	CHL	4	617	-	3/3/15/26	1/12/110/137	-
22	CLA	7	606	-	1/1/13/20	15/27/105/115	-
22	CLA	A	1101	-	1/1/15/20	15/37/115/115	-
25	BCR	5	503	-	-	12/29/63/63	0/2/2/2
40	CHL	5	611	-	3/3/17/26	3/21/119/137	-
40	CHL	2	613	-	3/3/17/26	5/21/119/137	-
22	CLA	9	601	-	1/1/14/20	14/31/109/115	-
22	CLA	9	605	-	-	6/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	1	603	-	1/1/15/20	15/37/115/115	-
25	BCR	J	4001	-	-	17/29/63/63	0/2/2/2
28	LMT	B	6101	-	-	10/21/61/61	0/2/2/2
22	CLA	B	1202	-	1/1/15/20	10/37/115/115	-
39	LUT	9	502	-	-	3/29/67/67	0/2/2/2
22	CLA	3	618	-	1/1/11/20	8/15/93/115	-
22	CLA	3	613	46	1/1/13/20	7/25/103/115	-
25	BCR	I	4001	-	-	13/29/63/63	0/2/2/2
22	CLA	Z	608	-	1/1/13/20	13/27/105/115	-
22	CLA	1	613	-	1/1/11/20	7/15/93/115	-
22	CLA	5	606	-	1/1/12/20	8/19/97/115	-
22	CLA	4	606	-	1/1/12/20	8/19/97/115	-
22	CLA	6	607	-	1/1/13/20	10/25/103/115	-
22	CLA	B	1236	-	1/1/15/20	25/37/115/115	-
25	BCR	4	503	-	-	15/29/63/63	0/2/2/2
22	CLA	A	1139	-	1/1/15/20	10/37/115/115	-
28	LMT	8	805	-	-	6/21/61/61	0/2/2/2
22	CLA	B	1219	-	1/1/13/20	15/30/108/115	-
22	CLA	B	1234	-	1/1/14/20	14/31/109/115	-
22	CLA	A	1137	-	1/1/15/20	15/37/115/115	-
26	LHG	7	801	-	-	22/41/41/53	-
22	CLA	Z	602	-	1/1/11/20	6/15/93/115	-
22	CLA	4	612	-	1/1/12/20	7/19/97/115	-
22	CLA	A	1128	-	1/1/15/20	19/37/115/115	-
40	CHL	Z	610	-	4/4/20/26	9/39/137/137	-
22	CLA	B	1232	-	1/1/11/20	3/13/91/115	-
40	CHL	8	613	-	5/5/20/26	11/39/137/137	-
22	CLA	7	613	-	1/1/10/20	4/10/88/115	-
22	CLA	2	601	-	1/1/14/20	14/31/109/115	-
22	CLA	B	1211	-	1/1/14/20	12/31/109/115	-
39	LUT	8	502	-	-	4/29/67/67	0/2/2/2
39	LUT	2	501	-	1/1/12/27	6/29/67/67	0/2/2/2
26	LHG	B	5002	-	-	13/22/22/53	-
22	CLA	A	1012	-	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	1	604	-	1/1/14/20	11/31/109/115	-
22	CLA	4	602	-	1/1/12/20	7/22/100/115	-
39	LUT	7	502	-	-	3/29/67/67	0/2/2/2
22	CLA	5	618	-	1/1/15/20	17/37/115/115	-
22	CLA	8	611	-	1/1/12/20	6/19/97/115	-
25	BCR	3	504	-	-	12/29/63/63	0/2/2/2
22	CLA	A	1112	-	1/1/14/20	9/31/109/115	-
22	CLA	A	1136	-	1/1/15/20	19/37/115/115	-
39	LUT	9	501	-	-	4/29/67/67	0/2/2/2
22	CLA	B	1201	-	1/1/11/20	4/13/91/115	-
22	CLA	J	1901	-	1/1/10/20	6/10/88/115	-
26	LHG	Z	801	-	-	29/47/47/53	-
22	CLA	A	1119	-	1/1/15/20	11/37/115/115	-
22	CLA	3	604	-	1/1/14/20	6/31/109/115	-
22	CLA	7	616	-	1/1/14/20	10/31/109/115	-
30	DAO	A	5007	-	-	3/11/11/11	-
22	CLA	F	1301	-	1/1/15/20	13/37/115/115	-
22	CLA	7	604	-	1/1/15/20	13/37/115/115	-
22	CLA	A	1103	-	1/1/15/20	11/37/115/115	-
22	CLA	1	605	-	1/1/13/20	7/25/103/115	-
25	BCR	L	4001	-	-	13/29/63/63	0/2/2/2
32	DGA	9	802	-	-	21/40/40/45	-
25	BCR	7	503	-	-	14/29/63/63	0/2/2/2
22	CLA	2	608	-	1/1/11/20	7/13/91/115	-
22	CLA	6	604	-	1/1/15/20	11/37/115/115	-
23	PQN	A	2001	-	-	5/23/43/43	0/2/2/2
22	CLA	5	613	-	1/1/13/20	10/25/103/115	-
22	CLA	1	615	12	1/1/15/20	9/37/115/115	-
40	CHL	6	610	-	4/4/18/26	4/27/125/137	-
22	CLA	A	1110	-	1/1/15/20	18/37/115/115	-
22	CLA	B	1205	-	1/1/15/20	12/37/115/115	-
28	LMT	A	5006	-	-	9/21/61/61	0/2/2/2
25	BCR	6	504	-	-	12/29/63/63	0/2/2/2
22	CLA	G	1601	-	1/1/12/20	9/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	SQD	1	802	-	-	17/43/63/69	0/1/1/1
22	CLA	9	609	20	1/1/11/20	7/15/93/115	-
22	CLA	8	607	-	1/1/13/20	13/25/103/115	-
22	CLA	B	1218	-	1/1/15/20	10/37/115/115	-
22	CLA	Z	612	-	1/1/15/20	15/37/115/115	-
27	NKP	8	802	-	-	12/28/28/28	-
22	CLA	9	608	-	1/1/11/20	6/13/91/115	-
22	CLA	K	1403	10	1/1/11/20	8/18/96/115	-
22	CLA	9	603	-	1/1/14/20	13/31/109/115	-
22	CLA	A	1132	-	1/1/15/20	12/37/115/115	-
22	CLA	6	608	-	1/1/13/20	10/25/103/115	-
22	CLA	3	603	-	1/1/15/20	17/37/115/115	-
39	LUT	Z	502	-	-	2/29/67/67	0/2/2/2
39	LUT	8	501	-	-	3/29/67/67	0/2/2/2
22	CLA	4	605	-	1/1/15/20	11/37/115/115	-
25	BCR	3	503	-	-	10/29/63/63	0/2/2/2
22	CLA	Z	601	-	1/1/14/20	11/31/109/115	-
22	CLA	7	608	-	1/1/10/20	5/11/89/115	-
25	BCR	A	4005	-	-	12/29/63/63	0/2/2/2
25	BCR	A	4002	-	-	8/29/63/63	0/2/2/2
26	LHG	6	801	-	-	37/53/53/53	-
22	CLA	6	615	-	1/1/14/20	14/33/111/115	-
28	LMT	F	5001	-	-	6/21/61/61	0/2/2/2
22	CLA	A	1115	-	1/1/14/20	11/31/109/115	-
22	CLA	4	615	-	1/1/10/20	4/8/86/115	-
26	LHG	4	801	-	-	30/53/53/53	-
26	LHG	8	801	-	-	23/42/42/53	-
25	BCR	8	503	-	-	11/29/63/63	0/2/2/2
35	T7X	B	5004	-	-	14/44/68/80	0/1/1/1
22	CLA	2	602	-	1/1/11/20	10/15/93/115	-
40	CHL	4	610	-	4/4/17/26	4/21/119/137	-
22	CLA	2	612	-	1/1/12/20	6/19/97/115	-
22	CLA	A	1141	26	1/1/12/20	8/22/100/115	-
22	CLA	9	606	-	1/1/12/20	11/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	1241	-	1/1/15/20	18/37/115/115	-
26	LHG	A	5001	22	-	16/39/39/53	-
22	CLA	A	1013	-	1/1/15/20	14/37/115/115	-
22	CLA	A	1113	-	1/1/15/20	9/37/115/115	-
40	CHL	6	617	-	3/3/15/26	2/12/110/137	-
22	CLA	B	1237	-	1/1/15/20	18/37/115/115	-
22	CLA	1	602	-	1/1/11/20	5/13/91/115	-
22	CLA	5	605	-	1/1/13/20	12/25/103/115	-
39	LUT	Z	501	-	-	4/29/67/67	0/2/2/2
26	LHG	9	801	-	-	20/37/37/53	-
22	CLA	9	604	-	1/1/15/20	13/37/115/115	-
22	CLA	A	1134	1	1/1/13/20	13/25/103/115	-
22	CLA	B	1212	-	1/1/13/20	14/28/106/115	-
22	CLA	B	1210	-	1/1/15/20	21/37/115/115	-
22	CLA	8	602	-	1/1/15/20	16/37/115/115	-
22	CLA	7	601	-	1/1/14/20	9/31/109/115	-
22	CLA	5	615	17	1/1/12/20	8/19/97/115	-
25	BCR	K	4001	-	-	16/29/63/63	0/2/2/2
22	CLA	8	609	15	1/1/15/20	15/37/115/115	-
22	CLA	6	602	-	1/1/12/20	6/22/100/115	-
25	BCR	A	4003	-	-	12/29/63/63	0/2/2/2
40	CHL	8	610	-	4/4/18/26	5/27/125/137	-
28	LMT	1	803	-	-	4/21/61/61	0/2/2/2
24	SF4	C	3002	3	-	-	0/6/5/5
22	CLA	A	1108	-	1/1/15/20	16/37/115/115	-
44	PLM	7	805	-	-	3/15/15/15	-
22	CLA	5	622	-	1/1/11/20	5/15/93/115	-
22	CLA	3	610	13	1/1/14/20	13/31/109/115	-
40	CHL	4	611	-	3/3/17/26	4/21/119/137	-
22	CLA	4	601	-	1/1/14/20	11/31/109/115	-
39	LUT	4	501	-	-	3/29/67/67	0/2/2/2
24	SF4	C	3003	3	-	-	0/6/5/5
40	CHL	Z	609	12	4/4/20/26	12/39/137/137	-
22	CLA	Z	611	-	1/1/13/20	8/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	DGA	A	5005	-	-	24/45/45/45	-
22	CLA	8	601	-	1/1/14/20	10/31/109/115	-
22	CLA	6	612	-	1/1/12/20	7/19/97/115	-
28	LMT	9	803	-	-	9/21/61/61	0/2/2/2
43	3PH	5	802	-	-	7/24/24/49	-
22	CLA	F	1302	-	1/1/11/20	3/13/91/115	-
22	CLA	A	1130	-	1/1/15/20	17/37/115/115	-
40	CHL	3	611	-	4/4/20/26	1/39/137/137	-
22	CLA	B	1223	-	1/1/15/20	21/37/115/115	-
22	CLA	B	1227	-	1/1/12/20	9/19/97/115	-
22	CLA	A	1133	-	1/1/15/20	15/37/115/115	-
22	CLA	A	1138	-	1/1/15/20	17/37/115/115	-
39	LUT	6	501	-	-	5/29/67/67	0/2/2/2
22	CLA	B	1221	-	1/1/15/20	12/37/115/115	-
22	CLA	8	608	-	1/1/13/20	8/25/103/115	-
22	CLA	6	609	18	1/1/15/20	11/37/115/115	-
22	CLA	3	605	-	1/1/15/20	8/37/115/115	-
22	CLA	6	603	-	1/1/15/20	17/37/115/115	-
22	CLA	4	608	-	1/1/13/20	14/25/103/115	-
39	LUT	1	502	-	-	2/29/67/67	0/2/2/2
21	CL0	A	1011	-	3/3/20/25	11/37/135/135	-
25	BCR	3	505	-	-	11/29/63/63	0/2/2/2
22	CLA	B	1209	-	1/1/15/20	16/37/115/115	-
26	LHG	3	801	-	-	13/22/22/53	-
22	CLA	B	1022	46	1/1/15/20	7/37/115/115	-
25	BCR	A	4004	-	-	14/29/63/63	0/2/2/2
26	LHG	1	801	-	-	26/47/47/53	-
22	CLA	A	1105	-	1/1/15/20	15/37/115/115	-
38	SPH	7	803	-	-	11/21/21/21	-
40	CHL	2	610	-	4/4/16/26	1/18/116/137	-
22	CLA	B	1215	-	1/1/14/20	14/31/109/115	-
25	BCR	B	4004	-	-	9/29/63/63	0/2/2/2
25	BCR	B	4002	-	-	13/29/63/63	0/2/2/2
22	CLA	8	604	-	1/1/14/20	6/34/112/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	1222	-	1/1/15/20	10/37/115/115	-
22	CLA	1	601	-	1/1/15/20	13/37/115/115	-
23	PQN	B	2002	-	-	8/23/43/43	0/2/2/2
22	CLA	4	609	16	1/1/14/20	12/31/109/115	-
22	CLA	B	1231	-	1/1/15/20	16/37/115/115	-
39	LUT	1	501	-	-	2/29/67/67	0/2/2/2
41	SQD	2	803	-	-	18/38/58/69	0/1/1/1
22	CLA	B	1023	-	1/1/15/20	13/37/115/115	-
39	LUT	3	502	-	-	3/29/67/67	0/2/2/2
22	CLA	5	603	-	1/1/13/20	8/27/105/115	-
39	LUT	2	503	-	1/1/12/27	9/29/67/67	0/2/2/2
25	BCR	7	504	-	-	12/29/63/63	0/2/2/2
22	CLA	6	606	-	1/1/15/20	17/37/115/115	-
22	CLA	3	612	-	1/1/14/20	9/31/109/115	-
22	CLA	7	612	-	1/1/12/20	9/19/97/115	-
22	CLA	4	607	-	1/1/13/20	9/25/103/115	-
22	CLA	3	616	-	1/1/13/20	11/27/105/115	-
22	CLA	4	603	-	1/1/15/20	14/37/115/115	-
25	BCR	A	4001	-	-	15/29/63/63	0/2/2/2
22	CLA	B	1208	-	1/1/13/20	10/27/105/115	-
22	CLA	B	1220	-	1/1/15/20	19/37/115/115	-
22	CLA	B	1213	-	1/1/15/20	17/37/115/115	-
22	CLA	6	619	18	1/1/15/20	17/37/115/115	-
22	CLA	A	1111	-	1/1/15/20	13/37/115/115	-
22	CLA	8	615	15	1/1/11/20	7/15/93/115	-
22	CLA	3	601	-	1/1/15/20	16/37/115/115	-
22	CLA	7	607	-	1/1/15/20	20/37/115/115	-

All (2148) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	1	503	C7Z	C25-C26	15.92	1.62	1.34
37	5	505	C7Z	C25-C26	15.89	1.62	1.34
37	J	4002	C7Z	C25-C26	15.74	1.61	1.34
37	5	505	C7Z	C5-C6	15.41	1.61	1.34
37	1	503	C7Z	C5-C6	15.37	1.61	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	F	4001	RRX	C26-C25	15.18	1.60	1.34
37	J	4002	C7Z	C5-C6	15.13	1.60	1.34
39	5	501	LUT	C24-C25	14.89	1.51	1.33
39	2	503	LUT	C24-C25	14.76	1.51	1.33
39	3	502	LUT	C24-C25	14.65	1.51	1.33
39	6	501	LUT	C24-C25	14.61	1.51	1.33
39	4	501	LUT	C24-C25	14.55	1.51	1.33
39	7	501	LUT	C24-C25	14.51	1.51	1.33
39	2	501	LUT	C24-C25	14.50	1.51	1.33
39	Z	501	LUT	C24-C25	14.46	1.51	1.33
39	Z	503	LUT	C24-C25	14.46	1.51	1.33
39	9	501	LUT	C24-C25	14.46	1.51	1.33
39	1	501	LUT	C24-C25	14.42	1.51	1.33
39	3	501	LUT	C24-C25	14.31	1.51	1.33
36	F	4001	RRX	C5-C6	14.28	1.59	1.34
39	6	502	LUT	C24-C25	14.21	1.50	1.33
39	1	502	LUT	C24-C25	14.20	1.50	1.33
39	2	502	LUT	C24-C25	14.18	1.50	1.33
39	7	502	LUT	C24-C25	14.16	1.50	1.33
39	8	501	LUT	C24-C25	14.10	1.50	1.33
39	4	502	LUT	C24-C25	13.99	1.50	1.33
39	8	502	LUT	C24-C25	13.96	1.50	1.33
39	5	502	LUT	C24-C25	13.80	1.50	1.33
39	Z	502	LUT	C24-C25	13.74	1.50	1.33
39	9	502	LUT	C24-C25	13.60	1.50	1.33
37	5	505	C7Z	C24-C23	11.78	1.72	1.52
37	1	503	C7Z	C24-C23	11.75	1.72	1.52
37	J	4002	C7Z	C24-C23	11.62	1.72	1.52
37	1	503	C7Z	C2-C3	-10.60	1.37	1.52
37	5	505	C7Z	C22-C23	-10.58	1.37	1.52
37	5	505	C7Z	C2-C3	-10.55	1.37	1.52
37	J	4002	C7Z	C22-C23	-10.53	1.37	1.52
37	J	4002	C7Z	C2-C3	-10.48	1.37	1.52
37	1	503	C7Z	C22-C23	-10.48	1.37	1.52
36	F	4001	RRX	C29-C28	-9.68	1.38	1.52
21	A	1011	CL0	MG-NA	8.97	2.27	2.06
37	J	4002	C7Z	C4-C3	8.57	1.67	1.52
37	5	505	C7Z	C4-C3	8.52	1.67	1.52
37	1	503	C7Z	C4-C3	8.41	1.66	1.52
36	F	4001	RRX	C27-C28	8.32	1.66	1.52
42	Z	504	QTB	C11-C12	-7.78	1.36	1.54
25	7	504	BCR	C10-C9	7.49	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	506	BCR	C10-C9	7.33	1.45	1.35
25	K	4001	BCR	C10-C9	7.12	1.45	1.35
25	6	504	BCR	C10-C9	7.11	1.45	1.35
25	4	503	BCR	C10-C9	7.11	1.45	1.35
25	3	505	BCR	C10-C9	7.02	1.45	1.35
25	A	4003	BCR	C10-C9	7.00	1.45	1.35
25	6	503	BCR	C10-C9	7.00	1.45	1.35
25	5	503	BCR	C10-C9	7.00	1.45	1.35
25	8	503	BCR	C10-C9	6.97	1.45	1.35
27	3	802	NKP	PAC-OAF	6.96	1.82	1.60
25	A	4005	BCR	C10-C9	6.95	1.45	1.35
25	B	4007	BCR	C10-C9	6.93	1.45	1.35
25	B	4005	BCR	C10-C9	6.93	1.45	1.35
27	A	5004	NKP	PAC-OAF	6.92	1.82	1.60
25	B	4004	BCR	C10-C9	6.89	1.44	1.35
25	G	4001	BCR	C10-C9	6.85	1.44	1.35
25	L	4002	BCR	C10-C9	6.82	1.44	1.35
25	A	4001	BCR	C10-C9	6.81	1.44	1.35
25	K	4002	BCR	C10-C9	6.80	1.44	1.35
25	3	504	BCR	C10-C9	6.77	1.44	1.35
27	8	802	NKP	PAC-OAF	6.77	1.82	1.60
25	I	4001	BCR	C10-C9	6.77	1.44	1.35
25	L	4001	BCR	C10-C9	6.75	1.44	1.35
25	7	503	BCR	C10-C9	6.74	1.44	1.35
25	B	4002	BCR	C10-C9	6.70	1.44	1.35
25	J	4001	BCR	C10-C9	6.70	1.44	1.35
40	9	613	CHL	C3A-C2A	-6.68	1.48	1.54
25	B	4006	BCR	C10-C9	6.65	1.44	1.35
25	3	503	BCR	C10-C9	6.65	1.44	1.35
25	5	504	BCR	C10-C9	6.62	1.44	1.35
25	B	4003	BCR	C10-C9	6.57	1.44	1.35
25	A	4002	BCR	C10-C9	6.54	1.44	1.35
22	A	1110	CLA	MG-NA	6.52	2.21	2.06
36	F	4001	RRX	C1-C6	-6.50	1.44	1.53
22	3	618	CLA	MG-NA	6.50	2.21	2.06
22	B	1240	CLA	MG-NA	6.48	2.21	2.06
22	2	605	CLA	MG-NA	6.48	2.21	2.06
22	5	604	CLA	MG-NA	6.48	2.21	2.06
22	A	1116	CLA	MG-NA	6.48	2.21	2.06
22	A	1123	CLA	MG-NA	6.47	2.21	2.06
22	B	1209	CLA	MG-NA	6.47	2.21	2.06
22	1	613	CLA	MG-NA	6.47	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	615	CLA	MG-NA	6.46	2.21	2.06
22	K	1401	CLA	MG-NA	6.46	2.21	2.06
22	7	615	CLA	MG-NA	6.45	2.21	2.06
22	3	605	CLA	MG-NA	6.45	2.21	2.06
22	6	605	CLA	MG-NA	6.45	2.21	2.06
22	A	1135	CLA	MG-NA	6.45	2.21	2.06
25	A	4004	BCR	C10-C9	6.45	1.44	1.35
22	8	605	CLA	MG-NA	6.45	2.21	2.06
22	3	603	CLA	MG-NA	6.45	2.21	2.06
22	A	1130	CLA	MG-NA	6.44	2.21	2.06
22	1	607	CLA	MG-NA	6.44	2.21	2.06
22	3	607	CLA	MG-NA	6.44	2.21	2.06
22	9	604	CLA	MG-NA	6.43	2.21	2.06
22	9	609	CLA	MG-NA	6.43	2.21	2.06
22	A	1107	CLA	MG-NA	6.43	2.21	2.06
22	3	602	CLA	MG-NA	6.43	2.21	2.06
22	7	605	CLA	MG-NA	6.43	2.21	2.06
22	8	609	CLA	MG-NA	6.43	2.21	2.06
22	4	605	CLA	MG-NA	6.42	2.21	2.06
22	7	604	CLA	MG-NA	6.42	2.21	2.06
22	B	1213	CLA	MG-NA	6.42	2.21	2.06
22	3	608	CLA	MG-NA	6.42	2.21	2.06
22	2	606	CLA	MG-NA	6.42	2.21	2.06
22	B	1236	CLA	MG-NA	6.42	2.21	2.06
22	6	604	CLA	MG-NA	6.42	2.21	2.06
22	9	605	CLA	MG-NA	6.41	2.21	2.06
22	4	607	CLA	MG-NA	6.41	2.21	2.06
22	A	1129	CLA	MG-NA	6.41	2.21	2.06
22	5	602	CLA	MG-NA	6.41	2.21	2.06
22	5	609	CLA	MG-NA	6.41	2.21	2.06
22	B	1221	CLA	MG-NA	6.40	2.21	2.06
22	Z	602	CLA	MG-NA	6.40	2.21	2.06
22	B	1232	CLA	MG-NA	6.40	2.21	2.06
22	5	622	CLA	MG-NA	6.40	2.21	2.06
22	4	604	CLA	MG-NA	6.40	2.21	2.06
22	4	603	CLA	MG-NA	6.40	2.21	2.06
22	2	607	CLA	MG-NA	6.39	2.21	2.06
22	K	1403	CLA	MG-NA	6.39	2.21	2.06
22	Z	604	CLA	MG-NA	6.39	2.21	2.06
22	5	613	CLA	MG-NA	6.39	2.21	2.06
22	4	602	CLA	MG-NA	6.39	2.21	2.06
22	A	1140	CLA	MG-NA	6.39	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	9	603	CLA	MG-NA	6.39	2.21	2.06
22	7	613	CLA	MG-NA	6.39	2.21	2.06
22	6	602	CLA	MG-NA	6.39	2.21	2.06
22	1	612	CLA	MG-NA	6.39	2.21	2.06
22	5	607	CLA	MG-NA	6.39	2.21	2.06
22	9	602	CLA	MG-NA	6.39	2.21	2.06
22	K	1402	CLA	MG-NA	6.38	2.21	2.06
22	3	616	CLA	MG-NA	6.38	2.21	2.06
22	7	603	CLA	MG-NA	6.38	2.21	2.06
22	A	1127	CLA	MG-NA	6.38	2.21	2.06
22	K	1404	CLA	MG-NA	6.38	2.21	2.06
22	A	1114	CLA	MG-NA	6.38	2.21	2.06
22	B	1207	CLA	MG-NA	6.37	2.21	2.06
22	A	1139	CLA	MG-NA	6.37	2.21	2.06
22	4	608	CLA	MG-NA	6.37	2.21	2.06
22	7	616	CLA	MG-NA	6.37	2.21	2.06
22	8	604	CLA	MG-NA	6.37	2.21	2.06
22	1	602	CLA	MG-NA	6.37	2.21	2.06
22	6	608	CLA	MG-NA	6.37	2.21	2.06
22	B	1234	CLA	MG-NA	6.37	2.21	2.06
22	B	1229	CLA	MG-NA	6.37	2.21	2.06
22	6	603	CLA	MG-NA	6.36	2.21	2.06
22	A	1112	CLA	MG-NA	6.36	2.21	2.06
22	Z	607	CLA	MG-NA	6.36	2.21	2.06
22	5	615	CLA	MG-NA	6.36	2.21	2.06
22	1	605	CLA	MG-NA	6.36	2.21	2.06
22	A	1101	CLA	MG-NA	6.36	2.21	2.06
22	4	615	CLA	MG-NA	6.36	2.21	2.06
22	6	607	CLA	MG-NA	6.36	2.21	2.06
22	6	615	CLA	MG-NA	6.36	2.21	2.06
22	B	1224	CLA	MG-NA	6.35	2.21	2.06
22	B	1227	CLA	MG-NA	6.35	2.21	2.06
22	A	1113	CLA	MG-NA	6.35	2.21	2.06
22	7	602	CLA	MG-NA	6.35	2.21	2.06
22	A	1105	CLA	MG-NA	6.35	2.21	2.06
22	8	603	CLA	MG-NA	6.35	2.21	2.06
22	1	604	CLA	MG-NA	6.35	2.21	2.06
22	Z	612	CLA	MG-NA	6.35	2.21	2.06
22	A	1134	CLA	MG-NA	6.34	2.21	2.06
22	B	1219	CLA	MG-NA	6.34	2.21	2.06
25	B	4001	BCR	C10-C9	6.34	1.44	1.35
22	A	1141	CLA	MG-NA	6.34	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	618	CLA	MG-NA	6.34	2.21	2.06
22	G	1602	CLA	MG-NA	6.34	2.21	2.06
22	A	1121	CLA	MG-NA	6.33	2.21	2.06
22	A	1104	CLA	MG-NA	6.33	2.21	2.06
22	2	603	CLA	MG-NA	6.33	2.21	2.06
22	2	602	CLA	MG-NA	6.33	2.21	2.06
22	8	615	CLA	MG-NA	6.33	2.21	2.06
22	6	601	CLA	MG-NA	6.33	2.21	2.06
22	Z	605	CLA	MG-NA	6.33	2.21	2.06
22	B	1206	CLA	MG-NA	6.33	2.21	2.06
22	5	608	CLA	MG-NA	6.33	2.21	2.06
22	6	606	CLA	MG-NA	6.33	2.21	2.06
22	5	603	CLA	MG-NA	6.33	2.21	2.06
22	9	607	CLA	MG-NA	6.33	2.21	2.06
22	B	1239	CLA	MG-NA	6.32	2.21	2.06
22	6	618	CLA	MG-NA	6.32	2.21	2.06
22	B	1226	CLA	MG-NA	6.32	2.21	2.06
22	B	1238	CLA	MG-NA	6.32	2.21	2.06
22	7	607	CLA	MG-NA	6.31	2.21	2.06
22	B	1228	CLA	MG-NA	6.31	2.21	2.06
22	8	602	CLA	MG-NA	6.31	2.21	2.06
22	2	608	CLA	MG-NA	6.31	2.21	2.06
22	L	1503	CLA	MG-NA	6.30	2.21	2.06
22	Z	615	CLA	MG-NA	6.30	2.21	2.06
22	A	1137	CLA	MG-NA	6.30	2.21	2.06
22	5	606	CLA	MG-NA	6.30	2.21	2.06
22	B	1223	CLA	MG-NA	6.30	2.21	2.06
22	A	1117	CLA	MG-NA	6.30	2.21	2.06
22	J	1901	CLA	MG-NA	6.30	2.21	2.06
22	A	1128	CLA	MG-NA	6.30	2.21	2.06
22	1	603	CLA	MG-NA	6.30	2.21	2.06
22	Z	611	CLA	MG-NA	6.29	2.21	2.06
22	A	1120	CLA	MG-NA	6.29	2.21	2.06
22	8	611	CLA	MG-NA	6.29	2.21	2.06
22	A	1122	CLA	MG-NA	6.29	2.21	2.06
22	2	612	CLA	MG-NA	6.29	2.21	2.06
22	8	607	CLA	MG-NA	6.29	2.21	2.06
22	9	608	CLA	MG-NA	6.29	2.21	2.06
22	F	1302	CLA	MG-NA	6.29	2.21	2.06
22	L	1502	CLA	MG-NA	6.29	2.21	2.06
22	A	1115	CLA	MG-NA	6.28	2.21	2.06
22	7	608	CLA	MG-NA	6.28	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	612	CLA	MG-NA	6.28	2.21	2.06
22	G	1601	CLA	MG-NA	6.27	2.21	2.06
22	A	1136	CLA	MG-NA	6.27	2.21	2.06
22	B	1214	CLA	MG-NA	6.27	2.21	2.06
22	B	1235	CLA	MG-NA	6.26	2.21	2.06
22	7	601	CLA	MG-NA	6.26	2.21	2.06
22	Z	603	CLA	MG-NA	6.26	2.21	2.06
22	B	1225	CLA	MG-NA	6.25	2.21	2.06
22	3	610	CLA	MG-NA	6.25	2.21	2.06
22	1	611	CLA	MG-NA	6.25	2.21	2.06
22	4	601	CLA	MG-NA	6.25	2.21	2.06
22	B	1237	CLA	MG-NA	6.25	2.21	2.06
22	4	606	CLA	MG-NA	6.25	2.21	2.06
22	3	601	CLA	MG-NA	6.25	2.21	2.06
22	B	1215	CLA	MG-NA	6.24	2.21	2.06
22	Z	606	CLA	MG-NA	6.24	2.21	2.06
22	8	608	CLA	MG-NA	6.24	2.21	2.06
22	5	605	CLA	MG-NA	6.24	2.21	2.06
22	4	609	CLA	MG-NA	6.24	2.21	2.06
22	6	609	CLA	MG-NA	6.24	2.21	2.06
22	B	1022	CLA	MG-NA	6.24	2.21	2.06
22	A	1108	CLA	MG-NA	6.23	2.21	2.06
22	8	606	CLA	MG-NA	6.23	2.21	2.06
22	9	606	CLA	MG-NA	6.23	2.21	2.06
22	B	1217	CLA	MG-NA	6.23	2.21	2.06
22	3	612	CLA	MG-NA	6.23	2.21	2.06
22	A	1126	CLA	MG-NA	6.22	2.21	2.06
22	F	1301	CLA	MG-NA	6.22	2.21	2.06
22	B	1212	CLA	MG-NA	6.22	2.21	2.06
22	9	601	CLA	MG-NA	6.22	2.21	2.06
22	A	1131	CLA	MG-NA	6.21	2.21	2.06
22	8	601	CLA	MG-NA	6.21	2.21	2.06
22	2	601	CLA	MG-NA	6.21	2.21	2.06
22	A	1012	CLA	MG-NA	6.20	2.21	2.06
22	B	1204	CLA	MG-NA	6.20	2.21	2.06
22	A	1102	CLA	MG-NA	6.20	2.21	2.06
22	B	1203	CLA	MG-NA	6.20	2.21	2.06
22	6	619	CLA	MG-NA	6.20	2.21	2.06
22	9	612	CLA	MG-NA	6.20	2.21	2.06
22	3	613	CLA	MG-NA	6.20	2.21	2.06
22	B	1218	CLA	MG-NA	6.20	2.21	2.06
22	A	1106	CLA	MG-NA	6.19	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1118	CLA	MG-NA	6.18	2.21	2.06
22	Z	608	CLA	MG-NA	6.18	2.21	2.06
22	5	601	CLA	MG-NA	6.18	2.21	2.06
22	7	611	CLA	MG-NA	6.18	2.21	2.06
22	A	1111	CLA	MG-NA	6.18	2.21	2.06
22	A	1125	CLA	MG-NA	6.18	2.21	2.06
22	4	612	CLA	MG-NA	6.17	2.20	2.06
22	A	1124	CLA	MG-NA	6.17	2.20	2.06
22	2	615	CLA	MG-NA	6.17	2.20	2.06
22	A	1132	CLA	MG-NA	6.17	2.20	2.06
22	7	606	CLA	MG-NA	6.17	2.20	2.06
22	1	601	CLA	MG-NA	6.17	2.20	2.06
22	B	1210	CLA	MG-NA	6.16	2.20	2.06
22	2	604	CLA	MG-NA	6.16	2.20	2.06
22	A	1109	CLA	MG-NA	6.16	2.20	2.06
22	B	1231	CLA	MG-NA	6.14	2.20	2.06
22	B	1208	CLA	MG-NA	6.13	2.20	2.06
22	B	1230	CLA	MG-NA	6.13	2.20	2.06
22	B	1216	CLA	MG-NA	6.13	2.20	2.06
22	1	606	CLA	MG-NA	6.13	2.20	2.06
22	A	1119	CLA	MG-NA	6.11	2.20	2.06
22	Z	601	CLA	MG-NA	6.11	2.20	2.06
22	A	1133	CLA	MG-NA	6.11	2.20	2.06
36	F	4001	RRX	C2-C3	-6.11	1.37	1.52
22	B	1220	CLA	MG-NA	6.11	2.20	2.06
22	8	612	CLA	MG-NA	6.10	2.20	2.06
22	A	1138	CLA	MG-NA	6.08	2.20	2.06
22	1	608	CLA	MG-NA	6.07	2.20	2.06
22	7	612	CLA	MG-NA	6.06	2.20	2.06
22	B	1241	CLA	MG-NA	6.06	2.20	2.06
22	3	606	CLA	MG-NA	6.06	2.20	2.06
22	7	609	CLA	MG-NA	6.06	2.20	2.06
22	B	1205	CLA	MG-NA	6.05	2.20	2.06
22	B	1222	CLA	MG-NA	6.04	2.20	2.06
22	5	612	CLA	MG-NA	6.02	2.20	2.06
22	B	1202	CLA	MG-NA	6.00	2.20	2.06
22	B	1021	CLA	MG-NA	5.97	2.20	2.06
22	A	1013	CLA	MG-NA	5.97	2.20	2.06
22	B	1201	CLA	MG-NA	5.90	2.20	2.06
25	3	506	BCR	C24-C23	5.88	1.50	1.33
22	B	1023	CLA	MG-NA	5.87	2.20	2.06
22	A	1103	CLA	MG-NA	5.86	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	504	BCR	C24-C23	5.85	1.50	1.33
22	3	604	CLA	MG-NA	5.81	2.20	2.06
37	J	4002	C7Z	C1-C6	-5.81	1.45	1.53
25	5	504	BCR	C24-C23	5.81	1.50	1.33
25	B	4003	BCR	C24-C23	5.80	1.50	1.33
37	5	505	C7Z	C12-C13	5.79	1.58	1.45
25	3	504	BCR	C24-C23	5.78	1.50	1.33
25	G	4001	BCR	C24-C23	5.77	1.50	1.33
25	K	4002	BCR	C24-C23	5.75	1.50	1.33
25	B	4004	BCR	C24-C23	5.73	1.50	1.33
25	4	503	BCR	C24-C23	5.73	1.50	1.33
25	7	503	BCR	C24-C23	5.70	1.50	1.33
22	B	1211	CLA	MG-NA	5.69	2.19	2.06
25	J	4001	BCR	C24-C23	5.69	1.50	1.33
25	3	505	BCR	C24-C23	5.68	1.50	1.33
25	5	503	BCR	C24-C23	5.67	1.50	1.33
25	B	4005	BCR	C24-C23	5.66	1.50	1.33
25	A	4001	BCR	C24-C23	5.65	1.50	1.33
25	B	4007	BCR	C24-C23	5.63	1.50	1.33
25	7	504	BCR	C24-C23	5.63	1.50	1.33
25	6	503	BCR	C24-C23	5.63	1.50	1.33
25	L	4002	BCR	C24-C23	5.62	1.50	1.33
25	8	503	BCR	C24-C23	5.62	1.50	1.33
36	F	4001	RRX	C30-C25	-5.61	1.46	1.53
25	K	4001	BCR	C24-C23	5.61	1.50	1.33
25	A	4002	BCR	C24-C23	5.61	1.50	1.33
25	L	4001	BCR	C24-C23	5.61	1.50	1.33
25	A	4004	BCR	C24-C23	5.60	1.50	1.33
25	3	503	BCR	C24-C23	5.60	1.50	1.33
25	B	4006	BCR	C24-C23	5.60	1.50	1.33
25	B	4001	BCR	C24-C23	5.59	1.50	1.33
25	A	4003	BCR	C24-C23	5.56	1.49	1.33
25	B	4001	BCR	C11-C12	-5.56	1.20	1.34
37	1	503	C7Z	C12-C13	5.55	1.57	1.45
25	B	4002	BCR	C24-C23	5.54	1.49	1.33
25	3	504	BCR	C11-C12	-5.51	1.20	1.34
25	A	4005	BCR	C24-C23	5.49	1.49	1.33
25	I	4001	BCR	C24-C23	5.49	1.49	1.33
25	B	4003	BCR	C11-C12	-5.48	1.20	1.34
25	A	4002	BCR	C11-C12	-5.48	1.20	1.34
37	J	4002	C7Z	C12-C13	5.47	1.57	1.45
25	A	4004	BCR	C11-C12	-5.44	1.20	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	5	505	C7Z	C1-C6	-5.43	1.46	1.53
37	1	503	C7Z	C1-C6	-5.41	1.46	1.53
25	6	504	BCR	C11-C12	-5.40	1.20	1.34
25	B	4002	BCR	C11-C12	-5.39	1.20	1.34
25	7	503	BCR	C11-C12	-5.39	1.20	1.34
25	3	503	BCR	C11-C12	-5.37	1.20	1.34
25	G	4001	BCR	C11-C12	-5.34	1.20	1.34
25	J	4001	BCR	C11-C12	-5.34	1.20	1.34
25	I	4001	BCR	C11-C12	-5.31	1.20	1.34
25	L	4002	BCR	C11-C12	-5.31	1.20	1.34
25	L	4001	BCR	C11-C12	-5.30	1.20	1.34
25	B	4005	BCR	C11-C12	-5.29	1.20	1.34
25	B	4007	BCR	C11-C12	-5.29	1.20	1.34
21	A	1011	CL0	O2A-C1	5.28	1.61	1.46
25	B	4006	BCR	C11-C12	-5.28	1.21	1.34
25	K	4002	BCR	C11-C12	-5.27	1.21	1.34
25	B	4004	BCR	C11-C12	-5.25	1.21	1.34
25	A	4001	BCR	C11-C12	-5.25	1.21	1.34
25	A	4005	BCR	C11-C12	-5.25	1.21	1.34
25	5	503	BCR	C11-C12	-5.24	1.21	1.34
36	F	4001	RRX	C2-C1	5.24	1.66	1.54
25	8	503	BCR	C11-C12	-5.23	1.21	1.34
25	3	505	BCR	C11-C12	-5.20	1.21	1.34
25	6	503	BCR	C11-C12	-5.18	1.21	1.34
25	5	504	BCR	C11-C12	-5.17	1.21	1.34
25	K	4001	BCR	C11-C12	-5.16	1.21	1.34
25	A	4003	BCR	C11-C12	-5.15	1.21	1.34
25	4	503	BCR	C11-C12	-5.13	1.21	1.34
37	1	503	C7Z	C28-C29	5.09	1.56	1.45
37	5	505	C7Z	C28-C29	5.07	1.56	1.45
25	7	504	BCR	C11-C12	-5.06	1.21	1.34
21	A	1011	CL0	CHC-C1C	5.04	1.47	1.35
25	3	506	BCR	C11-C12	-5.03	1.21	1.34
36	F	4001	RRX	C19-C18	5.02	1.56	1.45
21	A	1011	CL0	O2D-CGD	5.01	1.45	1.33
37	J	4002	C7Z	C28-C29	4.88	1.56	1.45
40	3	611	CHL	C3B-C2B	-4.87	1.33	1.40
37	J	4002	C7Z	C24-C25	-4.79	1.43	1.51
37	5	505	C7Z	C32-C33	4.78	1.56	1.45
37	1	503	C7Z	C32-C33	4.75	1.56	1.45
37	J	4002	C7Z	C32-C33	4.75	1.56	1.45
37	5	505	C7Z	C24-C25	-4.72	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	1	503	C7Z	C24-C25	-4.72	1.43	1.51
36	F	4001	RRX	C8-C9	4.66	1.56	1.45
21	A	1011	CL0	C3C-C2C	4.48	1.46	1.36
25	B	4005	BCR	C16-C17	-4.48	1.29	1.43
25	B	4001	BCR	C16-C17	-4.47	1.29	1.43
25	3	503	BCR	C16-C17	-4.47	1.29	1.43
25	A	4004	BCR	C16-C17	-4.46	1.29	1.43
25	B	4004	BCR	C16-C17	-4.45	1.29	1.43
25	B	4003	BCR	C16-C17	-4.44	1.29	1.43
21	A	1011	CL0	CHD-C1D	4.44	1.47	1.38
25	8	503	BCR	C16-C17	-4.44	1.29	1.43
25	I	4001	BCR	C16-C17	-4.44	1.29	1.43
25	5	504	BCR	C16-C17	-4.43	1.29	1.43
42	Z	504	QTB	C17-C11	-4.42	1.51	1.55
37	5	505	C7Z	C31-C30	4.42	1.57	1.43
25	6	504	BCR	C16-C17	-4.41	1.29	1.43
37	5	505	C7Z	C8-C9	4.41	1.55	1.45
22	A	1128	CLA	MG-ND	-4.40	1.97	2.05
25	K	4002	BCR	C16-C17	-4.39	1.29	1.43
25	A	4002	BCR	C16-C17	-4.39	1.29	1.43
36	F	4001	RRX	C27-C26	-4.38	1.44	1.51
21	A	1011	CL0	C3D-C4D	-4.38	1.34	1.44
25	B	4007	BCR	C16-C17	-4.38	1.29	1.43
25	7	503	BCR	C16-C17	-4.37	1.29	1.43
37	1	503	C7Z	C31-C30	4.37	1.57	1.43
25	A	4005	BCR	C16-C17	-4.36	1.29	1.43
25	L	4001	BCR	C16-C17	-4.36	1.29	1.43
22	B	1226	CLA	MG-ND	-4.35	1.97	2.05
25	6	503	BCR	C16-C17	-4.35	1.30	1.43
25	5	503	BCR	C16-C17	-4.34	1.30	1.43
25	4	503	BCR	C16-C17	-4.34	1.30	1.43
37	J	4002	C7Z	C31-C30	4.34	1.56	1.43
25	L	4002	BCR	C16-C17	-4.33	1.30	1.43
25	3	504	BCR	C16-C17	-4.33	1.30	1.43
25	B	4002	BCR	C16-C17	-4.32	1.30	1.43
25	A	4001	BCR	C16-C17	-4.32	1.30	1.43
36	F	4001	RRX	C12-C13	4.32	1.55	1.45
25	A	4003	BCR	C16-C17	-4.31	1.30	1.43
25	J	4001	BCR	C16-C17	-4.30	1.30	1.43
25	B	4006	BCR	C16-C17	-4.30	1.30	1.43
36	F	4001	RRX	C3-C4	4.29	1.66	1.52
25	G	4001	BCR	C16-C17	-4.29	1.30	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	K	4001	BCR	C16-C17	-4.28	1.30	1.43
25	3	505	BCR	C16-C17	-4.26	1.30	1.43
21	A	1011	CL0	C3B-C2B	4.25	1.46	1.40
37	J	4002	C7Z	C8-C9	4.25	1.55	1.45
33	B	5003	DGD	O1G-C1A	4.24	1.45	1.33
37	J	4002	C7Z	C4-C5	-4.23	1.44	1.51
37	1	503	C7Z	C8-C9	4.22	1.55	1.45
37	5	505	C7Z	C11-C10	4.21	1.56	1.43
25	3	506	BCR	C16-C17	-4.18	1.30	1.43
22	A	1127	CLA	MG-ND	-4.18	1.97	2.05
22	A	1012	CLA	MG-ND	-4.13	1.97	2.05
22	A	1013	CLA	MG-ND	-4.12	1.97	2.05
37	1	503	C7Z	C4-C5	-4.12	1.44	1.51
22	B	1022	CLA	MG-ND	-4.12	1.97	2.05
25	7	504	BCR	C16-C17	-4.10	1.30	1.43
22	9	612	CLA	MG-ND	-4.10	1.97	2.05
22	B	1224	CLA	MG-ND	-4.09	1.97	2.05
42	Z	504	QTB	C11-C10	-4.08	1.44	1.50
37	1	503	C7Z	C11-C10	4.02	1.55	1.43
22	B	1023	CLA	MG-ND	-4.02	1.97	2.05
22	A	1126	CLA	MG-ND	-4.01	1.97	2.05
22	B	1021	CLA	MG-ND	-4.01	1.97	2.05
22	B	1215	CLA	MG-ND	-4.00	1.97	2.05
22	A	1123	CLA	MG-ND	-4.00	1.97	2.05
22	B	1223	CLA	MG-ND	-4.00	1.97	2.05
22	B	1219	CLA	MG-ND	-3.98	1.97	2.05
36	F	4001	RRX	C23-C22	3.98	1.54	1.45
22	K	1404	CLA	MG-ND	-3.97	1.97	2.05
37	5	505	C7Z	C4-C5	-3.97	1.44	1.51
36	F	4001	RRX	C20-C21	3.97	1.55	1.43
37	J	4002	C7Z	C11-C10	3.96	1.55	1.43
22	2	606	CLA	MG-ND	-3.96	1.97	2.05
22	B	1225	CLA	MG-ND	-3.96	1.97	2.05
22	A	1116	CLA	MG-ND	-3.96	1.97	2.05
21	A	1011	CL0	C1D-ND	-3.96	1.32	1.37
22	1	607	CLA	MG-ND	-3.95	1.98	2.05
22	A	1107	CLA	MG-ND	-3.95	1.98	2.05
22	A	1125	CLA	MG-ND	-3.94	1.98	2.05
22	9	605	CLA	MG-ND	-3.94	1.98	2.05
22	7	601	CLA	MG-ND	-3.94	1.98	2.05
22	B	1221	CLA	MG-ND	-3.93	1.98	2.05
22	A	1131	CLA	MG-ND	-3.93	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	1205	CLA	MG-ND	-3.92	1.98	2.05
22	A	1117	CLA	MG-ND	-3.92	1.98	2.05
22	8	605	CLA	MG-ND	-3.92	1.98	2.05
22	B	1235	CLA	MG-ND	-3.91	1.98	2.05
22	B	1227	CLA	MG-ND	-3.90	1.98	2.05
22	A	1135	CLA	MG-ND	-3.90	1.98	2.05
22	A	1139	CLA	MG-ND	-3.90	1.98	2.05
22	A	1134	CLA	MG-ND	-3.90	1.98	2.05
22	B	1237	CLA	MG-ND	-3.89	1.98	2.05
22	9	608	CLA	MG-ND	-3.89	1.98	2.05
22	B	1208	CLA	MG-ND	-3.89	1.98	2.05
22	2	605	CLA	MG-ND	-3.89	1.98	2.05
22	1	613	CLA	MG-ND	-3.89	1.98	2.05
22	B	1212	CLA	C1C-NC	-3.89	1.32	1.37
22	2	615	CLA	MG-ND	-3.89	1.98	2.05
22	L	1502	CLA	MG-ND	-3.88	1.98	2.05
22	B	1241	CLA	MG-ND	-3.88	1.98	2.05
37	5	505	C7Z	C22-C21	3.88	1.67	1.54
22	3	618	CLA	MG-ND	-3.88	1.98	2.05
22	B	1203	CLA	MG-ND	-3.88	1.98	2.05
22	A	1130	CLA	MG-ND	-3.88	1.98	2.05
22	A	1132	CLA	MG-ND	-3.87	1.98	2.05
22	9	607	CLA	MG-ND	-3.87	1.98	2.05
22	A	1124	CLA	MG-ND	-3.87	1.98	2.05
22	9	602	CLA	MG-ND	-3.87	1.98	2.05
22	A	1133	CLA	MG-ND	-3.87	1.98	2.05
22	A	1136	CLA	MG-ND	-3.87	1.98	2.05
22	B	1206	CLA	MG-ND	-3.86	1.98	2.05
22	G	1602	CLA	MG-ND	-3.86	1.98	2.05
37	1	503	C7Z	C22-C21	3.86	1.66	1.54
22	7	613	CLA	MG-ND	-3.86	1.98	2.05
22	2	612	CLA	MG-ND	-3.86	1.98	2.05
22	9	609	CLA	MG-ND	-3.86	1.98	2.05
22	7	612	CLA	MG-ND	-3.86	1.98	2.05
22	8	601	CLA	MG-ND	-3.86	1.98	2.05
22	B	1213	CLA	MG-ND	-3.85	1.98	2.05
22	B	1217	CLA	MG-ND	-3.85	1.98	2.05
22	A	1115	CLA	MG-ND	-3.85	1.98	2.05
22	9	603	CLA	MG-ND	-3.85	1.98	2.05
22	B	1214	CLA	MG-ND	-3.85	1.98	2.05
22	2	603	CLA	MG-ND	-3.85	1.98	2.05
22	K	1403	CLA	MG-ND	-3.85	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	5	505	C7Z	C15-C14	3.85	1.55	1.43
22	B	1210	CLA	MG-ND	-3.85	1.98	2.05
22	8	612	CLA	MG-ND	-3.84	1.98	2.05
22	6	619	CLA	MG-ND	-3.84	1.98	2.05
22	9	601	CLA	MG-ND	-3.84	1.98	2.05
22	Z	604	CLA	MG-ND	-3.84	1.98	2.05
22	B	1209	CLA	MG-ND	-3.84	1.98	2.05
37	J	4002	C7Z	C22-C21	3.84	1.66	1.54
22	3	608	CLA	MG-ND	-3.84	1.98	2.05
22	1	602	CLA	MG-ND	-3.83	1.98	2.05
22	6	602	CLA	MG-ND	-3.83	1.98	2.05
22	5	613	CLA	MG-ND	-3.83	1.98	2.05
22	6	618	CLA	MG-ND	-3.83	1.98	2.05
22	2	608	CLA	MG-ND	-3.83	1.98	2.05
21	A	1011	CL0	CHD-C4C	3.83	1.48	1.39
22	4	608	CLA	MG-ND	-3.82	1.98	2.05
22	A	1114	CLA	MG-ND	-3.82	1.98	2.05
22	A	1102	CLA	MG-ND	-3.82	1.98	2.05
22	8	611	CLA	MG-ND	-3.82	1.98	2.05
22	B	1220	CLA	C1C-NC	-3.82	1.32	1.37
22	7	608	CLA	MG-ND	-3.82	1.98	2.05
22	7	615	CLA	MG-ND	-3.82	1.98	2.05
22	A	1137	CLA	MG-ND	-3.82	1.98	2.05
22	A	1112	CLA	MG-ND	-3.82	1.98	2.05
22	B	1218	CLA	MG-ND	-3.82	1.98	2.05
22	A	1118	CLA	MG-ND	-3.82	1.98	2.05
22	3	607	CLA	MG-ND	-3.82	1.98	2.05
22	4	607	CLA	MG-ND	-3.82	1.98	2.05
22	6	607	CLA	MG-ND	-3.81	1.98	2.05
22	5	618	CLA	MG-ND	-3.81	1.98	2.05
22	B	1210	CLA	C1C-NC	-3.81	1.32	1.37
22	A	1119	CLA	MG-ND	-3.81	1.98	2.05
22	A	1141	CLA	MG-ND	-3.81	1.98	2.05
22	B	1234	CLA	MG-ND	-3.81	1.98	2.05
22	1	615	CLA	MG-ND	-3.81	1.98	2.05
22	5	622	CLA	MG-ND	-3.81	1.98	2.05
22	6	608	CLA	MG-ND	-3.81	1.98	2.05
22	A	1111	CLA	MG-ND	-3.80	1.98	2.05
22	A	1113	CLA	MG-ND	-3.80	1.98	2.05
22	5	615	CLA	MG-ND	-3.80	1.98	2.05
22	A	1138	CLA	MG-ND	-3.80	1.98	2.05
22	J	1901	CLA	MG-ND	-3.80	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	F	1302	CLA	MG-ND	-3.79	1.98	2.05
22	2	601	CLA	MG-ND	-3.79	1.98	2.05
22	5	606	CLA	MG-ND	-3.79	1.98	2.05
22	6	615	CLA	MG-ND	-3.79	1.98	2.05
22	B	1204	CLA	MG-ND	-3.79	1.98	2.05
22	8	609	CLA	MG-ND	-3.79	1.98	2.05
22	8	607	CLA	MG-ND	-3.79	1.98	2.05
22	Z	602	CLA	MG-ND	-3.79	1.98	2.05
22	5	601	CLA	MG-ND	-3.78	1.98	2.05
22	B	1212	CLA	MG-ND	-3.78	1.98	2.05
22	B	1236	CLA	MG-ND	-3.78	1.98	2.05
22	9	606	CLA	MG-ND	-3.78	1.98	2.05
22	L	1503	CLA	MG-ND	-3.78	1.98	2.05
22	K	1401	CLA	MG-ND	-3.78	1.98	2.05
22	3	601	CLA	MG-ND	-3.78	1.98	2.05
22	4	603	CLA	MG-ND	-3.78	1.98	2.05
22	B	1228	CLA	MG-ND	-3.78	1.98	2.05
22	8	615	CLA	MG-ND	-3.78	1.98	2.05
22	3	610	CLA	MG-ND	-3.78	1.98	2.05
22	Z	612	CLA	MG-ND	-3.78	1.98	2.05
22	6	605	CLA	MG-ND	-3.78	1.98	2.05
22	1	612	CLA	MG-ND	-3.78	1.98	2.05
22	3	613	CLA	MG-ND	-3.78	1.98	2.05
22	Z	615	CLA	MG-ND	-3.77	1.98	2.05
22	B	1211	CLA	MG-ND	-3.77	1.98	2.05
22	2	602	CLA	MG-ND	-3.77	1.98	2.05
22	7	602	CLA	MG-ND	-3.77	1.98	2.05
22	B	1220	CLA	MG-ND	-3.77	1.98	2.05
22	2	604	CLA	MG-ND	-3.77	1.98	2.05
22	8	602	CLA	MG-ND	-3.77	1.98	2.05
22	1	604	CLA	MG-ND	-3.77	1.98	2.05
22	3	606	CLA	MG-ND	-3.77	1.98	2.05
22	4	615	CLA	MG-ND	-3.76	1.98	2.05
22	Z	611	CLA	MG-ND	-3.76	1.98	2.05
22	K	1402	CLA	MG-ND	-3.76	1.98	2.05
22	6	612	CLA	MG-ND	-3.76	1.98	2.05
22	Z	607	CLA	MG-ND	-3.76	1.98	2.05
22	B	1239	CLA	MG-ND	-3.75	1.98	2.05
22	F	1301	CLA	MG-ND	-3.75	1.98	2.05
22	G	1601	CLA	MG-ND	-3.75	1.98	2.05
22	6	603	CLA	MG-ND	-3.75	1.98	2.05
22	9	604	CLA	MG-ND	-3.75	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	606	CLA	MG-ND	-3.75	1.98	2.05
22	7	607	CLA	MG-ND	-3.75	1.98	2.05
22	4	601	CLA	MG-ND	-3.75	1.98	2.05
22	B	1201	CLA	MG-ND	-3.75	1.98	2.05
22	5	608	CLA	MG-ND	-3.75	1.98	2.05
22	A	1129	CLA	MG-ND	-3.74	1.98	2.05
22	5	609	CLA	MG-ND	-3.74	1.98	2.05
22	7	604	CLA	MG-ND	-3.74	1.98	2.05
22	A	1120	CLA	MG-ND	-3.74	1.98	2.05
22	B	1223	CLA	C1C-NC	-3.74	1.32	1.37
22	7	616	CLA	MG-ND	-3.74	1.98	2.05
22	1	606	CLA	MG-ND	-3.73	1.98	2.05
22	8	604	CLA	MG-ND	-3.73	1.98	2.05
22	6	601	CLA	MG-ND	-3.73	1.98	2.05
22	A	1103	CLA	MG-ND	-3.73	1.98	2.05
22	5	607	CLA	MG-ND	-3.73	1.98	2.05
22	7	603	CLA	MG-ND	-3.73	1.98	2.05
22	2	607	CLA	MG-ND	-3.73	1.98	2.05
22	4	609	CLA	MG-ND	-3.73	1.98	2.05
22	4	602	CLA	MG-ND	-3.73	1.98	2.05
22	4	606	CLA	MG-ND	-3.73	1.98	2.05
22	B	1202	CLA	MG-ND	-3.72	1.98	2.05
22	Z	601	CLA	MG-ND	-3.72	1.98	2.05
22	1	611	CLA	MG-ND	-3.72	1.98	2.05
22	4	604	CLA	MG-ND	-3.72	1.98	2.05
22	6	606	CLA	MG-ND	-3.72	1.98	2.05
22	1	601	CLA	MG-ND	-3.72	1.98	2.05
37	5	505	C7Z	C27-C26	3.72	1.58	1.45
22	A	1108	CLA	MG-ND	-3.72	1.98	2.05
22	B	1240	CLA	MG-ND	-3.72	1.98	2.05
22	B	1232	CLA	MG-ND	-3.71	1.98	2.05
22	6	604	CLA	MG-ND	-3.71	1.98	2.05
22	A	1104	CLA	MG-ND	-3.71	1.98	2.05
22	B	1231	CLA	MG-ND	-3.71	1.98	2.05
22	A	1101	CLA	MG-ND	-3.71	1.98	2.05
22	3	602	CLA	MG-ND	-3.71	1.98	2.05
37	1	503	C7Z	C15-C14	3.71	1.54	1.43
22	3	616	CLA	MG-ND	-3.71	1.98	2.05
22	1	603	CLA	MG-ND	-3.71	1.98	2.05
22	A	1121	CLA	MG-ND	-3.71	1.98	2.05
22	B	1207	CLA	MG-ND	-3.71	1.98	2.05
36	F	4001	RRX	C15-C14	3.71	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	605	CLA	MG-ND	-3.71	1.98	2.05
22	3	605	CLA	MG-ND	-3.71	1.98	2.05
22	A	1140	CLA	MG-ND	-3.70	1.98	2.05
22	B	1225	CLA	C1C-NC	-3.70	1.32	1.37
37	J	4002	C7Z	C27-C26	3.70	1.58	1.45
22	8	606	CLA	MG-ND	-3.70	1.98	2.05
22	Z	608	CLA	MG-ND	-3.70	1.98	2.05
22	8	608	CLA	MG-ND	-3.70	1.98	2.05
22	B	1216	CLA	MG-ND	-3.69	1.98	2.05
22	4	605	CLA	MG-ND	-3.69	1.98	2.05
22	3	612	CLA	MG-ND	-3.69	1.98	2.05
22	7	611	CLA	MG-ND	-3.69	1.98	2.05
22	Z	603	CLA	MG-ND	-3.68	1.98	2.05
22	4	612	CLA	MG-ND	-3.68	1.98	2.05
22	7	609	CLA	MG-ND	-3.68	1.98	2.05
22	6	609	CLA	MG-ND	-3.68	1.98	2.05
22	5	612	CLA	MG-ND	-3.67	1.98	2.05
22	3	604	CLA	MG-ND	-3.67	1.98	2.05
22	5	602	CLA	MG-ND	-3.66	1.98	2.05
22	3	603	CLA	MG-ND	-3.66	1.98	2.05
22	Z	605	CLA	MG-ND	-3.66	1.98	2.05
22	A	1109	CLA	MG-ND	-3.66	1.98	2.05
22	5	604	CLA	MG-ND	-3.66	1.98	2.05
22	B	1222	CLA	MG-ND	-3.66	1.98	2.05
37	5	505	C7Z	C35-C34	3.65	1.54	1.43
37	1	503	C7Z	C27-C26	3.65	1.58	1.45
22	1	605	CLA	MG-ND	-3.65	1.98	2.05
22	A	1110	CLA	MG-ND	-3.65	1.98	2.05
22	B	1239	CLA	C1C-NC	-3.64	1.32	1.37
22	B	1238	CLA	MG-ND	-3.64	1.98	2.05
22	5	603	CLA	MG-ND	-3.64	1.98	2.05
22	A	1106	CLA	MG-ND	-3.64	1.98	2.05
22	8	603	CLA	MG-ND	-3.64	1.98	2.05
22	A	1125	CLA	C1C-NC	-3.63	1.32	1.37
22	3	610	CLA	C1C-NC	-3.63	1.32	1.37
22	A	1132	CLA	C1C-NC	-3.63	1.32	1.37
22	7	605	CLA	MG-ND	-3.63	1.98	2.05
22	B	1211	CLA	C1C-NC	-3.62	1.32	1.37
21	A	1011	CL0	OBD-CAD	3.62	1.28	1.22
22	A	1124	CLA	C1C-NC	-3.61	1.32	1.37
22	Z	606	CLA	MG-ND	-3.61	1.98	2.05
22	A	1109	CLA	C1C-NC	-3.61	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	1230	CLA	MG-ND	-3.61	1.98	2.05
22	A	1111	CLA	C1C-NC	-3.61	1.32	1.37
22	6	609	CLA	C1C-NC	-3.61	1.32	1.37
22	A	1128	CLA	C1C-NC	-3.60	1.32	1.37
37	J	4002	C7Z	C15-C14	3.60	1.54	1.43
37	1	503	C7Z	C35-C34	3.60	1.54	1.43
22	A	1122	CLA	MG-ND	-3.59	1.98	2.05
22	B	1204	CLA	C1C-NC	-3.59	1.32	1.37
22	A	1105	CLA	MG-ND	-3.59	1.98	2.05
22	B	1214	CLA	C1C-NC	-3.58	1.32	1.37
22	B	1230	CLA	C1C-NC	-3.57	1.32	1.37
22	3	604	CLA	C1C-NC	-3.56	1.32	1.37
22	1	608	CLA	MG-ND	-3.55	1.98	2.05
22	B	1021	CLA	C1C-NC	-3.55	1.32	1.37
22	A	1115	CLA	C1C-NC	-3.53	1.32	1.37
22	A	1127	CLA	C1C-NC	-3.53	1.32	1.37
22	B	1226	CLA	C1C-NC	-3.53	1.32	1.37
22	4	609	CLA	C1C-NC	-3.52	1.32	1.37
22	B	1023	CLA	C1C-NC	-3.52	1.32	1.37
22	B	1205	CLA	C1C-NC	-3.52	1.32	1.37
37	J	4002	C7Z	C35-C34	3.51	1.54	1.43
22	A	1113	CLA	C1C-NC	-3.51	1.32	1.37
22	B	1234	CLA	C1C-NC	-3.51	1.32	1.37
22	A	1140	CLA	C1C-NC	-3.51	1.32	1.37
22	B	1208	CLA	C1C-NC	-3.50	1.32	1.37
22	B	1229	CLA	C1C-NC	-3.50	1.32	1.37
22	B	1222	CLA	C1C-NC	-3.49	1.32	1.37
22	A	1108	CLA	C1C-NC	-3.49	1.32	1.37
22	A	1137	CLA	C1C-NC	-3.49	1.32	1.37
22	B	1209	CLA	C1C-NC	-3.48	1.32	1.37
22	7	612	CLA	C1C-NC	-3.48	1.32	1.37
22	B	1203	CLA	C1C-NC	-3.48	1.32	1.37
32	A	5005	DGA	OG2-CB1	3.47	1.44	1.34
22	3	605	CLA	C1C-NC	-3.47	1.32	1.37
22	A	1110	CLA	C1C-NC	-3.47	1.32	1.37
22	3	613	CLA	C1C-NC	-3.47	1.32	1.37
22	A	1138	CLA	C1C-NC	-3.46	1.32	1.37
37	5	505	C7Z	C2-C1	3.45	1.65	1.54
22	B	1219	CLA	C1C-NC	-3.45	1.32	1.37
37	1	503	C7Z	C2-C1	3.45	1.65	1.54
37	5	505	C7Z	C7-C6	3.45	1.57	1.45
22	9	601	CLA	C1C-NC	-3.45	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	J	4002	C7Z	C2-C1	3.45	1.65	1.54
40	2	613	CHL	CBB-CAB	3.45	1.52	1.29
22	B	1202	CLA	C1C-NC	-3.45	1.32	1.37
32	A	5005	DGA	OG1-CA1	3.44	1.43	1.33
22	2	607	CLA	C1C-NC	-3.44	1.32	1.37
37	1	503	C7Z	C38-C25	3.44	1.56	1.50
22	A	1103	CLA	C1C-NC	-3.44	1.32	1.37
22	9	603	CLA	C1C-NC	-3.44	1.32	1.37
22	B	1228	CLA	C1C-NC	-3.44	1.32	1.37
22	B	1237	CLA	C1C-NC	-3.44	1.32	1.37
22	A	1107	CLA	C1C-NC	-3.44	1.32	1.37
40	6	611	CHL	CBB-CAB	3.43	1.52	1.29
22	G	1601	CLA	C1C-NC	-3.43	1.32	1.37
22	B	1217	CLA	C1C-NC	-3.42	1.32	1.37
40	4	613	CHL	CBB-CAB	3.42	1.52	1.29
22	B	1207	CLA	C1C-NC	-3.42	1.32	1.37
22	7	601	CLA	C1C-NC	-3.42	1.32	1.37
22	K	1403	CLA	C1C-NC	-3.42	1.32	1.37
22	B	1229	CLA	MG-ND	-3.41	1.99	2.05
22	B	1236	CLA	C1C-NC	-3.41	1.32	1.37
22	A	1106	CLA	C1C-NC	-3.40	1.32	1.37
22	A	1135	CLA	C1C-NC	-3.40	1.32	1.37
22	L	1503	CLA	CBB-CAB	3.40	1.51	1.29
36	F	4001	RRX	C4-C5	-3.40	1.44	1.51
22	B	1201	CLA	CBB-CAB	3.40	1.51	1.29
40	5	611	CHL	CBB-CAB	3.40	1.51	1.29
40	4	611	CHL	CBB-CAB	3.40	1.51	1.29
22	A	1119	CLA	C1C-NC	-3.39	1.32	1.37
22	B	1218	CLA	C1C-NC	-3.39	1.32	1.37
22	8	601	CLA	C1C-NC	-3.39	1.32	1.37
22	2	612	CLA	CBB-CAB	3.39	1.51	1.29
32	9	802	DGA	OG2-CB1	3.39	1.43	1.34
22	6	603	CLA	C1C-NC	-3.39	1.32	1.37
40	6	613	CHL	CBB-CAB	3.39	1.51	1.29
26	3	801	LHG	O7-C5	-3.39	1.42	1.46
22	B	1226	CLA	CBB-CAB	3.38	1.51	1.29
22	A	1128	CLA	CBB-CAB	3.38	1.51	1.29
22	B	1215	CLA	C1C-NC	-3.38	1.32	1.37
22	A	1102	CLA	CBB-CAB	3.38	1.51	1.29
22	F	1301	CLA	C1C-NC	-3.38	1.32	1.37
22	9	602	CLA	CBB-CAB	3.38	1.51	1.29
22	F	1302	CLA	C1C-NC	-3.38	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	605	CLA	CBB-CAB	3.38	1.51	1.29
22	A	1101	CLA	C1C-NC	-3.37	1.32	1.37
22	K	1404	CLA	CBB-CAB	3.37	1.51	1.29
22	B	1241	CLA	C1C-NC	-3.37	1.32	1.37
37	5	505	C7Z	C38-C25	3.37	1.56	1.50
22	6	605	CLA	CBB-CAB	3.37	1.51	1.29
22	9	609	CLA	C1C-NC	-3.37	1.32	1.37
22	Z	608	CLA	CBB-CAB	3.37	1.51	1.29
22	8	615	CLA	CBB-CAB	3.37	1.51	1.29
22	A	1112	CLA	C1C-NC	-3.37	1.32	1.37
22	8	606	CLA	CBB-CAB	3.37	1.51	1.29
22	5	606	CLA	CBB-CAB	3.37	1.51	1.29
22	7	612	CLA	CBB-CAB	3.37	1.51	1.29
22	5	615	CLA	CBB-CAB	3.37	1.51	1.29
22	A	1105	CLA	C1C-NC	-3.37	1.32	1.37
22	2	604	CLA	C1C-NC	-3.37	1.32	1.37
22	A	1122	CLA	C1C-NC	-3.36	1.32	1.37
36	F	4001	RRX	C11-C10	3.36	1.53	1.43
22	3	606	CLA	C1C-NC	-3.36	1.32	1.37
22	B	1213	CLA	C1C-NC	-3.36	1.32	1.37
22	5	602	CLA	CBB-CAB	3.36	1.51	1.29
22	5	615	CLA	C1C-NC	-3.36	1.32	1.37
22	8	612	CLA	CBB-CAB	3.36	1.51	1.29
22	2	608	CLA	CBB-CAB	3.36	1.51	1.29
22	A	1103	CLA	CBB-CAB	3.36	1.51	1.29
22	6	608	CLA	CBB-CAB	3.36	1.51	1.29
22	5	601	CLA	CBB-CAB	3.36	1.51	1.29
22	2	603	CLA	CBB-CAB	3.36	1.51	1.29
22	1	602	CLA	C1C-NC	-3.36	1.32	1.37
22	7	609	CLA	C1C-NC	-3.36	1.32	1.37
22	A	1138	CLA	CBB-CAB	3.36	1.51	1.29
22	6	619	CLA	CBB-CAB	3.36	1.51	1.29
22	A	1136	CLA	C1C-NC	-3.36	1.32	1.37
22	5	622	CLA	CBB-CAB	3.36	1.51	1.29
22	A	1129	CLA	CBB-CAB	3.36	1.51	1.29
22	K	1403	CLA	CBB-CAB	3.36	1.51	1.29
22	B	1238	CLA	C1C-NC	-3.35	1.32	1.37
22	Z	602	CLA	CBB-CAB	3.35	1.51	1.29
22	6	606	CLA	CBB-CAB	3.35	1.51	1.29
22	4	612	CLA	CBB-CAB	3.35	1.51	1.29
40	6	617	CHL	CBB-CAB	3.35	1.51	1.29
22	B	1207	CLA	CBB-CAB	3.35	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	605	CLA	CBB-CAB	3.35	1.51	1.29
40	Z	613	CHL	CBB-CAB	3.35	1.51	1.29
22	7	608	CLA	C1C-NC	-3.35	1.32	1.37
22	4	606	CLA	CBB-CAB	3.35	1.51	1.29
22	2	615	CLA	CBB-CAB	3.35	1.51	1.29
22	2	606	CLA	CBB-CAB	3.35	1.51	1.29
22	8	607	CLA	CBB-CAB	3.35	1.51	1.29
22	A	1139	CLA	C1C-NC	-3.35	1.32	1.37
22	6	601	CLA	CBB-CAB	3.35	1.51	1.29
22	9	608	CLA	CBB-CAB	3.35	1.51	1.29
22	3	607	CLA	CBB-CAB	3.35	1.51	1.29
22	B	1221	CLA	CBB-CAB	3.35	1.51	1.29
22	2	615	CLA	C1C-NC	-3.35	1.32	1.37
37	J	4002	C7Z	C7-C6	3.35	1.57	1.45
22	A	1123	CLA	CBB-CAB	3.35	1.51	1.29
22	7	613	CLA	CBB-CAB	3.35	1.51	1.29
22	4	609	CLA	CBB-CAB	3.35	1.51	1.29
22	A	1117	CLA	CBB-CAB	3.35	1.51	1.29
22	B	1228	CLA	CBB-CAB	3.35	1.51	1.29
22	7	606	CLA	CBB-CAB	3.35	1.51	1.29
22	5	607	CLA	CBB-CAB	3.35	1.51	1.29
22	8	609	CLA	CBB-CAB	3.35	1.51	1.29
22	1	602	CLA	CBB-CAB	3.35	1.51	1.29
22	B	1223	CLA	CBB-CAB	3.35	1.51	1.29
22	2	605	CLA	CBB-CAB	3.35	1.51	1.29
40	8	610	CHL	CBB-CAB	3.35	1.51	1.29
22	B	1202	CLA	CBB-CAB	3.35	1.51	1.29
22	Z	607	CLA	CBB-CAB	3.35	1.51	1.29
22	A	1133	CLA	C1C-NC	-3.35	1.32	1.37
22	Z	605	CLA	CBB-CAB	3.35	1.51	1.29
22	B	1213	CLA	CBB-CAB	3.34	1.51	1.29
22	2	601	CLA	C1C-NC	-3.34	1.32	1.37
22	B	1236	CLA	CBB-CAB	3.34	1.51	1.29
22	4	615	CLA	CBB-CAB	3.34	1.51	1.29
22	1	606	CLA	CBB-CAB	3.34	1.51	1.29
22	6	607	CLA	CBB-CAB	3.34	1.51	1.29
22	7	611	CLA	CBB-CAB	3.34	1.51	1.29
22	8	611	CLA	CBB-CAB	3.34	1.51	1.29
22	B	1222	CLA	CBB-CAB	3.34	1.51	1.29
22	A	1110	CLA	CBB-CAB	3.34	1.51	1.29
22	8	608	CLA	CBB-CAB	3.34	1.51	1.29
22	A	1121	CLA	CBB-CAB	3.34	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	1239	CLA	CBB-CAB	3.34	1.51	1.29
22	3	606	CLA	CBB-CAB	3.34	1.51	1.29
36	F	4001	RRX	C24-C25	3.34	1.57	1.45
22	3	608	CLA	CBB-CAB	3.34	1.51	1.29
22	4	602	CLA	CBB-CAB	3.34	1.51	1.29
22	5	612	CLA	CBB-CAB	3.34	1.51	1.29
22	9	603	CLA	CBB-CAB	3.34	1.51	1.29
22	B	1023	CLA	CBB-CAB	3.34	1.51	1.29
22	4	604	CLA	CBB-CAB	3.34	1.51	1.29
22	A	1118	CLA	CBB-CAB	3.34	1.51	1.29
22	A	1108	CLA	CBB-CAB	3.34	1.51	1.29
22	A	1114	CLA	CBB-CAB	3.34	1.51	1.29
22	B	1235	CLA	CBB-CAB	3.34	1.51	1.29
22	Z	615	CLA	CBB-CAB	3.34	1.51	1.29
22	Z	606	CLA	CBB-CAB	3.34	1.51	1.29
22	3	601	CLA	CBB-CAB	3.34	1.51	1.29
22	8	609	CLA	C1C-NC	-3.34	1.32	1.37
22	8	604	CLA	CBB-CAB	3.34	1.51	1.29
22	A	1122	CLA	CBB-CAB	3.34	1.51	1.29
22	1	608	CLA	CBB-CAB	3.34	1.51	1.29
22	6	612	CLA	CBB-CAB	3.34	1.51	1.29
22	9	607	CLA	CBB-CAB	3.34	1.51	1.29
22	6	602	CLA	CBB-CAB	3.34	1.51	1.29
22	1	607	CLA	CBB-CAB	3.34	1.51	1.29
22	4	601	CLA	CBB-CAB	3.34	1.51	1.29
22	6	609	CLA	CBB-CAB	3.34	1.51	1.29
22	A	1111	CLA	CBB-CAB	3.34	1.51	1.29
22	8	605	CLA	CBB-CAB	3.34	1.51	1.29
22	B	1206	CLA	CBB-CAB	3.34	1.51	1.29
22	1	611	CLA	CBB-CAB	3.33	1.51	1.29
22	1	612	CLA	CBB-CAB	3.33	1.51	1.29
22	7	615	CLA	CBB-CAB	3.33	1.51	1.29
22	1	613	CLA	CBB-CAB	3.33	1.51	1.29
22	9	605	CLA	CBB-CAB	3.33	1.51	1.29
22	B	1201	CLA	C1C-NC	-3.33	1.32	1.37
22	7	608	CLA	CBB-CAB	3.33	1.51	1.29
22	2	601	CLA	CBB-CAB	3.33	1.51	1.29
22	5	603	CLA	CBB-CAB	3.33	1.51	1.29
22	3	603	CLA	CBB-CAB	3.33	1.51	1.29
22	4	607	CLA	CBB-CAB	3.33	1.51	1.29
22	A	1119	CLA	CBB-CAB	3.33	1.51	1.29
22	B	1230	CLA	CBB-CAB	3.33	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	L	1503	CLA	C1C-NC	-3.33	1.32	1.37
22	7	606	CLA	C1C-NC	-3.33	1.32	1.37
22	9	612	CLA	C1C-NC	-3.33	1.32	1.37
40	4	617	CHL	CBB-CAB	3.33	1.51	1.29
22	K	1402	CLA	CBB-CAB	3.33	1.51	1.29
22	4	608	CLA	CBB-CAB	3.33	1.51	1.29
22	Z	604	CLA	CBB-CAB	3.33	1.51	1.29
22	5	602	CLA	C1C-NC	-3.33	1.32	1.37
22	G	1601	CLA	CBB-CAB	3.33	1.51	1.29
22	1	605	CLA	CBB-CAB	3.33	1.51	1.29
22	B	1234	CLA	CBB-CAB	3.33	1.51	1.29
22	3	618	CLA	CBB-CAB	3.33	1.51	1.29
22	5	618	CLA	CBB-CAB	3.33	1.51	1.29
22	9	601	CLA	CBB-CAB	3.33	1.51	1.29
22	B	1215	CLA	CBB-CAB	3.33	1.51	1.29
22	6	604	CLA	CBB-CAB	3.33	1.51	1.29
22	A	1132	CLA	CBB-CAB	3.33	1.51	1.29
22	Z	601	CLA	CBB-CAB	3.33	1.51	1.29
22	3	613	CLA	CBB-CAB	3.33	1.51	1.29
22	5	608	CLA	CBB-CAB	3.33	1.51	1.29
22	B	1209	CLA	CBB-CAB	3.33	1.51	1.29
22	A	1012	CLA	CBB-CAB	3.33	1.51	1.29
22	1	604	CLA	CBB-CAB	3.33	1.51	1.29
22	A	1120	CLA	CBB-CAB	3.33	1.51	1.29
22	A	1105	CLA	CBB-CAB	3.33	1.51	1.29
22	Z	615	CLA	C1C-NC	-3.33	1.32	1.37
22	Z	611	CLA	CBB-CAB	3.33	1.51	1.29
22	A	1013	CLA	CBB-CAB	3.33	1.51	1.29
22	6	615	CLA	CBB-CAB	3.33	1.51	1.29
22	2	607	CLA	CBB-CAB	3.33	1.51	1.29
22	L	1502	CLA	CBB-CAB	3.33	1.51	1.29
22	Z	603	CLA	CBB-CAB	3.33	1.51	1.29
22	7	607	CLA	CBB-CAB	3.33	1.51	1.29
22	5	609	CLA	CBB-CAB	3.33	1.51	1.29
22	9	609	CLA	CBB-CAB	3.33	1.51	1.29
22	B	1220	CLA	CBB-CAB	3.32	1.51	1.29
22	3	612	CLA	CBB-CAB	3.32	1.51	1.29
22	8	612	CLA	C1C-NC	-3.32	1.32	1.37
22	2	602	CLA	CBB-CAB	3.32	1.51	1.29
40	7	610	CHL	CBB-CAB	3.32	1.51	1.29
21	A	1011	CL0	MG-NC	3.32	2.14	2.06
22	B	1219	CLA	CBB-CAB	3.32	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	1206	CLA	C1C-NC	-3.32	1.32	1.37
22	A	1113	CLA	CBB-CAB	3.32	1.51	1.29
22	A	1109	CLA	CBB-CAB	3.32	1.51	1.29
22	8	601	CLA	CBB-CAB	3.32	1.51	1.29
22	5	613	CLA	CBB-CAB	3.32	1.51	1.29
22	B	1224	CLA	CBB-CAB	3.32	1.51	1.29
22	6	618	CLA	CBB-CAB	3.32	1.51	1.29
22	A	1137	CLA	CBB-CAB	3.32	1.51	1.29
22	A	1141	CLA	CBB-CAB	3.32	1.51	1.29
36	F	4001	RRX	C29-C30	3.32	1.65	1.54
22	7	602	CLA	CBB-CAB	3.32	1.51	1.29
22	B	1231	CLA	CBB-CAB	3.32	1.51	1.29
22	B	1224	CLA	C1C-NC	-3.32	1.32	1.37
22	7	609	CLA	CBB-CAB	3.32	1.51	1.29
22	1	615	CLA	CBB-CAB	3.32	1.51	1.29
22	1	615	CLA	C1C-NC	-3.32	1.32	1.37
22	B	1237	CLA	CBB-CAB	3.32	1.51	1.29
22	A	1131	CLA	CBB-CAB	3.32	1.51	1.29
22	G	1602	CLA	CBB-CAB	3.32	1.51	1.29
22	A	1115	CLA	CBB-CAB	3.32	1.51	1.29
22	7	616	CLA	CBB-CAB	3.32	1.51	1.29
22	A	1124	CLA	CBB-CAB	3.32	1.51	1.29
22	7	601	CLA	CBB-CAB	3.32	1.51	1.29
22	B	1240	CLA	CBB-CAB	3.32	1.51	1.29
22	3	602	CLA	CBB-CAB	3.32	1.51	1.29
22	6	603	CLA	CBB-CAB	3.32	1.51	1.29
22	A	1131	CLA	C1C-NC	-3.31	1.32	1.37
22	A	1140	CLA	CBB-CAB	3.31	1.51	1.29
22	K	1401	CLA	CBB-CAB	3.31	1.51	1.29
22	1	612	CLA	C1C-NC	-3.31	1.32	1.37
22	8	602	CLA	CBB-CAB	3.31	1.51	1.29
22	A	1101	CLA	CBB-CAB	3.31	1.51	1.29
22	8	603	CLA	CBB-CAB	3.31	1.51	1.29
22	3	601	CLA	C1C-NC	-3.31	1.32	1.37
22	1	603	CLA	CBB-CAB	3.31	1.51	1.29
22	Z	601	CLA	C1C-NC	-3.31	1.32	1.37
22	A	1107	CLA	CBB-CAB	3.31	1.51	1.29
22	B	1210	CLA	CBB-CAB	3.31	1.51	1.29
40	2	610	CHL	CBB-CAB	3.31	1.51	1.29
22	8	615	CLA	C1C-NC	-3.31	1.32	1.37
22	A	1139	CLA	CBB-CAB	3.31	1.51	1.29
22	4	603	CLA	CBB-CAB	3.31	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	5	617	CHL	CBB-CAB	3.31	1.51	1.29
22	B	1241	CLA	CBB-CAB	3.31	1.51	1.29
22	A	1126	CLA	CBB-CAB	3.31	1.51	1.29
22	4	605	CLA	C1C-NC	-3.31	1.32	1.37
22	A	1106	CLA	CBB-CAB	3.31	1.51	1.29
22	B	1214	CLA	CBB-CAB	3.31	1.51	1.29
22	B	1216	CLA	CBB-CAB	3.31	1.51	1.29
22	2	604	CLA	CBB-CAB	3.31	1.51	1.29
22	B	1217	CLA	CBB-CAB	3.31	1.51	1.29
22	B	1225	CLA	CBB-CAB	3.31	1.51	1.29
22	A	1134	CLA	CBB-CAB	3.31	1.51	1.29
22	B	1204	CLA	CBB-CAB	3.31	1.51	1.29
22	B	1211	CLA	CBB-CAB	3.31	1.51	1.29
22	B	1232	CLA	CBB-CAB	3.30	1.51	1.29
22	F	1302	CLA	CBB-CAB	3.30	1.51	1.29
22	A	1141	CLA	C1C-NC	-3.30	1.32	1.37
22	A	1127	CLA	CBB-CAB	3.30	1.51	1.29
22	9	612	CLA	CBB-CAB	3.30	1.51	1.29
22	A	1013	CLA	C1C-NC	-3.30	1.32	1.37
22	A	1133	CLA	CBB-CAB	3.30	1.51	1.29
22	B	1218	CLA	CBB-CAB	3.30	1.51	1.29
22	3	616	CLA	CBB-CAB	3.30	1.51	1.29
22	7	602	CLA	C1C-NC	-3.30	1.32	1.37
22	1	601	CLA	CBB-CAB	3.30	1.51	1.29
22	7	604	CLA	CBB-CAB	3.30	1.51	1.29
37	1	503	C7Z	C7-C6	3.30	1.56	1.45
22	A	1117	CLA	C1C-NC	-3.30	1.32	1.37
22	A	1120	CLA	C1C-NC	-3.30	1.32	1.37
22	B	1208	CLA	CBB-CAB	3.30	1.51	1.29
22	3	604	CLA	CBB-CAB	3.30	1.51	1.29
22	B	1203	CLA	CBB-CAB	3.30	1.51	1.29
22	7	607	CLA	C1C-NC	-3.30	1.32	1.37
22	5	605	CLA	C1C-NC	-3.30	1.32	1.37
22	5	622	CLA	C1C-NC	-3.30	1.32	1.37
22	A	1130	CLA	C1C-NC	-3.29	1.32	1.37
22	7	605	CLA	CBB-CAB	3.29	1.51	1.29
22	A	1104	CLA	CBB-CAB	3.29	1.51	1.29
22	3	605	CLA	CBB-CAB	3.29	1.51	1.29
22	B	1212	CLA	CBB-CAB	3.29	1.51	1.29
22	3	610	CLA	CBB-CAB	3.29	1.51	1.29
22	Z	612	CLA	CBB-CAB	3.29	1.51	1.29
22	K	1401	CLA	C1C-NC	-3.29	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Z	604	CLA	C1C-NC	-3.29	1.32	1.37
22	B	1229	CLA	CBB-CAB	3.29	1.51	1.29
22	B	1205	CLA	CBB-CAB	3.29	1.51	1.29
22	9	607	CLA	C1C-NC	-3.29	1.32	1.37
22	9	608	CLA	C1C-NC	-3.29	1.32	1.37
33	B	5003	DGD	CGB-CFB	-3.28	1.33	1.51
22	6	618	CLA	C1C-NC	-3.28	1.32	1.37
22	A	1112	CLA	CBB-CAB	3.28	1.51	1.29
40	1	609	CHL	C4B-NB	3.28	1.38	1.35
22	J	1901	CLA	CBB-CAB	3.28	1.51	1.29
22	B	1227	CLA	C1C-NC	-3.28	1.32	1.37
22	A	1125	CLA	CBB-CAB	3.28	1.51	1.29
33	B	5003	DGD	CAA-C9A	-3.28	1.33	1.51
22	8	606	CLA	C1C-NC	-3.28	1.32	1.37
22	B	1022	CLA	C1C-NC	-3.28	1.32	1.37
33	B	5003	DGD	CAB-C9B	-3.28	1.33	1.51
22	4	603	CLA	C1C-NC	-3.28	1.32	1.37
40	1	610	CHL	CBB-CAB	3.28	1.51	1.29
22	Z	602	CLA	C1C-NC	-3.28	1.32	1.37
22	A	1012	CLA	C1C-NC	-3.28	1.32	1.37
33	B	5003	DGD	CDB-CCB	-3.28	1.33	1.51
22	A	1130	CLA	CBB-CAB	3.28	1.51	1.29
22	F	1301	CLA	CBB-CAB	3.28	1.51	1.29
22	G	1602	CLA	C1C-NC	-3.28	1.32	1.37
22	5	612	CLA	C1C-NC	-3.27	1.32	1.37
22	B	1235	CLA	C1C-NC	-3.27	1.32	1.37
22	1	603	CLA	C1C-NC	-3.27	1.32	1.37
22	A	1121	CLA	C1C-NC	-3.27	1.32	1.37
22	2	606	CLA	C1C-NC	-3.27	1.32	1.37
22	3	603	CLA	C1C-NC	-3.27	1.32	1.37
40	9	610	CHL	CBB-CAB	3.27	1.51	1.29
22	A	1118	CLA	C1C-NC	-3.27	1.32	1.37
22	B	1238	CLA	CBB-CAB	3.27	1.51	1.29
22	A	1104	CLA	C1C-NC	-3.27	1.32	1.37
22	B	1021	CLA	CBB-CAB	3.27	1.51	1.29
22	8	602	CLA	C1C-NC	-3.27	1.32	1.37
22	9	602	CLA	C1C-NC	-3.27	1.32	1.37
22	A	1126	CLA	C1C-NC	-3.27	1.32	1.37
22	7	603	CLA	CBB-CAB	3.26	1.50	1.29
22	6	606	CLA	C1C-NC	-3.26	1.32	1.37
40	8	613	CHL	CBB-CAB	3.26	1.50	1.29
22	2	608	CLA	C1C-NC	-3.26	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	615	CLA	C1C-NC	-3.26	1.32	1.37
22	1	601	CLA	C1C-NC	-3.26	1.32	1.37
22	8	605	CLA	C1C-NC	-3.26	1.32	1.37
40	2	610	CHL	C4B-NB	3.26	1.38	1.35
33	B	5003	DGD	CGA-CFA	-3.26	1.33	1.51
40	Z	610	CHL	CBB-CAB	3.25	1.50	1.29
22	B	1227	CLA	CBB-CAB	3.25	1.50	1.29
22	8	604	CLA	C1C-NC	-3.25	1.33	1.37
22	1	606	CLA	C1C-NC	-3.25	1.33	1.37
22	7	604	CLA	C1C-NC	-3.25	1.33	1.37
22	6	602	CLA	C1C-NC	-3.25	1.33	1.37
22	B	1022	CLA	CBB-CAB	3.25	1.50	1.29
22	B	1231	CLA	C1C-NC	-3.25	1.33	1.37
22	5	603	CLA	C1C-NC	-3.25	1.33	1.37
22	6	601	CLA	C1C-NC	-3.25	1.33	1.37
40	4	610	CHL	CBB-CAB	3.25	1.50	1.29
22	2	603	CLA	C1C-NC	-3.25	1.33	1.37
37	J	4002	C7Z	C38-C25	3.24	1.56	1.50
22	A	1136	CLA	CBB-CAB	3.24	1.50	1.29
22	B	1216	CLA	C1C-NC	-3.24	1.33	1.37
22	3	612	CLA	C1C-NC	-3.24	1.33	1.37
22	2	612	CLA	C1C-NC	-3.24	1.33	1.37
22	4	612	CLA	C1C-NC	-3.24	1.33	1.37
22	6	608	CLA	C1C-NC	-3.23	1.33	1.37
22	8	607	CLA	C1C-NC	-3.23	1.33	1.37
22	1	604	CLA	C1C-NC	-3.23	1.33	1.37
22	5	608	CLA	C1C-NC	-3.23	1.33	1.37
40	9	613	CHL	CBB-CAB	3.23	1.50	1.29
22	J	1901	CLA	C1C-NC	-3.23	1.33	1.37
22	2	605	CLA	C1C-NC	-3.23	1.33	1.37
22	A	1116	CLA	CBB-CAB	3.23	1.50	1.29
40	1	609	CHL	CBB-CAB	3.22	1.50	1.29
22	1	611	CLA	C1C-NC	-3.22	1.33	1.37
32	9	802	DGA	OG1-CA1	3.22	1.42	1.33
22	5	618	CLA	C1C-NC	-3.22	1.33	1.37
22	1	608	CLA	C1C-NC	-3.22	1.33	1.37
22	5	604	CLA	CBB-CAB	3.22	1.50	1.29
22	9	604	CLA	C3B-C2B	-3.22	1.35	1.40
40	5	610	CHL	C3B-C2B	-3.22	1.35	1.40
22	7	611	CLA	C1C-NC	-3.21	1.33	1.37
40	5	617	CHL	C4B-NB	3.21	1.38	1.35
40	3	611	CHL	C4B-NB	3.21	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	616	CLA	C1C-NC	-3.21	1.33	1.37
22	6	619	CLA	C1C-NC	-3.21	1.33	1.37
22	K	1404	CLA	C1C-NC	-3.21	1.33	1.37
22	B	1240	CLA	C1C-NC	-3.21	1.33	1.37
22	4	601	CLA	C1C-NC	-3.21	1.33	1.37
22	1	605	CLA	C1C-NC	-3.21	1.33	1.37
22	A	1134	CLA	C1C-NC	-3.20	1.33	1.37
22	Z	612	CLA	C1C-NC	-3.20	1.33	1.37
22	B	1021	CLA	C3B-C2B	-3.20	1.35	1.40
22	A	1114	CLA	C1C-NC	-3.20	1.33	1.37
33	B	5003	DGD	CDA-CCA	-3.20	1.33	1.51
22	3	607	CLA	C1C-NC	-3.20	1.33	1.37
22	9	606	CLA	C3B-C2B	-3.20	1.35	1.40
40	4	617	CHL	C4B-NB	3.20	1.38	1.35
22	9	604	CLA	CBB-CAB	3.20	1.50	1.29
22	7	603	CLA	C1C-NC	-3.20	1.33	1.37
22	5	609	CLA	C1C-NC	-3.20	1.33	1.37
22	4	604	CLA	C1C-NC	-3.19	1.33	1.37
22	4	602	CLA	C1C-NC	-3.19	1.33	1.37
22	8	608	CLA	C1C-NC	-3.19	1.33	1.37
22	Z	611	CLA	C1C-NC	-3.19	1.33	1.37
22	5	601	CLA	C1C-NC	-3.19	1.33	1.37
22	Z	603	CLA	C1C-NC	-3.19	1.33	1.37
22	L	1502	CLA	C1C-NC	-3.19	1.33	1.37
22	7	613	CLA	C1C-NC	-3.19	1.33	1.37
22	8	603	CLA	C1C-NC	-3.19	1.33	1.37
40	6	610	CHL	CBB-CAB	3.18	1.50	1.29
22	5	606	CLA	C1C-NC	-3.18	1.33	1.37
22	6	612	CLA	C1C-NC	-3.18	1.33	1.37
22	7	605	CLA	C1C-NC	-3.18	1.33	1.37
22	4	608	CLA	C1C-NC	-3.18	1.33	1.37
22	9	606	CLA	C1C-NC	-3.18	1.33	1.37
40	6	617	CHL	C4B-NB	3.18	1.38	1.35
22	7	616	CLA	C1C-NC	-3.18	1.33	1.37
22	A	1135	CLA	C3B-C2B	-3.18	1.36	1.40
22	Z	606	CLA	C1C-NC	-3.17	1.33	1.37
22	4	615	CLA	C1C-NC	-3.17	1.33	1.37
22	9	605	CLA	C1C-NC	-3.17	1.33	1.37
36	F	4001	RRX	C16-C17	3.17	1.53	1.43
22	Z	608	CLA	C1C-NC	-3.17	1.33	1.37
22	K	1402	CLA	C1C-NC	-3.16	1.33	1.37
22	4	607	CLA	C1C-NC	-3.16	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	1221	CLA	C1C-NC	-3.16	1.33	1.37
22	A	1123	CLA	C1C-NC	-3.16	1.33	1.37
40	5	610	CHL	CBB-CAB	3.16	1.50	1.29
22	2	602	CLA	C1C-NC	-3.16	1.33	1.37
22	4	606	CLA	C1C-NC	-3.15	1.33	1.37
22	3	608	CLA	C1C-NC	-3.15	1.33	1.37
22	5	607	CLA	C1C-NC	-3.15	1.33	1.37
22	6	605	CLA	C1C-NC	-3.15	1.33	1.37
22	8	611	CLA	C1C-NC	-3.15	1.33	1.37
22	B	1022	CLA	C3B-C2B	-3.15	1.36	1.40
40	Z	609	CHL	CBB-CAB	3.15	1.50	1.29
40	9	613	CHL	C4B-NB	3.15	1.38	1.35
22	6	604	CLA	C1C-NC	-3.14	1.33	1.37
22	3	602	CLA	C1C-NC	-3.14	1.33	1.37
22	6	607	CLA	C1C-NC	-3.14	1.33	1.37
22	Z	605	CLA	C1C-NC	-3.14	1.33	1.37
22	7	615	CLA	C1C-NC	-3.14	1.33	1.37
22	Z	607	CLA	C1C-NC	-3.14	1.33	1.37
22	A	1135	CLA	CBB-CAB	3.14	1.50	1.29
22	A	1129	CLA	C1C-NC	-3.13	1.33	1.37
22	5	613	CLA	C1C-NC	-3.13	1.33	1.37
22	B	1232	CLA	C1C-NC	-3.13	1.33	1.37
22	3	618	CLA	C1C-NC	-3.13	1.33	1.37
22	A	1116	CLA	C1C-NC	-3.12	1.33	1.37
22	9	604	CLA	C1C-NC	-3.12	1.33	1.37
22	9	606	CLA	CBB-CAB	3.12	1.50	1.29
22	1	607	CLA	C1C-NC	-3.11	1.33	1.37
22	1	613	CLA	C1C-NC	-3.10	1.33	1.37
22	B	1225	CLA	C3B-C2B	-3.09	1.36	1.40
40	2	609	CHL	C3B-C2B	-3.06	1.36	1.40
22	A	1102	CLA	C1C-NC	-3.06	1.33	1.37
40	2	609	CHL	CBB-CAB	3.06	1.49	1.29
40	8	613	CHL	C4B-NB	3.03	1.37	1.35
22	9	604	CLA	CHC-C1C	3.02	1.42	1.35
22	5	604	CLA	C1C-NC	-3.02	1.33	1.37
40	7	610	CHL	C4B-NB	3.02	1.37	1.35
40	5	610	CHL	C4B-NB	3.01	1.37	1.35
40	Z	613	CHL	C4B-NB	3.00	1.37	1.35
22	3	616	CLA	C3B-C2B	-2.97	1.36	1.40
22	A	1116	CLA	CHC-C1C	2.97	1.42	1.35
40	2	613	CHL	C4B-NB	2.97	1.37	1.35
40	Z	609	CHL	C4B-NB	2.96	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	5002	LHG	O7-C5	-2.96	1.43	1.46
40	6	611	CHL	C4B-NB	2.96	1.37	1.35
22	B	1232	CLA	C3B-C2B	-2.96	1.36	1.40
40	9	610	CHL	C4B-NB	2.95	1.37	1.35
22	A	1127	CLA	C3B-C2B	-2.94	1.36	1.40
21	A	1011	CL0	C3D-C2D	2.94	1.47	1.39
40	3	611	CHL	CBB-CAB	2.94	1.48	1.29
22	B	1216	CLA	C3B-C2B	-2.92	1.36	1.40
36	F	4001	RRX	C7-C6	2.92	1.55	1.45
22	B	1229	CLA	C3B-C2B	-2.92	1.36	1.40
40	2	609	CHL	C4B-NB	2.91	1.37	1.35
22	B	1214	CLA	C3B-C2B	-2.91	1.36	1.40
22	B	1239	CLA	C3B-C2B	-2.90	1.36	1.40
40	6	613	CHL	C4B-NB	2.90	1.37	1.35
22	9	606	CLA	CHC-C1C	2.89	1.42	1.35
37	J	4002	C7Z	C21-C26	-2.88	1.49	1.53
22	5	604	CLA	C3B-C2B	-2.88	1.36	1.40
22	A	1102	CLA	CHC-C1C	2.87	1.42	1.35
22	B	1209	CLA	C3B-C2B	-2.87	1.36	1.40
22	5	604	CLA	CHC-C1C	2.85	1.42	1.35
22	F	1301	CLA	C3B-C2B	-2.85	1.36	1.40
22	5	601	CLA	CHC-C1C	2.84	1.42	1.35
22	1	615	CLA	C3B-C2B	-2.84	1.36	1.40
40	4	611	CHL	C4B-NB	2.83	1.37	1.35
22	B	1201	CLA	CHC-C1C	2.83	1.42	1.35
22	A	1106	CLA	C3B-C2B	-2.82	1.36	1.40
22	A	1012	CLA	C3B-C2B	-2.82	1.36	1.40
45	8	803	LPX	P1-O1	2.82	1.70	1.59
22	1	601	CLA	CHC-C1C	2.81	1.42	1.35
21	A	1011	CL0	C4D-CHA	2.81	1.48	1.38
22	5	605	CLA	CHC-C1C	2.81	1.42	1.35
40	1	610	CHL	C4B-NB	2.81	1.37	1.35
22	7	603	CLA	C3B-C2B	-2.79	1.36	1.40
22	B	1231	CLA	C3B-C2B	-2.79	1.36	1.40
22	A	1013	CLA	CHC-C1C	2.79	1.42	1.35
22	B	1211	CLA	CHC-C1C	2.79	1.42	1.35
22	3	604	CLA	CHC-C1C	2.78	1.42	1.35
22	A	1119	CLA	CHC-C1C	2.78	1.42	1.35
22	A	1116	CLA	C3B-C2B	-2.78	1.36	1.40
22	6	609	CLA	C3B-C2B	-2.77	1.36	1.40
22	3	610	CLA	C3B-C2B	-2.76	1.36	1.40
22	Z	608	CLA	CHC-C1C	2.75	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	9	609	CLA	C3B-C2B	-2.75	1.36	1.40
22	A	1012	CLA	CHC-C1C	2.75	1.42	1.35
22	A	1104	CLA	CHC-C1C	2.74	1.42	1.35
22	B	1222	CLA	CHC-C1C	2.74	1.42	1.35
22	3	603	CLA	C3B-C2B	-2.74	1.36	1.40
40	Z	610	CHL	C4B-NB	2.74	1.37	1.35
22	8	602	CLA	CHC-C1C	2.74	1.42	1.35
22	6	619	CLA	CHC-C1C	2.74	1.42	1.35
22	A	1105	CLA	CHC-C1C	2.74	1.42	1.35
22	A	1129	CLA	CHC-C1C	2.73	1.42	1.35
22	4	606	CLA	CHC-C1C	2.73	1.42	1.35
22	7	603	CLA	CHC-C1C	2.73	1.42	1.35
22	8	604	CLA	CHC-C1C	2.73	1.42	1.35
22	B	1232	CLA	CHC-C1C	2.73	1.42	1.35
22	B	1217	CLA	C3B-C2B	-2.73	1.36	1.40
22	5	613	CLA	CHC-C1C	2.73	1.42	1.35
22	4	601	CLA	CHC-C1C	2.73	1.42	1.35
22	2	612	CLA	CHC-C1C	2.73	1.42	1.35
22	6	605	CLA	CHC-C1C	2.73	1.42	1.35
22	7	609	CLA	CHC-C1C	2.72	1.41	1.35
22	Z	601	CLA	CHC-C1C	2.72	1.41	1.35
22	7	604	CLA	CHC-C1C	2.72	1.41	1.35
22	5	607	CLA	CHC-C1C	2.72	1.41	1.35
22	J	1901	CLA	CHC-C1C	2.72	1.41	1.35
40	5	611	CHL	C4B-NB	2.72	1.37	1.35
22	7	605	CLA	CHC-C1C	2.72	1.41	1.35
40	4	610	CHL	C4B-NB	2.72	1.37	1.35
22	1	606	CLA	CHC-C1C	2.72	1.41	1.35
22	9	609	CLA	CHC-C1C	2.72	1.41	1.35
22	3	601	CLA	CHC-C1C	2.71	1.41	1.35
22	5	612	CLA	CHC-C1C	2.71	1.41	1.35
22	6	601	CLA	CHC-C1C	2.71	1.41	1.35
22	2	606	CLA	C3B-C2B	-2.71	1.36	1.40
22	7	613	CLA	CHC-C1C	2.71	1.41	1.35
22	B	1241	CLA	CHC-C1C	2.70	1.41	1.35
22	B	1240	CLA	CHC-C1C	2.70	1.41	1.35
22	8	609	CLA	C3B-C2B	-2.70	1.36	1.40
22	4	604	CLA	CHC-C1C	2.70	1.41	1.35
28	1	803	LMT	O3'-C3'	-2.70	1.36	1.43
22	3	602	CLA	CHC-C1C	2.70	1.41	1.35
22	B	1231	CLA	CHC-C1C	2.70	1.41	1.35
22	A	1106	CLA	CHC-C1C	2.70	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	8	603	CLA	CHC-C1C	2.70	1.41	1.35
22	A	1139	CLA	C3B-C2B	-2.70	1.36	1.40
22	B	1208	CLA	CHC-C1C	2.70	1.41	1.35
22	8	608	CLA	CHC-C1C	2.70	1.41	1.35
22	A	1140	CLA	CHC-C1C	2.70	1.41	1.35
22	K	1402	CLA	CHC-C1C	2.69	1.41	1.35
22	F	1302	CLA	CHC-C1C	2.69	1.41	1.35
22	G	1602	CLA	C3B-C2B	-2.69	1.36	1.40
22	A	1112	CLA	CHC-C1C	2.69	1.41	1.35
22	9	602	CLA	CHC-C1C	2.69	1.41	1.35
27	8	802	NKP	OAF-CAG	-2.69	1.34	1.44
22	B	1227	CLA	CHC-C1C	2.69	1.41	1.35
22	7	606	CLA	CHC-C1C	2.69	1.41	1.35
22	7	616	CLA	CHC-C1C	2.69	1.41	1.35
22	A	1118	CLA	CHC-C1C	2.69	1.41	1.35
22	B	1235	CLA	CHC-C1C	2.68	1.41	1.35
22	2	605	CLA	CHC-C1C	2.68	1.41	1.35
22	A	1120	CLA	CHC-C1C	2.68	1.41	1.35
36	F	4001	RRX	C32-C1	2.68	1.59	1.53
22	7	609	CLA	C3B-C2B	-2.68	1.36	1.40
22	7	601	CLA	CHC-C1C	2.68	1.41	1.35
28	B	5005	LMT	O3'-C3'	-2.68	1.36	1.43
22	Z	606	CLA	CHC-C1C	2.68	1.41	1.35
22	Z	604	CLA	CHC-C1C	2.67	1.41	1.35
22	A	1111	CLA	CHC-C1C	2.67	1.41	1.35
22	7	611	CLA	CHC-C1C	2.67	1.41	1.35
22	4	603	CLA	CHC-C1C	2.66	1.41	1.35
22	5	609	CLA	CHC-C1C	2.66	1.41	1.35
22	1	605	CLA	CHC-C1C	2.66	1.41	1.35
22	B	1216	CLA	CHC-C1C	2.66	1.41	1.35
22	6	612	CLA	CHC-C1C	2.66	1.41	1.35
22	A	1139	CLA	CHC-C1C	2.66	1.41	1.35
21	A	1011	CL0	C1C-NC	-2.66	1.33	1.37
22	F	1301	CLA	CHC-C1C	2.66	1.41	1.35
22	1	608	CLA	CHC-C1C	2.65	1.41	1.35
22	B	1230	CLA	CHC-C1C	2.65	1.41	1.35
22	B	1221	CLA	CHC-C1C	2.65	1.41	1.35
22	G	1602	CLA	CHC-C1C	2.65	1.41	1.35
22	5	603	CLA	C3B-C2B	-2.65	1.36	1.40
22	K	1401	CLA	CHC-C1C	2.65	1.41	1.35
22	4	615	CLA	CHC-C1C	2.65	1.41	1.35
22	F	1302	CLA	C3B-C2B	-2.65	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1118	CLA	C3B-C2B	-2.65	1.36	1.40
22	1	608	CLA	C3B-C2B	-2.65	1.36	1.40
22	6	615	CLA	C3B-C2B	-2.65	1.36	1.40
22	3	605	CLA	CHC-C1C	2.65	1.41	1.35
28	4	803	LMT	O3'-C3'	-2.65	1.36	1.43
22	A	1109	CLA	CHC-C1C	2.64	1.41	1.35
40	8	610	CHL	C4B-NB	2.64	1.37	1.35
22	2	607	CLA	C3B-C2B	-2.64	1.36	1.40
22	B	1217	CLA	CHC-C1C	2.64	1.41	1.35
22	B	1205	CLA	C3B-C2B	-2.64	1.36	1.40
22	A	1124	CLA	CHC-C1C	2.64	1.41	1.35
22	B	1202	CLA	CHC-C1C	2.64	1.41	1.35
22	2	608	CLA	CHC-C1C	2.64	1.41	1.35
22	5	602	CLA	CHC-C1C	2.64	1.41	1.35
22	A	1132	CLA	C3B-C2B	-2.64	1.36	1.40
22	K	1401	CLA	C3B-C2B	-2.63	1.36	1.40
22	A	1110	CLA	C3B-C2B	-2.63	1.36	1.40
22	B	1234	CLA	CHC-C1C	2.63	1.41	1.35
21	A	1011	CL0	C1B-CHB	2.63	1.48	1.41
22	Z	603	CLA	CHC-C1C	2.63	1.41	1.35
28	9	803	LMT	O3'-C3'	-2.63	1.36	1.43
22	7	602	CLA	CHC-C1C	2.63	1.41	1.35
22	A	1110	CLA	CHC-C1C	2.63	1.41	1.35
22	6	618	CLA	CHC-C1C	2.63	1.41	1.35
22	9	612	CLA	CHC-C1C	2.63	1.41	1.35
22	A	1121	CLA	C3B-C2B	-2.63	1.36	1.40
22	8	607	CLA	CHC-C1C	2.63	1.41	1.35
22	B	1229	CLA	CHC-C1C	2.63	1.41	1.35
22	G	1601	CLA	C3B-C2B	-2.63	1.36	1.40
22	B	1236	CLA	CHC-C1C	2.63	1.41	1.35
22	A	1125	CLA	CHC-C1C	2.63	1.41	1.35
22	8	606	CLA	CHC-C1C	2.63	1.41	1.35
40	4	613	CHL	C4B-NB	2.63	1.37	1.35
40	6	610	CHL	C4B-NB	2.62	1.37	1.35
22	4	602	CLA	CHC-C1C	2.62	1.41	1.35
22	3	612	CLA	CHC-C1C	2.62	1.41	1.35
22	A	1121	CLA	CHC-C1C	2.62	1.41	1.35
22	B	1207	CLA	C3B-C2B	-2.62	1.36	1.40
28	F	5001	LMT	O3'-C3'	-2.62	1.36	1.43
22	A	1133	CLA	CHC-C1C	2.62	1.41	1.35
22	B	1220	CLA	CHC-C1C	2.62	1.41	1.35
22	8	603	CLA	C3B-C2B	-2.62	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	1213	CLA	CHC-C1C	2.62	1.41	1.35
22	A	1130	CLA	CHC-C1C	2.62	1.41	1.35
22	1	613	CLA	CHC-C1C	2.62	1.41	1.35
22	6	607	CLA	CHC-C1C	2.62	1.41	1.35
22	6	606	CLA	CHC-C1C	2.61	1.41	1.35
22	9	607	CLA	CHC-C1C	2.61	1.41	1.35
22	A	1138	CLA	CHC-C1C	2.61	1.41	1.35
22	3	613	CLA	CHC-C1C	2.61	1.41	1.35
22	1	612	CLA	CHC-C1C	2.61	1.41	1.35
22	2	603	CLA	CHC-C1C	2.61	1.41	1.35
22	2	602	CLA	CHC-C1C	2.61	1.41	1.35
28	B	5005	LMT	O2'-C2'	-2.61	1.36	1.43
22	8	605	CLA	CHC-C1C	2.61	1.41	1.35
22	6	602	CLA	CHC-C1C	2.61	1.41	1.35
27	A	5004	NKP	OAF-CAG	-2.61	1.34	1.44
22	1	602	CLA	CHC-C1C	2.60	1.41	1.35
28	8	805	LMT	O3'-C3'	-2.60	1.36	1.43
22	A	1105	CLA	C3B-C2B	-2.60	1.36	1.40
22	4	612	CLA	CHC-C1C	2.60	1.41	1.35
22	Z	607	CLA	CHC-C1C	2.60	1.41	1.35
22	6	608	CLA	CHC-C1C	2.60	1.41	1.35
22	8	612	CLA	CHC-C1C	2.60	1.41	1.35
22	A	1126	CLA	CHC-C1C	2.60	1.41	1.35
22	3	607	CLA	CHC-C1C	2.60	1.41	1.35
22	6	615	CLA	CHC-C1C	2.60	1.41	1.35
22	B	1022	CLA	CHC-C1C	2.60	1.41	1.35
22	B	1240	CLA	C3B-C2B	-2.60	1.36	1.40
22	4	609	CLA	C3B-C2B	-2.60	1.36	1.40
22	1	603	CLA	CHC-C1C	2.60	1.41	1.35
28	B	6101	LMT	O3'-C3'	-2.60	1.36	1.43
22	8	601	CLA	CHC-C1C	2.60	1.41	1.35
22	A	1140	CLA	C3B-C2B	-2.60	1.36	1.40
22	7	616	CLA	C3B-C2B	-2.60	1.36	1.40
27	3	802	NKP	OAF-CAG	-2.60	1.34	1.44
22	B	1023	CLA	CHC-C1C	2.60	1.41	1.35
37	5	505	C7Z	C21-C26	-2.59	1.50	1.53
22	K	1404	CLA	CHC-C1C	2.59	1.41	1.35
22	Z	611	CLA	CHC-C1C	2.59	1.41	1.35
22	A	1135	CLA	CHC-C1C	2.59	1.41	1.35
22	Z	602	CLA	CHC-C1C	2.59	1.41	1.35
22	2	601	CLA	CHC-C1C	2.59	1.41	1.35
22	A	1103	CLA	CHC-C1C	2.59	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	604	CLA	CHC-C1C	2.59	1.41	1.35
22	B	1228	CLA	CHC-C1C	2.59	1.41	1.35
22	6	603	CLA	C3B-C2B	-2.59	1.36	1.40
22	2	604	CLA	CHC-C1C	2.59	1.41	1.35
22	B	1238	CLA	CHC-C1C	2.59	1.41	1.35
22	5	608	CLA	CHC-C1C	2.59	1.41	1.35
22	3	605	CLA	C3B-C2B	-2.59	1.36	1.40
22	B	1209	CLA	CHC-C1C	2.59	1.41	1.35
22	2	607	CLA	CHC-C1C	2.59	1.41	1.35
22	A	1122	CLA	CHC-C1C	2.59	1.41	1.35
22	5	603	CLA	CHC-C1C	2.59	1.41	1.35
22	A	1101	CLA	C3B-C2B	-2.59	1.36	1.40
22	Z	605	CLA	CHC-C1C	2.59	1.41	1.35
22	8	609	CLA	CHC-C1C	2.59	1.41	1.35
22	7	612	CLA	CHC-C1C	2.59	1.41	1.35
22	1	604	CLA	CHC-C1C	2.58	1.41	1.35
22	A	1115	CLA	CHC-C1C	2.58	1.41	1.35
22	7	615	CLA	CHC-C1C	2.58	1.41	1.35
28	A	5006	LMT	O3'-C3'	-2.58	1.36	1.43
22	3	608	CLA	CHC-C1C	2.58	1.41	1.35
22	4	607	CLA	CHC-C1C	2.58	1.41	1.35
22	8	602	CLA	C3B-C2B	-2.58	1.36	1.40
22	7	605	CLA	C3B-C2B	-2.57	1.36	1.40
22	9	607	CLA	C3B-C2B	-2.57	1.36	1.40
22	B	1223	CLA	CHC-C1C	2.57	1.41	1.35
22	7	607	CLA	CHC-C1C	2.57	1.41	1.35
22	A	1130	CLA	C3B-C2B	-2.57	1.36	1.40
22	B	1212	CLA	CHC-C1C	2.57	1.41	1.35
22	3	616	CLA	CHC-C1C	2.57	1.41	1.35
22	Z	615	CLA	CHC-C1C	2.57	1.41	1.35
22	4	605	CLA	CHC-C1C	2.57	1.41	1.35
22	4	608	CLA	CHC-C1C	2.56	1.41	1.35
22	A	1114	CLA	CHC-C1C	2.56	1.41	1.35
22	1	615	CLA	CHC-C1C	2.56	1.41	1.35
22	B	1203	CLA	CHC-C1C	2.56	1.41	1.35
22	A	1122	CLA	C3B-C2B	-2.56	1.36	1.40
22	A	1134	CLA	CHC-C1C	2.56	1.41	1.35
22	9	601	CLA	CHC-C1C	2.56	1.41	1.35
22	3	603	CLA	CHC-C1C	2.55	1.41	1.35
22	G	1601	CLA	CHC-C1C	2.55	1.41	1.35
22	Z	612	CLA	CHC-C1C	2.55	1.41	1.35
22	Z	615	CLA	C3B-C2B	-2.55	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	605	CLA	C3B-C2B	-2.55	1.36	1.40
22	A	1131	CLA	CHC-C1C	2.55	1.41	1.35
22	A	1101	CLA	CHC-C1C	2.55	1.41	1.35
22	L	1503	CLA	CHC-C1C	2.55	1.41	1.35
22	B	1224	CLA	CHC-C1C	2.55	1.41	1.35
42	Z	504	QTB	C14-C12	-2.55	1.47	1.53
22	3	618	CLA	CHC-C1C	2.55	1.41	1.35
22	2	615	CLA	CHC-C1C	2.55	1.41	1.35
22	A	1126	CLA	C3B-C2B	-2.55	1.36	1.40
22	7	608	CLA	C3B-C2B	-2.55	1.36	1.40
22	B	1214	CLA	CHC-C1C	2.55	1.41	1.35
22	4	602	CLA	C3B-C2B	-2.55	1.36	1.40
22	5	602	CLA	C3B-C2B	-2.55	1.36	1.40
22	1	607	CLA	CHC-C1C	2.54	1.41	1.35
22	B	1021	CLA	CHC-C1C	2.54	1.41	1.35
22	1	611	CLA	CHC-C1C	2.54	1.41	1.35
22	7	615	CLA	C3B-C2B	-2.54	1.36	1.40
28	A	5006	LMT	O2'-C2'	-2.54	1.37	1.43
22	6	603	CLA	CHC-C1C	2.54	1.41	1.35
22	Z	612	CLA	C3B-C2B	-2.54	1.36	1.40
22	8	608	CLA	C3B-C2B	-2.54	1.36	1.40
22	8	611	CLA	CHC-C1C	2.54	1.41	1.35
22	B	1210	CLA	CHC-C1C	2.53	1.41	1.35
22	B	1225	CLA	CHC-C1C	2.53	1.41	1.35
22	5	606	CLA	CHC-C1C	2.53	1.41	1.35
22	9	605	CLA	CHC-C1C	2.53	1.41	1.35
22	B	1218	CLA	CHC-C1C	2.53	1.41	1.35
22	4	609	CLA	CHC-C1C	2.53	1.41	1.35
43	5	802	3PH	O31-C31	2.53	1.40	1.33
22	A	1113	CLA	CHC-C1C	2.53	1.41	1.35
22	3	602	CLA	C3B-C2B	-2.53	1.36	1.40
22	B	1238	CLA	C3B-C2B	-2.53	1.36	1.40
22	A	1137	CLA	CHC-C1C	2.53	1.41	1.35
22	L	1502	CLA	CHC-C1C	2.53	1.41	1.35
22	2	602	CLA	C3B-C2B	-2.53	1.36	1.40
22	5	618	CLA	CHC-C1C	2.53	1.41	1.35
22	B	1223	CLA	C3B-C2B	-2.53	1.36	1.40
22	B	1205	CLA	CHC-C1C	2.52	1.41	1.35
22	5	615	CLA	C3B-C2B	-2.52	1.36	1.40
22	5	609	CLA	C3B-C2B	-2.52	1.36	1.40
22	6	608	CLA	C3B-C2B	-2.52	1.36	1.40
37	J	4002	C7Z	C10-C9	-2.52	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	1227	CLA	C3B-C2B	-2.52	1.36	1.40
22	3	606	CLA	CHC-C1C	2.51	1.41	1.35
22	B	1207	CLA	CHC-C1C	2.51	1.41	1.35
22	A	1104	CLA	C3B-C2B	-2.51	1.36	1.40
22	7	608	CLA	CHC-C1C	2.51	1.41	1.35
40	9	613	CHL	C3B-C2B	-2.50	1.36	1.40
22	8	615	CLA	C3B-C2B	-2.50	1.36	1.40
43	8	806	3PH	O21-C2	-2.50	1.40	1.46
22	5	607	CLA	C3B-C2B	-2.50	1.36	1.40
40	9	610	CHL	C3B-C2B	-2.50	1.36	1.40
22	9	603	CLA	CHC-C1C	2.50	1.41	1.35
22	K	1403	CLA	C3B-C2B	-2.50	1.36	1.40
22	A	1123	CLA	CHC-C1C	2.50	1.41	1.35
22	2	605	CLA	C3B-C2B	-2.49	1.36	1.40
28	B	6101	LMT	O2'-C2'	-2.49	1.37	1.43
22	3	607	CLA	C3B-C2B	-2.49	1.36	1.40
22	A	1127	CLA	CHC-C1C	2.49	1.41	1.35
22	1	603	CLA	C3B-C2B	-2.49	1.36	1.40
37	5	505	C7Z	C20-C13	2.49	1.56	1.50
22	9	608	CLA	CHC-C1C	2.49	1.41	1.35
22	A	1107	CLA	CHC-C1C	2.49	1.41	1.35
28	F	5001	LMT	O2'-C2'	-2.49	1.37	1.43
22	A	1131	CLA	C3B-C2B	-2.48	1.36	1.40
22	K	1403	CLA	CHC-C1C	2.48	1.41	1.35
35	B	5004	T7X	O16-C8	-2.48	1.40	1.46
21	A	1011	CL0	C4B-CHC	2.48	1.47	1.41
22	A	1141	CLA	CHC-C1C	2.48	1.41	1.35
43	5	802	3PH	O21-C2	-2.48	1.40	1.46
22	A	1108	CLA	CHC-C1C	2.48	1.41	1.35
22	2	606	CLA	CHC-C1C	2.48	1.41	1.35
43	2	802	3PH	O31-C31	2.48	1.40	1.33
37	1	503	C7Z	C21-C26	-2.48	1.50	1.53
22	B	1237	CLA	CHC-C1C	2.48	1.41	1.35
22	A	1134	CLA	C3B-C2B	-2.48	1.36	1.40
22	5	622	CLA	C3B-C2B	-2.47	1.36	1.40
28	9	803	LMT	O3B-C3B	-2.47	1.37	1.43
22	B	1236	CLA	C3B-C2B	-2.47	1.36	1.40
40	7	610	CHL	C3B-C2B	-2.47	1.36	1.40
43	7	802	3PH	O31-C31	2.47	1.40	1.33
37	J	4002	C7Z	C20-C13	2.47	1.56	1.50
40	1	609	CHL	C3B-C2B	-2.46	1.36	1.40
28	1	803	LMT	O2'-C2'	-2.46	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	5006	LMT	O2B-C2B	-2.46	1.37	1.43
43	6	802	3PH	O31-C31	2.46	1.40	1.33
22	5	622	CLA	CHC-C1C	2.46	1.41	1.35
22	A	1117	CLA	CHC-C1C	2.46	1.41	1.35
22	B	1226	CLA	C3B-C2B	-2.46	1.37	1.40
28	4	803	LMT	O2B-C2B	-2.46	1.37	1.43
22	8	615	CLA	CHC-C1C	2.45	1.41	1.35
43	7	802	3PH	O21-C21	2.45	1.41	1.34
43	6	802	3PH	O21-C2	-2.45	1.40	1.46
22	6	609	CLA	CHC-C1C	2.45	1.41	1.35
22	B	1215	CLA	C3B-C2B	-2.45	1.37	1.40
22	A	1105	CLA	C1C-C2C	2.45	1.49	1.44
22	B	1226	CLA	C3D-C4D	-2.45	1.38	1.44
28	B	5005	LMT	O3B-C3B	-2.44	1.37	1.43
22	B	1219	CLA	CHC-C1C	2.44	1.41	1.35
22	5	613	CLA	C3B-C2B	-2.44	1.37	1.40
43	8	806	3PH	O31-C31	2.43	1.40	1.33
22	Z	603	CLA	C3B-C2B	-2.42	1.37	1.40
22	9	601	CLA	C3B-C2B	-2.42	1.37	1.40
22	B	1237	CLA	C3B-C2B	-2.42	1.37	1.40
28	1	803	LMT	O2B-C2B	-2.42	1.37	1.43
22	A	1136	CLA	CHC-C1C	2.42	1.41	1.35
22	9	608	CLA	C3B-C2B	-2.42	1.37	1.40
37	1	503	C7Z	C18-C5	2.41	1.54	1.50
22	3	610	CLA	CHC-C1C	2.41	1.41	1.35
22	5	615	CLA	CHC-C1C	2.41	1.41	1.35
22	A	1132	CLA	CHC-C1C	2.41	1.41	1.35
22	9	604	CLA	C1C-C2C	2.41	1.49	1.44
22	B	1215	CLA	CHC-C1C	2.40	1.41	1.35
28	8	805	LMT	O2B-C2B	-2.40	1.37	1.43
22	A	1128	CLA	C3B-C2B	-2.40	1.37	1.40
28	F	5001	LMT	O2B-C2B	-2.40	1.37	1.43
28	B	6101	LMT	O2B-C2B	-2.39	1.37	1.43
22	B	1241	CLA	C3B-C2B	-2.39	1.37	1.40
22	B	1204	CLA	CHC-C1C	2.39	1.41	1.35
28	A	5006	LMT	O3B-C3B	-2.39	1.37	1.43
28	B	6101	LMT	O3B-C3B	-2.38	1.37	1.43
22	B	1206	CLA	CHC-C1C	2.38	1.41	1.35
22	Z	601	CLA	C3B-C2B	-2.38	1.37	1.40
22	2	601	CLA	C3B-C2B	-2.38	1.37	1.40
22	A	1119	CLA	C3B-C2B	-2.38	1.37	1.40
22	L	1502	CLA	C3B-C2B	-2.38	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	F	4001	RRX	C35-C13	2.38	1.55	1.50
22	2	615	CLA	C3B-C2B	-2.37	1.37	1.40
22	8	611	CLA	C3B-C2B	-2.37	1.37	1.40
22	B	1023	CLA	C3B-C2B	-2.37	1.37	1.40
22	4	608	CLA	C3B-C2B	-2.37	1.37	1.40
22	5	604	CLA	C1C-C2C	2.37	1.49	1.44
22	A	1116	CLA	C1C-C2C	2.37	1.49	1.44
22	Z	607	CLA	C3B-C2B	-2.37	1.37	1.40
22	3	612	CLA	C3B-C2B	-2.36	1.37	1.40
28	B	5005	LMT	O2B-C2B	-2.35	1.37	1.43
22	A	1112	CLA	C3B-C2B	-2.35	1.37	1.40
28	8	805	LMT	O2'-C2'	-2.35	1.37	1.43
22	A	1141	CLA	C3B-C2B	-2.35	1.37	1.40
40	2	609	CHL	C3A-C2A	-2.35	1.47	1.54
28	4	803	LMT	O3B-C3B	-2.34	1.37	1.43
22	Z	611	CLA	C3B-C2B	-2.34	1.37	1.40
22	4	607	CLA	C3B-C2B	-2.34	1.37	1.40
37	J	4002	C7Z	C18-C5	2.34	1.54	1.50
22	9	606	CLA	C1C-C2C	2.34	1.49	1.44
35	B	5004	T7X	O18-C11	2.34	1.40	1.33
22	4	612	CLA	C1A-CHA	2.33	1.52	1.43
22	K	1404	CLA	C1A-CHA	2.33	1.52	1.43
22	A	1133	CLA	C3B-C2B	-2.33	1.37	1.40
22	A	1102	CLA	C1C-C2C	2.33	1.49	1.44
22	1	611	CLA	C3B-C2B	-2.33	1.37	1.40
22	8	607	CLA	C3B-C2B	-2.33	1.37	1.40
22	5	615	CLA	C1A-CHA	2.33	1.52	1.43
28	4	803	LMT	O2'-C2'	-2.32	1.37	1.43
28	9	803	LMT	O2B-C2B	-2.32	1.37	1.43
22	1	607	CLA	C1A-CHA	2.32	1.52	1.43
28	1	803	LMT	O3B-C3B	-2.32	1.37	1.43
22	A	1109	CLA	C3B-C2B	-2.32	1.37	1.40
40	5	617	CHL	C3B-C2B	-2.31	1.37	1.40
22	3	618	CLA	C3B-C2B	-2.31	1.37	1.40
22	B	1220	CLA	C3B-C2B	-2.31	1.37	1.40
22	2	603	CLA	C1A-CHA	2.31	1.52	1.43
22	9	605	CLA	C3B-C2B	-2.31	1.37	1.40
43	2	802	3PH	O21-C2	-2.31	1.40	1.46
22	B	1206	CLA	C1A-CHA	2.31	1.52	1.43
22	B	1239	CLA	CHC-C1C	2.31	1.40	1.35
22	3	608	CLA	C3B-C2B	-2.31	1.37	1.40
22	2	607	CLA	C1A-CHA	2.31	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	606	CLA	C3B-C2B	-2.31	1.37	1.40
22	1	613	CLA	C1C-C2C	2.31	1.49	1.44
22	3	607	CLA	C1A-CHA	2.30	1.52	1.43
28	8	805	LMT	O3B-C3B	-2.30	1.37	1.43
45	8	803	LPX	P1-O2	2.30	1.68	1.59
40	2	610	CHL	C3B-C2B	-2.30	1.37	1.40
22	A	1122	CLA	C1A-CHA	2.30	1.52	1.43
22	G	1601	CLA	C1A-CHA	2.30	1.52	1.43
22	K	1402	CLA	C3B-C2B	-2.30	1.37	1.40
22	1	601	CLA	C3B-C2B	-2.30	1.37	1.40
22	B	1203	CLA	C3B-C2B	-2.29	1.37	1.40
22	2	603	CLA	C3B-C2B	-2.28	1.37	1.40
28	F	5001	LMT	O3B-C3B	-2.28	1.37	1.43
22	A	1123	CLA	MG-NC	2.28	2.11	2.06
22	7	615	CLA	C1A-CHA	2.28	1.52	1.43
22	5	601	CLA	C3B-C2B	-2.28	1.37	1.40
22	Z	607	CLA	C1A-CHA	2.28	1.52	1.43
22	B	1022	CLA	C3D-C4D	-2.27	1.39	1.44
22	A	1012	CLA	C1C-C2C	2.27	1.49	1.44
22	B	1220	CLA	C1A-CHA	2.27	1.52	1.43
22	1	612	CLA	C1A-CHA	2.27	1.52	1.43
22	F	1301	CLA	C1A-CHA	2.27	1.52	1.43
22	6	607	CLA	C3B-C2B	-2.27	1.37	1.40
22	3	613	CLA	C3B-C2B	-2.27	1.37	1.40
22	1	601	CLA	C1C-C2C	2.27	1.49	1.44
22	3	616	CLA	C1A-CHA	2.27	1.52	1.43
22	5	601	CLA	C1A-CHA	2.27	1.52	1.43
40	Z	609	CHL	C3A-C2A	-2.27	1.48	1.54
22	B	1204	CLA	C3B-C2B	-2.27	1.37	1.40
22	K	1404	CLA	C3B-C2B	-2.27	1.37	1.40
22	A	1134	CLA	C1A-CHA	2.26	1.52	1.43
22	B	1219	CLA	C3B-C2B	-2.26	1.37	1.40
43	6	802	3PH	O21-C21	2.26	1.40	1.34
22	A	1108	CLA	C1A-CHA	2.26	1.52	1.43
22	8	609	CLA	C1A-CHA	2.26	1.52	1.43
22	B	1230	CLA	C3B-C2B	-2.26	1.37	1.40
40	8	613	CHL	C3B-C2B	-2.26	1.37	1.40
22	4	607	CLA	C1A-CHA	2.26	1.52	1.43
37	1	503	C7Z	C20-C13	2.26	1.55	1.50
22	9	609	CLA	C1C-C2C	2.26	1.48	1.44
22	1	603	CLA	C1A-CHA	2.26	1.52	1.43
22	A	1124	CLA	C3B-C2B	-2.26	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	8	607	CLA	C1A-CHA	2.26	1.52	1.43
22	3	610	CLA	C1A-CHA	2.26	1.52	1.43
22	B	1235	CLA	C3B-C2B	-2.26	1.37	1.40
22	A	1141	CLA	C1A-CHA	2.26	1.52	1.43
22	A	1121	CLA	C3D-C4D	-2.26	1.39	1.44
22	9	607	CLA	C1A-CHA	2.26	1.52	1.43
22	7	606	CLA	C3B-C2B	-2.25	1.37	1.40
28	8	805	LMT	O4'-C4B	-2.25	1.37	1.43
22	8	601	CLA	C1A-CHA	2.25	1.52	1.43
22	5	622	CLA	C1A-CHA	2.25	1.52	1.43
22	5	603	CLA	C1A-CHA	2.25	1.52	1.43
22	5	618	CLA	C3B-C2B	-2.25	1.37	1.40
39	5	501	LUT	C22-C21	-2.25	1.51	1.54
22	5	613	CLA	C1C-C2C	2.25	1.48	1.44
22	B	1224	CLA	C3B-C2B	-2.25	1.37	1.40
28	A	5006	LMT	O1'-C1'	-2.25	1.36	1.40
22	2	608	CLA	C1A-CHA	2.24	1.52	1.43
22	Z	606	CLA	C1A-CHA	2.24	1.52	1.43
22	7	607	CLA	C1A-CHA	2.24	1.52	1.43
22	8	615	CLA	C1A-CHA	2.24	1.52	1.43
22	A	1110	CLA	C1A-CHA	2.24	1.52	1.43
22	A	1106	CLA	C1C-C2C	2.24	1.48	1.44
28	A	5006	LMT	O4'-C4B	-2.24	1.37	1.43
22	7	603	CLA	C1C-C2C	2.24	1.48	1.44
22	6	618	CLA	C1C-C2C	2.24	1.48	1.44
22	K	1402	CLA	C1A-CHA	2.24	1.52	1.43
22	A	1118	CLA	C1C-C2C	2.23	1.48	1.44
43	8	806	3PH	O21-C21	2.23	1.40	1.34
28	9	803	LMT	O2'-C2'	-2.23	1.37	1.43
22	B	1023	CLA	C1A-CHA	2.23	1.52	1.43
22	3	603	CLA	C1A-CHA	2.23	1.52	1.43
22	6	615	CLA	C1A-CHA	2.23	1.52	1.43
22	6	618	CLA	C3B-C2B	-2.23	1.37	1.40
22	Z	603	CLA	C1A-CHA	2.23	1.52	1.43
22	7	607	CLA	C3B-C2B	-2.23	1.37	1.40
22	B	1213	CLA	C1A-CHA	2.23	1.52	1.43
22	Z	608	CLA	C3B-C2B	-2.23	1.37	1.40
22	5	618	CLA	C1A-CHA	2.22	1.52	1.43
22	6	605	CLA	C1A-CHA	2.22	1.52	1.43
22	A	1123	CLA	C1A-CHA	2.22	1.52	1.43
22	Z	612	CLA	C1A-CHA	2.22	1.52	1.43
22	4	615	CLA	C1A-CHA	2.22	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1117	CLA	C1A-CHA	2.22	1.52	1.43
22	4	601	CLA	C1A-CHA	2.22	1.52	1.43
22	1	601	CLA	C1A-CHA	2.22	1.52	1.43
22	Z	605	CLA	C3B-C2B	-2.22	1.37	1.40
22	B	1232	CLA	C1C-C2C	2.22	1.48	1.44
22	A	1139	CLA	C1A-CHA	2.22	1.52	1.43
43	2	802	3PH	O21-C21	2.22	1.40	1.34
22	6	619	CLA	C1A-CHA	2.22	1.52	1.43
22	6	607	CLA	C1A-CHA	2.22	1.52	1.43
22	B	1239	CLA	C1A-CHA	2.21	1.52	1.43
22	7	603	CLA	C1A-CHA	2.21	1.52	1.43
22	1	603	CLA	C1C-C2C	2.21	1.48	1.44
22	L	1502	CLA	C1A-CHA	2.21	1.52	1.43
22	B	1209	CLA	C1A-CHA	2.21	1.52	1.43
22	4	606	CLA	C1C-C2C	2.21	1.48	1.44
22	B	1226	CLA	CHD-C1D	2.21	1.42	1.38
22	A	1136	CLA	C1A-CHA	2.21	1.52	1.43
22	B	1212	CLA	C1A-CHA	2.21	1.52	1.43
22	7	613	CLA	C1C-C2C	2.21	1.48	1.44
22	5	607	CLA	C1A-CHA	2.20	1.52	1.43
22	6	606	CLA	C1A-CHA	2.20	1.52	1.43
37	5	505	C7Z	C18-C5	2.20	1.54	1.50
22	4	602	CLA	C1A-CHA	2.20	1.52	1.43
22	1	611	CLA	C1A-CHA	2.20	1.52	1.43
22	2	606	CLA	C1A-CHA	2.20	1.52	1.43
22	1	612	CLA	C3B-C2B	-2.20	1.37	1.40
22	2	612	CLA	C1C-C2C	2.20	1.48	1.44
22	B	1229	CLA	C1C-C2C	2.20	1.48	1.44
22	Z	601	CLA	C1A-CHA	2.20	1.52	1.43
35	B	5004	T7X	O16-C10	2.20	1.40	1.34
22	7	609	CLA	C1C-C2C	2.20	1.48	1.44
22	4	604	CLA	C1A-CHA	2.20	1.52	1.43
22	B	1212	CLA	C3B-C2B	-2.20	1.37	1.40
22	B	1219	CLA	C1A-CHA	2.20	1.52	1.43
22	K	1402	CLA	C1C-C2C	2.19	1.48	1.44
22	5	601	CLA	C1C-C2C	2.19	1.48	1.44
22	2	615	CLA	C1A-CHA	2.19	1.52	1.43
22	5	608	CLA	C3B-C2B	-2.19	1.37	1.40
22	B	1224	CLA	C1A-CHA	2.19	1.52	1.43
28	9	803	LMT	O4'-C4B	-2.19	1.37	1.43
22	J	1901	CLA	C1C-C2C	2.19	1.48	1.44
22	5	612	CLA	C3B-C2B	-2.19	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	K	1404	CLA	C1C-C2C	2.19	1.48	1.44
22	B	1217	CLA	C1A-CHA	2.19	1.52	1.43
22	B	1240	CLA	C1A-CHA	2.19	1.52	1.43
22	9	603	CLA	C1A-CHA	2.19	1.52	1.43
22	Z	603	CLA	C1C-C2C	2.19	1.48	1.44
28	1	803	LMT	O4'-C4B	-2.19	1.37	1.43
22	K	1403	CLA	C1A-CHA	2.19	1.52	1.43
22	6	608	CLA	C1A-CHA	2.19	1.52	1.43
22	Z	615	CLA	C1A-CHA	2.19	1.52	1.43
35	B	5004	T7X	O18-C9	-2.19	1.40	1.45
28	4	803	LMT	O4'-C4B	-2.19	1.37	1.43
22	B	1232	CLA	C1A-CHA	2.19	1.52	1.43
22	A	1128	CLA	CHC-C1C	2.19	1.40	1.35
22	B	1208	CLA	C1A-CHA	2.19	1.52	1.43
22	9	601	CLA	C1A-CHA	2.19	1.52	1.43
22	A	1138	CLA	C1A-CHA	2.18	1.52	1.43
22	5	602	CLA	C1C-C2C	2.18	1.48	1.44
22	A	1133	CLA	C1A-CHA	2.18	1.52	1.43
22	A	1109	CLA	C1A-CHA	2.18	1.52	1.43
22	A	1106	CLA	C1A-CHA	2.18	1.52	1.43
22	3	610	CLA	CHD-C1D	2.18	1.42	1.38
22	4	603	CLA	C1A-CHA	2.18	1.52	1.43
22	A	1113	CLA	C1A-CHA	2.18	1.52	1.43
22	3	601	CLA	C1A-CHA	2.18	1.52	1.43
22	7	606	CLA	C1C-C2C	2.18	1.48	1.44
22	7	608	CLA	C1A-CHA	2.18	1.52	1.43
22	A	1124	CLA	C1A-CHA	2.18	1.52	1.43
22	5	606	CLA	C1A-CHA	2.18	1.52	1.43
22	3	605	CLA	C1A-CHA	2.18	1.52	1.43
22	B	1230	CLA	C1A-CHA	2.18	1.52	1.43
22	A	1126	CLA	C1A-CHA	2.18	1.52	1.43
22	6	601	CLA	C1A-CHA	2.18	1.52	1.43
22	7	615	CLA	C1C-C2C	2.18	1.48	1.44
37	1	503	C7Z	C10-C9	-2.18	1.32	1.35
22	7	616	CLA	C1C-C2C	2.18	1.48	1.44
22	A	1107	CLA	C1A-CHA	2.18	1.52	1.43
22	B	1205	CLA	C1A-CHA	2.18	1.52	1.43
22	1	605	CLA	C1A-CHA	2.18	1.52	1.43
22	B	1210	CLA	C3D-C4D	-2.18	1.39	1.44
22	A	1132	CLA	C1A-CHA	2.18	1.52	1.43
22	3	608	CLA	C1A-CHA	2.18	1.52	1.43
22	6	612	CLA	C3B-C2B	-2.18	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	1206	CLA	C3B-C2B	-2.17	1.37	1.40
22	9	609	CLA	C1A-CHA	2.17	1.52	1.43
22	8	606	CLA	C1C-C2C	2.17	1.48	1.44
22	L	1503	CLA	C1A-CHA	2.17	1.52	1.43
22	B	1218	CLA	C1A-CHA	2.17	1.52	1.43
22	B	1236	CLA	C1C-C2C	2.17	1.48	1.44
22	8	612	CLA	C1A-CHA	2.17	1.52	1.43
43	5	802	3PH	O21-C21	2.17	1.40	1.34
22	6	604	CLA	C3B-C2B	-2.17	1.37	1.40
22	3	618	CLA	C1A-CHA	2.17	1.52	1.43
22	6	602	CLA	C3B-C2B	-2.17	1.37	1.40
22	B	1214	CLA	C1A-CHA	2.17	1.52	1.43
22	1	605	CLA	C3B-C2B	-2.17	1.37	1.40
22	B	1228	CLA	C1A-CHA	2.16	1.52	1.43
22	1	613	CLA	C3B-C2B	-2.16	1.37	1.40
22	1	613	CLA	C1A-CHA	2.16	1.52	1.43
22	B	1203	CLA	C1A-CHA	2.16	1.52	1.43
22	B	1221	CLA	C1A-CHA	2.16	1.52	1.43
22	A	1125	CLA	C3D-C4D	-2.16	1.39	1.44
22	A	1126	CLA	C1C-C2C	2.16	1.48	1.44
22	4	601	CLA	C3B-C2B	-2.16	1.37	1.40
22	1	602	CLA	C3B-C2B	-2.16	1.37	1.40
22	B	1226	CLA	CHC-C1C	2.16	1.40	1.35
22	A	1124	CLA	C1C-C2C	2.16	1.48	1.44
22	3	603	CLA	C1C-C2C	2.16	1.48	1.44
22	A	1102	CLA	C1A-CHA	2.16	1.52	1.43
28	B	6101	LMT	O4'-C4B	-2.16	1.37	1.43
22	L	1502	CLA	C1C-C2C	2.16	1.48	1.44
22	6	602	CLA	C1A-CHA	2.16	1.52	1.43
22	6	601	CLA	C3B-C2B	-2.16	1.37	1.40
22	4	615	CLA	C1C-C2C	2.16	1.48	1.44
22	B	1241	CLA	C1A-CHA	2.16	1.52	1.43
22	B	1238	CLA	C1A-CHA	2.16	1.52	1.43
22	A	1130	CLA	C1A-CHA	2.16	1.52	1.43
22	4	605	CLA	C1A-CHA	2.16	1.52	1.43
22	1	607	CLA	C3B-C2B	-2.16	1.37	1.40
22	A	1112	CLA	C1C-C2C	2.15	1.48	1.44
40	2	613	CHL	CHC-C1C	2.15	1.40	1.35
22	3	601	CLA	C1C-C2C	2.15	1.48	1.44
22	8	601	CLA	C3B-C2B	-2.15	1.37	1.40
22	4	603	CLA	C1C-C2C	2.15	1.48	1.44
22	A	1129	CLA	C3B-C2B	-2.15	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	1222	CLA	C1A-CHA	2.15	1.52	1.43
40	Z	609	CHL	C3B-C2B	-2.15	1.37	1.40
22	G	1602	CLA	C1A-CHA	2.15	1.52	1.43
22	2	608	CLA	C1C-C2C	2.15	1.48	1.44
22	B	1223	CLA	C1A-CHA	2.15	1.52	1.43
22	A	1127	CLA	C1A-CHA	2.15	1.52	1.43
22	7	601	CLA	C3D-C4D	-2.15	1.39	1.44
22	5	605	CLA	C3D-C4D	-2.15	1.39	1.44
22	3	606	CLA	C1A-CHA	2.15	1.52	1.43
22	5	608	CLA	C1A-CHA	2.15	1.52	1.43
22	7	605	CLA	C1A-CHA	2.15	1.52	1.43
22	1	606	CLA	C1C-C2C	2.15	1.48	1.44
22	6	607	CLA	C1C-C2C	2.15	1.48	1.44
22	Z	602	CLA	C1A-CHA	2.15	1.52	1.43
22	A	1118	CLA	C1A-CHA	2.15	1.52	1.43
22	F	1302	CLA	C1A-CHA	2.15	1.52	1.43
22	1	615	CLA	C1A-CHA	2.15	1.52	1.43
22	A	1119	CLA	C3D-C4D	-2.15	1.39	1.44
22	6	603	CLA	C1A-CHA	2.15	1.52	1.43
22	Z	611	CLA	C1A-CHA	2.14	1.52	1.43
22	A	1129	CLA	C1C-C2C	2.14	1.48	1.44
22	A	1131	CLA	C1A-CHA	2.14	1.52	1.43
22	K	1401	CLA	C1A-CHA	2.14	1.52	1.43
22	7	611	CLA	C1A-CHA	2.14	1.52	1.43
22	8	608	CLA	C1B-NB	2.14	1.37	1.35
22	9	605	CLA	C3D-C4D	-2.14	1.39	1.44
22	9	606	CLA	C3D-C4D	-2.14	1.39	1.44
22	Z	604	CLA	C1C-C2C	2.14	1.48	1.44
22	5	609	CLA	C1A-CHA	2.14	1.52	1.43
22	7	602	CLA	C1A-CHA	2.14	1.52	1.43
22	9	602	CLA	C1A-CHA	2.14	1.52	1.43
22	5	613	CLA	C1A-CHA	2.14	1.52	1.43
22	7	616	CLA	C1A-CHA	2.14	1.52	1.43
22	2	605	CLA	C1A-CHA	2.14	1.52	1.43
22	8	603	CLA	C1C-C2C	2.14	1.48	1.44
37	J	4002	C7Z	C40-C33	2.14	1.55	1.50
22	8	606	CLA	C1A-CHA	2.14	1.52	1.43
22	4	608	CLA	C1A-CHA	2.14	1.52	1.43
22	7	612	CLA	C1A-CHA	2.14	1.52	1.43
22	A	1129	CLA	C1A-CHA	2.13	1.52	1.43
22	A	1103	CLA	C1A-CHA	2.13	1.52	1.43
22	9	605	CLA	C1A-CHA	2.13	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	4	617	CHL	C3B-C2B	-2.13	1.37	1.40
22	F	1302	CLA	C1C-C2C	2.13	1.48	1.44
22	8	605	CLA	C1A-CHA	2.13	1.51	1.43
22	8	611	CLA	C1A-CHA	2.13	1.51	1.43
22	A	1111	CLA	C3D-C4D	-2.13	1.39	1.44
22	A	1140	CLA	C1C-C2C	2.13	1.48	1.44
22	B	1225	CLA	C1A-CHA	2.13	1.51	1.43
22	B	1240	CLA	C1C-C2C	2.13	1.48	1.44
22	3	612	CLA	C1A-CHA	2.13	1.51	1.43
22	A	1125	CLA	C1A-CHA	2.13	1.51	1.43
40	6	617	CHL	C3B-C2B	-2.13	1.37	1.40
22	3	613	CLA	C1A-CHA	2.13	1.51	1.43
22	7	601	CLA	C1A-CHA	2.13	1.51	1.43
22	2	604	CLA	C1A-CHA	2.13	1.51	1.43
22	B	1208	CLA	C1C-C2C	2.13	1.48	1.44
22	5	609	CLA	C1C-C2C	2.13	1.48	1.44
22	6	612	CLA	C1C-C2C	2.13	1.48	1.44
22	Z	601	CLA	C1C-C2C	2.13	1.48	1.44
22	3	608	CLA	C1C-C2C	2.13	1.48	1.44
22	4	604	CLA	C1C-C2C	2.12	1.48	1.44
22	A	1012	CLA	C3D-C4D	-2.12	1.39	1.44
22	8	603	CLA	C1A-CHA	2.12	1.51	1.43
22	6	618	CLA	C1A-CHA	2.12	1.51	1.43
22	A	1110	CLA	C1C-C2C	2.12	1.48	1.44
22	B	1204	CLA	C3D-C4D	-2.12	1.39	1.44
22	1	604	CLA	C1A-CHA	2.12	1.51	1.43
22	6	612	CLA	C1A-CHA	2.12	1.51	1.43
22	6	619	CLA	C1C-C2C	2.12	1.48	1.44
22	Z	605	CLA	C1A-CHA	2.12	1.51	1.43
22	3	602	CLA	C1A-CHA	2.12	1.51	1.43
28	B	5005	LMT	O1'-C1'	-2.12	1.36	1.40
22	A	1137	CLA	C1A-CHA	2.12	1.51	1.43
22	7	613	CLA	C1A-CHA	2.12	1.51	1.43
22	J	1901	CLA	C1A-CHA	2.12	1.51	1.43
22	8	602	CLA	C1A-CHA	2.12	1.51	1.43
22	A	1101	CLA	C3D-C4D	-2.11	1.39	1.44
22	6	605	CLA	C1C-C2C	2.11	1.48	1.44
22	A	1140	CLA	C1A-CHA	2.11	1.51	1.43
22	A	1013	CLA	C1A-CHA	2.11	1.51	1.43
22	A	1120	CLA	C1A-CHA	2.11	1.51	1.43
22	3	618	CLA	C1C-C2C	2.11	1.48	1.44
22	5	607	CLA	C1C-C2C	2.11	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	8	612	CLA	C3B-C2B	-2.11	1.37	1.40
43	2	802	3PH	O31-C3	-2.11	1.40	1.45
22	B	1201	CLA	C1A-CHA	2.11	1.51	1.43
22	B	1201	CLA	C1C-C2C	2.11	1.48	1.44
22	9	608	CLA	C1A-CHA	2.11	1.51	1.43
22	5	608	CLA	C1B-NB	2.11	1.37	1.35
32	9	802	DGA	OG2-CG2	-2.11	1.41	1.46
37	1	503	C7Z	C40-C33	2.11	1.55	1.50
25	B	4001	BCR	C12-C13	-2.11	1.41	1.45
22	Z	607	CLA	C1C-C2C	2.11	1.48	1.44
22	6	609	CLA	C1A-CHA	2.10	1.51	1.43
22	9	612	CLA	C3D-C4D	-2.10	1.39	1.44
22	5	605	CLA	C1C-C2C	2.10	1.48	1.44
22	5	602	CLA	C1A-CHA	2.10	1.51	1.43
28	B	5005	LMT	O4'-C4B	-2.10	1.38	1.43
22	A	1105	CLA	C1A-CHA	2.10	1.51	1.43
22	B	1225	CLA	C3D-C4D	-2.10	1.39	1.44
22	B	1241	CLA	C1C-C2C	2.10	1.48	1.44
22	2	604	CLA	C1C-C2C	2.10	1.48	1.44
22	2	607	CLA	C1B-NB	2.10	1.37	1.35
22	7	609	CLA	C1A-CHA	2.10	1.51	1.43
22	7	606	CLA	C1A-CHA	2.10	1.51	1.43
22	4	606	CLA	C1A-CHA	2.10	1.51	1.43
22	1	602	CLA	MG-NC	2.10	2.11	2.06
22	B	1231	CLA	C3D-C4D	-2.10	1.39	1.44
22	A	1114	CLA	C3D-C4D	-2.10	1.39	1.44
22	8	601	CLA	C1C-C2C	2.10	1.48	1.44
22	8	604	CLA	C1C-C2C	2.10	1.48	1.44
22	9	606	CLA	C1A-CHA	2.10	1.51	1.43
22	A	1115	CLA	C3D-C4D	-2.10	1.39	1.44
22	2	601	CLA	C1A-CHA	2.10	1.51	1.43
22	9	612	CLA	C1C-C2C	2.10	1.48	1.44
22	B	1207	CLA	C1A-CHA	2.10	1.51	1.43
22	Z	608	CLA	C1A-CHA	2.10	1.51	1.43
22	3	616	CLA	C1C-C2C	2.10	1.48	1.44
22	7	611	CLA	C1C-C2C	2.09	1.48	1.44
43	8	806	3PH	O31-C3	-2.09	1.40	1.45
22	4	602	CLA	C1C-C2C	2.09	1.48	1.44
22	Z	604	CLA	C1A-CHA	2.09	1.51	1.43
22	A	1128	CLA	C1A-CHA	2.09	1.51	1.43
22	8	601	CLA	C3D-C4D	-2.09	1.39	1.44
22	4	607	CLA	C1C-C2C	2.09	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	5005	DGA	OG2-CG2	-2.09	1.41	1.46
22	A	1135	CLA	C3D-C4D	-2.09	1.39	1.44
22	2	603	CLA	C1C-C2C	2.09	1.48	1.44
22	B	1223	CLA	C3D-C4D	-2.09	1.39	1.44
22	6	602	CLA	C1C-C2C	2.09	1.48	1.44
22	8	604	CLA	C3B-C2B	-2.09	1.37	1.40
22	2	605	CLA	C1C-C2C	2.09	1.48	1.44
22	1	608	CLA	C1A-CHA	2.09	1.51	1.43
22	9	609	CLA	C1B-NB	2.09	1.37	1.35
22	5	608	CLA	C1C-C2C	2.09	1.48	1.44
22	1	602	CLA	C1A-CHA	2.09	1.51	1.43
22	B	1211	CLA	C3D-C4D	-2.09	1.39	1.44
22	B	1215	CLA	C1A-CHA	2.08	1.51	1.43
22	1	607	CLA	MG-NC	2.08	2.11	2.06
22	2	612	CLA	C1A-CHA	2.08	1.51	1.43
22	Z	606	CLA	C3B-C2B	-2.08	1.37	1.40
22	A	1109	CLA	C3D-C4D	-2.08	1.39	1.44
22	B	1235	CLA	C1C-C2C	2.08	1.48	1.44
22	Z	611	CLA	C1C-C2C	2.08	1.48	1.44
22	A	1139	CLA	C1C-C2C	2.08	1.48	1.44
22	9	612	CLA	C1A-CHA	2.08	1.51	1.43
22	6	606	CLA	C3B-C2B	-2.08	1.37	1.40
22	4	601	CLA	C1C-C2C	2.08	1.48	1.44
22	B	1236	CLA	C3D-C4D	-2.08	1.39	1.44
22	B	1213	CLA	C1C-C2C	2.08	1.48	1.44
22	3	612	CLA	C1C-C2C	2.08	1.48	1.44
22	B	1237	CLA	C1A-CHA	2.08	1.51	1.43
22	A	1112	CLA	C1A-CHA	2.08	1.51	1.43
22	B	1216	CLA	C1A-CHA	2.08	1.51	1.43
22	1	606	CLA	C1A-CHA	2.08	1.51	1.43
30	A	5007	DAO	C2-C1	2.08	1.55	1.50
22	B	1234	CLA	C3D-C4D	-2.08	1.39	1.44
25	5	504	BCR	C12-C13	-2.08	1.41	1.45
22	A	1104	CLA	C1C-C2C	2.08	1.48	1.44
22	3	607	CLA	C1C-C2C	2.08	1.48	1.44
22	B	1219	CLA	C3D-C4D	-2.08	1.39	1.44
22	B	1227	CLA	C1C-C2C	2.07	1.48	1.44
22	7	607	CLA	C1C-C2C	2.07	1.48	1.44
22	3	605	CLA	C3D-C4D	-2.07	1.39	1.44
22	9	604	CLA	C3D-C4D	-2.07	1.39	1.44
22	A	1114	CLA	C1A-CHA	2.07	1.51	1.43
27	3	802	NKP	CAG-CAH	2.07	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1134	CLA	C1C-C2C	2.07	1.48	1.44
22	6	608	CLA	C3D-C4D	-2.07	1.39	1.44
22	A	1013	CLA	C1D-ND	-2.07	1.35	1.37
22	F	1301	CLA	C1C-C2C	2.07	1.48	1.44
22	5	612	CLA	C1A-CHA	2.07	1.51	1.43
22	A	1104	CLA	C1A-CHA	2.07	1.51	1.43
22	A	1135	CLA	C1C-C2C	2.07	1.48	1.44
22	B	1218	CLA	C1C-C2C	2.07	1.48	1.44
27	A	5004	NKP	CAG-CAH	2.07	1.58	1.51
22	7	604	CLA	C3B-C2B	-2.07	1.37	1.40
22	B	1238	CLA	C1C-C2C	2.07	1.48	1.44
22	B	1021	CLA	C3D-C4D	-2.07	1.39	1.44
43	7	802	3PH	O31-C3	-2.07	1.40	1.45
22	Z	604	CLA	C3D-C4D	-2.07	1.39	1.44
22	7	605	CLA	C1C-C2C	2.07	1.48	1.44
22	1	612	CLA	C1C-C2C	2.07	1.48	1.44
22	B	1235	CLA	C1A-CHA	2.07	1.51	1.43
22	4	605	CLA	C1C-C2C	2.07	1.48	1.44
22	B	1221	CLA	C3D-C4D	-2.07	1.39	1.44
22	B	1204	CLA	C1A-CHA	2.07	1.51	1.43
22	B	1202	CLA	C3D-C4D	-2.07	1.39	1.44
22	3	605	CLA	C1C-C2C	2.06	1.48	1.44
22	B	1224	CLA	C3D-C4D	-2.06	1.39	1.44
22	B	1228	CLA	C3B-C2B	-2.06	1.37	1.40
22	1	615	CLA	CHD-C1D	2.06	1.42	1.38
25	B	4003	BCR	C12-C13	-2.06	1.41	1.45
22	B	1221	CLA	MG-NC	2.06	2.11	2.06
22	B	1215	CLA	C3D-C4D	-2.06	1.39	1.44
25	3	504	BCR	C12-C13	-2.06	1.41	1.45
40	9	610	CHL	C3A-C2A	-2.06	1.48	1.54
22	B	1226	CLA	C1A-CHA	2.06	1.51	1.43
22	B	1229	CLA	C1A-CHA	2.06	1.51	1.43
22	B	1227	CLA	C3D-C4D	-2.06	1.39	1.44
22	4	612	CLA	C1C-C2C	2.06	1.48	1.44
22	5	604	CLA	C1A-CHA	2.06	1.51	1.43
22	B	1221	CLA	C1C-C2C	2.06	1.48	1.44
22	3	604	CLA	C1A-CHA	2.06	1.51	1.43
22	A	1135	CLA	MG-NC	2.06	2.11	2.06
22	A	1116	CLA	C1A-CHA	2.06	1.51	1.43
22	3	602	CLA	C1C-C2C	2.06	1.48	1.44
22	B	1214	CLA	C3D-C4D	-2.06	1.39	1.44
22	A	1013	CLA	C1C-C2C	2.06	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	604	CLA	C1A-CHA	2.06	1.51	1.43
22	A	1120	CLA	C1C-C2C	2.06	1.48	1.44
22	2	605	CLA	C3D-C4D	-2.06	1.39	1.44
22	Z	604	CLA	C3B-C2B	-2.05	1.37	1.40
22	J	1901	CLA	C3B-C2B	-2.05	1.37	1.40
22	B	1216	CLA	C3D-C4D	-2.05	1.39	1.44
22	A	1116	CLA	C3D-C4D	-2.05	1.39	1.44
22	4	612	CLA	C3B-C2B	-2.05	1.37	1.40
22	B	1234	CLA	C1C-C2C	2.05	1.48	1.44
22	G	1602	CLA	C1C-C2C	2.05	1.48	1.44
22	6	603	CLA	C1C-C2C	2.05	1.48	1.44
22	Z	605	CLA	C3D-C4D	-2.05	1.39	1.44
22	9	602	CLA	C1C-C2C	2.05	1.48	1.44
22	3	604	CLA	C1B-NB	2.05	1.37	1.35
22	4	607	CLA	MG-NC	2.05	2.11	2.06
22	B	1227	CLA	C1A-CHA	2.05	1.51	1.43
22	4	603	CLA	C3B-C2B	-2.05	1.37	1.40
22	A	1121	CLA	C1C-C2C	2.05	1.48	1.44
22	B	1236	CLA	C1A-CHA	2.05	1.51	1.43
22	8	605	CLA	C3B-C2B	-2.05	1.37	1.40
22	6	615	CLA	C1C-C2C	2.05	1.48	1.44
22	1	611	CLA	C3D-C4D	-2.05	1.39	1.44
22	Z	602	CLA	C1C-C2C	2.05	1.48	1.44
22	A	1138	CLA	C3B-C2B	-2.05	1.37	1.40
28	F	5001	LMT	O4'-C4B	-2.05	1.38	1.43
22	2	604	CLA	C3D-C4D	-2.05	1.39	1.44
22	6	604	CLA	C1C-C2C	2.05	1.48	1.44
22	2	607	CLA	MG-NC	2.04	2.11	2.06
22	8	609	CLA	C1C-C2C	2.04	1.48	1.44
22	4	609	CLA	C1A-CHA	2.04	1.51	1.43
22	B	1201	CLA	C3D-C4D	-2.04	1.39	1.44
22	B	1224	CLA	C1C-C2C	2.04	1.48	1.44
22	B	1234	CLA	C1A-CHA	2.04	1.51	1.43
22	4	608	CLA	C1C-C2C	2.04	1.48	1.44
22	2	601	CLA	C1C-C2C	2.04	1.48	1.44
28	F	5001	LMT	O1'-C1'	-2.04	1.36	1.40
22	A	1126	CLA	C3D-C4D	-2.04	1.39	1.44
22	B	1235	CLA	C3D-C4D	-2.04	1.39	1.44
22	A	1122	CLA	C1C-C2C	2.04	1.48	1.44
22	A	1117	CLA	C3D-C4D	-2.04	1.39	1.44
28	8	805	LMT	O1'-C1'	-2.04	1.36	1.40
22	7	604	CLA	C1C-C2C	2.04	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1136	CLA	C3D-C4D	-2.04	1.39	1.44
22	B	1203	CLA	C3D-C4D	-2.04	1.39	1.44
22	B	1210	CLA	C3B-C2B	-2.04	1.37	1.40
22	B	1217	CLA	C1C-C2C	2.04	1.48	1.44
22	7	601	CLA	C1C-C2C	2.04	1.48	1.44
25	A	4004	BCR	C12-C13	-2.04	1.41	1.45
22	8	604	CLA	C1A-CHA	2.04	1.51	1.43
22	4	606	CLA	C3B-C2B	-2.04	1.37	1.40
22	7	604	CLA	C1A-CHA	2.04	1.51	1.43
22	6	601	CLA	C1C-C2C	2.03	1.48	1.44
22	B	1217	CLA	C3D-C4D	-2.03	1.39	1.44
25	A	4002	BCR	C12-C13	-2.03	1.41	1.45
22	A	1119	CLA	C1C-C2C	2.03	1.48	1.44
22	7	601	CLA	C3B-C2B	-2.03	1.37	1.40
22	A	1111	CLA	C1A-CHA	2.03	1.51	1.43
22	B	1210	CLA	C1A-CHA	2.03	1.51	1.43
22	4	605	CLA	C3D-C4D	-2.03	1.39	1.44
22	A	1116	CLA	MG-NC	2.03	2.11	2.06
22	7	616	CLA	C1B-NB	2.03	1.37	1.35
22	6	619	CLA	C3B-C2B	-2.03	1.37	1.40
22	B	1021	CLA	C1A-CHA	2.03	1.51	1.43
22	6	606	CLA	C1C-C2C	2.03	1.48	1.44
22	7	608	CLA	C3D-C4D	-2.03	1.39	1.44
22	8	615	CLA	C1C-C2C	2.03	1.48	1.44
40	1	609	CHL	CHC-C1C	2.03	1.40	1.35
22	6	608	CLA	C1C-C2C	2.03	1.48	1.44
22	3	601	CLA	C3B-C2B	-2.03	1.37	1.40
43	6	802	3PH	O31-C3	-2.03	1.40	1.45
22	B	1237	CLA	C3D-C4D	-2.03	1.39	1.44
22	A	1104	CLA	C3D-C4D	-2.03	1.39	1.44
22	1	605	CLA	C1C-C2C	2.02	1.48	1.44
22	3	604	CLA	C3D-C4D	-2.02	1.39	1.44
22	A	1101	CLA	C1C-C2C	2.02	1.48	1.44
22	B	1202	CLA	C1A-CHA	2.02	1.51	1.43
22	A	1105	CLA	C1B-NB	2.02	1.37	1.35
22	3	608	CLA	C1B-NB	2.02	1.37	1.35
22	A	1135	CLA	C1A-CHA	2.02	1.51	1.43
22	1	605	CLA	C3D-C4D	-2.02	1.39	1.44
22	9	608	CLA	C1C-C2C	2.02	1.48	1.44
22	6	608	CLA	C1B-NB	2.02	1.37	1.35
22	Z	606	CLA	C1C-C2C	2.02	1.48	1.44
22	8	608	CLA	C1C-C2C	2.02	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	9	612	CLA	C3B-C2B	-2.02	1.37	1.40
22	Z	608	CLA	C3D-C4D	-2.02	1.39	1.44
22	3	606	CLA	C3D-C4D	-2.02	1.39	1.44
22	K	1402	CLA	C1B-NB	2.02	1.37	1.35
22	8	605	CLA	C3D-C4D	-2.02	1.39	1.44
22	1	613	CLA	C3D-C4D	-2.02	1.39	1.44
22	B	1241	CLA	C3D-C4D	-2.02	1.39	1.44
22	5	613	CLA	MG-NC	2.02	2.11	2.06
22	Z	605	CLA	C1C-C2C	2.02	1.48	1.44
22	9	608	CLA	C3D-C4D	-2.02	1.39	1.44
22	A	1115	CLA	C1C-C2C	2.01	1.48	1.44
22	8	605	CLA	C1C-C2C	2.01	1.48	1.44
22	2	602	CLA	C1A-CHA	2.01	1.51	1.43
22	2	601	CLA	C3D-C4D	-2.01	1.39	1.44
22	B	1218	CLA	MG-NC	2.01	2.11	2.06
22	Z	615	CLA	C1B-NB	2.01	1.37	1.35
22	3	612	CLA	C3D-C4D	-2.01	1.39	1.44
22	3	618	CLA	MG-NC	2.01	2.11	2.06
22	1	608	CLA	C3D-C4D	-2.01	1.39	1.44
22	B	1231	CLA	C1A-CHA	2.01	1.51	1.43
22	4	615	CLA	MG-NC	2.01	2.11	2.06
22	1	606	CLA	C3D-C4D	-2.01	1.39	1.44
22	8	611	CLA	C3D-C4D	-2.01	1.39	1.44
22	A	1129	CLA	C3D-C4D	-2.01	1.39	1.44
22	A	1106	CLA	C3D-C4D	-2.01	1.39	1.44
22	B	1208	CLA	C3D-C4D	-2.01	1.39	1.44
22	3	604	CLA	C1C-C2C	2.01	1.48	1.44
22	1	602	CLA	C3D-C4D	-2.01	1.39	1.44
22	Z	615	CLA	C1C-C2C	2.00	1.48	1.44
22	A	1141	CLA	MG-NC	2.00	2.11	2.06
22	3	603	CLA	MG-NC	2.00	2.11	2.06
22	5	622	CLA	MG-NC	2.00	2.11	2.06
22	Z	608	CLA	C1C-C2C	2.00	1.48	1.44
22	B	1213	CLA	C3B-C2B	-2.00	1.37	1.40
22	2	606	CLA	MG-NC	2.00	2.11	2.06
22	B	1222	CLA	C1C-C2C	2.00	1.48	1.44
42	Z	504	QTB	C03-C02	-2.00	1.33	1.35
22	1	604	CLA	C3D-C4D	-2.00	1.39	1.44
22	5	605	CLA	C1A-CHA	2.00	1.51	1.43
22	8	612	CLA	C3D-C4D	-2.00	1.39	1.44
22	5	615	CLA	C1C-C2C	2.00	1.48	1.44
22	3	607	CLA	MG-NC	2.00	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	609	CLA	C3D-C4D	-2.00	1.39	1.44

All (4938) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6	504	BCR	C10-C11-C12	18.05	179.54	123.22
25	5	504	BCR	C10-C11-C12	17.86	178.96	123.22
25	7	504	BCR	C10-C11-C12	17.63	178.24	123.22
25	3	504	BCR	C10-C11-C12	17.62	178.19	123.22
25	A	4002	BCR	C10-C11-C12	17.57	178.04	123.22
25	3	505	BCR	C10-C11-C12	17.56	178.03	123.22
25	6	503	BCR	C10-C11-C12	17.55	177.97	123.22
25	5	504	BCR	C16-C15-C14	17.53	159.38	123.47
25	5	503	BCR	C10-C11-C12	17.44	177.64	123.22
25	3	503	BCR	C10-C11-C12	17.43	177.61	123.22
25	K	4001	BCR	C10-C11-C12	17.31	177.24	123.22
25	4	503	BCR	C10-C11-C12	17.30	177.20	123.22
25	7	503	BCR	C10-C11-C12	17.29	177.16	123.22
25	8	503	BCR	C10-C11-C12	17.28	177.14	123.22
25	G	4001	BCR	C10-C11-C12	17.19	176.85	123.22
25	I	4001	BCR	C10-C11-C12	17.17	176.80	123.22
25	B	4007	BCR	C10-C11-C12	17.15	176.72	123.22
25	3	506	BCR	C10-C11-C12	17.14	176.69	123.22
25	B	4001	BCR	C10-C11-C12	17.13	176.69	123.22
25	B	4004	BCR	C10-C11-C12	17.09	176.55	123.22
25	K	4002	BCR	C10-C11-C12	17.07	176.47	123.22
25	B	4002	BCR	C10-C11-C12	17.05	176.43	123.22
25	A	4003	BCR	C10-C11-C12	17.00	176.27	123.22
25	L	4001	BCR	C10-C11-C12	17.00	176.27	123.22
25	B	4005	BCR	C10-C11-C12	16.77	175.54	123.22
25	L	4002	BCR	C10-C11-C12	16.76	175.53	123.22
25	J	4001	BCR	C10-C11-C12	16.72	175.40	123.22
25	A	4004	BCR	C10-C11-C12	16.63	175.11	123.22
25	A	4001	BCR	C10-C11-C12	16.62	175.08	123.22
25	B	4006	BCR	C10-C11-C12	16.57	174.94	123.22
25	B	4003	BCR	C10-C11-C12	16.54	174.84	123.22
25	A	4005	BCR	C10-C11-C12	16.10	173.45	123.22
25	7	504	BCR	C16-C15-C14	14.70	153.58	123.47
25	A	4005	BCR	C11-C10-C9	14.09	147.42	127.31
25	J	4001	BCR	C11-C10-C9	13.93	147.20	127.31
25	B	4003	BCR	C11-C10-C9	13.83	147.05	127.31
25	3	506	BCR	C11-C10-C9	13.83	147.05	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	4005	BCR	C11-C10-C9	13.71	146.88	127.31
25	6	503	BCR	C16-C15-C14	13.59	151.32	123.47
25	I	4001	BCR	C11-C10-C9	13.59	146.70	127.31
25	B	4002	BCR	C11-C10-C9	13.57	146.68	127.31
25	7	504	BCR	C11-C10-C9	13.51	146.59	127.31
25	3	505	BCR	C11-C10-C9	13.38	146.40	127.31
25	B	4005	BCR	C21-C20-C19	13.37	164.93	123.22
25	8	503	BCR	C11-C10-C9	13.34	146.35	127.31
25	G	4001	BCR	C21-C20-C19	13.33	164.83	123.22
25	7	503	BCR	C11-C10-C9	13.26	146.24	127.31
25	6	504	BCR	C11-C12-C13	13.25	163.62	126.42
25	B	4004	BCR	C11-C10-C9	13.24	146.21	127.31
25	A	4004	BCR	C11-C10-C9	13.22	146.18	127.31
25	L	4001	BCR	C11-C10-C9	13.19	146.14	127.31
25	3	506	BCR	C16-C15-C14	13.19	150.50	123.47
25	7	503	BCR	C16-C15-C14	13.11	150.33	123.47
25	K	4001	BCR	C11-C10-C9	13.04	145.93	127.31
25	5	503	BCR	C11-C10-C9	12.98	145.83	127.31
25	K	4001	BCR	C21-C20-C19	12.91	163.50	123.22
25	A	4003	BCR	C21-C20-C19	12.87	163.37	123.22
25	3	505	BCR	C16-C15-C14	12.87	149.83	123.47
25	8	503	BCR	C16-C15-C14	12.74	149.57	123.47
25	K	4002	BCR	C11-C10-C9	12.74	145.49	127.31
25	6	503	BCR	C11-C10-C9	12.74	145.49	127.31
25	A	4001	BCR	C11-C10-C9	12.73	145.47	127.31
25	B	4007	BCR	C11-C10-C9	12.73	145.47	127.31
25	B	4006	BCR	C21-C20-C19	12.69	162.82	123.22
25	L	4002	BCR	C11-C10-C9	12.68	145.41	127.31
25	6	504	BCR	C16-C15-C14	12.68	149.44	123.47
25	A	4003	BCR	C11-C10-C9	12.67	145.40	127.31
25	3	504	BCR	C11-C10-C9	12.65	145.37	127.31
25	4	503	BCR	C11-C10-C9	12.60	145.29	127.31
25	G	4001	BCR	C11-C10-C9	12.58	145.26	127.31
25	K	4001	BCR	C16-C15-C14	12.52	149.13	123.47
25	B	4006	BCR	C11-C10-C9	12.50	145.16	127.31
25	K	4002	BCR	C21-C20-C19	12.48	162.18	123.22
25	3	504	BCR	C21-C20-C19	12.47	162.12	123.22
25	7	504	BCR	C21-C20-C19	12.46	162.10	123.22
25	A	4005	BCR	C11-C12-C13	12.44	161.38	126.42
25	7	503	BCR	C21-C20-C19	12.39	161.87	123.22
25	B	4001	BCR	C21-C20-C19	12.37	161.81	123.22
25	3	506	BCR	C21-C20-C19	12.36	161.79	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	4004	BCR	C21-C20-C19	12.20	161.29	123.22
25	3	505	BCR	C21-C20-C19	12.17	161.20	123.22
25	B	4001	BCR	C11-C10-C9	12.12	144.60	127.31
25	J	4001	BCR	C21-C20-C19	12.10	160.98	123.22
25	A	4002	BCR	C11-C10-C9	12.01	144.45	127.31
25	L	4002	BCR	C21-C20-C19	11.90	160.36	123.22
25	3	503	BCR	C16-C15-C14	11.77	147.58	123.47
25	5	503	BCR	C21-C20-C19	11.75	159.87	123.22
25	B	4007	BCR	C16-C15-C14	11.73	147.50	123.47
25	A	4004	BCR	C11-C12-C13	11.73	159.37	126.42
25	B	4003	BCR	C11-C12-C13	11.72	159.35	126.42
25	I	4001	BCR	C16-C15-C14	11.70	147.44	123.47
25	A	4001	BCR	C21-C20-C19	11.67	159.64	123.22
25	5	503	BCR	C16-C15-C14	11.65	147.34	123.47
25	L	4001	BCR	C21-C20-C19	11.65	159.57	123.22
25	L	4001	BCR	C16-C15-C14	11.63	147.29	123.47
25	B	4004	BCR	C16-C15-C14	11.62	147.29	123.47
25	A	4003	BCR	C11-C12-C13	11.47	158.63	126.42
25	A	4002	BCR	C16-C15-C14	11.46	146.96	123.47
25	L	4002	BCR	C11-C12-C13	11.45	158.59	126.42
25	B	4002	BCR	C16-C15-C14	11.45	146.93	123.47
39	2	501	LUT	C21-C26-C27	11.44	127.16	112.70
25	3	503	BCR	C11-C12-C13	11.23	157.97	126.42
25	G	4001	BCR	C11-C12-C13	11.23	157.96	126.42
25	B	4001	BCR	C11-C12-C13	11.18	157.81	126.42
25	3	503	BCR	C11-C10-C9	11.15	143.22	127.31
25	L	4001	BCR	C11-C12-C13	11.14	157.70	126.42
25	L	4002	BCR	C16-C15-C14	11.13	146.27	123.47
25	K	4002	BCR	C11-C12-C13	11.13	157.67	126.42
25	A	4001	BCR	C11-C12-C13	11.12	157.66	126.42
25	A	4002	BCR	C21-C20-C19	11.12	157.91	123.22
25	B	4004	BCR	C11-C12-C13	11.11	157.62	126.42
25	6	504	BCR	C11-C10-C9	11.09	143.13	127.31
25	A	4003	BCR	C16-C15-C14	11.08	146.16	123.47
25	4	503	BCR	C16-C15-C14	11.08	146.16	123.47
25	3	504	BCR	C16-C15-C14	11.06	146.13	123.47
25	A	4004	BCR	C16-C15-C14	11.04	146.08	123.47
25	B	4003	BCR	C21-C20-C19	10.99	157.51	123.22
25	4	503	BCR	C21-C20-C19	10.98	157.47	123.22
25	K	4002	BCR	C16-C15-C14	10.89	145.78	123.47
25	B	4005	BCR	C11-C12-C13	10.85	156.90	126.42
25	B	4007	BCR	C11-C12-C13	10.83	156.84	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	K	4001	BCR	C11-C12-C13	10.81	156.78	126.42
25	B	4004	BCR	C21-C20-C19	10.81	156.94	123.22
25	B	4006	BCR	C11-C12-C13	10.79	156.73	126.42
25	B	4002	BCR	C11-C12-C13	10.68	156.42	126.42
25	B	4005	BCR	C16-C15-C14	10.66	145.31	123.47
25	3	504	BCR	C11-C12-C13	10.66	156.36	126.42
25	8	503	BCR	C21-C20-C19	10.65	156.45	123.22
25	B	4002	BCR	C21-C20-C19	10.62	156.35	123.22
25	6	503	BCR	C21-C20-C19	10.60	156.30	123.22
25	J	4001	BCR	C11-C12-C13	10.60	156.18	126.42
25	4	503	BCR	C11-C12-C13	10.58	156.14	126.42
25	A	4005	BCR	C21-C20-C19	10.55	156.13	123.22
25	A	4005	BCR	C16-C15-C14	10.51	145.00	123.47
25	A	4002	BCR	C11-C12-C13	10.47	155.84	126.42
25	I	4001	BCR	C11-C12-C13	10.43	155.72	126.42
25	J	4001	BCR	C16-C15-C14	10.42	144.82	123.47
25	3	503	BCR	C21-C20-C19	10.37	155.57	123.22
25	B	4003	BCR	C16-C15-C14	10.32	144.62	123.47
25	B	4007	BCR	C21-C20-C19	10.26	155.25	123.22
25	3	505	BCR	C11-C12-C13	10.23	155.16	126.42
25	A	4001	BCR	C16-C15-C14	10.17	144.32	123.47
25	8	503	BCR	C11-C12-C13	10.17	155.00	126.42
25	B	4001	BCR	C16-C15-C14	10.12	144.20	123.47
22	B	1211	CLA	C4A-NA-C1A	10.10	111.25	106.71
22	2	603	CLA	C4A-NA-C1A	10.09	111.24	106.71
22	B	1206	CLA	C4A-NA-C1A	10.08	111.24	106.71
25	3	506	BCR	C11-C12-C13	10.06	154.68	126.42
25	G	4001	BCR	C16-C15-C14	10.01	143.98	123.47
22	A	1103	CLA	C4A-NA-C1A	9.99	111.20	106.71
22	B	1214	CLA	C4A-NA-C1A	9.97	111.19	106.71
22	4	612	CLA	C4A-NA-C1A	9.94	111.17	106.71
25	7	504	BCR	C11-C12-C13	9.92	154.28	126.42
25	5	504	BCR	C21-C20-C19	9.91	154.15	123.22
22	5	603	CLA	C4A-NA-C1A	9.89	111.15	106.71
22	K	1404	CLA	C4A-NA-C1A	9.89	111.15	106.71
25	I	4001	BCR	C21-C20-C19	9.87	154.03	123.22
22	B	1218	CLA	C4A-NA-C1A	9.87	111.14	106.71
22	B	1023	CLA	C4A-NA-C1A	9.87	111.14	106.71
22	L	1502	CLA	C4A-NA-C1A	9.83	111.13	106.71
25	6	504	BCR	C21-C20-C19	9.77	153.70	123.22
25	B	4006	BCR	C16-C15-C14	9.76	143.47	123.47
25	5	503	BCR	C11-C12-C13	9.75	153.80	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1219	CLA	C4A-NA-C1A	9.73	111.08	106.71
22	1	603	CLA	C4A-NA-C1A	9.72	111.08	106.71
22	B	1205	CLA	C4A-NA-C1A	9.69	111.06	106.71
22	7	611	CLA	C4A-NA-C1A	9.68	111.06	106.71
22	5	615	CLA	C4A-NA-C1A	9.67	111.05	106.71
25	7	503	BCR	C11-C12-C13	9.66	153.56	126.42
22	B	1241	CLA	C4A-NA-C1A	9.65	111.05	106.71
22	A	1141	CLA	C4A-NA-C1A	9.65	111.04	106.71
22	3	603	CLA	C4A-NA-C1A	9.56	111.00	106.71
22	8	603	CLA	C4A-NA-C1A	9.54	111.00	106.71
22	8	615	CLA	C4A-NA-C1A	9.54	110.99	106.71
22	A	1118	CLA	C4A-NA-C1A	9.52	110.99	106.71
22	7	609	CLA	C4A-NA-C1A	9.50	110.97	106.71
22	4	603	CLA	C4A-NA-C1A	9.49	110.97	106.71
22	3	606	CLA	C4A-NA-C1A	9.48	110.97	106.71
22	B	1230	CLA	C4A-NA-C1A	9.47	110.97	106.71
22	A	1123	CLA	C4A-NA-C1A	9.45	110.95	106.71
22	B	1212	CLA	C4A-NA-C1A	9.44	110.95	106.71
22	Z	603	CLA	C4A-NA-C1A	9.44	110.95	106.71
22	2	615	CLA	C4A-NA-C1A	9.42	110.94	106.71
22	B	1221	CLA	C4A-NA-C1A	9.42	110.94	106.71
22	F	1301	CLA	C4A-NA-C1A	9.41	110.94	106.71
22	B	1213	CLA	C4A-NA-C1A	9.41	110.94	106.71
22	5	618	CLA	C4A-NA-C1A	9.40	110.93	106.71
22	A	1108	CLA	C4A-NA-C1A	9.40	110.93	106.71
22	A	1138	CLA	C4A-NA-C1A	9.39	110.93	106.71
22	3	616	CLA	C4A-NA-C1A	9.38	110.92	106.71
22	B	1238	CLA	C4A-NA-C1A	9.34	110.91	106.71
22	B	1217	CLA	C4A-NA-C1A	9.34	110.91	106.71
39	2	503	LUT	C21-C26-C27	9.28	124.44	112.70
22	8	611	CLA	C4A-NA-C1A	9.28	110.88	106.71
22	A	1139	CLA	C4A-NA-C1A	9.28	110.88	106.71
22	A	1136	CLA	C4A-NA-C1A	9.27	110.88	106.71
22	A	1134	CLA	C4A-NA-C1A	9.27	110.87	106.71
22	B	1239	CLA	C4A-NA-C1A	9.26	110.87	106.71
22	A	1109	CLA	C4A-NA-C1A	9.26	110.87	106.71
22	9	601	CLA	C4A-NA-C1A	9.26	110.87	106.71
25	B	4005	BCR	C20-C19-C18	9.25	152.41	126.42
22	B	1208	CLA	C4A-NA-C1A	9.25	110.87	106.71
22	1	612	CLA	C4A-NA-C1A	9.25	110.86	106.71
22	6	603	CLA	C4A-NA-C1A	9.24	110.86	106.71
22	B	1237	CLA	C4A-NA-C1A	9.23	110.86	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	6	618	CLA	C4A-NA-C1A	9.23	110.86	106.71
22	7	616	CLA	C4A-NA-C1A	9.23	110.85	106.71
22	A	1120	CLA	C4A-NA-C1A	9.22	110.85	106.71
22	6	615	CLA	C4A-NA-C1A	9.22	110.85	106.71
22	L	1503	CLA	C4A-NA-C1A	9.21	110.85	106.71
22	9	603	CLA	C4A-NA-C1A	9.21	110.85	106.71
22	A	1126	CLA	C4A-NA-C1A	9.21	110.84	106.71
22	4	601	CLA	C4A-NA-C1A	9.21	110.84	106.71
25	5	504	BCR	C11-C12-C13	9.19	152.24	126.42
22	8	612	CLA	C4A-NA-C1A	9.18	110.83	106.71
22	3	607	CLA	C4A-NA-C1A	9.17	110.83	106.71
22	2	608	CLA	C4A-NA-C1A	9.16	110.82	106.71
22	4	607	CLA	C4A-NA-C1A	9.16	110.82	106.71
22	B	1220	CLA	C4A-NA-C1A	9.15	110.82	106.71
25	6	503	BCR	C11-C12-C13	9.15	152.12	126.42
22	8	607	CLA	C4A-NA-C1A	9.14	110.82	106.71
22	1	607	CLA	C4A-NA-C1A	9.14	110.81	106.71
22	5	606	CLA	C4A-NA-C1A	9.14	110.81	106.71
22	6	606	CLA	C4A-NA-C1A	9.14	110.81	106.71
22	7	606	CLA	C4A-NA-C1A	9.14	110.81	106.71
22	3	612	CLA	C4A-NA-C1A	9.11	110.80	106.71
22	3	613	CLA	C4A-NA-C1A	9.10	110.80	106.71
22	A	1133	CLA	C4A-NA-C1A	9.09	110.79	106.71
22	3	608	CLA	C4A-NA-C1A	9.08	110.79	106.71
22	6	612	CLA	C4A-NA-C1A	9.08	110.79	106.71
22	5	601	CLA	C4A-NA-C1A	9.07	110.78	106.71
22	3	604	CLA	C4A-NA-C1A	9.06	110.78	106.71
22	B	1228	CLA	C4A-NA-C1A	9.06	110.78	106.71
22	7	607	CLA	C4A-NA-C1A	9.06	110.78	106.71
22	B	1202	CLA	C4A-NA-C1A	9.06	110.78	106.71
22	5	608	CLA	C4A-NA-C1A	9.05	110.78	106.71
22	A	1125	CLA	C4A-NA-C1A	9.05	110.78	106.71
22	Z	612	CLA	C4A-NA-C1A	9.04	110.77	106.71
22	Z	615	CLA	C4A-NA-C1A	9.04	110.77	106.71
22	3	618	CLA	C4A-NA-C1A	9.03	110.77	106.71
22	6	608	CLA	C4A-NA-C1A	9.03	110.77	106.71
22	1	608	CLA	C4A-NA-C1A	9.02	110.76	106.71
22	2	606	CLA	C4A-NA-C1A	9.02	110.76	106.71
22	1	611	CLA	C4A-NA-C1A	9.02	110.76	106.71
22	A	1131	CLA	C4A-NA-C1A	9.01	110.76	106.71
22	7	603	CLA	C4A-NA-C1A	9.01	110.76	106.71
22	Z	601	CLA	C4A-NA-C1A	9.00	110.75	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	8	606	CLA	C4A-NA-C1A	9.00	110.75	106.71
22	5	622	CLA	C4A-NA-C1A	8.99	110.75	106.71
22	8	601	CLA	C4A-NA-C1A	8.99	110.75	106.71
22	1	606	CLA	C4A-NA-C1A	8.98	110.74	106.71
22	Z	606	CLA	C4A-NA-C1A	8.98	110.74	106.71
22	G	1601	CLA	C4A-NA-C1A	8.98	110.74	106.71
22	4	608	CLA	C4A-NA-C1A	8.97	110.74	106.71
22	2	607	CLA	C4A-NA-C1A	8.97	110.74	106.71
22	B	1201	CLA	C4A-NA-C1A	8.97	110.74	106.71
22	3	601	CLA	C4A-NA-C1A	8.97	110.74	106.71
22	K	1402	CLA	C4A-NA-C1A	8.96	110.73	106.71
22	Z	607	CLA	C4A-NA-C1A	8.95	110.73	106.71
22	Z	602	CLA	C4A-NA-C1A	8.94	110.73	106.71
22	1	601	CLA	C4A-NA-C1A	8.94	110.72	106.71
22	A	1127	CLA	C4A-NA-C1A	8.93	110.72	106.71
22	7	608	CLA	C4A-NA-C1A	8.92	110.72	106.71
22	8	609	CLA	C4A-NA-C1A	8.92	110.72	106.71
22	A	1110	CLA	C4A-NA-C1A	8.92	110.72	106.71
22	B	1224	CLA	C4A-NA-C1A	8.92	110.72	106.71
22	B	1215	CLA	C4A-NA-C1A	8.91	110.71	106.71
22	6	602	CLA	C4A-NA-C1A	8.91	110.71	106.71
22	7	604	CLA	C4A-NA-C1A	8.91	110.71	106.71
25	4	503	BCR	C20-C19-C18	8.91	151.44	126.42
22	B	1222	CLA	C4A-NA-C1A	8.91	110.71	106.71
22	B	1021	CLA	C4A-NA-C1A	8.90	110.71	106.71
22	9	612	CLA	C4A-NA-C1A	8.89	110.70	106.71
22	4	605	CLA	C4A-NA-C1A	8.89	110.70	106.71
25	3	503	BCR	C20-C19-C18	8.89	151.38	126.42
22	2	604	CLA	C4A-NA-C1A	8.88	110.70	106.71
22	A	1113	CLA	C4A-NA-C1A	8.88	110.70	106.71
22	A	1122	CLA	C4A-NA-C1A	8.86	110.69	106.71
25	I	4001	BCR	C20-C19-C18	8.86	151.31	126.42
22	2	612	CLA	C4A-NA-C1A	8.83	110.68	106.71
22	4	609	CLA	C4A-NA-C1A	8.83	110.67	106.71
22	B	1210	CLA	C4A-NA-C1A	8.81	110.67	106.71
22	9	607	CLA	C4A-NA-C1A	8.80	110.66	106.71
22	1	605	CLA	C4A-NA-C1A	8.79	110.66	106.71
22	A	1124	CLA	C4A-NA-C1A	8.77	110.65	106.71
22	6	607	CLA	C4A-NA-C1A	8.77	110.65	106.71
22	7	612	CLA	C4A-NA-C1A	8.77	110.65	106.71
22	4	615	CLA	C4A-NA-C1A	8.76	110.65	106.71
22	8	604	CLA	C4A-NA-C1A	8.76	110.64	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1204	CLA	C4A-NA-C1A	8.76	110.64	106.71
22	2	601	CLA	C4A-NA-C1A	8.76	110.64	106.71
22	A	1132	CLA	C4A-NA-C1A	8.75	110.64	106.71
25	A	4005	BCR	C20-C19-C18	8.75	150.99	126.42
22	A	1111	CLA	C4A-NA-C1A	8.74	110.64	106.71
22	A	1137	CLA	C4A-NA-C1A	8.74	110.64	106.71
22	4	602	CLA	C4A-NA-C1A	8.74	110.63	106.71
22	A	1107	CLA	C4A-NA-C1A	8.73	110.63	106.71
22	9	609	CLA	C4A-NA-C1A	8.73	110.63	106.71
22	2	602	CLA	C4A-NA-C1A	8.71	110.62	106.71
25	B	4002	BCR	C20-C19-C18	8.71	150.89	126.42
22	4	604	CLA	C4A-NA-C1A	8.71	110.62	106.71
22	7	615	CLA	C4A-NA-C1A	8.70	110.62	106.71
22	6	604	CLA	C4A-NA-C1A	8.68	110.61	106.71
22	Z	605	CLA	C4A-NA-C1A	8.68	110.61	106.71
25	B	4004	BCR	C20-C19-C18	8.68	150.79	126.42
25	6	503	BCR	C20-C19-C18	8.67	150.78	126.42
22	B	1223	CLA	C4A-NA-C1A	8.67	110.60	106.71
22	1	604	CLA	C4A-NA-C1A	8.66	110.60	106.71
22	K	1403	CLA	C4A-NA-C1A	8.65	110.60	106.71
25	3	506	BCR	C20-C19-C18	8.65	150.73	126.42
22	5	607	CLA	C4A-NA-C1A	8.64	110.59	106.71
22	B	1203	CLA	C4A-NA-C1A	8.64	110.59	106.71
22	A	1112	CLA	C4A-NA-C1A	8.62	110.58	106.71
22	B	1216	CLA	C4A-NA-C1A	8.62	110.58	106.71
22	7	601	CLA	C4A-NA-C1A	8.62	110.58	106.71
22	4	606	CLA	C4A-NA-C1A	8.61	110.58	106.71
22	Z	604	CLA	C4A-NA-C1A	8.60	110.57	106.71
22	5	612	CLA	C4A-NA-C1A	8.60	110.57	106.71
22	9	608	CLA	C4A-NA-C1A	8.59	110.57	106.71
22	6	619	CLA	C4A-NA-C1A	8.59	110.57	106.71
22	Z	611	CLA	C4A-NA-C1A	8.58	110.56	106.71
22	6	601	CLA	C4A-NA-C1A	8.58	110.56	106.71
22	B	1235	CLA	C4A-NA-C1A	8.56	110.56	106.71
22	7	602	CLA	C4A-NA-C1A	8.56	110.56	106.71
22	A	1106	CLA	C4A-NA-C1A	8.53	110.54	106.71
22	B	1240	CLA	C4A-NA-C1A	8.53	110.54	106.71
22	5	609	CLA	C4A-NA-C1A	8.51	110.53	106.71
25	8	503	BCR	C20-C19-C18	8.51	150.31	126.42
22	A	1012	CLA	C4A-NA-C1A	8.51	110.53	106.71
22	9	602	CLA	C4A-NA-C1A	8.50	110.53	106.71
22	B	1236	CLA	C4A-NA-C1A	8.49	110.53	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1102	CLA	C4A-NA-C1A	8.49	110.52	106.71
22	3	610	CLA	C4A-NA-C1A	8.48	110.52	106.71
22	B	1225	CLA	C4A-NA-C1A	8.48	110.52	106.71
22	8	608	CLA	C4A-NA-C1A	8.47	110.51	106.71
22	A	1117	CLA	C4A-NA-C1A	8.46	110.51	106.71
22	7	605	CLA	C4A-NA-C1A	8.45	110.51	106.71
22	Z	608	CLA	C4A-NA-C1A	8.45	110.50	106.71
22	B	1234	CLA	C4A-NA-C1A	8.44	110.50	106.71
22	A	1013	CLA	C4A-NA-C1A	8.43	110.50	106.71
22	A	1104	CLA	C4A-NA-C1A	8.42	110.49	106.71
22	A	1121	CLA	C4A-NA-C1A	8.41	110.49	106.71
22	G	1602	CLA	C4A-NA-C1A	8.41	110.49	106.71
22	B	1207	CLA	C4A-NA-C1A	8.39	110.48	106.71
22	8	602	CLA	C4A-NA-C1A	8.38	110.47	106.71
22	J	1901	CLA	C4A-NA-C1A	8.38	110.47	106.71
22	B	1229	CLA	C4A-NA-C1A	8.38	110.47	106.71
22	6	609	CLA	C4A-NA-C1A	8.37	110.47	106.71
22	5	604	CLA	C4A-NA-C1A	8.36	110.47	106.71
22	1	613	CLA	C4A-NA-C1A	8.35	110.46	106.71
22	A	1105	CLA	C4A-NA-C1A	8.34	110.46	106.71
22	9	605	CLA	C4A-NA-C1A	8.34	110.46	106.71
22	3	602	CLA	C4A-NA-C1A	8.34	110.45	106.71
22	5	613	CLA	C4A-NA-C1A	8.33	110.45	106.71
22	8	605	CLA	C4A-NA-C1A	8.32	110.45	106.71
25	B	4007	BCR	C20-C19-C18	8.32	149.78	126.42
22	1	602	CLA	C4A-NA-C1A	8.31	110.44	106.71
22	B	1232	CLA	C4A-NA-C1A	8.30	110.44	106.71
22	K	1401	CLA	C4A-NA-C1A	8.29	110.43	106.71
22	A	1140	CLA	C4A-NA-C1A	8.28	110.43	106.71
22	1	615	CLA	C4A-NA-C1A	8.27	110.42	106.71
22	A	1128	CLA	C4A-NA-C1A	8.25	110.42	106.71
22	6	605	CLA	C4A-NA-C1A	8.25	110.41	106.71
22	A	1101	CLA	C4A-NA-C1A	8.23	110.41	106.71
22	A	1129	CLA	C4A-NA-C1A	8.23	110.40	106.71
22	F	1302	CLA	C4A-NA-C1A	8.22	110.40	106.71
25	B	4003	BCR	C20-C19-C18	8.20	149.46	126.42
22	B	1209	CLA	C4A-NA-C1A	8.20	110.39	106.71
22	A	1115	CLA	C4A-NA-C1A	8.16	110.38	106.71
22	2	605	CLA	C4A-NA-C1A	8.13	110.36	106.71
22	A	1114	CLA	C4A-NA-C1A	8.11	110.35	106.71
22	7	613	CLA	C4A-NA-C1A	8.11	110.35	106.71
25	5	504	BCR	C11-C10-C9	8.10	138.87	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	4002	BCR	C20-C19-C18	8.10	149.16	126.42
22	A	1130	CLA	C4A-NA-C1A	8.09	110.34	106.71
22	B	1231	CLA	C4A-NA-C1A	8.08	110.34	106.71
22	5	602	CLA	C4A-NA-C1A	8.07	110.33	106.71
22	B	1227	CLA	C4A-NA-C1A	8.06	110.33	106.71
22	5	605	CLA	C4A-NA-C1A	7.99	110.30	106.71
22	3	605	CLA	C4A-NA-C1A	7.92	110.27	106.71
22	B	1226	CLA	C4A-NA-C1A	7.92	110.27	106.71
22	A	1119	CLA	C4A-NA-C1A	7.91	110.26	106.71
25	L	4002	BCR	C20-C19-C18	7.89	148.59	126.42
25	5	504	BCR	C15-C14-C13	-7.85	116.11	127.31
22	9	606	CLA	C4A-NA-C1A	7.80	110.21	106.71
25	L	4001	BCR	C20-C19-C18	7.77	148.25	126.42
22	A	1135	CLA	C4A-NA-C1A	7.72	110.17	106.71
22	B	1022	CLA	C4A-NA-C1A	7.62	110.13	106.71
25	A	4001	BCR	C20-C19-C18	7.57	147.67	126.42
25	3	505	BCR	C20-C19-C18	7.54	147.60	126.42
25	J	4001	BCR	C20-C19-C18	7.53	147.57	126.42
25	5	503	BCR	C20-C19-C18	7.50	147.50	126.42
22	A	1116	CLA	C4A-NA-C1A	7.50	110.08	106.71
25	7	504	BCR	C20-C19-C18	7.46	147.36	126.42
21	A	1011	CL0	C4A-NA-C1A	7.46	110.06	106.71
22	9	604	CLA	C4A-NA-C1A	7.37	110.02	106.71
25	A	4004	BCR	C20-C19-C18	7.29	146.89	126.42
25	K	4002	BCR	C20-C19-C18	7.24	146.75	126.42
21	A	1011	CL0	CMD-C2D-C1D	7.01	137.07	124.71
22	8	603	CLA	O2A-C1-C2	7.00	127.03	108.64
25	7	503	BCR	C20-C19-C18	6.99	146.06	126.42
25	3	504	BCR	C20-C19-C18	6.97	145.99	126.42
22	6	603	CLA	O2A-C1-C2	6.96	126.92	108.64
22	B	1210	CLA	O2D-CGD-CBD	6.95	123.62	111.27
22	B	1209	CLA	O2A-C1-C2	6.92	126.82	108.64
25	A	4003	BCR	C20-C19-C18	6.84	145.65	126.42
37	1	503	C7Z	C35-C34-C33	-6.77	117.65	127.31
25	B	4001	BCR	C20-C19-C18	6.74	145.36	126.42
25	K	4001	BCR	C20-C19-C18	6.74	145.36	126.42
22	3	606	CLA	O2A-C1-C2	6.72	126.30	108.64
32	A	5005	DGA	CDB-CCB-CBB	-6.65	80.69	114.42
22	7	603	CLA	O2A-C1-C2	6.63	126.05	108.64
25	B	4006	BCR	C20-C19-C18	6.58	144.89	126.42
39	2	503	LUT	C31-C30-C29	-6.57	117.93	127.31
22	B	1226	CLA	CMD-C2D-C1D	6.55	136.26	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	9	802	DGA	CDB-CCB-CBB	-6.52	81.33	114.42
22	B	1213	CLA	O2A-C1-C2	6.49	125.69	108.64
22	2	604	CLA	O2A-C1-C2	6.41	125.48	108.64
22	7	601	CLA	O2A-C1-C2	6.40	125.46	108.64
25	6	504	BCR	C20-C19-C18	6.40	144.40	126.42
22	B	1205	CLA	O2A-C1-C2	6.39	125.43	108.64
22	3	603	CLA	O2A-C1-C2	6.38	125.41	108.64
22	5	603	CLA	O2A-C1-C2	6.38	125.39	108.64
22	2	604	CLA	CMD-C2D-C1D	6.35	135.90	124.71
22	A	1121	CLA	CMD-C2D-C1D	6.32	135.85	124.71
22	A	1116	CLA	O2A-C1-C2	6.32	125.24	108.64
22	6	619	CLA	O2D-CGD-CBD	6.29	122.45	111.27
22	B	1224	CLA	O2A-C1-C2	6.25	125.06	108.64
22	6	609	CLA	O2D-CGD-CBD	6.25	122.37	111.27
22	6	605	CLA	O2A-C1-C2	6.24	125.03	108.64
22	B	1221	CLA	O2D-CGD-CBD	6.19	122.28	111.27
22	Z	606	CLA	O2D-CGD-CBD	6.17	122.23	111.27
22	5	605	CLA	CMD-C2D-C1D	6.14	135.54	124.71
22	A	1122	CLA	O2A-C1-C2	6.12	124.73	108.64
22	A	1106	CLA	O2D-CGD-CBD	6.12	122.14	111.27
22	7	604	CLA	O2A-C1-C2	6.11	124.70	108.64
21	A	1011	CL0	C2D-C1D-ND	6.10	114.60	110.10
22	4	603	CLA	O2A-C1-C2	6.10	124.67	108.64
22	A	1111	CLA	O2D-CGD-CBD	6.10	122.11	111.27
22	B	1235	CLA	O2A-C1-C2	6.10	124.67	108.64
22	9	604	CLA	O2A-C1-C2	6.09	124.65	108.64
22	2	601	CLA	O2A-C1-C2	6.08	124.61	108.64
22	3	601	CLA	O2A-C1-C2	6.06	124.57	108.64
22	A	1125	CLA	O2A-C1-C2	6.04	124.51	108.64
22	1	608	CLA	CMD-C2D-C1D	6.04	135.36	124.71
22	B	1214	CLA	O2A-C1-C2	6.04	124.50	108.64
22	5	604	CLA	O2A-C1-C2	6.01	124.42	108.64
25	5	504	BCR	C20-C19-C18	6.00	143.28	126.42
22	A	1110	CLA	O2A-C1-C2	6.00	124.41	108.64
22	6	615	CLA	O2D-CGD-CBD	5.98	121.89	111.27
22	B	1211	CLA	O2A-C1-C2	5.97	124.33	108.64
25	G	4001	BCR	C20-C19-C18	5.97	143.19	126.42
22	B	1231	CLA	CMD-C2D-C1D	5.97	135.23	124.71
21	A	1011	CL0	C2C-C1C-NC	5.97	115.56	109.97
22	B	1210	CLA	O2A-C1-C2	5.96	124.31	108.64
22	6	601	CLA	O2A-C1-C2	5.95	124.26	108.64
22	A	1128	CLA	O2A-C1-C2	5.94	124.25	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	7	609	CLA	O2D-CGD-CBD	5.93	121.81	111.27
22	6	604	CLA	O2A-C1-C2	5.93	124.22	108.64
22	9	601	CLA	O2A-C1-C2	5.93	124.22	108.64
22	A	1135	CLA	O2D-CGD-CBD	5.93	121.81	111.27
22	3	607	CLA	O2A-C1-C2	5.93	124.21	108.64
22	1	611	CLA	CMD-C2D-C1D	5.93	135.16	124.71
22	6	608	CLA	CMD-C2D-C1D	5.92	135.14	124.71
22	A	1012	CLA	O2A-C1-C2	5.91	124.16	108.64
22	A	1101	CLA	O2D-CGD-CBD	5.90	121.75	111.27
22	B	1212	CLA	O2D-CGD-CBD	5.89	121.74	111.27
22	A	1132	CLA	O2D-CGD-CBD	5.87	121.70	111.27
22	3	607	CLA	O2D-CGD-CBD	5.86	121.68	111.27
22	8	601	CLA	CMD-C2D-C1D	5.85	135.02	124.71
22	Z	604	CLA	CMD-C2D-C1D	5.83	134.99	124.71
22	A	1101	CLA	O2A-C1-C2	5.83	123.96	108.64
22	A	1109	CLA	CMD-C2D-C1D	5.82	134.98	124.71
22	A	1120	CLA	O2D-CGD-CBD	5.82	121.62	111.27
22	1	606	CLA	CMD-C2D-C1D	5.81	134.96	124.71
22	8	609	CLA	O2A-C1-C2	5.79	123.85	108.64
22	B	1204	CLA	O2A-C1-C2	5.79	123.85	108.64
22	7	606	CLA	CMD-C2D-C1D	5.79	134.91	124.71
22	K	1404	CLA	O2D-CGD-CBD	5.78	121.54	111.27
22	A	1112	CLA	O2D-CGD-CBD	5.77	121.53	111.27
22	5	622	CLA	CMD-C2D-C1D	5.77	134.88	124.71
22	A	1114	CLA	CMD-C2D-C1D	5.77	134.88	124.71
22	Z	605	CLA	CMD-C2D-C1D	5.76	134.87	124.71
22	B	1023	CLA	O2A-C1-C2	5.75	123.74	108.64
22	1	605	CLA	CMD-C2D-C1D	5.73	134.81	124.71
22	9	606	CLA	CMD-C2D-C1D	5.73	134.81	124.71
22	5	601	CLA	CMD-C2D-C1D	5.73	134.81	124.71
22	Z	611	CLA	CMD-C2D-C1D	5.72	134.80	124.71
22	7	601	CLA	CMD-C2D-C1D	5.72	134.80	124.71
42	Z	504	QTB	C09-C02-C03	5.72	127.72	118.94
22	B	1221	CLA	CMD-C2D-C1D	5.72	134.79	124.71
22	7	605	CLA	CMD-C2D-C1D	5.72	134.79	124.71
22	9	603	CLA	O2D-CGD-CBD	5.71	121.42	111.27
36	F	4001	RRX	C15-C14-C13	-5.71	119.16	127.31
22	4	609	CLA	O2D-CGD-CBD	5.71	121.41	111.27
22	9	605	CLA	CMD-C2D-C1D	5.71	134.77	124.71
37	1	503	C7Z	C31-C30-C29	-5.70	119.17	127.31
39	Z	501	LUT	C21-C26-C25	5.70	121.62	111.42
22	9	603	CLA	O2A-C1-C2	5.69	123.59	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	613	CLA	CMD-C2D-C1D	5.69	134.74	124.71
25	B	4005	BCR	C23-C22-C21	5.68	127.66	118.94
22	3	616	CLA	O2A-C1-C2	5.68	123.56	108.64
22	A	1134	CLA	O2A-C1-C2	5.67	123.53	108.64
22	K	1402	CLA	O2D-CGD-CBD	5.66	121.33	111.27
39	8	501	LUT	C21-C26-C25	5.66	121.56	111.42
39	9	501	LUT	C21-C26-C25	5.66	121.56	111.42
39	1	501	LUT	C21-C26-C25	5.66	121.56	111.42
22	B	1023	CLA	O2D-CGD-CBD	5.66	121.32	111.27
22	Z	604	CLA	O2A-C1-C2	5.65	123.50	108.64
22	A	1118	CLA	O2D-CGD-CBD	5.65	121.31	111.27
22	3	606	CLA	CMD-C2D-C1D	5.65	134.67	124.71
22	8	604	CLA	O2A-C1-C2	5.65	123.48	108.64
22	6	601	CLA	CMD-C2D-C1D	5.65	134.66	124.71
22	B	1202	CLA	O2D-CGD-CBD	5.64	121.28	111.27
22	4	601	CLA	CMD-C2D-C1D	5.63	134.64	124.71
22	B	1221	CLA	O2A-C1-C2	5.62	123.41	108.64
22	8	611	CLA	O2A-C1-C2	5.62	123.41	108.64
22	Z	606	CLA	CMD-C2D-C1D	5.62	134.61	124.71
39	7	501	LUT	C21-C26-C25	5.62	121.48	111.42
22	3	610	CLA	O2D-CGD-CBD	5.62	121.25	111.27
22	B	1218	CLA	O2A-C1-C2	5.62	123.39	108.64
22	9	603	CLA	CMD-C2D-C1D	5.61	134.61	124.71
22	B	1228	CLA	O2A-C1-C2	5.61	123.39	108.64
22	7	615	CLA	O2A-C1-C2	5.61	123.38	108.64
22	2	605	CLA	CMD-C2D-C1D	5.61	134.60	124.71
22	1	604	CLA	CMD-C2D-C1D	5.61	134.60	124.71
22	8	609	CLA	CMD-C2D-C1D	5.61	134.59	124.71
22	B	1216	CLA	O2A-C1-C2	5.60	123.36	108.64
22	2	603	CLA	O2D-CGD-CBD	5.60	121.22	111.27
22	Z	601	CLA	CMD-C2D-C1D	5.59	134.56	124.71
39	3	501	LUT	C21-C26-C25	5.59	121.43	111.42
22	6	605	CLA	CMD-C2D-C1D	5.59	134.56	124.71
22	1	603	CLA	CMD-C2D-C1D	5.59	134.56	124.71
22	3	603	CLA	CMD-C2D-C1D	5.58	134.56	124.71
22	A	1134	CLA	O2D-CGD-CBD	5.58	121.19	111.27
22	1	615	CLA	CMD-C2D-C1D	5.58	134.55	124.71
22	Z	608	CLA	CMD-C2D-C1D	5.58	134.55	124.71
22	B	1230	CLA	O2D-CGD-CBD	5.58	121.19	111.27
22	A	1120	CLA	CMD-C2D-C1D	5.58	134.55	124.71
22	4	606	CLA	CMD-C2D-C1D	5.58	134.55	124.71
22	4	612	CLA	CMD-C2D-C1D	5.58	134.54	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1117	CLA	O2A-C1-C2	5.57	123.28	108.64
22	B	1229	CLA	CMD-C2D-C1D	5.57	134.53	124.71
39	Z	503	LUT	C35-C34-C33	-5.57	119.37	127.31
22	6	606	CLA	CMD-C2D-C1D	5.56	134.52	124.71
22	A	1122	CLA	CMD-C2D-C1D	5.56	134.51	124.71
22	6	603	CLA	CMD-C2D-C1D	5.56	134.51	124.71
22	F	1301	CLA	CMD-C2D-C1D	5.55	134.50	124.71
22	A	1138	CLA	O2D-CGD-CBD	5.55	121.13	111.27
22	6	609	CLA	CMD-C2D-C1D	5.54	134.48	124.71
22	5	605	CLA	O2A-C1-C2	5.54	123.19	108.64
25	B	4005	BCR	C37-C22-C21	-5.54	115.17	122.92
22	6	619	CLA	CMD-C2D-C1D	5.54	134.47	124.71
22	7	616	CLA	CMD-C2D-C1D	5.53	134.47	124.71
22	Z	611	CLA	O2A-C1-C2	5.53	123.17	108.64
22	A	1105	CLA	O2A-C1-C2	5.53	123.17	108.64
22	5	606	CLA	CMD-C2D-C1D	5.53	134.46	124.71
22	A	1105	CLA	CMD-C2D-C1D	5.53	134.45	124.71
22	A	1111	CLA	CMD-C2D-C1D	5.53	134.45	124.71
22	B	1202	CLA	CMD-C2D-C1D	5.53	134.45	124.71
22	9	606	CLA	O2A-C1-C2	5.52	123.16	108.64
22	B	1021	CLA	O2D-CGD-CBD	5.52	121.08	111.27
37	5	505	C7Z	C15-C14-C13	-5.52	119.43	127.31
22	B	1235	CLA	CMD-C2D-C1D	5.52	134.44	124.71
22	8	609	CLA	O2D-CGD-CBD	5.52	121.08	111.27
22	8	602	CLA	O2A-C1-C2	5.52	123.14	108.64
22	B	1213	CLA	CMD-C2D-C1D	5.52	134.44	124.71
22	B	1211	CLA	CMD-C2D-C1D	5.52	134.43	124.71
22	B	1214	CLA	O2D-CGD-CBD	5.51	121.06	111.27
22	A	1108	CLA	O2A-C1-C2	5.51	123.12	108.64
22	5	603	CLA	CMD-C2D-C1D	5.51	134.42	124.71
21	A	1011	CL0	C1C-C2C-C3C	-5.51	101.17	106.96
22	L	1502	CLA	O2A-C1-C2	5.51	123.11	108.64
22	A	1101	CLA	CMD-C2D-C1D	5.51	134.42	124.71
22	5	612	CLA	CMD-C2D-C1D	5.50	134.41	124.71
39	8	502	LUT	C21-C26-C25	5.50	121.27	111.42
22	9	604	CLA	O2D-CGD-CBD	5.50	121.04	111.27
22	3	610	CLA	CMD-C2D-C1D	5.50	134.40	124.71
22	A	1137	CLA	CMD-C2D-C1D	5.49	134.40	124.71
22	Z	603	CLA	CMD-C2D-C1D	5.49	134.40	124.71
22	A	1137	CLA	O2A-C1-C2	5.49	123.07	108.64
22	7	615	CLA	CMD-C2D-C1D	5.49	134.39	124.71
22	A	1102	CLA	CMD-C2D-C1D	5.49	134.39	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1112	CLA	CMD-C2D-C1D	5.49	134.39	124.71
22	L	1503	CLA	CMD-C2D-C1D	5.49	134.39	124.71
22	4	605	CLA	CMD-C2D-C1D	5.49	134.38	124.71
22	A	1130	CLA	CMD-C2D-C1D	5.49	134.38	124.71
22	Z	615	CLA	CMD-C2D-C1D	5.49	134.38	124.71
22	6	615	CLA	O2A-C1-C2	5.49	123.05	108.64
22	A	1132	CLA	CMD-C2D-C1D	5.48	134.38	124.71
37	5	505	C7Z	C38-C25-C26	-5.48	118.37	124.53
22	A	1125	CLA	CMD-C2D-C1D	5.48	134.38	124.71
22	B	1216	CLA	CMD-C2D-C1D	5.48	134.37	124.71
22	8	601	CLA	O2A-C1-C2	5.48	123.04	108.64
22	1	613	CLA	CMD-C2D-C1D	5.48	134.37	124.71
22	1	612	CLA	CMD-C2D-C1D	5.48	134.37	124.71
37	J	4002	C7Z	C31-C30-C29	-5.47	119.50	127.31
36	F	4001	RRX	C38-C26-C25	-5.47	118.38	124.53
39	3	502	LUT	C21-C26-C27	5.47	119.62	112.70
22	A	1108	CLA	CMD-C2D-C1D	5.47	134.36	124.71
22	8	605	CLA	O2A-C1-C2	5.47	123.02	108.64
22	6	606	CLA	O2A-C1-C2	5.47	123.02	108.64
22	B	1219	CLA	CMD-C2D-C1D	5.47	134.35	124.71
22	K	1401	CLA	CMD-C2D-C1D	5.46	134.33	124.71
22	8	611	CLA	CMD-C2D-C1D	5.46	134.33	124.71
22	7	606	CLA	O2A-C1-C2	5.46	122.98	108.64
22	A	1141	CLA	CMD-C2D-C1D	5.46	134.33	124.71
22	B	1212	CLA	CMD-C2D-C1D	5.46	134.33	124.71
22	B	1208	CLA	CMD-C2D-C1D	5.46	134.33	124.71
22	B	1238	CLA	O2A-C1-C2	5.45	122.97	108.64
22	B	1210	CLA	CMD-C2D-C1D	5.45	134.32	124.71
22	J	1901	CLA	CMD-C2D-C1D	5.45	134.32	124.71
22	A	1106	CLA	CMD-C2D-C1D	5.45	134.32	124.71
22	5	615	CLA	O2A-C1-C2	5.45	122.96	108.64
22	2	605	CLA	O2A-C1-C2	5.45	122.96	108.64
22	5	615	CLA	CMD-C2D-C1D	5.45	134.31	124.71
22	7	603	CLA	CMD-C2D-C1D	5.45	134.31	124.71
22	B	1208	CLA	O2A-C1-C2	5.45	122.95	108.64
22	9	612	CLA	O2D-CGD-CBD	5.44	120.94	111.27
22	B	1204	CLA	CMD-C2D-C1D	5.44	134.29	124.71
22	3	616	CLA	CMD-C2D-C1D	5.43	134.29	124.71
22	2	607	CLA	CMD-C2D-C1D	5.43	134.29	124.71
22	A	1119	CLA	CMD-C2D-C1D	5.43	134.28	124.71
22	2	606	CLA	O2D-CGD-CBD	5.43	120.92	111.27
22	B	1224	CLA	O2D-CGD-CBD	5.43	120.92	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1103	CLA	CMD-C2D-C1D	5.43	134.28	124.71
22	4	604	CLA	O2A-C1-C2	5.43	122.90	108.64
22	3	604	CLA	O2A-C1-C2	5.43	122.90	108.64
42	Z	504	QTB	C04-C03-C02	5.42	135.05	127.31
22	Z	605	CLA	O2D-CGD-CBD	5.42	120.91	111.27
22	8	603	CLA	CMD-C2D-C1D	5.42	134.27	124.71
22	3	612	CLA	CMD-C2D-C1D	5.42	134.27	124.71
22	B	1228	CLA	CMD-C2D-C1D	5.42	134.27	124.71
22	8	604	CLA	CMD-C2D-C1D	5.42	134.27	124.71
22	4	608	CLA	CMD-C2D-C1D	5.42	134.26	124.71
22	A	1134	CLA	CMD-C2D-C1D	5.42	134.26	124.71
22	4	602	CLA	O2A-C1-C2	5.42	122.87	108.64
22	B	1203	CLA	CMD-C2D-C1D	5.42	134.26	124.71
22	3	601	CLA	CMD-C2D-C1D	5.42	134.26	124.71
22	4	604	CLA	CMD-C2D-C1D	5.42	134.26	124.71
22	4	615	CLA	CMD-C2D-C1D	5.42	134.26	124.71
22	G	1602	CLA	O2D-CGD-CBD	5.41	120.89	111.27
22	1	601	CLA	CMD-C2D-C1D	5.41	134.25	124.71
22	2	602	CLA	CMD-C2D-C1D	5.41	134.25	124.71
22	3	607	CLA	CMD-C2D-C1D	5.41	134.25	124.71
22	9	608	CLA	CMD-C2D-C1D	5.41	134.24	124.71
22	B	1240	CLA	CMD-C2D-C1D	5.40	134.24	124.71
22	A	1140	CLA	CMD-C2D-C1D	5.40	134.23	124.71
22	A	1113	CLA	O2D-CGD-CBD	5.40	120.86	111.27
22	K	1403	CLA	CMD-C2D-C1D	5.40	134.22	124.71
22	B	1238	CLA	CMD-C2D-C1D	5.39	134.22	124.71
22	A	1012	CLA	O2D-CGD-CBD	5.39	120.85	111.27
22	B	1222	CLA	CMD-C2D-C1D	5.39	134.21	124.71
22	B	1209	CLA	CMD-C2D-C1D	5.39	134.21	124.71
22	B	1214	CLA	CMD-C2D-C1D	5.39	134.21	124.71
22	A	1121	CLA	O2A-C1-C2	5.39	122.79	108.64
39	1	502	LUT	C21-C26-C25	5.39	121.06	111.42
22	3	605	CLA	CMD-C2D-C1D	5.39	134.20	124.71
22	5	608	CLA	CMD-C2D-C1D	5.38	134.20	124.71
22	A	1104	CLA	O2A-C1-C2	5.38	122.78	108.64
22	A	1129	CLA	CMD-C2D-C1D	5.38	134.20	124.71
22	5	602	CLA	CMD-C2D-C1D	5.38	134.20	124.71
22	7	613	CLA	CMD-C2D-C1D	5.38	134.20	124.71
22	1	604	CLA	O2D-CGD-CBD	5.38	120.83	111.27
22	G	1602	CLA	CMD-C2D-C1D	5.38	134.19	124.71
22	7	611	CLA	CMD-C2D-C1D	5.38	134.19	124.71
22	6	604	CLA	CMD-C2D-C1D	5.38	134.19	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1212	CLA	O2A-C1-C2	5.37	122.75	108.64
22	7	608	CLA	CMD-C2D-C1D	5.37	134.17	124.71
22	2	608	CLA	O2D-CGD-CBD	5.37	120.80	111.27
22	9	607	CLA	CMD-C2D-C1D	5.36	134.17	124.71
22	B	1217	CLA	O2A-C1-C2	5.36	122.71	108.64
39	5	501	LUT	C21-C26-C25	5.35	121.01	111.42
22	B	1237	CLA	O2A-C1-C2	5.35	122.71	108.64
22	B	1236	CLA	O2A-C1-C2	5.35	122.69	108.64
22	8	606	CLA	CMD-C2D-C1D	5.35	134.14	124.71
22	4	603	CLA	CMD-C2D-C1D	5.35	134.14	124.71
22	2	608	CLA	CMD-C2D-C1D	5.34	134.13	124.71
22	9	609	CLA	CMD-C2D-C1D	5.34	134.13	124.71
22	B	1226	CLA	O2A-C1-C2	5.34	122.68	108.64
22	A	1138	CLA	O2A-C1-C2	5.34	122.67	108.64
22	5	606	CLA	O2D-CGD-CBD	5.34	120.75	111.27
22	2	602	CLA	O2D-CGD-CBD	5.34	120.75	111.27
22	Z	612	CLA	CMD-C2D-C1D	5.34	134.12	124.71
22	B	1231	CLA	O2D-CGD-CBD	5.33	120.75	111.27
22	9	601	CLA	CMD-C2D-C1D	5.33	134.12	124.71
22	8	615	CLA	CMD-C2D-C1D	5.33	134.11	124.71
22	B	1238	CLA	O2D-CGD-CBD	5.33	120.74	111.27
36	F	4001	RRX	C4-C5-C6	-5.33	114.99	122.73
22	A	1136	CLA	CMD-C2D-C1D	5.33	134.10	124.71
22	8	608	CLA	CMD-C2D-C1D	5.33	134.10	124.71
22	4	602	CLA	CMD-C2D-C1D	5.33	134.10	124.71
22	A	1131	CLA	CMD-C2D-C1D	5.33	134.10	124.71
22	F	1302	CLA	CMD-C2D-C1D	5.33	134.10	124.71
22	K	1402	CLA	CMD-C2D-C1D	5.33	134.10	124.71
22	B	1236	CLA	CMD-C2D-C1D	5.32	134.09	124.71
22	5	609	CLA	CMD-C2D-C1D	5.32	134.09	124.71
22	Z	602	CLA	O2D-CGD-CBD	5.32	120.72	111.27
36	F	4001	RRX	C11-C10-C9	-5.32	119.72	127.31
22	1	602	CLA	O2D-CGD-CBD	5.32	120.72	111.27
22	7	609	CLA	CMD-C2D-C1D	5.32	134.09	124.71
22	6	615	CLA	CMD-C2D-C1D	5.32	134.09	124.71
21	A	1011	CL0	O2A-C1-C2	5.32	122.61	108.64
22	K	1403	CLA	O2A-C1-C2	5.32	121.40	108.97
22	B	1234	CLA	O2D-CGD-CBD	5.31	120.71	111.27
22	B	1207	CLA	CMD-C2D-C1D	5.31	134.07	124.71
22	3	602	CLA	CMD-C2D-C1D	5.31	134.07	124.71
37	5	505	C7Z	C18-C5-C6	-5.31	118.56	124.53
22	B	1232	CLA	CMD-C2D-C1D	5.31	134.07	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1116	CLA	CMD-C2D-C1D	5.31	134.07	124.71
22	A	1123	CLA	CMD-C2D-C1D	5.31	134.07	124.71
22	7	612	CLA	CMD-C2D-C1D	5.31	134.06	124.71
22	B	1218	CLA	CMD-C2D-C1D	5.30	134.06	124.71
22	A	1104	CLA	CMD-C2D-C1D	5.30	134.06	124.71
22	1	606	CLA	O2D-CGD-CBD	5.30	120.69	111.27
22	G	1601	CLA	CMD-C2D-C1D	5.30	134.05	124.71
22	A	1139	CLA	CMD-C2D-C1D	5.30	134.05	124.71
22	B	1217	CLA	CMD-C2D-C1D	5.30	134.05	124.71
39	7	502	LUT	C21-C26-C25	5.29	120.90	111.42
22	8	605	CLA	O2D-CGD-CBD	5.29	120.67	111.27
22	A	1130	CLA	O2A-C1-C2	5.29	122.54	108.64
22	B	1239	CLA	CMD-C2D-C1D	5.29	134.04	124.71
22	8	605	CLA	CMD-C2D-C1D	5.29	134.04	124.71
22	5	604	CLA	CMD-C2D-C1D	5.29	134.03	124.71
22	B	1207	CLA	O2A-C1-C2	5.28	122.51	108.64
22	5	612	CLA	O2A-C1-C2	5.28	122.51	108.64
22	B	1211	CLA	O2D-CGD-CBD	5.28	120.64	111.27
22	K	1402	CLA	O2A-C1-C2	5.27	122.50	108.64
22	B	1218	CLA	O2D-CGD-CBD	5.27	120.64	111.27
22	B	1239	CLA	O2D-CGD-CBD	5.27	120.63	111.27
22	3	604	CLA	CMD-C2D-C1D	5.27	134.00	124.71
22	2	603	CLA	CMD-C2D-C1D	5.27	134.00	124.71
22	B	1230	CLA	O2A-C1-C2	5.27	122.48	108.64
22	7	604	CLA	CMD-C2D-C1D	5.27	133.99	124.71
22	A	1126	CLA	CMD-C2D-C1D	5.26	133.99	124.71
22	A	1110	CLA	CMD-C2D-C1D	5.26	133.98	124.71
22	5	618	CLA	O2A-C1-C2	5.25	122.44	108.64
22	A	1111	CLA	O2A-C1-C2	5.25	122.44	108.64
22	A	1137	CLA	O2D-CGD-CBD	5.25	120.60	111.27
22	9	606	CLA	O2D-CGD-CBD	5.25	120.60	111.27
22	A	1135	CLA	CMD-C2D-C1D	5.25	133.97	124.71
22	A	1116	CLA	O2D-CGD-CBD	5.24	120.59	111.27
22	2	612	CLA	CMD-C2D-C1D	5.24	133.96	124.71
22	A	1115	CLA	O2A-C1-C2	5.24	122.41	108.64
36	F	4001	RRX	C1-C6-C5	-5.24	115.23	122.61
22	2	601	CLA	CMD-C2D-C1D	5.24	133.95	124.71
22	B	1022	CLA	CMD-C2D-C1D	5.24	133.95	124.71
22	A	1105	CLA	O2D-CGD-CBD	5.24	120.58	111.27
22	A	1132	CLA	O2A-C1-C2	5.24	122.40	108.64
22	A	1133	CLA	CMD-C2D-C1D	5.24	133.94	124.71
22	B	1215	CLA	O2D-CGD-CBD	5.24	120.57	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1113	CLA	CMD-C2D-C1D	5.24	133.94	124.71
22	J	1901	CLA	O2D-CGD-CBD	5.23	120.56	111.27
39	Z	502	LUT	C21-C26-C25	5.23	120.79	111.42
22	A	1110	CLA	O2D-CGD-CBD	5.23	120.56	111.27
22	B	1022	CLA	O2A-C1-C2	5.23	122.37	108.64
22	7	607	CLA	CMD-C2D-C1D	5.23	133.93	124.71
22	A	1138	CLA	CMD-C2D-C1D	5.23	133.92	124.71
22	B	1201	CLA	CMD-C2D-C1D	5.22	133.92	124.71
22	7	612	CLA	O2A-C1-C2	5.22	122.36	108.64
22	B	1240	CLA	O2A-C1-C2	5.22	122.36	108.64
22	4	608	CLA	O2A-C1-C2	5.22	122.35	108.64
37	5	505	C7Z	C11-C10-C9	-5.22	119.86	127.31
22	5	606	CLA	O2A-C1-C2	5.22	122.34	108.64
22	Z	607	CLA	CMD-C2D-C1D	5.21	133.89	124.71
22	A	1135	CLA	O2A-C1-C2	5.21	122.31	108.64
22	1	605	CLA	O2D-CGD-CBD	5.20	120.52	111.27
22	2	605	CLA	O2D-CGD-CBD	5.20	120.52	111.27
22	B	1219	CLA	O2D-CGD-CBD	5.20	120.51	111.27
22	4	601	CLA	O2D-CGD-CBD	5.20	120.51	111.27
22	9	604	CLA	CMD-C2D-C1D	5.20	133.88	124.71
22	2	603	CLA	O2A-C1-C2	5.20	122.30	108.64
39	4	501	LUT	C21-C26-C25	5.20	120.73	111.42
22	A	1129	CLA	O2D-CGD-CBD	5.20	120.51	111.27
22	B	1235	CLA	O2D-CGD-CBD	5.19	120.50	111.27
22	B	1215	CLA	CMD-C2D-C1D	5.19	133.87	124.71
22	B	1220	CLA	CMD-C2D-C1D	5.19	133.87	124.71
21	A	1011	CL0	O2A-CGA-O1A	-5.19	110.49	123.59
22	6	612	CLA	CMD-C2D-C1D	5.19	133.86	124.71
22	7	616	CLA	O2A-C1-C2	5.19	122.28	108.64
22	1	605	CLA	O2A-C1-C2	5.19	122.27	108.64
22	A	1114	CLA	O2D-CGD-CBD	5.19	120.49	111.27
39	2	503	LUT	C22-C23-C24	-5.19	105.84	111.74
22	B	1241	CLA	CMD-C2D-C1D	5.19	133.85	124.71
22	6	609	CLA	O2A-C1-C2	5.19	122.26	108.64
22	4	601	CLA	O2A-C1-C2	5.18	122.25	108.64
22	B	1209	CLA	O2D-CGD-CBD	5.18	120.47	111.27
39	9	502	LUT	C21-C26-C27	5.18	119.25	112.70
22	6	602	CLA	O2D-CGD-CBD	5.18	120.47	111.27
22	3	613	CLA	O2D-CGD-CBD	5.17	120.46	111.27
21	A	1011	CL0	O2D-CGD-CBD	5.17	120.46	111.27
22	7	601	CLA	O2D-CGD-CBD	5.17	120.46	111.27
22	B	1205	CLA	CMD-C2D-C1D	5.17	133.83	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1230	CLA	CMD-C2D-C1D	5.17	133.83	124.71
22	A	1121	CLA	O2D-CGD-CBD	5.17	120.45	111.27
22	5	607	CLA	CMD-C2D-C1D	5.17	133.82	124.71
22	6	619	CLA	O2A-C1-C2	5.17	122.21	108.64
22	3	608	CLA	CMD-C2D-C1D	5.16	133.81	124.71
22	A	1104	CLA	O2D-CGD-CBD	5.16	120.43	111.27
22	8	602	CLA	O2D-CGD-CBD	5.16	120.43	111.27
22	A	1118	CLA	CMD-C2D-C1D	5.16	133.80	124.71
39	2	502	LUT	C21-C26-C25	5.15	120.65	111.42
22	7	602	CLA	O2D-CGD-CBD	5.15	120.42	111.27
22	5	613	CLA	O2D-CGD-CBD	5.15	120.42	111.27
22	7	616	CLA	O2D-CGD-CBD	5.15	120.42	111.27
22	A	1126	CLA	O2D-CGD-CBD	5.15	120.42	111.27
22	1	601	CLA	O2A-C1-C2	5.14	122.15	108.64
22	9	608	CLA	O2D-CGD-CBD	5.14	120.40	111.27
22	7	604	CLA	O2D-CGD-CBD	5.14	120.40	111.27
22	6	607	CLA	O2A-C1-C2	5.14	122.14	108.64
22	A	1131	CLA	O2D-CGD-CBD	5.14	120.39	111.27
22	6	606	CLA	O2D-CGD-CBD	5.14	120.39	111.27
22	B	1234	CLA	CMD-C2D-C1D	5.14	133.76	124.71
22	1	604	CLA	O2A-C1-C2	5.13	122.12	108.64
22	B	1229	CLA	O2D-CGD-CBD	5.13	120.39	111.27
22	1	613	CLA	O2D-CGD-CBD	5.13	120.39	111.27
22	A	1139	CLA	O2D-CGD-CBD	5.13	120.38	111.27
22	1	612	CLA	O2A-C1-C2	5.12	122.09	108.64
22	8	611	CLA	O2D-CGD-CBD	5.12	120.36	111.27
22	7	602	CLA	O2A-C1-C2	5.12	122.09	108.64
22	B	1223	CLA	CMD-C2D-C1D	5.12	133.73	124.71
22	6	602	CLA	CMD-C2D-C1D	5.12	133.73	124.71
22	B	1202	CLA	O2A-C1-C2	5.12	122.08	108.64
22	3	608	CLA	O2D-CGD-CBD	5.11	120.35	111.27
22	2	612	CLA	O2D-CGD-CBD	5.11	120.35	111.27
22	5	608	CLA	O2D-CGD-CBD	5.11	120.35	111.27
22	7	605	CLA	O2A-C1-C2	5.11	122.06	108.64
22	L	1503	CLA	O2A-C1-C2	5.11	122.05	108.64
22	5	607	CLA	O2A-C1-C2	5.10	122.05	108.64
22	A	1117	CLA	CMD-C2D-C1D	5.10	133.71	124.71
22	A	1141	CLA	O2A-C1-C2	5.10	122.04	108.64
22	A	1120	CLA	O2A-C1-C2	5.10	122.03	108.64
22	8	607	CLA	CMD-C2D-C1D	5.10	133.70	124.71
22	4	609	CLA	CMD-C2D-C1D	5.10	133.69	124.71
22	Z	601	CLA	O2A-C1-C2	5.09	122.02	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	9	602	CLA	O2D-CGD-CBD	5.09	120.31	111.27
22	B	1227	CLA	CMD-C2D-C1D	5.09	133.68	124.71
22	2	612	CLA	O2A-C1-C2	5.08	122.00	108.64
22	1	607	CLA	O2A-C1-C2	5.08	121.99	108.64
37	5	505	C7Z	C7-C8-C9	-5.08	118.56	126.23
22	Z	612	CLA	O2A-C1-C2	5.08	121.99	108.64
22	8	607	CLA	O2A-C1-C2	5.08	121.98	108.64
22	B	1204	CLA	O2D-CGD-CBD	5.08	120.29	111.27
22	3	602	CLA	O2D-CGD-CBD	5.08	120.29	111.27
22	B	1236	CLA	O2D-CGD-CBD	5.08	120.29	111.27
22	Z	607	CLA	O2D-CGD-CBD	5.07	120.29	111.27
39	3	502	LUT	C21-C26-C25	5.07	120.51	111.42
22	2	601	CLA	O2D-CGD-CBD	5.07	120.28	111.27
22	Z	608	CLA	O2A-C1-C2	5.07	121.97	108.64
22	9	605	CLA	O2D-CGD-CBD	5.07	120.28	111.27
22	8	604	CLA	O2D-CGD-CBD	5.07	120.28	111.27
22	8	602	CLA	CMD-C2D-C1D	5.07	133.65	124.71
22	L	1502	CLA	O2D-CGD-CBD	5.07	120.27	111.27
22	1	607	CLA	CMD-C2D-C1D	5.07	133.65	124.71
22	6	612	CLA	O2A-C1-C2	5.07	121.95	108.64
22	7	613	CLA	O2D-CGD-CBD	5.06	120.27	111.27
22	5	602	CLA	O2D-CGD-CBD	5.06	120.27	111.27
22	A	1128	CLA	O2D-CGD-CBD	5.06	120.27	111.27
22	4	607	CLA	O2A-C1-C2	5.05	121.92	108.64
22	9	607	CLA	O2A-C1-C2	5.05	121.92	108.64
22	B	1201	CLA	O2D-CGD-CBD	5.05	120.25	111.27
22	7	611	CLA	O2A-C1-C2	5.05	121.91	108.64
22	B	1206	CLA	O2D-CGD-CBD	5.05	120.25	111.27
22	B	1237	CLA	O2D-CGD-CBD	5.05	120.24	111.27
22	6	607	CLA	CMD-C2D-C1D	5.05	133.61	124.71
22	6	608	CLA	O2A-C1-C2	5.05	121.90	108.64
22	A	1107	CLA	O2A-C1-C2	5.04	121.89	108.64
22	B	1207	CLA	O2D-CGD-CBD	5.04	120.23	111.27
22	8	612	CLA	CMD-C2D-C1D	5.04	133.60	124.71
39	4	502	LUT	C21-C26-C25	5.04	120.45	111.42
22	4	612	CLA	O2A-C1-C2	5.04	121.89	108.64
22	5	607	CLA	O2D-CGD-CBD	5.04	120.22	111.27
22	3	601	CLA	O2D-CGD-CBD	5.04	120.22	111.27
22	5	601	CLA	O2D-CGD-CBD	5.04	120.22	111.27
22	1	601	CLA	O2D-CGD-CBD	5.04	120.22	111.27
22	B	1220	CLA	O2A-C1-C2	5.03	121.87	108.64
22	A	1106	CLA	O2A-C1-C2	5.03	121.86	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	K	1401	CLA	O2D-CGD-CBD	5.03	120.21	111.27
39	6	502	LUT	C21-C26-C25	5.03	120.43	111.42
22	Z	606	CLA	O2A-C1-C2	5.03	121.85	108.64
37	1	503	C7Z	C38-C25-C26	-5.03	118.88	124.53
22	1	606	CLA	O2A-C1-C2	5.03	121.84	108.64
22	2	604	CLA	O2D-CGD-CBD	5.02	120.20	111.27
22	4	605	CLA	O2D-CGD-CBD	5.02	120.19	111.27
39	Z	503	LUT	C11-C10-C9	-5.02	120.15	127.31
22	5	609	CLA	O2A-C1-C2	5.01	121.81	108.64
22	B	1240	CLA	O2D-CGD-CBD	5.01	120.17	111.27
22	Z	608	CLA	O2D-CGD-CBD	5.01	120.17	111.27
22	8	606	CLA	O2A-C1-C2	5.01	121.80	108.64
22	4	602	CLA	O2D-CGD-CBD	5.00	120.16	111.27
22	2	606	CLA	CMD-C2D-C1D	5.00	133.53	124.71
22	G	1601	CLA	O2A-C1-C2	5.00	121.78	108.64
22	Z	604	CLA	O2D-CGD-CBD	5.00	120.15	111.27
22	5	618	CLA	O2D-CGD-CBD	5.00	120.15	111.27
22	Z	602	CLA	CMD-C2D-C1D	4.99	133.51	124.71
26	3	801	LHG	O7-C7-O9	-4.99	119.21	125.57
22	1	611	CLA	O2D-CGD-CBD	4.99	120.14	111.27
22	6	607	CLA	O2D-CGD-CBD	4.99	120.14	111.27
22	B	1219	CLA	O2A-C1-C2	4.99	121.75	108.64
22	Z	607	CLA	O2A-C1-C2	4.99	121.74	108.64
22	8	606	CLA	O2D-CGD-CBD	4.99	120.13	111.27
22	5	612	CLA	O2D-CGD-CBD	4.99	120.13	111.27
22	A	1130	CLA	O2D-CGD-CBD	4.98	120.12	111.27
22	B	1241	CLA	O2D-CGD-CBD	4.98	120.11	111.27
22	3	616	CLA	O2D-CGD-CBD	4.98	120.11	111.27
22	5	618	CLA	CMD-C2D-C1D	4.98	133.48	124.71
22	B	1224	CLA	CMD-C2D-C1D	4.97	133.48	124.71
22	4	607	CLA	CMD-C2D-C1D	4.97	133.47	124.71
22	2	615	CLA	O2D-CGD-CBD	4.97	120.10	111.27
22	7	609	CLA	O2A-C1-C2	4.97	121.69	108.64
22	A	1140	CLA	O2A-C1-C2	4.97	121.69	108.64
22	3	606	CLA	O2D-CGD-CBD	4.96	120.09	111.27
22	4	607	CLA	O2D-CGD-CBD	4.96	120.09	111.27
22	9	605	CLA	O2A-C1-C2	4.96	121.67	108.64
22	B	1241	CLA	O2A-C1-C2	4.96	121.67	108.64
39	6	501	LUT	C21-C26-C25	4.96	120.30	111.42
22	7	602	CLA	CMD-C2D-C1D	4.96	133.45	124.71
22	A	1107	CLA	CMD-C2D-C1D	4.95	133.44	124.71
22	K	1403	CLA	O2D-CGD-CBD	4.95	120.06	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	7	607	CLA	O2D-CGD-CBD	4.94	120.05	111.27
22	A	1127	CLA	O2A-C1-C2	4.94	121.62	108.64
22	A	1136	CLA	O2A-C1-C2	4.94	121.61	108.64
22	A	1114	CLA	O2A-C1-C2	4.94	121.61	108.64
22	5	613	CLA	CMD-C2D-C1D	4.93	133.40	124.71
22	9	602	CLA	CMD-C2D-C1D	4.93	133.40	124.71
22	4	608	CLA	O2D-CGD-CBD	4.93	120.02	111.27
22	5	622	CLA	O2D-CGD-CBD	4.92	120.01	111.27
22	3	612	CLA	O2D-CGD-CBD	4.92	120.00	111.27
22	6	618	CLA	O2D-CGD-CBD	4.91	120.00	111.27
22	Z	611	CLA	O2D-CGD-CBD	4.91	120.00	111.27
22	Z	603	CLA	O2A-C1-C2	4.91	121.54	108.64
22	3	605	CLA	O2D-CGD-CBD	4.91	119.99	111.27
22	5	602	CLA	O2A-C1-C2	4.90	121.51	108.64
39	3	501	LUT	C21-C26-C27	4.90	118.89	112.70
22	A	1131	CLA	O2A-C1-C2	4.89	121.50	108.64
22	A	1112	CLA	O2A-C1-C2	4.89	121.49	108.64
22	6	602	CLA	O2A-C1-C2	4.89	121.48	108.64
22	4	609	CLA	O2A-C1-C2	4.89	121.48	108.64
22	4	606	CLA	O2D-CGD-CBD	4.89	119.95	111.27
22	B	1231	CLA	O2A-C1-C2	4.89	121.48	108.64
22	4	603	CLA	O2D-CGD-CBD	4.89	119.95	111.27
22	B	1223	CLA	O2A-C1-C2	4.88	121.47	108.64
22	A	1102	CLA	O2A-C1-C2	4.88	121.47	108.64
42	Z	504	QTB	C01-C02-C09	-4.88	110.39	118.08
22	B	1237	CLA	CMD-C2D-C1D	4.88	133.31	124.71
42	Z	504	QTB	C13-C12-C11	4.88	122.21	112.60
22	A	1125	CLA	O2D-CGD-CBD	4.87	119.93	111.27
22	L	1502	CLA	CMD-C2D-C1D	4.87	133.30	124.71
22	1	611	CLA	O2A-C1-C2	4.87	121.43	108.64
22	5	613	CLA	O2A-C1-C2	4.86	121.42	108.64
22	7	607	CLA	O2A-C1-C2	4.86	121.41	108.64
22	B	1206	CLA	O2A-C1-C2	4.86	121.40	108.64
22	1	602	CLA	CMD-C2D-C1D	4.86	133.27	124.71
22	Z	605	CLA	O2A-C1-C2	4.85	121.39	108.64
22	A	1118	CLA	O2A-C1-C2	4.85	121.39	108.64
22	Z	601	CLA	O2D-CGD-CBD	4.85	119.88	111.27
22	9	609	CLA	O2D-CGD-CBD	4.85	119.88	111.27
22	A	1107	CLA	O2D-CGD-CBD	4.84	119.88	111.27
22	A	1102	CLA	O2D-CGD-CBD	4.84	119.87	111.27
22	A	1133	CLA	O2D-CGD-CBD	4.84	119.87	111.27
22	9	601	CLA	O2D-CGD-CBD	4.84	119.86	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1234	CLA	O2A-C1-C2	4.83	121.34	108.64
37	1	503	C7Z	C27-C28-C29	-4.83	118.93	126.23
22	3	618	CLA	O2D-CGD-CBD	4.83	119.86	111.27
22	6	601	CLA	O2D-CGD-CBD	4.83	119.85	111.27
22	1	608	CLA	O2D-CGD-CBD	4.83	119.85	111.27
22	B	1223	CLA	O2D-CGD-CBD	4.83	119.85	111.27
39	5	502	LUT	C21-C26-C25	4.82	120.06	111.42
22	3	613	CLA	O2A-C1-C2	4.82	121.31	108.64
26	B	5002	LHG	O7-C7-O9	-4.82	119.43	125.57
22	A	1141	CLA	O2D-CGD-CBD	4.82	119.84	111.27
22	7	615	CLA	O2D-CGD-CBD	4.82	119.84	111.27
22	A	1129	CLA	O2A-C1-C2	4.82	121.31	108.64
22	4	606	CLA	O2A-C1-C2	4.82	121.31	108.64
22	B	1226	CLA	O2D-CGD-CBD	4.82	119.83	111.27
22	1	608	CLA	O2A-C1-C2	4.82	121.30	108.64
22	B	1208	CLA	O2D-CGD-CBD	4.82	119.83	111.27
39	9	502	LUT	C21-C26-C25	4.81	120.04	111.42
22	B	1022	CLA	O2D-CGD-CBD	4.81	119.82	111.27
22	B	1225	CLA	O2A-C1-C2	4.81	121.28	108.64
22	7	606	CLA	O2D-CGD-CBD	4.81	119.81	111.27
39	5	502	LUT	C21-C26-C27	4.80	118.77	112.70
22	3	605	CLA	O2A-C1-C2	4.80	121.25	108.64
22	8	601	CLA	O2D-CGD-CBD	4.80	119.79	111.27
22	5	609	CLA	O2D-CGD-CBD	4.80	119.79	111.27
22	5	605	CLA	O2D-CGD-CBD	4.79	119.79	111.27
22	B	1205	CLA	O2D-CGD-CBD	4.78	119.76	111.27
22	7	611	CLA	O2D-CGD-CBD	4.78	119.76	111.27
22	6	612	CLA	O2D-CGD-CBD	4.78	119.76	111.27
22	1	615	CLA	O2A-C1-C2	4.77	121.17	108.64
22	9	612	CLA	O2A-C1-C2	4.77	121.17	108.64
22	3	604	CLA	O2D-CGD-CBD	4.76	119.73	111.27
22	G	1601	CLA	O2D-CGD-CBD	4.76	119.73	111.27
22	B	1216	CLA	O2D-CGD-CBD	4.76	119.72	111.27
22	4	612	CLA	O2D-CGD-CBD	4.76	119.72	111.27
39	5	501	LUT	C22-C23-C24	-4.75	106.33	111.74
22	5	601	CLA	O2A-C1-C2	4.75	121.12	108.64
22	B	1206	CLA	CMD-C2D-C1D	4.74	133.07	124.71
22	3	603	CLA	O2D-CGD-CBD	4.74	119.70	111.27
22	3	612	CLA	O2A-C1-C2	4.74	121.10	108.64
22	K	1404	CLA	O2A-C1-C2	4.74	121.09	108.64
22	4	604	CLA	O2D-CGD-CBD	4.74	119.69	111.27
22	B	1229	CLA	O2A-C1-C2	4.74	121.08	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	2	615	CLA	CMD-C2D-C1D	4.73	133.05	124.71
22	8	615	CLA	O2D-CGD-CBD	4.73	119.67	111.27
22	K	1404	CLA	CMD-C2D-C1D	4.73	133.04	124.71
22	L	1503	CLA	O2D-CGD-CBD	4.73	119.67	111.27
22	A	1109	CLA	O2A-C1-C2	4.72	121.05	108.64
22	8	607	CLA	O2D-CGD-CBD	4.72	119.66	111.27
22	A	1124	CLA	O2D-CGD-CBD	4.72	119.66	111.27
22	B	1225	CLA	CMD-C2D-C1D	4.71	133.01	124.71
22	A	1136	CLA	O2D-CGD-CBD	4.71	119.64	111.27
22	Z	615	CLA	O2D-CGD-CBD	4.71	119.64	111.27
22	A	1109	CLA	O2D-CGD-CBD	4.71	119.63	111.27
22	B	1228	CLA	O2D-CGD-CBD	4.70	119.62	111.27
22	B	1217	CLA	O2D-CGD-CBD	4.70	119.62	111.27
22	B	1203	CLA	O2D-CGD-CBD	4.70	119.61	111.27
22	B	1213	CLA	O2D-CGD-CBD	4.70	119.61	111.27
22	A	1126	CLA	O2A-C1-C2	4.69	120.96	108.64
22	A	1113	CLA	O2A-C1-C2	4.69	120.96	108.64
22	A	1123	CLA	O2D-CGD-CBD	4.69	119.60	111.27
22	6	618	CLA	CMD-C2D-C1D	4.68	132.97	124.71
39	2	503	LUT	C21-C26-C25	4.68	119.80	111.42
22	7	605	CLA	O2D-CGD-CBD	4.68	119.58	111.27
22	A	1124	CLA	O2A-C1-C2	4.67	120.91	108.64
22	B	1227	CLA	O2D-CGD-CBD	4.67	119.56	111.27
22	7	608	CLA	O2D-CGD-CBD	4.67	119.56	111.27
22	6	605	CLA	O2D-CGD-CBD	4.67	119.56	111.27
22	6	608	CLA	O2D-CGD-CBD	4.66	119.55	111.27
22	4	615	CLA	O2D-CGD-CBD	4.66	119.55	111.27
22	8	608	CLA	O2A-C1-C2	4.66	120.87	108.64
22	A	1117	CLA	O2D-CGD-CBD	4.65	119.53	111.27
21	A	1011	CL0	O2A-CGA-CBA	4.65	126.49	111.91
22	4	605	CLA	O2A-C1-C2	4.64	120.84	108.64
22	F	1302	CLA	O2D-CGD-CBD	4.64	119.51	111.27
22	5	603	CLA	O2D-CGD-CBD	4.63	119.49	111.27
22	1	607	CLA	O2D-CGD-CBD	4.63	119.49	111.27
21	A	1011	CL0	C3D-C2D-C1D	-4.62	99.53	105.83
22	B	1215	CLA	O2A-C1-C2	4.61	120.75	108.64
39	Z	503	LUT	C21-C26-C27	4.61	118.52	112.70
22	1	615	CLA	O2D-CGD-CBD	4.60	119.45	111.27
22	3	610	CLA	O2A-C1-C2	4.60	120.73	108.64
22	A	1013	CLA	CMB-C2B-C3B	4.60	133.28	124.68
22	A	1128	CLA	CMB-C2B-C1B	-4.59	121.40	128.46
39	Z	502	LUT	C21-C26-C27	4.59	118.51	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	6	604	CLA	O2D-CGD-CBD	4.59	119.42	111.27
22	B	1021	CLA	O2A-C1-C2	4.58	120.68	108.64
22	A	1139	CLA	O2A-C1-C2	4.58	120.68	108.64
22	A	1013	CLA	CMB-C2B-C1B	-4.57	121.43	128.46
26	4	801	LHG	O7-C7-C8	4.57	121.36	111.50
39	7	502	LUT	C21-C26-C27	4.57	118.48	112.70
22	3	618	CLA	CMD-C2D-C1D	4.57	132.77	124.71
39	7	501	LUT	C21-C26-C27	4.57	118.48	112.70
25	5	504	BCR	C34-C9-C10	-4.57	116.52	122.92
22	6	603	CLA	O2D-CGD-CBD	4.57	119.38	111.27
22	A	1119	CLA	O2D-CGD-CBD	4.56	119.38	111.27
22	A	1140	CLA	O2D-CGD-CBD	4.56	119.38	111.27
22	1	603	CLA	O2D-CGD-CBD	4.56	119.37	111.27
22	8	603	CLA	O2D-CGD-CBD	4.56	119.37	111.27
22	A	1103	CLA	O2D-CGD-CBD	4.55	119.36	111.27
22	A	1012	CLA	CMD-C2D-C1D	4.54	132.72	124.71
21	A	1011	CL0	CHD-C1D-ND	-4.54	120.28	124.45
37	1	503	C7Z	C15-C14-C13	-4.54	120.84	127.31
22	2	607	CLA	O2D-CGD-CBD	4.53	119.32	111.27
22	B	1232	CLA	O2D-CGD-CBD	4.53	119.32	111.27
26	6	801	LHG	O7-C7-C8	4.53	121.26	111.50
37	J	4002	C7Z	C35-C34-C33	-4.53	120.85	127.31
22	1	612	CLA	O2D-CGD-CBD	4.52	119.30	111.27
22	B	1239	CLA	O2A-C1-C2	4.52	120.50	108.64
26	1	801	LHG	O7-C7-C8	4.51	121.22	111.50
43	2	802	3PH	O21-C21-C22	4.51	121.22	111.50
22	7	603	CLA	O2D-CGD-CBD	4.51	119.28	111.27
22	B	1023	CLA	CMD-C2D-C1D	4.51	132.66	124.71
37	J	4002	C7Z	C11-C12-C13	-4.51	113.76	126.42
22	A	1103	CLA	O2A-C1-C2	4.50	120.47	108.64
22	B	1227	CLA	O2A-C1-C2	4.50	120.45	108.64
22	B	1226	CLA	CMB-C2B-C1B	-4.49	121.56	128.46
22	A	1124	CLA	CMD-C2D-C1D	4.48	132.60	124.71
26	Z	801	LHG	O7-C7-C8	4.48	121.15	111.50
22	Z	603	CLA	O2D-CGD-CBD	4.47	119.22	111.27
39	6	502	LUT	C21-C26-C27	4.47	118.36	112.70
26	B	5001	LHG	O7-C7-C8	4.47	121.14	111.50
37	J	4002	C7Z	C18-C5-C6	-4.47	119.51	124.53
22	B	1021	CLA	CMD-C2D-C1D	4.46	132.58	124.71
22	1	603	CLA	O2A-C1-C2	4.46	120.36	108.64
22	A	1133	CLA	O2A-C1-C2	4.45	120.34	108.64
22	8	612	CLA	O2D-CGD-CBD	4.45	119.18	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	9	607	CLA	O2D-CGD-CBD	4.45	119.17	111.27
22	7	612	CLA	O2D-CGD-CBD	4.44	119.16	111.27
37	J	4002	C7Z	C27-C28-C29	-4.44	119.53	126.23
22	A	1123	CLA	O2A-C1-C2	4.43	120.29	108.64
25	A	4004	BCR	C27-C26-C25	-4.43	116.30	122.73
22	A	1127	CLA	O2D-CGD-CBD	4.42	119.12	111.27
36	F	4001	RRX	C7-C8-C9	-4.41	119.58	126.23
37	1	503	C7Z	C21-C26-C25	-4.40	116.42	122.61
22	5	604	CLA	O2D-CGD-CBD	4.40	119.08	111.27
22	Z	612	CLA	O2D-CGD-CBD	4.39	119.08	111.27
37	1	503	C7Z	C18-C5-C6	-4.39	119.60	124.53
31	J	5001	LMG	O7-C10-C11	4.37	120.93	111.50
26	B	5006	LHG	O7-C7-C8	4.37	120.92	111.50
42	Z	504	QTB	C19-C17-C11	-4.36	104.31	110.60
39	8	501	LUT	C21-C26-C27	4.36	118.21	112.70
26	2	801	LHG	O7-C7-C8	4.35	120.87	111.50
25	I	4001	BCR	C23-C24-C25	-4.34	115.01	127.20
22	8	608	CLA	O2D-CGD-CBD	4.34	118.97	111.27
25	3	504	BCR	C4-C5-C6	-4.32	116.46	122.73
22	9	612	CLA	C1-C2-C3	-4.31	119.78	126.75
22	A	1119	CLA	O2A-C1-C2	4.29	119.91	108.64
39	6	501	LUT	C35-C34-C33	-4.29	121.19	127.31
39	9	501	LUT	C7-C8-C9	-4.29	119.76	126.23
22	F	1301	CLA	O2D-CGD-CBD	4.28	118.87	111.27
43	6	802	3PH	O21-C21-C22	4.28	120.72	111.50
32	9	802	DGA	OG2-CB1-CB2	4.26	120.69	111.50
36	F	4001	RRX	C33-C5-C6	-4.26	119.74	124.53
22	B	1221	CLA	O2A-CGA-CBA	4.25	125.24	111.91
26	7	801	LHG	O7-C7-C8	4.24	120.65	111.50
22	A	1013	CLA	O2A-C1-C2	4.24	119.78	108.64
25	3	504	BCR	C1-C6-C5	-4.23	116.65	122.61
39	Z	503	LUT	C15-C14-C13	-4.23	121.28	127.31
22	A	1013	CLA	O2D-CGD-CBD	4.23	118.78	111.27
26	5	801	LHG	O7-C7-C8	4.21	120.58	111.50
22	B	1203	CLA	O2A-C1-C2	4.21	119.70	108.64
31	A	5003	LMG	O7-C10-C11	4.21	120.57	111.50
25	G	4001	BCR	C19-C18-C17	4.20	125.39	118.94
22	A	1115	CLA	O2D-CGD-CBD	4.20	118.73	111.27
22	2	604	CLA	C1-C2-C3	-4.20	118.78	126.04
39	Z	503	LUT	C21-C26-C25	4.19	118.92	111.42
26	A	5001	LHG	O7-C7-C8	4.18	120.52	111.50
22	B	1222	CLA	O2A-C1-C2	4.18	119.62	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	9	612	CLA	CMD-C2D-C1D	4.18	132.08	124.71
39	4	502	LUT	C21-C26-C27	4.17	117.98	112.70
43	5	802	3PH	O21-C21-C22	4.16	120.46	111.50
22	5	615	CLA	O2D-CGD-CBD	4.15	118.64	111.27
39	7	502	LUT	C7-C8-C9	-4.14	119.98	126.23
39	2	502	LUT	C11-C10-C9	-4.13	121.41	127.31
22	7	603	CLA	C1-C2-C3	-4.12	118.92	126.04
39	2	501	LUT	C39-C29-C28	4.11	124.55	118.08
22	A	1115	CLA	CMD-C2D-C1D	4.10	131.94	124.71
40	5	611	CHL	C4A-NA-C1A	4.09	108.55	106.71
37	J	4002	C7Z	C8-C7-C6	-4.09	115.72	127.20
22	A	1128	CLA	CMD-C2D-C1D	4.09	131.92	124.71
22	B	1225	CLA	O2D-CGD-CBD	4.08	118.52	111.27
40	3	611	CHL	CHD-C1D-ND	-4.08	120.71	124.45
22	B	1239	CLA	C2C-C1C-NC	4.07	113.78	109.97
39	5	501	LUT	C21-C26-C27	4.05	117.82	112.70
39	8	502	LUT	C35-C34-C33	-4.05	121.54	127.31
39	Z	502	LUT	C7-C8-C9	-4.04	120.13	126.23
22	A	1122	CLA	O2D-CGD-CBD	4.04	118.44	111.27
37	5	505	C7Z	C35-C34-C33	-4.03	121.55	127.31
33	B	5003	DGD	O2G-C1B-C2B	4.03	120.19	111.50
39	Z	501	LUT	C21-C26-C27	4.03	117.80	112.70
39	3	501	LUT	C22-C23-C24	-4.03	107.16	111.74
25	A	4003	BCR	C28-C27-C26	-4.03	106.89	114.08
22	2	604	CLA	CHD-C1D-ND	-4.02	120.76	124.45
37	J	4002	C7Z	C21-C26-C25	-4.02	116.95	122.61
39	9	501	LUT	C21-C26-C27	4.01	117.77	112.70
39	8	501	LUT	C7-C8-C9	-4.00	120.19	126.23
39	1	502	LUT	C7-C8-C9	-3.99	120.20	126.23
22	4	615	CLA	CAA-C2A-C3A	-3.99	106.78	116.10
39	2	503	LUT	C15-C14-C13	-3.98	121.63	127.31
39	2	502	LUT	C21-C26-C27	3.97	117.72	112.70
37	5	505	C7Z	C1-C6-C5	-3.97	117.02	122.61
26	9	801	LHG	O7-C7-C8	3.96	120.03	111.50
35	B	5004	T7X	O16-C10-C12	3.95	120.02	111.50
22	B	1211	CLA	CMB-C2B-C3B	3.92	132.02	124.68
26	8	801	LHG	O7-C7-C8	3.92	119.95	111.50
39	8	501	LUT	C22-C23-C24	-3.90	107.31	111.74
39	Z	501	LUT	C22-C23-C24	-3.89	107.31	111.74
39	8	502	LUT	C21-C26-C27	3.89	117.61	112.70
22	A	1121	CLA	CHD-C1D-ND	-3.88	120.89	124.45
22	2	601	CLA	C1-C2-C3	-3.88	119.34	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	5	504	BCR	C36-C18-C17	-3.88	117.49	122.92
39	7	502	LUT	C35-C34-C33	-3.88	121.78	127.31
21	A	1011	CL0	CAA-C2A-C3A	-3.87	102.18	112.78
40	9	613	CHL	CHD-C1D-ND	-3.87	120.90	124.45
39	7	501	LUT	C22-C23-C24	-3.87	107.34	111.74
32	A	5005	DGA	OG2-CB1-CB2	3.87	119.83	111.50
25	B	4006	BCR	C19-C18-C17	3.85	124.85	118.94
22	B	1226	CLA	C2C-C1C-NC	3.85	113.58	109.97
22	6	618	CLA	C2D-C1D-ND	3.85	112.94	110.10
22	A	1108	CLA	O2D-CGD-CBD	3.85	118.10	111.27
39	6	502	LUT	C15-C14-C13	-3.84	121.82	127.31
39	2	502	LUT	C15-C14-C13	-3.84	121.82	127.31
26	4	802	LHG	O7-C7-C8	3.84	119.77	111.50
22	B	1021	CLA	C1-C2-C3	-3.83	119.41	126.04
22	5	618	CLA	C2D-C1D-ND	3.83	112.93	110.10
39	7	501	LUT	C35-C34-C33	-3.83	121.84	127.31
39	5	502	LUT	C15-C14-C13	-3.83	121.84	127.31
22	A	1120	CLA	CHD-C1D-ND	-3.82	120.94	124.45
27	3	802	NKP	OAA-PAC-OAF	-3.81	96.59	106.73
22	A	1013	CLA	CMD-C2D-C1D	3.81	131.42	124.71
40	4	613	CHL	CHD-C1D-ND	-3.80	120.96	124.45
39	4	501	LUT	C35-C34-C33	-3.79	121.89	127.31
22	B	1211	CLA	CHD-C1D-ND	-3.78	120.98	124.45
22	B	1222	CLA	O2D-CGD-CBD	3.78	117.98	111.27
39	8	502	LUT	C7-C8-C9	-3.77	120.54	126.23
36	F	4001	RRX	C20-C21-C22	-3.77	121.93	127.31
21	A	1011	CL0	C1D-ND-C4D	-3.77	103.66	106.33
22	B	1220	CLA	O2D-CGD-CBD	3.76	117.95	111.27
22	A	1123	CLA	C2C-C1C-NC	3.76	113.50	109.97
40	3	611	CHL	C2C-C3C-C4C	3.76	109.17	106.49
39	7	502	LUT	C15-C14-C13	-3.75	121.96	127.31
40	6	611	CHL	CHD-C1D-ND	-3.75	121.01	124.45
39	Z	503	LUT	C31-C30-C29	-3.75	121.96	127.31
22	B	1231	CLA	CHD-C1D-ND	-3.74	121.02	124.45
22	5	612	CLA	CHD-C1D-ND	-3.74	121.02	124.45
22	B	1235	CLA	CHD-C1D-ND	-3.74	121.02	124.45
22	5	605	CLA	CHD-C1D-ND	-3.74	121.02	124.45
39	1	502	LUT	C21-C26-C27	3.73	117.42	112.70
22	B	1226	CLA	CMD-C2D-C3D	-3.73	119.03	127.61
25	3	504	BCR	C33-C5-C4	3.73	120.78	113.62
22	A	1127	CLA	C1-C2-C3	-3.73	119.59	126.04
40	4	610	CHL	C4A-NA-C1A	3.73	108.38	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	608	CLA	CHD-C1D-ND	-3.73	121.03	124.45
26	A	5002	LHG	O7-C7-C8	3.73	119.53	111.50
22	A	1123	CLA	CMA-C3A-C4A	3.72	121.78	111.77
40	7	610	CHL	C4A-NA-C1A	3.72	108.38	106.71
39	6	501	LUT	C7-C8-C9	-3.72	120.62	126.23
22	A	1102	CLA	CMB-C2B-C3B	3.71	131.62	124.68
40	4	611	CHL	CHD-C1D-ND	-3.71	121.05	124.45
22	4	612	CLA	CHD-C1D-ND	-3.71	121.05	124.45
37	J	4002	C7Z	C38-C25-C26	-3.70	120.38	124.53
22	9	606	CLA	C1-C2-C3	-3.70	120.77	126.75
40	1	609	CHL	CHD-C1D-ND	-3.70	121.06	124.45
43	7	802	3PH	O21-C21-C22	3.69	119.46	111.50
39	6	501	LUT	C35-C15-C14	-3.69	115.91	123.47
22	B	1222	CLA	CMB-C2B-C3B	3.69	131.58	124.68
22	A	1114	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
22	3	610	CLA	C2C-C1C-NC	3.68	113.42	109.97
40	2	609	CHL	CHB-C4A-NA	3.68	129.60	124.51
39	9	501	LUT	C35-C34-C33	-3.68	122.06	127.31
39	3	501	LUT	C35-C34-C33	-3.67	122.07	127.31
39	Z	503	LUT	C18-C5-C6	-3.67	120.40	124.53
22	G	1601	CLA	C1-C2-C3	-3.67	120.81	126.75
22	B	1202	CLA	CHD-C1D-ND	-3.67	121.08	124.45
40	9	610	CHL	CHD-C1D-ND	-3.67	121.08	124.45
22	B	1201	CLA	CMB-C2B-C3B	3.67	131.54	124.68
22	A	1109	CLA	CHD-C1D-ND	-3.66	121.09	124.45
22	3	604	CLA	CHD-C1D-ND	-3.66	121.09	124.45
37	J	4002	C7Z	C1-C6-C5	-3.66	117.46	122.61
39	6	502	LUT	C22-C23-C24	-3.66	107.58	111.74
39	1	501	LUT	C21-C26-C27	3.66	117.33	112.70
22	7	602	CLA	C1-C2-C3	-3.66	120.83	126.75
22	9	604	CLA	CMA-C3A-C4A	3.66	121.60	111.77
22	A	1128	CLA	C2C-C1C-NC	3.65	113.39	109.97
22	7	612	CLA	C1-C2-C3	-3.65	120.85	126.75
39	1	501	LUT	C22-C23-C24	-3.65	107.59	111.74
40	2	609	CHL	CHD-C1D-ND	-3.64	121.11	124.45
22	B	1222	CLA	CHD-C1D-ND	-3.64	121.11	124.45
22	8	603	CLA	CHD-C1D-ND	-3.64	121.11	124.45
22	9	606	CLA	CHD-C1D-ND	-3.64	121.11	124.45
39	2	502	LUT	C22-C23-C24	-3.64	107.60	111.74
22	9	603	CLA	CBA-CAA-C2A	3.64	124.59	113.86
25	I	4001	BCR	C27-C26-C25	-3.63	117.46	122.73
39	1	502	LUT	C35-C34-C33	-3.62	122.14	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	1	802	SQD	O7-S-C6	-3.62	102.64	106.94
22	8	608	CLA	CHD-C1D-ND	-3.62	121.13	124.45
22	2	607	CLA	C2C-C1C-NC	3.62	113.36	109.97
40	Z	613	CHL	CHD-C1D-ND	-3.62	121.13	124.45
25	G	4001	BCR	C36-C18-C17	-3.62	117.86	122.92
39	4	501	LUT	C22-C23-C24	-3.61	107.63	111.74
39	4	501	LUT	C7-C8-C9	-3.61	120.78	126.23
40	2	613	CHL	CHD-C1D-ND	-3.61	121.14	124.45
37	J	4002	C7Z	C31-C32-C33	-3.61	116.28	126.42
25	A	4004	BCR	C28-C27-C26	-3.61	107.63	114.08
36	F	4001	RRX	C30-C25-C26	-3.60	117.54	122.61
25	B	4006	BCR	C12-C13-C14	-3.59	113.43	118.94
22	5	603	CLA	O2A-CGA-CBA	3.59	123.18	111.91
39	5	501	LUT	C35-C15-C14	-3.59	116.12	123.47
40	8	613	CHL	CHD-C1D-ND	-3.58	121.16	124.45
22	2	606	CLA	CMA-C3A-C4A	3.57	121.38	111.77
39	4	502	LUT	C35-C34-C33	-3.57	122.22	127.31
22	B	1022	CLA	CHD-C1D-ND	-3.57	121.17	124.45
22	5	622	CLA	C2C-C1C-NC	3.57	113.31	109.97
22	3	612	CLA	CHD-C1D-ND	-3.57	121.18	124.45
40	4	610	CHL	CHD-C1D-ND	-3.57	121.18	124.45
22	B	1219	CLA	C2C-C1C-NC	3.57	113.31	109.97
40	4	610	CHL	CMA-C3A-C4A	3.56	121.34	111.77
39	1	501	LUT	C35-C34-C33	-3.56	122.23	127.31
22	Z	608	CLA	CHD-C1D-ND	-3.56	121.18	124.45
22	7	611	CLA	C2D-C1D-ND	3.56	112.72	110.10
22	1	611	CLA	CHD-C1D-ND	-3.56	121.19	124.45
22	A	1114	CLA	CMB-C2B-C3B	3.55	131.33	124.68
22	F	1301	CLA	C1-C2-C3	-3.55	119.90	126.04
22	A	1122	CLA	CHD-C1D-ND	-3.55	121.19	124.45
22	6	612	CLA	C1-C2-C3	-3.55	121.01	126.75
22	5	604	CLA	CMA-C3A-C4A	3.55	121.31	111.77
22	9	601	CLA	CAA-C2A-C3A	-3.55	103.06	112.78
22	B	1230	CLA	C2D-C1D-ND	3.55	112.72	110.10
22	7	616	CLA	CHD-C1D-ND	-3.54	121.20	124.45
22	A	1102	CLA	O2A-CGA-CBA	3.54	123.03	111.91
43	8	806	3PH	O21-C21-C22	3.54	120.68	110.80
40	5	610	CHL	C4A-NA-C1A	3.54	108.30	106.71
39	9	502	LUT	C15-C14-C13	-3.54	122.26	127.31
27	A	5004	NKP	OAF-PAC-OAD	-3.54	96.55	106.47
25	5	504	BCR	C19-C18-C17	3.54	124.37	118.94
22	9	603	CLA	CAA-C2A-C3A	-3.53	103.10	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1226	CLA	CMB-C2B-C3B	3.53	131.29	124.68
25	7	504	BCR	C15-C14-C13	-3.53	122.28	127.31
39	Z	502	LUT	C35-C34-C33	-3.53	122.28	127.31
22	B	1239	CLA	C1C-C2C-C3C	-3.52	103.25	106.96
22	B	1241	CLA	CAA-C2A-C3A	-3.52	103.13	112.78
22	7	612	CLA	CHD-C1D-ND	-3.52	121.22	124.45
22	B	1215	CLA	CHD-C1D-ND	-3.52	121.22	124.45
40	6	617	CHL	CHD-C1D-ND	-3.52	121.22	124.45
22	B	1223	CLA	C2D-C1D-ND	3.52	112.70	110.10
22	B	1206	CLA	C2C-C1C-NC	3.52	113.27	109.97
27	8	802	NKP	OAF-PAC-OAD	-3.51	96.62	106.47
39	2	501	LUT	C15-C14-C13	-3.51	122.30	127.31
39	2	501	LUT	C30-C31-C32	-3.51	112.26	123.22
25	B	4006	BCR	C36-C18-C17	-3.51	118.01	122.92
39	3	502	LUT	C22-C23-C24	-3.51	107.75	111.74
22	2	602	CLA	CHD-C1D-ND	-3.51	121.23	124.45
22	7	609	CLA	C2D-C1D-ND	3.51	112.69	110.10
22	A	1126	CLA	CHD-C1D-ND	-3.51	121.23	124.45
40	6	610	CHL	C1-O2A-CGA	3.50	125.64	116.44
22	4	601	CLA	CHD-C1D-ND	-3.50	121.24	124.45
22	L	1502	CLA	CMA-C3A-C4A	3.50	121.18	111.77
22	5	601	CLA	CHD-C1D-ND	-3.50	121.24	124.45
25	5	504	BCR	C8-C9-C10	3.49	124.30	118.94
22	L	1502	CLA	C2D-C1D-ND	3.49	112.68	110.10
22	1	603	CLA	CHD-C1D-ND	-3.49	121.25	124.45
22	6	619	CLA	CHD-C1D-ND	-3.49	121.25	124.45
39	5	501	LUT	C35-C34-C33	-3.49	122.33	127.31
22	A	1128	CLA	CMB-C2B-C3B	3.49	131.20	124.68
39	Z	502	LUT	C15-C14-C13	-3.48	122.34	127.31
22	1	606	CLA	CHD-C1D-ND	-3.47	121.26	124.45
39	Z	501	LUT	C7-C8-C9	-3.47	120.98	126.23
40	1	610	CHL	CHD-C1D-ND	-3.47	121.26	124.45
40	2	613	CHL	C1-C2-C3	-3.47	121.13	126.75
22	2	606	CLA	C2C-C1C-NC	3.47	113.22	109.97
22	A	1138	CLA	CHD-C1D-ND	-3.47	121.27	124.45
22	8	615	CLA	C2C-C1C-NC	3.47	113.22	109.97
40	3	611	CHL	C3C-C4C-NC	-3.47	106.68	110.57
39	3	501	LUT	C7-C8-C9	-3.47	121.00	126.23
22	B	1201	CLA	CHD-C1D-ND	-3.46	121.27	124.45
40	4	617	CHL	CHD-C1D-ND	-3.46	121.27	124.45
22	7	611	CLA	C1-C2-C3	-3.46	121.15	126.75
22	A	1102	CLA	CHD-C1D-ND	-3.46	121.27	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1103	CLA	CHD-C1D-ND	-3.46	121.27	124.45
22	A	1117	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
22	A	1137	CLA	CHD-C1D-ND	-3.46	121.28	124.45
22	Z	603	CLA	CHD-C1D-ND	-3.46	121.28	124.45
22	8	611	CLA	CHD-C1D-ND	-3.45	121.28	124.45
25	B	4003	BCR	C23-C22-C21	3.45	124.24	118.94
22	1	615	CLA	C2C-C1C-NC	3.45	113.20	109.97
22	B	1213	CLA	CHD-C1D-ND	-3.45	121.29	124.45
22	Z	601	CLA	CHD-C1D-ND	-3.45	121.29	124.45
25	L	4002	BCR	C33-C5-C6	-3.44	120.66	124.53
22	2	605	CLA	C1-C2-C3	-3.44	121.18	126.75
39	2	503	LUT	C31-C32-C33	-3.44	116.75	126.42
22	7	611	CLA	CHD-C1D-ND	-3.44	121.29	124.45
22	A	1136	CLA	C2C-C1C-NC	3.44	113.19	109.97
40	8	610	CHL	CHD-C1D-ND	-3.44	121.29	124.45
40	8	610	CHL	C4A-NA-C1A	3.44	108.25	106.71
22	Z	604	CLA	CHD-C1D-ND	-3.44	121.30	124.45
22	3	603	CLA	O2A-CGA-CBA	3.44	122.69	111.91
22	B	1218	CLA	CHD-C1D-ND	-3.44	121.30	124.45
22	5	615	CLA	C2C-C1C-NC	3.44	113.19	109.97
25	6	504	BCR	C19-C18-C17	3.44	124.21	118.94
22	B	1209	CLA	CHD-C1D-ND	-3.44	121.30	124.45
22	B	1235	CLA	C1-O2A-CGA	3.43	125.45	116.44
25	A	4005	BCR	C23-C24-C25	-3.43	117.56	127.20
22	6	603	CLA	CBA-CAA-C2A	3.43	123.99	113.86
37	5	505	C7Z	C27-C28-C29	-3.43	121.05	126.23
39	Z	501	LUT	C35-C34-C33	-3.43	122.42	127.31
22	3	606	CLA	CHD-C1D-ND	-3.43	121.31	124.45
22	A	1141	CLA	C2C-C1C-NC	3.43	113.18	109.97
22	A	1120	CLA	C2D-C1D-ND	3.42	112.63	110.10
22	1	607	CLA	C2C-C1C-NC	3.42	113.18	109.97
22	B	1210	CLA	C1-C2-C3	-3.42	120.14	126.04
22	A	1132	CLA	C2C-C1C-NC	3.41	113.17	109.97
22	4	606	CLA	CHD-C1D-ND	-3.41	121.32	124.45
22	B	1216	CLA	CHD-C1D-ND	-3.41	121.32	124.45
22	9	604	CLA	O2A-CGA-CBA	3.41	122.61	111.91
22	5	606	CLA	C1-C2-C3	-3.41	121.23	126.75
39	3	502	LUT	C15-C14-C13	-3.41	122.44	127.31
22	B	1202	CLA	CAA-C2A-C3A	-3.41	103.44	112.78
22	A	1127	CLA	CMD-C2D-C1D	3.41	130.72	124.71
22	9	604	CLA	CHD-C1D-ND	-3.41	121.32	124.45
25	B	4003	BCR	C34-C9-C10	-3.41	118.15	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1221	CLA	CMB-C2B-C3B	3.40	131.05	124.68
22	A	1121	CLA	CMA-C3A-C4A	3.40	120.92	111.77
22	1	603	CLA	CMA-C3A-C4A	3.40	120.92	111.77
40	8	613	CHL	CMA-C3A-C4A	3.40	120.92	111.77
22	6	612	CLA	C2D-C1D-ND	3.40	112.61	110.10
36	F	4001	RRX	C16-C17-C18	-3.40	122.46	127.31
22	B	1204	CLA	CHD-C1D-ND	-3.40	121.33	124.45
22	B	1228	CLA	CHD-C1D-ND	-3.40	121.33	124.45
22	6	603	CLA	O2A-CGA-CBA	3.39	122.56	111.91
22	8	603	CLA	C1-C2-C3	-3.39	120.18	126.04
25	B	4007	BCR	C23-C24-C25	-3.39	117.68	127.20
22	4	604	CLA	CMB-C2B-C3B	3.39	131.02	124.68
25	B	4002	BCR	C33-C5-C6	-3.39	120.72	124.53
22	1	605	CLA	C1-C2-C3	-3.39	120.18	126.04
22	B	1215	CLA	C2C-C1C-NC	3.39	113.15	109.97
22	1	607	CLA	CAA-C2A-C3A	-3.39	103.50	112.78
22	A	1125	CLA	C2D-C1D-ND	3.39	112.60	110.10
22	A	1112	CLA	CHD-C1D-ND	-3.39	121.34	124.45
22	6	606	CLA	CHD-C1D-ND	-3.39	121.34	124.45
22	A	1117	CLA	C1-C2-C3	-3.38	120.19	126.04
39	7	501	LUT	C7-C8-C9	-3.38	121.12	126.23
22	A	1118	CLA	C2D-C1D-ND	3.38	112.60	110.10
22	6	612	CLA	CHD-C1D-ND	-3.38	121.35	124.45
22	B	1241	CLA	C1-C2-C3	-3.38	120.20	126.04
22	A	1139	CLA	CHD-C1D-ND	-3.38	121.35	124.45
22	4	601	CLA	C1-C2-C3	-3.37	120.21	126.04
41	2	803	SQD	O7-S-C6	-3.37	102.93	106.94
37	5	505	C7Z	C31-C30-C29	-3.37	122.50	127.31
22	7	603	CLA	CHD-C1D-ND	-3.37	121.35	124.45
22	K	1403	CLA	C2C-C1C-NC	3.37	113.13	109.97
39	6	501	LUT	C22-C23-C24	-3.37	107.90	111.74
39	2	503	LUT	C40-C33-C34	-3.37	118.20	122.92
22	A	1133	CLA	CHD-C1D-ND	-3.37	121.36	124.45
22	1	601	CLA	CHD-C1D-ND	-3.37	121.36	124.45
22	6	604	CLA	CHD-C1D-ND	-3.37	121.36	124.45
40	Z	610	CHL	CHD-C1D-ND	-3.37	121.36	124.45
22	A	1115	CLA	CHD-C1D-ND	-3.37	121.36	124.45
22	3	613	CLA	CHD-C1D-ND	-3.37	121.36	124.45
22	2	612	CLA	C1-C2-C3	-3.37	121.30	126.75
22	A	1131	CLA	C2C-C1C-NC	3.37	113.13	109.97
40	4	611	CHL	C4A-NA-C1A	3.37	108.22	106.71
36	F	4001	RRX	C24-C23-C22	-3.37	121.15	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	602	CLA	C2C-C1C-NC	3.37	113.12	109.97
36	F	4001	RRX	C33-C5-C4	3.36	120.08	113.62
22	Z	612	CLA	C2C-C1C-NC	3.36	113.12	109.97
22	A	1107	CLA	C2C-C1C-NC	3.36	113.12	109.97
25	B	4005	BCR	C35-C13-C12	3.36	123.37	118.08
22	B	1210	CLA	CHD-C1D-ND	-3.36	121.37	124.45
22	B	1224	CLA	C2C-C1C-NC	3.36	113.12	109.97
22	7	608	CLA	C2C-C1C-NC	3.36	113.12	109.97
22	3	603	CLA	CHD-C1D-ND	-3.36	121.37	124.45
22	6	609	CLA	CHD-C1D-ND	-3.36	121.37	124.45
22	3	604	CLA	CAA-C2A-C3A	-3.35	103.59	112.78
22	B	1234	CLA	CMB-C2B-C3B	3.35	130.96	124.68
39	2	502	LUT	C38-C25-C24	-3.35	116.38	123.56
22	B	1208	CLA	CHD-C1D-ND	-3.35	121.37	124.45
25	6	504	BCR	C33-C5-C4	3.35	120.06	113.62
40	8	610	CHL	CHC-C1C-NC	3.35	129.29	124.20
22	B	1218	CLA	C2D-C1D-ND	3.35	112.57	110.10
22	8	603	CLA	CBA-CAA-C2A	3.35	123.74	113.86
39	5	501	LUT	C7-C8-C9	-3.34	121.18	126.23
22	6	604	CLA	O2A-CGA-CBA	3.34	122.40	111.91
22	B	1229	CLA	CHD-C1D-ND	-3.34	121.39	124.45
40	6	613	CHL	CHD-C1D-ND	-3.34	121.39	124.45
22	B	1218	CLA	C2C-C1C-NC	3.34	113.10	109.97
22	A	1113	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
22	A	1117	CLA	CMB-C2B-C3B	3.34	130.92	124.68
37	1	503	C7Z	C8-C7-C6	-3.33	117.84	127.20
22	2	615	CLA	C2D-C1D-ND	3.33	112.56	110.10
22	7	615	CLA	CHD-C1D-ND	-3.33	121.39	124.45
40	5	610	CHL	CHB-C4A-NA	3.33	129.12	124.51
39	4	502	LUT	C18-C5-C6	-3.33	120.79	124.53
22	3	604	CLA	O2A-CGA-CBA	3.33	122.34	111.91
22	B	1236	CLA	CHD-C1D-ND	-3.33	121.40	124.45
40	6	610	CHL	CHD-C1D-ND	-3.33	121.40	124.45
25	3	506	BCR	C33-C5-C6	-3.32	120.80	124.53
39	3	502	LUT	C35-C34-C33	-3.32	122.57	127.31
22	4	606	CLA	C1-C2-C3	-3.32	121.38	126.75
22	7	613	CLA	CMB-C2B-C3B	3.32	130.89	124.68
39	9	502	LUT	C22-C23-C24	-3.32	107.96	111.74
22	5	603	CLA	CHD-C1D-ND	-3.32	121.41	124.45
25	A	4005	BCR	C12-C13-C14	-3.32	113.85	118.94
22	B	1236	CLA	C2D-C1D-ND	3.32	112.55	110.10
22	5	618	CLA	CHD-C1D-ND	-3.31	121.41	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Z	601	CLA	C1-C2-C3	-3.31	120.31	126.04
39	8	501	LUT	C35-C34-C33	-3.31	122.58	127.31
22	B	1226	CLA	CHD-C1D-ND	-3.31	121.41	124.45
22	A	1122	CLA	C1-O2A-CGA	3.31	125.14	116.44
22	B	1229	CLA	C2D-C1D-ND	3.31	112.55	110.10
25	K	4001	BCR	C28-C27-C26	-3.31	108.17	114.08
22	Z	615	CLA	C2C-C1C-NC	3.31	113.07	109.97
39	1	502	LUT	C22-C23-C24	-3.30	107.98	111.74
22	B	1211	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
22	4	612	CLA	C1-C2-C3	-3.30	121.41	126.75
22	Z	612	CLA	CHD-C1D-ND	-3.30	121.42	124.45
22	3	601	CLA	CHD-C1D-ND	-3.30	121.42	124.45
22	7	612	CLA	CMB-C2B-C3B	3.30	130.85	124.68
39	2	501	LUT	C7-C8-C9	-3.30	121.25	126.23
22	7	601	CLA	CHD-C1D-ND	-3.30	121.42	124.45
22	Z	602	CLA	C2C-C1C-NC	3.30	113.06	109.97
22	A	1132	CLA	CHD-C1D-ND	-3.30	121.42	124.45
22	Z	611	CLA	CHD-C1D-ND	-3.30	121.42	124.45
25	3	506	BCR	C37-C22-C21	-3.30	118.31	122.92
22	2	603	CLA	C2D-C1D-ND	3.30	112.53	110.10
22	A	1117	CLA	C2C-C1C-NC	3.30	113.06	109.97
22	3	607	CLA	C2C-C1C-NC	3.30	113.06	109.97
22	A	1108	CLA	CHD-C1D-ND	-3.29	121.43	124.45
22	9	604	CLA	C2D-C1D-ND	3.29	112.53	110.10
22	L	1503	CLA	CHD-C1D-ND	-3.29	121.43	124.45
22	A	1101	CLA	CHD-C1D-ND	-3.29	121.43	124.45
22	6	608	CLA	C2C-C1C-NC	3.29	113.05	109.97
28	B	6101	LMT	C1'-O5'-C5'	-3.28	107.24	113.69
22	4	608	CLA	C2C-C1C-NC	3.28	113.05	109.97
22	B	1239	CLA	C1-C2-C3	-3.28	120.37	126.04
22	A	1129	CLA	C1-C2-C3	-3.28	121.44	126.75
22	A	1134	CLA	C2C-C1C-NC	3.28	113.05	109.97
22	5	603	CLA	C1-C2-C3	-3.28	120.37	126.04
40	Z	609	CHL	CMA-C3A-C4A	3.28	120.59	111.77
25	3	504	BCR	C36-C18-C17	-3.28	118.33	122.92
22	A	1105	CLA	CHD-C1D-ND	-3.28	121.44	124.45
22	A	1013	CLA	C2D-C1D-ND	3.28	112.52	110.10
22	J	1901	CLA	CHD-C1D-ND	-3.28	121.44	124.45
40	5	617	CHL	CHD-C1D-ND	-3.28	121.44	124.45
22	A	1104	CLA	C1-C2-C3	-3.28	120.38	126.04
22	1	601	CLA	C1-C2-C3	-3.28	120.38	126.04
22	6	608	CLA	CHD-C1D-ND	-3.28	121.44	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	606	CLA	C1-O2A-CGA	3.27	125.03	116.44
39	2	503	LUT	C7-C8-C9	3.27	131.18	126.23
28	8	805	LMT	C1'-O5'-C5'	-3.27	107.26	113.69
22	6	601	CLA	CHD-C1D-ND	-3.27	121.45	124.45
22	6	619	CLA	CMB-C2B-C3B	3.27	130.80	124.68
22	A	1103	CLA	C2D-C1D-ND	3.27	112.52	110.10
22	A	1110	CLA	O2A-CGA-CBA	3.27	122.17	111.91
22	4	608	CLA	CHD-C1D-ND	-3.27	121.45	124.45
22	5	608	CLA	C2C-C1C-NC	3.27	113.03	109.97
22	B	1215	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
22	3	618	CLA	C2C-C1C-NC	3.27	113.03	109.97
22	6	603	CLA	CHD-C1D-ND	-3.27	121.45	124.45
22	F	1301	CLA	O2A-C1-C2	3.27	117.22	108.64
22	Z	615	CLA	CHD-C1D-ND	-3.26	121.45	124.45
40	6	611	CHL	C4A-NA-C1A	3.26	108.17	106.71
22	7	613	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
22	5	606	CLA	C2C-C1C-NC	3.26	113.03	109.97
22	B	1204	CLA	C2C-C1C-NC	3.26	113.03	109.97
22	A	1117	CLA	CHD-C1D-ND	-3.26	121.46	124.45
22	A	1118	CLA	CHD-C1D-ND	-3.26	121.46	124.45
22	A	1140	CLA	C1-C2-C3	-3.26	120.41	126.04
22	K	1404	CLA	CMA-C3A-C4A	3.26	120.53	111.77
22	A	1102	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
39	Z	503	LUT	C31-C32-C33	-3.26	117.27	126.42
22	A	1106	CLA	C1-C2-C3	-3.26	120.41	126.04
22	9	605	CLA	C2C-C1C-NC	3.26	113.02	109.97
22	6	609	CLA	C2C-C1C-NC	3.25	113.02	109.97
39	2	501	LUT	C35-C34-C33	-3.25	122.67	127.31
22	8	612	CLA	CHD-C1D-ND	-3.25	121.46	124.45
25	5	503	BCR	C19-C18-C17	3.25	123.93	118.94
22	A	1130	CLA	CHD-C1D-ND	-3.25	121.47	124.45
22	7	603	CLA	CMA-C3A-C4A	3.25	120.50	111.77
22	7	603	CLA	CBA-CAA-C2A	3.25	123.45	113.86
22	7	613	CLA	CHD-C1D-ND	-3.25	121.47	124.45
22	9	607	CLA	C2C-C1C-NC	3.25	113.01	109.97
22	7	606	CLA	CHD-C1D-ND	-3.24	121.47	124.45
39	6	501	LUT	C18-C5-C6	-3.24	120.89	124.53
22	5	606	CLA	CHD-C1D-ND	-3.24	121.47	124.45
22	2	608	CLA	CHD-C1D-ND	-3.24	121.47	124.45
22	1	612	CLA	CHD-C1D-ND	-3.24	121.48	124.45
22	3	616	CLA	C2C-C1C-NC	3.24	113.01	109.97
22	4	603	CLA	C1-C2-C3	-3.24	120.44	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	4003	BCR	C33-C5-C4	3.24	119.84	113.62
40	7	610	CHL	CHD-C1D-ND	-3.24	121.48	124.45
22	A	1135	CLA	C1-C2-C3	-3.24	120.45	126.04
22	A	1114	CLA	C2C-C1C-NC	3.24	113.00	109.97
22	B	1212	CLA	C1-C2-C3	-3.24	120.45	126.04
23	A	2001	PQN	C14-C13-C15	3.23	120.71	115.27
22	8	601	CLA	CHD-C1D-ND	-3.23	121.48	124.45
39	7	502	LUT	C11-C10-C9	-3.23	122.70	127.31
22	3	610	CLA	CHD-C1D-ND	-3.23	121.48	124.45
22	A	1111	CLA	CMB-C2B-C3B	3.23	130.72	124.68
22	L	1503	CLA	C1-C2-C3	-3.23	121.53	126.75
22	B	1241	CLA	CHD-C1D-ND	-3.23	121.49	124.45
22	A	1137	CLA	C2C-C1C-NC	3.22	112.99	109.97
22	8	604	CLA	CHD-C1D-ND	-3.22	121.49	124.45
22	3	608	CLA	C2C-C1C-NC	3.22	112.99	109.97
22	3	604	CLA	CBA-CAA-C2A	3.22	123.38	113.86
22	5	604	CLA	CHD-C1D-ND	-3.22	121.49	124.45
22	B	1222	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
22	8	603	CLA	CMA-C3A-C4A	3.22	120.43	111.77
22	B	1208	CLA	C2D-C1D-ND	3.22	112.48	110.10
22	Z	606	CLA	CHD-C1D-ND	-3.22	121.50	124.45
22	3	604	CLA	C1D-ND-C4D	-3.22	104.05	106.33
22	5	605	CLA	CMB-C2B-C3B	3.22	130.70	124.68
22	A	1129	CLA	CHD-C1D-ND	-3.22	121.50	124.45
22	6	603	CLA	C2C-C1C-NC	3.22	112.99	109.97
22	B	1239	CLA	CHD-C1D-ND	-3.22	121.50	124.45
22	B	1202	CLA	CMB-C2B-C3B	3.22	130.70	124.68
22	Z	603	CLA	CMA-C3A-C4A	3.22	120.42	111.77
22	4	607	CLA	C2C-C1C-NC	3.22	112.98	109.97
22	6	602	CLA	C2C-C1C-NC	3.22	112.98	109.97
22	9	603	CLA	C2C-C1C-NC	3.22	112.98	109.97
22	4	605	CLA	C2C-C1C-NC	3.21	112.98	109.97
25	3	504	BCR	C19-C18-C17	3.21	123.87	118.94
22	A	1136	CLA	CHD-C1D-ND	-3.21	121.50	124.45
22	A	1107	CLA	CMB-C2B-C3B	3.21	130.68	124.68
22	A	1141	CLA	CHD-C1D-ND	-3.21	121.50	124.45
22	3	616	CLA	CHD-C1D-ND	-3.21	121.50	124.45
22	Z	606	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
22	B	1230	CLA	CHD-C1D-ND	-3.21	121.51	124.45
22	A	1135	CLA	C2C-C1C-NC	3.21	112.97	109.97
22	8	606	CLA	CHD-C1D-ND	-3.20	121.51	124.45
40	2	610	CHL	CMA-C3A-C4A	3.20	120.37	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	6	502	LUT	C35-C34-C33	-3.20	122.75	127.31
22	7	615	CLA	C2D-C1D-ND	3.20	112.46	110.10
22	B	1221	CLA	CHD-C1D-ND	-3.20	121.52	124.45
25	A	4003	BCR	C27-C26-C25	-3.20	118.09	122.73
22	B	1240	CLA	C1-C2-C3	-3.20	120.52	126.04
22	L	1503	CLA	C2C-C1C-NC	3.19	112.97	109.97
22	5	618	CLA	C1-C2-C3	-3.19	120.52	126.04
33	B	5003	DGD	O1G-C1A-C2A	3.19	121.93	111.91
22	8	601	CLA	C1-C2-C3	-3.19	120.52	126.04
22	2	612	CLA	CHD-C1D-ND	-3.19	121.52	124.45
22	3	604	CLA	C2D-C1D-ND	3.19	112.46	110.10
22	K	1402	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
22	7	609	CLA	CHD-C1D-ND	-3.19	121.52	124.45
22	K	1403	CLA	CHD-C1D-ND	-3.19	121.52	124.45
25	6	503	BCR	C15-C14-C13	-3.19	122.76	127.31
22	B	1214	CLA	C2D-C1D-ND	3.19	112.45	110.10
22	B	1238	CLA	C2C-C1C-NC	3.19	112.96	109.97
22	7	602	CLA	C2C-C1C-NC	3.19	112.96	109.97
22	2	607	CLA	CMA-C3A-C4A	3.19	120.34	111.77
39	9	501	LUT	C22-C23-C24	-3.19	108.11	111.74
22	7	604	CLA	O2A-CGA-CBA	3.19	121.91	111.91
25	J	4001	BCR	C36-C18-C17	-3.18	118.46	122.92
22	6	604	CLA	CMA-C3A-C4A	3.18	120.33	111.77
39	2	501	LUT	C21-C26-C25	3.18	117.12	111.42
22	G	1601	CLA	C2C-C1C-NC	3.18	112.95	109.97
22	7	608	CLA	CHD-C1D-ND	-3.18	121.53	124.45
25	8	503	BCR	C33-C5-C6	-3.18	120.96	124.53
25	6	503	BCR	C33-C5-C6	-3.18	120.96	124.53
22	A	1012	CLA	C2D-C1D-ND	3.18	112.45	110.10
22	6	607	CLA	C1-C2-C3	-3.18	120.54	126.04
22	1	603	CLA	C2D-C1D-ND	3.18	112.45	110.10
22	9	608	CLA	C2C-C1C-NC	3.18	112.95	109.97
22	A	1106	CLA	CHD-C1D-ND	-3.18	121.53	124.45
22	A	1114	CLA	CHD-C1D-ND	-3.18	121.53	124.45
22	A	1135	CLA	CHD-C1D-ND	-3.18	121.53	124.45
22	G	1602	CLA	C2C-C1C-NC	3.18	112.95	109.97
25	A	4004	BCR	C33-C5-C6	-3.17	120.96	124.53
40	Z	613	CHL	C2C-C3C-C4C	3.17	108.75	106.49
22	5	609	CLA	C2C-C1C-NC	3.17	112.95	109.97
22	B	1238	CLA	CHD-C1D-ND	-3.17	121.54	124.45
40	2	610	CHL	CHD-C1D-ND	-3.17	121.54	124.45
25	3	503	BCR	C23-C24-C25	-3.17	118.29	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1108	CLA	C2C-C1C-NC	3.17	112.94	109.97
22	A	1121	CLA	C2C-C1C-NC	3.17	112.94	109.97
22	7	616	CLA	O2A-CGA-CBA	3.17	121.86	111.91
22	A	1119	CLA	CHD-C1D-ND	-3.17	121.54	124.45
22	5	604	CLA	O2A-CGA-CBA	3.17	121.86	111.91
22	4	602	CLA	O2A-CGA-CBA	3.17	121.85	111.91
22	B	1232	CLA	CHD-C1D-ND	-3.17	121.54	124.45
22	8	609	CLA	C2C-C1C-NC	3.17	112.94	109.97
22	8	604	CLA	CMA-C3A-C4A	3.17	120.28	111.77
40	5	610	CHL	CHD-C1D-ND	-3.17	121.54	124.45
22	6	605	CLA	CMB-C2B-C3B	3.17	130.60	124.68
37	1	503	C7Z	C35-C15-C14	-3.17	116.99	123.47
22	6	607	CLA	C2C-C1C-NC	3.16	112.94	109.97
22	6	609	CLA	C1-C2-C3	-3.16	120.57	126.04
22	A	1122	CLA	C2C-C1C-NC	3.16	112.93	109.97
22	7	603	CLA	CAA-C2A-C3A	-3.16	104.12	112.78
22	F	1302	CLA	C2D-C1D-ND	3.16	112.43	110.10
22	2	603	CLA	CAA-C2A-C3A	-3.16	104.13	112.78
22	Z	603	CLA	C1-C2-C3	-3.16	121.64	126.75
22	6	606	CLA	C2C-C1C-NC	3.16	112.93	109.97
22	9	602	CLA	CMB-C2B-C3B	3.16	130.59	124.68
22	5	608	CLA	CHD-C1D-ND	-3.16	121.55	124.45
22	3	608	CLA	C2D-C1D-ND	3.16	112.43	110.10
22	6	615	CLA	C2C-C1C-NC	3.16	112.93	109.97
22	8	607	CLA	C2C-C1C-NC	3.16	112.93	109.97
22	B	1220	CLA	C2D-C1D-ND	3.16	112.43	110.10
22	8	603	CLA	C2D-C1D-ND	3.16	112.43	110.10
22	A	1111	CLA	CHD-C1D-ND	-3.16	121.55	124.45
22	9	608	CLA	CHD-C1D-ND	-3.15	121.56	124.45
22	B	1022	CLA	C2C-C1C-NC	3.15	112.92	109.97
40	4	613	CHL	C1-O2A-CGA	3.15	124.70	116.44
22	A	1130	CLA	C1-C2-C3	-3.15	120.60	126.04
22	9	612	CLA	CMB-C2B-C3B	3.15	130.57	124.68
22	B	1226	CLA	C1C-C2C-C3C	-3.15	103.65	106.96
22	B	1210	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
22	9	607	CLA	CHD-C1D-ND	-3.14	121.56	124.45
22	3	607	CLA	C1-O2A-CGA	3.14	124.69	116.44
22	1	615	CLA	CHD-C1D-ND	-3.14	121.57	124.45
22	B	1238	CLA	CMA-C3A-C4A	3.14	120.22	111.77
25	5	504	BCR	C30-C25-C26	-3.14	118.19	122.61
22	4	604	CLA	CHD-C1D-ND	-3.14	121.57	124.45
22	3	603	CLA	C2D-C1D-ND	3.14	112.42	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	6	618	CLA	CHD-C1D-ND	-3.14	121.57	124.45
22	1	601	CLA	C2D-C1D-ND	3.14	112.42	110.10
22	7	605	CLA	CHD-C1D-ND	-3.14	121.57	124.45
21	A	1011	CL0	CMC-C2C-C1C	3.14	129.82	125.04
22	B	1223	CLA	C1-C2-C3	-3.14	120.62	126.04
22	7	607	CLA	C2C-C1C-NC	3.14	112.91	109.97
22	5	604	CLA	C2D-C1D-ND	3.14	112.42	110.10
22	2	603	CLA	C2C-C1C-NC	3.13	112.91	109.97
39	Z	501	LUT	C18-C5-C6	-3.13	121.01	124.53
22	A	1109	CLA	CAA-C2A-C3A	-3.13	104.20	112.78
22	9	607	CLA	C1-C2-C3	-3.13	120.62	126.04
25	B	4003	BCR	C33-C5-C6	-3.13	121.01	124.53
22	A	1113	CLA	CMB-C2B-C3B	3.13	130.54	124.68
39	Z	503	LUT	C7-C8-C9	-3.13	121.50	126.23
22	8	604	CLA	O2A-CGA-CBA	3.13	121.74	111.91
25	B	4001	BCR	C23-C24-C25	-3.13	118.41	127.20
39	2	503	LUT	C18-C5-C6	-3.13	121.01	124.53
22	6	612	CLA	C2C-C1C-NC	3.13	112.91	109.97
22	Z	607	CLA	C2C-C1C-NC	3.13	112.90	109.97
22	3	605	CLA	C2C-C1C-NC	3.13	112.90	109.97
39	Z	502	LUT	C22-C23-C24	-3.13	108.18	111.74
22	5	608	CLA	C2D-C1D-ND	3.13	112.41	110.10
40	6	611	CHL	C1-C2-C3	-3.13	121.69	126.75
22	8	605	CLA	C2C-C1C-NC	3.13	112.90	109.97
22	B	1241	CLA	CMA-C3A-C4A	3.13	120.18	111.77
22	6	609	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
22	A	1115	CLA	C1-C2-C3	-3.13	120.63	126.04
22	A	1012	CLA	CHD-C1D-ND	-3.13	121.58	124.45
22	2	612	CLA	CMB-C2B-C3B	3.13	130.53	124.68
22	2	602	CLA	C2C-C1C-NC	3.13	112.90	109.97
22	B	1023	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
22	A	1113	CLA	CHD-C1D-ND	-3.12	121.58	124.45
40	4	610	CHL	C4D-CHA-C1A	3.12	125.05	121.25
25	7	503	BCR	C36-C18-C17	-3.12	118.55	122.92
22	8	611	CLA	C2C-C1C-NC	3.12	112.89	109.97
22	8	612	CLA	C2C-C1C-NC	3.12	112.89	109.97
22	B	1208	CLA	CMB-C2B-C3B	3.12	130.51	124.68
25	B	4003	BCR	C37-C22-C21	-3.12	118.55	122.92
22	A	1134	CLA	CHD-C1D-ND	-3.12	121.59	124.45
22	3	603	CLA	C2C-C1C-NC	3.12	112.89	109.97
22	1	604	CLA	C2C-C1C-NC	3.11	112.89	109.97
22	A	1134	CLA	C1-C2-C3	-3.11	120.66	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	6	602	CLA	C1-C2-C3	-3.11	120.66	126.04
22	B	1023	CLA	CAA-C2A-C3A	-3.11	104.25	112.78
39	4	501	LUT	C35-C15-C14	-3.11	117.10	123.47
22	B	1213	CLA	C2D-C1D-ND	3.11	112.40	110.10
22	A	1131	CLA	CHD-C1D-ND	-3.11	121.59	124.45
40	Z	613	CHL	C3C-C4C-NC	-3.11	107.08	110.57
40	6	610	CHL	C3C-C4C-NC	-3.11	107.08	110.57
22	B	1241	CLA	C2D-C1D-ND	3.11	112.40	110.10
22	F	1301	CLA	CHD-C1D-ND	-3.11	121.60	124.45
22	B	1234	CLA	C2C-C1C-NC	3.11	112.89	109.97
22	L	1502	CLA	C2C-C1C-NC	3.11	112.89	109.97
39	9	501	LUT	C18-C5-C6	-3.11	121.04	124.53
22	3	604	CLA	CMA-C3A-C4A	3.11	120.13	111.77
22	4	603	CLA	CMA-C3A-C4A	3.11	120.12	111.77
22	A	1111	CLA	C1-C2-C3	-3.11	120.67	126.04
22	K	1402	CLA	C1-C2-C3	-3.10	120.67	126.04
22	B	1203	CLA	C2C-C1C-NC	3.10	112.88	109.97
39	4	502	LUT	C22-C23-C24	-3.10	108.21	111.74
40	1	610	CHL	C4A-NA-C1A	3.10	108.10	106.71
25	5	503	BCR	C36-C18-C17	-3.10	118.58	122.92
22	3	603	CLA	CMA-C3A-C4A	3.10	120.11	111.77
22	9	605	CLA	C1-C2-C3	-3.10	120.68	126.04
22	4	602	CLA	C6-C5-C3	-3.10	109.55	114.62
22	K	1402	CLA	CHD-C1D-ND	-3.10	121.61	124.45
22	1	611	CLA	C2C-C1C-NC	3.10	112.88	109.97
25	5	503	BCR	C33-C5-C4	3.10	119.57	113.62
22	4	615	CLA	C2C-C1C-NC	3.10	112.87	109.97
22	4	603	CLA	CHD-C1D-ND	-3.09	121.61	124.45
22	A	1113	CLA	C1-C2-C3	-3.09	120.69	126.04
22	1	611	CLA	C1C-C2C-C3C	-3.09	103.70	106.96
22	L	1502	CLA	CHD-C1D-ND	-3.09	121.61	124.45
22	6	604	CLA	C2C-C1C-NC	3.09	112.87	109.97
22	2	604	CLA	C2C-C1C-NC	3.09	112.87	109.97
22	A	1124	CLA	C2D-C1D-ND	3.09	112.38	110.10
22	B	1234	CLA	C1-C2-C3	-3.09	120.70	126.04
25	A	4005	BCR	C35-C13-C12	3.09	122.94	118.08
22	J	1901	CLA	CAA-C2A-C3A	-3.09	106.54	114.26
22	2	601	CLA	CHD-C1D-ND	-3.09	121.62	124.45
22	9	603	CLA	CHD-C1D-ND	-3.09	121.62	124.45
22	B	1227	CLA	CHD-C1D-ND	-3.09	121.62	124.45
22	A	1105	CLA	C2D-C1D-ND	3.09	112.38	110.10
22	Z	603	CLA	C2D-C1D-ND	3.09	112.38	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1013	CLA	CHD-C1D-ND	-3.08	121.62	124.45
22	6	619	CLA	C1-C2-C3	-3.08	120.71	126.04
22	A	1140	CLA	C2C-C1C-NC	3.08	112.86	109.97
25	I	4001	BCR	C33-C5-C6	-3.08	121.07	124.53
22	2	608	CLA	C2C-C1C-NC	3.08	112.86	109.97
22	A	1141	CLA	C2D-C1D-ND	3.08	112.38	110.10
22	2	602	CLA	C2D-C1D-ND	3.08	112.38	110.10
22	B	1201	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
25	6	504	BCR	C15-C14-C13	-3.08	122.91	127.31
22	A	1141	CLA	C6-C5-C3	-3.08	109.58	114.62
39	8	501	LUT	C38-C25-C24	-3.08	116.97	123.56
22	A	1127	CLA	C2D-C1D-ND	3.08	112.37	110.10
22	Z	605	CLA	C2C-C1C-NC	3.08	112.86	109.97
22	4	609	CLA	C2C-C1C-NC	3.08	112.86	109.97
22	8	611	CLA	C1C-C2C-C3C	-3.08	103.72	106.96
22	B	1222	CLA	C2D-C1D-ND	3.08	112.37	110.10
22	9	601	CLA	CMA-C3A-C4A	3.08	120.04	111.77
25	3	503	BCR	C33-C5-C6	-3.08	121.07	124.53
22	B	1207	CLA	C2C-C1C-NC	3.08	112.85	109.97
22	B	1236	CLA	C2C-C1C-NC	3.08	112.85	109.97
22	1	602	CLA	C2D-C1D-ND	3.08	112.37	110.10
22	8	607	CLA	CHD-C1D-ND	-3.08	121.63	124.45
22	5	612	CLA	CAA-C2A-C3A	-3.08	104.36	112.78
22	6	619	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
22	Z	608	CLA	C1-C2-C3	-3.07	120.73	126.04
22	6	605	CLA	C2D-C1D-ND	3.07	112.37	110.10
40	4	611	CHL	CMA-C3A-C4A	3.07	120.03	111.77
22	1	612	CLA	C2C-C1C-NC	3.07	112.85	109.97
22	Z	605	CLA	C1C-C2C-C3C	-3.07	103.73	106.96
22	3	616	CLA	C2D-C1D-ND	3.07	112.37	110.10
22	3	608	CLA	CHD-C1D-ND	-3.07	121.63	124.45
22	7	604	CLA	CHD-C1D-ND	-3.07	121.63	124.45
22	A	1136	CLA	O2A-CGA-CBA	3.07	121.54	111.91
22	9	602	CLA	C2C-C1C-NC	3.07	112.85	109.97
22	Z	605	CLA	CHD-C1D-ND	-3.07	121.64	124.45
22	5	615	CLA	C2D-C1D-ND	3.07	112.36	110.10
40	1	609	CHL	C3C-C4C-NC	-3.07	107.13	110.57
22	3	602	CLA	CHD-C1D-ND	-3.07	121.64	124.45
25	B	4003	BCR	C33-C5-C4	3.06	119.50	113.62
22	5	602	CLA	C2D-C1D-ND	3.06	112.36	110.10
22	B	1023	CLA	CHD-C1D-ND	-3.06	121.64	124.45
22	B	1217	CLA	CHD-C1D-ND	-3.06	121.64	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1236	CLA	C1-C2-C3	-3.06	120.75	126.04
25	A	4002	BCR	C23-C24-C25	-3.06	118.60	127.20
25	A	4001	BCR	C19-C18-C17	3.06	123.64	118.94
40	8	610	CHL	C1-O2A-CGA	3.06	124.47	116.44
22	3	606	CLA	C2C-C1C-NC	3.06	112.84	109.97
22	F	1302	CLA	CHD-C1D-ND	-3.06	121.64	124.45
40	2	613	CHL	CMA-C3A-C4A	3.06	120.00	111.77
22	B	1209	CLA	O2A-CGA-CBA	3.06	121.51	111.91
22	3	607	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
22	A	1013	CLA	CAA-C2A-C3A	-3.06	104.40	112.78
39	7	502	LUT	C10-C11-C12	-3.06	113.67	123.22
25	6	503	BCR	C33-C5-C4	3.06	119.49	113.62
22	Z	604	CLA	C1-C2-C3	-3.06	120.75	126.04
22	K	1404	CLA	C2C-C1C-NC	3.06	112.84	109.97
22	5	618	CLA	C2C-C1C-NC	3.06	112.84	109.97
22	4	602	CLA	C2C-C1C-NC	3.06	112.83	109.97
22	8	609	CLA	CHD-C1D-ND	-3.05	121.65	124.45
40	9	613	CHL	CMA-C3A-C4A	3.05	119.98	111.77
22	A	1116	CLA	CHD-C1D-ND	-3.05	121.65	124.45
39	8	501	LUT	C35-C15-C14	-3.05	117.22	123.47
40	1	610	CHL	CMA-C3A-C4A	3.05	119.98	111.77
22	4	608	CLA	CMA-C3A-C4A	3.05	119.97	111.77
22	7	615	CLA	C2C-C1C-NC	3.05	112.83	109.97
22	4	605	CLA	C2D-C1D-ND	3.05	112.35	110.10
25	A	4003	BCR	C33-C5-C6	-3.05	121.10	124.53
25	A	4004	BCR	C38-C26-C27	3.05	119.47	113.62
22	6	615	CLA	C2D-C1D-ND	3.05	112.35	110.10
22	A	1130	CLA	C2C-C1C-NC	3.05	112.83	109.97
22	B	1225	CLA	C2C-C1C-NC	3.05	112.83	109.97
22	A	1138	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
22	B	1221	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
39	3	501	LUT	C15-C14-C13	-3.05	122.96	127.31
22	B	1211	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
22	Z	607	CLA	CHD-C1D-ND	-3.04	121.66	124.45
22	9	601	CLA	CHD-C1D-ND	-3.04	121.66	124.45
40	2	609	CHL	C3C-C4C-NC	-3.04	107.16	110.57
22	B	1207	CLA	CHD-C1D-ND	-3.04	121.66	124.45
39	4	501	LUT	C21-C26-C27	3.04	116.55	112.70
22	A	1113	CLA	C2C-C1C-NC	3.04	112.82	109.97
22	2	608	CLA	C2D-C1D-ND	3.04	112.34	110.10
22	A	1121	CLA	CMD-C2D-C3D	-3.04	120.63	127.61
39	8	502	LUT	C22-C23-C24	-3.04	108.28	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	4	603	CLA	C2C-C1C-NC	3.04	112.82	109.97
22	A	1102	CLA	C1-O2A-CGA	3.04	124.41	116.44
22	B	1203	CLA	CHD-C1D-ND	-3.03	121.67	124.45
22	3	604	CLA	CMB-C2B-C3B	3.03	130.36	124.68
22	K	1401	CLA	C2C-C1C-NC	3.03	112.81	109.97
22	5	602	CLA	C2C-C1C-NC	3.03	112.81	109.97
22	2	608	CLA	CMA-C3A-C4A	3.03	119.93	111.77
22	6	606	CLA	C1-C2-C3	-3.03	120.80	126.04
22	Z	611	CLA	C2C-C1C-NC	3.03	112.81	109.97
22	9	609	CLA	C2C-C1C-NC	3.03	112.81	109.97
22	7	606	CLA	C1-C2-C3	-3.03	120.80	126.04
22	A	1110	CLA	CMA-C3A-C4A	3.03	119.91	111.77
25	5	504	BCR	C33-C5-C6	-3.03	121.13	124.53
25	6	503	BCR	C23-C24-C25	-3.03	118.70	127.20
22	7	602	CLA	C2D-C1D-ND	3.02	112.33	110.10
22	B	1206	CLA	C1C-C2C-C3C	-3.02	103.78	106.96
22	B	1212	CLA	C2D-C1D-ND	3.02	112.33	110.10
22	3	602	CLA	C2C-C1C-NC	3.02	112.80	109.97
40	5	611	CHL	CMA-C3A-C4A	3.02	119.89	111.77
25	5	504	BCR	C37-C22-C23	3.02	122.83	118.08
22	A	1132	CLA	C1-C2-C3	-3.02	120.82	126.04
22	8	608	CLA	C1-C2-C3	-3.02	120.82	126.04
22	B	1205	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
22	3	612	CLA	C1-C2-C3	-3.02	120.82	126.04
22	B	1203	CLA	C2D-C1D-ND	3.02	112.33	110.10
22	Z	601	CLA	C2D-C1D-ND	3.02	112.33	110.10
22	8	605	CLA	C1-C2-C3	-3.02	120.82	126.04
22	A	1131	CLA	C1-C2-C3	-3.02	120.83	126.04
22	B	1212	CLA	CHD-C1D-ND	-3.02	121.68	124.45
25	A	4004	BCR	C30-C25-C26	-3.02	118.36	122.61
22	Z	606	CLA	C2C-C1C-NC	3.02	112.80	109.97
22	3	607	CLA	CMA-C3A-C4A	3.02	119.88	111.77
22	9	609	CLA	CMA-C3A-C4A	3.02	119.88	111.77
39	7	501	LUT	C35-C15-C14	-3.01	117.30	123.47
25	G	4001	BCR	C33-C5-C6	-3.01	121.14	124.53
22	B	1228	CLA	CMB-C2B-C3B	3.01	130.32	124.68
22	1	604	CLA	CHD-C1D-ND	-3.01	121.69	124.45
22	A	1125	CLA	C1-O2A-CGA	3.01	124.35	116.44
22	1	605	CLA	CHD-C1D-ND	-3.01	121.69	124.45
22	8	606	CLA	C2D-C1D-ND	3.01	112.32	110.10
22	A	1112	CLA	C2C-C1C-NC	3.01	112.79	109.97
22	A	1133	CLA	C2C-C1C-NC	3.01	112.79	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1124	CLA	CHD-C1D-ND	-3.01	121.69	124.45
22	4	603	CLA	CBA-CAA-C2A	3.01	122.75	113.86
39	1	501	LUT	C15-C14-C13	-3.01	123.02	127.31
22	B	1240	CLA	CHD-C1D-ND	-3.01	121.69	124.45
22	4	607	CLA	CMA-C3A-C4A	3.01	119.86	111.77
39	7	502	LUT	C22-C23-C24	-3.01	108.32	111.74
40	7	610	CHL	CHC-C1C-NC	3.00	128.76	124.20
22	B	1237	CLA	C1-C2-C3	-3.00	120.85	126.04
22	5	602	CLA	CHD-C1D-ND	-3.00	121.69	124.45
22	A	1121	CLA	C1-C2-C3	-3.00	120.85	126.04
22	J	1901	CLA	C2D-C1D-ND	3.00	112.32	110.10
22	B	1217	CLA	C2C-C1C-NC	3.00	112.78	109.97
22	2	604	CLA	CMB-C2B-C3B	3.00	130.29	124.68
22	4	602	CLA	C2D-C1D-ND	3.00	112.32	110.10
22	2	603	CLA	CHD-C1D-ND	-3.00	121.70	124.45
39	7	501	LUT	C38-C25-C24	-3.00	117.14	123.56
40	6	611	CHL	CMA-C3A-C4A	3.00	119.84	111.77
22	6	603	CLA	CMA-C3A-C4A	3.00	119.84	111.77
22	K	1401	CLA	CHD-C1D-ND	-3.00	121.70	124.45
22	4	615	CLA	CHD-C1D-ND	-3.00	121.70	124.45
22	K	1404	CLA	C2D-C1D-ND	3.00	112.31	110.10
22	7	612	CLA	C2C-C1C-NC	3.00	112.78	109.97
39	2	503	LUT	C38-C25-C24	-3.00	117.15	123.56
22	6	615	CLA	CHD-C1D-ND	-3.00	121.70	124.45
22	A	1118	CLA	C1-C2-C3	-3.00	120.86	126.04
22	Z	602	CLA	C2D-C1D-ND	3.00	112.31	110.10
22	B	1208	CLA	O2A-CGA-CBA	3.00	121.31	111.91
25	5	503	BCR	C33-C5-C6	-3.00	121.16	124.53
39	5	501	LUT	C18-C5-C6	-3.00	121.16	124.53
22	5	605	CLA	CMB-C2B-C1B	-3.00	123.86	128.46
25	A	4003	BCR	C1-C6-C5	-2.99	118.39	122.61
22	7	613	CLA	C2D-C1D-ND	2.99	112.31	110.10
22	2	615	CLA	CHD-C1D-ND	-2.99	121.70	124.45
39	3	501	LUT	C38-C25-C24	-2.99	117.16	123.56
22	A	1110	CLA	C2D-C1D-ND	2.99	112.31	110.10
22	A	1125	CLA	CMB-C2B-C3B	2.99	130.28	124.68
22	B	1209	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
22	A	1101	CLA	C1-O2A-CGA	2.99	124.29	116.44
22	4	604	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
22	5	622	CLA	CHD-C1D-ND	-2.99	121.71	124.45
22	1	607	CLA	CHD-C1D-ND	-2.99	121.71	124.45
22	5	603	CLA	CMA-C3A-C4A	2.99	119.80	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	2	609	CHL	C1-C2-C3	-2.99	121.92	126.75
22	8	611	CLA	C1-C2-C3	-2.98	121.92	126.75
22	B	1202	CLA	O2A-CGA-CBA	2.98	121.27	111.91
22	3	612	CLA	C2C-C1C-NC	2.98	112.77	109.97
22	5	607	CLA	C2C-C1C-NC	2.98	112.77	109.97
25	4	503	BCR	C33-C5-C4	2.98	119.35	113.62
22	B	1205	CLA	O2A-CGA-CBA	2.98	121.27	111.91
22	2	605	CLA	C2C-C1C-NC	2.98	112.77	109.97
22	A	1108	CLA	CMA-C3A-C4A	2.98	119.79	111.77
22	A	1132	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
22	F	1301	CLA	C2D-C1D-ND	2.98	112.30	110.10
22	4	607	CLA	CHD-C1D-ND	-2.98	121.72	124.45
22	3	616	CLA	CMA-C3A-C4A	2.98	119.78	111.77
22	5	615	CLA	CMA-C3A-C4A	2.98	119.78	111.77
22	7	607	CLA	CHD-C1D-ND	-2.98	121.72	124.45
22	9	601	CLA	C2C-C1C-NC	2.98	112.76	109.97
22	A	1117	CLA	CMA-C3A-C4A	2.98	119.78	111.77
22	A	1118	CLA	C2C-C1C-NC	2.98	112.76	109.97
22	9	609	CLA	CHD-C1D-ND	-2.98	121.72	124.45
22	1	605	CLA	C2C-C1C-NC	2.98	112.76	109.97
39	6	501	LUT	C21-C26-C27	2.98	116.46	112.70
37	5	505	C7Z	C21-C26-C25	-2.98	118.42	122.61
22	2	615	CLA	C2C-C1C-NC	2.97	112.76	109.97
22	5	601	CLA	C2D-C1D-ND	2.97	112.30	110.10
22	A	1101	CLA	C2C-C1C-NC	2.97	112.76	109.97
22	7	601	CLA	C1-O2A-CGA	2.97	124.25	116.44
22	A	1138	CLA	CMB-C2B-C3B	2.97	130.24	124.68
22	5	603	CLA	C2D-C1D-ND	2.97	112.30	110.10
22	Z	611	CLA	C1-C2-C3	-2.97	120.90	126.04
22	B	1234	CLA	CMB-C2B-C1B	-2.97	123.90	128.46
22	6	605	CLA	CHD-C1D-ND	-2.97	121.72	124.45
22	F	1301	CLA	C2C-C1C-NC	2.97	112.76	109.97
22	A	1137	CLA	CMB-C2B-C3B	2.97	130.24	124.68
25	A	4004	BCR	C12-C13-C14	-2.97	114.38	118.94
22	B	1238	CLA	C1-C2-C3	-2.97	120.91	126.04
22	3	618	CLA	C2D-C1D-ND	2.97	112.29	110.10
22	1	613	CLA	C2C-C1C-NC	2.97	112.75	109.97
40	5	617	CHL	CMA-C3A-C4A	2.97	119.75	111.77
22	8	608	CLA	C2C-C1C-NC	2.97	112.75	109.97
39	3	502	LUT	C2-C3-C4	-2.97	106.24	110.30
25	A	4001	BCR	C36-C18-C17	-2.97	118.77	122.92
22	2	612	CLA	C2D-C1D-ND	2.96	112.29	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	6	605	CLA	CMB-C2B-C1B	-2.96	123.91	128.46
22	B	1235	CLA	O2A-CGA-CBA	2.96	121.20	111.91
22	7	611	CLA	C1C-C2C-C3C	-2.96	103.84	106.96
22	2	601	CLA	C2C-C1C-NC	2.96	112.75	109.97
25	B	4002	BCR	C23-C24-C25	-2.96	118.89	127.20
22	Z	604	CLA	CMA-C3A-C4A	2.96	119.73	111.77
22	A	1104	CLA	CHD-C1D-ND	-2.96	121.73	124.45
22	4	609	CLA	C2D-C1D-ND	2.96	112.28	110.10
39	Z	501	LUT	C35-C15-C14	-2.96	117.42	123.47
22	A	1103	CLA	CMB-C2B-C3B	2.96	130.21	124.68
22	3	605	CLA	C1-C2-C3	-2.96	120.93	126.04
39	1	502	LUT	C38-C25-C24	-2.96	117.23	123.56
22	B	1219	CLA	CHD-C1D-ND	-2.96	121.74	124.45
22	8	602	CLA	CHD-C1D-ND	-2.96	121.74	124.45
25	A	4003	BCR	C19-C18-C17	2.96	123.48	118.94
22	5	603	CLA	C2C-C1C-NC	2.96	112.74	109.97
22	9	602	CLA	C2D-C1D-ND	2.96	112.28	110.10
25	3	505	BCR	C38-C26-C25	-2.95	121.21	124.53
22	1	604	CLA	C1-C2-C3	-2.95	120.93	126.04
22	B	1220	CLA	C1-C2-C3	-2.95	120.93	126.04
22	K	1402	CLA	C2C-C1C-NC	2.95	112.74	109.97
25	B	4007	BCR	C34-C9-C10	-2.95	118.79	122.92
22	7	606	CLA	C2C-C1C-NC	2.95	112.74	109.97
22	5	607	CLA	CHD-C1D-ND	-2.95	121.74	124.45
22	B	1222	CLA	CAA-C2A-C3A	-2.95	104.69	112.78
22	B	1227	CLA	C2C-C1C-NC	2.95	112.73	109.97
22	9	605	CLA	C1C-C2C-C3C	-2.95	103.86	106.96
22	5	613	CLA	C2C-C1C-NC	2.95	112.73	109.97
22	1	606	CLA	C1-C2-C3	-2.95	120.94	126.04
22	7	616	CLA	C1-C2-C3	-2.95	120.94	126.04
22	G	1602	CLA	CHD-C1D-ND	-2.95	121.75	124.45
22	3	601	CLA	C2D-C1D-ND	2.95	112.28	110.10
22	B	1237	CLA	CHD-C1D-ND	-2.95	121.75	124.45
29	A	5008	OCA	O1-C1-C2	-2.95	113.62	123.08
22	5	622	CLA	C1C-C2C-C3C	-2.94	103.86	106.96
22	8	615	CLA	CHD-C1D-ND	-2.94	121.75	124.45
40	4	610	CHL	C1-O2A-CGA	2.94	124.16	116.44
22	1	607	CLA	CMA-C3A-C4A	2.94	119.68	111.77
22	A	1138	CLA	O2A-CGA-CBA	2.94	121.14	111.91
22	4	602	CLA	CHD-C1D-ND	-2.94	121.75	124.45
22	4	603	CLA	C2D-C1D-ND	2.94	112.27	110.10
22	5	615	CLA	CHD-C1D-ND	-2.94	121.75	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1112	CLA	C1-C2-C3	-2.94	120.96	126.04
22	4	604	CLA	CMA-C3A-C4A	2.94	119.67	111.77
22	A	1123	CLA	C1-C2-C3	-2.94	120.96	126.04
22	4	607	CLA	C1-C2-C3	-2.94	120.96	126.04
22	A	1125	CLA	CHD-C1D-ND	-2.94	121.75	124.45
22	5	604	CLA	C1-O2A-CGA	2.93	124.14	116.44
22	B	1224	CLA	CHD-C1D-ND	-2.93	121.76	124.45
25	5	504	BCR	C33-C5-C4	2.93	119.25	113.62
22	8	611	CLA	O2A-CGA-CBA	2.93	121.12	111.91
25	B	4001	BCR	C36-C18-C17	-2.93	118.81	122.92
37	J	4002	C7Z	C15-C14-C13	-2.93	123.12	127.31
40	7	610	CHL	CMA-C3A-C4A	2.93	119.66	111.77
22	B	1220	CLA	CHD-C1D-ND	-2.93	121.76	124.45
40	2	609	CHL	C1B-CHB-C4A	-2.93	124.31	130.12
40	9	610	CHL	CHB-C4A-NA	2.93	128.56	124.51
22	6	605	CLA	C2C-C1C-NC	2.93	112.72	109.97
22	8	602	CLA	C2D-C1D-ND	2.93	112.26	110.10
22	A	1126	CLA	C2C-C1C-NC	2.93	112.72	109.97
22	7	605	CLA	C2D-C1D-ND	2.93	112.26	110.10
22	2	605	CLA	C1-O2A-CGA	2.93	124.12	116.44
22	A	1140	CLA	CHD-C1D-ND	-2.93	121.76	124.45
22	4	612	CLA	C1C-C2C-C3C	-2.93	103.88	106.96
39	4	501	LUT	C38-C25-C24	-2.93	117.30	123.56
22	B	1237	CLA	CMA-C3A-C4A	2.92	119.63	111.77
22	4	612	CLA	CMA-C3A-C4A	2.92	119.63	111.77
22	A	1110	CLA	CHD-C1D-ND	-2.92	121.77	124.45
22	A	1109	CLA	CMA-C3A-C4A	2.92	119.63	111.77
22	B	1213	CLA	C2C-C1C-NC	2.92	112.71	109.97
22	K	1402	CLA	C2D-C1D-ND	2.92	112.26	110.10
22	B	1205	CLA	CHD-C1D-ND	-2.92	121.77	124.45
22	7	616	CLA	C2D-C1D-ND	2.92	112.25	110.10
40	8	613	CHL	C1-C2-C3	-2.92	121.00	126.04
22	8	602	CLA	C2C-C1C-NC	2.92	112.70	109.97
40	4	610	CHL	C1B-CHB-C4A	-2.92	124.34	130.12
25	4	503	BCR	C4-C5-C6	-2.92	118.50	122.73
22	J	1901	CLA	C2C-C1C-NC	2.92	112.70	109.97
25	A	4003	BCR	C36-C18-C17	-2.92	118.84	122.92
22	B	1217	CLA	C2D-C1D-ND	2.92	112.25	110.10
22	A	1124	CLA	C2C-C1C-NC	2.92	112.70	109.97
40	Z	609	CHL	C3C-C4C-NC	-2.91	107.30	110.57
22	A	1120	CLA	CMA-C3A-C4A	2.91	119.60	111.77
40	Z	613	CHL	CMA-C3A-C4A	2.91	119.60	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	5	611	CHL	CHD-C1D-ND	-2.91	121.78	124.45
22	A	1136	CLA	CMA-C3A-C4A	2.91	119.60	111.77
22	9	601	CLA	O2A-CGA-CBA	2.91	121.04	111.91
39	2	502	LUT	C15-C35-C34	-2.91	117.51	123.47
40	1	609	CHL	CMA-C3A-C4A	2.91	119.59	111.77
22	B	1237	CLA	C2C-C1C-NC	2.91	112.70	109.97
22	A	1124	CLA	CAA-C2A-C3A	-2.91	104.81	112.78
36	F	4001	RRX	C29-C28-C27	2.91	114.29	110.30
22	B	1223	CLA	C2C-C1C-NC	2.91	112.70	109.97
39	3	502	LUT	C38-C25-C24	-2.91	117.34	123.56
22	B	1203	CLA	C1C-C2C-C3C	-2.91	103.90	106.96
22	G	1601	CLA	C2D-C1D-ND	2.91	112.25	110.10
25	B	4006	BCR	C15-C14-C13	2.91	131.46	127.31
25	L	4002	BCR	C34-C9-C10	-2.91	118.85	122.92
40	4	613	CHL	C3C-C4C-NC	-2.91	107.31	110.57
22	A	1012	CLA	C1-O2A-CGA	2.91	124.07	116.44
22	6	602	CLA	C2D-C1D-ND	2.91	112.25	110.10
22	L	1503	CLA	CMB-C2B-C3B	2.90	130.11	124.68
39	1	501	LUT	C38-C25-C24	-2.90	117.35	123.56
25	K	4002	BCR	C36-C18-C17	-2.90	118.86	122.92
22	9	609	CLA	C2D-C1D-ND	2.90	112.24	110.10
22	A	1107	CLA	CMB-C2B-C1B	-2.90	124.00	128.46
22	4	602	CLA	C1-C2-C3	-2.90	121.02	126.04
22	3	601	CLA	CAA-C2A-C3A	-2.90	104.83	112.78
22	2	604	CLA	CMD-C2D-C3D	-2.90	120.94	127.61
25	A	4005	BCR	C34-C9-C10	-2.90	118.86	122.92
22	3	613	CLA	C1-C2-C3	-2.90	121.03	126.04
22	A	1125	CLA	C2C-C1C-NC	2.90	112.69	109.97
22	6	618	CLA	C2C-C1C-NC	2.90	112.69	109.97
23	B	2002	PQN	C11-C12-C13	-2.90	121.97	126.79
22	B	1204	CLA	C2D-C1D-ND	2.90	112.24	110.10
25	4	503	BCR	C1-C6-C5	-2.90	118.53	122.61
22	B	1229	CLA	C2C-C1C-NC	2.90	112.69	109.97
22	3	607	CLA	CHD-C1D-ND	-2.90	121.79	124.45
25	6	504	BCR	C33-C5-C6	-2.90	121.28	124.53
22	8	615	CLA	C2D-C1D-ND	2.90	112.24	110.10
39	1	501	LUT	C10-C11-C12	-2.90	114.18	123.22
40	8	610	CHL	C3C-C4C-NC	-2.90	107.32	110.57
40	6	617	CHL	CMA-C3A-C4A	2.90	119.55	111.77
22	Z	611	CLA	CMA-C3A-C4A	2.89	119.55	111.77
40	3	611	CHL	CMA-C3A-C4A	2.89	119.55	111.77
22	8	612	CLA	C2D-C1D-ND	2.89	112.24	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	F	1302	CLA	C2C-C1C-NC	2.89	112.68	109.97
22	2	607	CLA	CHD-C1D-ND	-2.89	121.80	124.45
22	1	611	CLA	C1-C2-C3	-2.89	121.04	126.04
22	F	1301	CLA	O2A-CGA-CBA	2.89	120.99	111.91
22	7	611	CLA	CMB-C2B-C3B	2.89	130.09	124.68
22	B	1207	CLA	C1-C2-C3	-2.89	121.04	126.04
22	8	607	CLA	C1-C2-C3	-2.89	121.04	126.04
26	8	801	LHG	O8-C23-C24	2.89	120.98	111.91
22	Z	612	CLA	C1C-C2C-C3C	-2.89	103.92	106.96
22	4	606	CLA	C2D-C1D-ND	2.89	112.23	110.10
28	8	805	LMT	O1'-C1'-C2'	2.89	112.81	108.30
25	B	4003	BCR	C12-C13-C14	-2.89	114.51	118.94
22	A	1104	CLA	C2D-C1D-ND	2.89	112.23	110.10
21	A	1011	CL0	O2D-CGD-O1D	-2.89	118.19	123.84
22	B	1230	CLA	C1D-ND-C4D	-2.89	104.28	106.33
22	7	604	CLA	C2D-C1D-ND	2.89	112.23	110.10
22	7	616	CLA	C2C-C1C-NC	2.89	112.68	109.97
22	6	601	CLA	C2C-C1C-NC	2.89	112.68	109.97
40	1	609	CHL	C2C-C3C-C4C	2.89	108.55	106.49
22	A	1129	CLA	C2C-C1C-NC	2.89	112.67	109.97
22	B	1202	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
22	4	605	CLA	C1-C2-C3	-2.88	121.05	126.04
22	A	1117	CLA	C1C-C2C-C3C	-2.88	103.92	106.96
22	A	1127	CLA	C2C-C1C-NC	2.88	112.67	109.97
22	Z	603	CLA	C2C-C1C-NC	2.88	112.67	109.97
22	A	1139	CLA	CMA-C3A-C4A	2.88	119.52	111.77
22	3	602	CLA	C2D-C1D-ND	2.88	112.23	110.10
22	7	608	CLA	C2D-C1D-ND	2.88	112.23	110.10
39	3	501	LUT	C11-C10-C9	-2.88	123.19	127.31
22	B	1227	CLA	C1-C2-C3	-2.88	122.09	126.75
22	B	1218	CLA	C1C-C2C-C3C	-2.88	103.93	106.96
22	A	1120	CLA	CMB-C2B-C3B	2.88	130.07	124.68
22	8	602	CLA	C1-C2-C3	-2.88	121.06	126.04
22	Z	604	CLA	C2C-C1C-NC	2.88	112.67	109.97
22	B	1209	CLA	C1-O2A-CGA	2.88	123.99	116.44
22	B	1240	CLA	C2D-C1D-ND	2.87	112.22	110.10
22	Z	615	CLA	C2D-C1D-ND	2.87	112.22	110.10
22	7	607	CLA	CMA-C3A-C4A	2.87	119.49	111.77
22	5	607	CLA	CMA-C3A-C4A	2.87	119.49	111.77
40	6	613	CHL	CMA-C3A-C4A	2.87	119.49	111.77
22	A	1124	CLA	C1-C2-C3	-2.87	121.08	126.04
22	A	1118	CLA	CMA-C3A-C4A	2.87	119.49	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1122	CLA	CMA-C3A-C4A	2.87	119.49	111.77
22	3	618	CLA	CHD-C1D-ND	-2.87	121.82	124.45
25	B	4001	BCR	C33-C5-C6	-2.87	121.31	124.53
22	7	604	CLA	C1-O2A-CGA	2.87	123.97	116.44
22	6	612	CLA	CMA-C3A-C4A	2.87	119.48	111.77
25	A	4001	BCR	C35-C13-C12	2.87	122.59	118.08
22	3	606	CLA	C2D-C1D-ND	2.87	112.22	110.10
22	B	1228	CLA	C2C-C1C-NC	2.87	112.66	109.97
22	B	1228	CLA	C2D-C1D-ND	2.87	112.22	110.10
22	B	1023	CLA	CMB-C2B-C3B	2.87	130.04	124.68
22	2	601	CLA	CMA-C3A-C4A	2.86	119.47	111.77
22	B	1215	CLA	C2D-C1D-ND	2.86	112.21	110.10
22	8	606	CLA	C2C-C1C-NC	2.86	112.65	109.97
28	B	5005	LMT	O5'-C5'-C4'	2.86	115.79	109.75
40	2	610	CHL	C4A-NA-C1A	2.86	107.99	106.71
22	A	1116	CLA	C2D-C1D-ND	2.86	112.21	110.10
22	1	603	CLA	C1-C2-C3	-2.86	121.09	126.04
22	A	1133	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
22	4	604	CLA	C2C-C1C-NC	2.86	112.65	109.97
40	2	609	CHL	CHD-C4C-C3C	2.86	129.04	124.84
22	B	1209	CLA	C2C-C1C-NC	2.86	112.65	109.97
22	B	1211	CLA	C1-C2-C3	-2.86	121.10	126.04
22	5	605	CLA	C2D-C1D-ND	2.86	112.21	110.10
22	5	609	CLA	CHD-C1D-ND	-2.86	121.83	124.45
22	B	1226	CLA	CHA-C4D-ND	2.86	138.47	132.50
22	7	603	CLA	C2D-C1D-ND	2.86	112.21	110.10
22	9	607	CLA	CMA-C3A-C4A	2.86	119.45	111.77
22	4	604	CLA	C1-C2-C3	-2.86	121.11	126.04
22	3	618	CLA	C1C-C2C-C3C	-2.85	103.95	106.96
22	7	601	CLA	C2D-C1D-ND	2.85	112.21	110.10
22	A	1114	CLA	C1C-C2C-C3C	-2.85	103.96	106.96
25	L	4002	BCR	C36-C18-C17	-2.85	118.93	122.92
39	8	502	LUT	C35-C15-C14	-2.85	117.63	123.47
22	4	612	CLA	C2C-C1C-NC	2.85	112.64	109.97
39	2	503	LUT	C19-C9-C8	2.85	122.57	118.08
22	9	603	CLA	CMA-C3A-C4A	2.85	119.43	111.77
22	A	1104	CLA	C2C-C1C-NC	2.85	112.64	109.97
40	5	610	CHL	C1-O2A-CGA	2.85	123.91	116.44
22	B	1205	CLA	C2C-C1C-NC	2.84	112.64	109.97
22	1	603	CLA	C2C-C1C-NC	2.84	112.64	109.97
40	Z	610	CHL	CMA-C3A-C4A	2.84	119.42	111.77
22	1	606	CLA	CMB-C2B-C3B	2.84	130.00	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1127	CLA	CMA-C3A-C4A	2.84	119.42	111.77
22	Z	611	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
22	Z	612	CLA	C1-C2-C3	-2.84	121.13	126.04
39	5	502	LUT	C22-C23-C24	-2.84	108.51	111.74
39	4	502	LUT	C35-C15-C14	-2.84	117.65	123.47
22	B	1235	CLA	C2C-C1C-NC	2.84	112.63	109.97
22	A	1136	CLA	CMB-C2B-C3B	2.84	129.99	124.68
22	7	616	CLA	CMA-C3A-C4A	2.84	119.41	111.77
22	B	1224	CLA	C1-O2A-CGA	2.84	123.90	116.44
22	A	1128	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
22	A	1109	CLA	C2D-C1D-ND	2.84	112.20	110.10
22	6	607	CLA	CHD-C1D-ND	-2.84	121.84	124.45
22	4	615	CLA	CMA-C3A-C4A	2.84	119.40	111.77
22	6	605	CLA	C1-C2-C3	-2.84	121.13	126.04
22	2	604	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
25	L	4001	BCR	C28-C27-C26	-2.84	109.01	114.08
25	B	4007	BCR	C33-C5-C6	-2.84	121.34	124.53
22	B	1239	CLA	C2D-C1D-ND	2.84	112.19	110.10
22	1	608	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
27	8	802	NKP	OAB-PAC-OAA	2.84	118.48	107.64
22	5	605	CLA	CMA-C3A-C4A	2.84	119.40	111.77
22	6	609	CLA	C2D-C1D-ND	2.84	112.19	110.10
40	4	613	CHL	C4A-NA-C1A	2.84	107.98	106.71
22	B	1219	CLA	C1-C2-C3	-2.84	121.14	126.04
39	8	502	LUT	C15-C14-C13	-2.83	123.26	127.31
22	9	601	CLA	C1-O2A-CGA	2.83	123.88	116.44
22	A	1102	CLA	C2D-C1D-ND	2.83	112.19	110.10
22	5	613	CLA	CHD-C1D-ND	-2.83	121.85	124.45
22	A	1106	CLA	C2C-C1C-NC	2.83	112.63	109.97
22	8	603	CLA	C1D-ND-C4D	-2.83	104.32	106.33
22	4	604	CLA	C2D-C1D-ND	2.83	112.19	110.10
22	B	1228	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
22	A	1108	CLA	C2D-C1D-ND	2.83	112.19	110.10
22	B	1210	CLA	O1D-CGD-CBD	-2.83	118.69	124.48
22	B	1222	CLA	O2A-CGA-CBA	2.83	120.79	111.91
22	B	1202	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
22	B	1202	CLA	C2C-C1C-NC	2.83	112.62	109.97
22	4	609	CLA	C1-C2-C3	-2.83	121.15	126.04
40	Z	610	CHL	C3C-C4C-NC	-2.83	107.40	110.57
22	7	601	CLA	CAA-C2A-C3A	-2.83	105.04	112.78
39	8	502	LUT	C11-C10-C9	-2.83	123.28	127.31
22	B	1237	CLA	C2D-C1D-ND	2.83	112.19	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Z	602	CLA	CMB-C2B-C3B	2.83	129.97	124.68
39	6	502	LUT	C35-C15-C14	-2.83	117.69	123.47
22	7	609	CLA	C2C-C1C-NC	2.83	112.62	109.97
22	A	1136	CLA	C1C-C2C-C3C	-2.83	103.99	106.96
22	9	605	CLA	C2D-C1D-ND	2.83	112.19	110.10
22	A	1111	CLA	CMB-C2B-C1B	-2.82	124.12	128.46
22	B	1230	CLA	C1-C2-C3	-2.82	121.16	126.04
22	6	603	CLA	C2D-C1D-ND	2.82	112.19	110.10
22	1	613	CLA	CHD-C1D-ND	-2.82	121.86	124.45
22	8	604	CLA	C2C-C1C-NC	2.82	112.62	109.97
39	1	502	LUT	C11-C10-C9	-2.82	123.28	127.31
22	B	1215	CLA	CMA-C3A-C4A	2.82	119.36	111.77
22	B	1207	CLA	CMA-C3A-C4A	2.82	119.36	111.77
22	5	605	CLA	C1-C2-C3	-2.82	121.17	126.04
22	B	1214	CLA	OBD-CAD-C3D	-2.82	121.73	128.52
22	A	1101	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
22	B	1216	CLA	C2C-C1C-NC	2.82	112.61	109.97
22	3	601	CLA	C2C-C1C-NC	2.82	112.61	109.97
27	A	5004	NKP	OAB-PAC-OAA	2.82	118.41	107.64
22	B	1223	CLA	CMA-C3A-C4A	2.82	119.35	111.77
22	A	1105	CLA	CMA-C3A-C4A	2.82	119.35	111.77
22	7	602	CLA	CHD-C1D-ND	-2.82	121.86	124.45
39	1	502	LUT	C15-C14-C13	-2.82	123.29	127.31
22	5	612	CLA	C1-C2-C3	-2.82	121.17	126.04
22	B	1021	CLA	C2C-C1C-NC	2.82	112.61	109.97
25	B	4003	BCR	C36-C18-C17	-2.82	118.98	122.92
22	A	1137	CLA	C2D-C1D-ND	2.82	112.18	110.10
22	B	1023	CLA	C2D-C1D-ND	2.82	112.18	110.10
22	Z	608	CLA	C2C-C1C-NC	2.82	112.61	109.97
25	L	4002	BCR	C38-C26-C25	-2.82	121.36	124.53
22	6	619	CLA	CMB-C2B-C1B	-2.82	124.14	128.46
22	5	602	CLA	C1-C2-C3	-2.82	121.17	126.04
22	A	1120	CLA	C2C-C1C-NC	2.82	112.61	109.97
22	3	613	CLA	C2C-C1C-NC	2.82	112.61	109.97
40	9	610	CHL	C3C-C4C-NC	-2.82	107.41	110.57
39	3	501	LUT	C18-C5-C6	-2.82	121.37	124.53
22	7	604	CLA	C2C-C1C-NC	2.81	112.61	109.97
22	4	605	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
22	7	615	CLA	C1-C2-C3	-2.81	121.17	126.04
22	A	1140	CLA	C2D-C1D-ND	2.81	112.18	110.10
22	Z	604	CLA	C2D-C1D-ND	2.81	112.18	110.10
22	A	1110	CLA	C2C-C1C-NC	2.81	112.61	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6	504	BCR	C4-C5-C6	-2.81	118.65	122.73
22	A	1134	CLA	C2D-C1D-ND	2.81	112.18	110.10
22	4	607	CLA	C2D-C1D-ND	2.81	112.18	110.10
22	5	613	CLA	C2D-C1D-ND	2.81	112.18	110.10
22	A	1128	CLA	CHD-C1D-ND	-2.81	121.87	124.45
22	B	1226	CLA	CAC-C3C-C4C	2.81	128.46	124.81
22	B	1204	CLA	O2A-CGA-CBA	2.81	120.73	111.91
22	Z	612	CLA	CMA-C3A-C4A	2.81	119.33	111.77
22	A	1101	CLA	C2D-C1D-ND	2.81	112.17	110.10
22	6	608	CLA	CAA-C2A-C3A	-2.81	105.09	112.78
22	6	602	CLA	C6-C5-C3	-2.81	110.03	114.62
22	A	1129	CLA	CMB-C2B-C3B	2.81	129.93	124.68
22	7	613	CLA	C2C-C1C-NC	2.81	112.60	109.97
40	4	613	CHL	CMA-C3A-C4A	2.81	119.32	111.77
22	Z	606	CLA	C1-C2-C3	-2.81	121.19	126.04
22	A	1107	CLA	CMA-C3A-C4A	2.81	119.32	111.77
22	7	608	CLA	C1C-C2C-C3C	-2.81	104.01	106.96
22	3	601	CLA	O2A-CGA-CBA	2.81	120.71	111.91
40	Z	609	CHL	CAA-C2A-C3A	-2.81	105.09	112.78
39	2	503	LUT	C35-C34-C33	-2.81	123.31	127.31
22	7	601	CLA	C2C-C1C-NC	2.81	112.60	109.97
22	Z	605	CLA	C1-C2-C3	-2.80	121.19	126.04
22	A	1113	CLA	CMA-C3A-C4A	2.80	119.31	111.77
22	5	615	CLA	C1-C2-C3	-2.80	122.22	126.75
22	A	1122	CLA	C1C-C2C-C3C	-2.80	104.01	106.96
39	9	502	LUT	C10-C11-C12	-2.80	114.47	123.22
22	4	609	CLA	CHD-C1D-ND	-2.80	121.88	124.45
22	A	1114	CLA	CMA-C3A-C4A	2.80	119.31	111.77
22	9	612	CLA	CHD-C1D-ND	-2.80	121.88	124.45
22	B	1203	CLA	C1-C2-C3	-2.80	121.20	126.04
22	8	603	CLA	C2C-C1C-NC	2.80	112.60	109.97
22	A	1107	CLA	CHD-C1D-ND	-2.80	121.88	124.45
22	2	603	CLA	CBA-CAA-C2A	2.80	122.13	113.86
22	B	1213	CLA	O2A-CGA-CBA	2.80	120.69	111.91
22	B	1211	CLA	C1D-ND-C4D	-2.80	104.35	106.33
22	B	1241	CLA	C1D-ND-C4D	-2.80	104.35	106.33
25	B	4004	BCR	C33-C5-C6	-2.80	121.38	124.53
22	K	1403	CLA	CMA-C3A-C4A	2.80	119.30	111.77
28	4	803	LMT	C3'-C4'-C5'	-2.80	104.51	110.93
25	A	4001	BCR	C12-C13-C14	-2.80	114.65	118.94
22	B	1229	CLA	C1C-C2C-C3C	-2.80	104.02	106.96
22	2	615	CLA	C1C-C2C-C3C	-2.80	104.02	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1226	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
22	5	609	CLA	C2D-C1D-ND	2.80	112.17	110.10
25	B	4005	BCR	C27-C26-C25	-2.80	118.67	122.73
22	2	607	CLA	C2D-C1D-ND	2.80	112.16	110.10
22	A	1137	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
22	9	602	CLA	CMB-C2B-C1B	-2.79	124.17	128.46
22	8	602	CLA	CAA-C2A-C3A	-2.79	105.13	112.78
22	7	605	CLA	C2C-C1C-NC	2.79	112.59	109.97
22	2	603	CLA	C1-C2-C3	-2.79	121.21	126.04
22	6	615	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
22	6	618	CLA	CMA-C3A-C4A	2.79	119.28	111.77
22	A	1138	CLA	C2D-C1D-ND	2.79	112.16	110.10
22	B	1211	CLA	C2D-C1D-ND	2.79	112.16	110.10
22	2	606	CLA	CHD-C1D-ND	-2.79	121.89	124.45
22	9	605	CLA	CHD-C1D-ND	-2.79	121.89	124.45
22	A	1123	CLA	CMB-C2B-C3B	2.79	129.90	124.68
22	7	602	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
22	B	1210	CLA	C2D-C1D-ND	2.79	112.16	110.10
22	6	619	CLA	C2D-C1D-ND	2.79	112.16	110.10
22	6	605	CLA	O2A-CGA-CBA	2.79	120.66	111.91
22	8	611	CLA	C2D-C1D-ND	2.79	112.16	110.10
22	B	1218	CLA	CMA-C3A-C4A	2.79	119.27	111.77
22	8	604	CLA	C2D-C1D-ND	2.79	112.16	110.10
22	1	605	CLA	C1C-C2C-C3C	-2.79	104.03	106.96
22	A	1138	CLA	C2C-C1C-NC	2.79	112.58	109.97
22	A	1106	CLA	C2D-C1D-ND	2.79	112.16	110.10
25	A	4002	BCR	C36-C18-C17	-2.79	119.02	122.92
22	3	612	CLA	C1C-C2C-C3C	-2.79	104.03	106.96
22	7	605	CLA	O2A-CGA-CBA	2.79	120.65	111.91
22	5	606	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
25	B	4004	BCR	C35-C13-C12	2.78	122.46	118.08
22	9	612	CLA	O2A-CGA-CBA	2.78	120.64	111.91
31	J	5001	LMG	O8-C28-C29	2.78	120.64	111.91
22	A	1108	CLA	C1C-C2C-C3C	-2.78	104.03	106.96
22	A	1128	CLA	C1C-C2C-C3C	-2.78	104.03	106.96
22	3	616	CLA	C1C-C2C-C3C	-2.78	104.03	106.96
22	A	1113	CLA	C2D-C1D-ND	2.78	112.15	110.10
22	A	1140	CLA	C1C-C2C-C3C	-2.78	104.03	106.96
22	4	612	CLA	C2D-C1D-ND	2.78	112.15	110.10
39	Z	502	LUT	C38-C25-C24	-2.78	117.61	123.56
22	A	1101	CLA	O2A-CGA-CBA	2.78	120.63	111.91
22	2	605	CLA	O2A-CGA-CBA	2.78	120.63	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	7	503	BCR	C19-C18-C17	2.78	123.20	118.94
22	4	601	CLA	C2D-C1D-ND	2.78	112.15	110.10
39	8	501	LUT	C10-C11-C12	-2.78	114.55	123.22
22	8	603	CLA	C6-C5-C3	-2.78	106.17	113.45
22	8	606	CLA	CMB-C2B-C3B	2.78	129.87	124.68
22	A	1141	CLA	CMA-C3A-C4A	2.78	119.23	111.77
22	1	612	CLA	C1-C2-C3	-2.78	121.24	126.04
40	8	610	CHL	CHD-C4C-C3C	2.78	128.92	124.84
22	B	1216	CLA	C1-C2-C3	-2.78	121.24	126.04
25	L	4001	BCR	C33-C5-C6	-2.77	121.41	124.53
22	6	609	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
22	5	615	CLA	C1-O2A-CGA	2.77	123.72	116.44
39	2	502	LUT	C35-C34-C33	-2.77	123.35	127.31
22	B	1221	CLA	C2C-C1C-NC	2.77	112.57	109.97
40	5	610	CHL	CHC-C1C-NC	2.77	128.41	124.20
22	8	615	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
22	B	1234	CLA	CHD-C1D-ND	-2.77	121.91	124.45
22	3	608	CLA	CMA-C3A-C4A	2.77	119.22	111.77
22	B	1238	CLA	C2D-C1D-ND	2.77	112.15	110.10
22	9	603	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
22	3	601	CLA	C1-O2A-CGA	2.77	123.72	116.44
22	B	1217	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
22	B	1229	CLA	CAA-CBA-CGA	-2.77	105.15	113.25
22	8	605	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
37	J	4002	C7Z	C22-C23-C24	2.77	114.10	110.30
22	A	1137	CLA	C1-C2-C3	-2.77	121.25	126.04
40	6	610	CHL	C1B-CHB-C4A	-2.77	124.63	130.12
22	A	1116	CLA	CMA-C3A-C4A	2.77	119.22	111.77
22	B	1201	CLA	C2D-C1D-ND	2.77	112.14	110.10
40	Z	610	CHL	C1-O2A-CGA	2.77	123.71	116.44
22	8	615	CLA	CMA-C3A-C4A	2.77	119.21	111.77
22	B	1214	CLA	CHD-C1D-ND	-2.77	121.91	124.45
22	G	1602	CLA	C2D-C1D-ND	2.77	112.14	110.10
39	2	503	LUT	C18-C5-C4	2.77	119.48	114.36
26	2	801	LHG	O8-C23-C24	2.77	120.59	111.91
31	A	5003	LMG	O8-C28-C29	2.77	120.59	111.91
22	A	1138	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
22	G	1601	CLA	CHD-C1D-ND	-2.77	121.91	124.45
22	8	605	CLA	CHD-C1D-ND	-2.77	121.91	124.45
22	7	608	CLA	CMA-C3A-C4A	2.77	119.20	111.77
22	A	1115	CLA	C2C-C1C-NC	2.76	112.56	109.97
40	5	611	CHL	C1-O2A-CGA	2.76	123.70	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	608	CLA	C2C-C1C-NC	2.76	112.56	109.97
22	A	1123	CLA	CHD-C1D-ND	-2.76	121.92	124.45
40	9	610	CHL	C1-O2A-CGA	2.76	123.69	116.44
39	9	501	LUT	C35-C15-C14	-2.76	117.82	123.47
22	L	1502	CLA	C1-C2-C3	-2.76	121.27	126.04
26	4	801	LHG	O8-C23-C24	2.76	120.57	111.91
22	4	608	CLA	C1-C2-C3	-2.76	121.27	126.04
39	1	502	LUT	C10-C11-C12	-2.76	114.60	123.22
22	B	1234	CLA	C2D-C1D-ND	2.76	112.14	110.10
22	9	603	CLA	O2A-CGA-CBA	2.76	120.56	111.91
22	1	612	CLA	CMA-C3A-C4A	2.76	119.19	111.77
22	A	1129	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
25	5	504	BCR	C27-C26-C25	-2.76	118.73	122.73
22	A	1139	CLA	C2D-C1D-ND	2.76	112.14	110.10
22	A	1113	CLA	CMB-C2B-C1B	-2.76	124.23	128.46
22	6	607	CLA	CMA-C3A-C4A	2.76	119.18	111.77
22	B	1232	CLA	C2C-C1C-NC	2.76	112.55	109.97
22	8	612	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
22	Z	605	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
22	6	612	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
22	A	1111	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
22	2	605	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
28	B	5005	LMT	O5'-C1'-C2'	-2.75	104.53	110.35
22	4	601	CLA	C2C-C1C-NC	2.75	112.55	109.97
22	B	1213	CLA	C1-O2A-CGA	2.75	123.66	116.44
22	5	609	CLA	C1-C2-C3	-2.75	121.29	126.04
22	B	1206	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
22	B	1238	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
22	A	1139	CLA	CAA-C2A-C3A	-2.75	105.25	112.78
22	2	608	CLA	CMB-C2B-C3B	2.75	129.82	124.68
22	A	1120	CLA	C1C-C2C-C3C	-2.75	104.07	106.96
22	B	1231	CLA	CMD-C2D-C3D	-2.75	121.30	127.61
22	A	1105	CLA	C1-C2-C3	-2.75	121.29	126.04
22	8	606	CLA	C1-C2-C3	-2.75	121.29	126.04
22	A	1106	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
23	B	2002	PQN	C14-C13-C15	2.75	119.89	115.27
22	7	603	CLA	O2A-CGA-CBA	2.75	120.52	111.91
22	5	622	CLA	CMA-C3A-C4A	2.75	119.15	111.77
40	4	617	CHL	CMA-C3A-C4A	2.75	119.15	111.77
22	B	1226	CLA	CAA-C2A-C3A	-2.75	105.26	112.78
22	6	604	CLA	C2D-C1D-ND	2.74	112.13	110.10
22	6	603	CLA	C1-O2A-CGA	2.74	123.64	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	2	501	LUT	C28-C29-C30	-2.74	114.73	118.94
22	9	606	CLA	CAA-C2A-C3A	-2.74	105.27	112.78
25	B	4005	BCR	C33-C5-C4	2.74	118.88	113.62
22	B	1224	CLA	C1C-C2C-C3C	-2.74	104.08	106.96
22	A	1139	CLA	C2C-C1C-NC	2.74	112.54	109.97
22	B	1232	CLA	CMA-C3A-C4A	2.74	119.13	111.77
22	A	1126	CLA	C1-C2-C3	-2.74	121.31	126.04
22	9	612	CLA	C2C-C1C-NC	2.74	112.54	109.97
39	2	502	LUT	C40-C33-C32	2.74	122.39	118.08
22	1	613	CLA	CMA-C3A-C4A	2.74	119.13	111.77
22	B	1212	CLA	C2C-C1C-NC	2.74	112.53	109.97
22	A	1134	CLA	C1C-C2C-C3C	-2.74	104.08	106.96
22	5	612	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
22	B	1214	CLA	C2C-C1C-NC	2.73	112.53	109.97
22	4	606	CLA	C2C-C1C-NC	2.73	112.53	109.97
22	B	1232	CLA	C2D-C1D-ND	2.73	112.12	110.10
22	1	601	CLA	CMB-C2B-C3B	2.73	129.79	124.68
22	A	1135	CLA	CMA-C3A-C4A	2.73	119.12	111.77
22	A	1131	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
22	B	1204	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
22	5	618	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
22	A	1134	CLA	CMA-C3A-C4A	2.73	119.11	111.77
39	4	501	LUT	C10-C11-C12	-2.73	114.70	123.22
22	4	608	CLA	C2D-C1D-ND	2.73	112.12	110.10
22	6	607	CLA	C2D-C1D-ND	2.73	112.12	110.10
26	1	801	LHG	O8-C23-C24	2.73	120.47	111.91
22	Z	607	CLA	CMA-C3A-C4A	2.73	119.11	111.77
22	Z	607	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
22	1	608	CLA	CMD-C2D-C3D	-2.73	121.33	127.61
22	4	603	CLA	CAA-C2A-C3A	-2.73	105.30	112.78
22	7	605	CLA	C1-C2-C3	-2.73	121.32	126.04
22	8	601	CLA	C2D-C1D-ND	2.73	112.11	110.10
22	B	1218	CLA	CMB-C2B-C3B	2.73	129.78	124.68
22	7	613	CLA	CAA-C2A-C3A	-2.73	107.44	114.26
22	A	1122	CLA	C2D-C1D-ND	2.73	112.11	110.10
22	9	603	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
22	5	606	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
40	4	617	CHL	CHB-C4A-NA	2.73	128.28	124.51
22	B	1224	CLA	C2D-C1D-ND	2.73	112.11	110.10
22	1	605	CLA	C2D-C1D-ND	2.73	112.11	110.10
22	3	606	CLA	C1C-C2C-C3C	-2.72	104.09	106.96
22	5	605	CLA	C1C-C2C-C3C	-2.72	104.09	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1238	CLA	C1C-C2C-C3C	-2.72	104.09	106.96
22	L	1503	CLA	C2D-C1D-ND	2.72	112.11	110.10
22	6	601	CLA	O2A-CGA-CBA	2.72	120.45	111.91
40	8	610	CHL	CHB-C4A-NA	2.72	128.28	124.51
22	7	616	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
22	1	602	CLA	CHD-C1D-ND	-2.72	121.95	124.45
25	6	504	BCR	C36-C18-C17	-2.72	119.11	122.92
39	2	503	LUT	C36-C21-C22	-2.72	104.28	109.44
40	Z	609	CHL	CHB-C4A-NA	2.72	128.27	124.51
22	A	1121	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
40	8	610	CHL	C4D-CHA-C1A	2.72	124.56	121.25
22	1	607	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
22	1	612	CLA	C2D-C1D-ND	2.72	112.11	110.10
32	9	802	DGA	OG1-CA1-CA2	2.72	120.44	111.91
22	B	1240	CLA	C2C-C1C-NC	2.72	112.52	109.97
39	4	501	LUT	C18-C5-C6	-2.72	121.47	124.53
22	A	1132	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
22	6	603	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
22	A	1111	CLA	C2D-C1D-ND	2.72	112.11	110.10
22	9	608	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
22	6	615	CLA	C1-C2-C3	-2.72	121.34	126.04
22	B	1210	CLA	C2C-C1C-NC	2.72	112.52	109.97
22	J	1901	CLA	CMA-C3A-C4A	2.72	119.07	111.77
40	5	611	CHL	CHB-C4A-NA	2.72	128.27	124.51
22	Z	603	CLA	O2A-CGA-CBA	2.72	120.43	111.91
37	J	4002	C7Z	C2-C3-C4	2.72	114.02	110.30
22	A	1107	CLA	C2D-C1D-ND	2.72	112.11	110.10
22	2	605	CLA	CHD-C1D-ND	-2.71	121.96	124.45
22	5	615	CLA	C1C-C2C-C3C	-2.71	104.10	106.96
39	1	501	LUT	C7-C8-C9	-2.71	122.13	126.23
40	9	610	CHL	C1-C2-C3	-2.71	121.35	126.04
32	A	5005	DGA	OG1-CA1-CA2	2.71	120.42	111.91
43	6	802	3PH	O31-C31-C32	2.71	120.42	111.91
39	5	502	LUT	C10-C11-C12	-2.71	114.75	123.22
39	4	501	LUT	C15-C14-C13	-2.71	123.44	127.31
22	2	605	CLA	CHA-C4D-ND	2.71	138.17	132.50
22	Z	615	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
22	1	611	CLA	CMA-C3A-C4A	2.71	119.06	111.77
40	8	610	CHL	CMA-C3A-C4A	2.71	119.06	111.77
40	Z	609	CHL	CHD-C1D-ND	-2.71	121.96	124.45
22	A	1123	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
22	9	604	CLA	C1D-ND-C4D	-2.71	104.41	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1110	CLA	C1-C2-C3	-2.71	121.36	126.04
40	6	610	CHL	CHB-C4A-NA	2.71	128.26	124.51
22	2	612	CLA	CMB-C2B-C1B	-2.71	124.30	128.46
22	A	1110	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
22	6	615	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
40	Z	610	CHL	CHB-C4A-NA	2.71	128.25	124.51
25	I	4001	BCR	C38-C26-C27	2.71	118.81	113.62
25	B	4005	BCR	C12-C13-C14	-2.71	114.79	118.94
40	4	610	CHL	CHC-C1C-NC	2.71	128.31	124.20
22	7	609	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
45	8	803	LPX	O3-P1-O4	2.70	125.61	112.24
22	3	607	CLA	C2D-C1D-ND	2.70	112.10	110.10
22	2	606	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
37	5	505	C7Z	C28-C27-C26	-2.70	119.61	127.20
22	1	615	CLA	C1C-C2C-C3C	-2.70	104.11	106.96
22	K	1401	CLA	C2D-C1D-ND	2.70	112.10	110.10
22	9	606	CLA	C2D-C1D-ND	2.70	112.10	110.10
22	6	602	CLA	CHD-C1D-ND	-2.70	121.97	124.45
25	B	4005	BCR	C33-C5-C6	-2.70	121.49	124.53
40	2	613	CHL	CHB-C4A-NA	2.70	128.25	124.51
22	3	613	CLA	C2D-C1D-ND	2.70	112.09	110.10
22	4	612	CLA	CMB-C2B-C3B	2.70	129.73	124.68
22	8	603	CLA	O2A-CGA-CBA	2.70	120.38	111.91
22	B	1215	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
22	A	1125	CLA	C1-C2-C3	-2.70	121.38	126.04
22	3	607	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
22	8	608	CLA	C2D-C1D-ND	2.70	112.09	110.10
22	A	1141	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
22	4	608	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
37	1	503	C7Z	C1-C6-C5	-2.70	118.82	122.61
22	7	601	CLA	CMB-C2B-C3B	2.70	129.72	124.68
22	B	1227	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
22	B	1241	CLA	C2C-C1C-NC	2.70	112.50	109.97
22	6	608	CLA	C1C-C2C-C3C	-2.69	104.12	106.96
22	Z	607	CLA	C1C-C2C-C3C	-2.69	104.12	106.96
22	B	1202	CLA	C2D-C1D-ND	2.69	112.09	110.10
22	B	1208	CLA	C1-C2-C3	-2.69	121.39	126.04
22	B	1239	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
22	2	608	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
22	Z	602	CLA	CHD-C1D-ND	-2.69	121.98	124.45
22	2	603	CLA	CMA-C3A-C4A	2.69	119.01	111.77
22	A	1123	CLA	O2D-CGD-O1D	-2.69	118.58	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1116	CLA	O2A-CGA-CBA	2.69	120.36	111.91
22	7	612	CLA	CMB-C2B-C1B	-2.69	124.33	128.46
22	A	1121	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
25	J	4001	BCR	C30-C25-C24	2.69	123.39	115.78
22	Z	611	CLA	C2D-C1D-ND	2.69	112.09	110.10
22	8	605	CLA	C2D-C1D-ND	2.69	112.09	110.10
22	4	615	CLA	C2D-C1D-ND	2.69	112.09	110.10
40	Z	610	CHL	C2C-C3C-C4C	2.69	108.41	106.49
40	7	610	CHL	CHB-C4A-NA	2.69	128.23	124.51
22	5	612	CLA	C2C-C1C-NC	2.69	112.49	109.97
22	8	609	CLA	C2D-C1D-ND	2.69	112.09	110.10
22	3	608	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
40	8	610	CHL	C1B-CHB-C4A	-2.69	124.79	130.12
22	4	607	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
22	A	1129	CLA	C2D-C1D-ND	2.69	112.08	110.10
22	7	607	CLA	C2D-C1D-ND	2.69	112.08	110.10
22	A	1130	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
22	B	1224	CLA	O1D-CGD-CBD	-2.69	118.99	124.48
22	A	1107	CLA	O2A-CGA-CBA	2.69	120.34	111.91
22	7	601	CLA	O2A-CGA-CBA	2.69	120.34	111.91
22	2	606	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
26	Z	801	LHG	O8-C23-C24	2.69	120.33	111.91
22	B	1213	CLA	C1C-C2C-C3C	-2.68	104.13	106.96
22	5	613	CLA	C1C-C2C-C3C	-2.68	104.13	106.96
22	6	618	CLA	C1D-ND-C4D	-2.68	104.43	106.33
22	1	606	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
22	B	1201	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
40	6	610	CHL	C2C-C3C-C4C	2.68	108.40	106.49
22	8	605	CLA	CMB-C2B-C3B	2.68	129.70	124.68
22	A	1012	CLA	OBD-CAD-C3D	-2.68	122.06	128.52
22	B	1218	CLA	O2A-CGA-CBA	2.68	120.33	111.91
22	B	1229	CLA	CMA-C3A-C4A	2.68	118.98	111.77
22	G	1602	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
40	2	610	CHL	CHB-C4A-NA	2.68	128.22	124.51
22	6	619	CLA	C2C-C1C-NC	2.68	112.48	109.97
22	A	1115	CLA	CMA-C3A-C4A	2.68	118.98	111.77
22	6	608	CLA	CMD-C2D-C3D	-2.68	121.45	127.61
22	8	608	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
22	B	1231	CLA	C2C-C1C-NC	2.68	112.48	109.97
22	Z	602	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
22	3	603	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
26	7	801	LHG	C5-O7-C7	-2.68	111.19	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	F	4001	RRX	C30-C25-C24	2.68	123.36	115.78
39	2	502	LUT	C7-C8-C9	-2.68	122.19	126.23
22	B	1206	CLA	CHD-C1D-ND	-2.68	121.99	124.45
25	A	4003	BCR	C1-C6-C7	2.68	123.35	115.78
22	A	1135	CLA	C2D-C1D-ND	2.68	112.08	110.10
39	2	502	LUT	C39-C29-C28	2.68	122.29	118.08
43	8	806	3PH	O31-C31-C32	2.68	120.30	111.91
25	A	4004	BCR	C35-C13-C12	2.67	122.29	118.08
22	A	1132	CLA	CAA-C2A-C3A	-2.67	105.46	112.78
22	9	607	CLA	C2D-C1D-ND	2.67	112.07	110.10
22	B	1229	CLA	C1D-ND-C4D	-2.67	104.44	106.33
22	A	1138	CLA	C1-C2-C3	-2.67	121.42	126.04
22	B	1022	CLA	OBD-CAD-C3D	-2.67	122.09	128.52
22	1	611	CLA	C2D-C1D-ND	2.67	112.07	110.10
22	B	1208	CLA	CMB-C2B-C1B	-2.67	124.36	128.46
22	9	602	CLA	CHD-C1D-ND	-2.67	122.00	124.45
37	1	503	C7Z	C10-C11-C12	-2.67	114.88	123.22
22	A	1107	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
22	8	601	CLA	C2C-C1C-NC	2.67	112.47	109.97
39	2	501	LUT	C18-C5-C6	-2.67	121.53	124.53
22	A	1130	CLA	C2D-C1D-ND	2.67	112.07	110.10
22	2	605	CLA	C2D-C1D-ND	2.67	112.07	110.10
22	B	1221	CLA	O1D-CGD-CBD	-2.67	119.03	124.48
22	7	606	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
22	6	604	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
22	A	1130	CLA	CMA-C3A-C4A	2.67	118.94	111.77
22	9	605	CLA	CHA-C4D-ND	2.67	138.08	132.50
22	2	601	CLA	C2D-C1D-ND	2.67	112.07	110.10
22	B	1228	CLA	C1-C2-C3	-2.67	121.43	126.04
22	7	611	CLA	C1D-ND-C4D	-2.66	104.44	106.33
39	7	501	LUT	C15-C14-C13	-2.66	123.51	127.31
39	4	502	LUT	C15-C14-C13	-2.66	123.51	127.31
22	1	606	CLA	C2C-C1C-NC	2.66	112.47	109.97
25	7	504	BCR	C33-C5-C4	2.66	118.73	113.62
22	J	1901	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
25	4	503	BCR	C38-C26-C25	-2.66	121.54	124.53
22	4	603	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
22	A	1112	CLA	C2D-C1D-ND	2.66	112.07	110.10
43	7	802	3PH	O31-C31-C32	2.66	120.26	111.91
22	A	1118	CLA	C1D-ND-C4D	-2.66	104.44	106.33
22	Z	601	CLA	O2A-CGA-CBA	2.66	120.25	111.91
22	7	613	CLA	C1C-C2C-C3C	-2.66	104.16	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1115	CLA	C2D-C1D-ND	2.66	112.06	110.10
26	A	5002	LHG	O8-C23-C24	2.66	120.25	111.91
22	5	612	CLA	CMB-C2B-C3B	2.66	129.65	124.68
22	1	603	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
43	2	802	3PH	O31-C31-C32	2.66	120.25	111.91
22	3	612	CLA	C2D-C1D-ND	2.66	112.06	110.10
22	9	601	CLA	C2D-C1D-ND	2.66	112.06	110.10
22	B	1210	CLA	CMB-C2B-C3B	2.66	129.65	124.68
22	8	609	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
22	5	605	CLA	C2C-C1C-NC	2.66	112.46	109.97
22	7	611	CLA	CMA-C3A-C4A	2.66	118.91	111.77
39	6	502	LUT	C10-C11-C12	-2.66	114.93	123.22
22	K	1403	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
22	Z	606	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
22	4	609	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
22	B	1207	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
26	6	801	LHG	O8-C23-C24	2.65	120.24	111.91
22	8	607	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
22	A	1104	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
22	6	606	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
25	B	4006	BCR	C35-C13-C12	2.65	122.26	118.08
22	A	1120	CLA	C1-C2-C3	-2.65	121.45	126.04
25	6	504	BCR	C28-C27-C26	-2.65	109.34	114.08
22	6	607	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
22	A	1124	CLA	CAA-C2A-C1A	-2.65	103.28	111.97
22	3	605	CLA	CHA-C4D-ND	2.65	138.05	132.50
26	B	5006	LHG	O8-C23-C24	2.65	120.23	111.91
40	1	610	CHL	CHB-C4A-NA	2.65	128.18	124.51
22	2	607	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
22	B	1229	CLA	O2A-CGA-CBA	2.65	120.22	111.91
22	B	1223	CLA	CHA-C4D-ND	2.65	138.04	132.50
22	B	1231	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
22	A	1120	CLA	C1D-ND-C4D	-2.65	104.45	106.33
22	B	1222	CLA	CMA-C3A-C4A	2.65	118.89	111.77
22	B	1211	CLA	O2A-CGA-CBA	2.65	120.22	111.91
22	1	612	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
39	1	502	LUT	C35-C15-C14	-2.65	118.05	123.47
22	B	1212	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
22	7	604	CLA	CMA-C3A-C4A	2.65	118.89	111.77
25	B	4004	BCR	C37-C22-C23	2.65	122.25	118.08
22	A	1112	CLA	O2A-CGA-CBA	2.65	120.21	111.91
22	5	608	CLA	C1C-C2C-C3C	-2.65	104.17	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1137	CLA	O2D-CGD-O1D	-2.65	118.67	123.84
22	4	609	CLA	O2D-CGD-O1D	-2.65	118.67	123.84
22	B	1222	CLA	C1-O2A-CGA	2.65	123.38	116.44
22	L	1503	CLA	CMA-C3A-C4A	2.65	118.88	111.77
22	4	605	CLA	CHD-C1D-ND	-2.64	122.02	124.45
22	5	602	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
22	8	601	CLA	CHA-C4D-ND	2.64	138.03	132.50
22	B	1204	CLA	C1-C2-C3	-2.64	121.47	126.04
22	1	602	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
22	7	604	CLA	CAA-C2A-C1A	2.64	120.63	111.97
40	5	611	CHL	C1-C2-C3	-2.64	122.48	126.75
22	B	1234	CLA	CMA-C3A-C4A	2.64	118.87	111.77
22	5	605	CLA	CMD-C2D-C3D	-2.64	121.54	127.61
22	3	610	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
39	4	502	LUT	C38-C25-C24	-2.64	117.91	123.56
22	B	1234	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
39	2	503	LUT	C1-C6-C5	-2.64	118.90	122.61
25	5	504	BCR	C37-C22-C21	-2.64	119.23	122.92
22	B	1241	CLA	O2A-CGA-CBA	2.64	120.18	111.91
22	8	602	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
22	A	1101	CLA	C1C-C2C-C3C	-2.64	104.19	106.96
22	B	1208	CLA	C1C-C2C-C3C	-2.64	104.19	106.96
22	L	1502	CLA	C1C-C2C-C3C	-2.64	104.19	106.96
40	8	613	CHL	CHB-C4A-NA	2.64	128.16	124.51
26	A	5001	LHG	C5-O7-C7	-2.64	111.30	117.79
39	9	501	LUT	C10-C11-C12	-2.64	114.99	123.22
22	3	616	CLA	C1-C2-C3	-2.63	121.49	126.04
22	7	601	CLA	CHA-C4D-ND	2.63	138.01	132.50
25	K	4001	BCR	C2-C1-C6	2.63	114.54	110.48
22	B	1021	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
22	8	603	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
25	B	4001	BCR	C37-C22-C23	2.63	122.23	118.08
39	1	501	LUT	C35-C15-C14	-2.63	118.08	123.47
22	1	605	CLA	CMA-C3A-C4A	2.63	118.85	111.77
40	1	610	CHL	CHC-C1C-NC	2.63	128.20	124.20
22	B	1221	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
22	5	609	CLA	O2A-CGA-CBA	2.63	120.17	111.91
40	1	609	CHL	CHB-C4A-NA	2.63	128.15	124.51
22	B	1231	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
22	B	1240	CLA	CMA-C3A-C4A	2.63	118.84	111.77
22	B	1221	CLA	CHA-C4D-ND	2.63	138.00	132.50
22	A	1118	CLA	C1C-C2C-C3C	-2.63	104.19	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	7	607	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
22	Z	608	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
22	2	608	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
36	F	4001	RRX	C20-C19-C18	-2.63	119.04	126.42
22	A	1105	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
22	A	1118	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
36	F	4001	RRX	C15-C16-C17	-2.63	118.09	123.47
22	A	1105	CLA	C1C-C2C-C3C	-2.63	104.20	106.96
40	5	617	CHL	CHB-C4A-NA	2.63	128.14	124.51
25	3	503	BCR	C35-C13-C12	2.63	122.21	118.08
22	A	1111	CLA	C2C-C1C-NC	2.62	112.43	109.97
22	1	608	CLA	C2D-C1D-ND	2.62	112.04	110.10
22	1	607	CLA	CMB-C2B-C3B	2.62	129.59	124.68
22	A	1109	CLA	O2A-CGA-CBA	2.62	120.14	111.91
22	5	622	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
35	B	5004	T7X	C12-C13-C14	-2.62	108.55	113.23
40	3	611	CHL	C1-C2-C3	-2.62	121.51	126.04
25	K	4002	BCR	C31-C1-C6	-2.62	106.05	110.30
39	3	501	LUT	C35-C15-C14	-2.62	118.10	123.47
22	B	1205	CLA	C1-O2A-CGA	2.62	123.32	116.44
25	A	4002	BCR	C33-C5-C6	-2.62	121.58	124.53
22	Z	602	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
39	2	503	LUT	C32-C33-C34	2.62	122.96	118.94
39	5	502	LUT	C35-C34-C33	-2.62	123.57	127.31
22	6	606	CLA	C2D-C1D-ND	2.62	112.03	110.10
22	B	1230	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
22	B	1236	CLA	C1D-ND-C4D	-2.62	104.47	106.33
22	B	1022	CLA	CHA-C4D-ND	2.62	137.98	132.50
22	A	1012	CLA	CAA-C2A-C3A	-2.62	105.61	112.78
22	6	602	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
22	3	602	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
39	2	501	LUT	C10-C11-C12	-2.62	115.05	123.22
22	1	606	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
25	A	4002	BCR	C38-C26-C27	2.62	118.64	113.62
22	A	1133	CLA	C2D-C1D-ND	2.62	112.03	110.10
40	2	613	CHL	C1B-CHB-C4A	-2.62	124.93	130.12
40	4	611	CHL	C1-O2A-CGA	2.62	123.31	116.44
22	F	1301	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
22	B	1219	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
39	8	501	LUT	C18-C5-C6	-2.62	121.59	124.53
39	Z	501	LUT	C38-C25-C24	-2.62	117.96	123.56
22	5	609	CLA	C1C-C2C-C3C	-2.62	104.21	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1207	CLA	C2D-C1D-ND	2.61	112.03	110.10
22	5	607	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
22	6	605	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
22	B	1214	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
22	8	611	CLA	CMA-C3A-C4A	2.61	118.80	111.77
22	K	1402	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
22	9	607	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
40	4	611	CHL	C1-C2-C3	-2.61	122.53	126.75
22	5	608	CLA	CMA-C3A-C4A	2.61	118.79	111.77
22	4	605	CLA	CHA-C4D-ND	2.61	137.96	132.50
25	7	503	BCR	C15-C14-C13	-2.61	123.58	127.31
22	A	1105	CLA	C1D-ND-C4D	-2.61	104.48	106.33
22	7	603	CLA	C6-C5-C3	-2.61	106.61	113.45
22	A	1120	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
40	Z	610	CHL	C4D-CHA-C1A	2.61	124.43	121.25
22	A	1124	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
25	7	503	BCR	C33-C5-C6	-2.61	121.60	124.53
39	8	502	LUT	C10-C11-C12	-2.61	115.07	123.22
22	B	1205	CLA	C2D-C1D-ND	2.61	112.03	110.10
22	A	1116	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
22	B	1239	CLA	O2A-CGA-CBA	2.61	120.09	111.91
40	7	610	CHL	C3C-C4C-NC	-2.61	107.65	110.57
22	A	1128	CLA	C1-C2-C3	-2.61	121.53	126.04
22	A	1135	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
22	A	1109	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
28	F	5001	LMT	C1'-O5'-C5'	-2.61	108.57	113.69
22	2	601	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
22	A	1137	CLA	CMB-C2B-C1B	-2.61	124.46	128.46
22	A	1126	CLA	C2D-C1D-ND	2.60	112.02	110.10
40	6	613	CHL	CHB-C4A-NA	2.60	128.11	124.51
22	B	1207	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
22	8	606	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
22	B	1206	CLA	C2D-C1D-ND	2.60	112.02	110.10
22	A	1126	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
22	3	605	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
22	7	605	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
22	A	1012	CLA	C2C-C1C-NC	2.60	112.41	109.97
22	A	1105	CLA	C2C-C1C-NC	2.60	112.41	109.97
22	7	611	CLA	C2C-C1C-NC	2.60	112.41	109.97
37	J	4002	C7Z	C15-C35-C34	-2.60	118.15	123.47
22	7	606	CLA	CMD-C2D-C3D	-2.60	121.64	127.61
40	Z	609	CHL	C2C-C3C-C4C	2.60	108.34	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1219	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
22	B	1236	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
22	4	615	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
22	5	608	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
22	8	609	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
22	A	1102	CLA	C1-C2-C3	-2.60	121.55	126.04
22	7	615	CLA	C1C-C2C-C3C	-2.60	104.23	106.96
22	2	615	CLA	CMA-C3A-C4A	2.60	118.75	111.77
40	6	610	CHL	CMA-C3A-C4A	2.60	118.75	111.77
22	7	609	CLA	O2A-CGA-CBA	2.60	120.05	111.91
25	A	4002	BCR	C27-C26-C25	-2.60	118.96	122.73
22	K	1404	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
22	G	1601	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
40	4	613	CHL	CHB-C4A-NA	2.59	128.10	124.51
22	B	1231	CLA	CHA-C4D-ND	2.59	137.93	132.50
22	1	613	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
22	8	611	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
22	B	1202	CLA	C1-O2A-CGA	2.59	123.25	116.44
22	B	1021	CLA	C2D-C1D-ND	2.59	112.01	110.10
22	B	1217	CLA	C1-C2-C3	-2.59	121.56	126.04
22	B	1235	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
22	B	1209	CLA	CMA-C3A-C4A	2.59	118.73	111.77
22	A	1119	CLA	CMB-C2B-C3B	2.59	129.52	124.68
22	Z	605	CLA	C2D-C1D-ND	2.59	112.01	110.10
22	A	1124	CLA	O2A-CGA-CBA	2.59	120.03	111.91
22	L	1503	CLA	CMB-C2B-C1B	-2.59	124.48	128.46
22	Z	611	CLA	C1-O2A-CGA	2.59	123.24	116.44
25	A	4001	BCR	C23-C24-C25	-2.59	119.93	127.20
22	B	1216	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
39	4	502	LUT	C7-C8-C9	-2.59	122.32	126.23
22	A	1112	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
22	B	1215	CLA	CMB-C2B-C3B	2.59	129.52	124.68
22	A	1012	CLA	CHA-C4D-ND	2.59	137.91	132.50
39	9	502	LUT	C35-C34-C33	-2.59	123.62	127.31
22	1	606	CLA	CMD-C2D-C3D	-2.59	121.66	127.61
22	5	613	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
25	B	4007	BCR	C19-C18-C17	2.59	122.91	118.94
22	3	601	CLA	CMB-C2B-C3B	2.59	129.51	124.68
40	6	610	CHL	C4D-CHA-C1A	2.58	124.39	121.25
26	1	801	LHG	C5-O7-C7	-2.58	111.43	117.79
39	6	501	LUT	C39-C29-C28	2.58	122.15	118.08
39	3	502	LUT	C10-C11-C12	-2.58	115.16	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	5	609	CLA	CMA-C3A-C4A	2.58	118.71	111.77
22	A	1101	CLA	C1-C2-C3	-2.58	121.58	126.04
22	F	1301	CLA	C6-C5-C3	-2.58	106.69	113.45
39	3	502	LUT	C31-C30-C29	-2.58	123.63	127.31
22	6	619	CLA	CHA-C4D-ND	2.58	137.89	132.50
39	7	502	LUT	C35-C15-C14	-2.58	118.19	123.47
22	3	602	CLA	C1C-C2C-C3C	-2.58	104.25	106.96
22	3	605	CLA	C2D-C1D-ND	2.58	112.00	110.10
22	1	608	CLA	C1-C2-C3	-2.58	121.59	126.04
22	6	612	CLA	C1D-ND-C4D	-2.58	104.50	106.33
22	8	601	CLA	C1C-C2C-C3C	-2.58	104.25	106.96
22	2	603	CLA	C1C-C2C-C3C	-2.58	104.25	106.96
22	1	606	CLA	C2D-C1D-ND	2.58	112.00	110.10
22	B	1213	CLA	CMB-C2B-C3B	2.58	129.50	124.68
22	4	601	CLA	C1C-C2C-C3C	-2.58	104.25	106.96
22	K	1402	CLA	CMA-C3A-C4A	2.57	118.69	111.77
22	A	1109	CLA	C1D-ND-C4D	-2.57	104.51	106.33
22	B	1240	CLA	O2A-CGA-CBA	2.57	119.99	111.91
22	6	606	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
22	Z	606	CLA	C2D-C1D-ND	2.57	112.00	110.10
22	5	602	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
22	B	1205	CLA	C1-C2-C3	-2.57	121.59	126.04
26	4	802	LHG	O8-C23-C24	2.57	119.98	111.91
22	F	1301	CLA	CAA-C2A-C3A	-2.57	105.73	112.78
22	B	1203	CLA	CHA-C4D-ND	2.57	137.88	132.50
22	A	1106	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
22	6	618	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
22	9	603	CLA	C1-C2-C3	-2.57	121.59	126.04
22	3	601	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
22	6	601	CLA	C1-O2A-CGA	2.57	123.19	116.44
22	6	608	CLA	CHA-C4D-ND	2.57	137.88	132.50
22	B	1022	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
22	B	1209	CLA	C2D-C1D-ND	2.57	112.00	110.10
26	9	801	LHG	O8-C23-C24	2.57	119.97	111.91
40	6	611	CHL	C3C-C4C-NC	-2.57	107.69	110.57
22	A	1124	CLA	CMA-C3A-C4A	2.57	118.68	111.77
22	1	604	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
39	5	502	LUT	C7-C8-C9	-2.57	122.35	126.23
22	8	605	CLA	CHA-C4D-ND	2.57	137.87	132.50
39	6	502	LUT	C31-C30-C29	-2.57	123.64	127.31
22	5	618	CLA	C1D-ND-C4D	-2.57	104.51	106.33
22	7	616	CLA	C1C-C2C-C3C	-2.57	104.26	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1119	CLA	CHA-C4D-ND	2.57	137.87	132.50
22	A	1112	CLA	C1C-C2C-C3C	-2.57	104.26	106.96
25	B	4003	BCR	C8-C9-C10	2.57	122.88	118.94
22	F	1301	CLA	CHA-C4D-ND	2.57	137.87	132.50
39	6	501	LUT	C38-C25-C24	-2.57	118.07	123.56
22	8	606	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
25	8	503	BCR	C36-C18-C17	-2.56	119.33	122.92
22	A	1133	CLA	O2A-CGA-CBA	2.56	119.96	111.91
22	3	606	CLA	C1D-ND-C4D	-2.56	104.51	106.33
22	B	1209	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
22	A	1134	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
22	5	607	CLA	O2A-CGA-CBA	2.56	119.95	111.91
22	1	605	CLA	CHA-C4D-ND	2.56	137.86	132.50
22	B	1235	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
25	I	4001	BCR	C35-C13-C12	2.56	122.11	118.08
22	9	608	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
22	B	1227	CLA	C2D-C1D-ND	2.56	111.99	110.10
22	7	612	CLA	C2D-C1D-ND	2.56	111.99	110.10
22	2	602	CLA	C1D-ND-C4D	-2.56	104.52	106.33
22	9	602	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
22	B	1022	CLA	CAA-C2A-C3A	-2.56	105.77	112.78
25	3	505	BCR	C36-C18-C17	-2.56	119.34	122.92
22	1	613	CLA	CHA-C4D-ND	2.56	137.85	132.50
22	7	611	CLA	CMB-C2B-C1B	-2.56	124.53	128.46
25	3	506	BCR	C15-C14-C13	-2.56	123.66	127.31
22	8	604	CLA	C1-O2A-CGA	2.56	123.15	116.44
22	8	609	CLA	CHA-C4D-ND	2.56	137.85	132.50
22	3	608	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
22	B	1235	CLA	CMB-C2B-C3B	2.56	129.46	124.68
22	1	604	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
22	9	609	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
25	L	4001	BCR	C35-C13-C12	2.55	122.10	118.08
22	B	1218	CLA	C1-O2A-CGA	2.55	123.15	116.44
39	2	502	LUT	C30-C31-C32	-2.55	115.25	123.22
22	6	601	CLA	CAA-C2A-C3A	-2.55	105.78	112.78
22	A	1131	CLA	C2D-C1D-ND	2.55	111.99	110.10
22	A	1126	CLA	CMB-C2B-C3B	2.55	129.46	124.68
22	A	1103	CLA	C1D-ND-C4D	-2.55	104.52	106.33
22	A	1137	CLA	CMA-C3A-C4A	2.55	118.64	111.77
22	A	1125	CLA	C3D-C2D-C1D	-2.55	102.35	105.83
26	5	801	LHG	O8-C23-C24	2.55	119.92	111.91
22	A	1139	CLA	O2D-CGD-O1D	-2.55	118.85	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	Z	613	CHL	CHB-C4A-NA	2.55	128.04	124.51
22	5	601	CLA	C1-C2-C3	-2.55	121.63	126.04
25	3	506	BCR	C23-C22-C21	2.55	122.86	118.94
43	5	802	3PH	O31-C31-C32	2.55	119.92	111.91
22	Z	603	CLA	C1C-C2C-C3C	-2.55	104.27	106.96
22	5	622	CLA	CHA-C4D-ND	2.55	137.84	132.50
39	9	502	LUT	C18-C5-C6	-2.55	121.66	124.53
22	B	1213	CLA	C1-C2-C3	-2.55	121.63	126.04
22	A	1109	CLA	CMD-C2D-C3D	-2.55	121.75	127.61
22	7	609	CLA	C1D-ND-C4D	-2.55	104.52	106.33
22	B	1206	CLA	C1-C2-C3	-2.55	121.63	126.04
22	A	1134	CLA	CHA-C4D-ND	2.55	137.83	132.50
40	7	610	CHL	C1-C2-C3	-2.55	121.64	126.04
22	3	612	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
22	B	1237	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
22	B	1206	CLA	O2A-CGA-CBA	2.55	119.90	111.91
36	F	4001	RRX	C8-C7-C6	-2.55	120.05	127.20
22	G	1601	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
22	Z	607	CLA	C2D-C1D-ND	2.55	111.98	110.10
22	B	1208	CLA	C2C-C1C-NC	2.55	112.36	109.97
22	7	613	CLA	CMA-C3A-C4A	2.55	118.62	111.77
22	3	610	CLA	C1-C2-C3	-2.55	121.64	126.04
22	7	602	CLA	C1C-C2C-C3C	-2.54	104.28	106.96
22	3	607	CLA	CHA-C4D-ND	2.54	137.82	132.50
22	5	615	CLA	O2D-CGD-O1D	-2.54	118.86	123.84
22	A	1132	CLA	CMA-C3A-C4A	2.54	118.61	111.77
22	Z	605	CLA	CHA-C4D-ND	2.54	137.82	132.50
22	6	602	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
22	2	612	CLA	C2C-C1C-NC	2.54	112.35	109.97
28	A	5006	LMT	C1'-O5'-C5'	-2.54	108.70	113.69
22	B	1204	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
22	A	1116	CLA	CHA-C4D-ND	2.54	137.82	132.50
22	2	604	CLA	C2D-C1D-ND	2.54	111.98	110.10
22	9	603	CLA	C2D-C1D-ND	2.54	111.98	110.10
22	K	1401	CLA	CMA-C3A-C4A	2.54	118.60	111.77
22	B	1226	CLA	CHD-C4C-C3C	2.54	128.57	124.84
22	9	612	CLA	CMB-C2B-C1B	-2.54	124.56	128.46
22	Z	601	CLA	C2C-C1C-NC	2.54	112.35	109.97
22	B	1214	CLA	C1-O2A-CGA	2.54	123.10	116.44
22	A	1104	CLA	CHA-C4D-ND	2.54	137.81	132.50
22	A	1114	CLA	CMD-C2D-C3D	-2.54	121.78	127.61
22	A	1119	CLA	C2C-C1C-NC	2.54	112.35	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	8	601	CLA	CMB-C2B-C3B	2.54	129.43	124.68
22	6	605	CLA	C1-O2A-CGA	2.54	123.10	116.44
22	1	615	CLA	CHA-C4D-ND	2.54	137.81	132.50
22	8	605	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
22	K	1404	CLA	CHA-C4D-ND	2.54	137.80	132.50
22	5	605	CLA	C1-O2A-CGA	2.54	123.10	116.44
22	5	605	CLA	O2A-CGA-CBA	2.54	119.86	111.91
22	4	609	CLA	C1D-ND-C4D	-2.54	104.53	106.33
22	1	611	CLA	CMD-C2D-C3D	-2.54	121.78	127.61
22	A	1114	CLA	O2D-CGD-O1D	-2.53	118.88	123.84
22	3	616	CLA	O2D-CGD-O1D	-2.53	118.88	123.84
37	1	503	C7Z	C2-C3-C4	2.53	113.77	110.30
22	9	604	CLA	C1-O2A-CGA	2.53	123.09	116.44
22	G	1602	CLA	CHA-C4D-ND	2.53	137.80	132.50
22	3	606	CLA	CMB-C2B-C3B	2.53	129.42	124.68
22	Z	601	CLA	CAA-C2A-C3A	-2.53	105.84	112.78
22	Z	605	CLA	CMD-C2D-C3D	-2.53	121.79	127.61
22	A	1105	CLA	O2A-CGA-CBA	2.53	119.85	111.91
39	Z	502	LUT	C35-C15-C14	-2.53	118.29	123.47
22	2	604	CLA	CMB-C2B-C1B	-2.53	124.57	128.46
22	6	602	CLA	O2A-CGA-CBA	2.53	119.85	111.91
25	7	503	BCR	C38-C26-C25	-2.53	121.69	124.53
22	L	1503	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
37	J	4002	C7Z	C11-C10-C9	-2.53	123.70	127.31
25	A	4003	BCR	C4-C5-C6	-2.53	119.06	122.73
22	B	1232	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
40	1	610	CHL	C4D-CHA-C1A	2.53	124.33	121.25
22	K	1404	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
22	4	602	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
22	6	601	CLA	CHA-C4D-ND	2.53	137.79	132.50
25	5	503	BCR	C38-C26-C25	-2.53	121.69	124.53
39	Z	502	LUT	C10-C11-C12	-2.53	115.33	123.22
22	7	603	CLA	C2C-C1C-NC	2.53	112.34	109.97
25	A	4004	BCR	C34-C9-C10	-2.53	119.38	122.92
22	Z	606	CLA	CHA-C4D-ND	2.53	137.78	132.50
22	9	604	CLA	O1D-CGD-CBD	-2.53	119.31	124.48
22	7	605	CLA	CMA-C3A-C4A	2.53	118.56	111.77
28	8	805	LMT	O5'-C1'-C2'	-2.53	105.00	110.35
22	B	1229	CLA	C1-C2-C3	-2.52	121.68	126.04
22	J	1901	CLA	CMB-C2B-C3B	2.52	129.40	124.68
22	B	1219	CLA	CMA-C3A-C4A	2.52	118.56	111.77
22	A	1130	CLA	CHA-C4D-ND	2.52	137.78	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	9	502	LUT	C7-C8-C9	-2.52	122.42	126.23
22	Z	608	CLA	C2D-C1D-ND	2.52	111.96	110.10
22	B	1219	CLA	CHA-C4D-ND	2.52	137.78	132.50
22	B	1216	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
40	7	610	CHL	C4D-CHA-C1A	2.52	124.32	121.25
22	9	606	CLA	C1D-ND-C4D	-2.52	104.54	106.33
22	8	612	CLA	CMB-C2B-C3B	2.52	129.40	124.68
22	9	602	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
22	5	607	CLA	C2D-C1D-ND	2.52	111.96	110.10
22	A	1125	CLA	CMB-C2B-C1B	-2.52	124.59	128.46
22	B	1224	CLA	C1-C2-C3	-2.52	121.69	126.04
22	A	1135	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
22	B	1205	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
25	3	503	BCR	C36-C18-C17	-2.52	119.39	122.92
22	A	1111	CLA	CHA-C4D-ND	2.52	137.77	132.50
22	B	1223	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
22	1	607	CLA	C2A-C1A-CHA	2.52	128.26	123.86
25	I	4001	BCR	C36-C18-C17	-2.52	119.40	122.92
22	A	1109	CLA	C2C-C1C-NC	2.52	112.33	109.97
22	6	608	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
25	B	4007	BCR	C35-C13-C12	2.52	122.04	118.08
22	Z	606	CLA	CAA-C2A-C3A	-2.51	105.89	112.78
22	5	618	CLA	CMA-C3A-C4A	2.51	118.53	111.77
39	9	501	LUT	C38-C25-C24	-2.51	118.18	123.56
22	1	607	CLA	CHA-C4D-ND	2.51	137.76	132.50
26	A	5001	LHG	O8-C23-C24	2.51	119.80	111.91
22	3	605	CLA	CHD-C1D-ND	-2.51	122.14	124.45
22	8	605	CLA	CMA-C3A-C4A	2.51	118.53	111.77
22	B	1023	CLA	C2C-C1C-NC	2.51	112.33	109.97
22	5	607	CLA	C1C-C2C-C3C	-2.51	104.31	106.96
22	8	609	CLA	C1-C2-C3	-2.51	121.70	126.04
25	J	4001	BCR	C19-C18-C17	2.51	122.80	118.94
22	1	604	CLA	C2D-C1D-ND	2.51	111.95	110.10
22	5	606	CLA	C2D-C1D-ND	2.51	111.95	110.10
22	F	1302	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
22	5	605	CLA	C1D-ND-C4D	-2.51	104.55	106.33
22	B	1021	CLA	CHA-C4D-ND	2.51	137.75	132.50
40	6	613	CHL	C1-O2A-CGA	2.51	123.03	116.44
22	B	1224	CLA	CMB-C2B-C3B	2.51	129.38	124.68
25	L	4001	BCR	C27-C26-C25	-2.51	119.09	122.73
22	B	1220	CLA	C2C-C1C-NC	2.51	112.32	109.97
42	Z	504	QTB	C11-C10-C09	2.51	130.92	125.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	6	619	CLA	O2A-CGA-CBA	2.51	119.78	111.91
39	8	501	LUT	C15-C14-C13	-2.51	123.73	127.31
22	A	1112	CLA	CMA-C3A-C4A	2.51	118.52	111.77
22	B	1203	CLA	O2A-CGA-CBA	2.51	119.78	111.91
22	7	615	CLA	C1-O2A-CGA	2.51	123.02	116.44
35	B	5004	T7X	O18-C11-C31	2.51	119.78	111.91
39	7	501	LUT	C18-C5-C6	-2.51	121.71	124.53
22	A	1126	CLA	CMA-C3A-C4A	2.51	118.51	111.77
22	2	605	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
25	B	4005	BCR	C36-C18-C17	-2.51	119.41	122.92
22	B	1216	CLA	C2D-C1D-ND	2.51	111.95	110.10
22	G	1602	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
25	3	506	BCR	C38-C26-C25	-2.51	121.72	124.53
22	Z	612	CLA	C2D-C1D-ND	2.50	111.95	110.10
22	4	615	CLA	CHA-C4D-ND	2.50	137.74	132.50
22	A	1115	CLA	CMB-C2B-C3B	2.50	129.36	124.68
22	A	1125	CLA	CHA-C4D-ND	2.50	137.74	132.50
22	4	605	CLA	C1D-ND-C4D	-2.50	104.56	106.33
22	7	607	CLA	C1-C2-C3	-2.50	121.71	126.04
22	8	604	CLA	C1C-C2C-C3C	-2.50	104.32	106.96
22	B	1227	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
22	8	612	CLA	CHA-C4D-ND	2.50	137.73	132.50
22	2	612	CLA	CHA-C4D-ND	2.50	137.73	132.50
22	7	615	CLA	CMA-C3A-C4A	2.50	118.50	111.77
22	3	613	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
22	1	604	CLA	CHA-C4D-ND	2.50	137.73	132.50
22	3	606	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
22	A	1130	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
22	K	1401	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
22	A	1121	CLA	CHA-C4D-ND	2.50	137.73	132.50
22	K	1401	CLA	CHA-C4D-ND	2.50	137.73	132.50
22	K	1403	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
22	9	612	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
22	L	1502	CLA	C1D-ND-C4D	-2.50	104.56	106.33
22	B	1211	CLA	CMD-C2D-C3D	-2.50	121.86	127.61
22	2	601	CLA	C1C-C2C-C3C	-2.50	104.33	106.96
22	1	606	CLA	CHA-C4D-ND	2.50	137.72	132.50
25	A	4004	BCR	C36-C18-C17	-2.50	119.42	122.92
22	G	1601	CLA	CHA-C4D-ND	2.50	137.72	132.50
22	6	605	CLA	CHA-C4D-ND	2.50	137.72	132.50
22	B	1228	CLA	CMA-C3A-C4A	2.50	118.49	111.77
22	B	1214	CLA	CHA-C4D-ND	2.50	137.72	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	613	CLA	C2D-C1D-ND	2.50	111.94	110.10
22	Z	604	CLA	CHA-C4D-ND	2.50	137.72	132.50
22	2	612	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
25	G	4001	BCR	C37-C22-C21	-2.50	119.43	122.92
22	7	606	CLA	CHA-C4D-ND	2.50	137.72	132.50
40	6	610	CHL	C1-C2-C3	-2.50	121.73	126.04
22	B	1209	CLA	CHA-C4D-ND	2.50	137.72	132.50
22	9	609	CLA	C1C-C2C-C3C	-2.50	104.33	106.96
25	A	4003	BCR	C35-C13-C12	2.49	122.01	118.08
39	2	503	LUT	C36-C21-C26	2.49	113.32	109.55
22	8	608	CLA	CMA-C3A-C4A	2.49	118.48	111.77
22	F	1301	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
22	7	612	CLA	C1C-C2C-C3C	-2.49	104.33	106.96
22	K	1404	CLA	CHD-C1D-ND	-2.49	122.16	124.45
22	B	1222	CLA	C2C-C1C-NC	2.49	112.31	109.97
22	A	1114	CLA	CHA-C4D-ND	2.49	137.72	132.50
22	A	1129	CLA	CHA-C4D-ND	2.49	137.71	132.50
22	B	1218	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
22	A	1141	CLA	CHA-C4D-ND	2.49	137.71	132.50
22	9	612	CLA	C2D-C1D-ND	2.49	111.94	110.10
22	6	607	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
22	B	1234	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
22	A	1104	CLA	O2A-CGA-CBA	2.49	119.73	111.91
22	A	1129	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
22	6	619	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
22	B	1225	CLA	C2D-C1D-ND	2.49	111.94	110.10
22	5	622	CLA	CMD-C2D-C3D	-2.49	121.89	127.61
22	5	606	CLA	CHA-C4D-ND	2.49	137.71	132.50
22	9	609	CLA	CHA-C4D-ND	2.49	137.70	132.50
22	A	1103	CLA	CMB-C2B-C1B	-2.49	124.64	128.46
22	6	601	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
22	1	602	CLA	CHA-C4D-ND	2.49	137.70	132.50
22	A	1106	CLA	O1D-CGD-CBD	-2.49	119.40	124.48
22	4	604	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
22	2	602	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
25	J	4001	BCR	C34-C9-C10	-2.49	119.44	122.92
22	A	1102	CLA	CHA-C4D-ND	2.49	137.70	132.50
22	9	606	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
22	B	1241	CLA	OBD-CAD-C3D	-2.49	122.54	128.52
22	7	607	CLA	CHA-C4D-ND	2.49	137.70	132.50
22	5	607	CLA	CHA-C4D-ND	2.49	137.70	132.50
22	5	603	CLA	C1C-C2C-C3C	-2.48	104.34	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	7	801	LHG	O8-C23-C24	2.48	119.70	111.91
22	5	602	CLA	CHA-C4D-ND	2.48	137.70	132.50
40	4	613	CHL	C1-C2-C3	-2.48	121.75	126.04
22	3	610	CLA	O1D-CGD-CBD	-2.48	119.40	124.48
22	9	608	CLA	C2D-C1D-ND	2.48	111.93	110.10
22	6	609	CLA	C1D-ND-C4D	-2.48	104.57	106.33
22	A	1115	CLA	CGD-CBD-CAD	2.48	118.78	110.73
40	Z	610	CHL	C1B-CHB-C4A	-2.48	125.20	130.12
22	K	1404	CLA	C1-C2-C3	-2.48	121.75	126.04
22	4	606	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
25	K	4002	BCR	C35-C13-C12	2.48	121.99	118.08
22	A	1121	CLA	OBD-CAD-C3D	-2.48	122.55	128.52
22	B	1021	CLA	CAA-C2A-C3A	-2.48	105.98	112.78
22	A	1140	CLA	CHA-C4D-ND	2.48	137.69	132.50
22	9	603	CLA	CHA-C4D-ND	2.48	137.69	132.50
22	5	602	CLA	C1D-ND-C4D	-2.48	104.57	106.33
40	9	610	CHL	CHC-C1C-NC	2.48	127.97	124.20
22	3	612	CLA	CMA-C3A-C4A	2.48	118.44	111.77
22	B	1022	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
22	B	1217	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
22	B	1225	CLA	CMA-C3A-C4A	2.48	118.44	111.77
22	3	605	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
22	6	615	CLA	CHA-C4D-ND	2.48	137.69	132.50
22	3	618	CLA	CMA-C3A-C4A	2.48	118.44	111.77
22	A	1013	CLA	C2A-C1A-CHA	2.48	128.19	123.86
22	B	1202	CLA	C6-C5-C3	-2.48	106.96	113.45
22	B	1234	CLA	CHA-C4D-ND	2.48	137.68	132.50
25	7	504	BCR	C34-C9-C10	-2.48	119.45	122.92
40	5	610	CHL	C3C-C4C-NC	-2.48	107.79	110.57
39	6	501	LUT	C10-C11-C12	-2.48	115.49	123.22
25	A	4001	BCR	C31-C1-C6	-2.48	106.28	110.30
22	A	1114	CLA	O2A-CGA-CBA	2.48	119.68	111.91
22	7	607	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
25	5	504	BCR	C12-C13-C14	2.47	122.74	118.94
22	A	1102	CLA	C2C-C1C-NC	2.47	112.29	109.97
22	3	613	CLA	CHA-C4D-ND	2.47	137.68	132.50
22	B	1232	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
22	A	1135	CLA	O1D-CGD-CBD	-2.47	119.42	124.48
22	6	601	CLA	C2D-C1D-ND	2.47	111.93	110.10
22	F	1302	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
22	7	604	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
25	7	504	BCR	C36-C18-C17	-2.47	119.46	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	4004	BCR	C33-C5-C4	2.47	118.37	113.62
22	B	1230	CLA	O2A-CGA-CBA	2.47	119.67	111.91
22	A	1125	CLA	CMA-C3A-C4A	2.47	118.42	111.77
25	A	4001	BCR	C38-C26-C25	-2.47	121.75	124.53
22	6	602	CLA	CHA-C4D-ND	2.47	137.67	132.50
22	1	605	CLA	CMD-C2D-C3D	-2.47	121.93	127.61
22	A	1012	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
22	8	602	CLA	CHA-C4D-ND	2.47	137.67	132.50
22	B	1228	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
22	5	618	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
22	A	1116	CLA	C1-C2-C3	-2.47	121.77	126.04
22	4	608	CLA	O2A-CGA-CBA	2.47	119.66	111.91
22	A	1129	CLA	CMB-C2B-C1B	-2.47	124.67	128.46
22	7	607	CLA	CAA-C2A-C3A	-2.47	106.02	112.78
22	1	612	CLA	CHA-C4D-ND	2.47	137.66	132.50
22	4	602	CLA	CHA-C4D-ND	2.47	137.66	132.50
22	A	1111	CLA	O1D-CGD-CBD	-2.47	119.43	124.48
22	B	1203	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
36	F	4001	RRX	C35-C13-C14	-2.47	119.47	122.92
22	B	1214	CLA	CMA-C3A-C4A	2.47	118.40	111.77
22	B	1224	CLA	CHA-C4D-ND	2.47	137.66	132.50
22	2	604	CLA	CHA-C4D-ND	2.47	137.66	132.50
22	A	1139	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
22	6	612	CLA	O2D-CGD-O1D	-2.47	119.02	123.84
22	2	603	CLA	CHA-C4D-ND	2.47	137.66	132.50
40	6	617	CHL	CHB-C4A-NA	2.47	127.92	124.51
22	9	607	CLA	CHA-C4D-ND	2.46	137.66	132.50
39	9	501	LUT	C15-C14-C13	-2.46	123.79	127.31
22	7	605	CLA	CHA-C4D-ND	2.46	137.65	132.50
22	4	605	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
22	5	605	CLA	CHA-C4D-ND	2.46	137.65	132.50
22	1	611	CLA	C1-O2A-CGA	2.46	122.91	116.44
22	5	601	CLA	CHA-C4D-ND	2.46	137.65	132.50
22	A	1113	CLA	C1C-C2C-C3C	-2.46	104.37	106.96
22	B	1232	CLA	CHA-C4D-ND	2.46	137.65	132.50
22	K	1402	CLA	CHA-C4D-ND	2.46	137.65	132.50
22	6	602	CLA	CMA-C3A-C4A	2.46	118.39	111.77
39	9	502	LUT	C3-C4-C5	-2.46	106.95	111.85
22	8	603	CLA	CAA-C2A-C3A	-2.46	106.04	112.78
22	B	1227	CLA	CHA-C4D-ND	2.46	137.65	132.50
22	7	603	CLA	C1C-C2C-C3C	-2.46	104.37	106.96
22	7	605	CLA	C1D-ND-C4D	-2.46	104.59	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	4	611	CHL	CHB-C4A-NA	2.46	127.91	124.51
22	Z	612	CLA	CHA-C4D-ND	2.46	137.64	132.50
25	K	4002	BCR	C19-C18-C17	2.46	122.71	118.94
22	A	1110	CLA	CHA-C4D-ND	2.46	137.64	132.50
22	A	1102	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
22	3	602	CLA	CHA-C4D-ND	2.46	137.64	132.50
22	A	1128	CLA	CMA-C3A-C4A	2.46	118.37	111.77
22	9	612	CLA	CAA-CBA-CGA	-2.46	106.08	113.25
22	L	1502	CLA	O2D-CGD-O1D	-2.46	119.04	123.84
22	A	1116	CLA	C1-O2A-CGA	2.45	122.89	116.44
22	9	606	CLA	CMD-C2D-C3D	-2.45	121.97	127.61
22	7	608	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
22	2	603	CLA	O1D-CGD-CBD	-2.45	119.46	124.48
22	B	1208	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
22	B	1021	CLA	CHD-C1D-ND	-2.45	122.20	124.45
39	1	501	LUT	C20-C13-C12	2.45	121.94	118.08
22	Z	615	CLA	CHA-C4D-ND	2.45	137.63	132.50
22	A	1137	CLA	C1-O2A-CGA	2.45	122.88	116.44
22	B	1216	CLA	CHA-C4D-ND	2.45	137.63	132.50
22	Z	601	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
22	8	602	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
22	9	612	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
22	A	1139	CLA	CHA-C4D-ND	2.45	137.63	132.50
22	3	616	CLA	O2A-CGA-CBA	2.45	119.60	111.91
22	K	1403	CLA	C2D-C1D-ND	2.45	111.91	110.10
22	B	1212	CLA	CHA-C4D-ND	2.45	137.62	132.50
22	B	1222	CLA	CAA-C2A-C1A	-2.45	103.95	111.97
22	Z	608	CLA	CHA-C4D-ND	2.45	137.62	132.50
36	F	4001	RRX	C11-C12-C13	-2.45	119.53	126.42
22	4	607	CLA	O2A-CGA-CBA	2.45	119.59	111.91
22	B	1215	CLA	CMB-C2B-C1B	-2.45	124.70	128.46
22	B	1241	CLA	CAA-CBA-CGA	-2.45	106.09	113.25
25	8	503	BCR	C23-C24-C25	-2.45	120.32	127.20
22	Z	604	CLA	CMD-C2D-C3D	-2.45	121.98	127.61
22	4	607	CLA	CHA-C4D-ND	2.45	137.62	132.50
22	2	606	CLA	CHA-C4D-ND	2.45	137.62	132.50
22	5	605	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
22	Z	607	CLA	CHA-C4D-ND	2.45	137.62	132.50
39	9	502	LUT	C35-C15-C14	-2.45	118.46	123.47
22	1	608	CLA	CHA-C4D-ND	2.45	137.62	132.50
22	Z	602	CLA	CHA-C4D-ND	2.45	137.62	132.50
22	8	607	CLA	CHA-C4D-ND	2.45	137.62	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1140	CLA	CMA-C3A-C4A	2.45	118.35	111.77
22	A	1126	CLA	O1D-CGD-CBD	-2.45	119.48	124.48
39	Z	503	LUT	C22-C23-C24	-2.45	108.96	111.74
22	K	1401	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
22	3	603	CLA	C1D-ND-C4D	-2.45	104.60	106.33
22	2	606	CLA	C2D-C1D-ND	2.45	111.91	110.10
22	A	1106	CLA	CMA-C3A-C4A	2.45	118.34	111.77
22	A	1113	CLA	CHA-C4D-ND	2.45	137.61	132.50
22	4	601	CLA	CHA-C4D-ND	2.45	137.61	132.50
22	6	607	CLA	CHA-C4D-ND	2.45	137.61	132.50
22	Z	602	CLA	CMB-C2B-C1B	-2.45	124.71	128.46
22	5	612	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
22	A	1123	CLA	CHA-C4D-ND	2.44	137.61	132.50
22	5	612	CLA	CHA-C4D-ND	2.44	137.61	132.50
40	7	610	CHL	C1-O2A-CGA	2.44	122.86	116.44
22	5	613	CLA	CHA-C4D-ND	2.44	137.61	132.50
22	B	1220	CLA	CMA-C3A-C4A	2.44	118.34	111.77
22	A	1111	CLA	O2A-CGA-CBA	2.44	119.58	111.91
40	8	613	CHL	C1-O2A-CGA	2.44	122.86	116.44
22	4	602	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
22	4	608	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
22	B	1021	CLA	O1D-CGD-CBD	-2.44	119.48	124.48
22	A	1133	CLA	CHA-C4D-ND	2.44	137.61	132.50
22	2	604	CLA	CMA-C3A-C4A	2.44	118.34	111.77
22	1	608	CLA	C1D-ND-C4D	-2.44	104.60	106.33
22	1	601	CLA	C2C-C1C-NC	2.44	112.26	109.97
22	A	1103	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
22	B	1223	CLA	C3D-C2D-C1D	-2.44	102.50	105.83
22	7	612	CLA	CHA-C4D-ND	2.44	137.61	132.50
22	8	608	CLA	O2A-CGA-CBA	2.44	119.57	111.91
22	B	1202	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
22	Z	615	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
22	1	602	CLA	CAC-C3C-C4C	2.44	127.98	124.81
22	A	1121	CLA	CAA-C2A-C3A	-2.44	106.10	112.78
22	1	601	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
22	A	1101	CLA	CHA-C4D-ND	2.44	137.60	132.50
22	B	1240	CLA	CHA-C4D-ND	2.44	137.60	132.50
22	7	606	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
39	3	502	LUT	C37-C21-C26	2.44	113.24	109.55
22	B	1208	CLA	CMA-C3A-C4A	2.44	118.33	111.77
22	B	1229	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
22	A	1115	CLA	C1C-C2C-C3C	-2.44	104.39	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1206	CLA	CHA-C4D-ND	2.44	137.60	132.50
22	B	1217	CLA	CHA-C4D-ND	2.44	137.60	132.50
22	B	1236	CLA	CHA-C4D-ND	2.44	137.60	132.50
22	1	607	CLA	CHA-C1A-NA	-2.44	120.81	126.40
25	4	503	BCR	C35-C13-C12	2.44	121.92	118.08
21	A	1011	CL0	C1-C2-C3	-2.44	121.83	126.04
22	Z	606	CLA	CMD-C2D-C3D	-2.44	122.01	127.61
22	A	1102	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
22	5	604	CLA	C1D-ND-C4D	-2.44	104.60	106.33
25	J	4001	BCR	C35-C13-C12	2.44	121.92	118.08
37	J	4002	C7Z	C19-C9-C8	2.44	121.92	118.08
22	A	1106	CLA	CHA-C4D-ND	2.44	137.59	132.50
22	4	615	CLA	O2D-CGD-O1D	-2.44	119.08	123.84
25	J	4001	BCR	C38-C26-C25	-2.44	121.79	124.53
22	5	604	CLA	C2C-C1C-NC	2.43	112.25	109.97
22	7	605	CLA	C1-O2A-CGA	2.43	122.83	116.44
22	8	606	CLA	CMB-C2B-C1B	-2.43	124.72	128.46
22	8	615	CLA	CHA-C4D-ND	2.43	137.59	132.50
25	4	503	BCR	C36-C18-C17	-2.43	119.51	122.92
25	8	503	BCR	C27-C26-C25	-2.43	119.20	122.73
22	4	606	CLA	CHA-C4D-ND	2.43	137.59	132.50
22	2	608	CLA	CHA-C4D-ND	2.43	137.59	132.50
22	A	1102	CLA	CAA-CBA-CGA	-2.43	106.14	113.25
22	B	1226	CLA	C1-C2-C3	-2.43	121.83	126.04
22	A	1123	CLA	C2D-C1D-ND	2.43	111.90	110.10
22	A	1110	CLA	C1C-C2C-C3C	-2.43	104.40	106.96
22	9	601	CLA	CHA-C4D-ND	2.43	137.59	132.50
22	B	1210	CLA	O2A-CGA-CBA	2.43	119.54	111.91
39	4	502	LUT	C10-C11-C12	-2.43	115.63	123.22
22	1	611	CLA	CAA-C2A-C3A	-2.43	106.12	112.78
22	A	1119	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
22	5	609	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
22	A	1105	CLA	CMC-C2C-C1C	2.43	128.74	125.04
22	1	611	CLA	CHA-C4D-ND	2.43	137.58	132.50
22	A	1113	CLA	O2A-CGA-CBA	2.43	119.54	111.91
40	8	613	CHL	C3C-C4C-NC	-2.43	107.84	110.57
22	1	604	CLA	CMA-C3A-C4A	2.43	118.31	111.77
40	6	617	CHL	C4D-CHA-C1A	2.43	124.21	121.25
22	8	606	CLA	CHA-C4D-ND	2.43	137.58	132.50
25	3	505	BCR	C34-C9-C10	-2.43	119.52	122.92
22	5	601	CLA	CMB-C2B-C3B	2.43	129.22	124.68
22	B	1235	CLA	C2D-C1D-ND	2.43	111.89	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Z	611	CLA	CHA-C4D-ND	2.43	137.58	132.50
22	9	608	CLA	CMA-C3A-C4A	2.43	118.30	111.77
22	9	604	CLA	CMC-C2C-C1C	2.43	128.74	125.04
22	1	615	CLA	CMD-C2D-C3D	-2.43	122.03	127.61
22	B	1224	CLA	O2A-CGA-CBA	2.43	119.52	111.91
37	J	4002	C7Z	C38-C25-C24	2.43	118.85	114.36
22	8	604	CLA	CHA-C4D-ND	2.43	137.57	132.50
25	B	4007	BCR	C36-C18-C17	-2.43	119.53	122.92
22	2	601	CLA	O2A-CGA-CBA	2.43	119.52	111.91
22	7	615	CLA	CHA-C4D-ND	2.43	137.57	132.50
25	L	4001	BCR	C38-C26-C27	2.43	118.28	113.62
40	4	610	CHL	C1-C2-C3	-2.43	122.83	126.75
22	6	607	CLA	CAA-C2A-C3A	-2.43	106.14	112.78
22	9	612	CLA	CHA-C4D-ND	2.43	137.57	132.50
22	A	1136	CLA	C2D-C1D-ND	2.42	111.89	110.10
22	A	1136	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
22	B	1238	CLA	CHA-C4D-ND	2.42	137.57	132.50
22	Z	604	CLA	C1C-C2C-C3C	-2.42	104.41	106.96
37	J	4002	C7Z	C18-C5-C4	2.42	118.84	114.36
28	1	803	LMT	C3'-C4'-C5'	-2.42	105.37	110.93
22	A	1108	CLA	CAA-C2A-C3A	-2.42	106.14	112.78
22	7	601	CLA	C1C-C2C-C3C	-2.42	104.41	106.96
22	B	1239	CLA	CHA-C4D-ND	2.42	137.57	132.50
22	B	1225	CLA	CHD-C1D-ND	-2.42	122.23	124.45
22	7	613	CLA	CHA-C4D-ND	2.42	137.57	132.50
22	9	602	CLA	CHA-C4D-ND	2.42	137.57	132.50
22	A	1103	CLA	C1-C2-C3	-2.42	121.85	126.04
22	B	1240	CLA	CHA-C1A-NA	-2.42	120.85	126.40
22	1	607	CLA	C2D-C1D-ND	2.42	111.89	110.10
22	4	612	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
22	9	608	CLA	CHA-C4D-ND	2.42	137.56	132.50
22	3	601	CLA	O1D-CGD-CBD	-2.42	119.53	124.48
22	1	613	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
22	6	604	CLA	CBA-CAA-C2A	2.42	121.01	113.86
40	4	611	CHL	C4D-CHA-C1A	2.42	124.19	121.25
22	3	610	CLA	CHA-C4D-ND	2.42	137.56	132.50
22	B	1207	CLA	CAA-C2A-C3A	-2.42	106.15	112.78
22	A	1139	CLA	C1-O2A-CGA	2.42	122.79	116.44
22	B	1225	CLA	CHA-C4D-ND	2.42	137.56	132.50
22	J	1901	CLA	CHA-C4D-ND	2.42	137.56	132.50
22	2	607	CLA	CHA-C4D-ND	2.42	137.56	132.50
22	1	601	CLA	CHA-C4D-ND	2.42	137.56	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	7	609	CLA	CHA-C4D-ND	2.42	137.56	132.50
22	5	608	CLA	CHA-C4D-ND	2.42	137.56	132.50
22	5	601	CLA	CMD-C2D-C3D	-2.42	122.05	127.61
22	A	1102	CLA	CHA-C1A-NA	-2.42	120.86	126.40
22	A	1131	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
22	B	1212	CLA	CMB-C2B-C3B	2.42	129.20	124.68
22	A	1013	CLA	C1C-C2C-C3C	-2.42	104.42	106.96
22	A	1141	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
22	3	616	CLA	C1-O2A-CGA	2.42	122.78	116.44
22	B	1237	CLA	CHA-C4D-ND	2.42	137.55	132.50
22	A	1120	CLA	CMB-C2B-C1B	-2.42	124.75	128.46
22	Z	608	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
22	7	602	CLA	CHA-C4D-ND	2.42	137.55	132.50
22	6	604	CLA	CHA-C4D-ND	2.42	137.55	132.50
22	B	1241	CLA	C1C-C2C-C3C	-2.42	104.42	106.96
22	5	618	CLA	C3D-C2D-C1D	-2.42	102.53	105.83
25	A	4005	BCR	C37-C22-C23	2.41	121.88	118.08
40	4	617	CHL	C3C-C4C-NC	-2.41	107.86	110.57
22	B	1023	CLA	O2A-CGA-CBA	2.41	119.48	111.91
22	B	1221	CLA	CMD-C2D-C3D	-2.41	122.06	127.61
22	6	601	CLA	CMD-C2D-C3D	-2.41	122.06	127.61
22	A	1132	CLA	CHA-C4D-ND	2.41	137.54	132.50
22	6	606	CLA	CMA-C3A-C4A	2.41	118.25	111.77
22	A	1141	CLA	C1-C2-C3	-2.41	121.87	126.04
42	Z	504	QTB	C03-C04-C05	-2.41	115.70	123.22
22	3	606	CLA	CMD-C2D-C3D	-2.41	122.07	127.61
22	6	601	CLA	CMB-C2B-C3B	2.41	129.19	124.68
22	1	608	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
22	B	1221	CLA	CHA-C1A-NA	-2.41	120.88	126.40
22	B	1209	CLA	C1-C2-C3	-2.41	121.88	126.04
25	3	503	BCR	C34-C9-C10	-2.41	119.55	122.92
22	B	1208	CLA	CHA-C4D-ND	2.41	137.54	132.50
40	5	611	CHL	CHC-C1C-NC	2.41	127.86	124.20
22	A	1131	CLA	CHA-C4D-ND	2.41	137.54	132.50
22	1	605	CLA	O2A-CGA-CBA	2.41	119.47	111.91
22	5	601	CLA	C2C-C1C-NC	2.41	112.23	109.97
22	B	1202	CLA	CAA-C2A-C1A	-2.41	104.08	111.97
22	A	1127	CLA	CHA-C4D-ND	2.41	137.54	132.50
22	A	1123	CLA	CHA-C1A-NA	-2.41	120.88	126.40
22	7	604	CLA	CHA-C4D-ND	2.41	137.53	132.50
22	A	1116	CLA	CHA-C1A-NA	-2.41	120.89	126.40
39	5	501	LUT	C10-C11-C12	-2.41	115.70	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	4003	BCR	C35-C13-C12	2.41	121.87	118.08
22	A	1108	CLA	C1-C2-C3	-2.41	121.88	126.04
25	6	503	BCR	C38-C26-C25	-2.41	121.83	124.53
22	8	611	CLA	CHA-C4D-ND	2.41	137.53	132.50
22	B	1230	CLA	CMA-C3A-C4A	2.41	118.24	111.77
40	6	611	CHL	CHB-C4A-NA	2.41	127.84	124.51
22	6	615	CLA	O1D-CGD-CBD	-2.41	119.56	124.48
22	L	1503	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
22	5	604	CLA	CHA-C4D-ND	2.40	137.53	132.50
22	A	1013	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
25	B	4004	BCR	C37-C22-C21	-2.40	119.56	122.92
40	6	610	CHL	CHD-C4C-C3C	2.40	128.37	124.84
22	Z	608	CLA	CMD-C2D-C3D	-2.40	122.08	127.61
22	A	1123	CLA	CMB-C2B-C1B	-2.40	124.77	128.46
22	6	605	CLA	CHA-C1A-NA	-2.40	120.89	126.40
22	8	607	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
25	B	4001	BCR	C19-C18-C17	2.40	122.63	118.94
22	6	606	CLA	CHA-C4D-ND	2.40	137.53	132.50
22	3	618	CLA	CHA-C1A-NA	-2.40	120.90	126.40
22	5	603	CLA	CHA-C4D-ND	2.40	137.52	132.50
25	A	4004	BCR	C34-C9-C8	2.40	121.86	118.08
40	5	617	CHL	C3C-C4C-NC	-2.40	107.88	110.57
22	B	1210	CLA	CHA-C4D-ND	2.40	137.52	132.50
22	4	609	CLA	CHA-C4D-ND	2.40	137.52	132.50
22	3	610	CLA	CAA-C2A-C3A	-2.40	106.21	112.78
22	B	1221	CLA	C1C-C2C-C3C	-2.40	104.43	106.96
22	B	1231	CLA	O2A-CGA-CBA	2.40	119.44	111.91
40	Z	609	CHL	C1B-CHB-C4A	-2.40	125.37	130.12
22	K	1403	CLA	CHA-C4D-ND	2.40	137.51	132.50
22	5	609	CLA	CHA-C4D-ND	2.40	137.51	132.50
22	B	1237	CLA	C1C-C2C-C3C	-2.40	104.44	106.96
28	B	6101	LMT	O5B-C5B-C4B	2.40	114.05	109.69
22	J	1901	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
22	3	601	CLA	CHA-C4D-ND	2.40	137.51	132.50
39	6	502	LUT	C7-C8-C9	-2.40	122.61	126.23
22	A	1138	CLA	CHA-C4D-ND	2.40	137.51	132.50
22	4	606	CLA	CMA-C3A-C4A	2.40	118.21	111.77
22	9	607	CLA	O2A-CGA-CBA	2.40	119.42	111.91
22	8	609	CLA	C1-O2A-CGA	2.40	122.73	116.44
22	B	1228	CLA	CHA-C4D-ND	2.39	137.51	132.50
22	B	1204	CLA	CHA-C4D-ND	2.39	137.51	132.50
22	2	602	CLA	CHA-C4D-ND	2.39	137.51	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1135	CLA	CHA-C4D-ND	2.39	137.51	132.50
22	9	601	CLA	C1C-C2C-C3C	-2.39	104.44	106.96
40	7	610	CHL	CHD-C4C-C3C	2.39	128.36	124.84
22	B	1235	CLA	CHA-C4D-ND	2.39	137.50	132.50
25	5	503	BCR	C4-C5-C6	-2.39	119.26	122.73
22	4	607	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
22	9	605	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
22	B	1229	CLA	CHA-C4D-ND	2.39	137.50	132.50
22	B	1221	CLA	C2D-C1D-ND	2.39	111.87	110.10
39	4	502	LUT	C1-C6-C5	-2.39	119.24	122.61
25	7	504	BCR	C37-C22-C21	-2.39	119.57	122.92
22	4	601	CLA	CMD-C2D-C3D	-2.39	122.11	127.61
22	B	1201	CLA	CHA-C4D-ND	2.39	137.50	132.50
22	7	608	CLA	CHA-C4D-ND	2.39	137.50	132.50
22	A	1125	CLA	CAA-C2A-C3A	-2.39	106.23	112.78
22	B	1223	CLA	O2A-CGA-CBA	2.39	119.41	111.91
22	7	606	CLA	C2D-C1D-ND	2.39	111.87	110.10
22	4	615	CLA	CMB-C2B-C3B	2.39	129.15	124.68
22	A	1138	CLA	CMB-C2B-C1B	-2.39	124.79	128.46
22	B	1212	CLA	O1D-CGD-CBD	-2.39	119.59	124.48
22	6	618	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
22	8	605	CLA	CMB-C2B-C1B	-2.39	124.79	128.46
22	3	606	CLA	CHA-C4D-ND	2.39	137.50	132.50
22	5	615	CLA	CHA-C4D-ND	2.39	137.50	132.50
22	6	606	CLA	CAA-C2A-C3A	-2.39	106.24	112.78
22	B	1218	CLA	C1-C2-C3	-2.39	121.91	126.04
22	7	609	CLA	C1-C2-C3	-2.39	121.91	126.04
39	Z	502	LUT	C3-C4-C5	-2.39	107.10	111.85
22	4	608	CLA	CHA-C4D-ND	2.39	137.49	132.50
22	8	609	CLA	CMA-C3A-C4A	2.39	118.19	111.77
22	B	1213	CLA	CHA-C4D-ND	2.39	137.49	132.50
22	B	1213	CLA	CMA-C3A-C4A	2.39	118.19	111.77
22	3	618	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
22	Z	604	CLA	C1-O2A-CGA	2.38	122.70	116.44
22	B	1214	CLA	C1-C2-C3	-2.38	121.92	126.04
22	A	1112	CLA	CHA-C4D-ND	2.38	137.49	132.50
22	5	601	CLA	C1D-ND-C4D	-2.38	104.64	106.33
22	8	601	CLA	C2A-C1A-CHA	2.38	128.03	123.86
22	6	615	CLA	O2A-CGA-CBA	2.38	119.39	111.91
22	4	604	CLA	CHA-C4D-ND	2.38	137.48	132.50
22	Z	611	CLA	CMD-C2D-C3D	-2.38	122.13	127.61
22	6	612	CLA	CHA-C4D-ND	2.38	137.48	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	9	603	CLA	CMD-C2D-C3D	-2.38	122.14	127.61
22	3	616	CLA	CHA-C4D-ND	2.38	137.48	132.50
22	A	1126	CLA	O2A-CGA-CBA	2.38	119.38	111.91
39	2	503	LUT	C15-C35-C34	-2.38	118.60	123.47
25	J	4001	BCR	C12-C13-C14	-2.38	115.29	118.94
22	A	1137	CLA	CHA-C4D-ND	2.38	137.48	132.50
22	A	1107	CLA	C1-C2-C3	-2.38	121.92	126.04
22	Z	605	CLA	CMA-C3A-C4A	2.38	118.17	111.77
25	K	4002	BCR	C34-C9-C10	-2.38	119.59	122.92
22	3	604	CLA	CMB-C2B-C1B	-2.38	124.81	128.46
40	8	613	CHL	CMA-C3A-C2A	2.38	123.43	113.83
25	7	503	BCR	C33-C5-C4	2.38	118.19	113.62
22	7	605	CLA	CMD-C2D-C3D	-2.38	122.14	127.61
22	Z	608	CLA	CAA-C2A-C3A	-2.38	106.26	112.78
22	A	1101	CLA	CMA-C3A-C4A	2.38	118.17	111.77
22	5	601	CLA	C1-O2A-CGA	2.38	122.68	116.44
22	A	1107	CLA	CHA-C4D-ND	2.38	137.47	132.50
22	Z	601	CLA	CHA-C4D-ND	2.38	137.47	132.50
39	Z	502	LUT	C11-C10-C9	-2.38	123.92	127.31
37	1	503	C7Z	C31-C32-C33	-2.38	119.74	126.42
22	A	1139	CLA	O2A-CGA-CBA	2.38	119.37	111.91
22	B	1239	CLA	CMA-C3A-C4A	2.38	118.16	111.77
22	3	613	CLA	O2A-CGA-CBA	2.38	119.36	111.91
22	9	606	CLA	CHA-C4D-ND	2.38	137.47	132.50
22	B	1221	CLA	C1-C2-C3	-2.38	121.94	126.04
22	9	605	CLA	CMD-C2D-C3D	-2.38	122.15	127.61
39	6	501	LUT	C20-C13-C12	2.37	121.82	118.08
22	B	1215	CLA	CHA-C4D-ND	2.37	137.47	132.50
22	Z	608	CLA	CMB-C2B-C3B	2.37	129.12	124.68
22	A	1140	CLA	O2A-CGA-CBA	2.37	119.36	111.91
22	1	603	CLA	CHA-C4D-ND	2.37	137.47	132.50
22	3	603	CLA	CHA-C4D-ND	2.37	137.46	132.50
22	B	1219	CLA	O2A-CGA-CBA	2.37	119.36	111.91
22	A	1135	CLA	CHA-C1A-NA	-2.37	120.96	126.40
22	7	601	CLA	O1D-CGD-CBD	-2.37	119.63	124.48
22	5	601	CLA	C1C-C2C-C3C	-2.37	104.46	106.96
40	4	610	CHL	CHD-C4C-C3C	2.37	128.33	124.84
21	A	1011	CL0	C3D-C4D-ND	2.37	114.08	110.24
22	B	1220	CLA	O2A-CGA-CBA	2.37	119.35	111.91
22	2	602	CLA	CAC-C3C-C4C	2.37	127.89	124.81
22	3	612	CLA	CHA-C4D-ND	2.37	137.46	132.50
22	6	603	CLA	CHA-C4D-ND	2.37	137.46	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	7	616	CLA	CHA-C4D-ND	2.37	137.46	132.50
22	B	1228	CLA	C1C-C2C-C3C	-2.37	104.46	106.96
22	1	613	CLA	CHA-C1A-NA	-2.37	120.97	126.40
22	7	609	CLA	O1D-CGD-CBD	-2.37	119.64	124.48
22	3	610	CLA	CMD-C2D-C3D	-2.37	122.16	127.61
22	7	605	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
40	Z	609	CHL	C1-C2-C3	-2.37	121.95	126.04
22	Z	603	CLA	C1D-ND-C4D	-2.37	104.65	106.33
22	A	1125	CLA	C1C-C2C-C3C	-2.37	104.47	106.96
40	9	613	CHL	CHB-C4A-NA	2.37	127.79	124.51
22	A	1117	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
22	L	1503	CLA	CAA-C2A-C3A	-2.37	106.30	112.78
22	A	1109	CLA	CHA-C4D-ND	2.37	137.45	132.50
40	5	617	CHL	C4A-NA-C1A	2.37	107.77	106.71
22	K	1403	CLA	O2A-CGA-CBA	2.37	119.33	111.91
22	9	603	CLA	CMB-C2B-C3B	2.37	129.10	124.68
22	A	1122	CLA	CHA-C4D-ND	2.37	137.45	132.50
22	A	1110	CLA	C1D-ND-C4D	-2.36	104.66	106.33
22	B	1207	CLA	CHA-C4D-ND	2.36	137.45	132.50
22	5	607	CLA	C1-C2-C3	-2.36	121.95	126.04
22	B	1207	CLA	O2A-CGA-CBA	2.36	119.33	111.91
39	9	501	LUT	C11-C10-C9	-2.36	123.94	127.31
22	A	1120	CLA	O1D-CGD-CBD	-2.36	119.65	124.48
22	3	608	CLA	CHA-C4D-ND	2.36	137.44	132.50
22	A	1129	CLA	O2A-CGA-CBA	2.36	119.32	111.91
22	B	1211	CLA	C1C-C2C-C3C	-2.36	104.47	106.96
25	K	4001	BCR	C36-C18-C17	-2.36	119.61	122.92
22	9	604	CLA	O1A-CGA-CBA	-2.36	114.51	123.73
22	8	601	CLA	CMD-C2D-C3D	-2.36	122.18	127.61
22	A	1134	CLA	C1-O2A-CGA	2.36	122.64	116.44
22	A	1128	CLA	CHA-C4D-ND	2.36	137.44	132.50
22	B	1223	CLA	OBD-CAD-C3D	-2.36	122.84	128.52
40	9	613	CHL	C1B-CHB-C4A	-2.36	125.44	130.12
40	5	611	CHL	C3C-C4C-NC	-2.36	107.92	110.57
22	7	604	CLA	CHA-C1A-NA	-2.36	120.99	126.40
22	B	1229	CLA	C1-O2A-CGA	2.36	122.64	116.44
22	B	1226	CLA	CHA-C1A-NA	-2.36	121.00	126.40
39	5	501	LUT	C11-C10-C9	-2.36	123.94	127.31
22	B	1023	CLA	CHA-C4D-ND	2.36	137.43	132.50
22	2	604	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
40	2	609	CHL	CHC-C1C-NC	2.36	127.78	124.20
22	A	1117	CLA	CHA-C4D-ND	2.36	137.43	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	5	502	LUT	C3-C4-C5	-2.36	107.16	111.85
22	B	1235	CLA	CMD-C2D-C3D	-2.36	122.19	127.61
38	7	804	SPH	C3-C4-C5	-2.36	119.54	124.79
22	1	608	CLA	O2A-CGA-CBA	2.36	119.30	111.91
22	B	1214	CLA	O2A-CGA-CBA	2.36	119.30	111.91
22	A	1126	CLA	CHA-C4D-ND	2.36	137.43	132.50
22	4	603	CLA	CHA-C4D-ND	2.36	137.43	132.50
25	K	4001	BCR	C3-C4-C5	-2.35	109.87	114.08
22	4	612	CLA	CHA-C4D-ND	2.35	137.42	132.50
28	B	6101	LMT	O1'-C1'-C2'	2.35	111.98	108.30
22	A	1141	CLA	O2A-CGA-CBA	2.35	119.29	111.91
25	7	504	BCR	C4-C5-C6	-2.35	119.31	122.73
22	1	611	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
22	L	1503	CLA	CHA-C4D-ND	2.35	137.42	132.50
22	1	605	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
22	A	1012	CLA	C1C-C2C-C3C	-2.35	104.48	106.96
22	4	606	CLA	CAA-C2A-C3A	-2.35	106.34	112.78
25	L	4001	BCR	C36-C18-C17	-2.35	119.63	122.92
22	9	604	CLA	CHA-C4D-ND	2.35	137.42	132.50
22	K	1404	CLA	O1D-CGD-CBD	-2.35	119.67	124.48
22	2	612	CLA	CMA-C3A-C4A	2.35	118.09	111.77
22	7	613	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
22	A	1108	CLA	CHA-C4D-ND	2.35	137.42	132.50
39	9	501	LUT	C37-C21-C22	-2.35	104.98	109.44
40	6	617	CHL	C3C-C4C-NC	-2.35	107.94	110.57
22	A	1103	CLA	CMA-C3A-C4A	2.35	118.09	111.77
22	4	601	CLA	CMB-C2B-C3B	2.35	129.07	124.68
22	A	1131	CLA	O2A-CGA-CBA	2.35	119.28	111.91
25	B	4005	BCR	C38-C26-C27	2.35	118.13	113.62
39	8	502	LUT	C31-C32-C33	-2.35	119.81	126.42
22	A	1104	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
22	A	1124	CLA	CMB-C2B-C3B	2.35	129.07	124.68
40	4	617	CHL	C4A-NA-C1A	2.35	107.76	106.71
22	B	1225	CLA	C1C-C2C-C3C	-2.35	104.49	106.96
40	4	610	CHL	C3C-C4C-NC	-2.35	107.94	110.57
22	7	611	CLA	CHA-C4D-ND	2.35	137.41	132.50
22	1	604	CLA	CMD-C2D-C3D	-2.35	122.21	127.61
25	6	503	BCR	C36-C18-C17	-2.35	119.64	122.92
22	A	1135	CLA	O2A-CGA-CBA	2.35	119.27	111.91
22	2	602	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
22	A	1105	CLA	CHA-C4D-ND	2.35	137.41	132.50
22	B	1217	CLA	C1-O2A-CGA	2.35	122.60	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	6	609	CLA	O2A-CGA-CBA	2.35	119.27	111.91
22	3	618	CLA	CHA-C4D-ND	2.35	137.41	132.50
37	5	505	C7Z	C15-C35-C34	-2.35	118.67	123.47
22	8	607	CLA	C2D-C1D-ND	2.34	111.83	110.10
22	B	1230	CLA	C2C-C1C-NC	2.34	112.17	109.97
39	3	502	LUT	C18-C5-C6	-2.34	121.90	124.53
22	B	1217	CLA	CMA-C3A-C4A	2.34	118.07	111.77
22	A	1107	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
22	A	1112	CLA	O1D-CGD-CBD	-2.34	119.69	124.48
22	B	1218	CLA	C1D-ND-C4D	-2.34	104.67	106.33
40	6	617	CHL	C4A-NA-C1A	2.34	107.76	106.71
22	4	606	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
22	1	607	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
22	7	609	CLA	C1C-C2C-C3C	-2.34	104.50	106.96
22	G	1601	CLA	O2A-CGA-CBA	2.34	119.25	111.91
25	3	503	BCR	C38-C26-C25	-2.34	121.90	124.53
22	3	605	CLA	CMA-C3A-C4A	2.34	118.06	111.77
40	2	613	CHL	CMB-C2B-C1B	-2.34	124.87	128.46
22	A	1122	CLA	CMD-C2D-C3D	-2.34	122.23	127.61
22	B	1022	CLA	CHA-C1A-NA	-2.34	121.04	126.40
22	A	1136	CLA	CHA-C4D-ND	2.34	137.39	132.50
22	A	1112	CLA	CHA-C1A-NA	-2.34	121.04	126.40
22	7	603	CLA	CHA-C4D-ND	2.34	137.39	132.50
40	3	611	CHL	CHB-C4A-NA	2.34	127.74	124.51
25	K	4002	BCR	C37-C22-C21	-2.34	119.65	122.92
22	2	601	CLA	CHA-C4D-ND	2.34	137.39	132.50
22	A	1119	CLA	CMD-C2D-C3D	-2.34	122.24	127.61
22	7	615	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
22	6	601	CLA	C2A-C1A-CHA	2.34	127.94	123.86
22	A	1013	CLA	CHA-C4D-ND	2.34	137.39	132.50
22	A	1103	CLA	C2C-C1C-NC	2.34	112.16	109.97
22	6	609	CLA	CHA-C4D-ND	2.34	137.39	132.50
25	B	4001	BCR	C34-C9-C10	-2.34	119.65	122.92
22	B	1221	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
22	A	1109	CLA	C1C-C2C-C3C	-2.33	104.50	106.96
40	4	613	CHL	CHC-C1C-NC	2.33	127.74	124.20
22	5	605	CLA	CAA-C2A-C3A	-2.33	106.39	112.78
22	7	612	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
22	B	1205	CLA	CHA-C4D-ND	2.33	137.38	132.50
39	Z	502	LUT	C18-C5-C6	-2.33	121.91	124.53
22	8	615	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
22	Z	603	CLA	C1-O2A-CGA	2.33	122.56	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	5	504	BCR	C28-C27-C26	-2.33	109.92	114.08
22	A	1124	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
22	5	612	CLA	CMD-C2D-C3D	-2.33	122.25	127.61
39	8	501	LUT	C20-C13-C12	2.33	121.75	118.08
22	A	1132	CLA	O2A-CGA-CBA	2.33	119.22	111.91
22	A	1114	CLA	CHA-C1A-NA	-2.33	121.07	126.40
22	3	613	CLA	CMD-C2D-C3D	-2.33	122.26	127.61
22	6	619	CLA	O1D-CGD-CBD	-2.33	119.72	124.48
22	B	1211	CLA	C1-O2A-CGA	2.33	122.55	116.44
22	5	612	CLA	C2D-C1D-ND	2.33	111.82	110.10
22	6	608	CLA	C1-C2-C3	-2.33	122.02	126.04
22	A	1119	CLA	C1C-C2C-C3C	-2.33	104.51	106.96
22	B	1202	CLA	CHA-C4D-ND	2.33	137.36	132.50
22	Z	615	CLA	CMA-C3A-C4A	2.33	118.02	111.77
21	A	1011	CL0	CAA-CBA-CGA	-2.32	106.46	113.25
22	4	603	CLA	O2A-CGA-CBA	2.32	119.20	111.91
22	A	1012	CLA	CHA-C1A-NA	-2.32	121.08	126.40
22	6	601	CLA	CHA-C1A-NA	-2.32	121.08	126.40
22	A	1108	CLA	CMB-C2B-C3B	2.32	129.03	124.68
26	6	801	LHG	C5-O7-C7	-2.32	112.07	117.79
22	6	606	CLA	CMD-C2D-C3D	-2.32	122.27	127.61
25	6	504	BCR	C37-C22-C23	2.32	121.74	118.08
22	2	605	CLA	CMA-C3A-C4A	2.32	118.02	111.77
22	7	611	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
22	2	603	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
22	9	602	CLA	CHA-C1A-NA	-2.32	121.08	126.40
22	B	1219	CLA	CMD-C2D-C3D	-2.32	122.27	127.61
40	6	611	CHL	C4D-CHA-C1A	2.32	124.07	121.25
22	B	1223	CLA	CHD-C1D-ND	-2.32	122.32	124.45
25	3	506	BCR	C36-C18-C17	-2.32	119.67	122.92
22	B	1236	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
22	5	613	CLA	O2A-CGA-CBA	2.32	119.19	111.91
22	A	1133	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
22	Z	603	CLA	CHA-C4D-ND	2.32	137.35	132.50
22	1	612	CLA	CHA-C1A-NA	-2.32	121.09	126.40
22	A	1131	CLA	CMA-C3A-C4A	2.32	118.01	111.77
26	2	801	LHG	C5-O7-C7	-2.32	112.08	117.79
22	9	605	CLA	C1D-ND-C4D	-2.32	104.69	106.33
22	7	613	CLA	CHA-C1A-NA	-2.32	121.09	126.40
22	K	1401	CLA	CHA-C1A-NA	-2.32	121.09	126.40
39	9	501	LUT	C39-C29-C28	2.32	121.73	118.08
22	B	1241	CLA	O2D-CGD-O1D	-2.32	119.31	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1216	CLA	CMD-C2D-C3D	-2.32	122.29	127.61
40	2	613	CHL	C1-O2A-CGA	2.32	122.52	116.44
22	Z	604	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
22	A	1128	CLA	O2A-CGA-CBA	2.31	119.17	111.91
22	8	609	CLA	O2A-CGA-CBA	2.31	119.17	111.91
37	J	4002	C7Z	C28-C27-C26	-2.31	120.70	127.20
22	7	601	CLA	CMA-C3A-C4A	2.31	117.99	111.77
39	3	501	LUT	C10-C11-C12	-2.31	116.00	123.22
22	8	601	CLA	O2A-CGA-CBA	2.31	119.17	111.91
22	Z	605	CLA	C1D-ND-C4D	-2.31	104.69	106.33
25	K	4001	BCR	C34-C9-C10	-2.31	119.68	122.92
22	Z	601	CLA	CMA-C3A-C4A	2.31	117.99	111.77
22	A	1106	CLA	C1D-ND-C4D	-2.31	104.69	106.33
22	8	606	CLA	C1D-ND-C4D	-2.31	104.69	106.33
22	6	603	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
37	1	503	C7Z	C28-C27-C26	-2.31	120.71	127.20
39	8	502	LUT	C20-C13-C12	2.31	121.72	118.08
22	B	1241	CLA	CBA-CAA-C2A	2.31	120.68	113.86
22	B	1226	CLA	O2A-CGA-CBA	2.31	119.16	111.91
22	3	603	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
22	A	1101	CLA	C1D-ND-C4D	-2.31	104.69	106.33
22	B	1211	CLA	CHA-C4D-ND	2.31	137.33	132.50
22	3	610	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
22	5	606	CLA	O2A-CGA-CBA	2.31	119.16	111.91
25	5	503	BCR	C34-C9-C10	-2.31	119.69	122.92
40	6	613	CHL	CMB-C2B-C1B	-2.31	124.92	128.46
22	8	609	CLA	CMD-C2D-C3D	-2.31	122.30	127.61
22	5	622	CLA	C2D-C1D-ND	2.31	111.81	110.10
22	F	1302	CLA	CMA-C3A-C4A	2.31	117.98	111.77
22	B	1222	CLA	C1C-C2C-C3C	-2.31	104.53	106.96
22	4	606	CLA	CMB-C2B-C3B	2.31	129.00	124.68
22	A	1121	CLA	C1D-ND-C4D	-2.31	104.70	106.33
22	9	601	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
22	9	604	CLA	CHA-C1A-NA	-2.31	121.12	126.40
22	7	602	CLA	CMB-C2B-C3B	2.31	128.99	124.68
22	A	1118	CLA	CHA-C4D-ND	2.31	137.32	132.50
22	2	601	CLA	CAA-C2A-C3A	-2.31	106.47	112.78
22	B	1218	CLA	CHA-C4D-ND	2.31	137.32	132.50
22	6	615	CLA	CHA-C1A-NA	-2.31	121.12	126.40
39	7	502	LUT	C31-C30-C29	-2.30	124.02	127.31
22	4	606	CLA	C1D-ND-C4D	-2.30	104.70	106.33
39	5	501	LUT	C20-C13-C12	2.30	121.71	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	5	609	CLA	CHA-C1A-NA	-2.30	121.12	126.40
25	A	4001	BCR	C33-C5-C6	-2.30	121.94	124.53
22	L	1502	CLA	CHA-C4D-ND	2.30	137.32	132.50
22	9	605	CLA	CMA-C3A-C4A	2.30	117.96	111.77
25	I	4001	BCR	C37-C22-C23	2.30	121.71	118.08
22	1	602	CLA	C1C-C2C-C3C	-2.30	104.53	106.96
22	2	605	CLA	CMD-C2D-C3D	-2.30	122.32	127.61
22	8	608	CLA	CHA-C4D-ND	2.30	137.31	132.50
25	7	504	BCR	C33-C5-C6	-2.30	121.94	124.53
40	4	610	CHL	CHB-C4A-NA	2.30	127.69	124.51
22	A	1013	CLA	CHA-C1A-NA	-2.30	121.13	126.40
40	4	613	CHL	CMB-C2B-C1B	-2.30	124.93	128.46
22	A	1013	CLA	C1-O2A-CGA	2.30	122.48	116.44
22	4	609	CLA	O2A-CGA-CBA	2.30	119.12	111.91
22	2	603	CLA	C1D-ND-C4D	-2.30	104.70	106.33
25	I	4001	BCR	C34-C9-C10	-2.30	119.70	122.92
22	7	615	CLA	CHA-C1A-NA	-2.30	121.13	126.40
25	3	504	BCR	C23-C24-C25	-2.30	120.75	127.20
22	8	604	CLA	O1A-CGA-CBA	-2.30	114.77	123.73
25	L	4002	BCR	C12-C13-C14	-2.30	115.42	118.94
22	6	607	CLA	O2A-CGA-CBA	2.30	119.12	111.91
22	B	1219	CLA	CHA-C1A-NA	-2.30	121.14	126.40
22	B	1227	CLA	CAA-C2A-C3A	-2.30	106.49	112.78
22	Z	611	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
25	3	503	BCR	C12-C13-C14	-2.30	115.42	118.94
22	Z	607	CLA	C1-C2-C3	-2.30	122.07	126.04
40	9	610	CHL	CMA-C3A-C4A	2.30	117.94	111.77
22	B	1222	CLA	C1D-ND-C4D	-2.30	104.70	106.33
36	F	4001	RRX	C23-C24-C25	-2.30	120.75	127.20
22	B	1214	CLA	C3D-C2D-C1D	-2.30	102.70	105.83
22	B	1205	CLA	CMA-C3A-C4A	2.30	117.94	111.77
22	3	605	CLA	CMD-C2D-C3D	-2.30	122.33	127.61
39	2	502	LUT	C28-C29-C30	-2.30	115.42	118.94
37	5	505	C7Z	C38-C25-C24	2.30	118.61	114.36
37	J	4002	C7Z	C20-C13-C12	2.29	121.69	118.08
40	9	613	CHL	C3C-C4C-NC	-2.29	108.00	110.57
40	6	611	CHL	CMB-C2B-C1B	-2.29	124.94	128.46
25	B	4001	BCR	C12-C13-C14	-2.29	115.42	118.94
40	1	610	CHL	C1B-CHB-C4A	-2.29	125.58	130.12
22	2	615	CLA	C1D-ND-C4D	-2.29	104.71	106.33
28	1	803	LMT	C1'-O5'-C5'	-2.29	109.19	113.69
36	F	4001	RRX	C2-C1-C6	2.29	114.01	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1213	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
40	1	610	CHL	CMB-C2B-C1B	-2.29	124.94	128.46
22	B	1236	CLA	O2A-CGA-CBA	2.29	119.10	111.91
22	9	605	CLA	CMB-C2B-C3B	2.29	128.97	124.68
22	8	603	CLA	CHA-C4D-ND	2.29	137.29	132.50
22	1	613	CLA	CMD-C2D-C3D	-2.29	122.34	127.61
22	B	1231	CLA	C1-C2-C3	-2.29	122.08	126.04
40	9	613	CHL	C4D-CHA-C1A	2.29	124.04	121.25
25	L	4001	BCR	C12-C13-C14	-2.29	115.43	118.94
22	B	1219	CLA	C2D-C1D-ND	2.29	111.79	110.10
22	5	601	CLA	O1D-CGD-CBD	-2.29	119.80	124.48
25	3	503	BCR	C33-C5-C4	2.29	118.02	113.62
22	B	1210	CLA	CMA-C3A-C4A	2.29	117.93	111.77
25	A	4005	BCR	C33-C5-C6	-2.29	121.96	124.53
22	2	615	CLA	CHA-C4D-ND	2.29	137.29	132.50
40	Z	610	CHL	CMB-C2B-C1B	-2.29	124.95	128.46
22	B	1022	CLA	C2D-C1D-ND	2.29	111.79	110.10
22	5	613	CLA	CMA-C3A-C4A	2.29	117.92	111.77
22	B	1224	CLA	CMA-C3A-C4A	2.29	117.92	111.77
22	1	615	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
25	B	4006	BCR	C33-C5-C6	-2.29	121.96	124.53
22	8	604	CLA	CHA-C1A-NA	-2.29	121.16	126.40
26	Z	801	LHG	C6-C5-C4	-2.29	106.38	111.79
40	4	611	CHL	CMB-C2B-C1B	-2.29	124.95	128.46
22	6	603	CLA	C1D-ND-C4D	-2.29	104.71	106.33
40	1	610	CHL	C3C-C4C-NC	-2.29	108.01	110.57
40	4	611	CHL	C3C-C4C-NC	-2.29	108.01	110.57
22	5	603	CLA	C1D-ND-C4D	-2.28	104.71	106.33
22	9	608	CLA	CHA-C1A-NA	-2.28	121.17	126.40
39	7	502	LUT	C31-C32-C33	-2.28	120.00	126.42
22	1	615	CLA	O2A-CGA-CBA	2.28	119.07	111.91
22	6	618	CLA	C3D-C2D-C1D	-2.28	102.72	105.83
22	B	1204	CLA	C1D-ND-C4D	-2.28	104.71	106.33
22	4	612	CLA	CMD-C2D-C3D	-2.28	122.36	127.61
22	8	612	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
22	A	1137	CLA	CHA-C1A-NA	-2.28	121.17	126.40
22	A	1117	CLA	C2D-C1D-ND	2.28	111.78	110.10
40	6	610	CHL	CMB-C2B-C1B	-2.28	124.96	128.46
40	6	613	CHL	C4A-NA-C1A	2.28	107.73	106.71
22	7	604	CLA	O1A-CGA-CBA	-2.28	114.84	123.73
22	2	603	CLA	O2A-CGA-CBA	2.28	119.06	111.91
22	6	609	CLA	CMD-C2D-C3D	-2.28	122.37	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	7	504	BCR	C29-C28-C27	2.28	116.47	111.38
22	1	606	CLA	CMB-C2B-C1B	-2.28	124.96	128.46
22	G	1602	CLA	CHA-C1A-NA	-2.28	121.18	126.40
22	4	601	CLA	C1-O2A-CGA	2.28	122.42	116.44
22	8	605	CLA	O2A-CGA-CBA	2.28	119.05	111.91
22	2	612	CLA	O2A-CGA-CBA	2.28	119.05	111.91
22	A	1122	CLA	C1D-ND-C4D	-2.28	104.72	106.33
22	A	1119	CLA	C1-C2-C3	-2.28	122.11	126.04
41	1	802	SQD	O3-C3-C2	-2.28	105.09	110.35
22	A	1120	CLA	CHA-C4D-ND	2.28	137.26	132.50
22	6	603	CLA	CMD-C2D-C3D	-2.27	122.38	127.61
40	8	610	CHL	CMB-C2B-C1B	-2.27	124.97	128.46
22	A	1128	CLA	CHA-C1A-NA	-2.27	121.19	126.40
22	F	1302	CLA	CHA-C4D-ND	2.27	137.26	132.50
22	3	601	CLA	CMA-C3A-C4A	2.27	117.89	111.77
22	B	1234	CLA	O2A-CGA-CBA	2.27	119.04	111.91
22	A	1013	CLA	O2A-CGA-CBA	2.27	119.04	111.91
25	J	4001	BCR	C31-C1-C6	-2.27	106.61	110.30
22	L	1503	CLA	O2A-CGA-CBA	2.27	119.04	111.91
36	F	4001	RRX	C38-C26-C27	2.27	118.57	114.36
22	5	606	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
25	7	504	BCR	C38-C26-C25	-2.27	121.98	124.53
22	7	601	CLA	C3D-C2D-C1D	-2.27	102.73	105.83
22	Z	601	CLA	C1D-ND-C4D	-2.27	104.72	106.33
22	Z	601	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
25	G	4001	BCR	C35-C13-C12	2.27	121.65	118.08
22	1	611	CLA	C1D-ND-C4D	-2.27	104.72	106.33
22	3	616	CLA	C1D-ND-C4D	-2.27	104.72	106.33
22	6	608	CLA	C2D-C1D-ND	2.27	111.78	110.10
22	6	606	CLA	CMB-C2B-C3B	2.27	128.92	124.68
22	2	608	CLA	CMB-C2B-C1B	-2.27	124.98	128.46
22	2	612	CLA	CHA-C1A-NA	-2.27	121.20	126.40
22	9	603	CLA	CHA-C1A-NA	-2.27	121.21	126.40
22	4	606	CLA	CMD-C2D-C3D	-2.27	122.40	127.61
22	5	604	CLA	C1C-C2C-C3C	-2.27	104.57	106.96
39	Z	501	LUT	C10-C11-C12	-2.27	116.14	123.22
22	B	1203	CLA	CMB-C2B-C3B	2.27	128.92	124.68
22	7	601	CLA	CMB-C2B-C1B	-2.27	124.98	128.46
22	5	613	CLA	C1-C2-C3	-2.27	122.12	126.04
22	2	612	CLA	C1C-C2C-C3C	-2.27	104.57	106.96
25	3	504	BCR	C34-C9-C10	-2.27	119.75	122.92
22	B	1236	CLA	CHA-C1A-NA	-2.27	121.21	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	K	4001	BCR	C35-C13-C12	2.27	121.65	118.08
39	9	501	LUT	C20-C13-C12	2.27	121.65	118.08
40	1	609	CHL	C1-O2A-CGA	2.27	122.39	116.44
22	B	1208	CLA	C1D-ND-C4D	-2.26	104.73	106.33
22	F	1302	CLA	CHA-C1A-NA	-2.26	121.21	126.40
22	6	615	CLA	CMA-C3A-C4A	2.26	117.86	111.77
22	8	606	CLA	O2A-CGA-CBA	2.26	119.01	111.91
22	Z	604	CLA	C1D-ND-C4D	-2.26	104.73	106.33
22	5	606	CLA	CMB-C2B-C3B	2.26	128.91	124.68
22	4	601	CLA	O2A-CGA-CBA	2.26	119.01	111.91
22	Z	604	CLA	O2A-CGA-CBA	2.26	119.01	111.91
22	K	1403	CLA	CHA-C1A-NA	-2.26	121.22	126.40
22	B	1021	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
28	9	803	LMT	C3'-C4'-C5'	-2.26	105.74	110.93
22	Z	612	CLA	CHA-C1A-NA	-2.26	121.22	126.40
22	B	1218	CLA	CMB-C2B-C1B	-2.26	124.99	128.46
22	5	615	CLA	CHA-C1A-NA	-2.26	121.22	126.40
40	Z	613	CHL	CMB-C2B-C1B	-2.26	124.99	128.46
22	8	604	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
22	3	610	CLA	CMA-C3A-C4A	2.26	117.84	111.77
22	3	605	CLA	O2A-CGA-CBA	2.26	118.99	111.91
25	A	4001	BCR	C34-C9-C10	-2.26	119.76	122.92
22	9	607	CLA	CHA-C1A-NA	-2.26	121.23	126.40
40	5	617	CHL	CHC-C1C-NC	2.26	127.62	124.20
22	4	605	CLA	CMD-C2D-C3D	-2.26	122.43	127.61
22	B	1213	CLA	C1D-ND-C4D	-2.26	104.73	106.33
37	1	503	C7Z	C24-C25-C26	-2.26	115.82	120.85
22	A	1125	CLA	OBD-CAD-C3D	-2.25	123.09	128.52
22	3	602	CLA	CHA-C1A-NA	-2.25	121.23	126.40
22	B	1229	CLA	CHA-C1A-NA	-2.25	121.24	126.40
25	B	4004	BCR	C38-C26-C25	-2.25	122.00	124.53
22	9	607	CLA	CAA-C2A-C3A	-2.25	106.61	112.78
22	1	605	CLA	C1D-ND-C4D	-2.25	104.73	106.33
22	A	1120	CLA	C3D-C2D-C1D	-2.25	102.76	105.83
22	A	1117	CLA	C1-O2A-CGA	2.25	122.36	116.44
22	B	1222	CLA	C1-C2-C3	-2.25	122.15	126.04
22	A	1119	CLA	O2A-CGA-CBA	2.25	118.98	111.91
22	1	603	CLA	C1D-ND-C4D	-2.25	104.73	106.33
22	7	603	CLA	C1D-ND-C4D	-2.25	104.73	106.33
22	2	602	CLA	CMA-C3A-C4A	2.25	117.83	111.77
22	1	607	CLA	CMB-C2B-C1B	-2.25	125.00	128.46
40	4	610	CHL	CMB-C2B-C1B	-2.25	125.00	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1240	CLA	C1C-C2C-C3C	-2.25	104.59	106.96
22	B	1216	CLA	C1-O2A-CGA	2.25	122.35	116.44
22	1	602	CLA	CMA-C3A-C4A	2.25	117.82	111.77
22	6	618	CLA	CHA-C4D-ND	2.25	137.21	132.50
22	B	1209	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
22	B	1228	CLA	O2A-CGA-CBA	2.25	118.97	111.91
22	Z	607	CLA	CHA-C1A-NA	-2.25	121.25	126.40
22	B	1202	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
22	8	605	CLA	CHA-C1A-NA	-2.25	121.25	126.40
22	B	1023	CLA	C2A-C1A-CHA	2.25	127.79	123.86
22	8	601	CLA	OBD-CAD-C3D	-2.25	123.11	128.52
40	6	611	CHL	C1-O2A-CGA	2.25	122.34	116.44
22	A	1107	CLA	CHA-C1A-NA	-2.25	121.25	126.40
22	7	611	CLA	C3D-C2D-C1D	-2.25	102.76	105.83
25	B	4007	BCR	C37-C22-C23	2.25	121.62	118.08
22	A	1104	CLA	CAA-C2A-C3A	-2.25	106.62	112.78
22	A	1136	CLA	CMB-C2B-C1B	-2.25	125.01	128.46
22	A	1121	CLA	O2A-CGA-CBA	2.25	118.96	111.91
22	4	604	CLA	CHA-C1A-NA	-2.25	121.25	126.40
22	B	1206	CLA	C1-O2A-CGA	2.25	122.34	116.44
22	8	601	CLA	CHA-C1A-NA	-2.25	121.25	126.40
22	A	1136	CLA	OBD-CAD-C3D	-2.25	123.12	128.52
39	5	501	LUT	C39-C29-C28	2.25	121.61	118.08
39	3	502	LUT	C7-C8-C9	-2.25	122.84	126.23
22	3	607	CLA	C1-C2-C3	-2.25	122.16	126.04
39	9	502	LUT	C39-C29-C28	2.24	121.61	118.08
22	A	1137	CLA	O2A-CGA-CBA	2.24	118.95	111.91
22	1	615	CLA	CHA-C1A-NA	-2.24	121.26	126.40
22	A	1104	CLA	C1-O2A-CGA	2.24	122.33	116.44
22	Z	606	CLA	CMB-C2B-C3B	2.24	128.88	124.68
25	L	4002	BCR	C19-C18-C17	2.24	122.38	118.94
25	3	505	BCR	C37-C22-C21	-2.24	119.78	122.92
25	B	4003	BCR	C39-C30-C25	-2.24	106.66	110.30
22	7	612	CLA	O2A-CGA-CBA	2.24	118.95	111.91
26	5	801	LHG	C6-C5-C4	-2.24	106.48	111.79
22	Z	607	CLA	O2A-CGA-CBA	2.24	118.94	111.91
21	A	1011	CL0	C4D-C3D-CAD	2.24	110.74	108.10
22	4	601	CLA	O1D-CGD-CBD	-2.24	119.90	124.48
22	3	603	CLA	CMD-C2D-C3D	-2.24	122.46	127.61
22	A	1105	CLA	CMD-C2D-C3D	-2.24	122.46	127.61
40	5	611	CHL	CMB-C2B-C1B	-2.24	125.02	128.46
22	A	1130	CLA	CHA-C1A-NA	-2.24	121.27	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Z	603	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
22	9	606	CLA	C1C-C2C-C3C	-2.24	104.60	106.96
22	1	606	CLA	C1D-ND-C4D	-2.24	104.74	106.33
22	8	602	CLA	C1D-ND-C4D	-2.24	104.74	106.33
22	4	603	CLA	C1D-ND-C4D	-2.24	104.74	106.33
22	B	1237	CLA	O2A-CGA-CBA	2.24	118.94	111.91
39	1	502	LUT	C18-C5-C6	-2.24	122.01	124.53
22	A	1103	CLA	CHA-C4D-ND	2.24	137.19	132.50
22	9	605	CLA	CHA-C1A-NA	-2.24	121.27	126.40
22	L	1502	CLA	O2A-CGA-CBA	2.24	118.94	111.91
37	5	505	C7Z	C30-C31-C32	-2.24	116.23	123.22
22	9	609	CLA	CHA-C1A-NA	-2.24	121.27	126.40
25	A	4002	BCR	C33-C5-C4	2.24	117.92	113.62
22	6	609	CLA	O1D-CGD-CBD	-2.24	119.90	124.48
22	Z	603	CLA	CAA-C2A-C3A	-2.24	106.65	112.78
25	B	4004	BCR	C31-C1-C6	-2.24	106.67	110.30
40	7	610	CHL	C1B-CHB-C4A	-2.24	125.68	130.12
22	B	1216	CLA	O2A-CGA-CBA	2.24	118.93	111.91
39	4	501	LUT	C20-C13-C12	2.24	121.60	118.08
22	4	604	CLA	O2A-CGA-CBA	2.24	118.93	111.91
39	6	502	LUT	C18-C5-C6	-2.24	122.02	124.53
22	3	613	CLA	CHA-C1A-NA	-2.24	121.28	126.40
22	Z	607	CLA	CAA-C2A-C3A	-2.24	106.65	112.78
22	7	601	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
33	B	5003	DGD	C2G-O2G-C1B	-2.24	112.28	117.79
25	B	4003	BCR	C4-C5-C6	-2.24	119.48	122.73
22	1	612	CLA	O2D-CGD-O1D	-2.24	119.47	123.84
22	2	608	CLA	CHA-C1A-NA	-2.24	121.28	126.40
22	9	606	CLA	CHA-C1A-NA	-2.24	121.28	126.40
22	7	616	CLA	C1D-ND-C4D	-2.24	104.75	106.33
40	1	609	CHL	C1-C2-C3	-2.24	122.18	126.04
25	J	4001	BCR	C38-C26-C27	2.24	117.91	113.62
22	4	603	CLA	O2D-CGD-O1D	-2.24	119.47	123.84
25	3	506	BCR	C29-C28-C27	2.23	116.37	111.38
22	A	1103	CLA	CAC-C3C-C4C	2.23	127.71	124.81
25	K	4002	BCR	C12-C13-C14	-2.23	115.51	118.94
39	7	501	LUT	C10-C11-C12	-2.23	116.25	123.22
22	7	604	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
22	A	1106	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
39	7	501	LUT	C20-C13-C12	2.23	121.60	118.08
22	6	619	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
22	6	605	CLA	C1D-ND-C4D	-2.23	104.75	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	4	613	CHL	C4D-CHA-C1A	2.23	123.97	121.25
22	A	1132	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
40	3	611	CHL	C4D-CHA-C1A	2.23	123.97	121.25
22	8	602	CLA	CHA-C1A-NA	-2.23	121.29	126.40
22	1	601	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
22	A	1130	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
22	5	604	CLA	CMC-C2C-C1C	2.23	128.44	125.04
22	A	1140	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
22	A	1101	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
40	4	613	CHL	CHD-C4C-C3C	2.23	128.12	124.84
22	B	1219	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
22	2	606	CLA	CHA-C1A-NA	-2.23	121.29	126.40
41	2	803	SQD	O3-C3-C2	-2.23	105.20	110.35
25	8	503	BCR	C15-C14-C13	-2.23	124.13	127.31
25	3	504	BCR	C27-C26-C25	-2.23	119.50	122.73
22	B	1224	CLA	CHA-C1A-NA	-2.23	121.29	126.40
22	Z	604	CLA	CHA-C1A-NA	-2.23	121.29	126.40
22	4	609	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
22	7	616	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
25	J	4001	BCR	C30-C25-C26	-2.23	119.47	122.61
22	5	607	CLA	CAA-C2A-C3A	-2.23	106.68	112.78
22	A	1132	CLA	C2D-C1D-ND	2.23	111.75	110.10
22	4	605	CLA	O2A-CGA-CBA	2.23	118.90	111.91
22	6	605	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
22	8	603	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
39	9	502	LUT	C31-C32-C33	-2.23	120.16	126.42
22	7	602	CLA	CHA-C1A-NA	-2.23	121.30	126.40
22	7	609	CLA	C3D-C2D-C1D	-2.23	102.79	105.83
22	A	1115	CLA	CHA-C4D-ND	2.23	137.16	132.50
22	B	1220	CLA	CHA-C4D-ND	2.23	137.16	132.50
40	2	610	CHL	C1-O2A-CGA	2.23	123.20	116.73
40	3	611	CHL	C1-O2A-CGA	2.23	122.28	116.44
22	B	1229	CLA	CMD-C2D-C3D	-2.23	122.50	127.61
22	B	1022	CLA	C1-C2-C3	-2.22	122.20	126.04
22	5	604	CLA	CHA-C1A-NA	-2.22	121.30	126.40
22	B	1201	CLA	C1C-C2C-C3C	-2.22	104.62	106.96
22	6	606	CLA	CHA-C1A-NA	-2.22	121.31	126.40
22	L	1503	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
22	8	604	CLA	CAA-C2A-C1A	2.22	119.26	111.97
22	B	1220	CLA	C1D-ND-C4D	-2.22	104.76	106.33
22	3	604	CLA	C3A-C2A-C1A	2.22	104.67	101.34
22	8	601	CLA	C3D-C2D-C1D	-2.22	102.80	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1241	CLA	CHA-C4D-ND	2.22	137.15	132.50
40	6	617	CHL	CHC-C1C-NC	2.22	127.57	124.20
40	3	611	CHL	C1B-CHB-C4A	-2.22	125.72	130.12
22	B	1205	CLA	C6-C5-C3	-2.22	107.63	113.45
22	B	1230	CLA	CAA-CBA-CGA	-2.22	106.76	113.25
22	A	1112	CLA	CMD-C2D-C3D	-2.22	122.51	127.61
22	1	601	CLA	C1D-ND-C4D	-2.22	104.76	106.33
22	3	605	CLA	C1D-ND-C4D	-2.22	104.76	106.33
22	B	1225	CLA	O2A-CGA-CBA	2.22	118.87	111.91
22	B	1240	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
22	2	615	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
22	7	615	CLA	C3D-C2D-C1D	-2.22	102.80	105.83
22	A	1102	CLA	C2A-C1A-CHA	2.22	127.74	123.86
39	6	502	LUT	C31-C32-C33	-2.22	120.18	126.42
22	9	604	CLA	CBA-CAA-C2A	2.22	120.41	113.86
25	L	4002	BCR	C35-C13-C12	2.22	121.57	118.08
22	2	607	CLA	CHA-C1A-NA	-2.22	121.32	126.40
22	8	608	CLA	C1D-ND-C4D	-2.22	104.76	106.33
37	1	503	C7Z	C19-C9-C8	2.22	121.57	118.08
22	1	603	CLA	C1-O2A-CGA	2.22	122.26	116.44
22	6	601	CLA	C1-C2-C3	-2.22	122.21	126.04
25	6	503	BCR	C34-C9-C10	-2.22	119.82	122.92
22	1	603	CLA	CMD-C2D-C3D	-2.22	122.52	127.61
22	5	603	CLA	CMD-C2D-C3D	-2.22	122.52	127.61
22	B	1232	CLA	CHA-C1A-NA	-2.22	121.32	126.40
22	A	1129	CLA	CHA-C1A-NA	-2.22	121.33	126.40
22	F	1301	CLA	CMD-C2D-C3D	-2.21	122.52	127.61
22	5	603	CLA	CAC-C3C-C4C	2.21	127.68	124.81
22	B	1230	CLA	CHA-C4D-ND	2.21	137.13	132.50
22	5	601	CLA	C2A-C1A-CHA	2.21	127.73	123.86
39	5	501	LUT	C38-C25-C24	-2.21	118.82	123.56
22	A	1101	CLA	CHA-C1A-NA	-2.21	121.33	126.40
22	B	1212	CLA	CHA-C1A-NA	-2.21	121.33	126.40
22	A	1104	CLA	C1D-ND-C4D	-2.21	104.76	106.33
22	7	603	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
22	A	1119	CLA	C2D-C1D-ND	2.21	111.73	110.10
39	2	501	LUT	C37-C21-C26	2.21	112.89	109.55
22	A	1124	CLA	CHA-C4D-ND	2.21	137.12	132.50
39	5	502	LUT	C31-C30-C29	-2.21	124.16	127.31
22	5	622	CLA	CHA-C1A-NA	-2.21	121.34	126.40
22	B	1210	CLA	C1D-ND-C4D	-2.21	104.77	106.33
39	8	502	LUT	C38-C25-C24	-2.21	118.83	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1122	CLA	C1-C2-C3	-2.21	122.22	126.04
22	Z	601	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
37	1	503	C7Z	C18-C5-C4	2.21	118.45	114.36
22	A	1128	CLA	C1-O2A-CGA	2.21	122.24	116.44
22	2	604	CLA	C1D-ND-C4D	-2.21	104.77	106.33
22	4	609	CLA	CMA-C3A-C4A	2.21	117.70	111.77
22	6	604	CLA	CHA-C1A-NA	-2.21	121.34	126.40
22	B	1218	CLA	C3D-C2D-C1D	-2.21	102.82	105.83
22	6	601	CLA	O1D-CGD-CBD	-2.21	119.97	124.48
22	5	613	CLA	CHA-C1A-NA	-2.21	121.35	126.40
22	7	602	CLA	C1D-ND-C4D	-2.21	104.77	106.33
22	Z	603	CLA	CMD-C2D-C3D	-2.21	122.54	127.61
22	Z	602	CLA	CHA-C1A-NA	-2.21	121.35	126.40
39	Z	501	LUT	C39-C29-C28	2.21	121.55	118.08
22	A	1108	CLA	CMD-C2D-C3D	-2.20	122.54	127.61
22	6	608	CLA	CHA-C1A-NA	-2.20	121.35	126.40
22	B	1021	CLA	CHA-C1A-NA	-2.20	121.35	126.40
22	B	1223	CLA	CHA-C1A-NA	-2.20	121.35	126.40
22	K	1401	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
22	A	1133	CLA	CMB-C2B-C3B	2.20	128.80	124.68
22	F	1302	CLA	C1D-ND-C4D	-2.20	104.77	106.33
22	4	602	CLA	C1D-ND-C4D	-2.20	104.77	106.33
22	Z	612	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
22	6	605	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
21	A	1011	CL0	C3C-C4C-NC	2.20	113.04	110.57
22	3	608	CLA	CHA-C1A-NA	-2.20	121.36	126.40
22	A	1134	CLA	O1D-CGD-CBD	-2.20	119.98	124.48
22	5	618	CLA	CHA-C1A-NA	-2.20	121.36	126.40
22	Z	615	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
22	Z	608	CLA	O2A-CGA-CBA	2.20	118.81	111.91
22	1	603	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
22	3	604	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
25	K	4002	BCR	C38-C26-C25	-2.20	122.06	124.53
22	5	604	CLA	O1A-CGA-CBA	-2.20	115.15	123.73
22	A	1129	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
22	4	603	CLA	CHA-C1A-NA	-2.20	121.36	126.40
22	A	1104	CLA	CMA-C3A-C4A	2.20	117.68	111.77
22	J	1901	CLA	CHA-C1A-NA	-2.20	121.36	126.40
40	2	613	CHL	C3C-C4C-NC	-2.20	108.11	110.57
22	B	1222	CLA	CHA-C4D-ND	2.20	137.10	132.50
22	A	1118	CLA	O1D-CGD-CBD	-2.20	119.99	124.48
25	A	4003	BCR	C37-C22-C21	-2.20	119.85	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	2	602	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
22	5	608	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
39	8	501	LUT	C30-C31-C32	-2.20	116.36	123.22
22	1	604	CLA	C6-C5-C3	-2.20	107.70	113.45
22	A	1127	CLA	O2D-CGD-O1D	-2.20	119.55	123.84
22	A	1130	CLA	O2A-CGA-CBA	2.20	118.80	111.91
22	4	602	CLA	CHA-C1A-NA	-2.20	121.37	126.40
22	L	1503	CLA	CHA-C1A-NA	-2.20	121.37	126.40
40	6	613	CHL	C4D-CHA-C1A	2.19	123.92	121.25
40	6	617	CHL	C1B-CHB-C4A	-2.19	125.77	130.12
22	K	1402	CLA	C1-O2A-CGA	2.19	122.20	116.44
22	5	607	CLA	CHA-C1A-NA	-2.19	121.37	126.40
25	6	503	BCR	C4-C5-C6	-2.19	119.55	122.73
22	6	606	CLA	C1D-ND-C4D	-2.19	104.78	106.33
22	8	611	CLA	CHA-C1A-NA	-2.19	121.38	126.40
22	1	603	CLA	O2A-CGA-CBA	2.19	118.79	111.91
22	3	612	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
22	2	605	CLA	CHA-C1A-NA	-2.19	121.38	126.40
22	2	602	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
39	1	501	LUT	C18-C5-C6	-2.19	122.07	124.53
22	B	1236	CLA	CMA-C3A-C4A	2.19	117.66	111.77
22	A	1102	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
40	8	613	CHL	C1B-CHB-C4A	-2.19	125.78	130.12
22	B	1227	CLA	CMA-C3A-C4A	2.19	117.66	111.77
22	B	1201	CLA	CAA-C2A-C3A	-2.19	106.78	112.78
39	6	501	LUT	C28-C29-C30	-2.19	115.58	118.94
22	2	603	CLA	C2A-C1A-CHA	2.19	127.69	123.86
22	7	611	CLA	O2A-CGA-CBA	2.19	118.78	111.91
22	3	606	CLA	C1-C2-C3	-2.19	122.25	126.04
22	A	1117	CLA	CAA-C2A-C1A	-2.19	104.80	111.97
22	3	608	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
22	Z	606	CLA	C1-O2A-CGA	2.19	122.19	116.44
33	B	5003	DGD	O2G-C1B-O1B	-2.19	118.41	123.70
22	A	1116	CLA	OBD-CAD-C3D	-2.19	123.25	128.52
22	G	1601	CLA	CHA-C1A-NA	-2.19	121.39	126.40
22	3	602	CLA	C1D-ND-C4D	-2.19	104.78	106.33
22	1	601	CLA	CMB-C2B-C1B	-2.19	125.10	128.46
22	2	603	CLA	C3D-C2D-C1D	-2.19	102.85	105.83
39	6	501	LUT	C11-C10-C9	-2.19	124.19	127.31
22	5	608	CLA	CHA-C1A-NA	-2.19	121.39	126.40
22	4	601	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
39	8	502	LUT	C31-C30-C29	-2.19	124.19	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	Z	503	LUT	C35-C15-C14	-2.19	119.00	123.47
22	3	610	CLA	CHA-C1A-NA	-2.19	121.39	126.40
22	A	1118	CLA	O2A-CGA-CBA	2.18	118.76	111.91
22	A	1111	CLA	CMD-C2D-C3D	-2.18	122.59	127.61
25	L	4002	BCR	C29-C28-C27	2.18	116.26	111.38
25	B	4002	BCR	C33-C5-C4	2.18	117.81	113.62
22	8	615	CLA	CHA-C1A-NA	-2.18	121.40	126.40
22	Z	612	CLA	O2A-CGA-CBA	2.18	118.76	111.91
22	4	615	CLA	CHA-C1A-NA	-2.18	121.40	126.40
22	B	1023	CLA	CAC-C3C-C4C	2.18	127.64	124.81
25	A	4004	BCR	C30-C25-C24	2.18	121.95	115.78
22	Z	608	CLA	C1D-ND-C4D	-2.18	104.78	106.33
26	5	801	LHG	C5-O7-C7	-2.18	112.42	117.79
22	5	618	CLA	CHA-C4D-ND	2.18	137.06	132.50
22	1	612	CLA	CMD-C2D-C3D	-2.18	122.59	127.61
25	A	4002	BCR	C19-C18-C17	2.18	122.29	118.94
22	Z	606	CLA	C1D-ND-C4D	-2.18	104.78	106.33
22	A	1101	CLA	CMD-C2D-C3D	-2.18	122.59	127.61
40	8	613	CHL	CMB-C2B-C1B	-2.18	125.11	128.46
38	K	5001	SPH	C3-C4-C5	-2.18	119.92	124.79
40	9	613	CHL	CAA-C2A-C3A	-2.18	111.01	116.10
22	1	602	CLA	CHA-C1A-NA	-2.18	121.41	126.40
22	B	1205	CLA	CMD-C2D-C3D	-2.18	122.60	127.61
25	3	504	BCR	C3-C4-C5	-2.18	110.19	114.08
22	1	603	CLA	CAA-C2A-C3A	-2.18	106.81	112.78
22	9	604	CLA	CAA-C2A-C3A	-2.18	106.81	112.78
25	L	4002	BCR	C37-C22-C21	-2.18	119.87	122.92
22	A	1116	CLA	CMB-C2B-C3B	2.18	128.75	124.68
22	A	1139	CLA	CHA-C1A-NA	-2.18	121.41	126.40
22	B	1239	CLA	CHA-C1A-NA	-2.18	121.41	126.40
22	4	605	CLA	CHA-C1A-NA	-2.18	121.41	126.40
22	A	1106	CLA	C1-O2A-CGA	2.18	122.16	116.44
22	3	607	CLA	CHA-C1A-NA	-2.18	121.41	126.40
22	K	1403	CLA	CMD-C2D-C3D	-2.18	122.61	127.61
22	7	612	CLA	CMD-C2D-C3D	-2.18	122.61	127.61
22	5	615	CLA	C2A-C1A-CHA	2.18	127.67	123.86
22	6	604	CLA	C1-O2A-CGA	2.18	122.15	116.44
39	9	502	LUT	C18-C5-C4	2.18	118.39	114.36
22	3	612	CLA	CHA-C1A-NA	-2.18	121.41	126.40
22	B	1238	CLA	CMD-C2D-C3D	-2.18	122.61	127.61
22	9	604	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
22	Z	602	CLA	CMA-C3A-C4A	2.18	117.62	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	5	604	CLA	CAA-C2A-C3A	-2.17	106.82	112.78
22	5	615	CLA	C3D-C2D-C1D	-2.17	102.86	105.83
22	5	606	CLA	CHA-C1A-NA	-2.17	121.42	126.40
22	L	1503	CLA	C1D-ND-C4D	-2.17	104.79	106.33
22	4	601	CLA	C1D-ND-C4D	-2.17	104.79	106.33
22	4	612	CLA	O2A-CGA-CBA	2.17	118.73	111.91
22	3	612	CLA	O2A-CGA-CBA	2.17	118.73	111.91
22	8	604	CLA	CMB-C2B-C3B	2.17	128.74	124.68
22	A	1125	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
22	2	607	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
25	5	504	BCR	C38-C26-C27	2.17	117.79	113.62
22	6	604	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
22	A	1117	CLA	CBA-CAA-C2A	2.17	120.27	113.86
22	A	1111	CLA	CHA-C1A-NA	-2.17	121.42	126.40
22	6	607	CLA	CHA-C1A-NA	-2.17	121.42	126.40
22	3	607	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
22	B	1228	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
22	A	1122	CLA	CAA-C2A-C3A	-2.17	106.84	112.78
36	F	4001	RRX	C2-C3-C4	2.17	116.22	111.38
25	K	4002	BCR	C33-C5-C6	-2.17	122.09	124.53
22	6	602	CLA	CHA-C1A-NA	-2.17	121.43	126.40
40	Z	609	CHL	CHD-C4C-C3C	2.17	128.03	124.84
40	4	617	CHL	CHC-C1C-NC	2.17	127.49	124.20
22	5	612	CLA	CMA-C3A-C4A	2.17	117.60	111.77
22	3	607	CLA	O2A-CGA-CBA	2.17	118.71	111.91
25	8	503	BCR	C34-C9-C10	-2.17	119.89	122.92
26	4	801	LHG	C5-O7-C7	-2.17	112.46	117.79
22	2	601	CLA	C1D-ND-C4D	-2.17	104.80	106.33
39	Z	501	LUT	C20-C13-C12	2.17	121.49	118.08
22	6	609	CLA	CMA-C3A-C4A	2.17	117.59	111.77
22	4	604	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
25	7	504	BCR	C1-C6-C5	-2.17	119.56	122.61
22	4	607	CLA	CHA-C1A-NA	-2.17	121.44	126.40
22	F	1302	CLA	C3D-C2D-C1D	-2.17	102.88	105.83
22	5	603	CLA	C6-C5-C3	-2.16	107.78	113.45
25	3	505	BCR	C19-C18-C17	2.16	122.26	118.94
22	5	612	CLA	O2A-CGA-CBA	2.16	118.70	111.91
40	9	610	CHL	C1B-CHB-C4A	-2.16	125.83	130.12
25	B	4004	BCR	C12-C13-C14	-2.16	115.62	118.94
22	8	609	CLA	CHA-C1A-NA	-2.16	121.44	126.40
40	Z	613	CHL	C1B-CHB-C4A	-2.16	125.83	130.12
22	8	607	CLA	CHA-C1A-NA	-2.16	121.44	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1141	CLA	C3D-C2D-C1D	-2.16	102.88	105.83
22	2	603	CLA	CHA-C1A-NA	-2.16	121.45	126.40
25	I	4001	BCR	C12-C13-C14	-2.16	115.62	118.94
22	7	608	CLA	C3D-C2D-C1D	-2.16	102.88	105.83
22	4	608	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
39	1	501	LUT	C39-C29-C28	2.16	121.48	118.08
22	Z	608	CLA	CHA-C1A-NA	-2.16	121.45	126.40
22	B	1213	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
40	1	609	CHL	CMB-C2B-C1B	-2.16	125.14	128.46
38	K	5001	SPH	O3-C3-C2	2.16	110.74	107.31
22	A	1109	CLA	OBD-CAD-C3D	-2.16	123.32	128.52
22	B	1236	CLA	C3D-C2D-C1D	-2.16	102.88	105.83
22	9	608	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
22	8	604	CLA	C1D-ND-C4D	-2.16	104.80	106.33
22	B	1204	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
22	9	609	CLA	CAA-C2A-C3A	-2.16	106.87	112.78
25	G	4001	BCR	C23-C24-C25	-2.16	121.14	127.20
22	A	1136	CLA	CHA-C1A-NA	-2.16	121.45	126.40
22	B	1225	CLA	CHA-C1A-NA	-2.16	121.45	126.40
22	B	1206	CLA	CHA-C1A-NA	-2.16	121.46	126.40
22	9	607	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
22	4	612	CLA	CMB-C2B-C1B	-2.16	125.15	128.46
25	8	503	BCR	C38-C26-C27	2.16	117.76	113.62
39	Z	501	LUT	C11-C10-C9	-2.16	124.23	127.31
22	A	1137	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
22	A	1136	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
22	B	1210	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
22	3	604	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
37	5	505	C7Z	C22-C23-C24	2.16	113.25	110.30
22	8	604	CLA	CBA-CAA-C2A	2.15	120.22	113.86
22	Z	615	CLA	CHA-C1A-NA	-2.15	121.47	126.40
22	1	613	CLA	CMB-C2B-C3B	2.15	128.71	124.68
31	A	5003	LMG	C8-O7-C10	-2.15	112.49	117.79
36	F	4001	RRX	C36-C18-C19	2.15	121.47	118.08
25	K	4001	BCR	C19-C18-C17	2.15	122.25	118.94
22	8	604	CLA	CMD-C2D-C3D	-2.15	122.66	127.61
22	6	605	CLA	C3D-C2D-C1D	-2.15	102.89	105.83
22	Z	611	CLA	CHA-C1A-NA	-2.15	121.47	126.40
22	A	1116	CLA	C3D-C2D-C1D	-2.15	102.89	105.83
21	A	1011	CL0	CBC-CAC-C3C	-2.15	106.50	112.43
22	A	1140	CLA	C1D-ND-C4D	-2.15	104.81	106.33
22	3	601	CLA	C1D-ND-C4D	-2.15	104.81	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	4	617	CHL	CMB-C2B-C1B	-2.15	125.16	128.46
22	A	1140	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
39	8	501	LUT	C39-C29-C28	2.15	121.46	118.08
22	7	605	CLA	CHA-C1A-NA	-2.15	121.47	126.40
22	K	1402	CLA	C1D-ND-C4D	-2.15	104.81	106.33
22	1	615	CLA	C2D-C1D-ND	2.15	111.69	110.10
22	B	1022	CLA	C1-O2A-CGA	2.15	122.08	116.44
22	Z	612	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
22	4	615	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
22	Z	611	CLA	CAA-C2A-C3A	-2.15	106.89	112.78
25	7	504	BCR	C23-C24-C25	-2.15	121.17	127.20
25	B	4001	BCR	C35-C13-C12	2.15	121.46	118.08
25	5	504	BCR	C4-C5-C6	-2.15	119.61	122.73
22	8	612	CLA	CHA-C1A-NA	-2.15	121.48	126.40
40	1	610	CHL	C1-O2A-CGA	2.15	122.97	116.73
22	G	1602	CLA	CMD-C2D-C3D	-2.15	122.68	127.61
22	7	612	CLA	CAC-C3C-C4C	2.15	127.59	124.81
22	2	608	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
22	B	1022	CLA	O2A-CGA-CBA	2.15	118.64	111.91
22	L	1502	CLA	C1-O2A-CGA	2.15	122.08	116.44
22	4	605	CLA	CMA-C3A-C4A	2.15	117.54	111.77
22	A	1012	CLA	C1D-ND-C4D	-2.15	104.81	106.33
22	B	1230	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
27	3	802	NKP	OAB-PAC-OAF	-2.15	101.03	106.73
22	Z	601	CLA	C3D-C2D-C1D	-2.14	102.90	105.83
22	9	612	CLA	CHA-C1A-NA	-2.14	121.49	126.40
22	1	612	CLA	C2A-C1A-CHA	2.14	127.61	123.86
39	2	503	LUT	C39-C29-C30	-2.14	119.92	122.92
22	5	605	CLA	CHA-C1A-NA	-2.14	121.49	126.40
22	6	612	CLA	O2A-CGA-CBA	2.14	118.64	111.91
27	A	5004	NKP	OAB-PAC-OAF	-2.14	101.03	106.73
22	A	1137	CLA	CAA-CBA-CGA	-2.14	106.99	113.25
22	B	1227	CLA	C1D-ND-C4D	-2.14	104.81	106.33
27	8	802	NKP	OAB-PAC-OAF	-2.14	101.03	106.73
25	B	4005	BCR	C4-C5-C6	-2.14	119.62	122.73
39	4	501	LUT	C39-C29-C28	2.14	121.45	118.08
22	A	1140	CLA	CHA-C1A-NA	-2.14	121.49	126.40
22	B	1234	CLA	CHA-C1A-NA	-2.14	121.49	126.40
22	B	1202	CLA	C1D-ND-C4D	-2.14	104.81	106.33
22	A	1133	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
22	6	604	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
22	A	1114	CLA	C1-C2-C3	-2.14	122.34	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	1	501	LUT	C30-C31-C32	-2.14	116.53	123.22
22	7	604	CLA	O1D-CGD-CBD	-2.14	120.10	124.48
22	F	1301	CLA	CHA-C1A-NA	-2.14	121.49	126.40
39	6	502	LUT	C38-C25-C24	-2.14	118.98	123.56
28	B	5005	LMT	O1'-C1'-C2'	2.14	111.65	108.30
22	A	1103	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
22	B	1214	CLA	C1D-ND-C4D	-2.14	104.81	106.33
22	B	1240	CLA	C1D-ND-C4D	-2.14	104.81	106.33
22	B	1226	CLA	CMA-C3A-C4A	2.14	117.53	111.77
22	K	1404	CLA	CHA-C1A-NA	-2.14	121.50	126.40
22	3	616	CLA	CHA-C1A-NA	-2.14	121.50	126.40
22	B	1212	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
22	J	1901	CLA	C1D-ND-C4D	-2.14	104.81	106.33
22	Z	611	CLA	C1D-ND-C4D	-2.14	104.81	106.33
22	A	1120	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
22	B	1215	CLA	O2A-CGA-CBA	2.14	118.62	111.91
39	7	502	LUT	C20-C13-C12	2.14	121.45	118.08
22	B	1207	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
22	B	1220	CLA	CMB-C2B-C3B	2.14	128.68	124.68
22	B	1208	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
22	A	1108	CLA	CHA-C1A-NA	-2.14	121.50	126.40
22	9	612	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
40	6	611	CHL	C1B-CHB-C4A	-2.14	125.88	130.12
22	8	608	CLA	CMD-C2D-C3D	-2.14	122.70	127.61
22	4	607	CLA	CAA-C2A-C3A	-2.14	106.92	112.78
22	3	610	CLA	C2A-C1A-CHA	2.14	127.59	123.86
22	2	602	CLA	CHA-C1A-NA	-2.14	121.50	126.40
39	2	503	LUT	C10-C11-C12	-2.14	116.55	123.22
22	1	601	CLA	C3D-C2D-C1D	-2.14	102.92	105.83
39	3	502	LUT	C35-C15-C14	-2.14	119.10	123.47
22	5	618	CLA	O2A-CGA-CBA	2.14	118.61	111.91
22	B	1228	CLA	C1D-ND-C4D	-2.14	104.82	106.33
22	B	1232	CLA	CMD-C2D-C3D	-2.14	122.70	127.61
39	2	503	LUT	C11-C10-C9	-2.13	124.26	127.31
22	B	1230	CLA	C1C-C2C-C3C	-2.13	104.71	106.96
22	A	1123	CLA	O2A-CGA-CBA	2.13	118.61	111.91
22	3	605	CLA	CHA-C1A-NA	-2.13	121.51	126.40
22	B	1213	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
25	3	503	BCR	C29-C28-C27	2.13	116.14	111.38
26	B	5006	LHG	O7-C7-O9	-2.13	118.55	123.70
22	7	608	CLA	CHA-C1A-NA	-2.13	121.51	126.40
22	1	605	CLA	CHA-C1A-NA	-2.13	121.52	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	7	609	CLA	CHA-C1A-NA	-2.13	121.52	126.40
25	K	4001	BCR	C37-C22-C21	-2.13	119.94	122.92
37	5	505	C7Z	C20-C13-C14	-2.13	119.94	122.92
22	5	605	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
22	B	1210	CLA	CMB-C2B-C1B	-2.13	125.19	128.46
22	5	602	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
22	B	1203	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
22	8	605	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
22	A	1114	CLA	C2D-C1D-ND	2.13	111.67	110.10
22	5	602	CLA	O2A-CGA-CBA	2.13	118.59	111.91
22	B	1234	CLA	C1D-ND-C4D	-2.13	104.82	106.33
22	5	603	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
22	A	1012	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
22	B	1021	CLA	O2A-CGA-CBA	2.13	118.59	111.91
22	4	603	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
22	4	604	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
22	1	603	CLA	C3D-C2D-C1D	-2.13	102.93	105.83
40	4	611	CHL	C1B-CHB-C4A	-2.13	125.90	130.12
22	A	1108	CLA	C1D-ND-C4D	-2.13	104.82	106.33
22	J	1901	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
22	A	1141	CLA	CHA-C1A-NA	-2.13	121.52	126.40
22	A	1118	CLA	C3D-C2D-C1D	-2.13	102.93	105.83
22	7	606	CLA	O2A-CGA-CBA	2.13	118.58	111.91
22	B	1213	CLA	CMB-C2B-C1B	-2.13	125.19	128.46
22	A	1122	CLA	CHA-C1A-NA	-2.13	121.53	126.40
22	B	1220	CLA	C3D-C2D-C1D	-2.13	102.93	105.83
22	7	613	CLA	C3D-C2D-C1D	-2.13	102.93	105.83
22	Z	615	CLA	C1D-ND-C4D	-2.13	104.82	106.33
22	A	1127	CLA	CHA-C1A-NA	-2.13	121.53	126.40
22	A	1123	CLA	C2A-C1A-CHA	2.13	127.58	123.86
22	A	1110	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
22	B	1022	CLA	CMA-C3A-C4A	2.13	117.49	111.77
40	Z	609	CHL	CMB-C2B-C1B	-2.13	125.20	128.46
22	7	606	CLA	CMB-C2B-C3B	2.13	128.66	124.68
22	8	607	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
22	6	619	CLA	CHA-C1A-NA	-2.13	121.53	126.40
22	5	622	CLA	C2A-C1A-CHA	2.13	127.58	123.86
22	8	611	CLA	CMD-C2D-C3D	-2.12	122.73	127.61
28	9	803	LMT	C1'-O5'-C5'	-2.12	109.52	113.69
22	6	604	CLA	O1A-CGA-CBA	-2.12	115.44	123.73
22	A	1127	CLA	C1C-C2C-C3C	-2.12	104.72	106.96
25	B	4002	BCR	C36-C18-C17	-2.12	119.95	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	2	612	CLA	C3D-C2D-C1D	-2.12	102.93	105.83
22	A	1125	CLA	C1D-ND-C4D	-2.12	104.83	106.33
22	B	1203	CLA	C1D-ND-C4D	-2.12	104.83	106.33
22	B	1223	CLA	C1D-ND-C4D	-2.12	104.83	106.33
22	1	602	CLA	C1D-ND-C4D	-2.12	104.83	106.33
22	6	609	CLA	CHA-C1A-NA	-2.12	121.54	126.40
40	2	610	CHL	CMB-C2B-C1B	-2.12	125.20	128.46
22	B	1227	CLA	CHA-C1A-NA	-2.12	121.54	126.40
22	B	1232	CLA	CAA-C2A-C3A	-2.12	106.97	112.78
22	9	601	CLA	CMD-C2D-C3D	-2.12	122.73	127.61
40	2	609	CHL	CMB-C2B-C1B	-2.12	125.20	128.46
22	5	609	CLA	C1D-ND-C4D	-2.12	104.83	106.33
22	A	1131	CLA	CHA-C1A-NA	-2.12	121.54	126.40
22	B	1240	CLA	CMD-C2D-C3D	-2.12	122.73	127.61
22	6	612	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
22	3	616	CLA	CMD-C2D-C3D	-2.12	122.74	127.61
22	B	1230	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
22	4	604	CLA	C1-O2A-CGA	2.12	122.00	116.44
22	3	606	CLA	O2A-CGA-CBA	2.12	118.56	111.91
39	Z	503	LUT	C11-C12-C13	-2.12	120.46	126.42
22	8	603	CLA	O1A-CGA-CBA	-2.12	115.46	123.73
22	3	601	CLA	CMD-C2D-C3D	-2.12	122.74	127.61
25	L	4001	BCR	C19-C18-C17	2.12	122.19	118.94
22	3	604	CLA	O1A-CGA-CBA	-2.12	115.47	123.73
25	K	4002	BCR	C3-C4-C5	-2.12	110.30	114.08
22	9	603	CLA	O1D-CGD-CBD	-2.12	120.15	124.48
25	3	504	BCR	C38-C26-C27	2.12	117.68	113.62
22	7	604	CLA	C1D-ND-C4D	-2.12	104.83	106.33
22	9	602	CLA	C1D-ND-C4D	-2.12	104.83	106.33
22	8	611	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
22	9	602	CLA	CMA-C3A-C4A	2.12	117.46	111.77
22	1	611	CLA	CHA-C1A-NA	-2.12	121.55	126.40
22	8	603	CLA	O2D-CGD-O1D	-2.12	119.70	123.84
22	K	1404	CLA	O2A-CGA-CBA	2.12	118.55	111.91
40	6	617	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
22	Z	612	CLA	CAA-C2A-C3A	-2.12	106.99	112.78
22	4	608	CLA	CHA-C1A-NA	-2.11	121.56	126.40
22	1	612	CLA	O2A-CGA-CBA	2.11	118.54	111.91
40	4	613	CHL	C1B-CHB-C4A	-2.11	125.93	130.12
22	8	609	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
25	4	503	BCR	C33-C5-C6	-2.11	122.15	124.53
22	A	1139	CLA	CMD-C2D-C3D	-2.11	122.75	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	6	618	CLA	CAA-C2A-C3A	-2.11	106.99	112.78
22	A	1134	CLA	CHA-C1A-NA	-2.11	121.56	126.40
22	1	604	CLA	O2A-CGA-CBA	2.11	118.54	111.91
22	1	601	CLA	C2A-C1A-CHA	2.11	127.56	123.86
22	9	604	CLA	C2C-C1C-NC	2.11	111.95	109.97
25	3	503	BCR	C37-C22-C23	2.11	121.41	118.08
22	A	1116	CLA	CAC-C3C-C4C	2.11	127.55	124.81
22	A	1140	CLA	CAA-C2A-C3A	-2.11	107.00	112.78
22	A	1134	CLA	CMB-C2B-C3B	2.11	128.63	124.68
22	A	1120	CLA	O2A-CGA-CBA	2.11	118.53	111.91
22	B	1212	CLA	CMD-C2D-C3D	-2.11	122.76	127.61
22	K	1402	CLA	CHA-C1A-NA	-2.11	121.56	126.40
22	A	1137	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
22	B	1210	CLA	CHA-C1A-NA	-2.11	121.56	126.40
22	Z	601	CLA	CMB-C2B-C3B	2.11	128.63	124.68
22	B	1222	CLA	CMD-C2D-C3D	-2.11	122.76	127.61
22	B	1208	CLA	CMD-C2D-C3D	-2.11	122.76	127.61
25	A	4003	BCR	C38-C26-C27	2.11	117.67	113.62
22	8	606	CLA	CMD-C2D-C3D	-2.11	122.76	127.61
22	7	603	CLA	CHA-C1A-NA	-2.11	121.57	126.40
22	Z	605	CLA	O2A-CGA-CBA	2.11	118.53	111.91
22	4	601	CLA	C2A-C1A-CHA	2.11	127.55	123.86
40	4	613	CHL	C2C-C3C-C4C	2.11	107.99	106.49
40	5	617	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
22	B	1220	CLA	CAC-C3C-C4C	2.11	127.55	124.81
22	G	1602	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
22	A	1111	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
22	A	1124	CLA	C1D-ND-C4D	-2.11	104.84	106.33
40	9	610	CHL	C4A-NA-C1A	2.11	107.65	106.71
22	2	615	CLA	CHA-C1A-NA	-2.11	121.57	126.40
22	A	1134	CLA	C3D-C2D-C1D	-2.11	102.96	105.83
22	G	1601	CLA	C1D-ND-C4D	-2.11	104.84	106.33
22	B	1207	CLA	CHA-C1A-NA	-2.11	121.58	126.40
40	9	613	CHL	CMB-C2B-C1B	-2.11	125.23	128.46
22	J	1901	CLA	C3D-C2D-C1D	-2.11	102.96	105.83
22	7	603	CLA	O2D-CGD-O1D	-2.11	119.72	123.84
40	4	617	CHL	C4D-CHA-C1A	2.11	123.81	121.25
22	8	608	CLA	O2D-CGD-O1D	-2.10	119.72	123.84
22	7	602	CLA	O2A-CGA-CBA	2.10	118.51	111.91
26	6	801	LHG	O7-C7-O9	-2.10	118.62	123.70
22	B	1226	CLA	CBA-CAA-C2A	2.10	120.07	113.86
22	7	601	CLA	CHA-C1A-NA	-2.10	121.58	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	607	CLA	O2A-CGA-CBA	2.10	118.51	111.91
22	A	1125	CLA	CHA-C1A-NA	-2.10	121.58	126.40
22	B	1222	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
22	6	602	CLA	C1D-ND-C4D	-2.10	104.84	106.33
37	1	503	C7Z	C40-C33-C34	-2.10	119.98	122.92
22	B	1212	CLA	CMA-C3A-C4A	2.10	117.42	111.77
22	6	605	CLA	CMA-C3A-C4A	2.10	117.42	111.77
39	5	502	LUT	C35-C15-C14	-2.10	119.17	123.47
22	A	1134	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
22	A	1121	CLA	C2D-C1D-ND	2.10	111.65	110.10
22	F	1301	CLA	C2A-C1A-CHA	2.10	127.53	123.86
22	F	1301	CLA	C1D-ND-C4D	-2.10	104.84	106.33
22	B	1231	CLA	C2D-C1D-ND	2.10	111.65	110.10
22	B	1209	CLA	CHA-C1A-NA	-2.10	121.59	126.40
22	Z	602	CLA	C1D-ND-C4D	-2.10	104.84	106.33
22	4	604	CLA	C1D-ND-C4D	-2.10	104.84	106.33
22	B	1227	CLA	CMD-C2D-C3D	-2.10	122.79	127.61
22	B	1203	CLA	CHA-C1A-NA	-2.10	121.59	126.40
22	9	604	CLA	C1C-C2C-C3C	-2.10	104.75	106.96
25	K	4002	BCR	C38-C26-C27	2.10	117.65	113.62
25	B	4001	BCR	C23-C22-C21	-2.10	115.72	118.94
22	A	1141	CLA	CMD-C2D-C3D	-2.10	122.79	127.61
22	A	1113	CLA	CHA-C1A-NA	-2.10	121.59	126.40
22	A	1119	CLA	CMB-C2B-C1B	-2.10	125.24	128.46
40	9	610	CHL	CMB-C2B-C1B	-2.10	125.24	128.46
22	5	602	CLA	CHA-C1A-NA	-2.10	121.60	126.40
22	B	1214	CLA	CHA-C1A-NA	-2.10	121.60	126.40
22	B	1229	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
22	9	604	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
40	7	610	CHL	CMB-C2B-C1B	-2.09	125.24	128.46
22	A	1012	CLA	C1-C2-C3	-2.09	122.42	126.04
40	4	610	CHL	CMA-C3A-C2A	2.09	122.28	113.83
39	2	501	LUT	C40-C33-C32	2.09	121.38	118.08
22	9	605	CLA	CMB-C2B-C1B	-2.09	125.25	128.46
22	B	1212	CLA	C2A-C1A-CHA	2.09	127.52	123.86
22	7	604	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
22	B	1214	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
22	A	1104	CLA	CMD-C2D-C3D	-2.09	122.80	127.61
22	B	1231	CLA	CHA-C1A-NA	-2.09	121.60	126.40
22	B	1205	CLA	C1D-ND-C4D	-2.09	104.85	106.33
22	7	615	CLA	C1D-ND-C4D	-2.09	104.85	106.33
22	1	605	CLA	CMB-C2B-C3B	2.09	128.59	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1223	CLA	CAA-C2A-C3A	-2.09	107.05	112.78
22	5	605	CLA	CAA-CBA-CGA	-2.09	107.14	113.25
22	A	1121	CLA	CHA-C1A-NA	-2.09	121.61	126.40
22	2	601	CLA	CMD-C2D-C3D	-2.09	122.80	127.61
25	4	503	BCR	C34-C9-C10	-2.09	119.99	122.92
22	Z	606	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
22	3	616	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
22	8	601	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
22	7	615	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
22	B	1201	CLA	C2C-C1C-NC	2.09	111.93	109.97
39	3	502	LUT	C30-C31-C32	-2.09	116.69	123.22
22	7	607	CLA	CMB-C2B-C3B	2.09	128.59	124.68
40	5	610	CHL	C1B-CHB-C4A	-2.09	125.98	130.12
25	3	505	BCR	C31-C1-C6	-2.09	106.91	110.30
25	8	503	BCR	C29-C28-C27	2.09	116.05	111.38
22	3	601	CLA	C2A-C1A-CHA	2.09	127.51	123.86
22	5	604	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
39	Z	501	LUT	C15-C14-C13	-2.09	124.33	127.31
22	A	1103	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
25	K	4002	BCR	C2-C1-C6	2.09	113.70	110.48
22	B	1202	CLA	CMA-C3A-C4A	2.09	117.39	111.77
22	B	1241	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
22	1	602	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
25	7	503	BCR	C30-C25-C24	2.09	121.68	115.78
22	7	607	CLA	CHA-C1A-NA	-2.09	121.62	126.40
22	B	1220	CLA	CAA-CBA-CGA	-2.09	107.16	113.25
22	A	1103	CLA	C1-O2A-CGA	2.09	121.92	116.44
22	F	1301	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
22	4	612	CLA	C1D-ND-C4D	-2.09	104.85	106.33
22	6	604	CLA	C1D-ND-C4D	-2.09	104.85	106.33
22	3	605	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
22	3	602	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
39	2	503	LUT	C28-C29-C30	2.09	122.14	118.94
40	Z	610	CHL	CHD-C4C-C3C	2.09	127.91	124.84
22	B	1203	CLA	CMD-C2D-C3D	-2.08	122.82	127.61
25	8	503	BCR	C19-C18-C17	2.08	122.14	118.94
22	6	615	CLA	CMD-C2D-C3D	-2.08	122.82	127.61
22	A	1101	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
22	8	605	CLA	C1-O2A-CGA	2.08	121.91	116.44
22	K	1401	CLA	C1D-ND-C4D	-2.08	104.86	106.33
22	3	603	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
22	6	604	CLA	CMB-C2B-C3B	2.08	128.57	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	4	602	CLA	CMD-C2D-C3D	-2.08	122.82	127.61
22	5	615	CLA	CMD-C2D-C3D	-2.08	122.82	127.61
40	5	610	CHL	CMB-C2B-C1B	-2.08	125.26	128.46
22	5	604	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
22	A	1111	CLA	C1D-ND-C4D	-2.08	104.86	106.33
22	B	1238	CLA	C1D-ND-C4D	-2.08	104.86	106.33
22	A	1116	CLA	C2C-C1C-NC	2.08	111.92	109.97
22	5	601	CLA	CHA-C1A-NA	-2.08	121.63	126.40
22	5	607	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
40	4	617	CHL	C1B-CHB-C4A	-2.08	126.00	130.12
22	1	601	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
22	1	604	CLA	CMB-C2B-C3B	2.08	128.57	124.68
22	A	1123	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
39	7	502	LUT	C38-C25-C24	-2.08	119.11	123.56
22	B	1023	CLA	CHA-C1A-NA	-2.08	121.64	126.40
22	B	1221	CLA	CMA-C3A-C2A	2.08	122.21	113.83
22	B	1201	CLA	C1D-ND-C4D	-2.08	104.86	106.33
22	1	606	CLA	O2A-CGA-CBA	2.08	118.43	111.91
22	1	604	CLA	CHA-C1A-NA	-2.08	121.64	126.40
22	A	1122	CLA	O2D-CGD-O1D	-2.08	119.78	123.84
22	3	601	CLA	CMB-C2B-C1B	-2.08	125.27	128.46
22	8	615	CLA	C3D-C2D-C1D	-2.08	103.00	105.83
25	4	503	BCR	C3-C4-C5	-2.08	110.37	114.08
22	A	1131	CLA	CMD-C2D-C3D	-2.08	122.84	127.61
39	3	501	LUT	C30-C31-C32	-2.08	116.74	123.22
22	B	1023	CLA	CMB-C2B-C1B	-2.08	125.27	128.46
22	L	1502	CLA	C3D-C2D-C1D	-2.08	103.00	105.83
22	3	618	CLA	C3D-C2D-C1D	-2.08	103.00	105.83
25	5	503	BCR	C35-C13-C12	2.08	121.35	118.08
22	A	1139	CLA	CBA-CAA-C2A	2.08	119.99	113.86
22	B	1207	CLA	C1D-ND-C4D	-2.07	104.86	106.33
22	B	1212	CLA	C1D-ND-C4D	-2.07	104.86	106.33
22	1	605	CLA	O1D-CGD-CBD	-2.07	120.24	124.48
25	G	4001	BCR	C34-C9-C10	-2.07	120.02	122.92
22	6	603	CLA	O1A-CGA-CBA	-2.07	115.64	123.73
22	A	1013	CLA	C2C-C1C-NC	2.07	111.92	109.97
22	B	1226	CLA	CAC-C3C-C2C	-2.07	123.98	127.53
22	9	609	CLA	CMD-C2D-C3D	-2.07	122.84	127.61
22	B	1228	CLA	C1-O2A-CGA	2.07	121.88	116.44
22	3	601	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
22	3	613	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
22	9	606	CLA	C2C-C1C-NC	2.07	111.91	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	4	606	CLA	CHA-C1A-NA	-2.07	121.65	126.40
22	9	608	CLA	CAA-C2A-C3A	-2.07	107.10	112.78
25	8	503	BCR	C33-C5-C4	2.07	117.60	113.62
26	A	5001	LHG	C9-C8-C7	-2.07	106.09	113.62
22	B	1235	CLA	CMA-C3A-C4A	2.07	117.34	111.77
22	B	1221	CLA	C2A-C1A-CHA	2.07	127.48	123.86
39	7	501	LUT	C31-C30-C29	-2.07	124.35	127.31
22	Z	611	CLA	O2A-CGA-CBA	2.07	118.41	111.91
26	1	801	LHG	O7-C7-O9	-2.07	118.70	123.70
23	A	2001	PQN	C11-C12-C13	-2.07	123.34	126.79
22	7	604	CLA	CBA-CAA-C2A	2.07	119.97	113.86
22	5	609	CLA	CMD-C2D-C3D	-2.07	122.85	127.61
40	6	611	CHL	CHC-C1C-NC	2.07	127.34	124.20
22	7	611	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
22	4	603	CLA	CMB-C2B-C3B	2.07	128.55	124.68
22	B	1215	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
22	A	1138	CLA	CMD-C2D-C3D	-2.07	122.86	127.61
22	2	604	CLA	CHA-C1A-NA	-2.07	121.66	126.40
22	G	1601	CLA	CMD-C2D-C3D	-2.07	122.86	127.61
26	4	801	LHG	O7-C7-O9	-2.07	118.71	123.70
22	Z	607	CLA	CMD-C2D-C3D	-2.07	122.86	127.61
40	3	611	CHL	CMB-C2B-C1B	-2.07	125.29	128.46
22	K	1402	CLA	CMD-C2D-C3D	-2.07	122.86	127.61
39	6	501	LUT	C15-C14-C13	-2.06	124.36	127.31
37	5	505	C7Z	C19-C9-C10	-2.06	120.03	122.92
22	B	1201	CLA	CHA-C1A-NA	-2.06	121.67	126.40
22	2	601	CLA	CHA-C1A-NA	-2.06	121.67	126.40
22	A	1118	CLA	CAA-C2A-C3A	-2.06	107.12	112.78
22	9	612	CLA	CAA-C2A-C3A	-2.06	107.12	112.78
22	B	1239	CLA	C3D-C2D-C1D	-2.06	103.01	105.83
22	3	610	CLA	O2A-CGA-CBA	2.06	118.39	111.91
22	B	1227	CLA	O2A-CGA-CBA	2.06	118.38	111.91
22	B	1240	CLA	C2A-C1A-CHA	2.06	127.46	123.86
22	3	607	CLA	C2A-C1A-CHA	2.06	127.46	123.86
22	6	612	CLA	CHA-C1A-NA	-2.06	121.68	126.40
39	9	502	LUT	C38-C25-C24	-2.06	119.15	123.56
22	3	610	CLA	C2D-C1D-ND	2.06	111.62	110.10
39	6	502	LUT	C19-C9-C8	2.06	121.32	118.08
22	B	1210	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
22	A	1119	CLA	CHA-C1A-NA	-2.06	121.68	126.40
37	5	505	C7Z	C11-C12-C13	-2.06	120.63	126.42
22	7	613	CLA	CMD-C2D-C3D	-2.06	122.88	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	8	604	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
37	1	503	C7Z	C7-C8-C9	-2.06	123.12	126.23
25	K	4001	BCR	C15-C14-C13	-2.06	124.37	127.31
22	A	1115	CLA	C1-O2A-CGA	2.06	121.84	116.44
40	4	611	CHL	CHC-C1C-NC	2.06	127.33	124.20
22	1	615	CLA	C1-C2-C3	-2.06	122.48	126.04
40	Z	613	CHL	C4D-CHA-C1A	2.06	123.75	121.25
37	1	503	C7Z	C38-C25-C24	2.06	118.17	114.36
22	3	601	CLA	CHA-C1A-NA	-2.06	121.69	126.40
22	B	1217	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
37	5	505	C7Z	C24-C25-C26	-2.06	116.26	120.85
22	B	1219	CLA	C2A-C1A-CHA	2.06	127.46	123.86
22	A	1123	CLA	CAC-C3C-C4C	2.06	127.48	124.81
40	2	609	CHL	C1-O2A-CGA	2.06	121.84	116.44
22	Z	604	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
22	B	1214	CLA	CAA-CBA-CGA	-2.06	107.24	113.25
22	4	604	CLA	C3D-C2D-C1D	-2.06	103.03	105.83
22	9	609	CLA	C3D-C2D-C1D	-2.06	103.03	105.83
22	5	605	CLA	OBD-CAD-C3D	-2.06	123.57	128.52
22	5	613	CLA	C1D-ND-C4D	-2.06	104.88	106.33
22	B	1230	CLA	C1-O2A-CGA	2.06	121.84	116.44
22	B	1240	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
22	1	601	CLA	O2A-CGA-CBA	2.05	118.36	111.91
22	6	608	CLA	C1-O2A-CGA	2.05	121.83	116.44
25	G	4001	BCR	C12-C13-C14	-2.05	115.79	118.94
22	8	615	CLA	CMD-C2D-C3D	-2.05	122.89	127.61
22	B	1216	CLA	C1D-ND-C4D	-2.05	104.88	106.33
22	5	608	CLA	C1D-ND-C4D	-2.05	104.88	106.33
22	B	1234	CLA	CAA-C2A-C3A	-2.05	107.15	112.78
22	J	1901	CLA	O1D-CGD-CBD	-2.05	120.28	124.48
40	6	610	CHL	C4A-NA-C1A	2.05	107.63	106.71
22	B	1234	CLA	OBD-CAD-C3D	-2.05	123.58	128.52
22	A	1134	CLA	O2A-CGA-CBA	2.05	118.35	111.91
22	B	1222	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
40	6	610	CHL	CMB-C2B-C3B	2.05	128.52	124.68
22	A	1132	CLA	O1D-CGD-CBD	-2.05	120.28	124.48
39	9	501	LUT	C30-C31-C32	-2.05	116.81	123.22
25	3	506	BCR	C33-C5-C4	2.05	117.56	113.62
28	9	803	LMT	O1B-C1B-C2B	2.05	113.42	108.10
22	6	618	CLA	CHA-C1A-NA	-2.05	121.70	126.40
25	I	4001	BCR	C19-C18-C17	2.05	122.09	118.94
22	5	612	CLA	CMB-C2B-C1B	-2.05	125.31	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1118	CLA	CHA-C1A-NA	-2.05	121.70	126.40
25	B	4006	BCR	C34-C9-C10	-2.05	120.05	122.92
22	A	1114	CLA	C1-O2A-CGA	2.05	121.82	116.44
22	1	608	CLA	CHA-C1A-NA	-2.05	121.71	126.40
22	6	604	CLA	CAA-C2A-C3A	-2.05	107.17	112.78
22	A	1126	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
22	A	1120	CLA	C1-O2A-CGA	2.05	121.82	116.44
25	7	503	BCR	C35-C13-C12	2.05	121.30	118.08
22	7	616	CLA	CHA-C1A-NA	-2.05	121.71	126.40
22	A	1102	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
22	K	1402	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
22	B	1238	CLA	O2A-CGA-CBA	2.05	118.33	111.91
22	5	615	CLA	O2A-CGA-CBA	2.05	118.33	111.91
22	G	1601	CLA	C2A-C1A-CHA	2.05	127.44	123.86
22	Z	605	CLA	C1-O2A-CGA	2.05	121.81	116.44
22	B	1241	CLA	CMB-C2B-C3B	2.05	128.50	124.68
22	6	615	CLA	C1D-ND-C4D	-2.05	104.88	106.33
22	B	1231	CLA	C1-O2A-CGA	2.05	121.81	116.44
25	5	503	BCR	C38-C26-C27	2.04	117.54	113.62
22	A	1129	CLA	C1D-ND-C4D	-2.04	104.88	106.33
22	1	612	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
22	8	605	CLA	C1D-ND-C4D	-2.04	104.88	106.33
22	B	1217	CLA	CHA-C1A-NA	-2.04	121.72	126.40
22	1	601	CLA	O2D-CGD-O1D	-2.04	119.85	123.84
25	8	503	BCR	C37-C22-C21	-2.04	120.06	122.92
22	A	1108	CLA	C2A-C1A-CHA	2.04	127.43	123.86
22	9	605	CLA	O2A-CGA-CBA	2.04	118.31	111.91
22	2	608	CLA	C1D-ND-C4D	-2.04	104.89	106.33
22	7	605	CLA	CAA-C2A-C3A	-2.04	107.19	112.78
38	7	803	SPH	O3-C3-C2	2.04	110.55	107.31
22	7	616	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
22	A	1108	CLA	O2A-CGA-CBA	2.04	118.31	111.91
22	7	604	CLA	CMB-C2B-C3B	2.04	128.50	124.68
22	A	1120	CLA	CHA-C1A-NA	-2.04	121.73	126.40
22	8	615	CLA	C1D-ND-C4D	-2.04	104.89	106.33
22	A	1132	CLA	CHA-C1A-NA	-2.04	121.73	126.40
22	9	606	CLA	C1-O2A-CGA	2.04	121.79	116.44
22	1	613	CLA	CAA-C2A-C3A	-2.04	107.19	112.78
22	A	1115	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
22	A	1133	CLA	C1-O2A-CGA	2.04	121.79	116.44
22	8	607	CLA	O2A-CGA-CBA	2.04	118.30	111.91
25	3	506	BCR	C34-C9-C10	-2.04	120.07	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	7	608	CLA	CMD-C2D-C3D	-2.04	122.93	127.61
22	8	602	CLA	O2A-CGA-CBA	2.04	118.30	111.91
22	B	1217	CLA	CMD-C2D-C3D	-2.04	122.93	127.61
22	A	1012	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
22	6	619	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
22	B	1227	CLA	CMB-C2B-C3B	2.04	128.49	124.68
22	B	1212	CLA	C1-O2A-CGA	2.04	121.79	116.44
22	A	1113	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
22	4	606	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
22	8	611	CLA	CMB-C2B-C3B	2.04	128.49	124.68
25	7	504	BCR	C19-C18-C17	2.04	122.06	118.94
22	A	1104	CLA	O1D-CGD-CBD	-2.04	120.32	124.48
22	B	1240	CLA	O1D-CGD-CBD	-2.04	120.32	124.48
22	2	612	CLA	CAA-C2A-C3A	-2.04	107.20	112.78
22	5	609	CLA	C3D-C2D-C1D	-2.03	103.05	105.83
22	7	606	CLA	C1D-ND-C4D	-2.03	104.89	106.33
22	4	609	CLA	CHA-C1A-NA	-2.03	121.74	126.40
22	2	615	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
22	B	1211	CLA	CAA-CBA-CGA	-2.03	107.31	113.25
22	B	1213	CLA	O1A-CGA-CBA	-2.03	115.80	123.73
22	5	603	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
22	B	1201	CLA	CMD-C2D-C3D	-2.03	122.94	127.61
22	Z	605	CLA	CAA-C2A-C3A	-2.03	107.22	112.78
22	B	1204	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
22	7	602	CLA	CMA-C3A-C4A	2.03	117.23	111.77
25	4	503	BCR	C1-C6-C7	2.03	121.52	115.78
25	7	503	BCR	C29-C28-C27	2.03	115.91	111.38
22	A	1141	CLA	CAC-C3C-C4C	2.03	127.44	124.81
22	B	1210	CLA	CAC-C3C-C4C	2.03	127.44	124.81
22	1	611	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
40	6	613	CHL	C1B-CHB-C4A	-2.03	126.10	130.12
22	9	601	CLA	C1D-ND-C4D	-2.03	104.89	106.33
22	A	1131	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
22	Z	603	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
22	B	1239	CLA	CMD-C2D-C3D	-2.03	122.95	127.61
22	B	1214	CLA	C1C-C2C-C3C	-2.03	104.83	106.96
22	Z	611	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
40	5	611	CHL	C4D-CHA-C1A	2.03	123.72	121.25
22	Z	604	CLA	CMB-C2B-C3B	2.03	128.47	124.68
22	3	604	CLA	C1C-C2C-C3C	-2.03	104.83	106.96
22	Z	615	CLA	C3D-C2D-C1D	-2.03	103.07	105.83
26	Z	801	LHG	C5-O7-C7	-2.03	112.80	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	2	607	CLA	C1D-ND-C4D	-2.03	104.90	106.33
22	4	601	CLA	CHA-C1A-NA	-2.03	121.76	126.40
22	4	601	CLA	CMA-C3A-C4A	2.02	117.22	111.77
22	9	607	CLA	O2D-CGD-O1D	-2.02	119.88	123.84
22	A	1138	CLA	C1D-ND-C4D	-2.02	104.90	106.33
22	2	615	CLA	CAA-C2A-C3A	-2.02	107.24	112.78
22	B	1022	CLA	CMD-C2D-C3D	-2.02	122.96	127.61
22	1	613	CLA	CMC-C2C-C1C	2.02	128.12	125.04
22	1	601	CLA	CMA-C3A-C4A	2.02	117.21	111.77
22	A	1135	CLA	CMD-C2D-C3D	-2.02	122.96	127.61
22	7	605	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
22	4	615	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
22	4	603	CLA	C1-O2A-CGA	2.02	121.75	116.44
25	A	4004	BCR	C19-C18-C17	2.02	122.04	118.94
22	8	604	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
22	B	1217	CLA	O2A-CGA-CBA	2.02	118.25	111.91
22	9	605	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
22	5	608	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
25	5	504	BCR	C30-C25-C24	2.02	121.50	115.78
22	2	604	CLA	O2A-CGA-CBA	2.02	118.25	111.91
40	2	610	CHL	C3C-C4C-NC	-2.02	108.31	110.57
22	7	601	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
22	4	602	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
22	2	605	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
22	2	608	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
25	A	4003	BCR	C23-C24-C25	-2.02	121.53	127.20
22	A	1135	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
22	B	1240	CLA	CMC-C2C-C1C	2.02	128.11	125.04
22	A	1127	CLA	O2A-CGA-CBA	2.02	118.24	111.91
39	8	502	LUT	C39-C29-C28	2.02	121.26	118.08
22	A	1117	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
22	A	1126	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
22	7	611	CLA	CHA-C1A-NA	-2.02	121.78	126.40
22	6	615	CLA	C2A-C1A-CHA	2.02	127.39	123.86
22	7	602	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
22	1	604	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
39	1	502	LUT	C31-C30-C29	-2.02	124.43	127.31
22	5	604	CLA	CMD-C2D-C3D	-2.02	122.98	127.61
22	8	607	CLA	CMB-C2B-C3B	2.02	128.45	124.68
22	1	601	CLA	CHA-C1A-NA	-2.02	121.78	126.40
40	8	613	CHL	CHC-C1C-NC	2.02	127.26	124.20
22	1	606	CLA	CHA-C1A-NA	-2.02	121.78	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1202	CLA	C1-C2-C3	-2.01	122.56	126.04
25	B	4004	BCR	C36-C18-C17	-2.01	120.10	122.92
22	8	606	CLA	CHA-C1A-NA	-2.01	121.79	126.40
22	B	1226	CLA	C2A-C1A-CHA	2.01	127.38	123.86
22	B	1217	CLA	C1D-ND-C4D	-2.01	104.91	106.33
22	B	1212	CLA	C1C-C2C-C3C	-2.01	104.84	106.96
39	2	501	LUT	C35-C15-C14	-2.01	119.35	123.47
22	3	604	CLA	CHA-C4D-ND	2.01	136.71	132.50
22	7	607	CLA	CMD-C2D-C3D	-2.01	122.98	127.61
22	B	1022	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
22	8	607	CLA	CMA-C3A-C4A	2.01	117.18	111.77
44	7	805	PLM	C3-C2-C1	-2.01	109.40	114.47
22	A	1111	CLA	C1-O2A-CGA	2.01	121.72	116.44
22	B	1215	CLA	CHA-C1A-NA	-2.01	121.79	126.40
25	6	504	BCR	C1-C6-C5	-2.01	119.78	122.61
22	8	612	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
39	4	502	LUT	C39-C29-C28	2.01	121.25	118.08
25	K	4002	BCR	C23-C24-C25	-2.01	121.56	127.20
22	B	1221	CLA	CMA-C3A-C4A	2.01	117.18	111.77
22	1	607	CLA	CMD-C2D-C3D	-2.01	122.99	127.61
22	A	1126	CLA	CHA-C1A-NA	-2.01	121.80	126.40
22	3	618	CLA	C2A-C1A-CHA	2.01	127.37	123.86
22	K	1403	CLA	CAA-C2A-C3A	-2.01	107.28	112.78
22	A	1110	CLA	CHA-C1A-NA	-2.01	121.80	126.40
22	7	607	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
22	B	1224	CLA	CMB-C2B-C1B	-2.01	125.38	128.46
22	A	1127	CLA	C1D-ND-C4D	-2.01	104.91	106.33
22	A	1110	CLA	CMC-C2C-C1C	2.01	128.10	125.04
22	A	1105	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
22	G	1601	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
22	4	612	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
22	B	1223	CLA	CAA-CBA-CGA	-2.01	107.38	113.25
39	1	502	LUT	C20-C13-C12	2.01	121.24	118.08
39	2	503	LUT	C37-C21-C36	2.01	110.85	107.89
22	5	602	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
22	8	606	CLA	CMA-C3A-C4A	2.01	117.17	111.77
22	B	1232	CLA	C1D-ND-C4D	-2.01	104.91	106.33
22	2	612	CLA	C1D-ND-C4D	-2.01	104.91	106.33
22	B	1235	CLA	CMB-C2B-C1B	-2.01	125.38	128.46
22	B	1206	CLA	C2A-C1A-CHA	2.01	127.37	123.86
39	5	502	LUT	C18-C5-C4	2.01	118.07	114.36
25	A	4002	BCR	C37-C22-C23	2.01	121.24	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	5	606	CLA	CAC-C3C-C4C	2.01	127.41	124.81
22	4	608	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
22	6	615	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
22	8	608	CLA	CAA-C2A-C3A	-2.01	107.29	112.78
39	8	502	LUT	C18-C5-C6	-2.01	122.28	124.53
39	Z	503	LUT	C40-C33-C34	-2.01	120.11	122.92
22	B	1210	CLA	CAA-C2A-C3A	-2.01	107.29	112.78
22	2	607	CLA	C3D-C2D-C1D	-2.00	103.09	105.83
22	7	613	CLA	C1D-ND-C4D	-2.00	104.91	106.33
22	B	1235	CLA	CHA-C1A-NA	-2.00	121.81	126.40
39	1	502	LUT	C3-C4-C5	-2.00	107.86	111.85
22	8	606	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
22	B	1216	CLA	CHA-C1A-NA	-2.00	121.81	126.40
22	B	1228	CLA	CHA-C1A-NA	-2.00	121.81	126.40
22	Z	605	CLA	CHA-C1A-NA	-2.00	121.81	126.40
22	B	1224	CLA	C2A-C1A-CHA	2.00	127.36	123.86
40	6	613	CHL	C3C-C4C-NC	-2.00	108.33	110.57
22	A	1113	CLA	CMD-C2D-C3D	-2.00	123.01	127.61
22	4	606	CLA	O2A-CGA-CBA	2.00	118.19	111.91
25	B	4006	BCR	C33-C5-C4	2.00	117.46	113.62
40	5	611	CHL	C1B-CHB-C4A	-2.00	126.15	130.12
22	B	1218	CLA	CHA-C1A-NA	-2.00	121.81	126.40
22	7	612	CLA	CHA-C1A-NA	-2.00	121.81	126.40
22	A	1108	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
22	Z	607	CLA	C2A-C1A-CHA	2.00	127.36	123.86
22	7	615	CLA	C2A-C1A-CHA	2.00	127.36	123.86
22	F	1301	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
22	3	603	CLA	O1A-CGA-CBA	-2.00	115.93	123.73
25	A	4004	BCR	C37-C22-C21	-2.00	120.12	122.92

All (315) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	A	1011	CL0	NA
21	A	1011	CL0	NC
21	A	1011	CL0	ND
22	A	1012	CLA	ND
22	A	1102	CLA	ND
22	A	1103	CLA	ND
22	A	1104	CLA	ND
22	A	1105	CLA	ND
22	A	1106	CLA	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
22	A	1107	CLA	ND
22	A	1108	CLA	ND
22	A	1109	CLA	ND
22	A	1110	CLA	ND
22	A	1111	CLA	ND
22	A	1112	CLA	ND
22	A	1113	CLA	ND
22	A	1114	CLA	ND
22	A	1115	CLA	ND
22	A	1116	CLA	ND
22	A	1117	CLA	ND
22	A	1118	CLA	ND
22	A	1119	CLA	ND
22	A	1120	CLA	ND
22	A	1121	CLA	ND
22	A	1122	CLA	ND
22	A	1123	CLA	ND
22	A	1124	CLA	ND
22	A	1125	CLA	ND
22	A	1126	CLA	ND
22	A	1127	CLA	ND
22	A	1128	CLA	ND
22	A	1129	CLA	ND
22	A	1130	CLA	ND
22	A	1131	CLA	ND
22	A	1132	CLA	ND
22	A	1133	CLA	ND
22	A	1134	CLA	ND
22	A	1135	CLA	ND
22	A	1136	CLA	ND
22	A	1137	CLA	ND
22	A	1138	CLA	ND
22	A	1139	CLA	ND
22	A	1141	CLA	ND
22	A	1013	CLA	ND
22	A	1140	CLA	ND
22	A	1101	CLA	ND
22	B	1022	CLA	ND
22	B	1237	CLA	ND
22	B	1021	CLA	ND
22	B	1023	CLA	ND
22	B	1201	CLA	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
22	B	1202	CLA	ND
22	B	1203	CLA	ND
22	B	1204	CLA	ND
22	B	1205	CLA	ND
22	B	1206	CLA	ND
22	B	1207	CLA	ND
22	B	1208	CLA	ND
22	B	1209	CLA	ND
22	B	1210	CLA	ND
22	B	1211	CLA	ND
22	B	1212	CLA	ND
22	B	1213	CLA	ND
22	B	1214	CLA	ND
22	B	1215	CLA	ND
22	B	1216	CLA	ND
22	B	1217	CLA	ND
22	B	1218	CLA	ND
22	B	1219	CLA	ND
22	B	1220	CLA	ND
22	B	1221	CLA	ND
22	B	1222	CLA	ND
22	B	1223	CLA	ND
22	B	1224	CLA	ND
22	B	1225	CLA	ND
22	B	1226	CLA	ND
22	B	1227	CLA	ND
22	B	1228	CLA	ND
22	B	1229	CLA	ND
22	B	1230	CLA	ND
22	B	1231	CLA	ND
22	B	1232	CLA	ND
22	B	1234	CLA	ND
22	B	1235	CLA	ND
22	B	1236	CLA	ND
22	B	1238	CLA	ND
22	B	1239	CLA	ND
22	B	1240	CLA	ND
22	B	1241	CLA	ND
22	F	1301	CLA	ND
22	F	1302	CLA	ND
22	G	1601	CLA	ND
22	G	1602	CLA	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
22	J	1901	CLA	ND
22	K	1401	CLA	ND
22	K	1402	CLA	ND
22	K	1403	CLA	ND
22	K	1404	CLA	ND
22	L	1502	CLA	ND
22	L	1503	CLA	ND
22	1	601	CLA	ND
22	1	602	CLA	ND
22	1	603	CLA	ND
22	1	604	CLA	ND
22	1	605	CLA	ND
22	1	606	CLA	ND
22	1	607	CLA	ND
22	1	608	CLA	ND
22	1	611	CLA	ND
22	1	612	CLA	ND
22	1	613	CLA	ND
22	1	615	CLA	ND
22	Z	601	CLA	ND
22	Z	602	CLA	ND
22	Z	603	CLA	ND
22	Z	604	CLA	ND
22	Z	605	CLA	ND
22	Z	606	CLA	ND
22	Z	607	CLA	ND
22	Z	608	CLA	ND
22	Z	611	CLA	ND
22	Z	612	CLA	ND
22	Z	615	CLA	ND
22	3	601	CLA	ND
22	3	602	CLA	ND
22	3	603	CLA	ND
22	3	604	CLA	ND
22	3	605	CLA	ND
22	3	606	CLA	ND
22	3	607	CLA	ND
22	3	608	CLA	ND
22	3	610	CLA	ND
22	3	612	CLA	ND
22	3	613	CLA	ND
22	3	618	CLA	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
22	3	616	CLA	ND
22	7	609	CLA	ND
22	7	601	CLA	ND
22	7	602	CLA	ND
22	7	603	CLA	ND
22	7	604	CLA	ND
22	7	605	CLA	ND
22	7	606	CLA	ND
22	7	607	CLA	ND
22	7	608	CLA	ND
22	7	611	CLA	ND
22	7	612	CLA	ND
22	7	613	CLA	ND
22	7	615	CLA	ND
22	7	616	CLA	ND
22	8	605	CLA	ND
22	8	609	CLA	ND
22	8	601	CLA	ND
22	8	602	CLA	ND
22	8	603	CLA	ND
22	8	604	CLA	ND
22	8	606	CLA	ND
22	8	607	CLA	ND
22	8	608	CLA	ND
22	8	611	CLA	ND
22	8	612	CLA	ND
22	8	615	CLA	ND
22	4	601	CLA	ND
22	4	602	CLA	ND
22	4	603	CLA	ND
22	4	604	CLA	ND
22	4	605	CLA	ND
22	4	606	CLA	ND
22	4	607	CLA	ND
22	4	608	CLA	ND
22	4	612	CLA	ND
22	4	615	CLA	ND
22	4	609	CLA	ND
22	5	601	CLA	ND
22	5	602	CLA	ND
22	5	603	CLA	ND
22	5	604	CLA	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
22	5	605	CLA	ND
22	5	606	CLA	ND
22	5	607	CLA	ND
22	5	608	CLA	ND
22	5	609	CLA	ND
22	5	612	CLA	ND
22	5	613	CLA	ND
22	5	615	CLA	ND
22	5	618	CLA	ND
22	5	622	CLA	ND
22	6	608	CLA	ND
22	6	609	CLA	ND
22	6	601	CLA	ND
22	6	602	CLA	ND
22	6	603	CLA	ND
22	6	604	CLA	ND
22	6	605	CLA	ND
22	6	606	CLA	ND
22	6	607	CLA	ND
22	6	612	CLA	ND
22	6	615	CLA	ND
22	6	618	CLA	ND
22	6	619	CLA	ND
22	2	601	CLA	ND
22	2	602	CLA	ND
22	2	603	CLA	ND
22	2	604	CLA	ND
22	2	605	CLA	ND
22	2	606	CLA	ND
22	2	607	CLA	ND
22	2	608	CLA	ND
22	2	612	CLA	ND
22	2	615	CLA	ND
22	9	601	CLA	ND
22	9	602	CLA	ND
22	9	603	CLA	ND
22	9	604	CLA	ND
22	9	606	CLA	ND
22	9	607	CLA	ND
22	9	608	CLA	ND
22	9	609	CLA	ND
22	9	612	CLA	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
36	F	4001	RRX	C28
37	J	4002	C7Z	C3
37	1	503	C7Z	C3
37	5	505	C7Z	C3
39	2	501	LUT	C26
39	2	503	LUT	C26
40	1	610	CHL	NA
40	1	610	CHL	NC
40	1	610	CHL	ND
40	1	609	CHL	NA
40	1	609	CHL	NC
40	1	609	CHL	C8
40	1	609	CHL	ND
40	Z	610	CHL	NA
40	Z	610	CHL	NC
40	Z	610	CHL	C8
40	Z	610	CHL	ND
40	Z	613	CHL	NA
40	Z	613	CHL	NC
40	Z	613	CHL	ND
40	Z	609	CHL	NA
40	Z	609	CHL	NC
40	Z	609	CHL	C8
40	Z	609	CHL	ND
40	3	611	CHL	NA
40	3	611	CHL	NC
40	3	611	CHL	C8
40	3	611	CHL	ND
40	7	610	CHL	NA
40	7	610	CHL	NC
40	7	610	CHL	ND
40	8	610	CHL	NA
40	8	610	CHL	NC
40	8	610	CHL	C8
40	8	610	CHL	ND
40	8	613	CHL	NC
40	8	613	CHL	NA
40	8	613	CHL	C3A
40	8	613	CHL	ND
40	8	613	CHL	C8
40	4	610	CHL	NA
40	4	610	CHL	NC

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
40	4	610	CHL	C3A
40	4	610	CHL	ND
40	4	611	CHL	NA
40	4	611	CHL	NC
40	4	611	CHL	ND
40	4	613	CHL	NA
40	4	613	CHL	NC
40	4	613	CHL	C8
40	4	613	CHL	ND
40	4	617	CHL	NA
40	4	617	CHL	NC
40	4	617	CHL	ND
40	5	610	CHL	NA
40	5	610	CHL	NC
40	5	610	CHL	C8
40	5	610	CHL	ND
40	5	611	CHL	NA
40	5	611	CHL	NC
40	5	611	CHL	ND
40	5	617	CHL	NA
40	5	617	CHL	NC
40	5	617	CHL	ND
40	6	610	CHL	NA
40	6	610	CHL	NC
40	6	610	CHL	C8
40	6	610	CHL	ND
40	6	611	CHL	NA
40	6	611	CHL	NC
40	6	611	CHL	ND
40	6	613	CHL	NA
40	6	613	CHL	NC
40	6	613	CHL	C8
40	6	613	CHL	ND
40	6	617	CHL	NA
40	6	617	CHL	NC
40	6	617	CHL	ND
40	2	609	CHL	NA
40	2	609	CHL	NC
40	2	609	CHL	ND
40	2	610	CHL	NA
40	2	610	CHL	NC
40	2	610	CHL	C3A

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Mol	Chain	Res	Type	Atom
40	2	610	CHL	ND
40	2	613	CHL	NA
40	2	613	CHL	NC
40	2	613	CHL	ND
40	9	610	CHL	NA
40	9	610	CHL	NC
40	9	610	CHL	C8
40	9	610	CHL	ND
40	9	613	CHL	NA
40	9	613	CHL	NC
40	9	613	CHL	ND
42	Z	504	QTB	C11

All (3914) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	1012	CLA	CBD-CGD-O2D-CED
22	A	1012	CLA	C2-C3-C5-C6
22	A	1012	CLA	C4-C3-C5-C6
22	A	1102	CLA	CBA-CGA-O2A-C1
22	A	1102	CLA	O1A-CGA-O2A-C1
22	A	1103	CLA	C1A-C2A-CAA-CBA
22	A	1103	CLA	C3A-C2A-CAA-CBA
22	A	1103	CLA	CHA-CBD-CGD-O1D
22	A	1103	CLA	CHA-CBD-CGD-O2D
22	A	1105	CLA	C1A-C2A-CAA-CBA
22	A	1105	CLA	C3A-C2A-CAA-CBA
22	A	1106	CLA	C3A-C2A-CAA-CBA
22	A	1108	CLA	C1A-C2A-CAA-CBA
22	A	1108	CLA	C2-C1-O2A-CGA
22	A	1108	CLA	CHA-CBD-CGD-O1D
22	A	1108	CLA	CHA-CBD-CGD-O2D
22	A	1109	CLA	C1A-C2A-CAA-CBA
22	A	1111	CLA	CHA-CBD-CGD-O1D
22	A	1111	CLA	C2-C3-C5-C6
22	A	1111	CLA	C4-C3-C5-C6
22	A	1114	CLA	CBD-CGD-O2D-CED
22	A	1116	CLA	C1A-C2A-CAA-CBA
22	A	1116	CLA	C3A-C2A-CAA-CBA
22	A	1116	CLA	C2-C1-O2A-CGA
22	A	1116	CLA	CBD-CGD-O2D-CED
22	A	1117	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	A	1117	CLA	C3A-C2A-CAA-CBA
22	A	1117	CLA	CHA-CBD-CGD-O1D
22	A	1117	CLA	CHA-CBD-CGD-O2D
22	A	1119	CLA	CHA-CBD-CGD-O1D
22	A	1119	CLA	CHA-CBD-CGD-O2D
22	A	1120	CLA	C1A-C2A-CAA-CBA
22	A	1120	CLA	C3A-C2A-CAA-CBA
22	A	1121	CLA	C1A-C2A-CAA-CBA
22	A	1121	CLA	C2A-CAA-CBA-CGA
22	A	1121	CLA	CBD-CGD-O2D-CED
22	A	1122	CLA	CHA-CBD-CGD-O1D
22	A	1122	CLA	CHA-CBD-CGD-O2D
22	A	1122	CLA	C4-C3-C5-C6
22	A	1123	CLA	C1A-C2A-CAA-CBA
22	A	1123	CLA	C3A-C2A-CAA-CBA
22	A	1123	CLA	C2-C1-O2A-CGA
22	A	1123	CLA	CBD-CGD-O2D-CED
22	A	1125	CLA	C1A-C2A-CAA-CBA
22	A	1125	CLA	CHA-CBD-CGD-O1D
22	A	1125	CLA	CHA-CBD-CGD-O2D
22	A	1126	CLA	CHA-CBD-CGD-O1D
22	A	1126	CLA	CHA-CBD-CGD-O2D
22	A	1128	CLA	CBD-CGD-O2D-CED
22	A	1129	CLA	C1A-C2A-CAA-CBA
22	A	1129	CLA	C3A-C2A-CAA-CBA
22	A	1129	CLA	C2-C1-O2A-CGA
22	A	1130	CLA	C1A-C2A-CAA-CBA
22	A	1132	CLA	CBD-CGD-O2D-CED
22	A	1135	CLA	C1A-C2A-CAA-CBA
22	A	1136	CLA	C1A-C2A-CAA-CBA
22	A	1136	CLA	C3A-C2A-CAA-CBA
22	A	1136	CLA	C2-C3-C5-C6
22	A	1136	CLA	C4-C3-C5-C6
22	A	1136	CLA	C14-C13-C15-C16
22	A	1137	CLA	C2-C1-O2A-CGA
22	A	1137	CLA	CHA-CBD-CGD-O1D
22	A	1137	CLA	CHA-CBD-CGD-O2D
22	A	1138	CLA	C1A-C2A-CAA-CBA
22	A	1138	CLA	C3A-C2A-CAA-CBA
22	A	1139	CLA	C1A-C2A-CAA-CBA
22	A	1139	CLA	C3A-C2A-CAA-CBA
22	A	1139	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	A	1139	CLA	C4-C3-C5-C6
22	A	1141	CLA	CHA-CBD-CGD-O1D
22	A	1141	CLA	CHA-CBD-CGD-O2D
22	A	1140	CLA	CBD-CGD-O2D-CED
22	A	1101	CLA	C1A-C2A-CAA-CBA
22	A	1101	CLA	C2-C1-O2A-CGA
22	A	1101	CLA	C11-C10-C8-C9
22	B	1022	CLA	CBD-CGD-O2D-CED
22	B	1237	CLA	C2-C1-O2A-CGA
22	B	1021	CLA	CHA-CBD-CGD-O1D
22	B	1021	CLA	CHA-CBD-CGD-O2D
22	B	1021	CLA	CBD-CGD-O2D-CED
22	B	1023	CLA	C2-C1-O2A-CGA
22	B	1023	CLA	CHA-CBD-CGD-O1D
22	B	1023	CLA	CHA-CBD-CGD-O2D
22	B	1023	CLA	CBD-CGD-O2D-CED
22	B	1201	CLA	CBD-CGD-O2D-CED
22	B	1202	CLA	C1A-C2A-CAA-CBA
22	B	1202	CLA	C3A-C2A-CAA-CBA
22	B	1204	CLA	C1A-C2A-CAA-CBA
22	B	1205	CLA	C1A-C2A-CAA-CBA
22	B	1205	CLA	C3A-C2A-CAA-CBA
22	B	1206	CLA	C1A-C2A-CAA-CBA
22	B	1206	CLA	C3A-C2A-CAA-CBA
22	B	1207	CLA	CBD-CGD-O2D-CED
22	B	1208	CLA	C1A-C2A-CAA-CBA
22	B	1208	CLA	C3A-C2A-CAA-CBA
22	B	1208	CLA	CBD-CGD-O2D-CED
22	B	1209	CLA	C2-C1-O2A-CGA
22	B	1210	CLA	CHA-CBD-CGD-O1D
22	B	1210	CLA	CHA-CBD-CGD-O2D
22	B	1211	CLA	C2-C1-O2A-CGA
22	B	1211	CLA	CBD-CGD-O2D-CED
22	B	1212	CLA	C1A-C2A-CAA-CBA
22	B	1212	CLA	C2-C1-O2A-CGA
22	B	1213	CLA	CHA-CBD-CGD-O1D
22	B	1213	CLA	CHA-CBD-CGD-O2D
22	B	1213	CLA	CBD-CGD-O2D-CED
22	B	1214	CLA	C1A-C2A-CAA-CBA
22	B	1214	CLA	C3A-C2A-CAA-CBA
22	B	1214	CLA	C2-C1-O2A-CGA
22	B	1214	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	B	1215	CLA	C1A-C2A-CAA-CBA
22	B	1215	CLA	C3A-C2A-CAA-CBA
22	B	1215	CLA	C2-C3-C5-C6
22	B	1215	CLA	C4-C3-C5-C6
22	B	1216	CLA	C1A-C2A-CAA-CBA
22	B	1216	CLA	C3A-C2A-CAA-CBA
22	B	1216	CLA	CHA-CBD-CGD-O1D
22	B	1216	CLA	CHA-CBD-CGD-O2D
22	B	1217	CLA	C1A-C2A-CAA-CBA
22	B	1217	CLA	C3A-C2A-CAA-CBA
22	B	1217	CLA	CBD-CGD-O2D-CED
22	B	1219	CLA	C1A-C2A-CAA-CBA
22	B	1219	CLA	C3A-C2A-CAA-CBA
22	B	1219	CLA	CBD-CGD-O2D-CED
22	B	1220	CLA	C1A-C2A-CAA-CBA
22	B	1220	CLA	C3A-C2A-CAA-CBA
22	B	1220	CLA	CHA-CBD-CGD-O1D
22	B	1220	CLA	CHA-CBD-CGD-O2D
22	B	1223	CLA	C1A-C2A-CAA-CBA
22	B	1223	CLA	C3A-C2A-CAA-CBA
22	B	1223	CLA	CHA-CBD-CGD-O1D
22	B	1223	CLA	CHA-CBD-CGD-O2D
22	B	1224	CLA	C1A-C2A-CAA-CBA
22	B	1224	CLA	C3A-C2A-CAA-CBA
22	B	1224	CLA	C2-C1-O2A-CGA
22	B	1224	CLA	CHA-CBD-CGD-O1D
22	B	1224	CLA	CHA-CBD-CGD-O2D
22	B	1224	CLA	CBD-CGD-O2D-CED
22	B	1225	CLA	C1A-C2A-CAA-CBA
22	B	1225	CLA	C3A-C2A-CAA-CBA
22	B	1226	CLA	C1A-C2A-CAA-CBA
22	B	1226	CLA	C3A-C2A-CAA-CBA
22	B	1226	CLA	CBD-CGD-O2D-CED
22	B	1226	CLA	C2-C3-C5-C6
22	B	1226	CLA	C4-C3-C5-C6
22	B	1227	CLA	CHA-CBD-CGD-O1D
22	B	1227	CLA	CHA-CBD-CGD-O2D
22	B	1228	CLA	C2A-CAA-CBA-CGA
22	B	1228	CLA	C2-C1-O2A-CGA
22	B	1229	CLA	C2-C1-O2A-CGA
22	B	1231	CLA	C2-C1-O2A-CGA
22	B	1234	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	B	1234	CLA	C3A-C2A-CAA-CBA
22	B	1234	CLA	CBD-CGD-O2D-CED
22	B	1235	CLA	C1A-C2A-CAA-CBA
22	B	1235	CLA	C3A-C2A-CAA-CBA
22	B	1235	CLA	C2-C1-O2A-CGA
22	B	1235	CLA	C2-C3-C5-C6
22	B	1235	CLA	C4-C3-C5-C6
22	B	1236	CLA	C1A-C2A-CAA-CBA
22	B	1240	CLA	C3A-C2A-CAA-CBA
22	B	1240	CLA	C2A-CAA-CBA-CGA
22	B	1240	CLA	CHA-CBD-CGD-O1D
22	B	1240	CLA	CHA-CBD-CGD-O2D
22	B	1240	CLA	C2-C3-C5-C6
22	B	1240	CLA	C4-C3-C5-C6
22	B	1241	CLA	C1A-C2A-CAA-CBA
22	F	1301	CLA	C1A-C2A-CAA-CBA
22	F	1301	CLA	CAD-CBD-CGD-O1D
22	F	1301	CLA	CAD-CBD-CGD-O2D
22	F	1302	CLA	CBD-CGD-O2D-CED
22	G	1601	CLA	CHA-CBD-CGD-O1D
22	G	1601	CLA	CHA-CBD-CGD-O2D
22	G	1601	CLA	CBD-CGD-O2D-CED
22	G	1602	CLA	CBA-CGA-O2A-C1
22	J	1901	CLA	C1A-C2A-CAA-CBA
22	J	1901	CLA	CBD-CGD-O2D-CED
22	K	1401	CLA	CBA-CGA-O2A-C1
22	K	1402	CLA	C1A-C2A-CAA-CBA
22	K	1402	CLA	C3A-C2A-CAA-CBA
22	K	1403	CLA	CBD-CGD-O2D-CED
22	K	1404	CLA	CBD-CGD-O2D-CED
22	L	1502	CLA	C1A-C2A-CAA-CBA
22	L	1502	CLA	C3A-C2A-CAA-CBA
22	L	1502	CLA	CHA-CBD-CGD-O1D
22	L	1502	CLA	CHA-CBD-CGD-O2D
22	L	1503	CLA	C1A-C2A-CAA-CBA
22	1	601	CLA	C1A-C2A-CAA-CBA
22	1	601	CLA	C3A-C2A-CAA-CBA
22	1	602	CLA	CBD-CGD-O2D-CED
22	1	603	CLA	CHA-CBD-CGD-O1D
22	1	603	CLA	CHA-CBD-CGD-O2D
22	1	604	CLA	C1A-C2A-CAA-CBA
22	1	604	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	1	607	CLA	C1A-C2A-CAA-CBA
22	1	607	CLA	C3A-C2A-CAA-CBA
22	1	607	CLA	CHA-CBD-CGD-O1D
22	1	607	CLA	CHA-CBD-CGD-O2D
22	1	608	CLA	C3A-C2A-CAA-CBA
22	1	608	CLA	CHA-CBD-CGD-O1D
22	1	608	CLA	CHA-CBD-CGD-O2D
22	1	611	CLA	CHA-CBD-CGD-O1D
22	1	611	CLA	CHA-CBD-CGD-O2D
22	1	612	CLA	C1A-C2A-CAA-CBA
22	1	612	CLA	C3A-C2A-CAA-CBA
22	1	612	CLA	CHA-CBD-CGD-O1D
22	1	612	CLA	CHA-CBD-CGD-O2D
22	1	613	CLA	CBA-CGA-O2A-C1
22	1	613	CLA	CBD-CGD-O2D-CED
22	1	615	CLA	C2-C1-O2A-CGA
22	1	615	CLA	CHA-CBD-CGD-O1D
22	1	615	CLA	CHA-CBD-CGD-O2D
22	1	615	CLA	CBD-CGD-O2D-CED
22	Z	601	CLA	CHA-CBD-CGD-O1D
22	Z	601	CLA	CHA-CBD-CGD-O2D
22	Z	601	CLA	CBD-CGD-O2D-CED
22	Z	603	CLA	CHA-CBD-CGD-O1D
22	Z	603	CLA	CHA-CBD-CGD-O2D
22	Z	604	CLA	C3A-C2A-CAA-CBA
22	Z	606	CLA	CHA-CBD-CGD-O1D
22	Z	606	CLA	CHA-CBD-CGD-O2D
22	Z	607	CLA	CHA-CBD-CGD-O1D
22	Z	607	CLA	CHA-CBD-CGD-O2D
22	Z	608	CLA	CHA-CBD-CGD-O1D
22	Z	608	CLA	CHA-CBD-CGD-O2D
22	Z	611	CLA	CHA-CBD-CGD-O1D
22	Z	611	CLA	CHA-CBD-CGD-O2D
22	Z	615	CLA	CBA-CGA-O2A-C1
22	Z	615	CLA	CBD-CGD-O2D-CED
22	3	601	CLA	C1A-C2A-CAA-CBA
22	3	602	CLA	CBD-CGD-O2D-CED
22	3	603	CLA	CHA-CBD-CGD-O1D
22	3	603	CLA	CHA-CBD-CGD-O2D
22	3	605	CLA	CBD-CGD-O2D-CED
22	3	606	CLA	C3A-C2A-CAA-CBA
22	3	606	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	3	606	CLA	CHA-CBD-CGD-O2D
22	3	607	CLA	C2-C1-O2A-CGA
22	3	607	CLA	CBD-CGD-O2D-CED
22	3	608	CLA	CBD-CGD-O2D-CED
22	3	610	CLA	C2-C1-O2A-CGA
22	3	612	CLA	C3A-C2A-CAA-CBA
22	3	612	CLA	CBD-CGD-O2D-CED
22	3	613	CLA	CBD-CGD-O2D-CED
22	3	618	CLA	C1A-C2A-CAA-CBA
22	3	616	CLA	C2-C1-O2A-CGA
22	3	616	CLA	CBD-CGD-O2D-CED
22	7	601	CLA	C1A-C2A-CAA-CBA
22	7	602	CLA	CBD-CGD-O2D-CED
22	7	603	CLA	C1A-C2A-CAA-CBA
22	7	603	CLA	CHA-CBD-CGD-O1D
22	7	603	CLA	CHA-CBD-CGD-O2D
22	7	603	CLA	CBD-CGD-O2D-CED
22	7	604	CLA	C1A-C2A-CAA-CBA
22	7	605	CLA	CBA-CGA-O2A-C1
22	7	605	CLA	O1A-CGA-O2A-C1
22	7	606	CLA	C2-C1-O2A-CGA
22	7	606	CLA	CHA-CBD-CGD-O1D
22	7	606	CLA	CHA-CBD-CGD-O2D
22	7	607	CLA	CHA-CBD-CGD-O1D
22	7	607	CLA	CHA-CBD-CGD-O2D
22	7	608	CLA	CHA-CBD-CGD-O1D
22	7	608	CLA	CHA-CBD-CGD-O2D
22	7	612	CLA	C3A-C2A-CAA-CBA
22	7	612	CLA	CHA-CBD-CGD-O1D
22	7	612	CLA	CHA-CBD-CGD-O2D
22	7	613	CLA	C1A-C2A-CAA-CBA
22	7	613	CLA	C3A-C2A-CAA-CBA
22	7	613	CLA	CBD-CGD-O2D-CED
22	7	615	CLA	C3A-C2A-CAA-CBA
22	7	615	CLA	CBD-CGD-O2D-CED
22	7	616	CLA	CBD-CGD-O2D-CED
22	8	609	CLA	CHA-CBD-CGD-O1D
22	8	609	CLA	CHA-CBD-CGD-O2D
22	8	601	CLA	C1A-C2A-CAA-CBA
22	8	601	CLA	C3A-C2A-CAA-CBA
22	8	601	CLA	C2-C3-C5-C6
22	8	601	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	8	602	CLA	CBD-CGD-O2D-CED
22	8	603	CLA	C1A-C2A-CAA-CBA
22	8	603	CLA	CHA-CBD-CGD-O1D
22	8	603	CLA	CHA-CBD-CGD-O2D
22	8	603	CLA	CBD-CGD-O2D-CED
22	8	604	CLA	C1A-C2A-CAA-CBA
22	8	606	CLA	C1A-C2A-CAA-CBA
22	8	607	CLA	C1A-C2A-CAA-CBA
22	8	607	CLA	C3A-C2A-CAA-CBA
22	8	607	CLA	CHA-CBD-CGD-O1D
22	8	607	CLA	CHA-CBD-CGD-O2D
22	8	608	CLA	CHA-CBD-CGD-O1D
22	8	608	CLA	CHA-CBD-CGD-O2D
22	8	611	CLA	C2-C1-O2A-CGA
22	8	611	CLA	CBD-CGD-O2D-CED
22	8	612	CLA	C1A-C2A-CAA-CBA
22	8	612	CLA	C3A-C2A-CAA-CBA
22	8	612	CLA	CBA-CGA-O2A-C1
22	8	612	CLA	CHA-CBD-CGD-O1D
22	8	612	CLA	CHA-CBD-CGD-O2D
22	8	615	CLA	CBA-CGA-O2A-C1
22	8	615	CLA	CHA-CBD-CGD-O1D
22	8	615	CLA	CHA-CBD-CGD-O2D
22	4	601	CLA	C1A-C2A-CAA-CBA
22	4	601	CLA	C3A-C2A-CAA-CBA
22	4	602	CLA	C2-C1-O2A-CGA
22	4	602	CLA	C3-C5-C6-C7
22	4	603	CLA	C1A-C2A-CAA-CBA
22	4	603	CLA	C3A-C2A-CAA-CBA
22	4	604	CLA	C1A-C2A-CAA-CBA
22	4	604	CLA	C3A-C2A-CAA-CBA
22	4	605	CLA	CBD-CGD-O2D-CED
22	4	606	CLA	CHA-CBD-CGD-O1D
22	4	606	CLA	CHA-CBD-CGD-O2D
22	4	607	CLA	CHA-CBD-CGD-O1D
22	4	607	CLA	CBD-CGD-O2D-CED
22	4	612	CLA	C1A-C2A-CAA-CBA
22	4	612	CLA	C3A-C2A-CAA-CBA
22	4	612	CLA	CHA-CBD-CGD-O1D
22	4	612	CLA	CHA-CBD-CGD-O2D
22	4	612	CLA	CBD-CGD-O2D-CED
22	5	601	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	5	601	CLA	C3A-C2A-CAA-CBA
22	5	601	CLA	C2-C3-C5-C6
22	5	601	CLA	C4-C3-C5-C6
22	5	602	CLA	CBD-CGD-O2D-CED
22	5	603	CLA	CHA-CBD-CGD-O1D
22	5	603	CLA	CHA-CBD-CGD-O2D
22	5	603	CLA	CBD-CGD-O2D-CED
22	5	604	CLA	C1A-C2A-CAA-CBA
22	5	604	CLA	CHA-CBD-CGD-O1D
22	5	604	CLA	CHA-CBD-CGD-O2D
22	5	605	CLA	CHA-CBD-CGD-O1D
22	5	605	CLA	CHA-CBD-CGD-O2D
22	5	606	CLA	C2A-CAA-CBA-CGA
22	5	606	CLA	CHA-CBD-CGD-O1D
22	5	606	CLA	CHA-CBD-CGD-O2D
22	5	609	CLA	CHA-CBD-CGD-O1D
22	5	609	CLA	CHA-CBD-CGD-O2D
22	5	612	CLA	C2-C1-O2A-CGA
22	5	613	CLA	C2-C1-O2A-CGA
22	5	613	CLA	CBD-CGD-O2D-CED
22	5	618	CLA	C3A-C2A-CAA-CBA
22	5	618	CLA	CHA-CBD-CGD-O1D
22	5	618	CLA	CHA-CBD-CGD-O2D
22	5	622	CLA	CBD-CGD-O2D-CED
22	6	608	CLA	C1A-C2A-CAA-CBA
22	6	601	CLA	C1A-C2A-CAA-CBA
22	6	603	CLA	CHA-CBD-CGD-O1D
22	6	603	CLA	CHA-CBD-CGD-O2D
22	6	603	CLA	CBD-CGD-O2D-CED
22	6	604	CLA	C1A-C2A-CAA-CBA
22	6	605	CLA	C2-C1-O2A-CGA
22	6	606	CLA	C1A-C2A-CAA-CBA
22	6	606	CLA	CHA-CBD-CGD-O1D
22	6	606	CLA	CHA-CBD-CGD-O2D
22	6	606	CLA	CBD-CGD-O2D-CED
22	6	612	CLA	C3A-C2A-CAA-CBA
22	6	612	CLA	CHA-CBD-CGD-O1D
22	6	612	CLA	CHA-CBD-CGD-O2D
22	6	615	CLA	C1A-C2A-CAA-CBA
22	6	615	CLA	C3A-C2A-CAA-CBA
22	6	618	CLA	C1A-C2A-CAA-CBA
22	6	619	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	6	619	CLA	CBD-CGD-O2D-CED
22	2	602	CLA	CBA-CGA-O2A-C1
22	2	602	CLA	CBD-CGD-O2D-CED
22	2	603	CLA	C1A-C2A-CAA-CBA
22	2	603	CLA	C3A-C2A-CAA-CBA
22	2	603	CLA	CHA-CBD-CGD-O2D
22	2	603	CLA	CBD-CGD-O2D-CED
22	2	604	CLA	C1A-C2A-CAA-CBA
22	2	604	CLA	C3A-C2A-CAA-CBA
22	2	604	CLA	CHA-CBD-CGD-O1D
22	2	604	CLA	CHA-CBD-CGD-O2D
22	2	606	CLA	CBA-CGA-O2A-C1
22	2	606	CLA	CBD-CGD-O2D-CED
22	2	607	CLA	CHA-CBD-CGD-O1D
22	2	607	CLA	CHA-CBD-CGD-O2D
22	2	608	CLA	CBD-CGD-O2D-CED
22	2	612	CLA	CBD-CGD-O2D-CED
22	2	615	CLA	CBA-CGA-O2A-C1
22	9	601	CLA	C1A-C2A-CAA-CBA
22	9	601	CLA	CHA-CBD-CGD-O1D
22	9	601	CLA	CHA-CBD-CGD-O2D
22	9	603	CLA	C1A-C2A-CAA-CBA
22	9	603	CLA	CBD-CGD-O2D-CED
22	9	604	CLA	C1A-C2A-CAA-CBA
22	9	606	CLA	C1A-C2A-CAA-CBA
22	9	606	CLA	C2-C1-O2A-CGA
22	9	606	CLA	CHA-CBD-CGD-O1D
22	9	606	CLA	CHA-CBD-CGD-O2D
22	9	607	CLA	CHA-CBD-CGD-O1D
22	9	607	CLA	CHA-CBD-CGD-O2D
22	9	608	CLA	CBD-CGD-O2D-CED
22	9	609	CLA	CBA-CGA-O2A-C1
22	9	609	CLA	CHA-CBD-CGD-O1D
25	A	4001	BCR	C11-C10-C9-C8
25	A	4001	BCR	C11-C10-C9-C34
25	A	4001	BCR	C10-C11-C12-C13
25	A	4001	BCR	C11-C12-C13-C14
25	A	4001	BCR	C11-C12-C13-C35
25	A	4002	BCR	C7-C8-C9-C10
25	A	4002	BCR	C7-C8-C9-C34
25	A	4002	BCR	C11-C10-C9-C8
25	A	4002	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
25	A	4002	BCR	C10-C11-C12-C13
25	A	4003	BCR	C5-C6-C7-C8
25	A	4003	BCR	C7-C8-C9-C10
25	A	4003	BCR	C7-C8-C9-C34
25	A	4004	BCR	C7-C8-C9-C10
25	A	4004	BCR	C7-C8-C9-C34
25	A	4004	BCR	C11-C10-C9-C8
25	A	4004	BCR	C11-C10-C9-C34
25	A	4004	BCR	C23-C24-C25-C26
25	A	4005	BCR	C7-C8-C9-C10
25	A	4005	BCR	C7-C8-C9-C34
25	A	4005	BCR	C11-C10-C9-C8
25	A	4005	BCR	C11-C10-C9-C34
25	A	4005	BCR	C36-C18-C19-C20
25	A	4005	BCR	C21-C22-C23-C24
25	A	4005	BCR	C37-C22-C23-C24
25	B	4001	BCR	C1-C6-C7-C8
25	B	4001	BCR	C11-C10-C9-C8
25	B	4001	BCR	C11-C10-C9-C34
25	B	4001	BCR	C17-C18-C19-C20
25	B	4001	BCR	C36-C18-C19-C20
25	B	4001	BCR	C21-C22-C23-C24
25	B	4001	BCR	C37-C22-C23-C24
25	B	4001	BCR	C23-C24-C25-C30
25	B	4002	BCR	C7-C8-C9-C34
25	B	4002	BCR	C11-C10-C9-C8
25	B	4002	BCR	C11-C10-C9-C34
25	B	4002	BCR	C10-C11-C12-C13
25	B	4002	BCR	C36-C18-C19-C20
25	B	4002	BCR	C21-C22-C23-C24
25	B	4002	BCR	C37-C22-C23-C24
25	B	4004	BCR	C7-C8-C9-C10
25	B	4004	BCR	C7-C8-C9-C34
25	B	4004	BCR	C11-C10-C9-C8
25	B	4004	BCR	C11-C10-C9-C34
25	B	4004	BCR	C10-C11-C12-C13
25	B	4004	BCR	C23-C24-C25-C30
25	B	4005	BCR	C11-C10-C9-C8
25	B	4005	BCR	C11-C10-C9-C34
25	B	4005	BCR	C10-C11-C12-C13
25	B	4005	BCR	C11-C12-C13-C14
25	B	4005	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
25	B	4007	BCR	C11-C10-C9-C8
25	B	4007	BCR	C11-C10-C9-C34
25	B	4007	BCR	C9-C10-C11-C12
25	B	4007	BCR	C10-C11-C12-C13
25	B	4006	BCR	C10-C11-C12-C13
25	G	4001	BCR	C7-C8-C9-C10
25	G	4001	BCR	C7-C8-C9-C34
25	G	4001	BCR	C11-C10-C9-C8
25	G	4001	BCR	C11-C10-C9-C34
25	G	4001	BCR	C10-C11-C12-C13
25	I	4001	BCR	C11-C10-C9-C8
25	I	4001	BCR	C11-C10-C9-C34
25	I	4001	BCR	C10-C11-C12-C13
25	I	4001	BCR	C17-C18-C19-C20
25	I	4001	BCR	C36-C18-C19-C20
25	J	4001	BCR	C7-C8-C9-C10
25	J	4001	BCR	C7-C8-C9-C34
25	J	4001	BCR	C11-C10-C9-C8
25	J	4001	BCR	C11-C10-C9-C34
25	J	4001	BCR	C10-C11-C12-C13
25	J	4001	BCR	C11-C12-C13-C14
25	J	4001	BCR	C11-C12-C13-C35
25	J	4001	BCR	C17-C18-C19-C20
25	J	4001	BCR	C36-C18-C19-C20
25	J	4001	BCR	C21-C22-C23-C24
25	J	4001	BCR	C37-C22-C23-C24
25	K	4001	BCR	C7-C8-C9-C34
25	K	4001	BCR	C11-C10-C9-C8
25	K	4001	BCR	C11-C10-C9-C34
25	K	4001	BCR	C10-C11-C12-C13
25	K	4001	BCR	C21-C22-C23-C24
25	K	4001	BCR	C37-C22-C23-C24
25	K	4001	BCR	C23-C24-C25-C26
25	K	4001	BCR	C23-C24-C25-C30
25	K	4002	BCR	C11-C10-C9-C8
25	K	4002	BCR	C11-C10-C9-C34
25	K	4002	BCR	C10-C11-C12-C13
25	L	4001	BCR	C7-C8-C9-C10
25	L	4001	BCR	C7-C8-C9-C34
25	L	4001	BCR	C11-C10-C9-C8
25	L	4001	BCR	C11-C10-C9-C34
25	L	4001	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
25	L	4001	BCR	C23-C24-C25-C26
25	L	4001	BCR	C23-C24-C25-C30
25	L	4002	BCR	C11-C10-C9-C8
25	L	4002	BCR	C11-C10-C9-C34
25	L	4002	BCR	C23-C24-C25-C30
25	3	503	BCR	C5-C6-C7-C8
25	3	503	BCR	C7-C8-C9-C10
25	3	503	BCR	C7-C8-C9-C34
25	3	503	BCR	C11-C10-C9-C8
25	3	503	BCR	C11-C10-C9-C34
25	3	503	BCR	C23-C24-C25-C30
25	3	504	BCR	C7-C8-C9-C10
25	3	504	BCR	C7-C8-C9-C34
25	3	504	BCR	C11-C10-C9-C8
25	3	504	BCR	C11-C10-C9-C34
25	3	504	BCR	C21-C22-C23-C24
25	3	504	BCR	C37-C22-C23-C24
25	3	505	BCR	C7-C8-C9-C10
25	3	505	BCR	C7-C8-C9-C34
25	3	505	BCR	C11-C10-C9-C8
25	3	505	BCR	C11-C10-C9-C34
25	3	505	BCR	C10-C11-C12-C13
25	3	506	BCR	C7-C8-C9-C10
25	3	506	BCR	C7-C8-C9-C34
25	3	506	BCR	C11-C10-C9-C8
25	3	506	BCR	C11-C10-C9-C34
25	3	506	BCR	C10-C11-C12-C13
25	3	506	BCR	C21-C22-C23-C24
25	3	506	BCR	C37-C22-C23-C24
25	3	506	BCR	C23-C24-C25-C26
25	3	506	BCR	C23-C24-C25-C30
25	7	503	BCR	C11-C10-C9-C8
25	7	503	BCR	C11-C10-C9-C34
25	7	503	BCR	C10-C11-C12-C13
25	7	503	BCR	C23-C24-C25-C26
25	7	503	BCR	C23-C24-C25-C30
25	7	504	BCR	C11-C10-C9-C8
25	7	504	BCR	C11-C10-C9-C34
25	7	504	BCR	C9-C10-C11-C12
25	7	504	BCR	C10-C11-C12-C13
25	7	504	BCR	C21-C22-C23-C24
25	7	504	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
25	7	504	BCR	C23-C24-C25-C30
25	8	503	BCR	C5-C6-C7-C8
25	8	503	BCR	C7-C8-C9-C34
25	8	503	BCR	C11-C10-C9-C8
25	8	503	BCR	C11-C10-C9-C34
25	8	503	BCR	C10-C11-C12-C13
25	4	503	BCR	C11-C10-C9-C8
25	4	503	BCR	C11-C10-C9-C34
25	4	503	BCR	C10-C11-C12-C13
25	4	503	BCR	C21-C22-C23-C24
25	4	503	BCR	C37-C22-C23-C24
25	4	503	BCR	C23-C24-C25-C26
25	4	503	BCR	C23-C24-C25-C30
25	5	503	BCR	C11-C10-C9-C8
25	5	503	BCR	C11-C10-C9-C34
25	5	503	BCR	C9-C10-C11-C12
25	5	503	BCR	C10-C11-C12-C13
25	5	503	BCR	C23-C24-C25-C26
25	5	504	BCR	C10-C11-C12-C13
25	6	504	BCR	C7-C8-C9-C10
25	6	504	BCR	C7-C8-C9-C34
25	6	504	BCR	C9-C10-C11-C12
25	6	504	BCR	C11-C12-C13-C14
25	6	504	BCR	C11-C12-C13-C35
25	6	503	BCR	C7-C8-C9-C10
25	6	503	BCR	C7-C8-C9-C34
25	6	503	BCR	C11-C10-C9-C8
25	6	503	BCR	C11-C10-C9-C34
25	6	503	BCR	C10-C11-C12-C13
26	A	5001	LHG	C4-O6-P-O3
26	A	5001	LHG	C4-O6-P-O4
26	A	5001	LHG	C4-O6-P-O5
26	A	5001	LHG	O6-C4-C5-O7
26	A	5002	LHG	C3-O3-P-O6
26	A	5002	LHG	C4-O6-P-O4
26	B	5001	LHG	C4-O6-P-O3
26	B	5001	LHG	C4-O6-P-O4
26	B	5001	LHG	C4-O6-P-O5
26	B	5001	LHG	O9-C7-O7-C5
26	B	5001	LHG	C8-C7-O7-C5
26	B	5002	LHG	C3-O3-P-O5
26	B	5002	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
26	B	5002	LHG	O9-C7-O7-C5
26	B	5006	LHG	C1-C2-C3-O3
26	B	5006	LHG	C3-O3-P-O5
26	B	5006	LHG	C4-O6-P-O4
26	B	5006	LHG	O9-C7-O7-C5
26	1	801	LHG	O1-C1-C2-C3
26	1	801	LHG	C3-O3-P-O5
26	Z	801	LHG	C1-C2-C3-O3
26	Z	801	LHG	C4-O6-P-O3
26	Z	801	LHG	C4-O6-P-O5
26	Z	801	LHG	C8-C7-O7-C5
26	3	801	LHG	C1-C2-C3-O3
26	3	801	LHG	C4-O6-P-O5
26	3	801	LHG	O9-C7-O7-C5
26	7	801	LHG	C3-O3-P-O5
26	7	801	LHG	C4-O6-P-O4
26	8	801	LHG	C1-C2-C3-O3
26	8	801	LHG	C4-O6-P-O3
26	4	801	LHG	O2-C2-C3-O3
26	4	801	LHG	C4-O6-P-O5
26	4	801	LHG	C8-C7-O7-C5
26	4	802	LHG	O1-C1-C2-C3
26	4	802	LHG	C1-C2-C3-O3
26	4	802	LHG	C3-O3-P-O4
26	4	802	LHG	C3-O3-P-O5
26	4	802	LHG	C3-O3-P-O6
26	4	802	LHG	C4-O6-P-O4
26	4	802	LHG	O7-C5-C6-O8
26	5	801	LHG	O1-C1-C2-C3
26	5	801	LHG	C1-C2-C3-O3
26	5	801	LHG	O2-C2-C3-O3
26	5	801	LHG	C3-O3-P-O5
26	5	801	LHG	C4-O6-P-O3
26	5	801	LHG	C4-O6-P-O4
26	5	801	LHG	C4-O6-P-O5
26	5	801	LHG	O7-C5-C6-O8
26	6	801	LHG	C1-C2-C3-O3
26	6	801	LHG	C3-O3-P-O5
26	6	801	LHG	C3-O3-P-O6
26	6	801	LHG	C4-O6-P-O5
26	6	801	LHG	O6-C4-C5-O7
26	6	801	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
26	2	801	LHG	C3-O3-P-O5
26	9	801	LHG	O1-C1-C2-C3
26	9	801	LHG	C1-C2-C3-O3
26	9	801	LHG	C3-O3-P-O5
26	9	801	LHG	C3-O3-P-O6
27	A	5004	NKP	CAG-CAH-CAI-OAJ
27	3	802	NKP	OAF-CAG-CAH-CAI
27	8	802	NKP	CAG-OAF-PAC-OAA
27	8	802	NKP	CAG-OAF-PAC-OAB
27	8	802	NKP	OAF-CAG-CAH-CAI
27	8	802	NKP	OBC-CAH-CAI-OAJ
28	A	5006	LMT	C2'-C1'-O1'-C1
28	A	5006	LMT	O5'-C1'-O1'-C1
28	B	5005	LMT	C2-C1-O1'-C1'
28	F	5001	LMT	C2-C1-O1'-C1'
28	8	805	LMT	C2-C1-O1'-C1'
28	9	803	LMT	O5'-C1'-O1'-C1
31	A	5003	LMG	C2-C1-O1-C7
31	A	5003	LMG	O6-C1-O1-C7
31	J	5001	LMG	C11-C10-O7-C8
32	A	5005	DGA	CG1-CG2-CG3-OXT
32	A	5005	DGA	OG2-CG2-CG3-OXT
32	9	802	DGA	CG1-CG2-CG3-OXT
32	9	802	DGA	OG2-CG2-CG3-OXT
33	B	5003	DGD	O1B-C1B-O2G-C2G
37	J	4002	C7Z	C31-C32-C33-C40
37	5	505	C7Z	C21-C26-C27-C28
37	5	505	C7Z	C11-C12-C13-C20
37	5	505	C7Z	C11-C12-C13-C14
37	5	505	C7Z	C27-C28-C29-C30
37	5	505	C7Z	C27-C28-C29-C39
38	K	5001	SPH	C1-C2-C3-O3
38	K	5001	SPH	C1-C2-C3-C4
38	K	5001	SPH	N2-C2-C3-O3
38	K	5001	SPH	N2-C2-C3-C4
38	7	803	SPH	C1-C2-C3-O3
38	7	803	SPH	C1-C2-C3-C4
38	7	803	SPH	N2-C2-C3-O3
38	7	803	SPH	N2-C2-C3-C4
38	7	803	SPH	C2-C3-C4-C5
38	7	803	SPH	O3-C3-C4-C5
39	Z	503	LUT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
39	Z	503	LUT	C27-C28-C29-C39
39	7	502	LUT	C25-C26-C27-C28
39	8	502	LUT	C25-C26-C27-C28
39	4	501	LUT	C25-C26-C27-C28
39	5	501	LUT	C21-C26-C27-C28
39	2	501	LUT	C21-C26-C27-C28
39	2	502	LUT	C7-C8-C9-C10
39	2	502	LUT	C7-C8-C9-C19
39	2	502	LUT	C25-C26-C27-C28
39	2	503	LUT	C7-C8-C9-C10
39	2	503	LUT	C7-C8-C9-C19
39	2	503	LUT	C21-C26-C27-C28
39	2	503	LUT	C25-C26-C27-C28
40	1	610	CHL	C2A-CAA-CBA-CGA
40	Z	609	CHL	C1A-C2A-CAA-CBA
40	7	610	CHL	C1A-C2A-CAA-CBA
40	8	613	CHL	C1A-C2A-CAA-CBA
40	4	610	CHL	C2A-CAA-CBA-CGA
40	5	611	CHL	C1A-C2A-CAA-CBA
40	6	610	CHL	CHA-CBD-CGD-O1D
40	6	611	CHL	C1A-C2A-CAA-CBA
40	6	611	CHL	C3A-C2A-CAA-CBA
40	6	617	CHL	CHA-CBD-CGD-O1D
40	6	617	CHL	CHA-CBD-CGD-O2D
40	2	609	CHL	CHA-CBD-CGD-O1D
40	2	609	CHL	CHA-CBD-CGD-O2D
40	2	613	CHL	C1A-C2A-CAA-CBA
40	2	613	CHL	C3A-C2A-CAA-CBA
40	2	613	CHL	CHA-CBD-CGD-O1D
40	2	613	CHL	CHA-CBD-CGD-O2D
41	1	802	SQD	C8-C7-O47-C45
41	2	803	SQD	C2-C1-O6-C44
41	2	803	SQD	O5-C1-O6-C44
41	2	803	SQD	C5-C6-S-O9
42	Z	504	QTB	C01-C02-C09-C10
42	Z	504	QTB	C03-C02-C09-C10
42	Z	504	QTB	C04-C05-C06-C08
42	Z	504	QTB	C04-C05-C06-O07
42	Z	504	QTB	C09-C10-C11-C17
43	8	806	3PH	C1-O11-P-O13
43	8	806	3PH	C1-O11-P-O14
43	8	806	3PH	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
43	8	806	3PH	O22-C21-O21-C2
43	8	806	3PH	C22-C21-O21-C2
43	5	802	3PH	O11-C1-C2-O21
43	5	802	3PH	O22-C21-O21-C2
43	5	802	3PH	C22-C21-O21-C2
43	6	802	3PH	O22-C21-O21-C2
43	6	802	3PH	C22-C21-O21-C2
43	2	802	3PH	C1-O11-P-O13
43	2	802	3PH	C1-O11-P-O14
43	2	802	3PH	C1-O11-P-O12
43	2	802	3PH	O32-C31-O31-C3
45	8	803	LPX	O1-C3-C4-O5
45	8	803	LPX	C3-O1-P1-O3
45	8	803	LPX	C1-O2-P1-O1
45	8	803	LPX	C1-O2-P1-O3
45	8	803	LPX	C1-O2-P1-O4
22	A	1138	CLA	O1D-CGD-O2D-CED
22	A	1140	CLA	O1D-CGD-O2D-CED
22	K	1402	CLA	O1D-CGD-O2D-CED
22	L	1503	CLA	O1D-CGD-O2D-CED
22	1	603	CLA	O1D-CGD-O2D-CED
22	5	605	CLA	O1D-CGD-O2D-CED
22	6	605	CLA	O1D-CGD-O2D-CED
22	B	1021	CLA	O1D-CGD-O2D-CED
22	B	1023	CLA	O1D-CGD-O2D-CED
22	1	612	CLA	O1D-CGD-O2D-CED
22	Z	603	CLA	O1D-CGD-O2D-CED
22	Z	612	CLA	O1D-CGD-O2D-CED
22	7	605	CLA	O1D-CGD-O2D-CED
22	5	615	CLA	O1D-CGD-O2D-CED
22	6	619	CLA	O1D-CGD-O2D-CED
22	A	1109	CLA	CBD-CGD-O2D-CED
22	A	1115	CLA	CBD-CGD-O2D-CED
22	A	1119	CLA	CBD-CGD-O2D-CED
22	A	1126	CLA	CBD-CGD-O2D-CED
22	A	1131	CLA	CBD-CGD-O2D-CED
22	A	1138	CLA	CBD-CGD-O2D-CED
22	A	1139	CLA	CBD-CGD-O2D-CED
22	A	1141	CLA	CBD-CGD-O2D-CED
22	B	1203	CLA	CBD-CGD-O2D-CED
22	B	1205	CLA	CBD-CGD-O2D-CED
22	B	1206	CLA	CBD-CGD-O2D-CED

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
22	B	1216	CLA	CBD-CGD-O2D-CED
22	B	1218	CLA	CBD-CGD-O2D-CED
22	B	1232	CLA	CBD-CGD-O2D-CED
22	B	1236	CLA	CBD-CGD-O2D-CED
22	B	1239	CLA	CBD-CGD-O2D-CED
22	B	1241	CLA	CBD-CGD-O2D-CED
22	K	1402	CLA	CBD-CGD-O2D-CED
22	L	1502	CLA	CBD-CGD-O2D-CED
22	L	1503	CLA	CBD-CGD-O2D-CED
22	1	603	CLA	CBD-CGD-O2D-CED
22	1	605	CLA	CBD-CGD-O2D-CED
22	1	606	CLA	CBD-CGD-O2D-CED
22	1	611	CLA	CBD-CGD-O2D-CED
22	1	612	CLA	CBD-CGD-O2D-CED
22	Z	602	CLA	CBD-CGD-O2D-CED
22	Z	603	CLA	CBD-CGD-O2D-CED
22	Z	605	CLA	CBD-CGD-O2D-CED
22	Z	607	CLA	CBD-CGD-O2D-CED
22	Z	611	CLA	CBD-CGD-O2D-CED
22	Z	612	CLA	CBD-CGD-O2D-CED
22	3	603	CLA	CBD-CGD-O2D-CED
22	3	606	CLA	CBD-CGD-O2D-CED
22	3	618	CLA	CBD-CGD-O2D-CED
22	7	605	CLA	CBD-CGD-O2D-CED
22	7	606	CLA	CBD-CGD-O2D-CED
22	7	611	CLA	CBD-CGD-O2D-CED
22	8	605	CLA	CBD-CGD-O2D-CED
22	8	606	CLA	CBD-CGD-O2D-CED
22	8	615	CLA	CBD-CGD-O2D-CED
22	4	602	CLA	CBD-CGD-O2D-CED
22	4	603	CLA	CBD-CGD-O2D-CED
22	4	606	CLA	CBD-CGD-O2D-CED
22	4	608	CLA	CBD-CGD-O2D-CED
22	4	615	CLA	CBD-CGD-O2D-CED
22	5	605	CLA	CBD-CGD-O2D-CED
22	5	606	CLA	CBD-CGD-O2D-CED
22	5	608	CLA	CBD-CGD-O2D-CED
22	5	609	CLA	CBD-CGD-O2D-CED
22	5	615	CLA	CBD-CGD-O2D-CED
22	6	608	CLA	CBD-CGD-O2D-CED
22	6	602	CLA	CBD-CGD-O2D-CED
22	6	605	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	6	612	CLA	CBD-CGD-O2D-CED
22	6	618	CLA	CBD-CGD-O2D-CED
22	2	601	CLA	CBD-CGD-O2D-CED
22	2	605	CLA	CBD-CGD-O2D-CED
22	2	607	CLA	CBD-CGD-O2D-CED
22	9	602	CLA	CBD-CGD-O2D-CED
22	9	605	CLA	CBD-CGD-O2D-CED
22	9	609	CLA	CBD-CGD-O2D-CED
22	A	1113	CLA	O1A-CGA-O2A-C1
22	A	1133	CLA	O1A-CGA-O2A-C1
22	B	1207	CLA	O1A-CGA-O2A-C1
22	B	1222	CLA	O1A-CGA-O2A-C1
22	1	615	CLA	O1A-CGA-O2A-C1
22	Z	612	CLA	O1A-CGA-O2A-C1
22	4	606	CLA	O1A-CGA-O2A-C1
22	5	605	CLA	O1A-CGA-O2A-C1
22	K	1401	CLA	O1A-CGA-O2A-C1
22	Z	615	CLA	O1A-CGA-O2A-C1
22	8	612	CLA	O1A-CGA-O2A-C1
22	8	615	CLA	O1A-CGA-O2A-C1
22	2	606	CLA	O1A-CGA-O2A-C1
22	2	615	CLA	O1A-CGA-O2A-C1
22	A	1114	CLA	O1D-CGD-O2D-CED
22	A	1126	CLA	O1D-CGD-O2D-CED
22	A	1132	CLA	O1D-CGD-O2D-CED
22	B	1207	CLA	O1D-CGD-O2D-CED
22	B	1213	CLA	O1D-CGD-O2D-CED
22	B	1232	CLA	O1D-CGD-O2D-CED
22	F	1302	CLA	O1D-CGD-O2D-CED
22	Z	611	CLA	O1D-CGD-O2D-CED
22	3	606	CLA	O1D-CGD-O2D-CED
22	3	607	CLA	O1D-CGD-O2D-CED
22	3	608	CLA	O1D-CGD-O2D-CED
22	3	616	CLA	O1D-CGD-O2D-CED
22	7	606	CLA	O1D-CGD-O2D-CED
22	8	611	CLA	O1D-CGD-O2D-CED
22	8	615	CLA	O1D-CGD-O2D-CED
22	4	608	CLA	O1D-CGD-O2D-CED
22	4	615	CLA	O1D-CGD-O2D-CED
22	5	603	CLA	O1D-CGD-O2D-CED
22	9	602	CLA	O1D-CGD-O2D-CED
22	A	1012	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	A	1123	CLA	O1D-CGD-O2D-CED
22	A	1141	CLA	O1D-CGD-O2D-CED
22	B	1201	CLA	O1D-CGD-O2D-CED
22	B	1214	CLA	O1D-CGD-O2D-CED
22	B	1217	CLA	O1D-CGD-O2D-CED
22	B	1224	CLA	O1D-CGD-O2D-CED
22	B	1226	CLA	O1D-CGD-O2D-CED
22	B	1241	CLA	O1D-CGD-O2D-CED
22	J	1901	CLA	O1D-CGD-O2D-CED
22	K	1403	CLA	O1D-CGD-O2D-CED
22	1	602	CLA	O1D-CGD-O2D-CED
22	1	611	CLA	O1D-CGD-O2D-CED
22	1	613	CLA	O1D-CGD-O2D-CED
22	1	615	CLA	O1D-CGD-O2D-CED
22	Z	601	CLA	O1D-CGD-O2D-CED
22	Z	615	CLA	O1D-CGD-O2D-CED
22	3	612	CLA	O1D-CGD-O2D-CED
22	7	602	CLA	O1D-CGD-O2D-CED
22	7	603	CLA	O1D-CGD-O2D-CED
22	7	613	CLA	O1D-CGD-O2D-CED
22	7	616	CLA	O1D-CGD-O2D-CED
22	8	602	CLA	O1D-CGD-O2D-CED
22	8	603	CLA	O1D-CGD-O2D-CED
22	4	605	CLA	O1D-CGD-O2D-CED
22	4	606	CLA	O1D-CGD-O2D-CED
22	4	612	CLA	O1D-CGD-O2D-CED
22	5	602	CLA	O1D-CGD-O2D-CED
22	5	622	CLA	O1D-CGD-O2D-CED
22	6	603	CLA	O1D-CGD-O2D-CED
22	2	603	CLA	O1D-CGD-O2D-CED
22	2	608	CLA	O1D-CGD-O2D-CED
22	9	608	CLA	O1D-CGD-O2D-CED
22	A	1113	CLA	CBA-CGA-O2A-C1
22	Z	612	CLA	CBA-CGA-O2A-C1
22	4	606	CLA	CBA-CGA-O2A-C1
22	5	605	CLA	CBA-CGA-O2A-C1
22	A	1105	CLA	CBD-CGD-O2D-CED
22	A	1107	CLA	CBD-CGD-O2D-CED
22	A	1113	CLA	CBD-CGD-O2D-CED
22	A	1129	CLA	CBD-CGD-O2D-CED
22	A	1130	CLA	CBD-CGD-O2D-CED
22	A	1133	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	A	1136	CLA	CBD-CGD-O2D-CED
22	A	1137	CLA	CBD-CGD-O2D-CED
22	B	1237	CLA	CBD-CGD-O2D-CED
22	B	1212	CLA	CBD-CGD-O2D-CED
22	B	1215	CLA	CBD-CGD-O2D-CED
22	B	1223	CLA	CBD-CGD-O2D-CED
22	B	1228	CLA	CBD-CGD-O2D-CED
22	B	1229	CLA	CBD-CGD-O2D-CED
22	B	1230	CLA	CBD-CGD-O2D-CED
22	B	1231	CLA	CBD-CGD-O2D-CED
22	B	1235	CLA	CBD-CGD-O2D-CED
22	B	1238	CLA	CBD-CGD-O2D-CED
22	G	1602	CLA	CBD-CGD-O2D-CED
22	K	1401	CLA	CBD-CGD-O2D-CED
22	1	601	CLA	CBD-CGD-O2D-CED
22	1	604	CLA	CBD-CGD-O2D-CED
22	1	607	CLA	CBD-CGD-O2D-CED
22	Z	604	CLA	CBD-CGD-O2D-CED
22	Z	608	CLA	CBD-CGD-O2D-CED
22	3	601	CLA	CBD-CGD-O2D-CED
22	8	607	CLA	CBD-CGD-O2D-CED
22	4	601	CLA	CBD-CGD-O2D-CED
22	6	609	CLA	CBD-CGD-O2D-CED
22	2	604	CLA	CBD-CGD-O2D-CED
22	2	615	CLA	CBD-CGD-O2D-CED
22	9	606	CLA	CBD-CGD-O2D-CED
22	A	1104	CLA	O1A-CGA-O2A-C1
22	A	1114	CLA	O1A-CGA-O2A-C1
22	A	1101	CLA	O1A-CGA-O2A-C1
22	B	1202	CLA	O1A-CGA-O2A-C1
22	B	1206	CLA	O1A-CGA-O2A-C1
22	B	1218	CLA	O1A-CGA-O2A-C1
22	B	1220	CLA	O1A-CGA-O2A-C1
22	B	1228	CLA	O1A-CGA-O2A-C1
22	B	1240	CLA	O1A-CGA-O2A-C1
22	K	1404	CLA	O1A-CGA-O2A-C1
22	1	604	CLA	O1A-CGA-O2A-C1
22	1	605	CLA	O1A-CGA-O2A-C1
22	Z	604	CLA	O1A-CGA-O2A-C1
22	7	607	CLA	O1A-CGA-O2A-C1
22	4	604	CLA	O1A-CGA-O2A-C1
22	4	605	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	2	601	CLA	O1A-CGA-O2A-C1
22	2	605	CLA	O1A-CGA-O2A-C1
27	A	5004	NKP	OAE-CAK-OAJ-CAI
27	3	802	NKP	OAE-CAK-OAJ-CAI
31	A	5003	LMG	O10-C28-O8-C9
41	1	802	SQD	O10-C23-O48-C46
41	2	803	SQD	O10-C23-O48-C46
43	7	802	3PH	O32-C31-O31-C3
43	8	806	3PH	O32-C31-O31-C3
22	G	1602	CLA	O1A-CGA-O2A-C1
22	1	613	CLA	O1A-CGA-O2A-C1
22	A	1116	CLA	O1D-CGD-O2D-CED
22	A	1121	CLA	O1D-CGD-O2D-CED
22	B	1022	CLA	O1D-CGD-O2D-CED
22	B	1234	CLA	O1D-CGD-O2D-CED
22	K	1404	CLA	O1D-CGD-O2D-CED
22	3	602	CLA	O1D-CGD-O2D-CED
22	3	605	CLA	O1D-CGD-O2D-CED
22	3	613	CLA	O1D-CGD-O2D-CED
22	7	615	CLA	O1D-CGD-O2D-CED
22	4	607	CLA	O1D-CGD-O2D-CED
22	5	613	CLA	O1D-CGD-O2D-CED
22	6	606	CLA	O1D-CGD-O2D-CED
22	2	602	CLA	O1D-CGD-O2D-CED
22	2	612	CLA	O1D-CGD-O2D-CED
22	A	1115	CLA	O1D-CGD-O2D-CED
22	A	1128	CLA	O1D-CGD-O2D-CED
22	B	1203	CLA	O1D-CGD-O2D-CED
22	B	1208	CLA	O1D-CGD-O2D-CED
22	B	1219	CLA	O1D-CGD-O2D-CED
22	G	1601	CLA	O1D-CGD-O2D-CED
22	3	618	CLA	O1D-CGD-O2D-CED
22	7	611	CLA	O1D-CGD-O2D-CED
22	8	605	CLA	O1D-CGD-O2D-CED
22	2	606	CLA	O1D-CGD-O2D-CED
22	9	603	CLA	O1D-CGD-O2D-CED
22	A	1106	CLA	CBD-CGD-O2D-CED
22	B	1209	CLA	CBD-CGD-O2D-CED
22	Z	606	CLA	CBD-CGD-O2D-CED
22	7	608	CLA	CBD-CGD-O2D-CED
22	A	1131	CLA	O1D-CGD-O2D-CED
22	B	1211	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	Z	602	CLA	O1D-CGD-O2D-CED
22	4	603	CLA	O1D-CGD-O2D-CED
26	1	801	LHG	O9-C7-O7-C5
26	6	801	LHG	O9-C7-O7-C5
31	J	5001	LMG	O9-C10-O7-C8
41	1	802	SQD	O49-C7-O47-C45
43	7	802	3PH	O22-C21-O21-C2
22	3	618	CLA	CBA-CGA-O2A-C1
22	2	607	CLA	O1A-CGA-O2A-C1
22	5	609	CLA	O1D-CGD-O2D-CED
22	A	1115	CLA	C3-C5-C6-C7
22	A	1118	CLA	C3-C5-C6-C7
22	A	1124	CLA	C3-C5-C6-C7
22	A	1126	CLA	C3-C5-C6-C7
22	A	1131	CLA	C3-C5-C6-C7
22	A	1136	CLA	C3-C5-C6-C7
22	B	1237	CLA	C3-C5-C6-C7
22	B	1215	CLA	C3-C5-C6-C7
22	B	1224	CLA	C3-C5-C6-C7
22	B	1226	CLA	C3-C5-C6-C7
22	B	1240	CLA	C3-C5-C6-C7
22	B	1241	CLA	C3-C5-C6-C7
22	1	605	CLA	C3-C5-C6-C7
22	1	611	CLA	C3-C5-C6-C7
22	Z	605	CLA	C3-C5-C6-C7
22	Z	607	CLA	C3-C5-C6-C7
22	Z	608	CLA	C3-C5-C6-C7
22	3	607	CLA	C3-C5-C6-C7
22	3	610	CLA	C3-C5-C6-C7
22	3	616	CLA	C3-C5-C6-C7
22	7	605	CLA	C3-C5-C6-C7
22	7	606	CLA	C3-C5-C6-C7
22	7	615	CLA	C3-C5-C6-C7
22	7	616	CLA	C3-C5-C6-C7
22	8	605	CLA	C3-C5-C6-C7
22	8	607	CLA	C3-C5-C6-C7
22	8	608	CLA	C3-C5-C6-C7
22	5	603	CLA	C3-C5-C6-C7
22	A	1104	CLA	CBA-CGA-O2A-C1
22	A	1130	CLA	CBA-CGA-O2A-C1
22	A	1133	CLA	CBA-CGA-O2A-C1
22	A	1139	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	A	1101	CLA	CBA-CGA-O2A-C1
22	B	1202	CLA	CBA-CGA-O2A-C1
22	B	1207	CLA	CBA-CGA-O2A-C1
22	B	1218	CLA	CBA-CGA-O2A-C1
22	B	1222	CLA	CBA-CGA-O2A-C1
22	B	1227	CLA	CBA-CGA-O2A-C1
22	B	1228	CLA	CBA-CGA-O2A-C1
22	B	1240	CLA	CBA-CGA-O2A-C1
22	K	1404	CLA	CBA-CGA-O2A-C1
22	1	605	CLA	CBA-CGA-O2A-C1
22	1	615	CLA	CBA-CGA-O2A-C1
22	Z	603	CLA	CBA-CGA-O2A-C1
22	4	605	CLA	CBA-CGA-O2A-C1
22	5	607	CLA	CBA-CGA-O2A-C1
22	5	613	CLA	CBA-CGA-O2A-C1
22	2	605	CLA	CBA-CGA-O2A-C1
22	2	612	CLA	CBA-CGA-O2A-C1
27	A	5004	NKP	CAL-CAK-OAJ-CAI
31	A	5003	LMG	C29-C28-O8-C9
41	2	803	SQD	C24-C23-O48-C46
43	7	802	3PH	C32-C31-O31-C3
43	2	802	3PH	C32-C31-O31-C3
26	B	5006	LHG	C8-C7-O7-C5
26	1	801	LHG	C8-C7-O7-C5
33	B	5003	DGD	C2B-C1B-O2G-C2G
43	7	802	3PH	C22-C21-O21-C2
22	1	606	CLA	O1D-CGD-O2D-CED
22	4	602	CLA	O1D-CGD-O2D-CED
22	5	608	CLA	O1D-CGD-O2D-CED
22	6	602	CLA	O1D-CGD-O2D-CED
22	2	605	CLA	O1D-CGD-O2D-CED
22	9	605	CLA	O1D-CGD-O2D-CED
22	9	609	CLA	O1D-CGD-O2D-CED
22	A	1124	CLA	CBD-CGD-O2D-CED
22	F	1301	CLA	O1A-CGA-O2A-C1
22	Z	606	CLA	O1A-CGA-O2A-C1
22	5	618	CLA	O1A-CGA-O2A-C1
28	B	5005	LMT	O5'-C5'-C6'-O6'
22	3	618	CLA	O1A-CGA-O2A-C1
22	9	609	CLA	O1A-CGA-O2A-C1
22	B	1239	CLA	O1D-CGD-O2D-CED
22	2	607	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	6	602	CLA	C3-C5-C6-C7
22	A	1122	CLA	C2-C3-C5-C6
22	A	1103	CLA	CBD-CGD-O2D-CED
22	B	1202	CLA	CBD-CGD-O2D-CED
22	B	1240	CLA	CBD-CGD-O2D-CED
22	F	1301	CLA	CBD-CGD-O2D-CED
22	5	601	CLA	CBD-CGD-O2D-CED
22	A	1105	CLA	C2A-CAA-CBA-CGA
22	A	1106	CLA	C2A-CAA-CBA-CGA
22	A	1111	CLA	C2A-CAA-CBA-CGA
22	A	1119	CLA	C2A-CAA-CBA-CGA
22	A	1120	CLA	C2A-CAA-CBA-CGA
22	A	1122	CLA	C2A-CAA-CBA-CGA
22	A	1127	CLA	C2A-CAA-CBA-CGA
22	A	1131	CLA	C2A-CAA-CBA-CGA
22	A	1133	CLA	C2A-CAA-CBA-CGA
22	A	1141	CLA	C2A-CAA-CBA-CGA
22	B	1206	CLA	C2A-CAA-CBA-CGA
22	B	1207	CLA	C2A-CAA-CBA-CGA
22	B	1211	CLA	C2A-CAA-CBA-CGA
22	B	1214	CLA	C2A-CAA-CBA-CGA
22	B	1226	CLA	C2A-CAA-CBA-CGA
22	B	1238	CLA	C2A-CAA-CBA-CGA
22	Z	607	CLA	C2A-CAA-CBA-CGA
22	8	606	CLA	C2A-CAA-CBA-CGA
22	8	612	CLA	C2A-CAA-CBA-CGA
22	5	615	CLA	C2A-CAA-CBA-CGA
22	6	603	CLA	C2A-CAA-CBA-CGA
22	6	606	CLA	C2A-CAA-CBA-CGA
22	2	601	CLA	C2A-CAA-CBA-CGA
22	2	606	CLA	C2A-CAA-CBA-CGA
22	2	607	CLA	C2A-CAA-CBA-CGA
40	8	613	CHL	C2A-CAA-CBA-CGA
22	A	1123	CLA	O1A-CGA-O2A-C1
33	B	5003	DGD	C8A-C9A-CAA-CBA
33	B	5003	DGD	CBA-CCA-CDA-CEA
22	A	1127	CLA	C3-C5-C6-C7
22	A	1134	CLA	C3-C5-C6-C7
22	A	1140	CLA	C3-C5-C6-C7
22	B	1206	CLA	C3-C5-C6-C7
22	B	1236	CLA	C3-C5-C6-C7
22	1	607	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	7	607	CLA	C3-C5-C6-C7
22	5	609	CLA	C3-C5-C6-C7
22	A	1111	CLA	CBA-CGA-O2A-C1
22	A	1114	CLA	CBA-CGA-O2A-C1
22	A	1119	CLA	CBA-CGA-O2A-C1
22	A	1123	CLA	CBA-CGA-O2A-C1
22	A	1124	CLA	CBA-CGA-O2A-C1
22	A	1128	CLA	CBA-CGA-O2A-C1
22	A	1129	CLA	CBA-CGA-O2A-C1
22	B	1237	CLA	CBA-CGA-O2A-C1
22	B	1203	CLA	CBA-CGA-O2A-C1
22	B	1206	CLA	CBA-CGA-O2A-C1
22	B	1216	CLA	CBA-CGA-O2A-C1
22	B	1220	CLA	CBA-CGA-O2A-C1
22	B	1230	CLA	CBA-CGA-O2A-C1
22	B	1231	CLA	CBA-CGA-O2A-C1
22	1	601	CLA	CBA-CGA-O2A-C1
22	1	604	CLA	CBA-CGA-O2A-C1
22	Z	604	CLA	CBA-CGA-O2A-C1
22	Z	606	CLA	CBA-CGA-O2A-C1
22	Z	607	CLA	CBA-CGA-O2A-C1
22	7	606	CLA	CBA-CGA-O2A-C1
22	7	607	CLA	CBA-CGA-O2A-C1
22	8	601	CLA	CBA-CGA-O2A-C1
22	4	602	CLA	CBA-CGA-O2A-C1
22	4	604	CLA	CBA-CGA-O2A-C1
22	4	607	CLA	CBA-CGA-O2A-C1
22	5	601	CLA	CBA-CGA-O2A-C1
22	5	606	CLA	CBA-CGA-O2A-C1
22	6	607	CLA	CBA-CGA-O2A-C1
22	2	601	CLA	CBA-CGA-O2A-C1
22	9	607	CLA	CBA-CGA-O2A-C1
27	3	802	NKP	CAL-CAK-OAJ-CAI
32	A	5005	DGA	CA2-CA1-OG1-CG1
41	1	802	SQD	C24-C23-O48-C46
43	8	806	3PH	C32-C31-O31-C3
22	A	1119	CLA	O1D-CGD-O2D-CED
22	B	1216	CLA	O1D-CGD-O2D-CED
22	B	1218	CLA	O1D-CGD-O2D-CED
22	1	605	CLA	O1D-CGD-O2D-CED
22	Z	605	CLA	O1D-CGD-O2D-CED
22	8	606	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	A	1109	CLA	O1D-CGD-O2D-CED
22	B	1206	CLA	O1D-CGD-O2D-CED
22	2	607	CLA	O1D-CGD-O2D-CED
28	8	805	LMT	O5'-C5'-C6'-O6'
26	Z	801	LHG	O9-C7-O7-C5
26	4	801	LHG	O9-C7-O7-C5
28	9	803	LMT	C4B-C5B-C6B-O6B
22	A	1119	CLA	O1A-CGA-O2A-C1
22	A	1126	CLA	O1A-CGA-O2A-C1
22	A	1129	CLA	O1A-CGA-O2A-C1
22	A	1130	CLA	O1A-CGA-O2A-C1
22	A	1139	CLA	O1A-CGA-O2A-C1
22	B	1237	CLA	O1A-CGA-O2A-C1
22	B	1203	CLA	O1A-CGA-O2A-C1
22	B	1227	CLA	O1A-CGA-O2A-C1
22	1	601	CLA	O1A-CGA-O2A-C1
22	Z	603	CLA	O1A-CGA-O2A-C1
22	Z	607	CLA	O1A-CGA-O2A-C1
22	8	601	CLA	O1A-CGA-O2A-C1
22	4	601	CLA	O1A-CGA-O2A-C1
22	4	602	CLA	O1A-CGA-O2A-C1
22	4	608	CLA	O1A-CGA-O2A-C1
22	5	601	CLA	O1A-CGA-O2A-C1
22	5	606	CLA	O1A-CGA-O2A-C1
22	5	607	CLA	O1A-CGA-O2A-C1
22	2	612	CLA	O1A-CGA-O2A-C1
22	9	612	CLA	O1A-CGA-O2A-C1
32	A	5005	DGA	OA1-CA1-OG1-CG1
22	2	602	CLA	O1A-CGA-O2A-C1
22	B	1205	CLA	O1D-CGD-O2D-CED
22	Z	607	CLA	O1D-CGD-O2D-CED
22	5	606	CLA	O1D-CGD-O2D-CED
22	6	618	CLA	O1D-CGD-O2D-CED
25	K	4001	BCR	C19-C20-C21-C22
25	3	505	BCR	C9-C10-C11-C12
25	8	503	BCR	C13-C14-C15-C16
25	6	504	BCR	C13-C14-C15-C16
25	6	503	BCR	C9-C10-C11-C12
36	F	4001	RRX	C19-C20-C21-C22
37	J	4002	C7Z	C9-C10-C11-C12
37	5	505	C7Z	C13-C14-C15-C35
39	2	501	LUT	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
28	4	803	LMT	O5'-C5'-C6'-O6'
22	A	1104	CLA	CBD-CGD-O2D-CED
22	A	1110	CLA	CBD-CGD-O2D-CED
22	A	1117	CLA	CBD-CGD-O2D-CED
22	A	1101	CLA	CBD-CGD-O2D-CED
22	B	1221	CLA	CBD-CGD-O2D-CED
22	B	1227	CLA	CBD-CGD-O2D-CED
22	7	609	CLA	CBD-CGD-O2D-CED
22	7	607	CLA	CBD-CGD-O2D-CED
22	8	609	CLA	CBD-CGD-O2D-CED
22	6	615	CLA	CBD-CGD-O2D-CED
22	9	601	CLA	CBD-CGD-O2D-CED
22	9	604	CLA	CBD-CGD-O2D-CED
22	6	612	CLA	O1D-CGD-O2D-CED
22	2	601	CLA	O1D-CGD-O2D-CED
26	A	5001	LHG	O2-C2-C3-O3
26	Z	801	LHG	O2-C2-C3-O3
26	8	801	LHG	O2-C2-C3-O3
26	2	801	LHG	O2-C2-C3-O3
26	9	801	LHG	O2-C2-C3-O3
27	3	802	NKP	OAF-CAG-CAH-OBC
22	A	1120	CLA	C3-C5-C6-C7
22	B	1204	CLA	C3-C5-C6-C7
22	B	1209	CLA	C3-C5-C6-C7
22	B	1228	CLA	C3-C5-C6-C7
22	B	1229	CLA	C3-C5-C6-C7
22	L	1502	CLA	C3-C5-C6-C7
22	1	604	CLA	C3-C5-C6-C7
22	5	601	CLA	C3-C5-C6-C7
22	A	1117	CLA	CBA-CGA-O2A-C1
22	A	1121	CLA	CBA-CGA-O2A-C1
22	A	1126	CLA	CBA-CGA-O2A-C1
22	A	1137	CLA	CBA-CGA-O2A-C1
22	B	1215	CLA	CBA-CGA-O2A-C1
22	B	1236	CLA	CBA-CGA-O2A-C1
22	3	613	CLA	CBA-CGA-O2A-C1
22	8	606	CLA	CBA-CGA-O2A-C1
22	8	611	CLA	CBA-CGA-O2A-C1
22	6	608	CLA	CBA-CGA-O2A-C1
22	6	602	CLA	CBA-CGA-O2A-C1
22	A	1111	CLA	O1A-CGA-O2A-C1
22	A	1128	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	4	607	CLA	O1A-CGA-O2A-C1
22	5	613	CLA	O1A-CGA-O2A-C1
22	9	607	CLA	O1A-CGA-O2A-C1
22	B	1236	CLA	O1D-CGD-O2D-CED
22	6	608	CLA	O1D-CGD-O2D-CED
22	5	622	CLA	CBA-CGA-O2A-C1
22	7	601	CLA	CBD-CGD-O2D-CED
22	4	609	CLA	CBD-CGD-O2D-CED
22	5	607	CLA	CBD-CGD-O2D-CED
28	1	803	LMT	O5B-C5B-C6B-O6B
22	A	1137	CLA	O1A-CGA-O2A-C1
26	5	801	LHG	C28-C29-C30-C31
28	B	5005	LMT	C4'-C5'-C6'-O6'
22	A	1133	CLA	O1D-CGD-O2D-CED
22	3	603	CLA	O1D-CGD-O2D-CED
22	A	1013	CLA	CBD-CGD-O2D-CED
22	1	612	CLA	C3-C5-C6-C7
22	B	1210	CLA	CBA-CGA-O2A-C1
22	F	1301	CLA	CBA-CGA-O2A-C1
22	4	601	CLA	CBA-CGA-O2A-C1
22	4	608	CLA	CBA-CGA-O2A-C1
22	5	618	CLA	CBA-CGA-O2A-C1
22	9	612	CLA	CBA-CGA-O2A-C1
22	L	1502	CLA	O1D-CGD-O2D-CED
28	A	5006	LMT	O5'-C5'-C6'-O6'
22	A	1121	CLA	O1A-CGA-O2A-C1
22	A	1124	CLA	O1A-CGA-O2A-C1
22	B	1215	CLA	O1A-CGA-O2A-C1
22	B	1230	CLA	O1A-CGA-O2A-C1
22	3	613	CLA	O1A-CGA-O2A-C1
22	7	606	CLA	O1A-CGA-O2A-C1
22	8	606	CLA	O1A-CGA-O2A-C1
22	8	611	CLA	O1A-CGA-O2A-C1
22	6	602	CLA	O1A-CGA-O2A-C1
28	9	803	LMT	O5B-C5B-C6B-O6B
22	A	1115	CLA	C4-C3-C5-C6
28	4	803	LMT	C4B-C5B-C6B-O6B
22	A	1115	CLA	C2-C3-C5-C6
22	A	1112	CLA	CBD-CGD-O2D-CED
22	B	1241	CLA	C2A-CAA-CBA-CGA
22	A	1136	CLA	O1D-CGD-O2D-CED
22	A	1139	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	A	1117	CLA	O1A-CGA-O2A-C1
22	B	1210	CLA	O1A-CGA-O2A-C1
22	B	1216	CLA	O1A-CGA-O2A-C1
22	B	1231	CLA	O1A-CGA-O2A-C1
22	B	1236	CLA	O1A-CGA-O2A-C1
22	Z	605	CLA	O1A-CGA-O2A-C1
22	6	607	CLA	O1A-CGA-O2A-C1
22	A	1131	CLA	CBA-CGA-O2A-C1
22	B	1217	CLA	CBA-CGA-O2A-C1
22	Z	605	CLA	CBA-CGA-O2A-C1
22	6	606	CLA	CBA-CGA-O2A-C1
22	5	618	CLA	CBD-CGD-O2D-CED
22	4	601	CLA	O1D-CGD-O2D-CED
22	A	1105	CLA	O1D-CGD-O2D-CED
22	A	1137	CLA	O1D-CGD-O2D-CED
22	B	1237	CLA	O1D-CGD-O2D-CED
22	B	1229	CLA	O1D-CGD-O2D-CED
22	1	604	CLA	O1D-CGD-O2D-CED
22	2	604	CLA	O1D-CGD-O2D-CED
22	6	608	CLA	O1A-CGA-O2A-C1
32	9	802	DGA	CB2-CB1-OG2-CG2
22	B	1212	CLA	O1D-CGD-O2D-CED
22	B	1228	CLA	O1D-CGD-O2D-CED
22	B	1231	CLA	O1D-CGD-O2D-CED
22	G	1602	CLA	O1D-CGD-O2D-CED
22	1	601	CLA	O1D-CGD-O2D-CED
22	Z	604	CLA	O1D-CGD-O2D-CED
22	3	601	CLA	O1D-CGD-O2D-CED
26	7	801	LHG	C1-C2-C3-O3
28	8	805	LMT	O5B-C5B-C6B-O6B
22	B	1217	CLA	O1A-CGA-O2A-C1
22	6	606	CLA	O1A-CGA-O2A-C1
22	A	1104	CLA	C3-C5-C6-C7
22	B	1217	CLA	C3-C5-C6-C7
22	B	1218	CLA	C3-C5-C6-C7
22	Z	611	CLA	C3-C5-C6-C7
22	A	1106	CLA	CBA-CGA-O2A-C1
22	A	1108	CLA	CBA-CGA-O2A-C1
22	A	1116	CLA	CBA-CGA-O2A-C1
22	A	1120	CLA	CBA-CGA-O2A-C1
22	B	1211	CLA	CBA-CGA-O2A-C1
22	B	1214	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	B	1219	CLA	CBA-CGA-O2A-C1
22	B	1224	CLA	CBA-CGA-O2A-C1
22	B	1229	CLA	CBA-CGA-O2A-C1
22	B	1239	CLA	CBA-CGA-O2A-C1
22	K	1403	CLA	CBA-CGA-O2A-C1
22	L	1502	CLA	CBA-CGA-O2A-C1
22	1	607	CLA	CBA-CGA-O2A-C1
22	3	610	CLA	CBA-CGA-O2A-C1
22	8	607	CLA	CBA-CGA-O2A-C1
22	5	609	CLA	CBA-CGA-O2A-C1
22	5	612	CLA	CBA-CGA-O2A-C1
22	6	605	CLA	CBA-CGA-O2A-C1
32	9	802	DGA	CA2-CA1-OG1-CG1
22	7	612	CLA	CBD-CGD-O2D-CED
28	8	805	LMT	C4B-C5B-C6B-O6B
22	A	1113	CLA	O1D-CGD-O2D-CED
25	I	4001	BCR	C15-C16-C17-C18
26	A	5002	LHG	C7-C8-C9-C10
26	4	801	LHG	C7-C8-C9-C10
22	A	1125	CLA	C8-C10-C11-C12
22	3	610	CLA	C5-C6-C7-C8
22	8	609	CLA	C15-C16-C17-C18
28	4	803	LMT	C4'-C5'-C6'-O6'
26	4	801	LHG	O6-C4-C5-O7
21	A	1011	CL0	C5-C6-C7-C8
22	B	1203	CLA	C8-C10-C11-C12
22	B	1210	CLA	C8-C10-C11-C12
22	3	603	CLA	C13-C15-C16-C17
22	3	612	CLA	C8-C10-C11-C12
22	8	606	CLA	C8-C10-C11-C12
40	Z	609	CHL	C5-C6-C7-C8
26	B	5006	LHG	O2-C2-C3-O3
26	7	801	LHG	O2-C2-C3-O3
26	6	801	LHG	O2-C2-C3-O3
27	8	802	NKP	OAF-CAG-CAH-OBC
32	9	802	DGA	OG1-CG1-CG2-OG2
26	A	5002	LHG	C28-C29-C30-C31
22	A	1120	CLA	O1A-CGA-O2A-C1
22	B	1214	CLA	O1A-CGA-O2A-C1
22	K	1403	CLA	O1A-CGA-O2A-C1
22	8	607	CLA	O1A-CGA-O2A-C1
22	B	1236	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	A	1104	CLA	C6-C7-C8-C9
22	A	1110	CLA	C14-C13-C15-C16
22	A	1121	CLA	C11-C10-C8-C9
22	B	1209	CLA	C6-C7-C8-C9
22	B	1215	CLA	C6-C7-C8-C9
22	1	611	CLA	C6-C7-C8-C9
22	Z	604	CLA	C14-C13-C15-C16
22	8	605	CLA	C14-C13-C15-C16
22	5	609	CLA	C11-C10-C8-C9
22	9	603	CLA	C6-C7-C8-C9
40	Z	610	CHL	C11-C12-C13-C14
40	Z	609	CHL	C14-C13-C15-C16
40	9	610	CHL	C11-C12-C13-C14
22	A	1107	CLA	O1D-CGD-O2D-CED
22	B	1223	CLA	O1D-CGD-O2D-CED
22	B	1235	CLA	O1D-CGD-O2D-CED
22	B	1238	CLA	O1D-CGD-O2D-CED
22	6	609	CLA	O1D-CGD-O2D-CED
22	2	615	CLA	O1D-CGD-O2D-CED
22	A	1134	CLA	CBD-CGD-O2D-CED
22	3	603	CLA	C5-C6-C7-C8
22	3	610	CLA	C2A-CAA-CBA-CGA
22	4	608	CLA	C2A-CAA-CBA-CGA
22	9	608	CLA	C2A-CAA-CBA-CGA
25	A	4001	BCR	C36-C18-C19-C20
25	B	4001	BCR	C7-C8-C9-C34
25	B	4007	BCR	C7-C8-C9-C34
25	B	4006	BCR	C11-C12-C13-C35
25	B	4006	BCR	C36-C18-C19-C20
25	I	4001	BCR	C7-C8-C9-C34
25	K	4002	BCR	C7-C8-C9-C34
25	L	4001	BCR	C37-C22-C23-C24
25	7	504	BCR	C7-C8-C9-C34
25	4	503	BCR	C7-C8-C9-C34
25	4	503	BCR	C11-C12-C13-C35
25	5	503	BCR	C37-C22-C23-C24
25	6	504	BCR	C37-C22-C23-C24
25	6	503	BCR	C36-C18-C19-C20
36	F	4001	RRX	C36-C18-C19-C20
37	J	4002	C7Z	C7-C8-C9-C19
37	J	4002	C7Z	C27-C28-C29-C39
37	1	503	C7Z	C7-C8-C9-C19

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Mol	Chain	Res	Type	Atoms
37	5	505	C7Z	C31-C32-C33-C40
39	Z	503	LUT	C31-C32-C33-C40
39	2	501	LUT	C27-C28-C29-C39
39	2	502	LUT	C31-C32-C33-C40
39	2	503	LUT	C11-C12-C13-C20
25	A	4004	BCR	C21-C22-C23-C24
25	A	4005	BCR	C17-C18-C19-C20
25	B	4002	BCR	C7-C8-C9-C10
25	B	4006	BCR	C11-C12-C13-C14
25	I	4001	BCR	C7-C8-C9-C10
25	K	4001	BCR	C7-C8-C9-C10
25	L	4001	BCR	C21-C22-C23-C24
25	7	504	BCR	C7-C8-C9-C10
25	8	503	BCR	C7-C8-C9-C10
25	5	503	BCR	C21-C22-C23-C24
25	6	504	BCR	C21-C22-C23-C24
36	F	4001	RRX	C17-C18-C19-C20
37	J	4002	C7Z	C7-C8-C9-C10
37	J	4002	C7Z	C11-C12-C13-C14
37	J	4002	C7Z	C31-C32-C33-C34
37	J	4002	C7Z	C27-C28-C29-C30
39	2	501	LUT	C27-C28-C29-C30
26	2	801	LHG	C8-C7-O7-C5
28	1	803	LMT	C4B-C5B-C6B-O6B
22	A	1106	CLA	O1A-CGA-O2A-C1
22	A	1108	CLA	O1A-CGA-O2A-C1
22	B	1211	CLA	O1A-CGA-O2A-C1
22	B	1219	CLA	O1A-CGA-O2A-C1
22	B	1229	CLA	O1A-CGA-O2A-C1
22	B	1239	CLA	O1A-CGA-O2A-C1
22	L	1502	CLA	O1A-CGA-O2A-C1
22	5	612	CLA	O1A-CGA-O2A-C1
22	6	605	CLA	O1A-CGA-O2A-C1
22	B	1021	CLA	C13-C15-C16-C17
22	B	1204	CLA	C15-C16-C17-C18
22	B	1207	CLA	C15-C16-C17-C18
22	B	1213	CLA	C15-C16-C17-C18
22	B	1222	CLA	C13-C15-C16-C17
22	B	1224	CLA	C13-C15-C16-C17
22	B	1241	CLA	C5-C6-C7-C8
22	9	603	CLA	C5-C6-C7-C8
40	Z	609	CHL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
22	K	1401	CLA	O1D-CGD-O2D-CED
22	Z	608	CLA	O1D-CGD-O2D-CED
28	8	805	LMT	C4'-C5'-C6'-O6'
22	A	1129	CLA	O1D-CGD-O2D-CED
22	Z	606	CLA	C3-C5-C6-C7
22	3	606	CLA	CBA-CGA-O2A-C1
22	3	607	CLA	CBA-CGA-O2A-C1
22	3	616	CLA	CBA-CGA-O2A-C1
22	A	1104	CLA	C5-C6-C7-C8
22	A	1110	CLA	C8-C10-C11-C12
22	A	1117	CLA	C13-C15-C16-C17
22	A	1118	CLA	C10-C11-C12-C13
22	A	1136	CLA	C5-C6-C7-C8
22	B	1213	CLA	C8-C10-C11-C12
22	B	1229	CLA	C13-C15-C16-C17
22	B	1231	CLA	C8-C10-C11-C12
22	B	1236	CLA	C15-C16-C17-C18
22	1	611	CLA	C15-C16-C17-C18
22	1	612	CLA	C5-C6-C7-C8
22	Z	604	CLA	C10-C11-C12-C13
22	3	607	CLA	C10-C11-C12-C13
22	7	603	CLA	C15-C16-C17-C18
22	8	601	CLA	C10-C11-C12-C13
22	6	609	CLA	C8-C10-C11-C12
22	6	619	CLA	C8-C10-C11-C12
22	2	603	CLA	C5-C6-C7-C8
26	A	5002	LHG	C23-C24-C25-C26
35	B	5004	T7X	C10-C12-C13-C14
43	8	806	3PH	C31-C32-C33-C34
22	A	1130	CLA	O1D-CGD-O2D-CED
22	B	1230	CLA	O1D-CGD-O2D-CED
22	8	607	CLA	O1D-CGD-O2D-CED
22	9	606	CLA	O1D-CGD-O2D-CED
22	1	608	CLA	CBD-CGD-O2D-CED
22	6	601	CLA	CBD-CGD-O2D-CED
22	9	607	CLA	CBD-CGD-O2D-CED
22	A	1012	CLA	C5-C6-C7-C8
22	A	1106	CLA	C15-C16-C17-C18
22	A	1107	CLA	C8-C10-C11-C12
22	A	1107	CLA	C10-C11-C12-C13
22	A	1109	CLA	C13-C15-C16-C17
22	A	1113	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
22	A	1116	CLA	C10-C11-C12-C13
22	A	1124	CLA	C15-C16-C17-C18
22	A	1127	CLA	C10-C11-C12-C13
22	A	1130	CLA	C10-C11-C12-C13
22	A	1131	CLA	C5-C6-C7-C8
22	A	1101	CLA	C8-C10-C11-C12
22	B	1205	CLA	C15-C16-C17-C18
22	B	1209	CLA	C5-C6-C7-C8
22	B	1210	CLA	C10-C11-C12-C13
22	B	1216	CLA	C8-C10-C11-C12
22	B	1216	CLA	C10-C11-C12-C13
22	B	1218	CLA	C13-C15-C16-C17
22	B	1220	CLA	C5-C6-C7-C8
22	B	1230	CLA	C5-C6-C7-C8
22	B	1241	CLA	C10-C11-C12-C13
22	B	1241	CLA	C15-C16-C17-C18
22	F	1301	CLA	C10-C11-C12-C13
22	1	612	CLA	C13-C15-C16-C17
22	Z	605	CLA	C8-C10-C11-C12
22	Z	611	CLA	C5-C6-C7-C8
22	9	601	CLA	C10-C11-C12-C13
22	5	622	CLA	O1A-CGA-O2A-C1
22	3	610	CLA	O1A-CGA-O2A-C1
26	7	801	LHG	C7-C8-C9-C10
26	6	801	LHG	C23-C24-C25-C26
26	2	801	LHG	C7-C8-C9-C10
26	9	801	LHG	C7-C8-C9-C10
26	9	801	LHG	C23-C24-C25-C26
35	B	5004	T7X	C11-C31-C32-C33
28	4	803	LMT	O5B-C5B-C6B-O6B
22	B	1209	CLA	O1D-CGD-O2D-CED
22	1	607	CLA	O1D-CGD-O2D-CED
22	A	1119	CLA	C8-C10-C11-C12
22	A	1120	CLA	C5-C6-C7-C8
22	A	1128	CLA	C5-C6-C7-C8
22	A	1128	CLA	C15-C16-C17-C18
22	B	1239	CLA	C15-C16-C17-C18
22	K	1404	CLA	C5-C6-C7-C8
22	1	601	CLA	C15-C16-C17-C18
22	1	615	CLA	C15-C16-C17-C18
22	3	601	CLA	C13-C15-C16-C17
22	3	601	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	3	610	CLA	C10-C11-C12-C13
22	7	615	CLA	C5-C6-C7-C8
22	8	605	CLA	C13-C15-C16-C17
22	6	609	CLA	C5-C6-C7-C8
22	B	1023	CLA	CBA-CGA-O2A-C1
22	B	1215	CLA	O1D-CGD-O2D-CED
22	7	608	CLA	O1D-CGD-O2D-CED
21	A	1011	CL0	C2-C1-O2A-CGA
22	A	1012	CLA	C2-C1-O2A-CGA
22	A	1112	CLA	C2-C1-O2A-CGA
22	A	1114	CLA	C2-C1-O2A-CGA
22	A	1122	CLA	C2-C1-O2A-CGA
22	A	1126	CLA	C2-C1-O2A-CGA
22	A	1128	CLA	C2-C1-O2A-CGA
22	A	1130	CLA	C2-C1-O2A-CGA
22	B	1205	CLA	C2-C1-O2A-CGA
22	B	1216	CLA	C2-C1-O2A-CGA
22	B	1226	CLA	C2-C1-O2A-CGA
22	B	1227	CLA	C2-C1-O2A-CGA
22	B	1230	CLA	C2-C1-O2A-CGA
22	G	1601	CLA	C2-C1-O2A-CGA
22	K	1403	CLA	C2-C1-O2A-CGA
22	Z	605	CLA	C2-C1-O2A-CGA
22	3	601	CLA	C2-C1-O2A-CGA
22	3	606	CLA	C2-C1-O2A-CGA
22	7	601	CLA	C2-C1-O2A-CGA
22	7	602	CLA	C2-C1-O2A-CGA
22	7	604	CLA	C2-C1-O2A-CGA
22	7	615	CLA	C2-C1-O2A-CGA
22	8	609	CLA	C2-C1-O2A-CGA
22	8	602	CLA	C2-C1-O2A-CGA
22	8	604	CLA	C2-C1-O2A-CGA
22	4	608	CLA	C2-C1-O2A-CGA
22	5	604	CLA	C2-C1-O2A-CGA
22	5	606	CLA	C2-C1-O2A-CGA
22	6	601	CLA	C2-C1-O2A-CGA
22	6	603	CLA	C2-C1-O2A-CGA
22	6	606	CLA	C2-C1-O2A-CGA
22	2	604	CLA	C2-C1-O2A-CGA
22	2	612	CLA	C2-C1-O2A-CGA
22	9	601	CLA	C2-C1-O2A-CGA
22	9	604	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
28	4	803	LMT	O1'-C1-C2-C3
22	A	1109	CLA	C15-C16-C17-C18
22	A	1111	CLA	C13-C15-C16-C17
22	A	1122	CLA	C8-C10-C11-C12
22	A	1138	CLA	C8-C10-C11-C12
22	A	1013	CLA	C15-C16-C17-C18
22	B	1240	CLA	C10-C11-C12-C13
22	F	1301	CLA	C5-C6-C7-C8
22	3	605	CLA	C15-C16-C17-C18
22	4	601	CLA	C8-C10-C11-C12
26	4	801	LHG	C23-C24-C25-C26
26	5	801	LHG	C23-C24-C25-C26
22	Z	612	CLA	C10-C11-C12-C13
22	7	607	CLA	C5-C6-C7-C8
22	6	606	CLA	C5-C6-C7-C8
23	A	2001	PQN	C25-C26-C27-C28
40	Z	610	CHL	C13-C15-C16-C17
22	F	1301	CLA	O1D-CGD-O2D-CED
22	A	1104	CLA	C12-C13-C15-C16
22	A	1106	CLA	C12-C13-C15-C16
22	A	1111	CLA	C6-C7-C8-C10
22	A	1112	CLA	C6-C7-C8-C10
22	A	1124	CLA	C11-C10-C8-C7
22	B	1237	CLA	C11-C10-C8-C7
22	1	607	CLA	C6-C7-C8-C10
22	8	606	CLA	C11-C10-C8-C7
22	4	603	CLA	C11-C12-C13-C15
22	5	607	CLA	C6-C7-C8-C10
22	5	609	CLA	C6-C7-C8-C10
22	4	603	CLA	C3-C5-C6-C7
22	1	607	CLA	O1A-CGA-O2A-C1
22	3	607	CLA	O1A-CGA-O2A-C1
25	B	4007	BCR	C13-C14-C15-C16
25	3	504	BCR	C9-C10-C11-C12
25	7	503	BCR	C9-C10-C11-C12
25	7	504	BCR	C13-C14-C15-C16
37	1	503	C7Z	C29-C30-C31-C32
39	Z	503	LUT	C29-C30-C31-C32
27	8	802	NKP	CAK-CAL-CAM-CAN
22	B	1216	CLA	C2A-CAA-CBA-CGA
22	B	1239	CLA	C2A-CAA-CBA-CGA
22	8	609	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	6	612	CLA	C2A-CAA-CBA-CGA
22	6	615	CLA	C2A-CAA-CBA-CGA
40	6	611	CHL	C2A-CAA-CBA-CGA
40	9	610	CHL	C2A-CAA-CBA-CGA
22	A	1106	CLA	O1D-CGD-O2D-CED
22	Z	606	CLA	O1D-CGD-O2D-CED
22	5	601	CLA	O1D-CGD-O2D-CED
22	A	1124	CLA	C10-C11-C12-C13
22	A	1133	CLA	C15-C16-C17-C18
22	A	1101	CLA	C13-C15-C16-C17
22	B	1203	CLA	C10-C11-C12-C13
22	B	1224	CLA	C15-C16-C17-C18
22	B	1236	CLA	C13-C15-C16-C17
22	7	616	CLA	C8-C10-C11-C12
22	4	605	CLA	C15-C16-C17-C18
22	5	609	CLA	C8-C10-C11-C12
22	6	601	CLA	C8-C10-C11-C12
22	6	619	CLA	C10-C11-C12-C13
22	9	605	CLA	C5-C6-C7-C8
22	3	602	CLA	CBA-CGA-O2A-C1
22	B	1224	CLA	O1A-CGA-O2A-C1
22	5	609	CLA	O1A-CGA-O2A-C1
32	9	802	DGA	OA1-CA1-OG1-CG1
28	4	803	LMT	O5'-C1'-O1'-C1
22	B	1203	CLA	C5-C6-C7-C8
22	B	1231	CLA	C15-C16-C17-C18
22	Z	612	CLA	C5-C6-C7-C8
22	7	607	CLA	C13-C15-C16-C17
28	1	803	LMT	O1'-C1-C2-C3
44	7	805	PLM	C1-C2-C3-C4
25	A	4004	BCR	C10-C11-C12-C13
25	L	4002	BCR	C10-C11-C12-C13
26	B	5002	LHG	O2-C2-C3-O3
26	3	801	LHG	O2-C2-C3-O3
26	2	801	LHG	O9-C7-O7-C5
32	9	802	DGA	OB1-CB1-OG2-CG2
22	1	615	CLA	C3-C5-C6-C7
22	B	1212	CLA	C8-C10-C11-C12
22	Z	606	CLA	C8-C10-C11-C12
40	1	609	CHL	C8-C10-C11-C12
22	A	1111	CLA	C15-C16-C17-C18
22	A	1112	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	A	1125	CLA	C15-C16-C17-C18
22	A	1132	CLA	C5-C6-C7-C8
22	A	1136	CLA	C15-C16-C17-C18
22	B	1207	CLA	C10-C11-C12-C13
22	B	1210	CLA	C13-C15-C16-C17
22	B	1215	CLA	C8-C10-C11-C12
22	B	1221	CLA	C13-C15-C16-C17
22	B	1228	CLA	C5-C6-C7-C8
22	1	606	CLA	C5-C6-C7-C8
22	Z	601	CLA	C10-C11-C12-C13
22	Z	612	CLA	C15-C16-C17-C18
22	7	605	CLA	C5-C6-C7-C8
22	7	607	CLA	C15-C16-C17-C18
22	A	1116	CLA	O1A-CGA-O2A-C1
22	A	1131	CLA	O1A-CGA-O2A-C1
22	3	616	CLA	O1A-CGA-O2A-C1
22	6	618	CLA	CBA-CGA-O2A-C1
22	A	1012	CLA	C8-C10-C11-C12
22	A	1110	CLA	C10-C11-C12-C13
22	A	1121	CLA	C5-C6-C7-C8
22	B	1217	CLA	C5-C6-C7-C8
22	1	612	CLA	C10-C11-C12-C13
22	3	606	CLA	C15-C16-C17-C18
22	8	605	CLA	C8-C10-C11-C12
22	8	605	CLA	C10-C11-C12-C13
22	4	603	CLA	C10-C11-C12-C13
26	B	5002	LHG	C24-C23-O8-C6
22	5	612	CLA	CBD-CGD-O2D-CED
22	3	606	CLA	O1A-CGA-O2A-C1
31	A	5003	LMG	C11-C10-O7-C8
22	A	1102	CLA	C5-C6-C7-C8
22	A	1112	CLA	C8-C10-C11-C12
22	B	1220	CLA	C10-C11-C12-C13
22	B	1225	CLA	C8-C10-C11-C12
22	B	1231	CLA	C13-C15-C16-C17
22	Z	612	CLA	C8-C10-C11-C12
22	3	606	CLA	C8-C10-C11-C12
22	7	601	CLA	C8-C10-C11-C12
22	7	616	CLA	C5-C6-C7-C8
22	4	601	CLA	C10-C11-C12-C13
22	6	619	CLA	C5-C6-C7-C8
22	9	604	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
26	A	5002	LHG	C4-O6-P-O3
26	B	5006	LHG	C4-O6-P-O3
26	1	801	LHG	C4-O6-P-O3
26	7	801	LHG	C4-O6-P-O3
26	4	802	LHG	C4-O6-P-O3
45	8	803	LPX	C3-O1-P1-O2
22	A	1111	CLA	C3-C5-C6-C7
22	7	603	CLA	C3-C5-C6-C7
32	A	5005	DGA	CB9-CAB-CBB-CCB
22	B	1212	CLA	CBA-CGA-O2A-C1
22	8	604	CLA	CBA-CGA-O2A-C1
22	8	608	CLA	CBA-CGA-O2A-C1
22	6	601	CLA	CBA-CGA-O2A-C1
27	8	802	NKP	CAL-CAK-OAJ-CAI
22	A	1107	CLA	C5-C6-C7-C8
22	B	1219	CLA	C5-C6-C7-C8
22	B	1229	CLA	C15-C16-C17-C18
22	8	601	CLA	C8-C10-C11-C12
22	4	609	CLA	C5-C6-C7-C8
22	2	601	CLA	C5-C6-C7-C8
26	2	801	LHG	C23-C24-C25-C26
22	A	1103	CLA	O1D-CGD-O2D-CED
22	A	1124	CLA	O1D-CGD-O2D-CED
26	A	5001	LHG	C1-C2-C3-O3
26	B	5002	LHG	C1-C2-C3-O3
26	4	801	LHG	C1-C2-C3-O3
45	8	803	LPX	O1-C3-C4-C5
31	A	5003	LMG	O9-C10-O7-C8
22	A	1128	CLA	C4-C3-C5-C6
22	B	1216	CLA	C4-C3-C5-C6
22	B	1231	CLA	C5-C6-C7-C8
22	B	1238	CLA	C5-C6-C7-C8
22	L	1502	CLA	C10-C11-C12-C13
22	Z	604	CLA	C5-C6-C7-C8
22	5	601	CLA	C10-C11-C12-C13
22	A	1104	CLA	C2A-CAA-CBA-CGA
22	A	1128	CLA	C2A-CAA-CBA-CGA
22	B	1237	CLA	C2A-CAA-CBA-CGA
22	B	1023	CLA	C2A-CAA-CBA-CGA
22	3	616	CLA	C2A-CAA-CBA-CGA
22	7	606	CLA	C2A-CAA-CBA-CGA
22	7	612	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	8	607	CLA	C2A-CAA-CBA-CGA
22	2	604	CLA	C2A-CAA-CBA-CGA
22	A	1102	CLA	C6-C7-C8-C10
22	B	1213	CLA	C16-C17-C18-C19
22	1	612	CLA	C16-C17-C18-C20
22	K	1402	CLA	C3-C5-C6-C7
22	5	602	CLA	C3-C5-C6-C7
22	6	615	CLA	C3-C5-C6-C7
22	A	1112	CLA	CBA-CGA-O2A-C1
22	K	1402	CLA	CBA-CGA-O2A-C1
22	7	604	CLA	CBA-CGA-O2A-C1
22	A	1013	CLA	C10-C11-C12-C13
22	B	1206	CLA	C5-C6-C7-C8
22	2	601	CLA	C8-C10-C11-C12
25	A	4005	BCR	C19-C20-C21-C22
25	B	4005	BCR	C19-C20-C21-C22
25	3	503	BCR	C13-C14-C15-C16
25	3	506	BCR	C9-C10-C11-C12
25	5	504	BCR	C9-C10-C11-C12
42	Z	504	QTB	C02-C03-C04-C05
26	B	5006	LHG	C7-C8-C9-C10
26	7	801	LHG	C23-C24-C25-C26
22	A	1108	CLA	C15-C16-C17-C18
22	3	603	CLA	C8-C10-C11-C12
25	A	4003	BCR	C11-C10-C9-C34
25	B	4003	BCR	C11-C10-C9-C34
32	9	802	DGA	CB9-CAB-CBB-CCB
22	A	1110	CLA	O1D-CGD-O2D-CED
22	A	1110	CLA	C16-C17-C18-C20
22	A	1126	CLA	C16-C17-C18-C19
22	A	1133	CLA	C16-C17-C18-C19
22	3	607	CLA	C11-C12-C13-C15
22	6	609	CLA	C16-C17-C18-C19
40	6	613	CHL	C6-C7-C8-C10
22	1	611	CLA	CBA-CGA-O2A-C1
22	Z	608	CLA	CBA-CGA-O2A-C1
26	A	5001	LHG	C11-C10-C9-C8
26	8	801	LHG	C12-C13-C14-C15
26	A	5002	LHG	C25-C26-C27-C28
26	8	801	LHG	C28-C29-C30-C31
27	A	5004	NKP	CAX-CAY-CAZ-CBA
32	A	5005	DGA	CA7-CA8-CA9-CAA

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Mol	Chain	Res	Type	Atoms
32	A	5005	DGA	CCA-CDA-CEA-CFA
43	7	802	3PH	C22-C23-C24-C25
22	B	1202	CLA	O1D-CGD-O2D-CED
22	B	1221	CLA	O1D-CGD-O2D-CED
22	B	1240	CLA	O1D-CGD-O2D-CED
26	7	801	LHG	C2-C3-O3-P
28	F	5001	LMT	O5'-C5'-C6'-O6'
26	A	5001	LHG	C9-C10-C11-C12
22	A	1124	CLA	C13-C15-C16-C17
22	Z	604	CLA	C15-C16-C17-C18
26	5	801	LHG	C11-C12-C13-C14
38	7	804	SPH	C9-C10-C11-C12
22	9	603	CLA	C3-C5-C6-C7
26	8	801	LHG	C23-C24-C25-C26
43	2	802	3PH	C21-C22-C23-C24
22	A	1117	CLA	O1D-CGD-O2D-CED
22	B	1227	CLA	O1D-CGD-O2D-CED
22	6	615	CLA	O1D-CGD-O2D-CED
25	A	4003	BCR	C11-C10-C9-C8
25	B	4003	BCR	C11-C10-C9-C8
22	B	1226	CLA	CBA-CGA-O2A-C1
22	5	604	CLA	CBA-CGA-O2A-C1
22	5	615	CLA	CBA-CGA-O2A-C1
26	Z	801	LHG	C28-C29-C30-C31
22	B	1209	CLA	C13-C15-C16-C17
22	B	1023	CLA	O1A-CGA-O2A-C1
22	8	608	CLA	O1A-CGA-O2A-C1
27	8	802	NKP	OAE-CAK-OAJ-CAI
22	A	1107	CLA	C16-C17-C18-C20
22	A	1115	CLA	C11-C12-C13-C14
22	A	1134	CLA	C6-C7-C8-C10
22	B	1223	CLA	C16-C17-C18-C19
22	B	1236	CLA	C16-C17-C18-C20
22	1	612	CLA	C16-C17-C18-C19
22	7	607	CLA	C16-C17-C18-C19
22	7	616	CLA	C11-C12-C13-C14
22	4	604	CLA	C11-C12-C13-C15
22	5	613	CLA	C6-C7-C8-C10
40	8	610	CHL	C6-C7-C8-C10
22	A	1104	CLA	O1D-CGD-O2D-CED
22	A	1101	CLA	O1D-CGD-O2D-CED
22	7	609	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	8	609	CLA	O1D-CGD-O2D-CED
22	6	603	CLA	C4-C3-C5-C6
22	6	605	CLA	C4-C3-C5-C6
26	4	801	LHG	C28-C29-C30-C31
26	4	802	LHG	C11-C10-C9-C8
26	4	802	LHG	C11-C12-C13-C14
26	6	801	LHG	C11-C12-C13-C14
41	1	802	SQD	C17-C18-C19-C20
41	2	803	SQD	C9-C10-C11-C12
22	A	1105	CLA	C11-C12-C13-C14
22	A	1140	CLA	C6-C7-C8-C9
22	B	1238	CLA	C6-C7-C8-C9
22	1	612	CLA	C14-C13-C15-C16
22	3	601	CLA	C6-C7-C8-C9
22	6	603	CLA	C6-C7-C8-C9
22	6	615	CLA	C11-C10-C8-C9
43	7	802	3PH	C21-C22-C23-C24
22	B	1214	CLA	C10-C11-C12-C13
26	7	801	LHG	C28-C29-C30-C31
28	A	5006	LMT	C3-C4-C5-C6
22	1	603	CLA	C15-C16-C17-C18
22	K	1404	CLA	C2A-CAA-CBA-CGA
22	8	602	CLA	C2A-CAA-CBA-CGA
22	9	606	CLA	C2A-CAA-CBA-CGA
22	B	1212	CLA	O1A-CGA-O2A-C1
22	6	601	CLA	O1A-CGA-O2A-C1
25	A	4004	BCR	C37-C22-C23-C24
25	B	4005	BCR	C36-C18-C19-C20
25	G	4001	BCR	C37-C22-C23-C24
25	5	504	BCR	C37-C22-C23-C24
36	F	4001	RRX	C37-C22-C23-C24
37	J	4002	C7Z	C11-C12-C13-C20
26	6	801	LHG	C16-C17-C18-C19
32	9	802	DGA	CAB-CBB-CCB-CDB
38	7	804	SPH	C10-C11-C12-C13
26	A	5001	LHG	O1-C1-C2-C3
26	B	5002	LHG	O1-C1-C2-C3
26	Z	801	LHG	O1-C1-C2-C3
26	3	801	LHG	O1-C1-C2-C3
26	8	801	LHG	O1-C1-C2-C3
26	4	801	LHG	O1-C1-C2-C3
26	6	801	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
26	2	801	LHG	O1-C1-C2-C3
25	B	4001	BCR	C7-C8-C9-C10
25	B	4005	BCR	C17-C18-C19-C20
25	G	4001	BCR	C21-C22-C23-C24
25	5	504	BCR	C21-C22-C23-C24
36	F	4001	RRX	C21-C22-C23-C24
22	A	1113	CLA	C3-C5-C6-C7
22	B	1216	CLA	C3-C5-C6-C7
22	1	606	CLA	C3-C5-C6-C7
27	A	5004	NKP	OBC-CAH-CAI-OAJ
22	A	1126	CLA	C15-C16-C17-C18
22	B	1216	CLA	C15-C16-C17-C18
26	5	801	LHG	C8-C7-O7-C5
26	5	801	LHG	C11-C10-C9-C8
26	6	801	LHG	C12-C13-C14-C15
26	1	801	LHG	C23-C24-C25-C26
26	8	801	LHG	C11-C10-C9-C8
26	6	801	LHG	C11-C10-C9-C8
26	6	801	LHG	C13-C14-C15-C16
28	A	5006	LMT	C5-C6-C7-C8
32	9	802	DGA	CDB-CEB-CFB-CGB
38	7	804	SPH	C6-C7-C8-C9
22	A	1102	CLA	C6-C7-C8-C9
22	A	1133	CLA	C16-C17-C18-C20
22	7	616	CLA	C11-C12-C13-C15
40	8	610	CHL	C6-C7-C8-C9
40	6	613	CHL	C6-C7-C8-C9
28	B	6101	LMT	O5'-C1'-O1'-C1
41	1	802	SQD	O5-C1-O6-C44
22	B	1223	CLA	C10-C11-C12-C13
22	B	1230	CLA	C8-C10-C11-C12
22	1	603	CLA	C8-C10-C11-C12
22	5	602	CLA	C5-C6-C7-C8
22	5	618	CLA	C8-C10-C11-C12
22	7	601	CLA	O1D-CGD-O2D-CED
26	Z	801	LHG	C13-C14-C15-C16
26	7	801	LHG	C11-C12-C13-C14
26	8	801	LHG	C25-C26-C27-C28
26	6	801	LHG	C30-C31-C32-C33
28	1	803	LMT	C11-C10-C9-C8
38	K	5001	SPH	C12-C13-C14-C15
22	6	607	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	A	1013	CLA	O1D-CGD-O2D-CED
26	A	5002	LHG	C13-C14-C15-C16
26	6	801	LHG	C34-C35-C36-C37
22	7	609	CLA	C5-C6-C7-C8
26	4	801	LHG	C10-C11-C12-C13
26	4	801	LHG	C11-C12-C13-C14
26	4	801	LHG	C29-C30-C31-C32
22	9	601	CLA	O1D-CGD-O2D-CED
22	B	1212	CLA	C3-C5-C6-C7
22	5	612	CLA	C3-C5-C6-C7
22	A	1122	CLA	CBA-CGA-O2A-C1
22	3	601	CLA	CBA-CGA-O2A-C1
22	8	605	CLA	CBA-CGA-O2A-C1
22	6	604	CLA	CBA-CGA-O2A-C1
22	9	601	CLA	CBA-CGA-O2A-C1
26	4	801	LHG	C13-C14-C15-C16
22	5	607	CLA	O1D-CGD-O2D-CED
22	A	1104	CLA	C3A-C2A-CAA-CBA
22	A	1108	CLA	C3A-C2A-CAA-CBA
22	A	1109	CLA	C3A-C2A-CAA-CBA
22	A	1125	CLA	C3A-C2A-CAA-CBA
22	A	1131	CLA	C3A-C2A-CAA-CBA
22	A	1135	CLA	C3A-C2A-CAA-CBA
22	A	1101	CLA	C3A-C2A-CAA-CBA
22	B	1207	CLA	C3A-C2A-CAA-CBA
22	B	1212	CLA	C3A-C2A-CAA-CBA
22	B	1236	CLA	C3A-C2A-CAA-CBA
22	B	1241	CLA	C3A-C2A-CAA-CBA
22	K	1404	CLA	C3A-C2A-CAA-CBA
22	1	613	CLA	C3A-C2A-CAA-CBA
22	3	608	CLA	C3A-C2A-CAA-CBA
22	3	618	CLA	C3A-C2A-CAA-CBA
22	7	603	CLA	C3A-C2A-CAA-CBA
22	7	604	CLA	C3A-C2A-CAA-CBA
22	8	602	CLA	C3A-C2A-CAA-CBA
22	8	603	CLA	C3A-C2A-CAA-CBA
22	8	604	CLA	C3A-C2A-CAA-CBA
22	5	605	CLA	C3A-C2A-CAA-CBA
22	5	609	CLA	C3A-C2A-CAA-CBA
22	6	608	CLA	C3A-C2A-CAA-CBA
22	6	601	CLA	C3A-C2A-CAA-CBA
22	6	618	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	2	602	CLA	C3A-C2A-CAA-CBA
22	9	603	CLA	C3A-C2A-CAA-CBA
40	Z	613	CHL	C3A-C2A-CAA-CBA
40	8	613	CHL	C3A-C2A-CAA-CBA
40	4	613	CHL	C3A-C2A-CAA-CBA
22	B	1214	CLA	C8-C10-C11-C12
22	B	1228	CLA	C13-C15-C16-C17
22	F	1301	CLA	C8-C10-C11-C12
22	7	607	CLA	O1D-CGD-O2D-CED
22	4	609	CLA	O1D-CGD-O2D-CED
22	8	604	CLA	O1A-CGA-O2A-C1
22	A	1110	CLA	C16-C17-C18-C19
22	A	1117	CLA	C16-C17-C18-C19
22	A	1117	CLA	C16-C17-C18-C20
22	B	1207	CLA	C16-C17-C18-C19
22	B	1207	CLA	C16-C17-C18-C20
22	B	1236	CLA	C16-C17-C18-C19
22	3	607	CLA	C11-C12-C13-C14
22	4	601	CLA	C11-C12-C13-C15
22	6	609	CLA	C16-C17-C18-C20
26	1	801	LHG	C11-C10-C9-C8
22	5	618	CLA	O1D-CGD-O2D-CED
26	4	801	LHG	C9-C10-C11-C12
27	8	802	NKP	CAM-CAN-CAO-CAP
32	A	5005	DGA	CB7-CB8-CB9-CAB
22	4	608	CLA	C3-C5-C6-C7
26	A	5001	LHG	C23-C24-C25-C26
43	7	802	3PH	C31-C32-C33-C34
22	A	1125	CLA	C4-C3-C5-C6
22	B	1231	CLA	C4-C3-C5-C6
22	9	604	CLA	CBA-CGA-O2A-C1
22	A	1125	CLA	C2-C3-C5-C6
22	B	1231	CLA	C2-C3-C5-C6
22	6	603	CLA	C2-C3-C5-C6
22	6	605	CLA	C2-C3-C5-C6
26	A	5002	LHG	C8-C7-O7-C5
22	A	1125	CLA	C2A-CAA-CBA-CGA
22	B	1225	CLA	C2A-CAA-CBA-CGA
26	B	5002	LHG	O1-C1-C2-O2
26	1	801	LHG	O1-C1-C2-O2
26	Z	801	LHG	O1-C1-C2-O2
26	8	801	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
26	4	801	LHG	O1-C1-C2-O2
26	5	801	LHG	O1-C1-C2-O2
26	2	801	LHG	O1-C1-C2-O2
32	A	5005	DGA	CA6-CA7-CA8-CA9
41	1	802	SQD	C10-C11-C12-C13
41	1	802	SQD	C11-C12-C13-C14
26	4	802	LHG	C23-C24-C25-C26
22	A	1112	CLA	O1A-CGA-O2A-C1
22	1	611	CLA	O1A-CGA-O2A-C1
22	7	604	CLA	O1A-CGA-O2A-C1
22	A	1107	CLA	C16-C17-C18-C19
22	A	1126	CLA	C16-C17-C18-C20
22	B	1216	CLA	C16-C17-C18-C20
28	4	803	LMT	C3-C4-C5-C6
28	B	6101	LMT	C1-C2-C3-C4
26	4	802	LHG	O2-C2-C3-O3
22	A	1124	CLA	C8-C10-C11-C12
22	B	1213	CLA	C5-C6-C7-C8
22	1	603	CLA	C5-C6-C7-C8
22	8	606	CLA	C10-C11-C12-C13
22	8	607	CLA	C5-C6-C7-C8
22	A	1109	CLA	CBA-CGA-O2A-C1
22	K	1402	CLA	O1A-CGA-O2A-C1
22	5	615	CLA	O1A-CGA-O2A-C1
43	5	802	3PH	C21-C22-C23-C24
22	B	1234	CLA	C5-C6-C7-C8
22	9	603	CLA	C8-C10-C11-C12
22	B	1220	CLA	CBD-CGD-O2D-CED
26	2	801	LHG	C1-C2-C3-O3
26	A	5001	LHG	C11-C12-C13-C14
32	9	802	DGA	CB2-CB3-CB4-CB5
26	5	801	LHG	O9-C7-O7-C5
22	A	1103	CLA	C2-C1-O2A-CGA
22	A	1120	CLA	C2-C1-O2A-CGA
22	A	1121	CLA	C2-C1-O2A-CGA
22	A	1125	CLA	C2-C1-O2A-CGA
22	A	1134	CLA	C2-C1-O2A-CGA
22	A	1141	CLA	C2-C1-O2A-CGA
22	B	1022	CLA	C2-C1-O2A-CGA
22	B	1206	CLA	C2-C1-O2A-CGA
22	B	1210	CLA	C2-C1-O2A-CGA
22	B	1213	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
22	B	1215	CLA	C2-C1-O2A-CGA
22	B	1218	CLA	C2-C1-O2A-CGA
22	B	1220	CLA	C2-C1-O2A-CGA
22	K	1404	CLA	C2-C1-O2A-CGA
22	L	1502	CLA	C2-C1-O2A-CGA
22	L	1503	CLA	C2-C1-O2A-CGA
22	1	607	CLA	C2-C1-O2A-CGA
22	1	611	CLA	C2-C1-O2A-CGA
22	Z	607	CLA	C2-C1-O2A-CGA
22	Z	608	CLA	C2-C1-O2A-CGA
22	Z	611	CLA	C2-C1-O2A-CGA
22	Z	612	CLA	C2-C1-O2A-CGA
22	3	603	CLA	C2-C1-O2A-CGA
22	3	604	CLA	C2-C1-O2A-CGA
22	3	605	CLA	C2-C1-O2A-CGA
22	3	613	CLA	C2-C1-O2A-CGA
22	8	601	CLA	C2-C1-O2A-CGA
22	8	606	CLA	C2-C1-O2A-CGA
22	4	606	CLA	C2-C1-O2A-CGA
22	4	609	CLA	C2-C1-O2A-CGA
22	6	604	CLA	C2-C1-O2A-CGA
22	6	607	CLA	C2-C1-O2A-CGA
22	2	605	CLA	C2-C1-O2A-CGA
26	6	801	LHG	C31-C32-C33-C34
32	9	802	DGA	CA6-CA7-CA8-CA9
41	1	802	SQD	C9-C10-C11-C12
22	K	1402	CLA	C5-C6-C7-C8
22	9	603	CLA	C10-C11-C12-C13
22	Z	608	CLA	O1A-CGA-O2A-C1
22	8	605	CLA	O1A-CGA-O2A-C1
32	9	802	DGA	CB5-CB6-CB7-CB8
43	7	802	3PH	C25-C26-C27-C28
22	7	607	CLA	C16-C17-C18-C20
22	5	613	CLA	C6-C7-C8-C9
25	A	4003	BCR	C1-C6-C7-C8
25	A	4003	BCR	C23-C24-C25-C26
25	A	4003	BCR	C23-C24-C25-C30
25	A	4004	BCR	C1-C6-C7-C8
25	A	4004	BCR	C5-C6-C7-C8
25	A	4004	BCR	C23-C24-C25-C30
25	B	4001	BCR	C5-C6-C7-C8
25	B	4001	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
25	B	4004	BCR	C23-C24-C25-C26
25	B	4005	BCR	C23-C24-C25-C26
25	B	4005	BCR	C23-C24-C25-C30
25	B	4006	BCR	C23-C24-C25-C26
25	B	4006	BCR	C23-C24-C25-C30
25	G	4001	BCR	C1-C6-C7-C8
25	G	4001	BCR	C5-C6-C7-C8
25	G	4001	BCR	C23-C24-C25-C26
25	G	4001	BCR	C23-C24-C25-C30
25	I	4001	BCR	C1-C6-C7-C8
25	I	4001	BCR	C5-C6-C7-C8
25	J	4001	BCR	C23-C24-C25-C26
25	J	4001	BCR	C23-C24-C25-C30
25	K	4001	BCR	C1-C6-C7-C8
25	K	4002	BCR	C5-C6-C7-C8
25	K	4002	BCR	C23-C24-C25-C26
25	K	4002	BCR	C23-C24-C25-C30
25	L	4002	BCR	C1-C6-C7-C8
25	L	4002	BCR	C5-C6-C7-C8
25	L	4002	BCR	C23-C24-C25-C26
25	3	503	BCR	C1-C6-C7-C8
25	3	505	BCR	C23-C24-C25-C26
25	3	505	BCR	C23-C24-C25-C30
25	7	504	BCR	C23-C24-C25-C26
25	8	503	BCR	C1-C6-C7-C8
25	4	503	BCR	C1-C6-C7-C8
25	4	503	BCR	C5-C6-C7-C8
25	5	503	BCR	C23-C24-C25-C30
25	5	504	BCR	C23-C24-C25-C26
25	5	504	BCR	C23-C24-C25-C30
25	6	504	BCR	C23-C24-C25-C26
25	6	504	BCR	C23-C24-C25-C30
25	6	503	BCR	C23-C24-C25-C30
36	F	4001	RRX	C23-C24-C25-C30
36	F	4001	RRX	C23-C24-C25-C26
37	J	4002	C7Z	C21-C26-C27-C28
37	1	503	C7Z	C5-C6-C7-C8
37	1	503	C7Z	C25-C26-C27-C28
39	Z	503	LUT	C1-C6-C7-C8
26	A	5001	LHG	C13-C14-C15-C16
28	F	5001	LMT	C3-C4-C5-C6
32	A	5005	DGA	CB4-CB5-CB6-CB7

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Mol	Chain	Res	Type	Atoms
43	2	802	3PH	C36-C37-C38-C39
22	A	1115	CLA	CBA-CGA-O2A-C1
22	A	1013	CLA	CBA-CGA-O2A-C1
22	7	601	CLA	CBA-CGA-O2A-C1
22	7	602	CLA	CBA-CGA-O2A-C1
21	A	1011	CL0	C15-C16-C17-C18
22	A	1115	CLA	C10-C11-C12-C13
22	A	1137	CLA	C10-C11-C12-C13
22	B	1023	CLA	C13-C15-C16-C17
22	7	604	CLA	C13-C15-C16-C17
22	8	602	CLA	C13-C15-C16-C17
28	4	803	LMT	C1-C2-C3-C4
28	F	5001	LMT	C2-C3-C4-C5
22	1	611	CLA	C8-C10-C11-C12
22	1	612	CLA	C8-C10-C11-C12
22	7	604	CLA	C5-C6-C7-C8
22	7	604	CLA	C8-C10-C11-C12
22	B	1211	CLA	C4-C3-C5-C6
22	A	1102	CLA	C2-C3-C5-C6
22	A	1103	CLA	C11-C12-C13-C15
22	A	1105	CLA	C11-C12-C13-C15
22	A	1110	CLA	C12-C13-C15-C16
22	A	1140	CLA	C6-C7-C8-C10
22	B	1203	CLA	C11-C10-C8-C7
22	B	1209	CLA	C6-C7-C8-C10
22	B	1211	CLA	C2-C3-C5-C6
22	B	1222	CLA	C6-C7-C8-C10
22	1	603	CLA	C11-C10-C8-C7
22	1	612	CLA	C12-C13-C15-C16
22	Z	607	CLA	C6-C7-C8-C10
22	Z	608	CLA	C6-C7-C8-C10
22	3	601	CLA	C6-C7-C8-C10
22	8	605	CLA	C2-C3-C5-C6
22	4	604	CLA	C11-C10-C8-C7
22	5	609	CLA	C11-C10-C8-C7
22	6	603	CLA	C6-C7-C8-C10
22	6	615	CLA	C11-C10-C8-C7
22	9	603	CLA	C6-C7-C8-C10
23	B	2002	PQN	C21-C22-C23-C25
40	Z	610	CHL	C11-C10-C8-C7
40	Z	609	CHL	C11-C12-C13-C15
40	Z	609	CHL	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	B	1219	CLA	C3-C5-C6-C7
22	2	601	CLA	C3-C5-C6-C7
22	9	605	CLA	C3-C5-C6-C7
22	A	1122	CLA	O1A-CGA-O2A-C1
22	B	1226	CLA	O1A-CGA-O2A-C1
22	3	601	CLA	O1A-CGA-O2A-C1
22	5	604	CLA	O1A-CGA-O2A-C1
22	9	601	CLA	O1A-CGA-O2A-C1
44	7	805	PLM	C2-C3-C4-C5
22	A	1105	CLA	C13-C15-C16-C17
25	8	503	BCR	C9-C10-C11-C12
39	9	502	LUT	C29-C30-C31-C32
22	A	1115	CLA	C11-C12-C13-C15
22	A	1134	CLA	C6-C7-C8-C9
22	B	1223	CLA	C16-C17-C18-C20
22	4	604	CLA	C11-C12-C13-C14
26	A	5001	LHG	C7-C8-C9-C10
26	1	801	LHG	C7-C8-C9-C10
26	Z	801	LHG	C7-C8-C9-C10
41	1	802	SQD	C7-C8-C9-C10
22	G	1601	CLA	CBA-CGA-O2A-C1
22	1	603	CLA	CBA-CGA-O2A-C1
22	4	609	CLA	CBA-CGA-O2A-C1
26	A	5002	LHG	C24-C23-O8-C6
22	A	1118	CLA	C2A-CAA-CBA-CGA
22	B	1022	CLA	C2A-CAA-CBA-CGA
22	3	607	CLA	C2A-CAA-CBA-CGA
22	3	612	CLA	C2A-CAA-CBA-CGA
22	3	618	CLA	C2A-CAA-CBA-CGA
22	7	615	CLA	C2A-CAA-CBA-CGA
40	Z	613	CHL	C2A-CAA-CBA-CGA
40	5	611	CHL	C2A-CAA-CBA-CGA
22	A	1104	CLA	C8-C10-C11-C12
22	A	1126	CLA	C5-C6-C7-C8
22	5	605	CLA	C5-C6-C7-C8
22	6	601	CLA	C10-C11-C12-C13
22	6	605	CLA	C5-C6-C7-C8
26	4	801	LHG	C30-C31-C32-C33
43	6	802	3PH	C22-C23-C24-C25
27	8	802	NKP	CAG-CAH-CAI-OAJ
22	A	1112	CLA	O1D-CGD-O2D-CED
22	7	612	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	6	601	CLA	O1D-CGD-O2D-CED
22	B	1222	CLA	C10-C11-C12-C13
22	8	606	CLA	C5-C6-C7-C8
22	6	606	CLA	C13-C15-C16-C17
38	K	5001	SPH	C11-C12-C13-C14
43	7	802	3PH	C24-C25-C26-C27
22	A	1110	CLA	C3-C5-C6-C7
22	7	609	CLA	C3-C5-C6-C7
22	7	602	CLA	O1A-CGA-O2A-C1
22	9	606	CLA	CBA-CGA-O2A-C1
22	2	601	CLA	C11-C12-C13-C15
22	B	1205	CLA	C10-C11-C12-C13
22	B	1239	CLA	C13-C15-C16-C17
22	1	607	CLA	C5-C6-C7-C8
26	Z	801	LHG	C23-C24-C25-C26
26	4	802	LHG	C7-C8-C9-C10
26	7	801	LHG	C8-C7-O7-C5
26	4	802	LHG	C8-C7-O7-C5
41	2	803	SQD	C8-C7-O47-C45
26	1	801	LHG	O6-C4-C5-O7
27	A	5004	NKP	CAV-CAW-CAX-CAY
22	3	603	CLA	C15-C16-C17-C18
22	4	609	CLA	C8-C10-C11-C12
22	A	1013	CLA	O1A-CGA-O2A-C1
26	A	5002	LHG	O9-C7-O7-C5
41	2	803	SQD	O49-C7-O47-C45
43	5	802	3PH	C22-C23-C24-C25
28	B	6101	LMT	C2'-C1'-O1'-C1
32	A	5005	DGA	CA2-CA3-CA4-CA5
22	A	1111	CLA	C8-C10-C11-C12
22	1	601	CLA	C10-C11-C12-C13
35	B	5004	T7X	C12-C13-C14-C15
22	A	1102	CLA	C4-C3-C5-C6
22	B	1229	CLA	C4-C3-C5-C6
26	6	801	LHG	C7-C8-C9-C10
22	A	1128	CLA	C2-C3-C5-C6
22	B	1216	CLA	C2-C3-C5-C6
22	B	1221	CLA	C2-C3-C5-C6
22	B	1229	CLA	C2-C3-C5-C6
22	B	1236	CLA	C2-C3-C5-C6
27	8	802	NKP	CAL-CAM-CAN-CAO
28	8	805	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
22	A	1103	CLA	C11-C12-C13-C14
22	A	1104	CLA	C14-C13-C15-C16
22	A	1105	CLA	C14-C13-C15-C16
22	A	1106	CLA	C11-C12-C13-C14
22	A	1106	CLA	C14-C13-C15-C16
22	A	1111	CLA	C6-C7-C8-C9
22	A	1112	CLA	C6-C7-C8-C9
22	A	1114	CLA	C6-C7-C8-C9
22	A	1128	CLA	C14-C13-C15-C16
22	A	1136	CLA	C6-C7-C8-C9
22	A	1101	CLA	C11-C12-C13-C14
22	B	1237	CLA	C11-C10-C8-C9
22	B	1023	CLA	C11-C12-C13-C14
22	B	1207	CLA	C11-C10-C8-C9
22	B	1222	CLA	C6-C7-C8-C9
22	B	1223	CLA	C11-C10-C8-C9
22	B	1231	CLA	C14-C13-C15-C16
22	1	607	CLA	C6-C7-C8-C9
22	Z	607	CLA	C6-C7-C8-C9
22	Z	608	CLA	C6-C7-C8-C9
22	3	603	CLA	C11-C12-C13-C14
22	8	606	CLA	C11-C10-C8-C9
22	4	603	CLA	C11-C12-C13-C14
22	4	604	CLA	C11-C10-C8-C9
22	5	609	CLA	C6-C7-C8-C9
22	6	619	CLA	C6-C7-C8-C9
22	9	604	CLA	C11-C10-C8-C9
23	B	2002	PQN	C21-C22-C23-C24
40	Z	609	CHL	C11-C12-C13-C14
26	B	5002	LHG	O10-C23-O8-C6
22	A	1102	CLA	CBD-CGD-O2D-CED
22	6	604	CLA	O1A-CGA-O2A-C1
38	K	5001	SPH	C7-C8-C9-C10
22	A	1012	CLA	C2A-CAA-CBA-CGA
22	A	1013	CLA	C2A-CAA-CBA-CGA
22	B	1210	CLA	C2A-CAA-CBA-CGA
22	1	606	CLA	C2A-CAA-CBA-CGA
22	3	606	CLA	C2A-CAA-CBA-CGA
22	7	609	CLA	C2A-CAA-CBA-CGA
26	A	5002	LHG	C31-C32-C33-C34
22	B	1238	CLA	CBA-CGA-O2A-C1
25	A	4004	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
37	1	503	C7Z	C27-C28-C29-C39
22	1	608	CLA	O1D-CGD-O2D-CED
22	Z	601	CLA	C5-C6-C7-C8
22	4	601	CLA	C5-C6-C7-C8
26	1	801	LHG	C27-C28-C29-C30
37	1	503	C7Z	C27-C28-C29-C30
39	2	502	LUT	C31-C32-C33-C34
22	A	1115	CLA	O1A-CGA-O2A-C1
22	1	603	CLA	O1A-CGA-O2A-C1
22	7	601	CLA	O1A-CGA-O2A-C1
22	A	1104	CLA	C1A-C2A-CAA-CBA
22	A	1106	CLA	C1A-C2A-CAA-CBA
22	A	1118	CLA	C1A-C2A-CAA-CBA
22	A	1122	CLA	C1A-C2A-CAA-CBA
22	A	1126	CLA	C1A-C2A-CAA-CBA
22	A	1131	CLA	C1A-C2A-CAA-CBA
22	A	1132	CLA	C1A-C2A-CAA-CBA
22	B	1207	CLA	C1A-C2A-CAA-CBA
22	B	1209	CLA	C1A-C2A-CAA-CBA
22	B	1227	CLA	C1A-C2A-CAA-CBA
22	B	1229	CLA	C1A-C2A-CAA-CBA
22	B	1239	CLA	C1A-C2A-CAA-CBA
22	B	1240	CLA	C1A-C2A-CAA-CBA
22	K	1404	CLA	C1A-C2A-CAA-CBA
22	1	606	CLA	C1A-C2A-CAA-CBA
22	1	608	CLA	C1A-C2A-CAA-CBA
22	1	611	CLA	C1A-C2A-CAA-CBA
22	1	613	CLA	C1A-C2A-CAA-CBA
22	Z	601	CLA	C1A-C2A-CAA-CBA
22	Z	604	CLA	C1A-C2A-CAA-CBA
22	Z	606	CLA	C1A-C2A-CAA-CBA
22	Z	607	CLA	C1A-C2A-CAA-CBA
22	Z	608	CLA	C1A-C2A-CAA-CBA
22	3	604	CLA	C1A-C2A-CAA-CBA
22	3	606	CLA	C1A-C2A-CAA-CBA
22	3	607	CLA	C1A-C2A-CAA-CBA
22	3	608	CLA	C1A-C2A-CAA-CBA
22	3	610	CLA	C1A-C2A-CAA-CBA
22	3	612	CLA	C1A-C2A-CAA-CBA
22	7	609	CLA	C1A-C2A-CAA-CBA
22	7	607	CLA	C1A-C2A-CAA-CBA
22	7	608	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	7	612	CLA	C1A-C2A-CAA-CBA
22	7	615	CLA	C1A-C2A-CAA-CBA
22	8	602	CLA	C1A-C2A-CAA-CBA
22	5	605	CLA	C1A-C2A-CAA-CBA
22	5	618	CLA	C1A-C2A-CAA-CBA
22	6	609	CLA	C1A-C2A-CAA-CBA
22	6	607	CLA	C1A-C2A-CAA-CBA
22	6	612	CLA	C1A-C2A-CAA-CBA
22	2	601	CLA	C1A-C2A-CAA-CBA
22	2	602	CLA	C1A-C2A-CAA-CBA
22	9	607	CLA	C1A-C2A-CAA-CBA
22	9	608	CLA	C1A-C2A-CAA-CBA
40	Z	613	CHL	C1A-C2A-CAA-CBA
40	4	613	CHL	C1A-C2A-CAA-CBA
40	2	610	CHL	C1A-C2A-CAA-CBA
22	B	1216	CLA	C16-C17-C18-C19
22	4	601	CLA	C11-C12-C13-C14
22	2	601	CLA	C11-C12-C13-C14
26	7	801	LHG	O9-C7-O7-C5
25	A	4001	BCR	C9-C10-C11-C12
25	B	4003	BCR	C19-C20-C21-C22
39	7	502	LUT	C29-C30-C31-C32
22	3	602	CLA	O1A-CGA-O2A-C1
22	A	1133	CLA	C10-C11-C12-C13
28	F	5001	LMT	C1-C2-C3-C4
26	B	5002	LHG	C4-O6-P-O3
26	B	5006	LHG	C3-O3-P-O6
22	B	1222	CLA	CBD-CGD-O2D-CED
22	B	1231	CLA	C3-C5-C6-C7
22	3	612	CLA	C3-C5-C6-C7
38	7	804	SPH	C7-C8-C9-C10
22	A	1109	CLA	O1A-CGA-O2A-C1
22	A	1137	CLA	C5-C6-C7-C8
22	1	607	CLA	C8-C10-C11-C12
21	A	1011	CL0	CBA-CGA-O2A-C1
26	4	801	LHG	O6-C4-C5-C6
26	6	801	LHG	O6-C4-C5-C6
43	5	802	3PH	O11-C1-C2-C3
22	A	1134	CLA	O1D-CGD-O2D-CED
43	8	806	3PH	C37-C38-C39-C3A
22	9	604	CLA	O1D-CGD-O2D-CED
32	9	802	DGA	CB3-CB4-CB5-CB6

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Mol	Chain	Res	Type	Atoms
22	9	607	CLA	O1D-CGD-O2D-CED
26	4	802	LHG	C13-C14-C15-C16
22	B	1223	CLA	C8-C10-C11-C12
22	4	603	CLA	C8-C10-C11-C12
22	5	604	CLA	C5-C6-C7-C8
43	8	806	3PH	C34-C35-C36-C37
26	4	802	LHG	O9-C7-O7-C5
22	8	605	CLA	C4-C3-C5-C6
22	J	1901	CLA	C3A-C2A-CAA-CBA
22	B	1224	CLA	C10-C11-C12-C13
22	B	1228	CLA	C15-C16-C17-C18
22	L	1502	CLA	C13-C15-C16-C17
26	9	801	LHG	C11-C10-C9-C8
32	A	5005	DGA	CA5-CA6-CA7-CA8
38	K	5001	SPH	C9-C10-C11-C12
22	G	1601	CLA	O1A-CGA-O2A-C1
22	4	609	CLA	O1A-CGA-O2A-C1
22	9	604	CLA	O1A-CGA-O2A-C1
26	A	5002	LHG	O10-C23-O8-C6
22	A	1107	CLA	C2A-CAA-CBA-CGA
22	B	1213	CLA	C16-C17-C18-C20
22	6	605	CLA	C6-C7-C8-C9
22	A	1133	CLA	C3-C5-C6-C7
22	B	1203	CLA	C3-C5-C6-C7
22	3	603	CLA	C3-C5-C6-C7
26	B	5006	LHG	C4-C5-C6-O8
26	1	801	LHG	C4-C5-C6-O8
26	Z	801	LHG	C4-C5-C6-O8
26	4	801	LHG	C4-C5-C6-O8
32	9	802	DGA	OG1-CG1-CG2-CG3
33	B	5003	DGD	O1G-C1G-C2G-C3G
35	B	5004	T7X	C7-C8-C9-O18
22	3	606	CLA	C10-C11-C12-C13
22	8	602	CLA	C15-C16-C17-C18
43	2	802	3PH	C22-C23-C24-C25
22	A	1104	CLA	C13-C15-C16-C17
22	A	1123	CLA	C13-C15-C16-C17
22	A	1137	CLA	C15-C16-C17-C18
22	3	605	CLA	C8-C10-C11-C12
22	7	616	CLA	C10-C11-C12-C13
22	4	608	CLA	C5-C6-C7-C8
22	5	609	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	A	1127	CLA	CAA-CBA-CGA-O2A
22	B	1205	CLA	CAA-CBA-CGA-O2A
43	6	802	3PH	C29-C2A-C2B-C2C
22	A	1133	CLA	C13-C15-C16-C17
22	B	1204	CLA	C5-C6-C7-C8
22	B	1219	CLA	C11-C12-C13-C14
26	6	801	LHG	C28-C29-C30-C31
26	2	801	LHG	C25-C26-C27-C28
26	4	802	LHG	O1-C1-C2-O2
26	6	801	LHG	O1-C1-C2-O2
26	9	801	LHG	O1-C1-C2-O2
31	J	5001	LMG	C8-C9-O8-C28
26	B	5001	LHG	C7-C8-C9-C10
22	1	608	CLA	CAA-CBA-CGA-O2A
21	A	1011	CL0	C4-C3-C5-C6
22	A	1141	CLA	C4-C3-C5-C6
22	B	1221	CLA	C4-C3-C5-C6
22	5	602	CLA	C4-C3-C5-C6
26	9	801	LHG	C11-C12-C13-C14
22	B	1209	CLA	C2-C3-C5-C6
21	A	1011	CL0	C16-C17-C18-C20
22	Z	601	CLA	CBA-CGA-O2A-C1
26	6	801	LHG	C19-C20-C21-C22
22	Z	604	CLA	C13-C15-C16-C17
22	6	603	CLA	C13-C15-C16-C17
22	6	618	CLA	O1A-CGA-O2A-C1
31	J	5001	LMG	C7-C8-O7-C10
43	7	802	3PH	C3-C2-O21-C21
22	7	601	CLA	C10-C11-C12-C13
22	7	606	CLA	C5-C6-C7-C8
22	A	1105	CLA	C2-C1-O2A-CGA
22	B	1204	CLA	C2-C1-O2A-CGA
22	B	1223	CLA	C2-C1-O2A-CGA
22	1	606	CLA	C2-C1-O2A-CGA
22	1	608	CLA	C2-C1-O2A-CGA
22	Z	606	CLA	C2-C1-O2A-CGA
22	5	602	CLA	C2-C1-O2A-CGA
22	5	615	CLA	C2-C1-O2A-CGA
22	2	601	CLA	C2-C1-O2A-CGA
22	9	603	CLA	C2-C1-O2A-CGA
26	1	801	LHG	C11-C12-C13-C14
22	A	1121	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	B	1220	CLA	C3-C5-C6-C7
26	4	801	LHG	C19-C20-C21-C22
28	B	6101	LMT	C9-C10-C11-C12
22	8	609	CLA	C13-C15-C16-C17
27	8	802	NKP	CAG-OAF-PAC-OAD
43	5	802	3PH	C1-O11-P-O12
26	5	801	LHG	C13-C14-C15-C16
22	3	604	CLA	CBA-CGA-O2A-C1
22	5	602	CLA	CBA-CGA-O2A-C1
22	5	612	CLA	O1D-CGD-O2D-CED
22	6	605	CLA	C6-C7-C8-C10
26	A	5002	LHG	C11-C12-C13-C14
28	A	5006	LMT	C4'-C5'-C6'-O6'
22	B	1213	CLA	C10-C11-C12-C13
28	B	6101	LMT	C2-C3-C4-C5
22	5	607	CLA	C5-C6-C7-C8
38	7	803	SPH	C9-C10-C11-C12
43	8	806	3PH	C3A-C3B-C3C-C3D
22	1	611	CLA	C13-C15-C16-C17
22	9	606	CLA	O1A-CGA-O2A-C1
22	8	607	CLA	C6-C7-C8-C10
22	A	1132	CLA	C4-C3-C5-C6
22	B	1209	CLA	C4-C3-C5-C6
22	B	1021	CLA	C8-C10-C11-C12
22	3	610	CLA	C8-C10-C11-C12
21	A	1011	CL0	C2-C3-C5-C6
22	A	1012	CLA	C11-C12-C13-C15
22	A	1105	CLA	C12-C13-C15-C16
22	A	1106	CLA	C11-C12-C13-C15
22	A	1110	CLA	C6-C7-C8-C10
22	A	1114	CLA	C6-C7-C8-C10
22	A	1117	CLA	C6-C7-C8-C10
22	A	1128	CLA	C12-C13-C15-C16
22	A	1130	CLA	C11-C10-C8-C7
22	A	1132	CLA	C11-C12-C13-C15
22	A	1136	CLA	C6-C7-C8-C10
22	A	1138	CLA	C11-C10-C8-C7
22	A	1141	CLA	C2-C3-C5-C6
22	A	1101	CLA	C11-C12-C13-C15
22	B	1023	CLA	C11-C12-C13-C15
22	B	1203	CLA	C12-C13-C15-C16
22	B	1204	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	B	1207	CLA	C11-C10-C8-C7
22	B	1209	CLA	C11-C10-C8-C7
22	B	1210	CLA	C12-C13-C15-C16
22	B	1223	CLA	C11-C10-C8-C7
22	B	1228	CLA	C11-C10-C8-C7
22	B	1231	CLA	C12-C13-C15-C16
22	B	1234	CLA	C6-C7-C8-C10
22	B	1234	CLA	C11-C10-C8-C7
22	B	1238	CLA	C6-C7-C8-C10
22	B	1240	CLA	C11-C12-C13-C15
22	1	606	CLA	C6-C7-C8-C10
22	1	611	CLA	C11-C10-C8-C7
22	1	612	CLA	C11-C12-C13-C15
22	3	603	CLA	C11-C12-C13-C15
22	3	607	CLA	C6-C7-C8-C10
22	3	610	CLA	C11-C10-C8-C7
22	7	609	CLA	C11-C12-C13-C15
22	7	607	CLA	C11-C10-C8-C7
22	8	605	CLA	C11-C12-C13-C15
22	8	605	CLA	C12-C13-C15-C16
22	4	609	CLA	C11-C10-C8-C7
22	5	602	CLA	C2-C3-C5-C6
22	5	602	CLA	C6-C7-C8-C10
22	5	609	CLA	C11-C12-C13-C15
22	6	619	CLA	C6-C7-C8-C10
22	6	619	CLA	C11-C10-C8-C7
22	9	604	CLA	C11-C10-C8-C7
23	B	2002	PQN	C17-C18-C20-C21
40	Z	610	CHL	C11-C12-C13-C15
40	8	613	CHL	C11-C12-C13-C15
26	B	5001	LHG	C24-C23-O8-C6
22	B	1235	CLA	CAA-CBA-CGA-O2A
22	A	1012	CLA	C11-C12-C13-C14
22	A	1107	CLA	C11-C10-C8-C9
22	A	1109	CLA	C14-C13-C15-C16
22	A	1110	CLA	C6-C7-C8-C9
22	A	1117	CLA	C11-C10-C8-C9
22	A	1117	CLA	C11-C12-C13-C14
22	A	1119	CLA	C14-C13-C15-C16
22	A	1121	CLA	C14-C13-C15-C16
22	A	1122	CLA	C6-C7-C8-C9
22	A	1126	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	A	1130	CLA	C11-C10-C8-C9
22	A	1130	CLA	C11-C12-C13-C14
22	A	1132	CLA	C11-C12-C13-C14
22	A	1133	CLA	C6-C7-C8-C9
22	A	1138	CLA	C14-C13-C15-C16
22	A	1101	CLA	C14-C13-C15-C16
22	B	1203	CLA	C14-C13-C15-C16
22	B	1204	CLA	C11-C10-C8-C9
22	B	1209	CLA	C11-C10-C8-C9
22	B	1210	CLA	C14-C13-C15-C16
22	B	1212	CLA	C6-C7-C8-C9
22	B	1213	CLA	C6-C7-C8-C9
22	B	1234	CLA	C6-C7-C8-C9
22	B	1234	CLA	C11-C10-C8-C9
22	B	1235	CLA	C11-C12-C13-C14
22	B	1235	CLA	C14-C13-C15-C16
22	B	1236	CLA	C11-C12-C13-C14
22	L	1502	CLA	C11-C10-C8-C9
22	1	603	CLA	C11-C10-C8-C9
22	3	610	CLA	C11-C10-C8-C9
22	3	616	CLA	C6-C7-C8-C9
22	7	603	CLA	C14-C13-C15-C16
22	7	607	CLA	C11-C10-C8-C9
22	8	602	CLA	C11-C10-C8-C9
22	4	605	CLA	C6-C7-C8-C9
22	4	609	CLA	C11-C10-C8-C9
22	5	601	CLA	C6-C7-C8-C9
22	5	602	CLA	C6-C7-C8-C9
22	5	607	CLA	C6-C7-C8-C9
22	5	609	CLA	C11-C12-C13-C14
22	6	603	CLA	C14-C13-C15-C16
22	2	601	CLA	C6-C7-C8-C9
40	Z	610	CHL	C11-C10-C8-C9
40	8	613	CHL	C11-C12-C13-C14
40	5	610	CHL	C11-C10-C8-C9
40	9	610	CHL	C11-C10-C8-C9
22	4	612	CLA	C2A-CAA-CBA-CGA
26	2	801	LHG	C28-C29-C30-C31
22	6	607	CLA	O1D-CGD-O2D-CED
21	A	1011	CL0	O1A-CGA-O2A-C1
25	B	4006	BCR	C37-C22-C23-C24
39	Z	503	LUT	C7-C8-C9-C19

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Mol	Chain	Res	Type	Atoms
22	A	1116	CLA	C11-C12-C13-C14
22	B	1214	CLA	C11-C12-C13-C14
25	B	4006	BCR	C21-C22-C23-C24
39	Z	503	LUT	C27-C28-C29-C30
39	Z	503	LUT	C31-C32-C33-C34
26	4	801	LHG	C35-C36-C37-C38
30	A	5007	DAO	C3-C4-C5-C6
38	7	804	SPH	C15-C16-C17-C18
38	7	803	SPH	C7-C8-C9-C10
22	A	1121	CLA	C15-C16-C17-C18
22	B	1229	CLA	C5-C6-C7-C8
22	8	605	CLA	C5-C6-C7-C8
22	5	618	CLA	C5-C6-C7-C8
26	B	5006	LHG	C11-C12-C13-C14
26	1	801	LHG	C31-C32-C33-C34
43	8	806	3PH	C3C-C3D-C3E-C3F
22	B	1241	CLA	CBA-CGA-O2A-C1
31	J	5001	LMG	C29-C28-O8-C9
22	A	1128	CLA	C10-C11-C12-C13
26	2	801	LHG	C11-C12-C13-C14
22	A	1110	CLA	C13-C15-C16-C17
26	B	5001	LHG	O6-C4-C5-C6
26	1	801	LHG	O6-C4-C5-C6
26	4	802	LHG	O6-C4-C5-C6
26	5	801	LHG	O6-C4-C5-C6
43	7	802	3PH	O11-C1-C2-C3
43	6	802	3PH	O11-C1-C2-C3
22	B	1215	CLA	C5-C6-C7-C8
22	8	603	CLA	C8-C10-C11-C12
22	A	1117	CLA	C4-C3-C5-C6
22	B	1237	CLA	C4-C3-C5-C6
22	1	603	CLA	C4-C3-C5-C6
22	A	1132	CLA	C2-C3-C5-C6
22	1	603	CLA	C2-C3-C5-C6
22	7	615	CLA	C8-C10-C11-C12
22	9	604	CLA	C13-C15-C16-C17
22	2	604	CLA	C11-C10-C8-C9
22	B	1238	CLA	O1A-CGA-O2A-C1
22	5	602	CLA	O1A-CGA-O2A-C1
26	8	801	LHG	C30-C31-C32-C33
26	4	801	LHG	C18-C19-C20-C21
22	A	1013	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	6	608	CLA	C6-C7-C8-C10
22	Z	607	CLA	C8-C10-C11-C12
32	9	802	DGA	CB4-CB5-CB6-CB7
22	B	1220	CLA	C15-C16-C17-C18
22	8	603	CLA	C15-C16-C17-C18
22	8	602	CLA	CBA-CGA-O2A-C1
41	2	803	SQD	C7-C8-C9-C10
22	A	1126	CLA	C3A-C2A-CAA-CBA
22	A	1130	CLA	C3A-C2A-CAA-CBA
22	A	1133	CLA	C3A-C2A-CAA-CBA
22	A	1134	CLA	C3A-C2A-CAA-CBA
22	B	1204	CLA	C3A-C2A-CAA-CBA
22	B	1209	CLA	C3A-C2A-CAA-CBA
22	B	1230	CLA	C3A-C2A-CAA-CBA
22	1	606	CLA	C3A-C2A-CAA-CBA
22	3	607	CLA	C3A-C2A-CAA-CBA
22	7	606	CLA	C3A-C2A-CAA-CBA
22	7	616	CLA	C3A-C2A-CAA-CBA
22	8	606	CLA	C3A-C2A-CAA-CBA
22	5	615	CLA	C3A-C2A-CAA-CBA
22	6	609	CLA	C3A-C2A-CAA-CBA
40	7	610	CHL	C3A-C2A-CAA-CBA
40	5	611	CHL	C3A-C2A-CAA-CBA
25	A	4002	BCR	C13-C14-C15-C16
25	B	4005	BCR	C9-C10-C11-C12
25	I	4001	BCR	C9-C10-C11-C12
25	I	4001	BCR	C19-C20-C21-C22
25	J	4001	BCR	C9-C10-C11-C12
25	3	505	BCR	C13-C14-C15-C16
39	Z	502	LUT	C29-C30-C31-C32
39	3	502	LUT	C29-C30-C31-C32
39	4	502	LUT	C29-C30-C31-C32
28	B	6101	LMT	C2-C1-O1'-C1'
26	8	801	LHG	C13-C14-C15-C16
22	Z	601	CLA	O1A-CGA-O2A-C1
26	2	801	LHG	C26-C27-C28-C29
43	8	806	3PH	C39-C3A-C3B-C3C
22	A	1108	CLA	C10-C11-C12-C13
22	A	1122	CLA	C5-C6-C7-C8
22	A	1126	CLA	C8-C10-C11-C12
22	B	1220	CLA	C13-C15-C16-C17
22	B	1229	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
26	A	5002	LHG	C4-C5-C6-O8
26	4	802	LHG	C4-C5-C6-O8
31	J	5001	LMG	O1-C7-C8-C9
41	2	803	SQD	O6-C44-C45-C46
43	6	802	3PH	C1-C2-C3-O31
26	7	801	LHG	C25-C26-C27-C28
33	B	5003	DGD	CAA-CBA-CCA-CDA
26	6	801	LHG	C35-C36-C37-C38
22	6	604	CLA	C13-C15-C16-C17
27	3	802	NKP	OBC-CAH-CAI-OAJ
26	Z	801	LHG	C16-C17-C18-C19
31	J	5001	LMG	C30-C31-C32-C33
26	2	801	LHG	C3-O3-P-O6
35	B	5004	T7X	C15-C16-C17-C18
35	B	5004	T7X	C21-C22-C23-C24
35	B	5004	T7X	C22-C23-C24-C25
33	B	5003	DGD	C1A-C2A-C3A-C4A
40	Z	610	CHL	C2A-CAA-CBA-CGA
40	4	611	CHL	C2A-CAA-CBA-CGA
40	2	613	CHL	C2A-CAA-CBA-CGA
22	A	1138	CLA	C13-C15-C16-C17
22	B	1209	CLA	C10-C11-C12-C13
26	A	5002	LHG	C29-C30-C31-C32
26	A	5002	LHG	O6-C4-C5-O7
26	Z	801	LHG	O6-C4-C5-O7
26	9	801	LHG	O6-C4-C5-O7
22	A	1132	CLA	CBA-CGA-O2A-C1
22	B	1241	CLA	O1A-CGA-O2A-C1
21	A	1011	CL0	C16-C17-C18-C19
22	A	1116	CLA	C11-C12-C13-C15
22	6	603	CLA	C15-C16-C17-C18
26	1	801	LHG	C16-C17-C18-C19
22	A	1013	CLA	C8-C10-C11-C12
31	J	5001	LMG	O10-C28-O8-C9
41	1	802	SQD	C16-C17-C18-C19
26	A	5002	LHG	O7-C5-C6-O8
26	Z	801	LHG	O7-C5-C6-O8
33	B	5003	DGD	O1G-C1G-C2G-O2G
33	B	5003	DGD	O2G-C2G-C3G-O3G
43	8	806	3PH	O21-C2-C3-O31
43	6	802	3PH	O21-C2-C3-O31
25	8	503	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
28	B	5005	LMT	C4-C5-C6-C7
21	A	1011	CL0	CBD-CGD-O2D-CED
26	A	5002	LHG	C35-C36-C37-C38
35	B	5004	T7X	C27-C28-C29-C30
22	B	1224	CLA	C4-C3-C5-C6
22	1	605	CLA	C2-C1-O2A-CGA
22	A	1117	CLA	C2-C3-C5-C6
22	B	1224	CLA	C2-C3-C5-C6
22	A	1108	CLA	C14-C13-C15-C16
22	A	1109	CLA	C11-C10-C8-C9
22	B	1021	CLA	C11-C10-C8-C9
22	B	1023	CLA	C11-C10-C8-C9
22	B	1205	CLA	C11-C10-C8-C9
22	B	1209	CLA	C11-C12-C13-C14
22	B	1210	CLA	C11-C12-C13-C14
22	B	1216	CLA	C14-C13-C15-C16
22	B	1223	CLA	C14-C13-C15-C16
22	B	1228	CLA	C11-C10-C8-C9
22	3	606	CLA	C6-C7-C8-C9
22	3	607	CLA	C6-C7-C8-C9
22	7	609	CLA	C14-C13-C15-C16
22	7	603	CLA	C11-C10-C8-C9
22	5	618	CLA	C14-C13-C15-C16
22	6	606	CLA	C14-C13-C15-C16
22	6	619	CLA	C11-C10-C8-C9
22	9	601	CLA	C11-C10-C8-C9
40	Z	609	CHL	C11-C10-C8-C9
22	B	1230	CLA	C10-C11-C12-C13
26	Z	801	LHG	C11-C10-C9-C8
26	B	5002	LHG	C2-C3-O3-P
26	1	801	LHG	C2-C3-O3-P
26	Z	801	LHG	C2-C3-O3-P
26	8	801	LHG	C2-C3-O3-P
26	6	801	LHG	C2-C3-O3-P
22	8	602	CLA	O1A-CGA-O2A-C1
26	1	801	LHG	C9-C10-C11-C12
22	F	1302	CLA	C2A-CAA-CBA-CGA
22	Z	604	CLA	C2A-CAA-CBA-CGA
22	6	608	CLA	C6-C7-C8-C9
22	6	606	CLA	C16-C17-C18-C20
25	A	4001	BCR	C23-C24-C25-C26
25	B	4007	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	B	4007	BCR	C5-C6-C7-C8
25	K	4001	BCR	C5-C6-C7-C8
25	K	4002	BCR	C1-C6-C7-C8
25	L	4001	BCR	C1-C6-C7-C8
25	L	4001	BCR	C5-C6-C7-C8
25	3	503	BCR	C23-C24-C25-C26
25	3	506	BCR	C5-C6-C7-C8
25	6	503	BCR	C23-C24-C25-C26
37	J	4002	C7Z	C5-C6-C7-C8
39	1	501	LUT	C1-C6-C7-C8
39	Z	501	LUT	C5-C6-C7-C8
39	7	501	LUT	C1-C6-C7-C8
39	7	501	LUT	C5-C6-C7-C8
39	8	501	LUT	C5-C6-C7-C8
39	2	501	LUT	C1-C6-C7-C8
39	2	501	LUT	C5-C6-C7-C8
22	A	1139	CLA	C10-C11-C12-C13
22	7	603	CLA	C10-C11-C12-C13
22	6	609	CLA	C15-C16-C17-C18
22	6	603	CLA	C5-C6-C7-C8
28	B	5005	LMT	C3-C4-C5-C6
22	K	1402	CLA	CAA-CBA-CGA-O2A
25	A	4001	BCR	C37-C22-C23-C24
25	3	504	BCR	C36-C18-C19-C20
25	7	503	BCR	C11-C12-C13-C35
25	B	4002	BCR	C17-C18-C19-C20
25	B	4007	BCR	C7-C8-C9-C10
25	B	4006	BCR	C17-C18-C19-C20
25	K	4001	BCR	C17-C18-C19-C20
25	K	4002	BCR	C7-C8-C9-C10
25	4	503	BCR	C7-C8-C9-C10
25	4	503	BCR	C11-C12-C13-C14
37	1	503	C7Z	C7-C8-C9-C10
37	5	505	C7Z	C31-C32-C33-C34
39	2	503	LUT	C11-C12-C13-C14
22	A	1105	CLA	C10-C11-C12-C13
22	A	1114	CLA	C5-C6-C7-C8
22	A	1127	CLA	C13-C15-C16-C17
22	B	1239	CLA	C8-C10-C11-C12
22	8	607	CLA	C6-C7-C8-C9
42	Z	504	QTB	C09-C10-C11-C12
22	B	1219	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	B	1223	CLA	C13-C15-C16-C17
26	4	802	LHG	C12-C13-C14-C15
28	B	6101	LMT	O1'-C1-C2-C3
22	4	604	CLA	C8-C10-C11-C12
22	6	615	CLA	C5-C6-C7-C8
26	A	5001	LHG	O6-C4-C5-C6
26	A	5002	LHG	O6-C4-C5-C6
26	3	801	LHG	O6-C4-C5-C6
26	4	802	LHG	C9-C10-C11-C12
22	A	1012	CLA	C11-C10-C8-C7
22	A	1104	CLA	C6-C7-C8-C10
22	A	1104	CLA	C11-C12-C13-C15
22	A	1107	CLA	C11-C10-C8-C7
22	A	1108	CLA	C12-C13-C15-C16
22	A	1109	CLA	C11-C10-C8-C7
22	A	1109	CLA	C12-C13-C15-C16
22	A	1117	CLA	C11-C10-C8-C7
22	A	1117	CLA	C11-C12-C13-C15
22	A	1119	CLA	C12-C13-C15-C16
22	A	1121	CLA	C12-C13-C15-C16
22	A	1122	CLA	C6-C7-C8-C10
22	A	1122	CLA	C12-C13-C15-C16
22	A	1126	CLA	C6-C7-C8-C10
22	A	1126	CLA	C11-C12-C13-C15
22	A	1130	CLA	C6-C7-C8-C10
22	A	1133	CLA	C6-C7-C8-C10
22	A	1136	CLA	C12-C13-C15-C16
22	A	1137	CLA	C11-C10-C8-C7
22	A	1138	CLA	C12-C13-C15-C16
22	A	1013	CLA	C11-C10-C8-C7
22	A	1101	CLA	C11-C10-C8-C7
22	A	1101	CLA	C12-C13-C15-C16
22	B	1237	CLA	C6-C7-C8-C10
22	B	1021	CLA	C11-C10-C8-C7
22	B	1023	CLA	C11-C10-C8-C7
22	B	1205	CLA	C11-C10-C8-C7
22	B	1212	CLA	C6-C7-C8-C10
22	B	1213	CLA	C6-C7-C8-C10
22	B	1216	CLA	C6-C7-C8-C10
22	B	1216	CLA	C11-C12-C13-C15
22	B	1216	CLA	C12-C13-C15-C16
22	B	1218	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	B	1223	CLA	C11-C12-C13-C15
22	B	1223	CLA	C12-C13-C15-C16
22	B	1235	CLA	C11-C12-C13-C15
22	B	1235	CLA	C12-C13-C15-C16
22	B	1236	CLA	C6-C7-C8-C10
22	B	1236	CLA	C11-C12-C13-C15
22	L	1502	CLA	C11-C10-C8-C7
22	1	611	CLA	C6-C7-C8-C10
22	1	612	CLA	C11-C10-C8-C7
22	3	603	CLA	C11-C10-C8-C7
22	3	606	CLA	C6-C7-C8-C10
22	3	616	CLA	C6-C7-C8-C10
22	7	609	CLA	C12-C13-C15-C16
22	7	603	CLA	C11-C10-C8-C7
22	7	603	CLA	C12-C13-C15-C16
22	7	607	CLA	C11-C12-C13-C15
22	8	609	CLA	C12-C13-C15-C16
22	8	602	CLA	C11-C10-C8-C7
22	8	602	CLA	C12-C13-C15-C16
22	5	601	CLA	C6-C7-C8-C10
22	5	612	CLA	C11-C12-C13-C15
22	5	618	CLA	C12-C13-C15-C16
22	6	603	CLA	C12-C13-C15-C16
22	6	604	CLA	C11-C12-C13-C15
22	6	606	CLA	C12-C13-C15-C16
22	2	601	CLA	C6-C7-C8-C10
22	9	601	CLA	C11-C10-C8-C7
22	9	603	CLA	C11-C10-C8-C7
23	B	2002	PQN	C16-C17-C18-C20
40	Z	609	CHL	C11-C10-C8-C7
40	8	613	CHL	C11-C10-C8-C7
40	5	610	CHL	C11-C10-C8-C7
40	5	610	CHL	C12-C13-C15-C16
40	9	610	CHL	C11-C10-C8-C7
25	A	4002	BCR	C9-C10-C11-C12
25	B	4007	BCR	C19-C20-C21-C22
25	I	4001	BCR	C13-C14-C15-C16
25	K	4002	BCR	C19-C20-C21-C22
25	L	4001	BCR	C13-C14-C15-C16
25	L	4002	BCR	C13-C14-C15-C16
25	4	503	BCR	C9-C10-C11-C12
25	5	503	BCR	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	6	503	BCR	C19-C20-C21-C22
37	J	4002	C7Z	C29-C30-C31-C32
39	1	502	LUT	C29-C30-C31-C32
39	7	501	LUT	C29-C30-C31-C32
39	6	501	LUT	C29-C30-C31-C32
39	9	501	LUT	C29-C30-C31-C32
26	4	801	LHG	C31-C32-C33-C34
22	B	1227	CLA	C2A-CAA-CBA-CGA
22	Z	601	CLA	C2A-CAA-CBA-CGA
25	5	504	BCR	C11-C10-C9-C34
26	A	5001	LHG	C10-C11-C12-C13
22	B	1240	CLA	C16-C17-C18-C19
22	A	1105	CLA	C5-C6-C7-C8
22	B	1211	CLA	C10-C11-C12-C13
22	L	1502	CLA	C15-C16-C17-C18
22	8	601	CLA	C5-C6-C7-C8
22	5	609	CLA	C13-C15-C16-C17
32	9	802	DGA	CBB-CAB-CB9-CB8
22	A	1124	CLA	CAD-CBD-CGD-O2D
22	A	1132	CLA	CAD-CBD-CGD-O2D
22	B	1205	CLA	CAD-CBD-CGD-O2D
22	B	1211	CLA	CAD-CBD-CGD-O2D
22	B	1212	CLA	CAD-CBD-CGD-O2D
22	B	1218	CLA	CAD-CBD-CGD-O2D
22	B	1221	CLA	CAD-CBD-CGD-O2D
22	G	1602	CLA	CAD-CBD-CGD-O2D
22	K	1402	CLA	CAD-CBD-CGD-O2D
22	K	1404	CLA	CAD-CBD-CGD-O2D
22	Z	604	CLA	CAD-CBD-CGD-O2D
22	3	607	CLA	CAD-CBD-CGD-O2D
22	8	605	CLA	CAD-CBD-CGD-O2D
22	2	608	CLA	CAD-CBD-CGD-O2D
40	6	613	CHL	CAD-CBD-CGD-O2D
22	3	605	CLA	CBA-CGA-O2A-C1
22	2	604	CLA	CBA-CGA-O2A-C1
22	8	602	CLA	C4-C3-C5-C6
26	3	801	LHG	C2-C3-O3-P
26	3	801	LHG	C4-C5-C6-O8
26	8	801	LHG	C4-C5-C6-O8
26	5	801	LHG	C4-C5-C6-O8
41	2	803	SQD	C44-C45-C46-O48
26	B	5006	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
26	4	802	LHG	O6-C4-C5-O7
26	5	801	LHG	O6-C4-C5-O7
43	7	802	3PH	O11-C1-C2-O21
22	B	1220	CLA	C8-C10-C11-C12
26	5	801	LHG	O8-C23-C24-C25
28	9	803	LMT	C2B-C1B-O1B-C4'
22	5	605	CLA	C2A-CAA-CBA-CGA
38	7	803	SPH	C11-C12-C13-C14
22	Z	602	CLA	CBA-CGA-O2A-C1
28	9	803	LMT	C3-C4-C5-C6
22	B	1222	CLA	O1D-CGD-O2D-CED
22	A	1106	CLA	CHA-CBD-CGD-O1D
22	A	1106	CLA	CHA-CBD-CGD-O2D
22	A	1111	CLA	CHA-CBD-CGD-O2D
22	A	1129	CLA	CHA-CBD-CGD-O1D
22	A	1134	CLA	CHA-CBD-CGD-O1D
22	A	1134	CLA	CHA-CBD-CGD-O2D
22	A	1138	CLA	CHA-CBD-CGD-O1D
22	Z	605	CLA	CHA-CBD-CGD-O1D
22	Z	605	CLA	CHA-CBD-CGD-O2D
22	Z	615	CLA	CHA-CBD-CGD-O1D
22	Z	615	CLA	CHA-CBD-CGD-O2D
22	7	609	CLA	CHA-CBD-CGD-O1D
22	7	609	CLA	CHA-CBD-CGD-O2D
22	7	611	CLA	CHA-CBD-CGD-O1D
22	7	611	CLA	CHA-CBD-CGD-O2D
22	4	607	CLA	CHA-CBD-CGD-O2D
22	6	615	CLA	CHA-CBD-CGD-O1D
22	6	615	CLA	CHA-CBD-CGD-O2D
22	2	603	CLA	CHA-CBD-CGD-O1D
22	2	605	CLA	CHA-CBD-CGD-O1D
22	2	605	CLA	CHA-CBD-CGD-O2D
22	2	606	CLA	CHA-CBD-CGD-O1D
22	2	606	CLA	CHA-CBD-CGD-O2D
22	9	604	CLA	CHA-CBD-CGD-O2D
22	9	609	CLA	CHA-CBD-CGD-O2D
40	1	610	CHL	CHA-CBD-CGD-O1D
40	1	610	CHL	CHA-CBD-CGD-O2D
40	6	610	CHL	CHA-CBD-CGD-O2D
40	6	610	CHL	C3-C5-C6-C7
22	A	1132	CLA	O1A-CGA-O2A-C1
25	5	504	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
28	9	803	LMT	C2'-C1'-O1'-C1
41	1	802	SQD	C2-C1-O6-C44
43	7	802	3PH	C39-C3A-C3B-C3C
43	6	802	3PH	C24-C25-C26-C27
26	B	5001	LHG	O7-C5-C6-O8
26	3	801	LHG	O7-C5-C6-O8
26	6	801	LHG	O7-C5-C6-O8
41	2	803	SQD	O6-C44-C45-O47
22	7	607	CLA	C8-C10-C11-C12
22	3	604	CLA	O1A-CGA-O2A-C1
26	A	5002	LHG	O1-C1-C2-O2
26	7	801	LHG	O1-C1-C2-O2
38	K	5001	SPH	C6-C7-C8-C9
22	A	1128	CLA	C3-C5-C6-C7
22	B	1202	CLA	C4-C3-C5-C6
22	B	1228	CLA	C4-C3-C5-C6
26	A	5002	LHG	C16-C17-C18-C19
22	A	1102	CLA	O1D-CGD-O2D-CED
26	Z	801	LHG	C30-C31-C32-C33
22	A	1012	CLA	C11-C10-C8-C9
22	A	1104	CLA	C11-C12-C13-C14
22	A	1130	CLA	C6-C7-C8-C9
22	A	1137	CLA	C11-C10-C8-C9
22	B	1237	CLA	C6-C7-C8-C9
22	B	1231	CLA	C11-C12-C13-C14
22	Z	605	CLA	C6-C7-C8-C9
22	7	605	CLA	C11-C12-C13-C14
22	8	602	CLA	C14-C13-C15-C16
38	7	804	SPH	C12-C13-C14-C15
41	2	803	SQD	C5-C6-S-O8
32	A	5005	DGA	CB5-CB6-CB7-CB8
33	B	5003	DGD	C7A-C8A-C9A-CAA
22	A	1109	CLA	C2A-CAA-CBA-CGA
22	B	1206	CLA	C8-C10-C11-C12
25	A	4003	BCR	C37-C22-C23-C24
25	K	4001	BCR	C36-C18-C19-C20
25	L	4002	BCR	C37-C22-C23-C24
25	7	503	BCR	C37-C22-C23-C24
25	5	503	BCR	C36-C18-C19-C20
22	6	609	CLA	C13-C15-C16-C17
28	9	803	LMT	C11-C10-C9-C8
25	A	4003	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
25	L	4002	BCR	C21-C22-C23-C24
25	7	503	BCR	C11-C12-C13-C14
25	7	503	BCR	C21-C22-C23-C24
25	6	503	BCR	C17-C18-C19-C20
39	Z	503	LUT	C7-C8-C9-C10
22	A	1107	CLA	C1A-C2A-CAA-CBA
22	B	1230	CLA	C1A-C2A-CAA-CBA
22	B	1232	CLA	C1A-C2A-CAA-CBA
22	Z	611	CLA	C1A-C2A-CAA-CBA
22	Z	615	CLA	C1A-C2A-CAA-CBA
22	7	606	CLA	C1A-C2A-CAA-CBA
22	4	606	CLA	C1A-C2A-CAA-CBA
22	4	607	CLA	C1A-C2A-CAA-CBA
22	5	607	CLA	C1A-C2A-CAA-CBA
22	5	608	CLA	C1A-C2A-CAA-CBA
22	5	615	CLA	C1A-C2A-CAA-CBA
22	2	608	CLA	C1A-C2A-CAA-CBA
33	B	5003	DGD	C1B-C2B-C3B-C4B
22	B	1210	CLA	C16-C17-C18-C19
22	B	1226	CLA	C16-C17-C18-C19
22	A	1121	CLA	C13-C15-C16-C17
32	9	802	DGA	CA7-CA8-CA9-CAA
22	A	1110	CLA	C2-C1-O2A-CGA
22	A	1127	CLA	C2-C1-O2A-CGA
22	A	1136	CLA	C2-C1-O2A-CGA
22	7	607	CLA	C2-C1-O2A-CGA
22	7	611	CLA	C2-C1-O2A-CGA
22	5	603	CLA	C2-C1-O2A-CGA
22	6	619	CLA	C2-C1-O2A-CGA
37	1	503	C7Z	C13-C14-C15-C35
39	8	502	LUT	C29-C30-C31-C32
26	3	801	LHG	C3-O3-P-O6
26	3	801	LHG	C4-O6-P-O3
26	4	801	LHG	C4-O6-P-O3
26	5	801	LHG	C3-O3-P-O6
26	9	801	LHG	C4-O6-P-O3
43	7	802	3PH	C27-C28-C29-C2A
45	8	803	LPX	C4-C3-O1-P1
26	A	5002	LHG	C3-O3-P-O4
26	B	5002	LHG	C4-O6-P-O4
26	1	801	LHG	C4-O6-P-O5
26	8	801	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
26	4	802	LHG	C4-O6-P-O5
22	A	1118	CLA	C11-C12-C13-C14
22	1	608	CLA	C11-C12-C13-C14
22	4	605	CLA	C16-C17-C18-C20
22	6	619	CLA	C16-C17-C18-C20
22	9	605	CLA	C6-C7-C8-C9
22	B	1221	CLA	CBA-CGA-O2A-C1
26	B	5006	LHG	O6-C4-C5-C6
26	7	801	LHG	O6-C4-C5-C6
26	9	801	LHG	O6-C4-C5-C6
22	8	612	CLA	O1D-CGD-O2D-CED
22	A	1140	CLA	C8-C10-C11-C12
22	6	608	CLA	C2A-CAA-CBA-CGA
22	A	1114	CLA	C3-C5-C6-C7
22	B	1222	CLA	C3-C5-C6-C7
22	3	605	CLA	O1A-CGA-O2A-C1
22	B	1021	CLA	C16-C17-C18-C20
22	3	601	CLA	C16-C17-C18-C19
22	4	603	CLA	C16-C17-C18-C19
35	B	5004	T7X	C31-C32-C33-C34
22	B	1234	CLA	CAD-CBD-CGD-O1D
22	Z	605	CLA	CAD-CBD-CGD-O1D
22	Z	606	CLA	CAD-CBD-CGD-O1D
22	7	609	CLA	CAD-CBD-CGD-O1D
22	8	609	CLA	CAD-CBD-CGD-O1D
22	6	615	CLA	CAD-CBD-CGD-O1D
22	2	605	CLA	CAD-CBD-CGD-O1D
22	2	606	CLA	CAD-CBD-CGD-O1D
40	1	610	CHL	CAD-CBD-CGD-O1D
41	2	803	SQD	C5-C6-S-O7
26	4	801	LHG	C33-C34-C35-C36
22	8	612	CLA	CBD-CGD-O2D-CED
27	A	5004	NKP	CAK-CAL-CAM-CAN
26	6	801	LHG	C27-C28-C29-C30
22	B	1208	CLA	CBA-CGA-O2A-C1
22	A	1122	CLA	C16-C17-C18-C20
22	A	1110	CLA	C4-C3-C5-C6
22	A	1105	CLA	C6-C7-C8-C10
22	A	1125	CLA	C12-C13-C15-C16
22	B	1203	CLA	C11-C12-C13-C15
22	B	1206	CLA	C6-C7-C8-C10
22	B	1206	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	B	1208	CLA	C6-C7-C8-C10
22	B	1215	CLA	C6-C7-C8-C10
22	B	1217	CLA	C6-C7-C8-C10
22	B	1219	CLA	C6-C7-C8-C10
22	B	1220	CLA	C6-C7-C8-C10
22	B	1221	CLA	C12-C13-C15-C16
22	B	1241	CLA	C11-C10-C8-C7
22	1	604	CLA	C6-C7-C8-C10
22	1	611	CLA	C12-C13-C15-C16
22	Z	604	CLA	C6-C7-C8-C10
22	Z	612	CLA	C6-C7-C8-C10
22	Z	612	CLA	C11-C10-C8-C7
22	4	605	CLA	C6-C7-C8-C10
22	5	602	CLA	C11-C12-C13-C15
26	B	5001	LHG	O6-C4-C5-O7
26	3	801	LHG	O6-C4-C5-O7
26	7	801	LHG	O6-C4-C5-O7
39	1	502	LUT	C25-C26-C27-C28
39	Z	502	LUT	C25-C26-C27-C28
39	Z	503	LUT	C25-C26-C27-C28
39	4	502	LUT	C25-C26-C27-C28
39	5	502	LUT	C25-C26-C27-C28
39	6	501	LUT	C25-C26-C27-C28
39	6	502	LUT	C25-C26-C27-C28
39	9	502	LUT	C25-C26-C27-C28
43	6	802	3PH	O11-C1-C2-O21
22	6	619	CLA	C3-C5-C6-C7
41	1	802	SQD	C13-C14-C15-C16
25	G	4001	BCR	C9-C10-C11-C12
39	Z	501	LUT	C29-C30-C31-C32
39	6	502	LUT	C29-C30-C31-C32
28	A	5006	LMT	C2-C3-C4-C5
22	5	612	CLA	C10-C11-C12-C13
26	1	801	LHG	C26-C27-C28-C29
22	A	1137	CLA	C13-C15-C16-C17
22	1	612	CLA	C2A-CAA-CBA-CGA
22	5	604	CLA	C16-C17-C18-C20
32	9	802	DGA	CB1-CB2-CB3-CB4
26	B	5001	LHG	C4-C5-C6-O8
38	7	804	SPH	O1-C1-C2-N2
43	7	802	3PH	C1-C2-C3-O31
43	8	806	3PH	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
43	6	802	3PH	C28-C29-C2A-C2B
26	B	5006	LHG	O7-C5-C6-O8
26	1	801	LHG	O7-C5-C6-O8
26	8	801	LHG	O7-C5-C6-O8
26	4	801	LHG	O7-C5-C6-O8
31	A	5003	LMG	O1-C7-C8-O7
35	B	5004	T7X	O16-C8-C9-O18
41	2	803	SQD	O47-C45-C46-O48
43	7	802	3PH	O21-C2-C3-O31
28	F	5001	LMT	C11-C10-C9-C8
21	A	1011	CL0	O1D-CGD-O2D-CED
22	2	604	CLA	O1A-CGA-O2A-C1
31	J	5001	LMG	C8-C7-O1-C1
22	6	606	CLA	C16-C17-C18-C19
22	A	1123	CLA	C15-C16-C17-C18
22	A	1132	CLA	C10-C11-C12-C13
22	B	1202	CLA	C15-C16-C17-C18
22	5	607	CLA	C10-C11-C12-C13
22	5	618	CLA	C15-C16-C17-C18
22	6	608	CLA	C3-C5-C6-C7
22	A	1120	CLA	O1D-CGD-O2D-CED
22	7	609	CLA	C13-C15-C16-C17
22	5	613	CLA	C5-C6-C7-C8
22	A	1108	CLA	C4-C3-C5-C6
40	7	610	CHL	C4-C3-C5-C6
22	A	1135	CLA	CBA-CGA-O2A-C1
22	B	1228	CLA	C2-C3-C5-C6
22	A	1117	CLA	C6-C7-C8-C9
22	A	1122	CLA	C14-C13-C15-C16
22	A	1131	CLA	C6-C7-C8-C9
22	A	1013	CLA	C11-C10-C8-C9
22	B	1207	CLA	C14-C13-C15-C16
22	B	1216	CLA	C11-C12-C13-C14
22	B	1218	CLA	C6-C7-C8-C9
22	B	1223	CLA	C11-C12-C13-C14
22	B	1236	CLA	C6-C7-C8-C9
22	B	1241	CLA	C11-C10-C8-C9
22	1	606	CLA	C6-C7-C8-C9
22	1	612	CLA	C11-C10-C8-C9
22	3	603	CLA	C11-C10-C8-C9
22	7	604	CLA	C11-C10-C8-C9
22	7	607	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	8	609	CLA	C14-C13-C15-C16
22	5	612	CLA	C11-C12-C13-C14
22	6	604	CLA	C11-C12-C13-C14
22	9	603	CLA	C11-C10-C8-C9
23	B	2002	PQN	C16-C17-C18-C19
40	3	611	CHL	C6-C7-C8-C9
40	8	613	CHL	C11-C10-C8-C9
40	5	610	CHL	C14-C13-C15-C16
22	B	1234	CLA	O1A-CGA-O2A-C1
22	B	1240	CLA	C16-C17-C18-C20
26	3	801	LHG	O1-C1-C2-O2
32	9	802	DGA	CB6-CB7-CB8-CB9
25	B	4005	BCR	C18-C19-C20-C21
25	3	506	BCR	C18-C19-C20-C21
25	5	504	BCR	C18-C19-C20-C21
25	6	504	BCR	C18-C19-C20-C21
25	A	4003	BCR	C36-C18-C19-C20
25	3	504	BCR	C11-C12-C13-C35
22	A	1122	CLA	C15-C16-C17-C18
22	B	1208	CLA	O1A-CGA-O2A-C1
26	Z	801	LHG	C11-C12-C13-C14
26	6	801	LHG	C10-C11-C12-C13
45	8	803	LPX	C11-C12-C13-C14
26	8	801	LHG	C26-C27-C28-C29
22	B	1220	CLA	O1D-CGD-O2D-CED
25	A	4001	BCR	C17-C18-C19-C20
26	6	801	LHG	C33-C34-C35-C36
40	8	610	CHL	CAA-CBA-CGA-O2A
22	A	1118	CLA	C5-C6-C7-C8
22	7	607	CLA	C10-C11-C12-C13
22	B	1204	CLA	C13-C15-C16-C17
22	3	612	CLA	C5-C6-C7-C8
22	A	1125	CLA	O1A-CGA-O2A-C1
22	A	1136	CLA	CAA-CBA-CGA-O2A
22	B	1221	CLA	CAA-CBA-CGA-O2A
38	7	803	SPH	C13-C14-C15-C16
43	8	806	3PH	C38-C39-C3A-C3B
22	L	1502	CLA	C8-C10-C11-C12
22	B	1208	CLA	C2A-CAA-CBA-CGA
22	7	605	CLA	C2A-CAA-CBA-CGA
22	6	609	CLA	C2A-CAA-CBA-CGA
22	A	1135	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	B	1234	CLA	CBA-CGA-O2A-C1
22	Z	601	CLA	C2-C1-O2A-CGA
22	A	1120	CLA	CBD-CGD-O2D-CED
22	B	1221	CLA	O1A-CGA-O2A-C1
26	4	802	LHG	C2-C3-O3-P
26	B	5006	LHG	O8-C23-C24-C25
22	B	1210	CLA	C16-C17-C18-C20
22	7	609	CLA	C4-C3-C5-C6
22	A	1122	CLA	O1D-CGD-O2D-CED
25	A	4001	BCR	C23-C24-C25-C30
25	B	4002	BCR	C5-C6-C7-C8
25	3	506	BCR	C1-C6-C7-C8
39	1	501	LUT	C5-C6-C7-C8
39	Z	501	LUT	C1-C6-C7-C8
39	3	502	LUT	C1-C6-C7-C8
39	3	502	LUT	C5-C6-C7-C8
22	B	1237	CLA	C2-C3-C5-C6
22	B	1202	CLA	C2-C3-C5-C6
22	8	602	CLA	C2-C3-C5-C6
22	B	1235	CLA	C5-C6-C7-C8
22	A	1121	CLA	C16-C17-C18-C20
22	4	608	CLA	C6-C7-C8-C10
31	J	5001	LMG	O1-C7-C8-O7
41	1	802	SQD	O47-C45-C46-O48
30	A	5007	DAO	C6-C7-C8-C9
26	A	5001	LHG	C3-O3-P-O6
26	1	801	LHG	C3-O3-P-O6
26	Z	801	LHG	C3-O3-P-O6
26	7	801	LHG	C3-O3-P-O6
26	8	801	LHG	C3-O3-P-O6
26	4	801	LHG	C3-O3-P-O6
26	6	801	LHG	C4-O6-P-O3
26	2	801	LHG	C4-O6-P-O3
35	B	5004	T7X	C7-O13-P1-O1
26	6	801	LHG	C24-C25-C26-C27
32	9	802	DGA	CB7-CB8-CB9-CAB
38	K	5001	SPH	C10-C11-C12-C13
33	B	5003	DGD	C1G-C2G-C3G-O3G
41	1	802	SQD	C44-C45-C46-O48
43	6	802	3PH	C27-C28-C29-C2A
22	A	1108	CLA	C5-C6-C7-C8
22	B	1234	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	A	1130	CLA	C11-C12-C13-C15
22	Z	605	CLA	C6-C7-C8-C10
22	7	605	CLA	C11-C12-C13-C15
22	A	1124	CLA	C11-C10-C8-C9
22	A	1125	CLA	C14-C13-C15-C16
22	A	1126	CLA	C6-C7-C8-C9
22	A	1138	CLA	C11-C10-C8-C9
22	B	1203	CLA	C11-C12-C13-C14
22	B	1206	CLA	C6-C7-C8-C9
22	B	1208	CLA	C6-C7-C8-C9
22	B	1216	CLA	C6-C7-C8-C9
22	B	1217	CLA	C6-C7-C8-C9
22	B	1219	CLA	C6-C7-C8-C9
22	B	1240	CLA	C11-C12-C13-C14
22	1	604	CLA	C6-C7-C8-C9
22	1	611	CLA	C11-C10-C8-C9
22	1	611	CLA	C14-C13-C15-C16
22	1	612	CLA	C11-C12-C13-C14
22	Z	604	CLA	C6-C7-C8-C9
22	Z	612	CLA	C11-C10-C8-C9
22	7	609	CLA	C11-C12-C13-C14
22	8	605	CLA	C11-C12-C13-C14
22	5	602	CLA	C11-C12-C13-C14
25	B	4002	BCR	C9-C10-C11-C12
25	B	4002	BCR	C13-C14-C15-C16
25	B	4006	BCR	C9-C10-C11-C12
25	J	4001	BCR	C19-C20-C21-C22
25	3	503	BCR	C19-C20-C21-C22
25	4	503	BCR	C19-C20-C21-C22
39	8	501	LUT	C29-C30-C31-C32
32	A	5005	DGA	OB1-CB1-OG2-CG2
22	B	1203	CLA	C2A-CAA-CBA-CGA
22	3	601	CLA	C16-C17-C18-C20
28	B	6101	LMT	C7-C8-C9-C10
26	5	801	LHG	C12-C13-C14-C15
35	B	5004	T7X	O16-C10-C12-C13
25	A	4004	BCR	C17-C18-C19-C20
22	3	613	CLA	C3-C5-C6-C7
22	2	604	CLA	C11-C10-C8-C7
27	A	5004	NKP	OAF-CAG-CAH-CAI
22	B	1203	CLA	C13-C15-C16-C17
22	B	1230	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	1	612	CLA	C4-C3-C5-C6
22	A	1118	CLA	C11-C12-C13-C15
22	4	603	CLA	C16-C17-C18-C20
22	A	1125	CLA	CBA-CGA-O2A-C1
22	8	604	CLA	C5-C6-C7-C8
26	A	5002	LHG	C32-C33-C34-C35
22	1	612	CLA	CBA-CGA-O2A-C1
22	1	608	CLA	C11-C12-C13-C15
28	B	5005	LMT	O5'-C1'-O1'-C1
25	A	4002	BCR	C19-C20-C21-C22
25	A	4004	BCR	C19-C20-C21-C22
25	K	4001	BCR	C15-C16-C17-C18
25	3	505	BCR	C15-C16-C17-C18
25	6	503	BCR	C15-C16-C17-C18
37	5	505	C7Z	C9-C10-C11-C12
37	5	505	C7Z	C33-C34-C35-C15
39	3	501	LUT	C29-C30-C31-C32
39	5	502	LUT	C29-C30-C31-C32
22	3	605	CLA	C10-C11-C12-C13
22	B	1211	CLA	C3-C5-C6-C7
22	5	618	CLA	C4-C3-C5-C6
22	B	1210	CLA	C15-C16-C17-C18
23	A	2001	PQN	C15-C16-C17-C18
22	A	1117	CLA	C8-C10-C11-C12
22	A	1139	CLA	C2-C1-O2A-CGA
22	B	1241	CLA	C2-C1-O2A-CGA
22	K	1402	CLA	C2-C1-O2A-CGA
26	Z	801	LHG	C9-C10-C11-C12
22	B	1235	CLA	C13-C15-C16-C17
22	1	607	CLA	C10-C11-C12-C13
22	B	1228	CLA	C16-C17-C18-C20
22	A	1127	CLA	CAA-CBA-CGA-O1A
22	B	1236	CLA	C2A-CAA-CBA-CGA
22	Z	603	CLA	C2A-CAA-CBA-CGA
32	A	5005	DGA	OG1-CG1-CG2-OG2
32	A	5005	DGA	CA4-CA5-CA6-CA7
22	A	1110	CLA	C3A-C2A-CAA-CBA
22	A	1128	CLA	C3A-C2A-CAA-CBA
22	L	1503	CLA	C3A-C2A-CAA-CBA
22	3	616	CLA	C3A-C2A-CAA-CBA
22	5	603	CLA	C3A-C2A-CAA-CBA
40	Z	609	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	A	1138	CLA	CAA-CBA-CGA-O2A
25	B	4004	BCR	C19-C20-C21-C22
25	3	505	BCR	C19-C20-C21-C22
22	B	1213	CLA	C4-C3-C5-C6
22	8	609	CLA	C3-C5-C6-C7
22	4	607	CLA	C3-C5-C6-C7
22	A	1105	CLA	C6-C7-C8-C9
22	B	1203	CLA	C11-C10-C8-C9
22	B	1207	CLA	C11-C12-C13-C14
22	B	1221	CLA	C14-C13-C15-C16
22	L	1502	CLA	C11-C12-C13-C14
22	Z	604	CLA	C11-C12-C13-C14
22	3	612	CLA	C6-C7-C8-C9
22	9	601	CLA	C6-C7-C8-C9
40	Z	610	CHL	C6-C7-C8-C9
22	4	605	CLA	C16-C17-C18-C19
22	6	619	CLA	C16-C17-C18-C19
31	J	5001	LMG	C11-C12-C13-C14
26	B	5001	LHG	O10-C23-O8-C6
22	B	1228	CLA	C8-C10-C11-C12
25	A	4005	BCR	C16-C17-C18-C36
25	B	4003	BCR	C20-C21-C22-C37
25	5	504	BCR	C16-C17-C18-C36
26	6	801	LHG	C4-C5-C6-O8
31	A	5003	LMG	O1-C7-C8-C9
36	F	4001	RRX	C35-C13-C14-C15
39	Z	501	LUT	C21-C26-C27-C28
39	2	503	LUT	C40-C33-C34-C35
39	9	501	LUT	C21-C26-C27-C28
22	9	602	CLA	CAA-CBA-CGA-O1A
22	A	1134	CLA	C2A-CAA-CBA-CGA
40	2	609	CHL	C2A-CAA-CBA-CGA
26	7	801	LHG	C30-C31-C32-C33
22	B	1205	CLA	CAA-CBA-CGA-O1A
22	1	608	CLA	CAA-CBA-CGA-O1A
22	4	608	CLA	C6-C7-C8-C9
22	5	604	CLA	C16-C17-C18-C19
25	B	4005	BCR	C37-C22-C23-C24
25	B	4007	BCR	C36-C18-C19-C20
22	A	1119	CLA	C13-C15-C16-C17
38	K	5001	SPH	C11-C10-C9-C8
22	B	1237	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	A	1110	CLA	C1A-C2A-CAA-CBA
22	A	1133	CLA	C1A-C2A-CAA-CBA
22	A	1134	CLA	C1A-C2A-CAA-CBA
22	B	1222	CLA	C1A-C2A-CAA-CBA
22	K	1403	CLA	C1A-C2A-CAA-CBA
22	7	616	CLA	C1A-C2A-CAA-CBA
22	8	608	CLA	C1A-C2A-CAA-CBA
22	8	615	CLA	C1A-C2A-CAA-CBA
22	4	609	CLA	C1A-C2A-CAA-CBA
22	5	603	CLA	C1A-C2A-CAA-CBA
22	5	609	CLA	C1A-C2A-CAA-CBA
22	9	609	CLA	C1A-C2A-CAA-CBA
26	1	801	LHG	C13-C14-C15-C16
22	A	1121	CLA	C11-C10-C8-C7
22	A	1131	CLA	C6-C7-C8-C10
22	B	1231	CLA	C11-C12-C13-C15
22	L	1502	CLA	C12-C13-C15-C16
22	3	601	CLA	C11-C12-C13-C15
22	3	606	CLA	C11-C10-C8-C7
22	7	604	CLA	C6-C7-C8-C10
35	B	5004	T7X	C13-C14-C15-C16
22	3	606	CLA	C13-C15-C16-C17
28	A	5006	LMT	C5'-C4'-O1B-C1B
25	A	4001	BCR	C15-C16-C17-C18
25	7	503	BCR	C15-C16-C17-C18
26	A	5002	LHG	C11-C10-C9-C8
40	Z	613	CHL	CAA-CBA-CGA-O1A
40	Z	613	CHL	CAA-CBA-CGA-O2A
22	B	1206	CLA	C10-C11-C12-C13
22	B	1238	CLA	C16-C17-C18-C19
40	8	610	CHL	C2A-CAA-CBA-CGA
22	A	1130	CLA	C13-C15-C16-C17
22	B	1228	CLA	C10-C11-C12-C13
22	2	612	CLA	CAA-CBA-CGA-O2A
26	5	801	LHG	C29-C30-C31-C32
22	A	1013	CLA	C5-C6-C7-C8
43	7	802	3PH	C34-C35-C36-C37
22	1	612	CLA	O1A-CGA-O2A-C1
26	5	801	LHG	C7-C8-C9-C10
22	A	1108	CLA	C2-C3-C5-C6
22	B	1213	CLA	C2-C3-C5-C6
40	7	610	CHL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	L	1503	CLA	CBA-CGA-O2A-C1
22	B	1221	CLA	C15-C16-C17-C18
45	8	803	LPX	C14-C15-C16-C17
25	A	4005	BCR	C16-C17-C18-C19
25	B	4003	BCR	C20-C21-C22-C23
25	5	504	BCR	C16-C17-C18-C19
36	F	4001	RRX	C12-C13-C14-C15
39	2	503	LUT	C32-C33-C34-C35
25	L	4001	BCR	C9-C10-C11-C12
39	7	502	LUT	C9-C10-C11-C12
39	2	503	LUT	C9-C10-C11-C12
22	1	602	CLA	CAA-CBA-CGA-O1A
41	2	803	SQD	C11-C12-C13-C14
22	A	1123	CLA	C10-C11-C12-C13
22	A	1136	CLA	C13-C15-C16-C17
22	1	602	CLA	CAA-CBA-CGA-O2A
22	B	1022	CLA	C4-C3-C5-C6
22	B	1220	CLA	C4-C3-C5-C6
43	7	802	3PH	C37-C38-C39-C3A
22	A	1107	CLA	C2-C1-O2A-CGA
40	5	610	CHL	C2-C1-O2A-CGA
40	6	613	CHL	C2-C1-O2A-CGA
22	7	612	CLA	O1A-CGA-O2A-C1
40	5	610	CHL	C13-C15-C16-C17
22	9	602	CLA	CAA-CBA-CGA-O2A
26	4	801	LHG	C26-C27-C28-C29
22	A	1113	CLA	C14-C13-C15-C16
22	A	1127	CLA	C5-C6-C7-C8
26	4	801	LHG	C16-C17-C18-C19
22	B	1208	CLA	CAA-CBA-CGA-O2A
40	1	610	CHL	CAA-CBA-CGA-O2A
22	A	1126	CLA	C10-C11-C12-C13
22	A	1124	CLA	C2A-CAA-CBA-CGA
22	2	603	CLA	C6-C7-C8-C9
22	7	612	CLA	CBA-CGA-O2A-C1
25	A	4001	BCR	C1-C6-C7-C8
25	A	4001	BCR	C5-C6-C7-C8
25	A	4005	BCR	C23-C24-C25-C30
25	B	4002	BCR	C1-C6-C7-C8
25	J	4001	BCR	C1-C6-C7-C8
25	8	503	BCR	C23-C24-C25-C30
39	8	501	LUT	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
39	8	502	LUT	C1-C6-C7-C8
39	4	501	LUT	C1-C6-C7-C8
39	4	501	LUT	C5-C6-C7-C8
39	5	501	LUT	C1-C6-C7-C8
39	6	501	LUT	C1-C6-C7-C8
39	6	501	LUT	C5-C6-C7-C8
39	6	502	LUT	C1-C6-C7-C8
39	9	501	LUT	C1-C6-C7-C8
39	9	502	LUT	C1-C6-C7-C8
26	9	801	LHG	C26-C27-C28-C29
25	7	503	BCR	C7-C8-C9-C34
22	5	609	CLA	C15-C16-C17-C18
25	L	4002	BCR	C19-C20-C21-C22
25	7	503	BCR	C13-C14-C15-C16
25	7	504	BCR	C19-C20-C21-C22
22	B	1241	CLA	C4-C3-C5-C6
22	4	608	CLA	C4-C3-C5-C6
22	5	607	CLA	C4-C3-C5-C6
22	6	619	CLA	C4-C3-C5-C6
25	3	504	BCR	C11-C12-C13-C14
25	3	504	BCR	C17-C18-C19-C20
22	K	1404	CLA	C6-C7-C8-C9
22	A	1103	CLA	C5-C6-C7-C8
32	A	5005	DGA	CBB-CCB-CDB-CEB
22	1	612	CLA	C2-C3-C5-C6
22	5	618	CLA	C3-C5-C6-C7
22	B	1240	CLA	C13-C15-C16-C17
26	8	801	LHG	C7-C8-C9-C10
22	7	615	CLA	CAA-CBA-CGA-O2A
22	A	1121	CLA	C16-C17-C18-C19
23	A	2001	PQN	C26-C27-C28-C30
22	A	1107	CLA	C15-C16-C17-C18
22	B	1240	CLA	C5-C6-C7-C8
22	4	602	CLA	CAA-CBA-CGA-O2A
22	A	1138	CLA	C4-C3-C5-C6
23	B	2002	PQN	C14-C13-C15-C16
40	9	610	CHL	C4-C3-C5-C6
22	A	1122	CLA	C11-C10-C8-C7
22	B	1207	CLA	C12-C13-C15-C16
22	B	1210	CLA	C11-C12-C13-C15
22	9	608	CLA	CAA-CBA-CGA-O1A
26	B	5006	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
22	L	1503	CLA	O1A-CGA-O2A-C1
25	B	4004	BCR	C9-C10-C11-C12
25	K	4001	BCR	C9-C10-C11-C12
25	6	504	BCR	C15-C16-C17-C18
26	7	801	LHG	C26-C27-C28-C29
22	9	608	CLA	CAA-CBA-CGA-O2A
26	7	801	LHG	O7-C5-C6-O8
22	7	609	CLA	CAA-CBA-CGA-O2A
40	2	609	CHL	CAA-CBA-CGA-O2A
40	8	613	CHL	C10-C11-C12-C13
28	B	6101	LMT	C4B-C5B-C6B-O6B
22	A	1137	CLA	CAA-CBA-CGA-O2A
22	G	1601	CLA	CAA-CBA-CGA-O2A
22	L	1502	CLA	CAA-CBA-CGA-O2A
22	4	605	CLA	CAA-CBA-CGA-O2A
22	B	1234	CLA	C3-C5-C6-C7
22	1	606	CLA	C4-C3-C5-C6
22	8	609	CLA	C4-C3-C5-C6
40	Z	610	CHL	C4-C3-C5-C6
26	8	801	LHG	C9-C10-C11-C12
32	A	5005	DGA	CEA-CFA-CGA-CHA
22	B	1220	CLA	C2-C3-C5-C6
22	5	618	CLA	C2-C3-C5-C6
22	B	1207	CLA	CAA-CBA-CGA-O2A
22	2	607	CLA	CAA-CBA-CGA-O2A
22	A	1138	CLA	C6-C7-C8-C9
22	B	1206	CLA	C11-C12-C13-C14
22	B	1220	CLA	C6-C7-C8-C9
22	Z	612	CLA	C6-C7-C8-C9
22	3	606	CLA	C11-C10-C8-C9
23	B	2002	PQN	C19-C18-C20-C21
22	3	601	CLA	C3A-C2A-CAA-CBA
22	7	601	CLA	C3A-C2A-CAA-CBA
22	5	604	CLA	C3A-C2A-CAA-CBA
22	6	605	CLA	C3A-C2A-CAA-CBA
22	9	604	CLA	C3A-C2A-CAA-CBA
26	1	801	LHG	O2-C2-C3-O3
26	9	801	LHG	O8-C23-C24-C25
27	A	5004	NKP	CAQ-CAR-CAS-CAT
22	A	1104	CLA	CAD-CBD-CGD-O2D
22	A	1138	CLA	CAD-CBD-CGD-O2D
22	1	602	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	1	605	CLA	CAD-CBD-CGD-O2D
22	5	622	CLA	CAD-CBD-CGD-O2D
22	9	605	CLA	CAD-CBD-CGD-O2D
40	4	617	CHL	CAD-CBD-CGD-O2D
22	B	1240	CLA	C8-C10-C11-C12
22	B	1240	CLA	C15-C16-C17-C18
25	L	4002	BCR	C9-C10-C11-C12
22	2	602	CLA	C2A-CAA-CBA-CGA
28	4	803	LMT	C2-C1-O1'-C1'
22	5	604	CLA	C10-C11-C12-C13
26	6	801	LHG	C26-C27-C28-C29
22	A	1104	CLA	CAA-CBA-CGA-O2A
22	B	1216	CLA	CAA-CBA-CGA-O2A
22	Z	602	CLA	CAA-CBA-CGA-O2A
22	3	610	CLA	CAA-CBA-CGA-O2A
26	Z	801	LHG	O7-C7-C8-C9
22	B	1235	CLA	CAA-CBA-CGA-O1A
22	A	1122	CLA	CBD-CGD-O2D-CED
28	9	803	LMT	C9-C10-C11-C12
22	7	606	CLA	C4-C3-C5-C6
22	6	607	CLA	C4-C3-C5-C6
22	A	1127	CLA	C16-C17-C18-C20
22	1	601	CLA	C5-C6-C7-C8
22	B	1241	CLA	C2-C3-C5-C6
22	1	603	CLA	CAA-CBA-CGA-O2A
22	6	615	CLA	CAA-CBA-CGA-O2A
32	A	5005	DGA	OG1-CA1-CA2-CA3
40	8	613	CHL	CAA-CBA-CGA-O2A
44	7	805	PLM	CC-CD-CE-CF
25	A	4001	BCR	C21-C22-C23-C24
25	A	4003	BCR	C17-C18-C19-C20
25	B	4005	BCR	C7-C8-C9-C10
25	3	506	BCR	C11-C12-C13-C14
25	7	503	BCR	C7-C8-C9-C10
25	5	503	BCR	C7-C8-C9-C10
25	5	503	BCR	C17-C18-C19-C20
38	7	803	SPH	C4-C5-C6-C7
43	6	802	3PH	C32-C33-C34-C35
22	Z	602	CLA	O1A-CGA-O2A-C1
26	B	5001	LHG	C2-C3-O3-P
26	9	801	LHG	C5-C4-O6-P
40	1	610	CHL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
22	B	1206	CLA	CAA-CBA-CGA-O2A
22	L	1503	CLA	CAA-CBA-CGA-O2A
22	5	612	CLA	CAA-CBA-CGA-O2A
26	6	801	LHG	O8-C23-C24-C25
40	6	611	CHL	CAA-CBA-CGA-O2A
40	8	610	CHL	O2A-C1-C2-C3
40	4	610	CHL	O2A-C1-C2-C3
40	6	610	CHL	O2A-C1-C2-C3
32	A	5005	DGA	CB6-CB7-CB8-CB9
22	4	609	CLA	CAA-CBA-CGA-O2A
22	A	1012	CLA	CHA-CBD-CGD-O1D
22	A	1012	CLA	CHA-CBD-CGD-O2D
22	A	1118	CLA	CHA-CBD-CGD-O1D
22	A	1118	CLA	CHA-CBD-CGD-O2D
22	A	1127	CLA	CHA-CBD-CGD-O1D
22	A	1127	CLA	CHA-CBD-CGD-O2D
22	A	1129	CLA	CHA-CBD-CGD-O2D
22	A	1136	CLA	CHA-CBD-CGD-O1D
22	A	1136	CLA	CHA-CBD-CGD-O2D
22	A	1138	CLA	CHA-CBD-CGD-O2D
22	A	1013	CLA	CHA-CBD-CGD-O1D
22	A	1013	CLA	CHA-CBD-CGD-O2D
22	A	1140	CLA	CHA-CBD-CGD-O1D
22	A	1140	CLA	CHA-CBD-CGD-O2D
22	B	1022	CLA	CHA-CBD-CGD-O1D
22	B	1022	CLA	CHA-CBD-CGD-O2D
22	B	1237	CLA	CHA-CBD-CGD-O1D
22	B	1237	CLA	CHA-CBD-CGD-O2D
22	B	1201	CLA	CHA-CBD-CGD-O1D
22	B	1201	CLA	CHA-CBD-CGD-O2D
22	B	1204	CLA	CHA-CBD-CGD-O1D
22	B	1204	CLA	CHA-CBD-CGD-O2D
22	B	1206	CLA	CHA-CBD-CGD-O1D
22	B	1206	CLA	CHA-CBD-CGD-O2D
22	B	1228	CLA	CHA-CBD-CGD-O2D
22	B	1230	CLA	CHA-CBD-CGD-O1D
22	B	1230	CLA	CHA-CBD-CGD-O2D
22	B	1236	CLA	CHA-CBD-CGD-O2D
22	B	1239	CLA	CHA-CBD-CGD-O2D
22	F	1301	CLA	CHA-CBD-CGD-O1D
22	F	1301	CLA	CHA-CBD-CGD-O2D
22	J	1901	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	J	1901	CLA	CHA-CBD-CGD-O2D
22	K	1401	CLA	CHA-CBD-CGD-O1D
22	K	1401	CLA	CHA-CBD-CGD-O2D
22	K	1402	CLA	CHA-CBD-CGD-O1D
22	L	1503	CLA	CHA-CBD-CGD-O1D
22	L	1503	CLA	CHA-CBD-CGD-O2D
22	1	601	CLA	CHA-CBD-CGD-O1D
22	1	601	CLA	CHA-CBD-CGD-O2D
22	Z	612	CLA	CHA-CBD-CGD-O1D
22	Z	612	CLA	CHA-CBD-CGD-O2D
22	3	604	CLA	CHA-CBD-CGD-O2D
22	7	605	CLA	CHA-CBD-CGD-O1D
22	7	605	CLA	CHA-CBD-CGD-O2D
22	7	615	CLA	CHA-CBD-CGD-O1D
22	7	615	CLA	CHA-CBD-CGD-O2D
22	8	606	CLA	CHA-CBD-CGD-O1D
22	8	606	CLA	CHA-CBD-CGD-O2D
22	4	603	CLA	CHA-CBD-CGD-O1D
22	4	603	CLA	CHA-CBD-CGD-O2D
22	4	604	CLA	CHA-CBD-CGD-O2D
22	4	615	CLA	CHA-CBD-CGD-O1D
22	4	615	CLA	CHA-CBD-CGD-O2D
22	5	613	CLA	CHA-CBD-CGD-O1D
22	5	613	CLA	CHA-CBD-CGD-O2D
22	6	604	CLA	CHA-CBD-CGD-O1D
22	6	604	CLA	CHA-CBD-CGD-O2D
22	6	605	CLA	CHA-CBD-CGD-O1D
22	6	605	CLA	CHA-CBD-CGD-O2D
22	6	618	CLA	CHA-CBD-CGD-O1D
22	6	618	CLA	CHA-CBD-CGD-O2D
22	2	602	CLA	CHA-CBD-CGD-O1D
22	2	602	CLA	CHA-CBD-CGD-O2D
22	2	608	CLA	CHA-CBD-CGD-O1D
22	9	604	CLA	CHA-CBD-CGD-O1D
40	1	609	CHL	CHA-CBD-CGD-O1D
40	4	610	CHL	CHA-CBD-CGD-O1D
40	4	610	CHL	CHA-CBD-CGD-O2D
22	A	1106	CLA	C13-C15-C16-C17
22	A	1120	CLA	C4-C3-C5-C6
22	L	1502	CLA	C4-C3-C5-C6
22	A	1108	CLA	CAA-CBA-CGA-O2A
22	3	607	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	6	619	CLA	C2-C3-C5-C6
40	Z	610	CHL	C2-C3-C5-C6
22	9	601	CLA	C8-C10-C11-C12
26	Z	801	LHG	O6-C4-C5-C6
22	1	604	CLA	C11-C12-C13-C15
22	3	601	CLA	C8-C10-C11-C12
22	A	1121	CLA	CAA-CBA-CGA-O2A
22	A	1131	CLA	CAA-CBA-CGA-O2A
22	A	1134	CLA	CAA-CBA-CGA-O2A
22	8	609	CLA	CAA-CBA-CGA-O2A
40	4	611	CHL	CAA-CBA-CGA-O2A
27	A	5004	NKP	CAO-CAP-CAQ-CAR
26	9	801	LHG	O7-C5-C6-O8
22	A	1125	CLA	CAA-CBA-CGA-O2A
22	A	1128	CLA	CAA-CBA-CGA-O2A
22	Z	603	CLA	CAA-CBA-CGA-O2A
22	Z	608	CLA	CAA-CBA-CGA-O2A
22	9	607	CLA	CAA-CBA-CGA-O2A
28	B	6101	LMT	C5'-C4'-O1B-C1B
22	6	602	CLA	C2A-CAA-CBA-CGA
22	A	1131	CLA	C13-C15-C16-C17
22	A	1136	CLA	C8-C10-C11-C12
22	B	1241	CLA	CAA-CBA-CGA-O2A
22	8	611	CLA	CAA-CBA-CGA-O2A
22	2	604	CLA	CAA-CBA-CGA-O2A
22	B	1238	CLA	C4-C3-C5-C6
28	9	803	LMT	O5B-C1B-O1B-C4'
22	A	1110	CLA	C2-C3-C5-C6
22	A	1115	CLA	C6-C7-C8-C10
23	A	2001	PQN	C21-C22-C23-C25
22	B	1226	CLA	C13-C15-C16-C17
22	B	1237	CLA	CAA-CBA-CGA-O2A
22	5	605	CLA	CAA-CBA-CGA-O2A
22	6	601	CLA	CAA-CBA-CGA-O2A
22	6	603	CLA	CAA-CBA-CGA-O2A
26	5	801	LHG	O7-C7-C8-C9
31	J	5001	LMG	O8-C28-C29-C30
33	B	5003	DGD	O1G-C1A-C2A-C3A
40	1	610	CHL	C2C-C3C-CAC-CBC
22	A	1124	CLA	C14-C13-C15-C16
22	B	1219	CLA	C11-C10-C8-C9
22	L	1502	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	7	604	CLA	C11-C12-C13-C14
23	A	2001	PQN	C21-C22-C23-C24
25	3	506	BCR	C19-C20-C21-C22
25	6	503	BCR	C13-C14-C15-C16
39	5	501	LUT	C29-C30-C31-C32
26	A	5002	LHG	C27-C28-C29-C30
22	B	1212	CLA	CAA-CBA-CGA-O2A
22	A	1137	CLA	CAA-CBA-CGA-O1A
41	2	803	SQD	C4-C5-C6-S
41	1	802	SQD	C29-C30-C31-C32
32	A	5005	DGA	CB2-CB1-OG2-CG2
22	2	605	CLA	C2A-CAA-CBA-CGA
22	B	1206	CLA	CAA-CBA-CGA-O1A
32	A	5005	DGA	OA1-CA1-CA2-CA3
26	6	801	LHG	C17-C18-C19-C20
26	8	801	LHG	O7-C7-C8-C9
38	K	5001	SPH	C13-C14-C15-C16
26	A	5002	LHG	C24-C25-C26-C27
26	9	801	LHG	C27-C28-C29-C30
22	2	607	CLA	CAA-CBA-CGA-O1A
26	Z	801	LHG	C31-C32-C33-C34
33	B	5003	DGD	CFA-CGA-CHA-CIA
26	A	5002	LHG	O1-C1-C2-C3
26	7	801	LHG	O1-C1-C2-C3
22	A	1138	CLA	C2-C3-C5-C6
22	4	608	CLA	C2-C3-C5-C6
26	B	5006	LHG	C9-C10-C11-C12
22	G	1601	CLA	CAA-CBA-CGA-O1A
22	Z	602	CLA	CAA-CBA-CGA-O1A
43	8	806	3PH	C32-C33-C34-C35
22	A	1128	CLA	C1A-C2A-CAA-CBA
22	B	1203	CLA	C1A-C2A-CAA-CBA
22	B	1210	CLA	C1A-C2A-CAA-CBA
22	B	1213	CLA	C1A-C2A-CAA-CBA
22	3	603	CLA	C1A-C2A-CAA-CBA
22	3	616	CLA	C1A-C2A-CAA-CBA
22	6	605	CLA	C1A-C2A-CAA-CBA
40	4	611	CHL	C1A-C2A-CAA-CBA
22	L	1502	CLA	CAA-CBA-CGA-O1A
22	4	605	CLA	CAA-CBA-CGA-O1A
22	5	612	CLA	CAA-CBA-CGA-O1A
22	6	615	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
41	1	802	SQD	C25-C26-C27-C28
40	8	613	CHL	C2-C1-O2A-CGA
26	2	801	LHG	C27-C28-C29-C30
22	B	1207	CLA	CAA-CBA-CGA-O1A
22	7	609	CLA	CAA-CBA-CGA-O1A
26	5	801	LHG	O9-C7-C8-C9
26	6	801	LHG	O10-C23-C24-C25
31	J	5001	LMG	O10-C28-C29-C30
32	A	5005	DGA	OG1-CG1-CG2-CG3
22	1	604	CLA	C2A-CAA-CBA-CGA
22	B	1238	CLA	C16-C17-C18-C20
22	A	1104	CLA	CAA-CBA-CGA-O1A
22	A	1108	CLA	CAA-CBA-CGA-O1A
22	B	1216	CLA	CAA-CBA-CGA-O1A
22	L	1503	CLA	CAA-CBA-CGA-O1A
32	A	5005	DGA	CA3-CA4-CA5-CA6
22	6	607	CLA	CAA-CBA-CGA-O2A
22	A	1130	CLA	C15-C16-C17-C18
22	B	1223	CLA	C15-C16-C17-C18
22	B	1236	CLA	C10-C11-C12-C13
22	A	1125	CLA	C3-C5-C6-C7
22	6	605	CLA	C3-C5-C6-C7
22	A	1131	CLA	CAA-CBA-CGA-O1A
22	Z	603	CLA	CAA-CBA-CGA-O1A
22	B	1230	CLA	C2-C3-C5-C6
22	7	609	CLA	C2-C3-C5-C6
22	2	608	CLA	CAA-CBA-CGA-O2A
26	A	5002	LHG	C4-O6-P-O5
26	Z	801	LHG	C3-O3-P-O5
26	8	801	LHG	C3-O3-P-O5
26	4	801	LHG	C3-O3-P-O5
22	K	1404	CLA	C6-C7-C8-C10
26	B	5002	LHG	O7-C5-C6-O8
22	A	1134	CLA	CAA-CBA-CGA-O1A
22	B	1237	CLA	CAA-CBA-CGA-O1A
22	1	603	CLA	CAA-CBA-CGA-O1A
22	3	610	CLA	CAA-CBA-CGA-O1A
22	4	609	CLA	CAA-CBA-CGA-O1A
22	6	603	CLA	CAA-CBA-CGA-O1A
22	9	607	CLA	CAA-CBA-CGA-O1A
40	6	611	CHL	CAA-CBA-CGA-O1A
22	7	605	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	9	606	CLA	CAA-CBA-CGA-O2A
22	A	1140	CLA	O1A-CGA-O2A-C1
25	B	4007	BCR	C23-C24-C25-C30
25	J	4001	BCR	C5-C6-C7-C8
39	8	502	LUT	C5-C6-C7-C8
39	6	502	LUT	C5-C6-C7-C8
39	9	501	LUT	C5-C6-C7-C8
26	A	5002	LHG	C9-C10-C11-C12
22	B	1210	CLA	C5-C6-C7-C8
22	5	605	CLA	CAA-CBA-CGA-O1A
26	Z	801	LHG	O9-C7-C8-C9
22	B	1219	CLA	CAA-CBA-CGA-O2A
22	7	606	CLA	CAA-CBA-CGA-O2A
26	7	801	LHG	O8-C23-C24-C25
22	B	1228	CLA	C16-C17-C18-C19
25	3	504	BCR	C10-C11-C12-C13
22	4	604	CLA	C2A-CAA-CBA-CGA
22	Z	608	CLA	CAA-CBA-CGA-O1A
22	3	607	CLA	CAA-CBA-CGA-O1A
26	4	802	LHG	C10-C11-C12-C13
22	K	1402	CLA	CAA-CBA-CGA-O1A
26	9	801	LHG	O10-C23-C24-C25
22	K	1402	CLA	C4-C3-C5-C6
25	K	4002	BCR	C9-C10-C11-C12
23	B	2002	PQN	C12-C13-C15-C16
22	A	1012	CLA	CAD-CBD-CGD-O1D
22	A	1120	CLA	CAD-CBD-CGD-O1D
22	A	1135	CLA	C2-C3-C5-C6
22	B	1206	CLA	CAD-CBD-CGD-O1D
22	B	1236	CLA	CAD-CBD-CGD-O1D
22	B	1239	CLA	CAD-CBD-CGD-O1D
22	1	601	CLA	CAD-CBD-CGD-O1D
22	3	604	CLA	CAD-CBD-CGD-O1D
22	3	613	CLA	CAD-CBD-CGD-O1D
22	8	606	CLA	CAD-CBD-CGD-O1D
22	6	619	CLA	CAD-CBD-CGD-O1D
40	1	609	CHL	CAD-CBD-CGD-O1D
40	Z	609	CHL	CAD-CBD-CGD-O1D
41	2	803	SQD	O5-C5-C6-S
22	A	1128	CLA	CAA-CBA-CGA-O1A
40	8	613	CHL	CAA-CBA-CGA-O1A
22	1	613	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
31	J	5001	LMG	O7-C10-C11-C12
22	A	1103	CLA	C14-C13-C15-C16
22	A	1122	CLA	C11-C10-C8-C9
22	A	1123	CLA	C11-C12-C13-C14
22	B	1210	CLA	C11-C10-C8-C9
22	B	1223	CLA	C6-C7-C8-C9
22	B	1236	CLA	C14-C13-C15-C16
22	3	601	CLA	C11-C12-C13-C14
22	7	604	CLA	C6-C7-C8-C9
35	B	5004	T7X	C26-C27-C28-C29
22	2	608	CLA	CAA-CBA-CGA-O1A
22	4	603	CLA	C5-C6-C7-C8
30	A	5007	DAO	C1-C2-C3-C4
22	A	1113	CLA	CAA-CBA-CGA-O2A
22	A	1135	CLA	CAA-CBA-CGA-O2A
22	B	1211	CLA	CAA-CBA-CGA-O2A
22	K	1403	CLA	CAA-CBA-CGA-O2A
22	Z	607	CLA	CAA-CBA-CGA-O2A
22	8	608	CLA	CAA-CBA-CGA-O2A
22	4	607	CLA	CAA-CBA-CGA-O2A
22	4	608	CLA	CAA-CBA-CGA-O2A
22	5	618	CLA	CAA-CBA-CGA-O2A
40	Z	609	CHL	CAA-CBA-CGA-O2A
26	8	801	LHG	O9-C7-C8-C9
22	B	1210	CLA	CAA-CBA-CGA-O2A
22	5	607	CLA	CAA-CBA-CGA-O2A
26	9	801	LHG	O7-C7-C8-C9
22	A	1130	CLA	C8-C10-C11-C12
22	1	606	CLA	C8-C10-C11-C12
22	Z	605	CLA	C13-C15-C16-C17
22	A	1121	CLA	CAA-CBA-CGA-O1A
43	7	802	3PH	C3C-C3D-C3E-C3F
22	A	1104	CLA	C4-C3-C5-C6
22	A	1121	CLA	C3A-C2A-CAA-CBA
22	A	1121	CLA	C6-C7-C8-C10
22	A	1123	CLA	C11-C12-C13-C15
22	A	1124	CLA	C12-C13-C15-C16
22	A	1128	CLA	C11-C10-C8-C7
22	A	1140	CLA	C11-C10-C8-C7
22	B	1210	CLA	C3A-C2A-CAA-CBA
22	B	1213	CLA	C3A-C2A-CAA-CBA
22	B	1219	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	B	1223	CLA	C6-C7-C8-C10
22	B	1236	CLA	C12-C13-C15-C16
22	1	601	CLA	C11-C10-C8-C7
22	7	604	CLA	C11-C12-C13-C15
22	5	607	CLA	C2-C3-C5-C6
22	6	604	CLA	C3A-C2A-CAA-CBA
22	6	606	CLA	C3A-C2A-CAA-CBA
22	9	601	CLA	C3A-C2A-CAA-CBA
43	8	806	3PH	O11-C1-C2-O21
22	B	1212	CLA	CAA-CBA-CGA-O1A
22	B	1236	CLA	CAA-CBA-CGA-O1A
22	8	609	CLA	CAA-CBA-CGA-O1A
22	9	606	CLA	CAA-CBA-CGA-O1A
27	A	5004	NKP	OAE-CAK-CAL-CAM
22	5	608	CLA	CAA-CBA-CGA-O2A
22	B	1239	CLA	CAA-CBA-CGA-O2A
22	6	604	CLA	CAA-CBA-CGA-O2A
22	2	602	CLA	CAA-CBA-CGA-O2A
22	2	615	CLA	CAA-CBA-CGA-O2A
26	A	5002	LHG	O8-C23-C24-C25
27	A	5004	NKP	OAJ-CAK-CAL-CAM
33	B	5003	DGD	C2B-C3B-C4B-C5B
26	Z	801	LHG	C26-C27-C28-C29
25	B	4005	BCR	C21-C22-C23-C24
25	B	4007	BCR	C17-C18-C19-C20
25	B	4006	BCR	C7-C8-C9-C10
25	L	4002	BCR	C17-C18-C19-C20
39	6	501	LUT	C27-C28-C29-C30
22	A	1113	CLA	CAA-CBA-CGA-O1A
22	7	606	CLA	CAA-CBA-CGA-O1A
22	4	608	CLA	CAA-CBA-CGA-O1A
22	6	601	CLA	CAA-CBA-CGA-O1A
22	2	615	CLA	CAA-CBA-CGA-O1A
25	G	4001	BCR	C19-C20-C21-C22
37	J	4002	C7Z	C13-C14-C15-C35
28	A	5006	LMT	C2-C1-O1'-C1'
22	6	605	CLA	CAA-CBA-CGA-O2A
33	B	5003	DGD	O6E-C1E-O5D-C6D
22	A	1127	CLA	C15-C16-C17-C18
43	8	806	3PH	C36-C37-C38-C39
22	A	1125	CLA	CAA-CBA-CGA-O1A
22	B	1241	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
22	Z	607	CLA	CAA-CBA-CGA-O1A
26	5	801	LHG	O10-C23-C24-C25
40	4	611	CHL	CAA-CBA-CGA-O1A
26	6	801	LHG	C29-C30-C31-C32
22	A	1110	CLA	C15-C16-C17-C18
22	B	1202	CLA	CAA-CBA-CGA-O2A
22	B	1228	CLA	CAA-CBA-CGA-O2A
22	B	1236	CLA	CAA-CBA-CGA-O2A
22	3	603	CLA	CAA-CBA-CGA-O2A
22	6	606	CLA	CAA-CBA-CGA-O2A
26	Z	801	LHG	O8-C23-C24-C25
26	1	801	LHG	C24-C25-C26-C27
22	A	1135	CLA	CAA-CBA-CGA-O1A
22	B	1239	CLA	CAA-CBA-CGA-O1A
22	K	1403	CLA	CAA-CBA-CGA-O1A
22	3	603	CLA	CAA-CBA-CGA-O1A
22	6	607	CLA	CAA-CBA-CGA-O1A
22	6	607	CLA	C2A-CAA-CBA-CGA
22	3	608	CLA	CAA-CBA-CGA-O2A
22	F	1301	CLA	C13-C15-C16-C17
22	8	608	CLA	CAA-CBA-CGA-O1A
22	B	1204	CLA	CAA-CBA-CGA-O2A
22	3	618	CLA	CAA-CBA-CGA-O2A
26	1	801	LHG	O8-C23-C24-C25

There are no ring outliers.

300 monomers are involved in 666 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	J	5001	LMG	1	0
22	A	1122	CLA	2	0
22	5	601	CLA	3	0
22	A	1109	CLA	5	0
22	8	603	CLA	1	0
22	A	1131	CLA	1	0
22	Z	605	CLA	6	0
39	5	502	LUT	5	0
22	A	1116	CLA	7	0
22	B	1206	CLA	2	0
22	3	607	CLA	1	0
22	A	1121	CLA	3	0
28	B	5005	LMT	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	Z	503	LUT	3	0
22	2	606	CLA	1	0
26	A	5002	LHG	4	0
22	B	1226	CLA	3	0
25	K	4002	BCR	4	0
22	4	604	CLA	4	0
22	8	612	CLA	1	0
39	3	501	LUT	2	0
25	5	504	BCR	3	0
22	K	1401	CLA	4	0
22	2	605	CLA	1	0
40	1	609	CHL	1	0
22	1	608	CLA	5	0
39	5	501	LUT	4	0
22	2	603	CLA	3	0
22	B	1204	CLA	1	0
45	8	803	LPX	1	0
22	A	1120	CLA	3	0
22	Z	607	CLA	2	0
22	7	602	CLA	1	0
22	B	1240	CLA	9	0
22	2	607	CLA	3	0
25	3	506	BCR	2	0
40	6	611	CHL	1	0
22	A	1104	CLA	4	0
25	B	4005	BCR	2	0
25	B	4007	BCR	3	0
22	5	607	CLA	3	0
22	8	605	CLA	3	0
40	7	610	CHL	3	0
22	A	1107	CLA	4	0
40	5	617	CHL	1	0
22	1	607	CLA	3	0
22	8	606	CLA	3	0
25	B	4003	BCR	2	0
39	2	502	LUT	5	0
38	7	804	SPH	1	0
22	5	602	CLA	2	0
25	B	4006	BCR	2	0
25	B	4001	BCR	3	0
22	K	1402	CLA	2	0
31	A	5003	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	2	609	CHL	3	0
40	Z	613	CHL	6	0
22	B	1225	CLA	4	0
22	B	1239	CLA	3	0
22	A	1126	CLA	12	0
36	F	4001	RRX	1	0
22	B	1230	CLA	5	0
22	5	612	CLA	2	0
38	K	5001	SPH	1	0
22	1	612	CLA	2	0
22	A	1127	CLA	6	0
22	6	618	CLA	1	0
22	5	609	CLA	3	0
22	A	1102	CLA	2	0
28	4	803	LMT	1	0
22	Z	606	CLA	2	0
22	B	1238	CLA	4	0
40	1	610	CHL	2	0
39	7	501	LUT	2	0
22	A	1124	CLA	5	0
22	9	612	CLA	2	0
22	B	1203	CLA	4	0
26	2	801	LHG	2	0
40	6	613	CHL	1	0
22	7	611	CLA	1	0
22	7	615	CLA	1	0
22	B	1229	CLA	2	0
33	B	5003	DGD	4	0
22	B	1235	CLA	3	0
22	3	606	CLA	4	0
22	A	1140	CLA	2	0
22	B	1216	CLA	6	0
22	6	601	CLA	4	0
25	G	4001	BCR	1	0
22	A	1123	CLA	1	0
22	Z	604	CLA	6	0
40	9	613	CHL	1	0
22	B	1207	CLA	3	0
22	A	1125	CLA	4	0
22	2	604	CLA	2	0
43	7	802	3PH	1	0
22	B	1214	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	L	1502	CLA	2	0
22	A	1114	CLA	5	0
22	Z	615	CLA	1	0
22	5	604	CLA	3	0
40	4	613	CHL	2	0
25	L	4002	BCR	2	0
22	K	1404	CLA	2	0
22	1	611	CLA	4	0
26	B	5001	LHG	2	0
22	B	1224	CLA	4	0
22	A	1106	CLA	3	0
22	B	1217	CLA	2	0
40	5	610	CHL	7	0
22	A	1117	CLA	4	0
22	7	603	CLA	5	0
22	A	1118	CLA	3	0
22	3	608	CLA	2	0
22	7	609	CLA	3	0
39	6	502	LUT	1	0
22	9	602	CLA	1	0
22	6	605	CLA	2	0
39	4	502	LUT	6	0
22	A	1129	CLA	3	0
25	6	503	BCR	3	0
26	B	5006	LHG	1	0
22	B	1021	CLA	9	0
40	9	610	CHL	1	0
40	4	617	CHL	1	0
22	7	606	CLA	1	0
22	A	1101	CLA	2	0
25	5	503	BCR	4	0
40	5	611	CHL	2	0
40	2	613	CHL	2	0
22	9	601	CLA	2	0
22	9	605	CLA	3	0
22	1	603	CLA	3	0
25	J	4001	BCR	4	0
28	B	6101	LMT	2	0
22	B	1202	CLA	2	0
39	9	502	LUT	2	0
22	3	618	CLA	4	0
22	3	613	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	I	4001	BCR	3	0
22	1	613	CLA	2	0
22	5	606	CLA	2	0
22	4	606	CLA	1	0
22	6	607	CLA	1	0
22	B	1236	CLA	6	0
25	4	503	BCR	2	0
22	A	1139	CLA	4	0
22	B	1234	CLA	3	0
22	A	1137	CLA	4	0
26	7	801	LHG	2	0
22	4	612	CLA	4	0
22	A	1128	CLA	7	0
40	Z	610	CHL	6	0
22	B	1232	CLA	1	0
40	8	613	CHL	3	0
22	7	613	CLA	2	0
22	2	601	CLA	1	0
39	8	502	LUT	2	0
39	2	501	LUT	1	0
22	A	1012	CLA	9	0
22	1	604	CLA	3	0
22	4	602	CLA	1	0
39	7	502	LUT	1	0
22	5	618	CLA	6	0
22	8	611	CLA	1	0
25	3	504	BCR	4	0
22	A	1112	CLA	2	0
22	A	1136	CLA	2	0
39	9	501	LUT	4	0
22	B	1201	CLA	2	0
22	J	1901	CLA	3	0
26	Z	801	LHG	1	0
22	A	1119	CLA	4	0
22	3	604	CLA	4	0
22	7	616	CLA	5	0
22	F	1301	CLA	3	0
22	7	604	CLA	1	0
22	A	1103	CLA	5	0
22	1	605	CLA	2	0
25	L	4001	BCR	1	0
32	9	802	DGA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	7	503	BCR	3	0
22	6	604	CLA	2	0
23	A	2001	PQN	1	0
22	5	613	CLA	3	0
22	1	615	CLA	3	0
40	6	610	CHL	3	0
22	A	1110	CLA	2	0
22	B	1205	CLA	3	0
28	A	5006	LMT	1	0
25	6	504	BCR	1	0
41	1	802	SQD	1	0
22	8	607	CLA	3	0
22	B	1218	CLA	2	0
22	Z	612	CLA	2	0
22	9	603	CLA	3	0
22	A	1132	CLA	1	0
22	6	608	CLA	2	0
22	3	603	CLA	3	0
39	Z	502	LUT	4	0
39	8	501	LUT	4	0
22	4	605	CLA	4	0
25	3	503	BCR	1	0
22	Z	601	CLA	3	0
25	A	4005	BCR	5	0
25	A	4002	BCR	4	0
26	6	801	LHG	4	0
22	6	615	CLA	2	0
22	A	1115	CLA	4	0
26	4	801	LHG	1	0
25	8	503	BCR	1	0
22	2	602	CLA	1	0
40	4	610	CHL	4	0
22	2	612	CLA	1	0
22	A	1141	CLA	1	0
22	9	606	CLA	1	0
22	B	1241	CLA	3	0
26	A	5001	LHG	4	0
22	A	1013	CLA	4	0
22	A	1113	CLA	1	0
40	6	617	CHL	1	0
22	B	1237	CLA	4	0
22	1	602	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	5	605	CLA	3	0
39	Z	501	LUT	1	0
22	9	604	CLA	5	0
22	A	1134	CLA	3	0
22	B	1212	CLA	2	0
22	B	1210	CLA	7	0
22	8	602	CLA	2	0
22	7	601	CLA	3	0
22	5	615	CLA	4	0
25	K	4001	BCR	2	0
22	8	609	CLA	2	0
25	A	4003	BCR	3	0
40	8	610	CHL	1	0
28	1	803	LMT	3	0
22	A	1108	CLA	2	0
22	5	622	CLA	1	0
22	3	610	CLA	1	0
40	4	611	CHL	1	0
22	4	601	CLA	4	0
39	4	501	LUT	5	0
24	C	3003	SF4	1	0
40	Z	609	CHL	3	0
22	Z	611	CLA	3	0
32	A	5005	DGA	4	0
22	8	601	CLA	5	0
22	6	612	CLA	4	0
28	9	803	LMT	3	0
22	F	1302	CLA	3	0
22	A	1130	CLA	4	0
40	3	611	CHL	4	0
22	B	1227	CLA	3	0
22	A	1133	CLA	7	0
22	A	1138	CLA	5	0
39	6	501	LUT	3	0
22	B	1221	CLA	5	0
22	8	608	CLA	5	0
22	6	609	CLA	8	0
22	3	605	CLA	3	0
22	6	603	CLA	3	0
22	4	608	CLA	1	0
39	1	502	LUT	4	0
21	A	1011	CL0	5	0

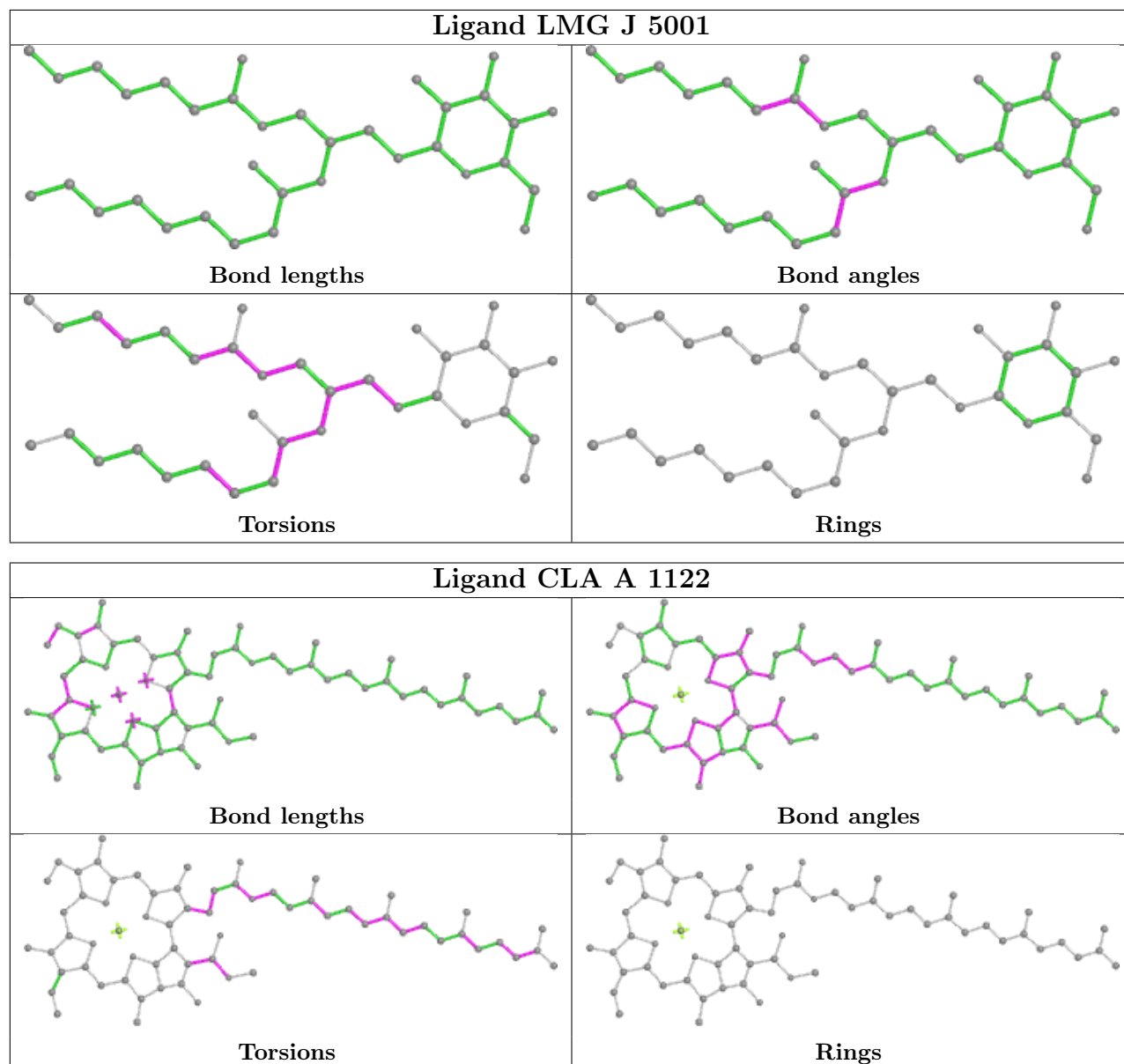
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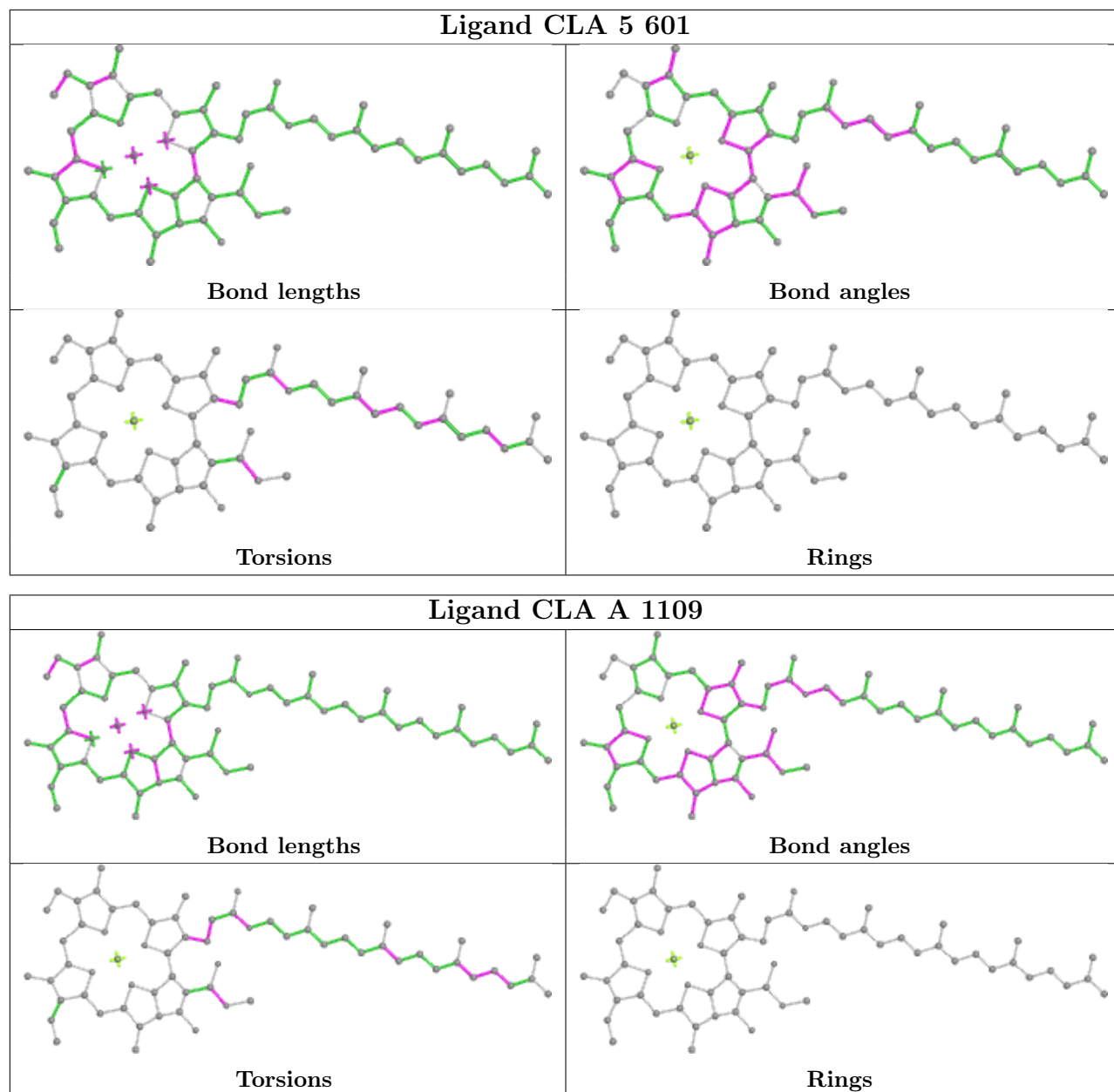
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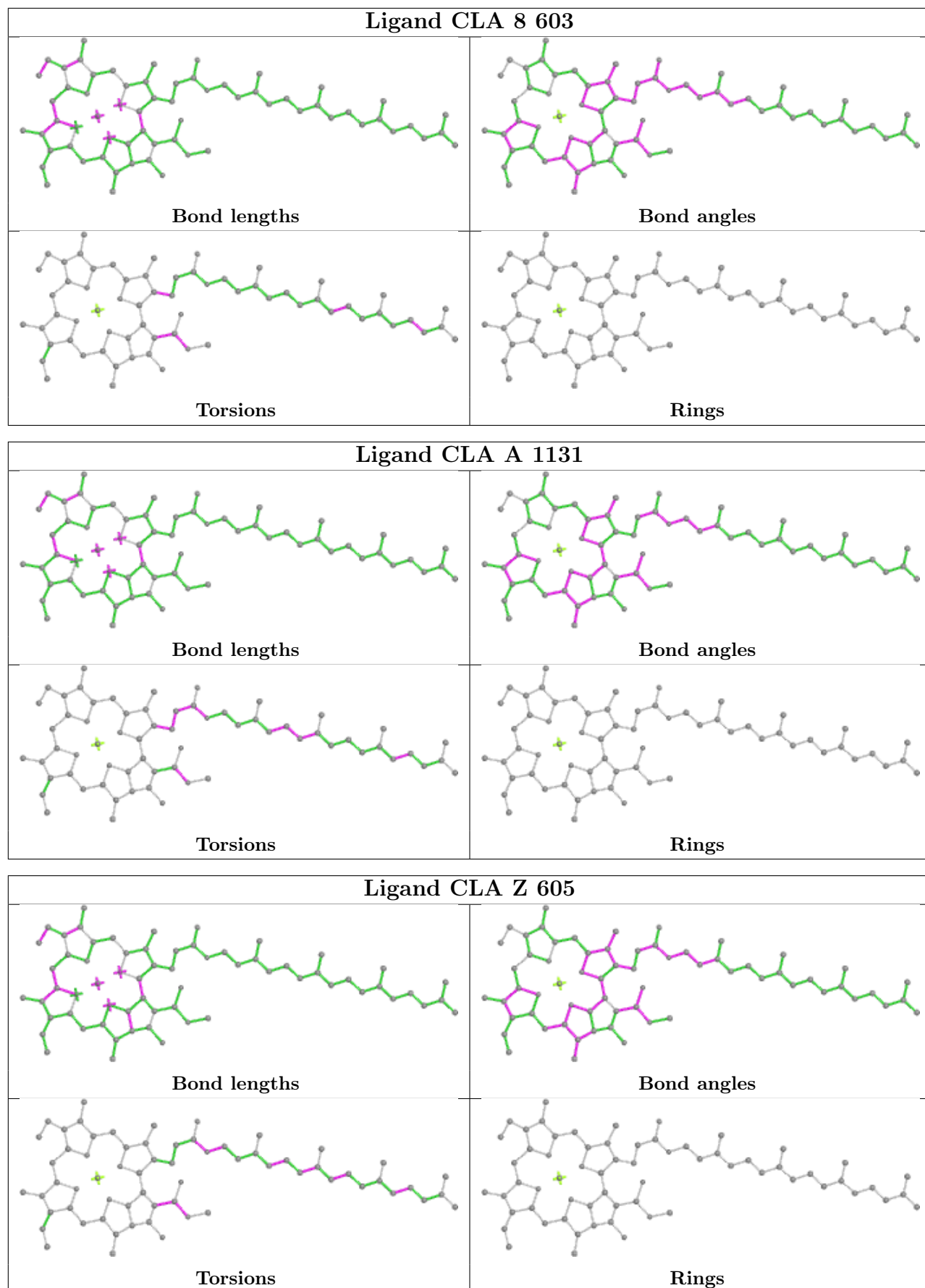
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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25	3	505	BCR	3	0
22	B	1022	CLA	3	0
25	A	4004	BCR	3	0
26	1	801	LHG	1	0
22	A	1105	CLA	3	0
38	7	803	SPH	1	0
40	2	610	CHL	2	0
22	B	1215	CLA	3	0
25	B	4004	BCR	4	0
25	B	4002	BCR	3	0
22	8	604	CLA	1	0
22	B	1222	CLA	4	0
22	1	601	CLA	5	0
22	4	609	CLA	5	0
22	B	1231	CLA	2	0
39	1	501	LUT	2	0
41	2	803	SQD	2	0
22	B	1023	CLA	5	0
39	3	502	LUT	5	0
22	5	603	CLA	3	0
39	2	503	LUT	1	0
25	7	504	BCR	1	0
22	6	606	CLA	1	0
22	3	612	CLA	5	0
22	7	612	CLA	2	0
22	3	616	CLA	1	0
25	A	4001	BCR	1	0
22	B	1208	CLA	5	0
22	B	1220	CLA	5	0
22	B	1213	CLA	4	0
22	6	619	CLA	3	0
22	A	1111	CLA	7	0
22	3	601	CLA	3	0
22	7	607	CLA	3	0

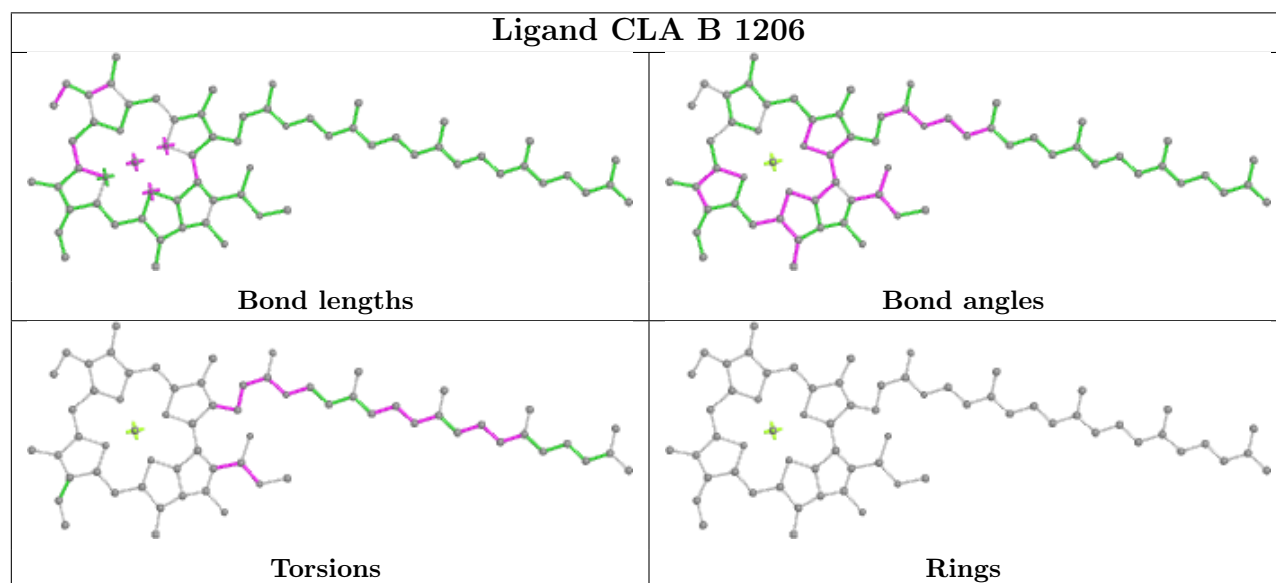
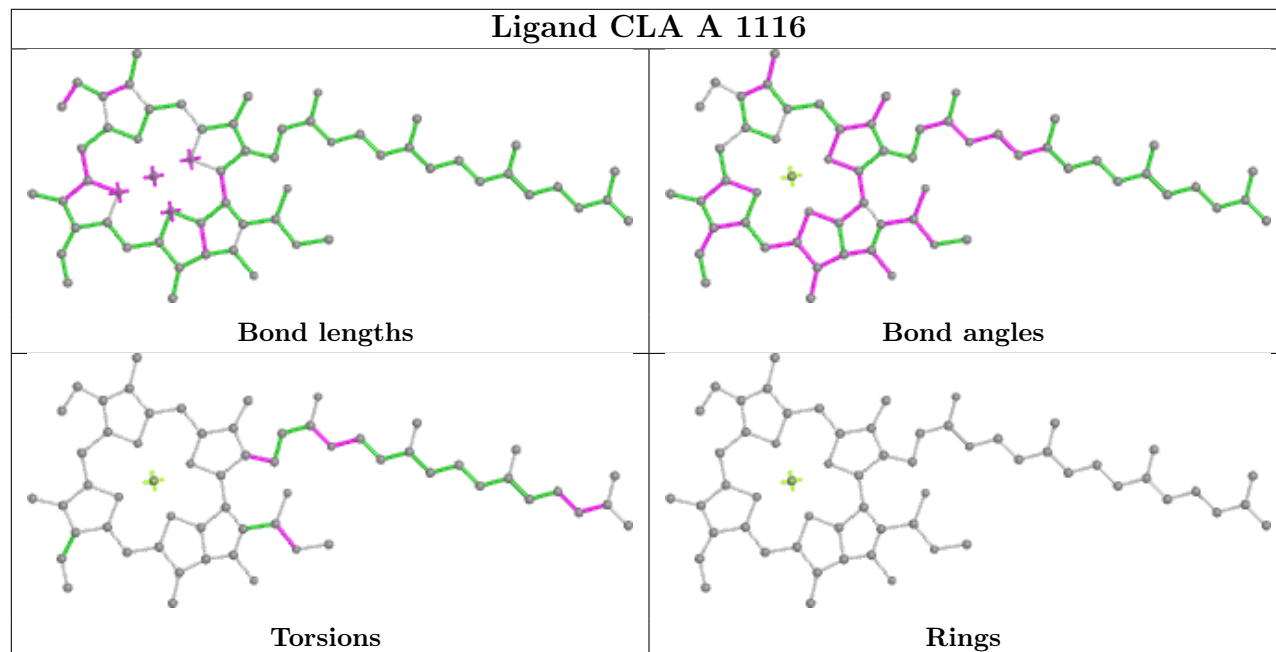
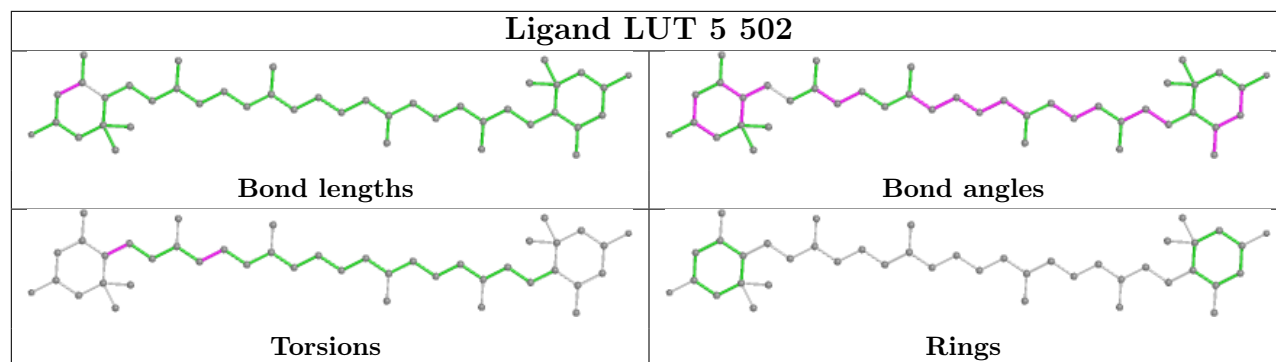
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

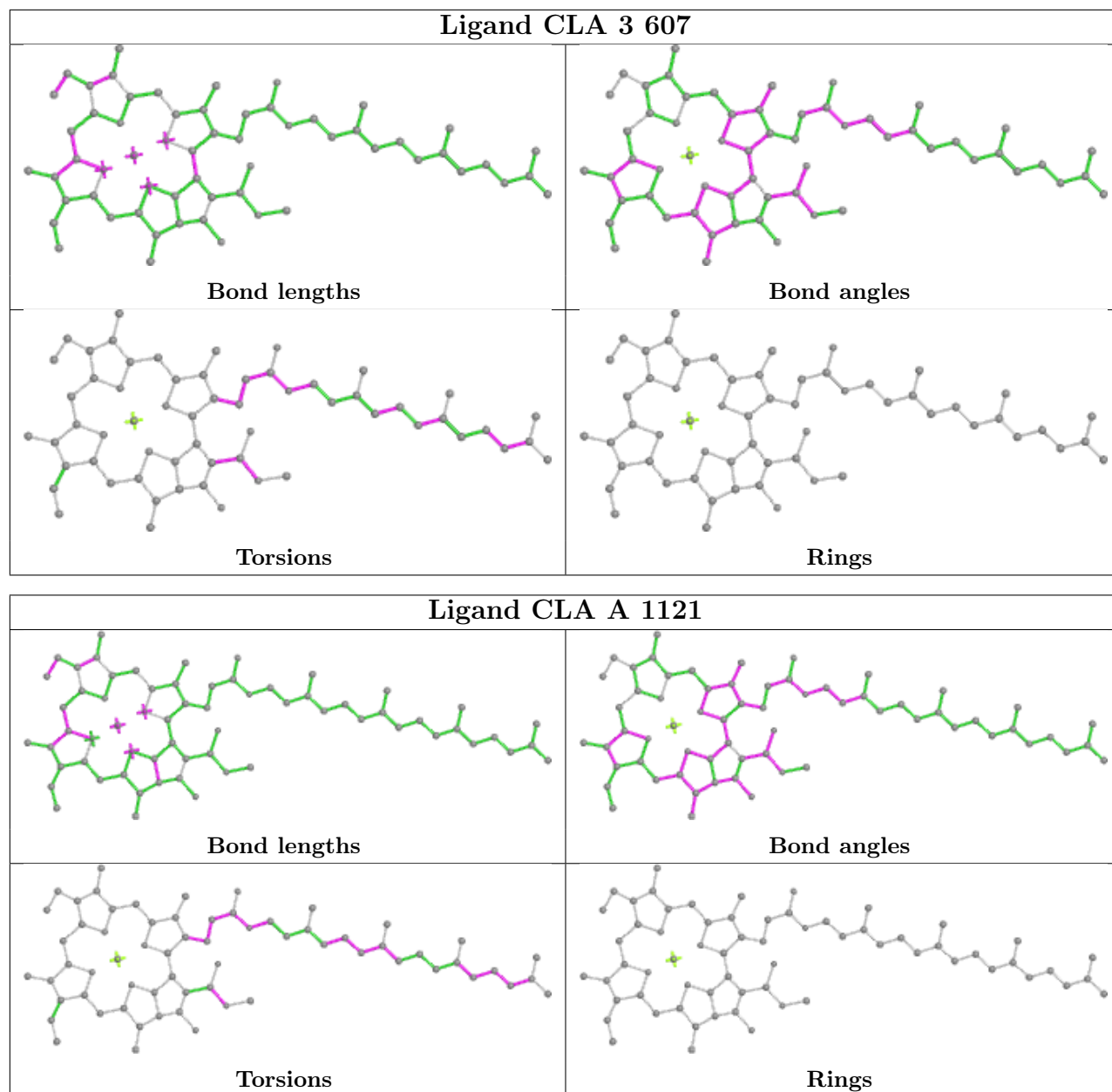
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

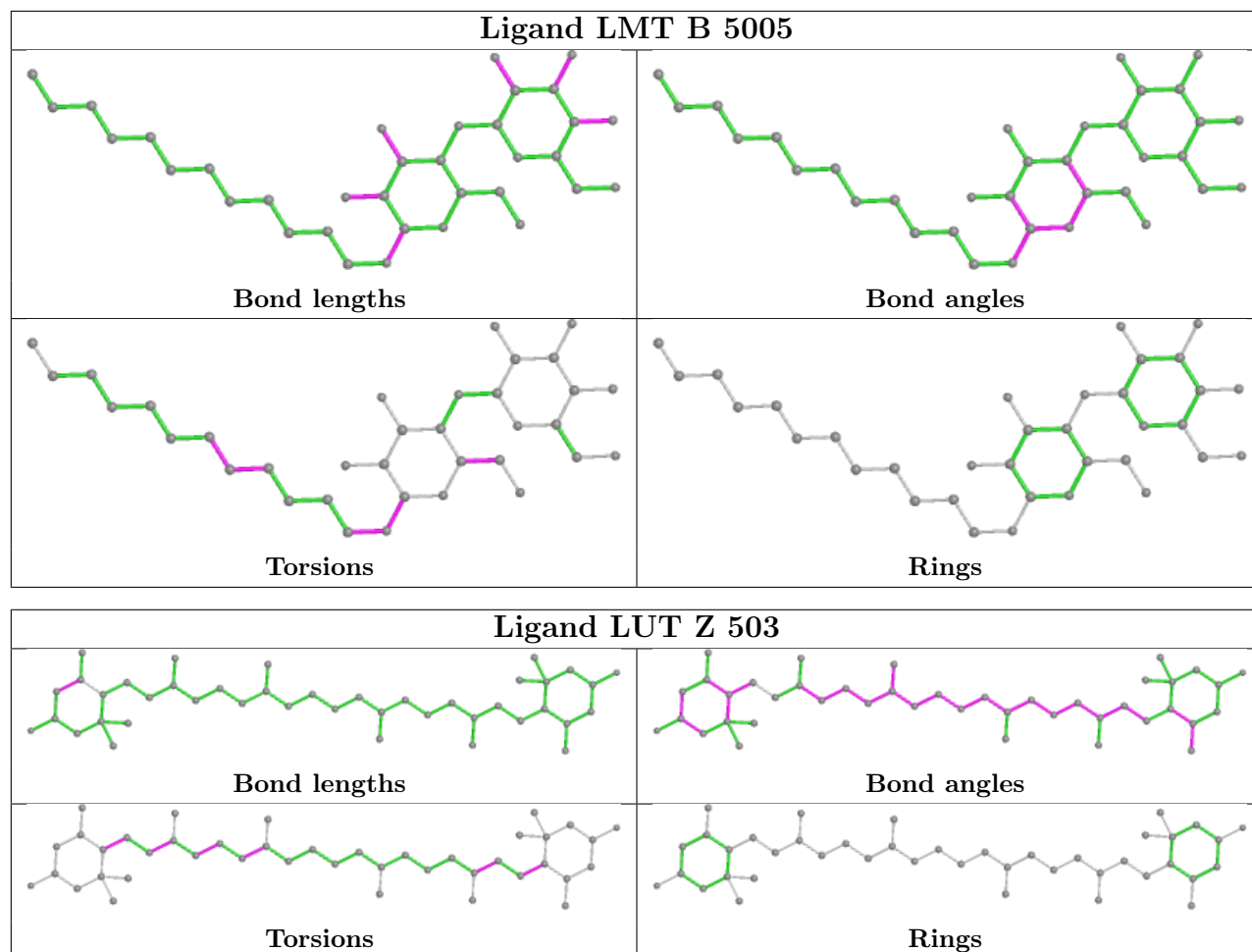




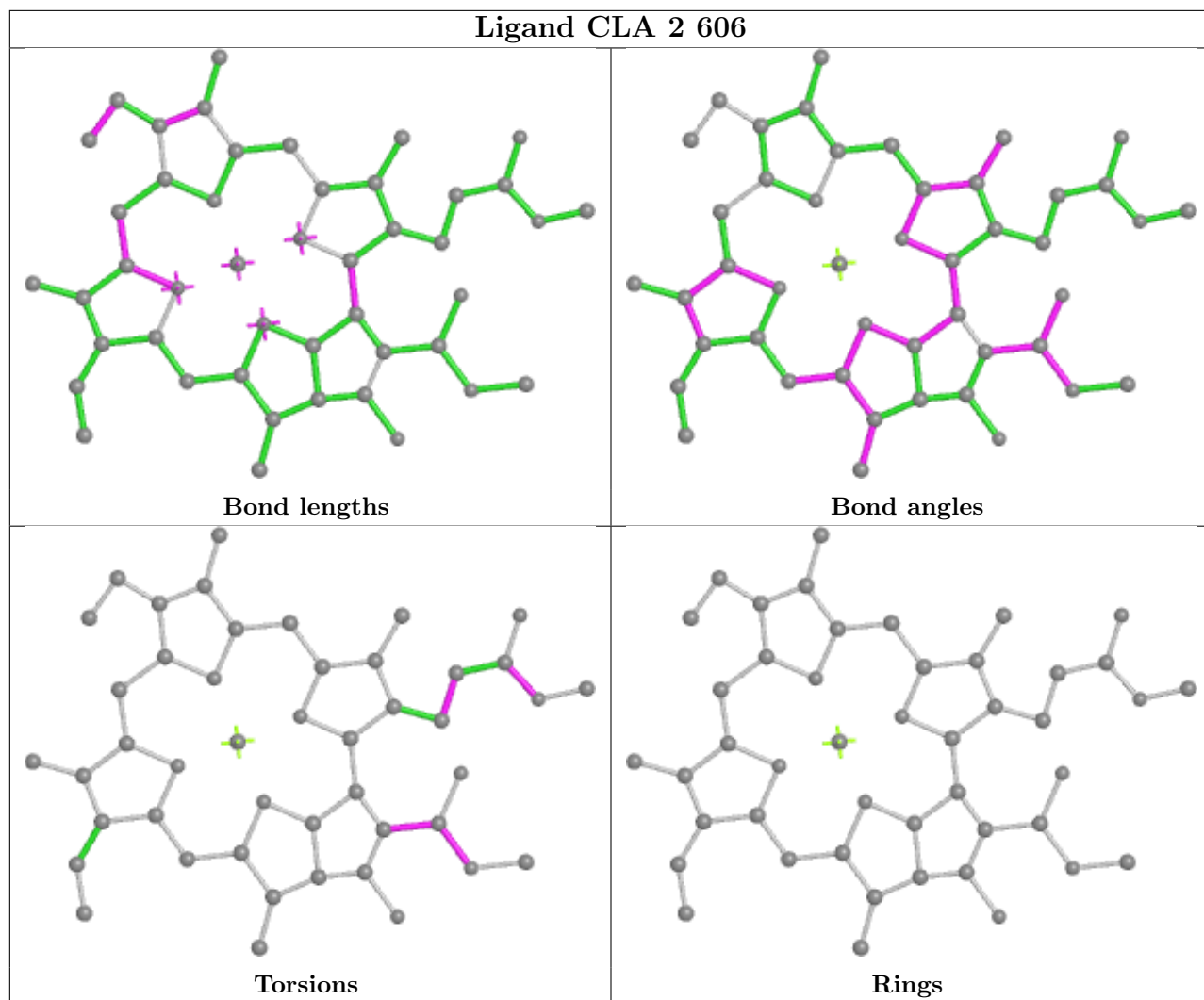


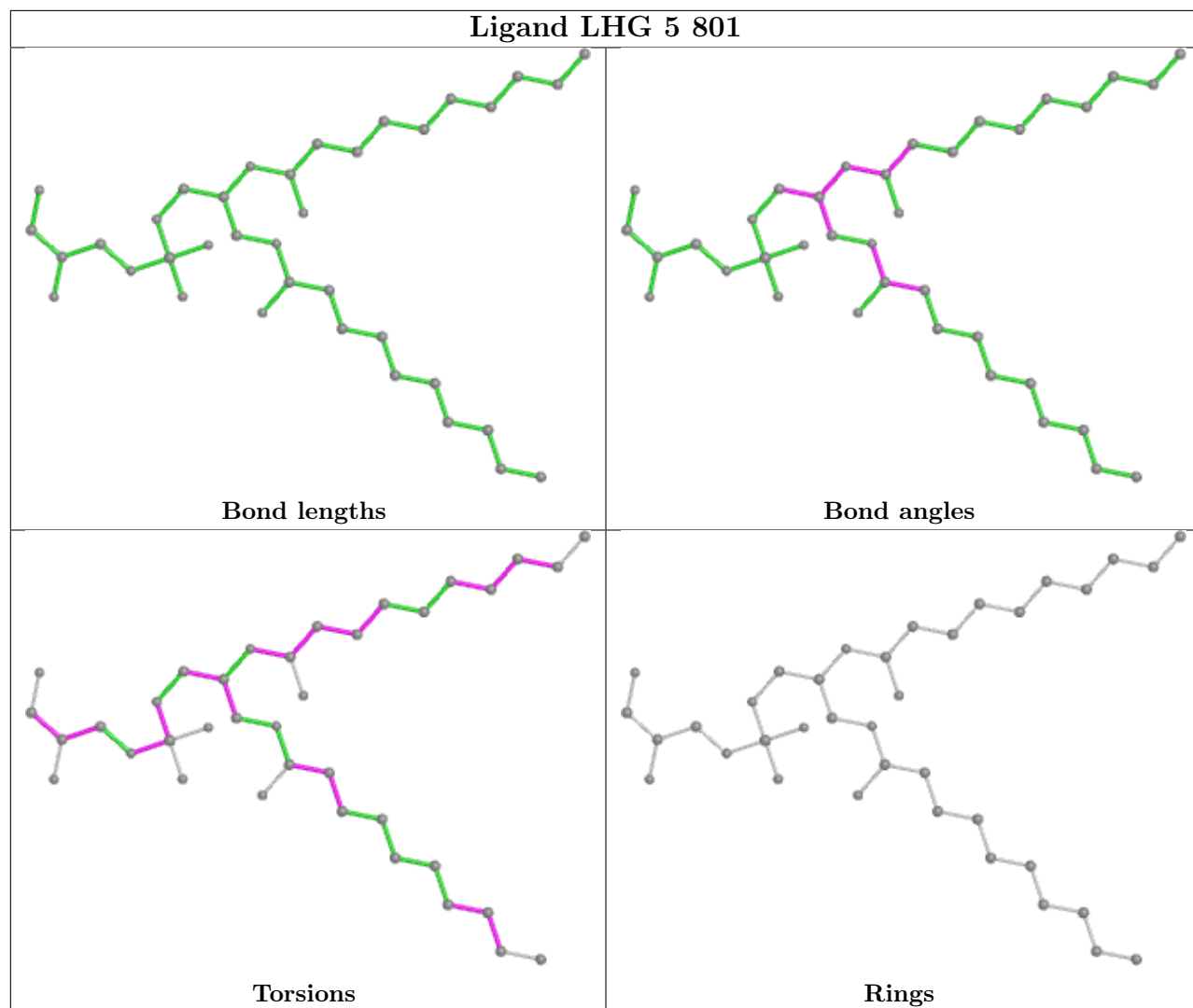


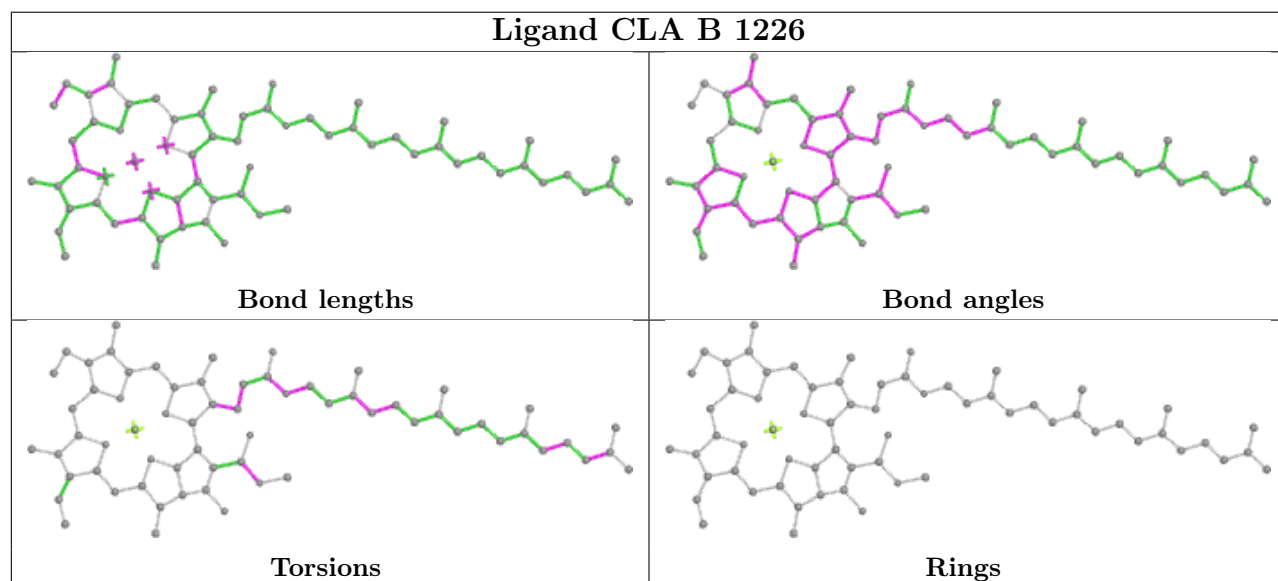
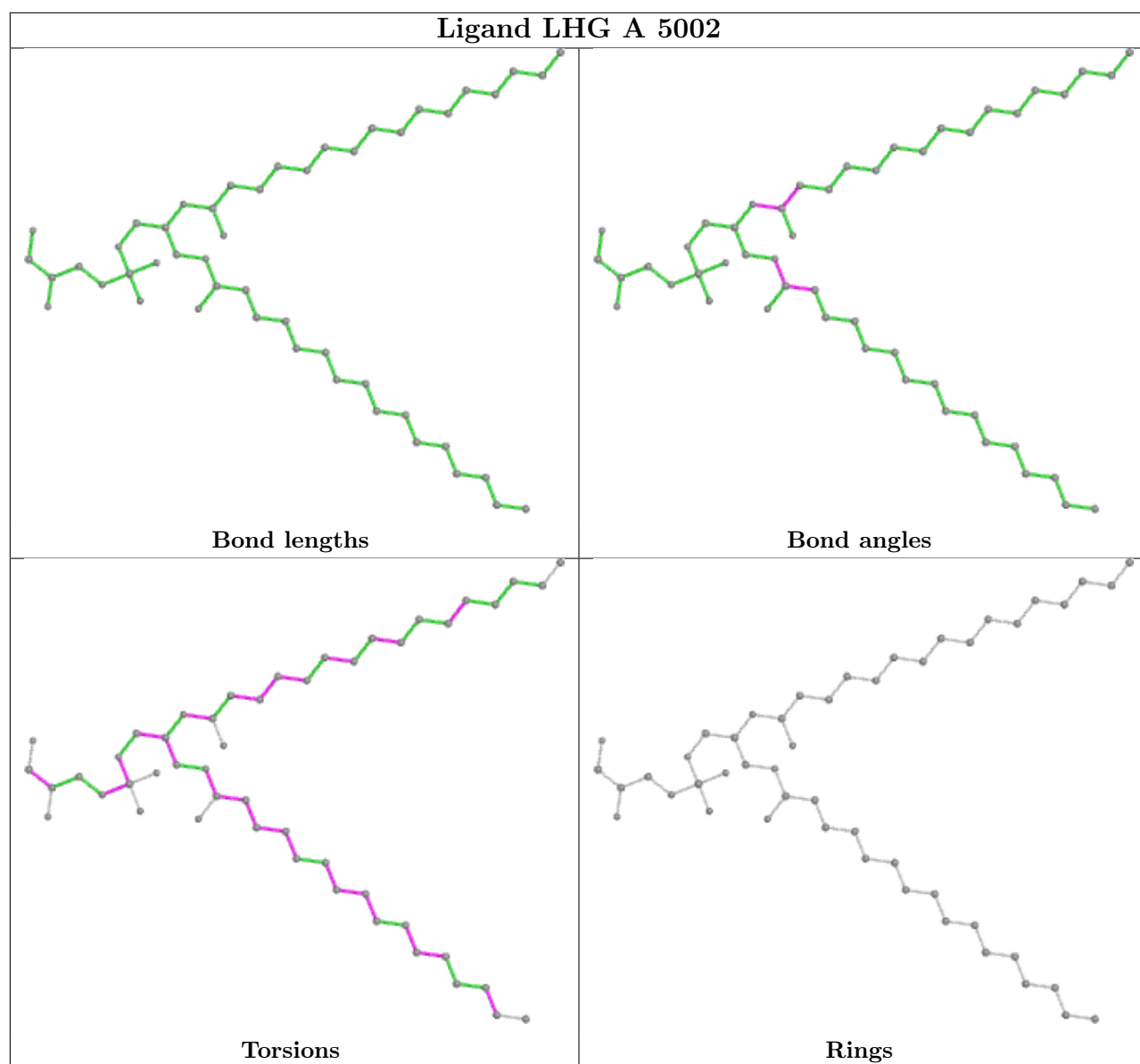


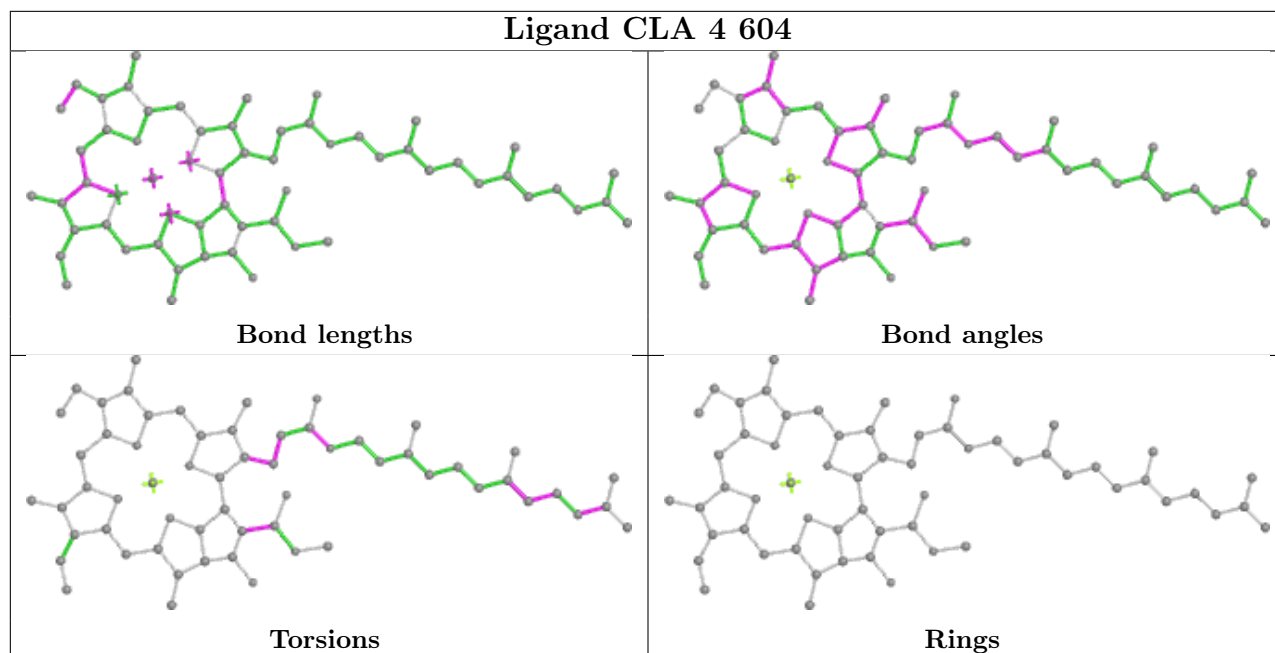
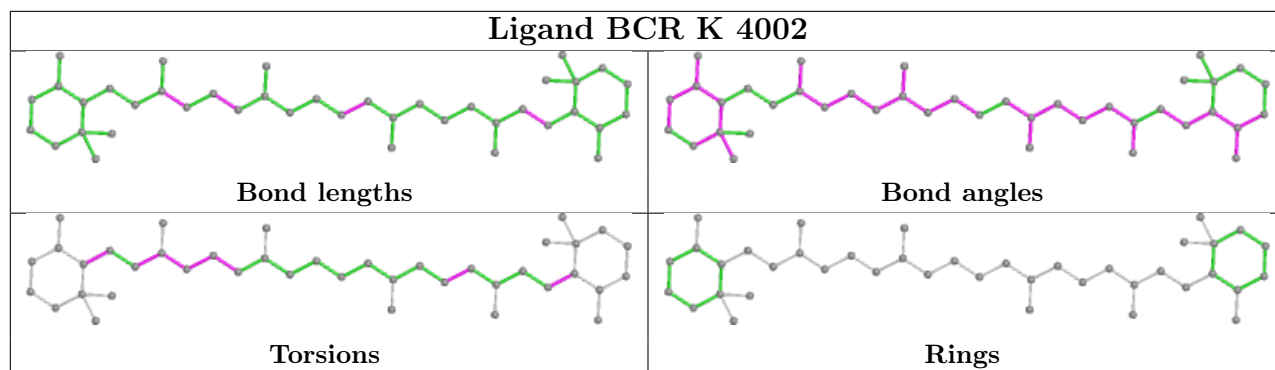


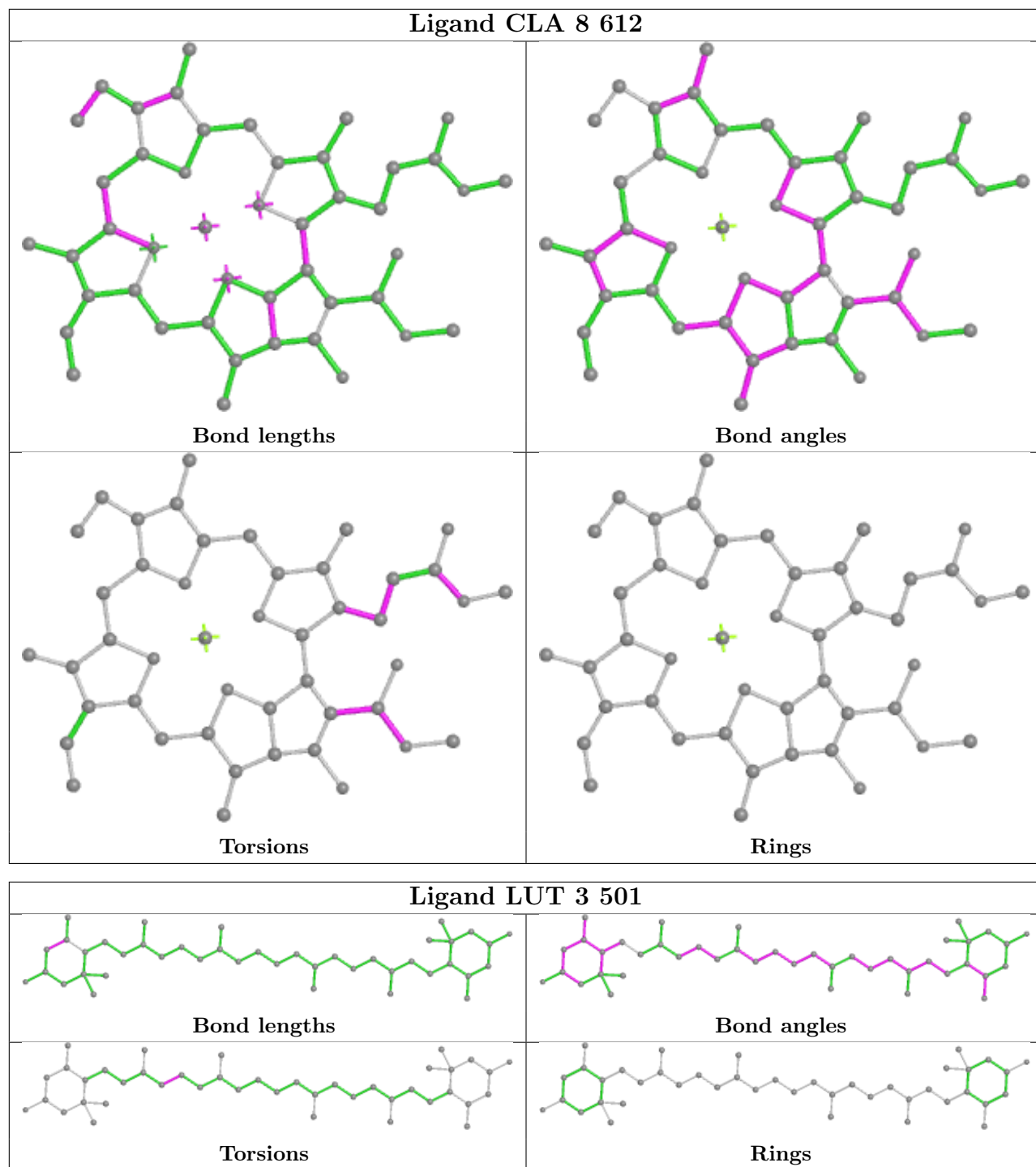


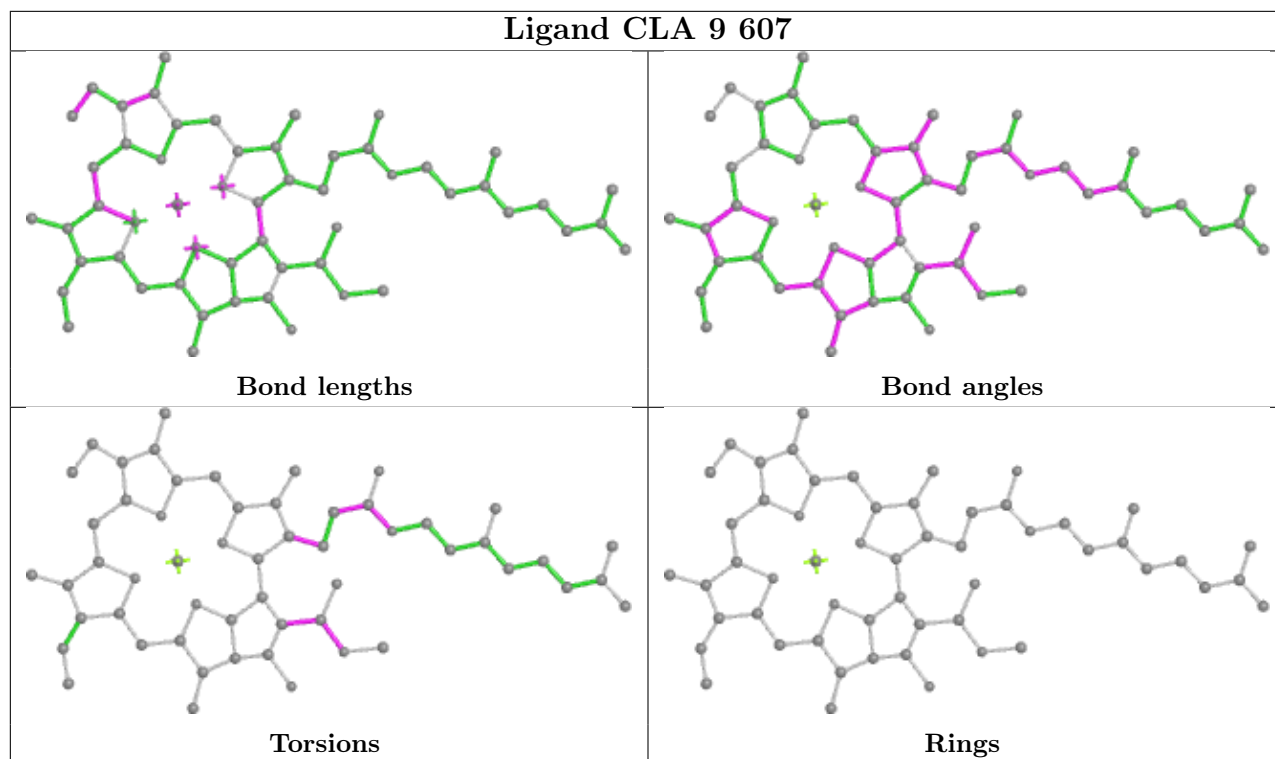
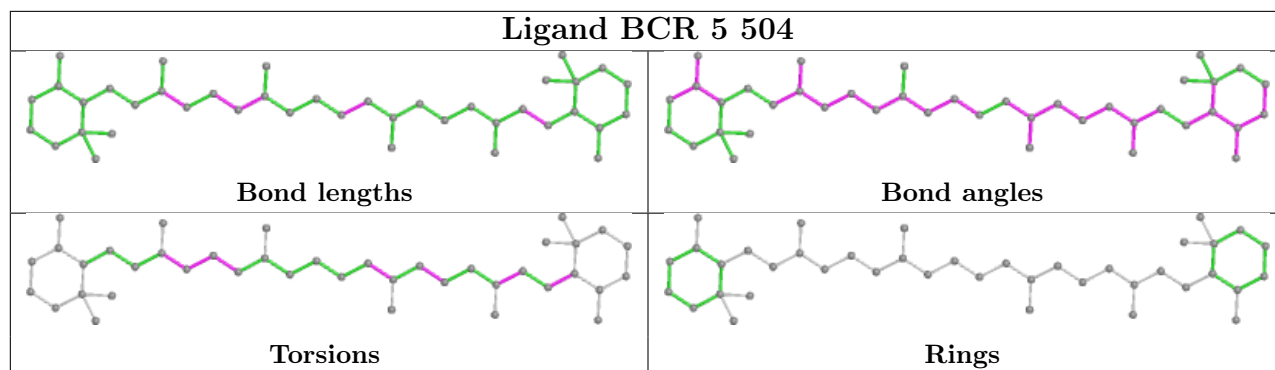


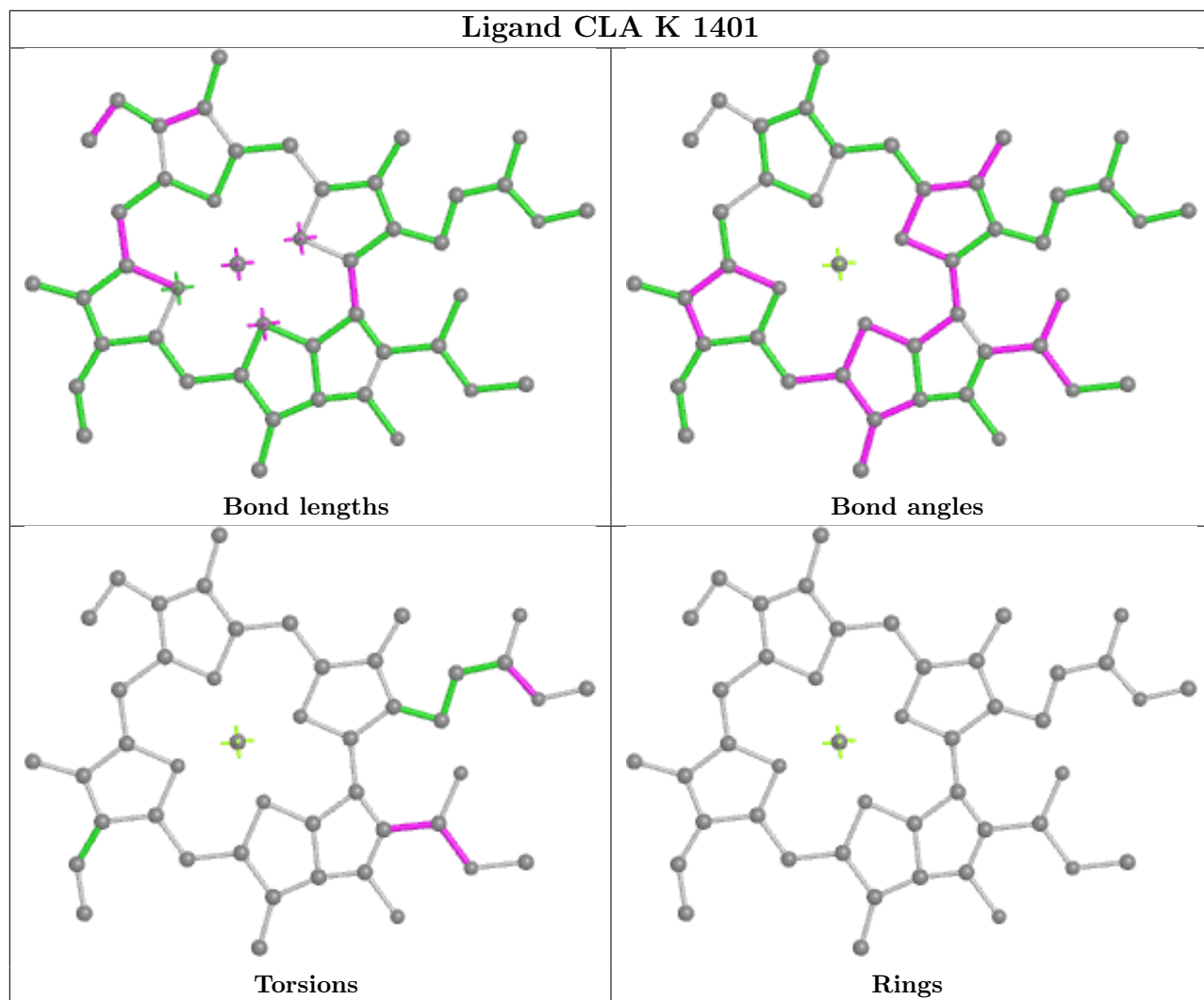


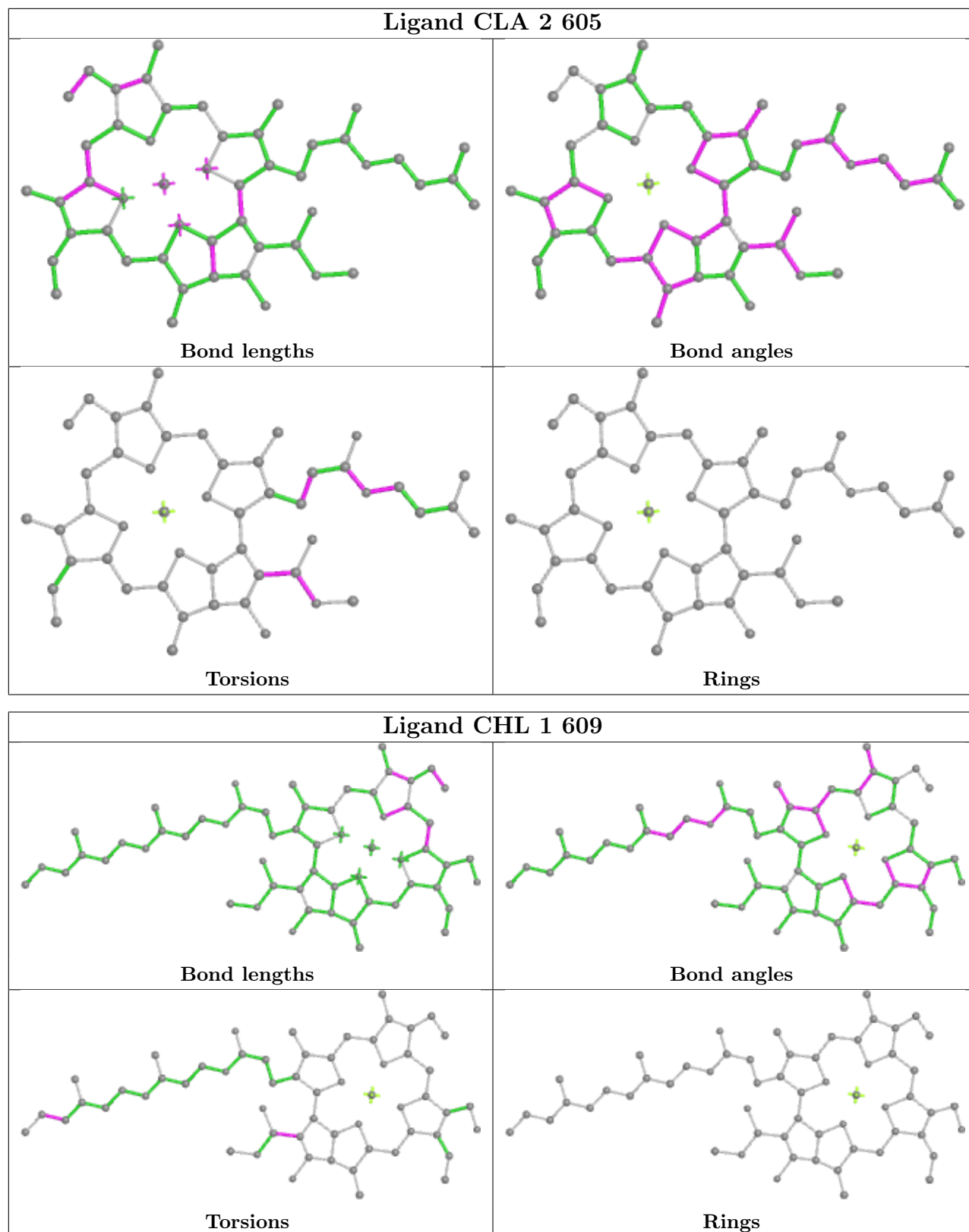




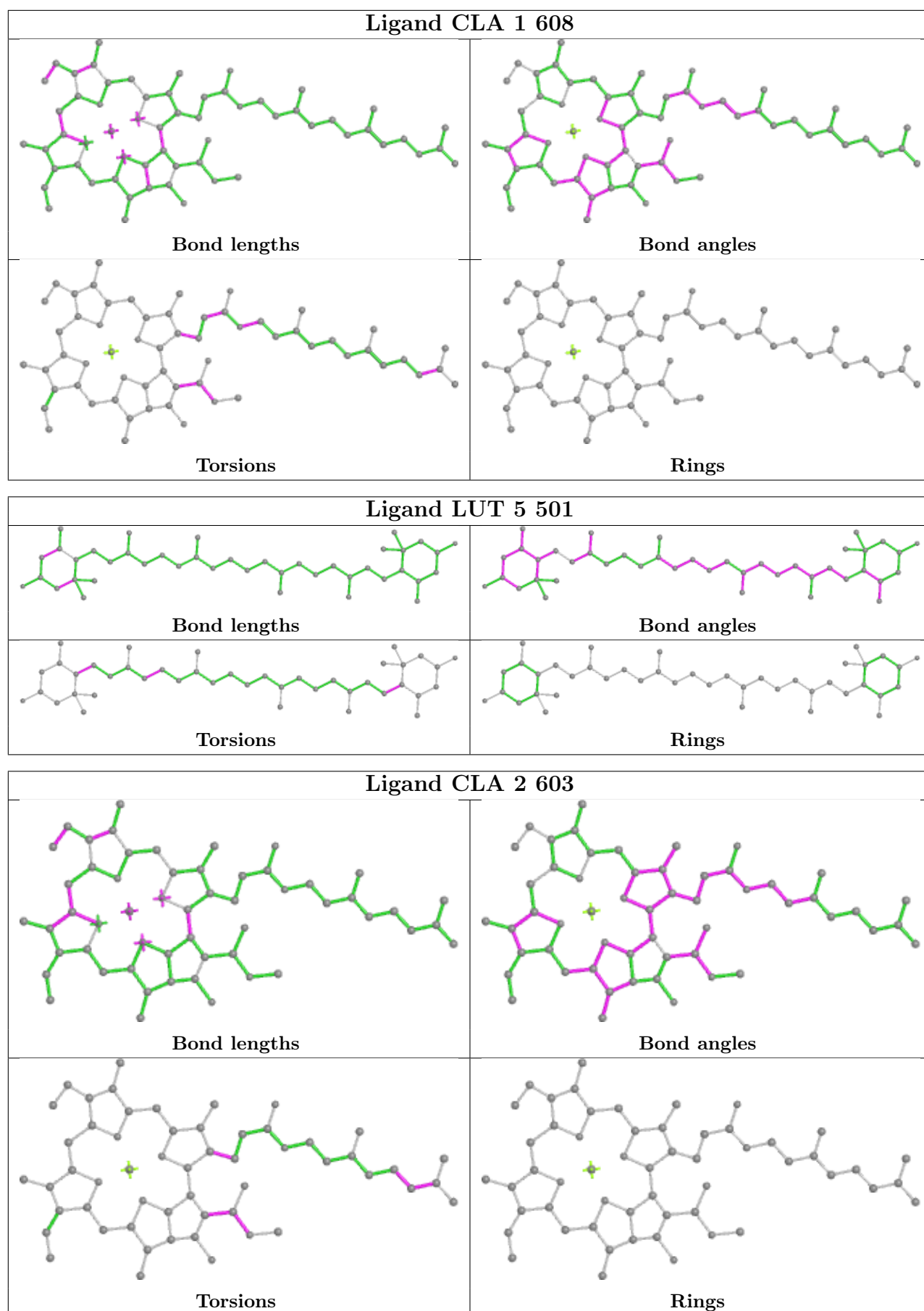


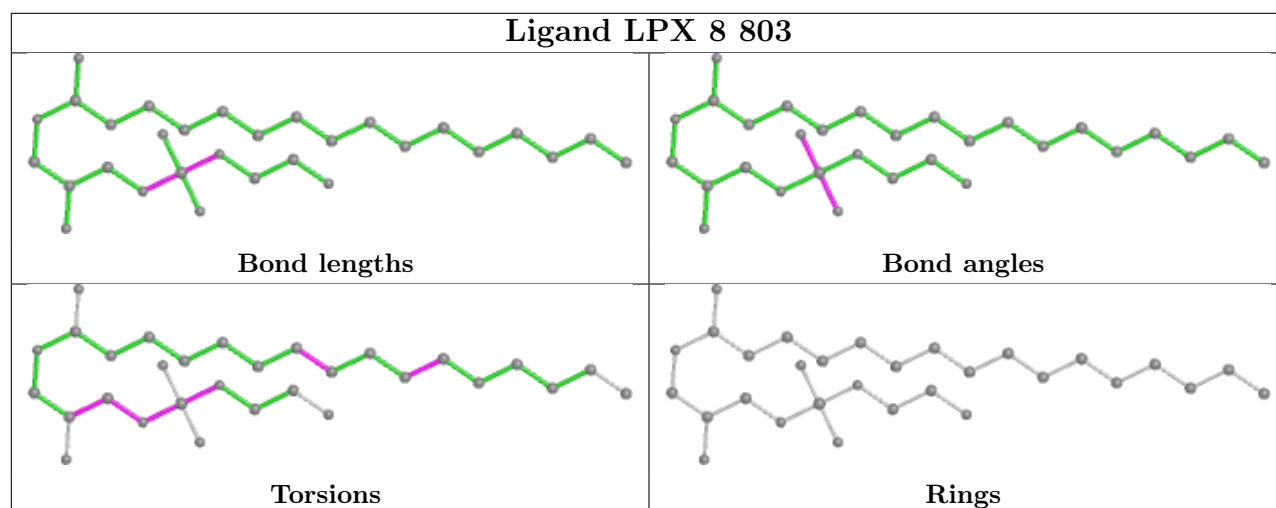
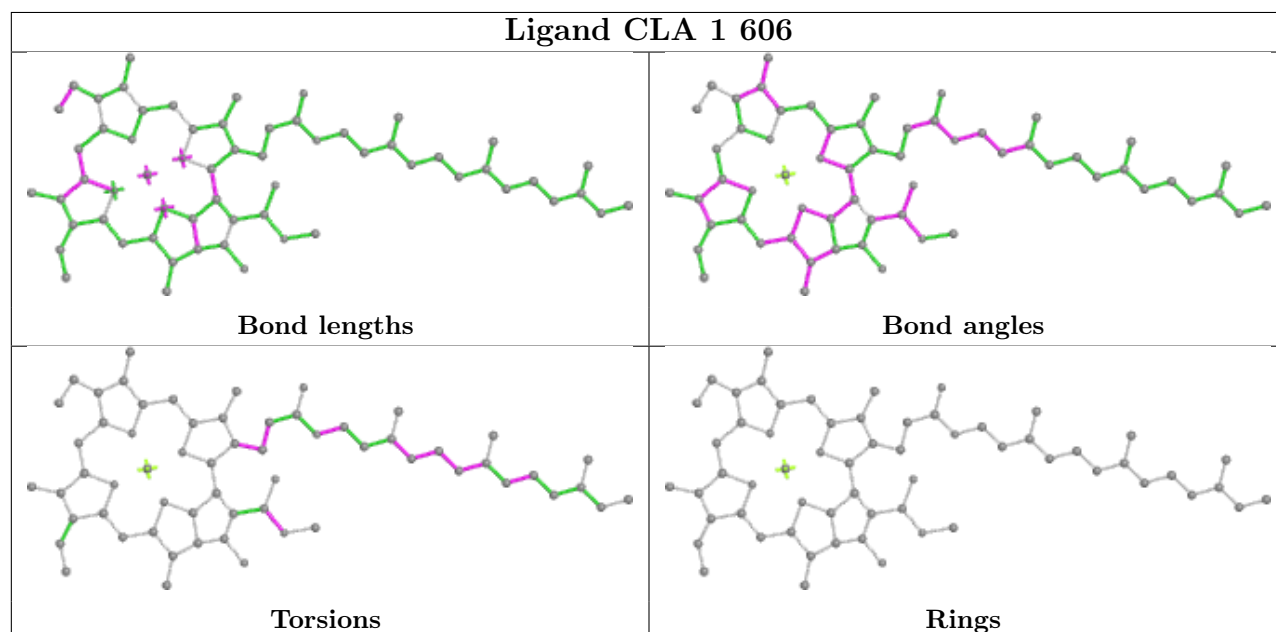
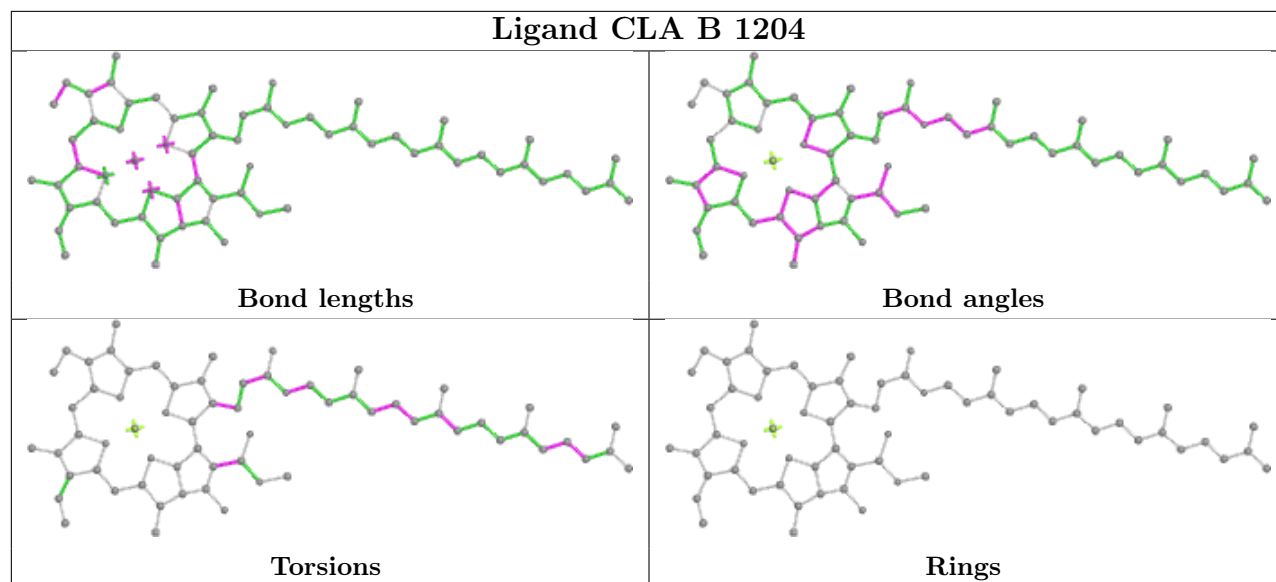


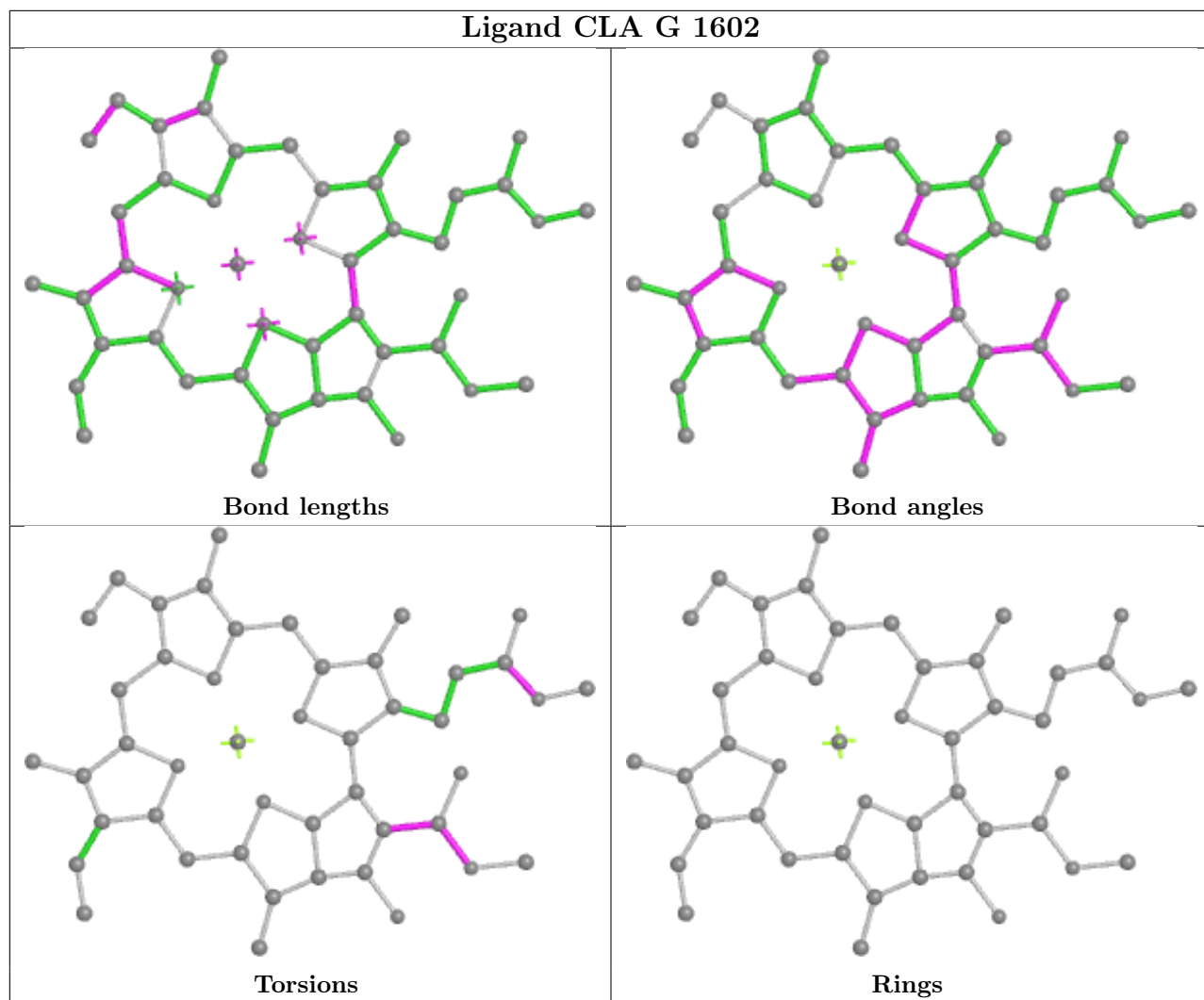


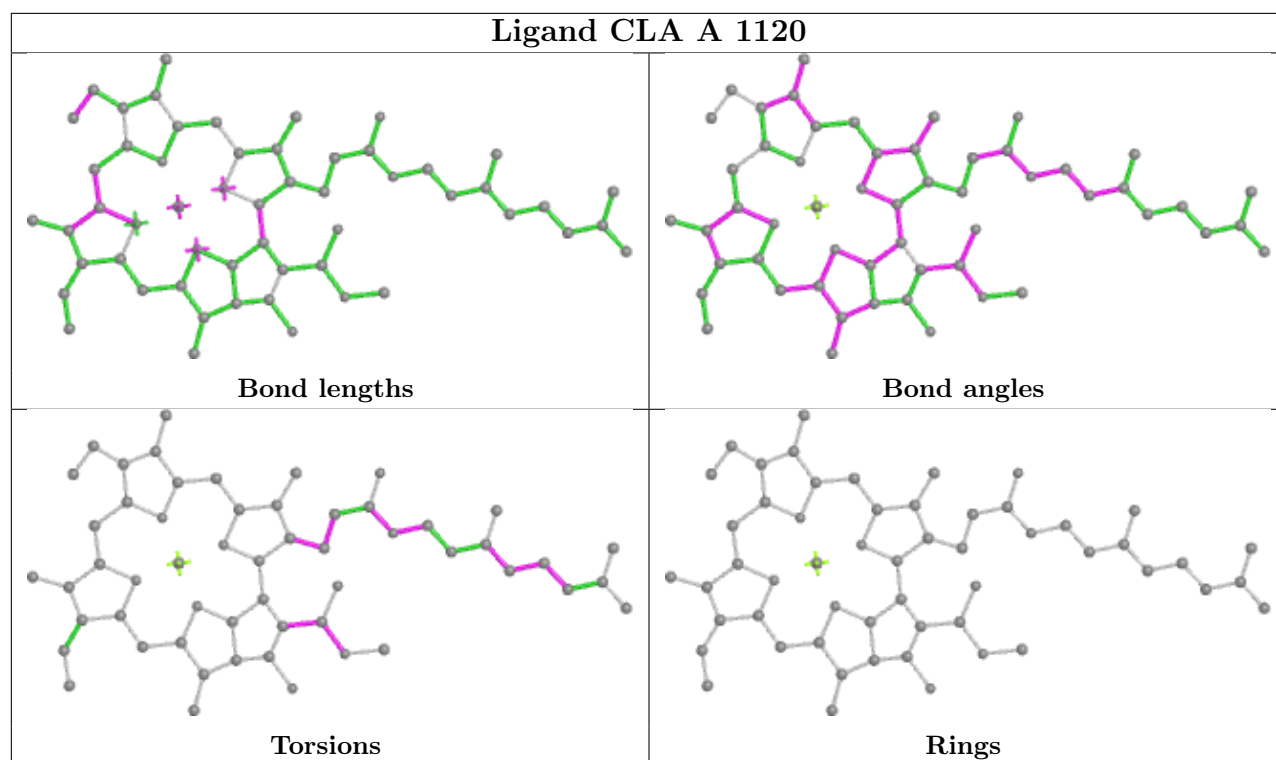
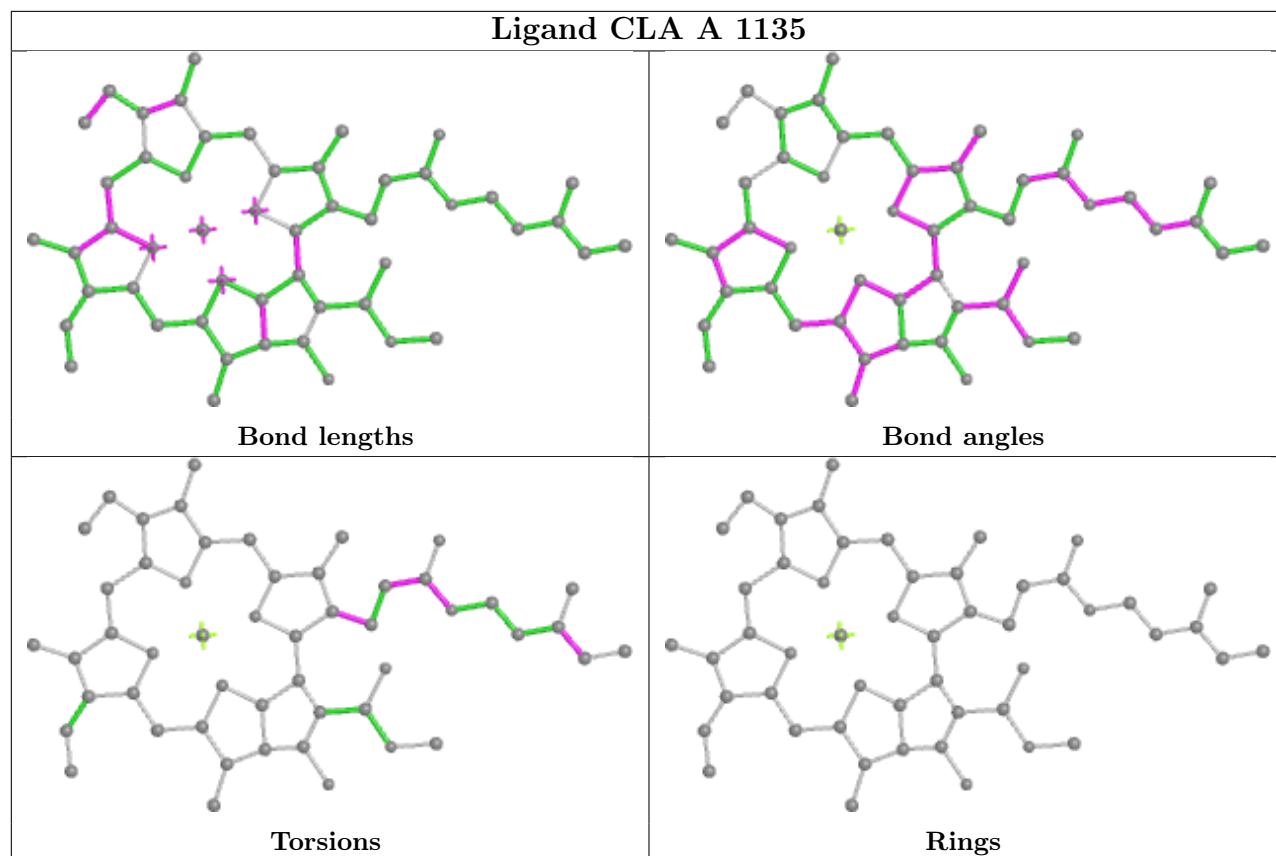


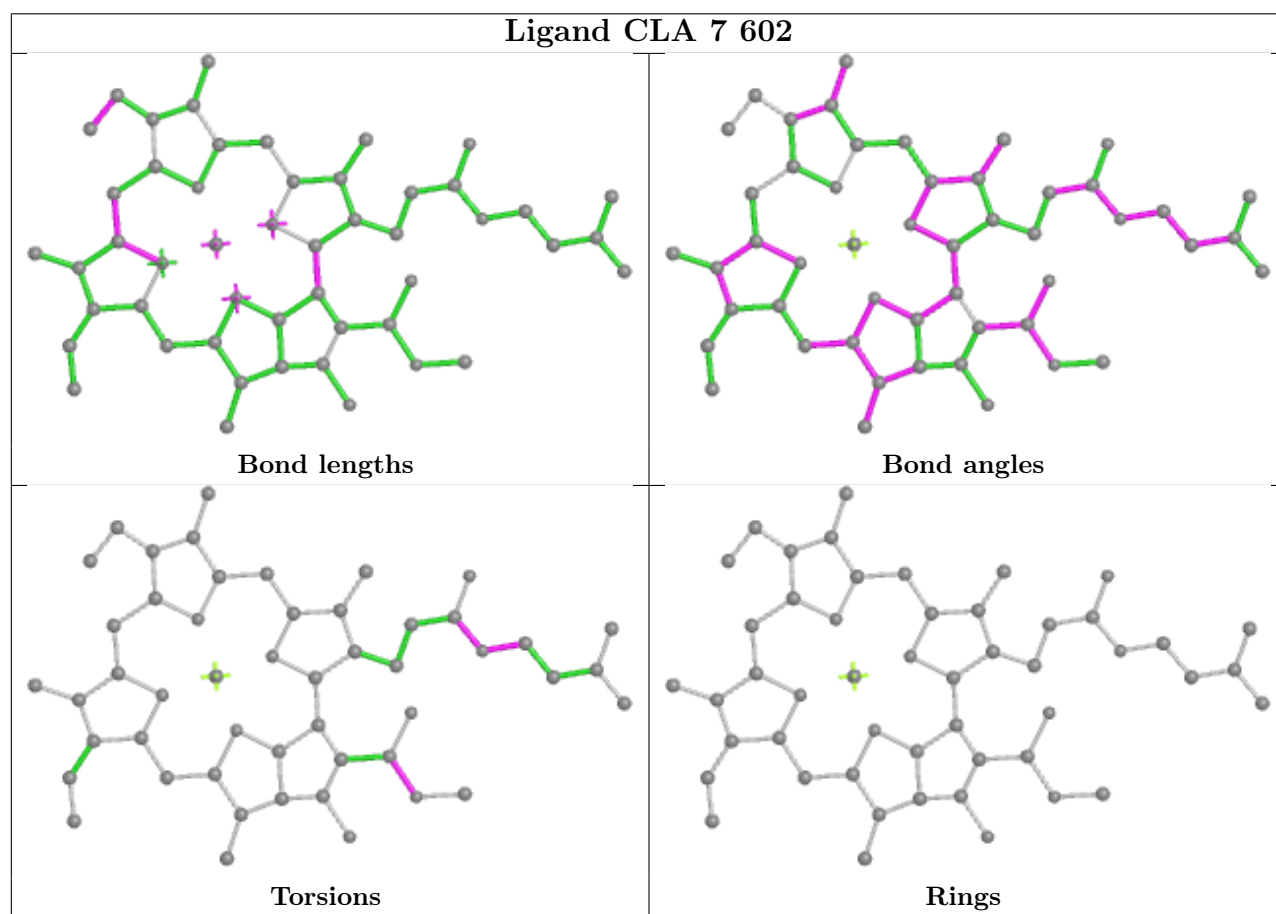
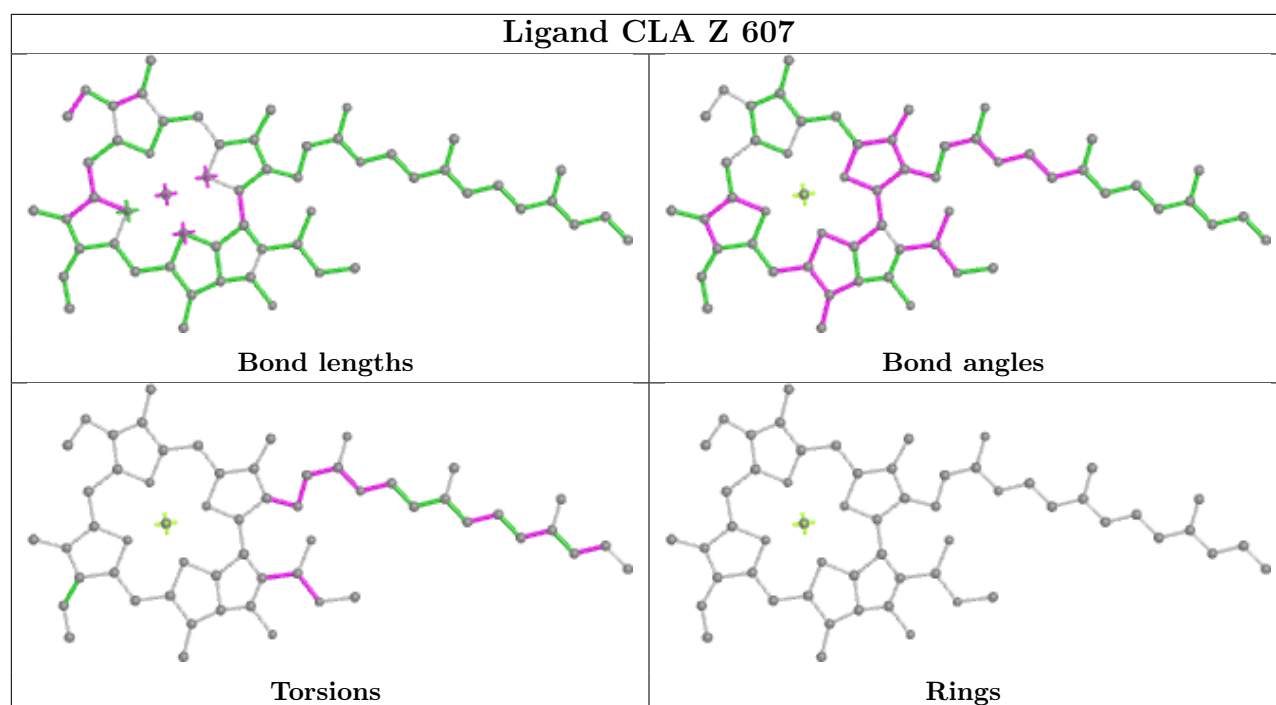


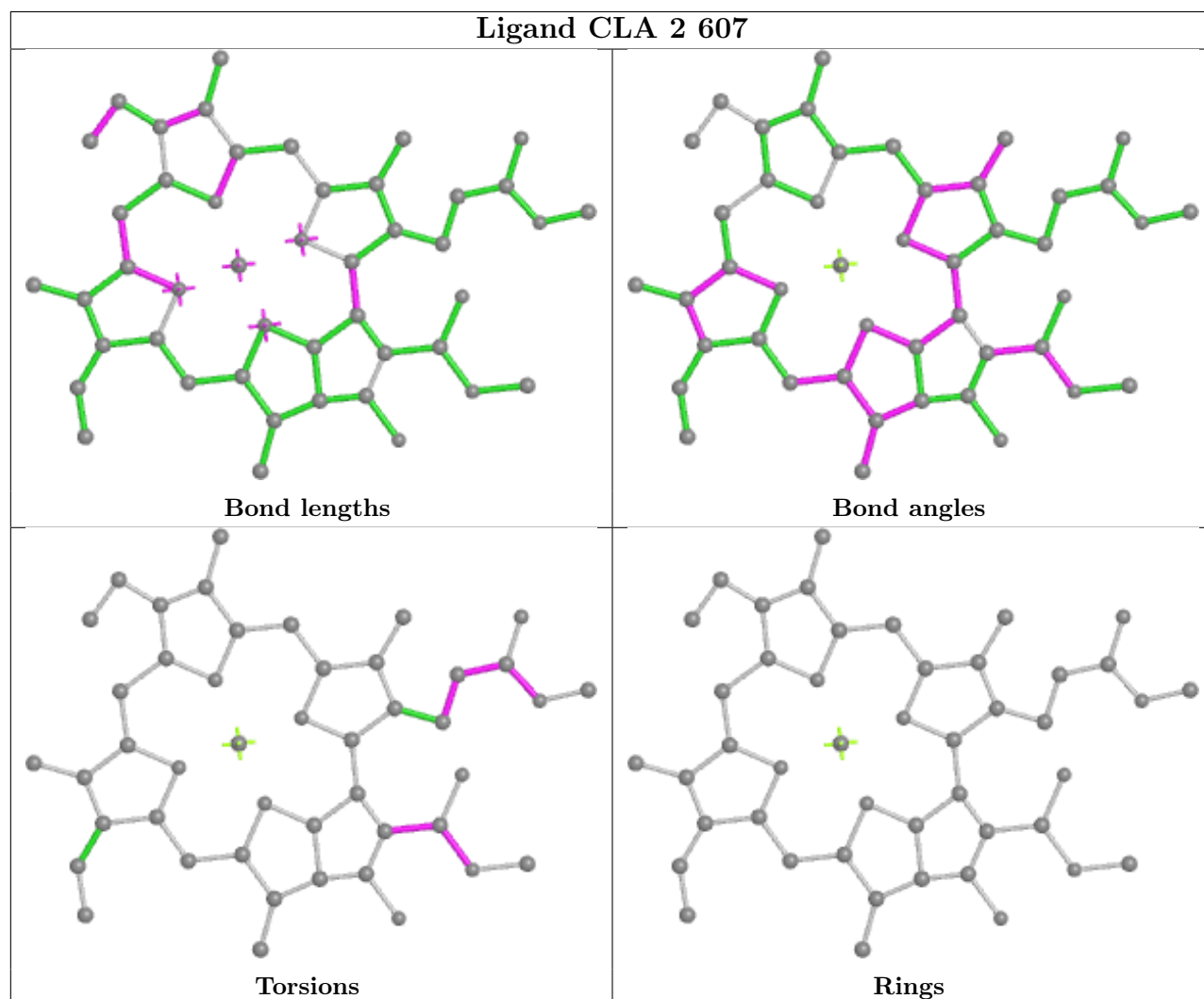
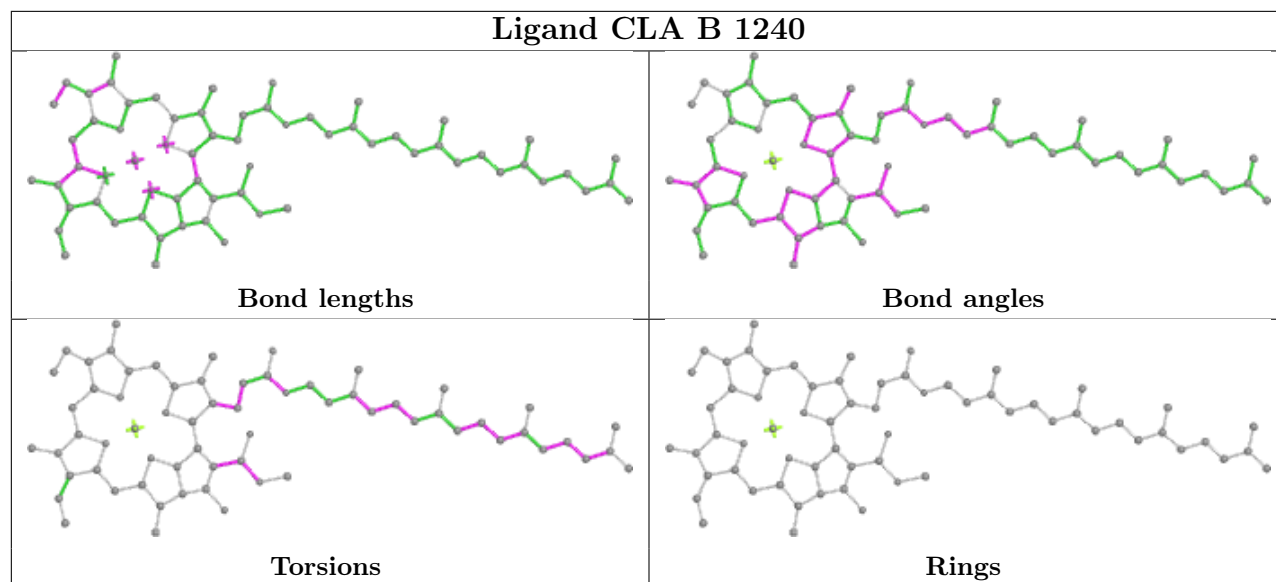


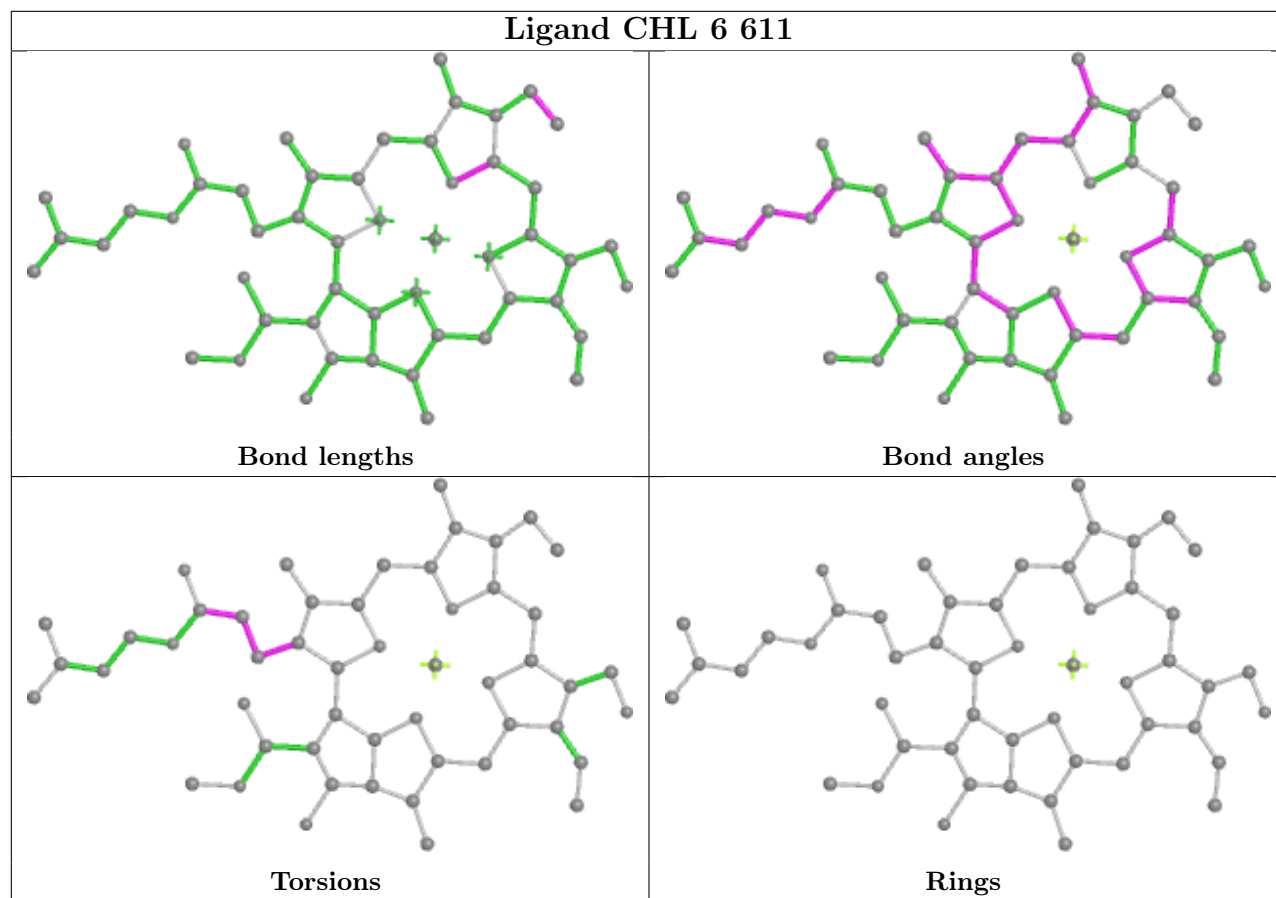
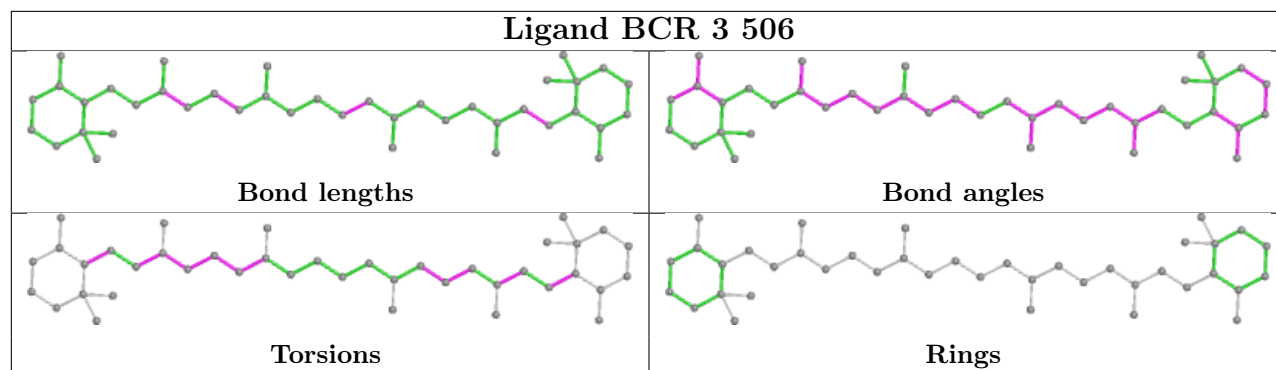


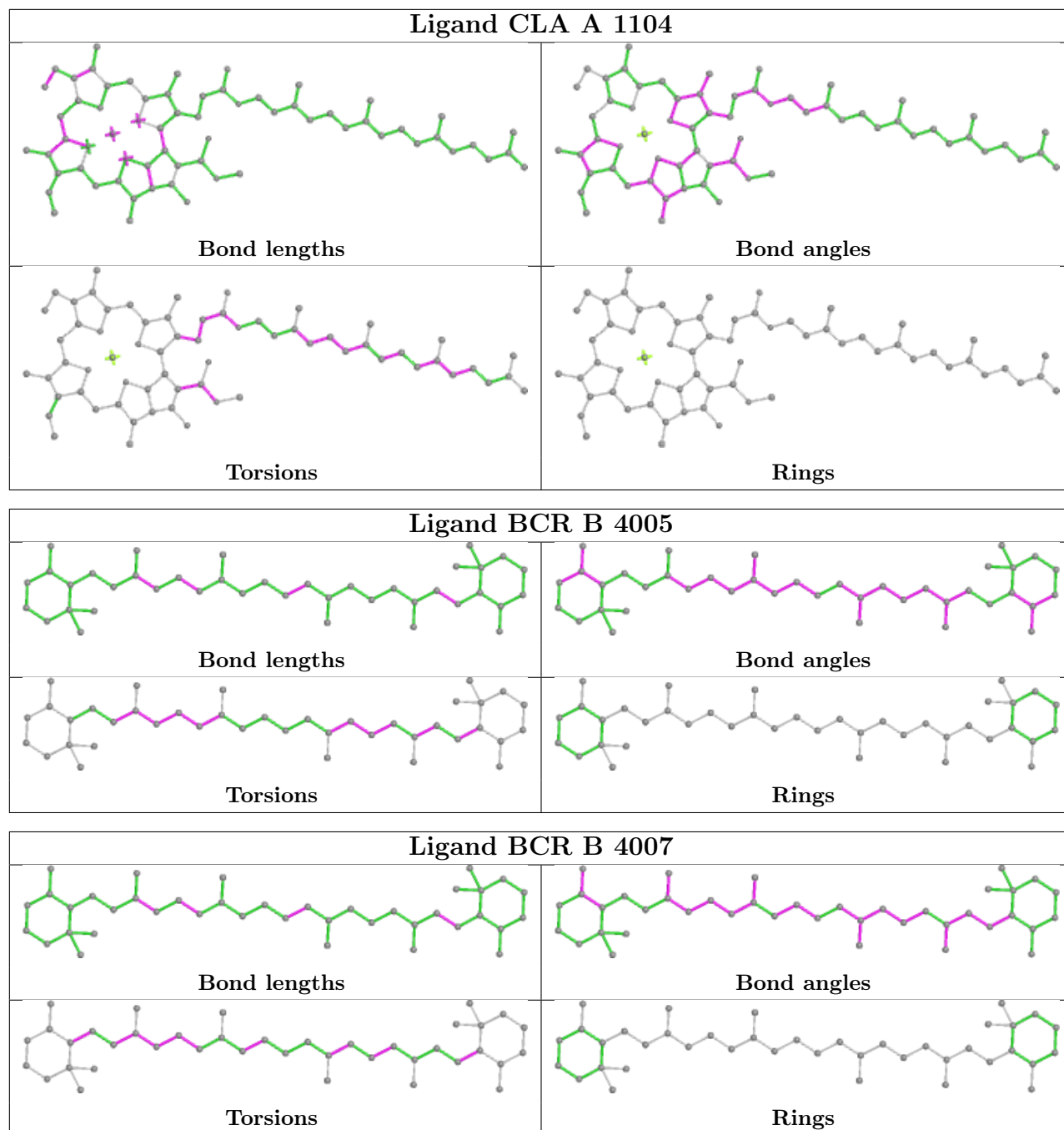




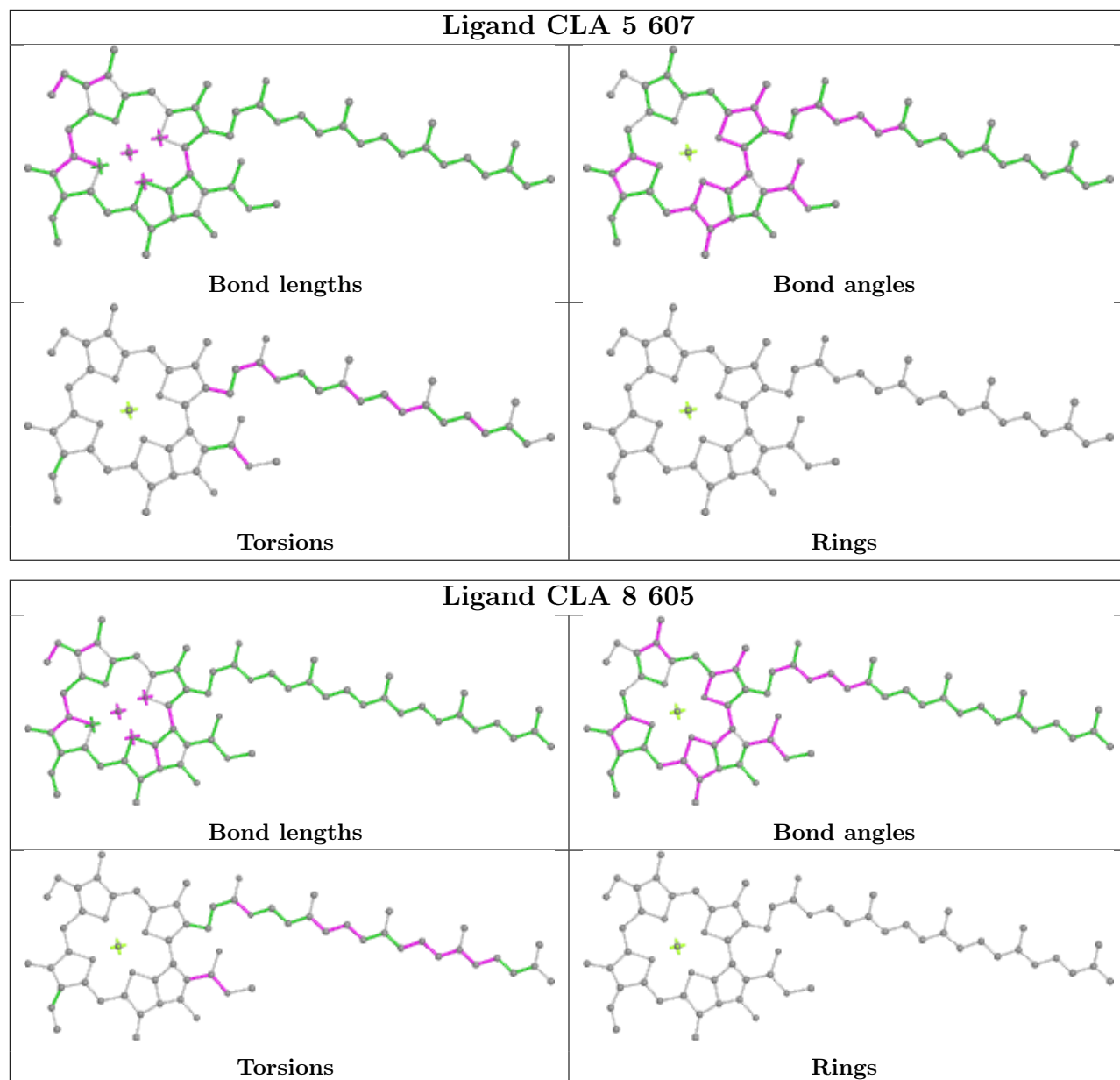


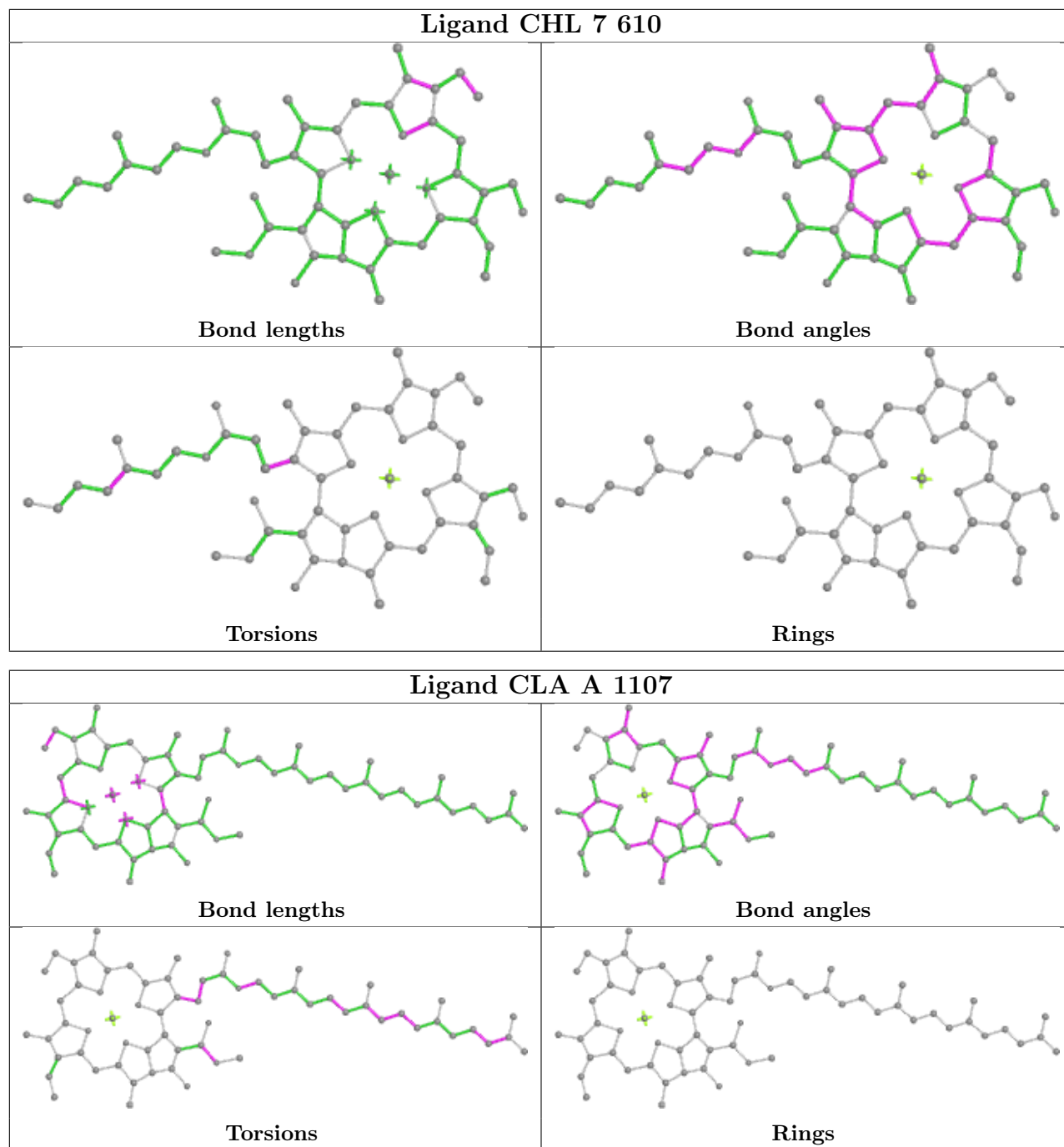


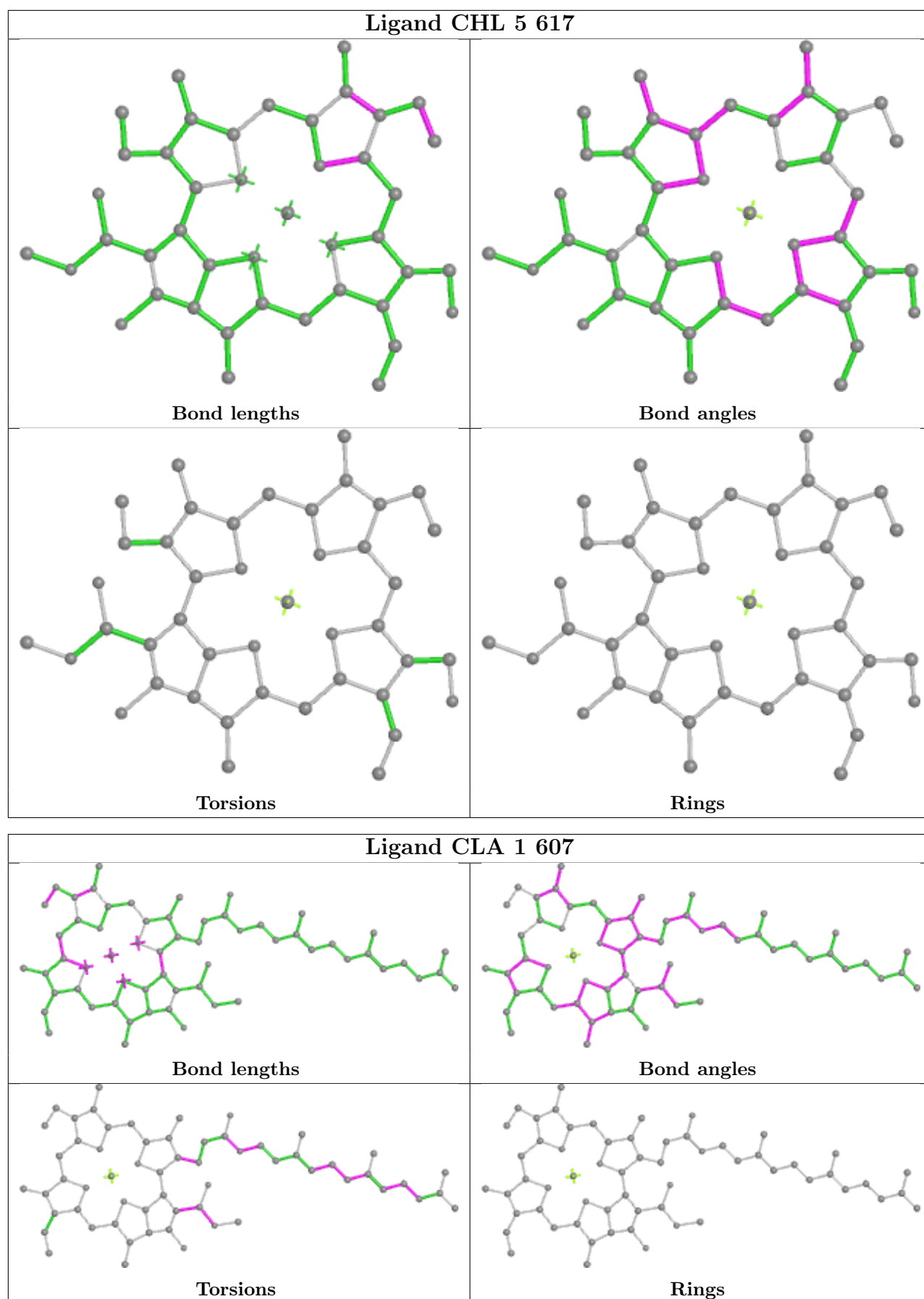


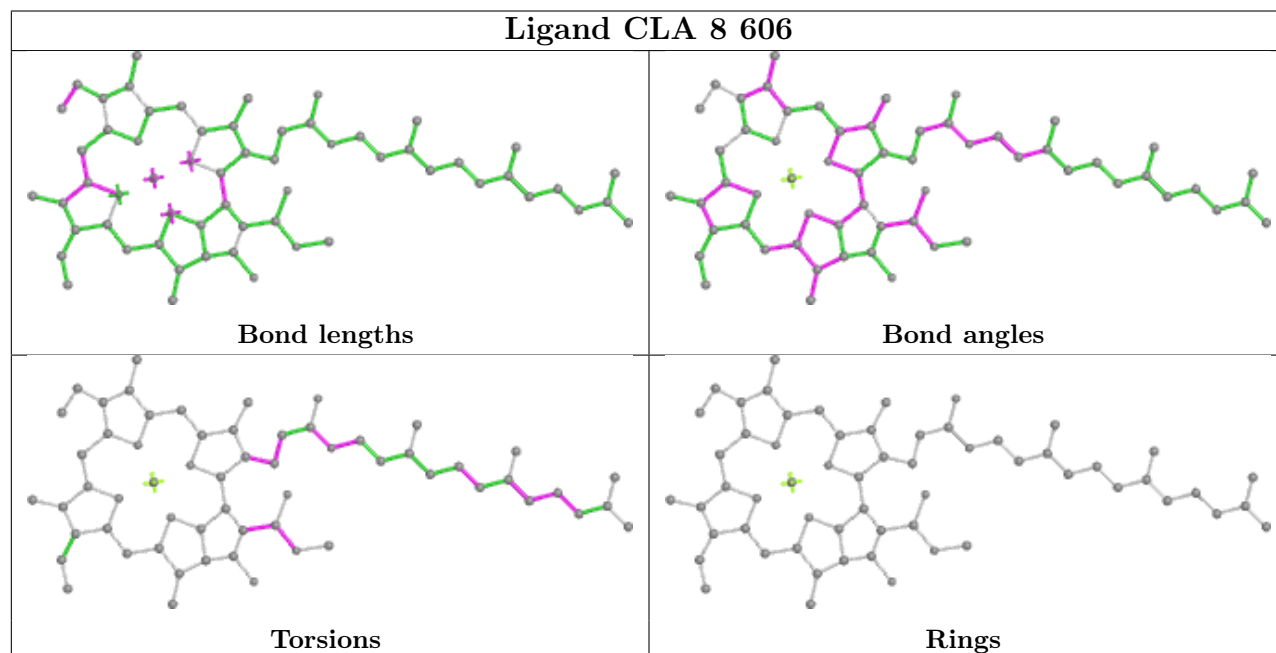
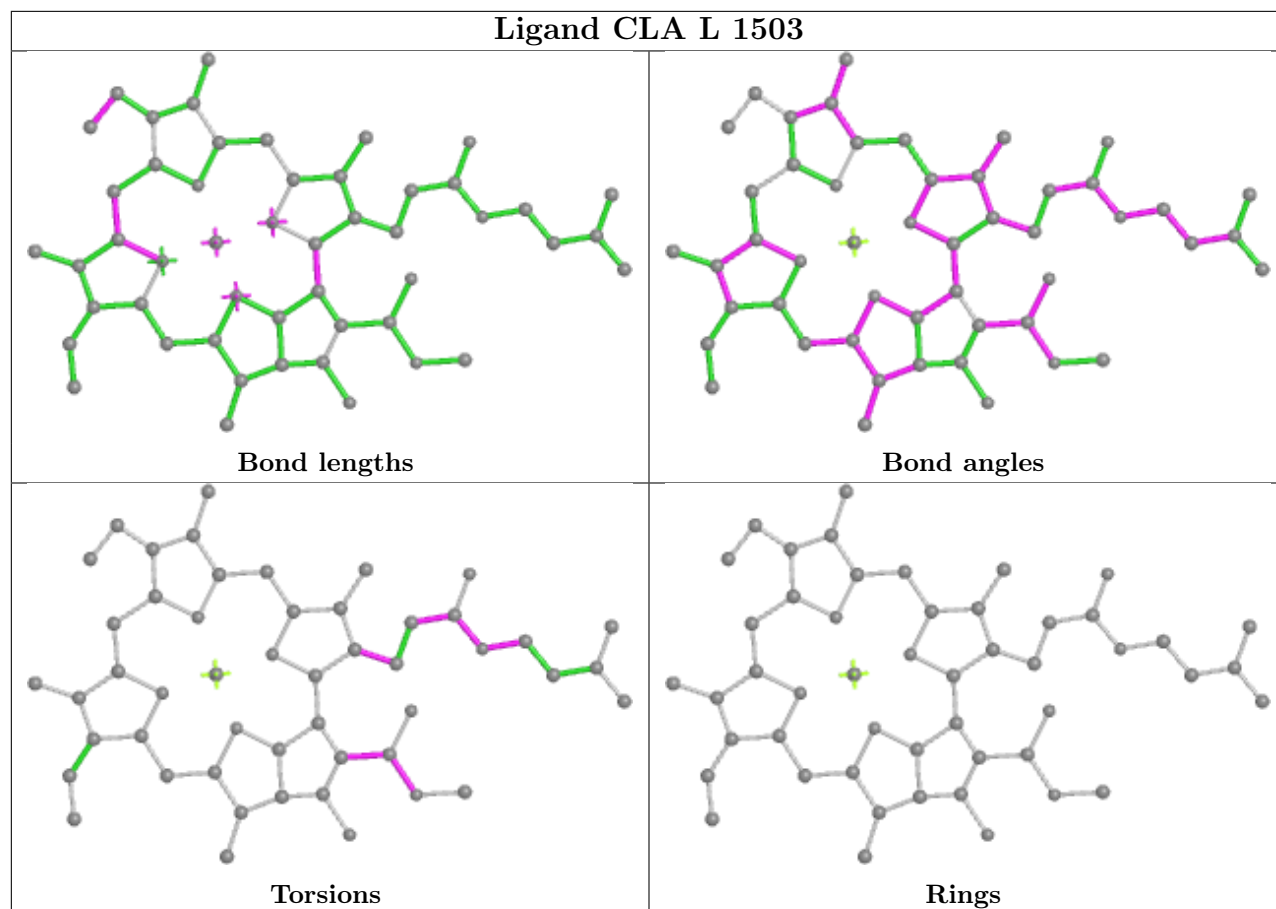


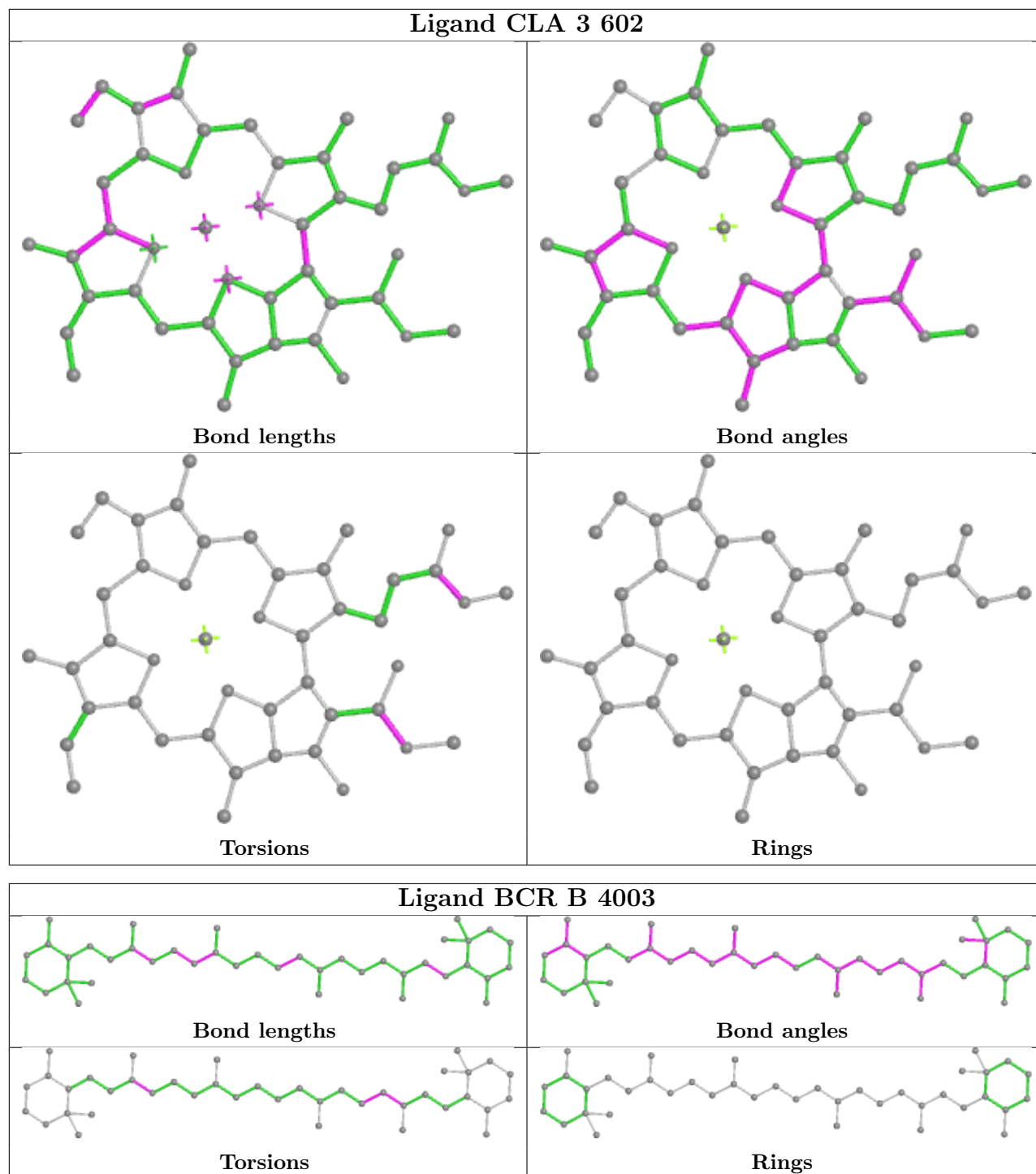


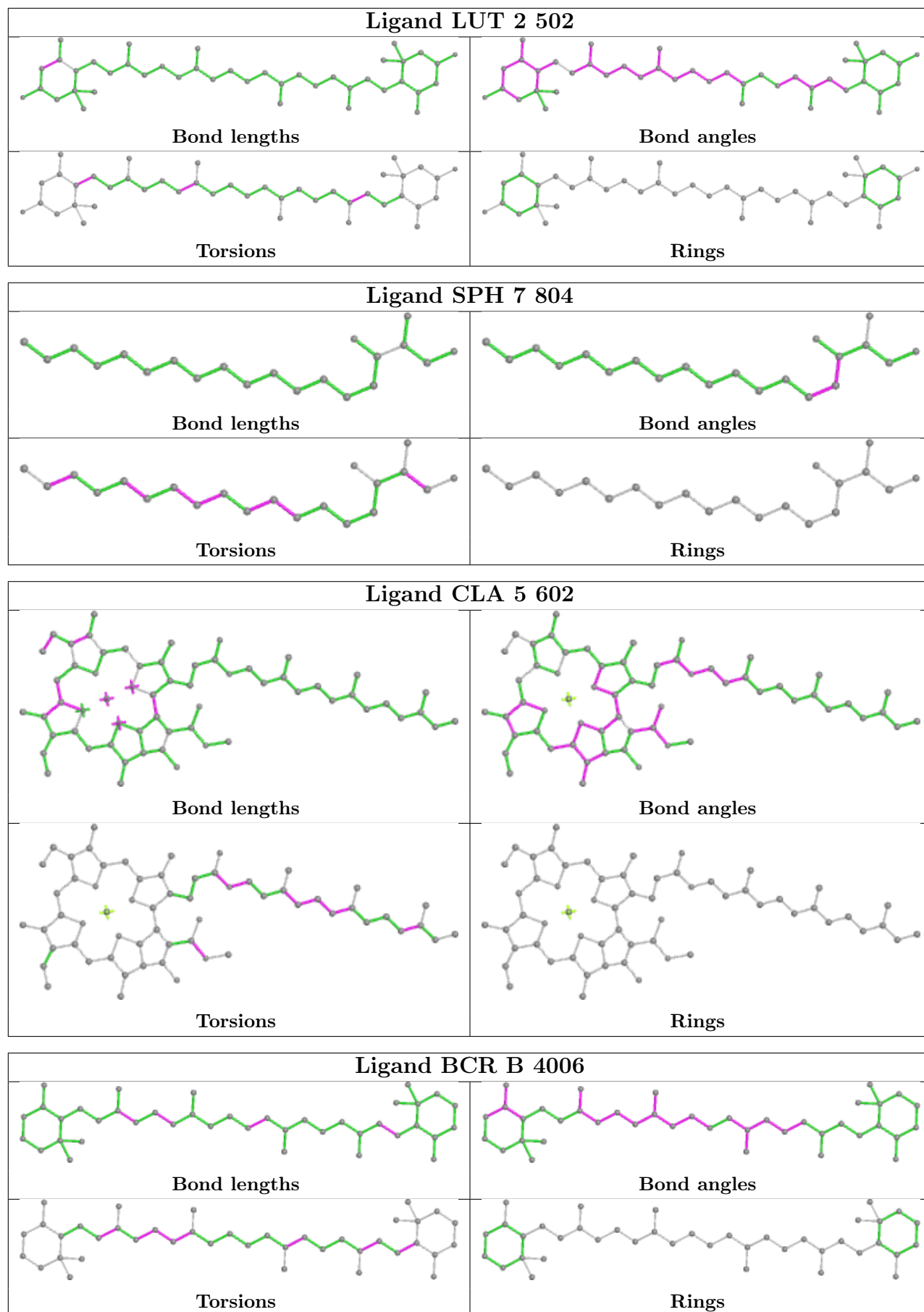


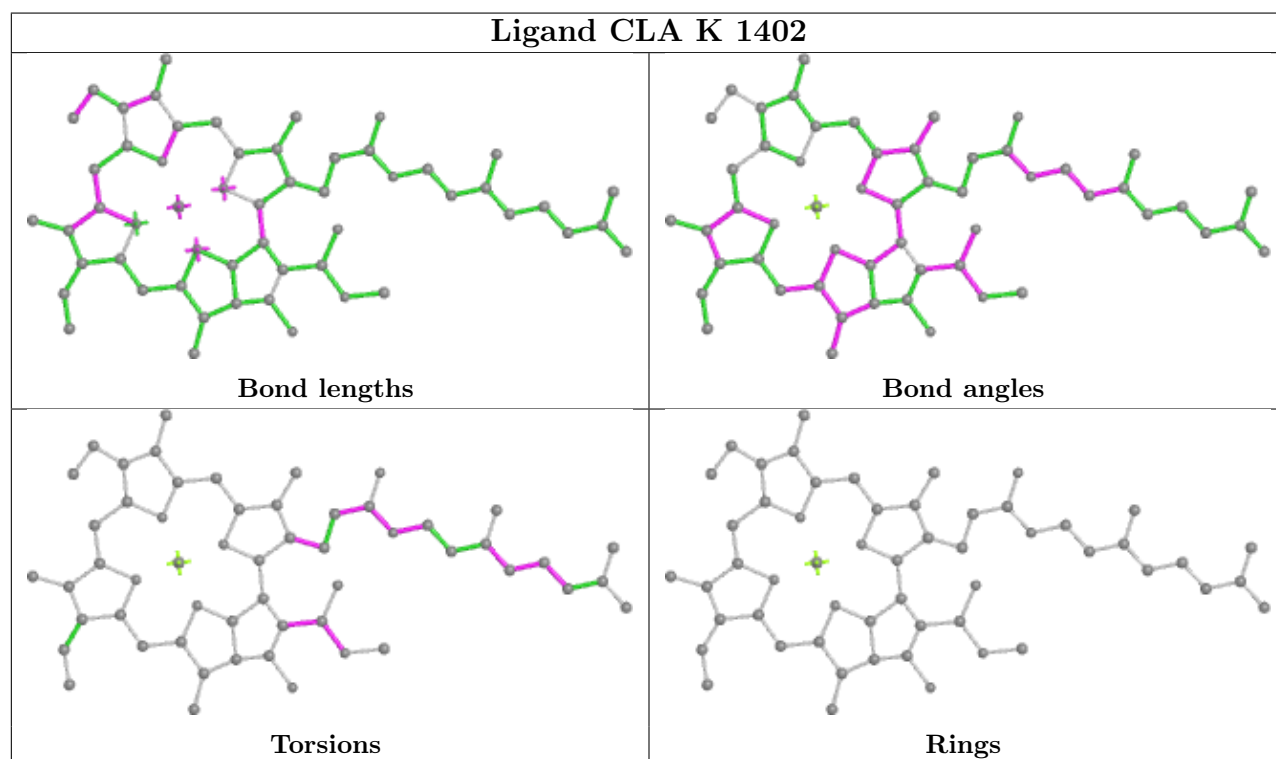
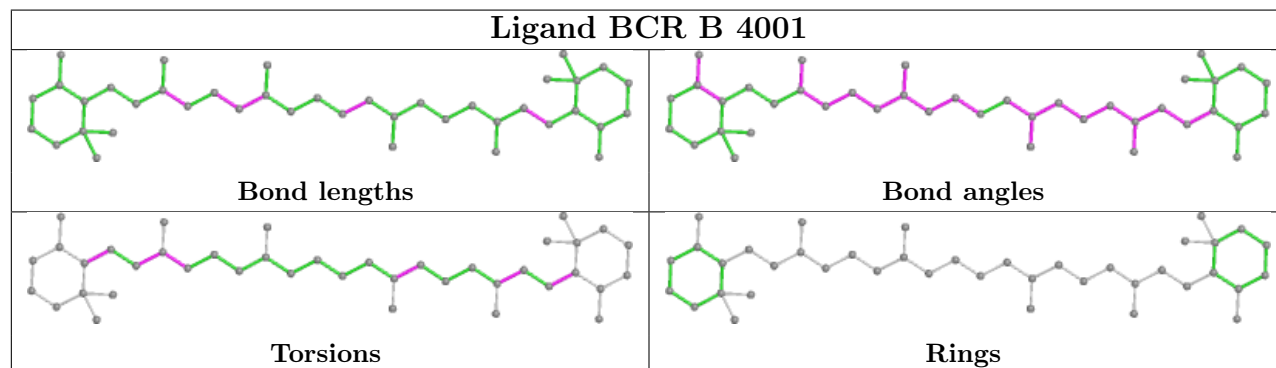
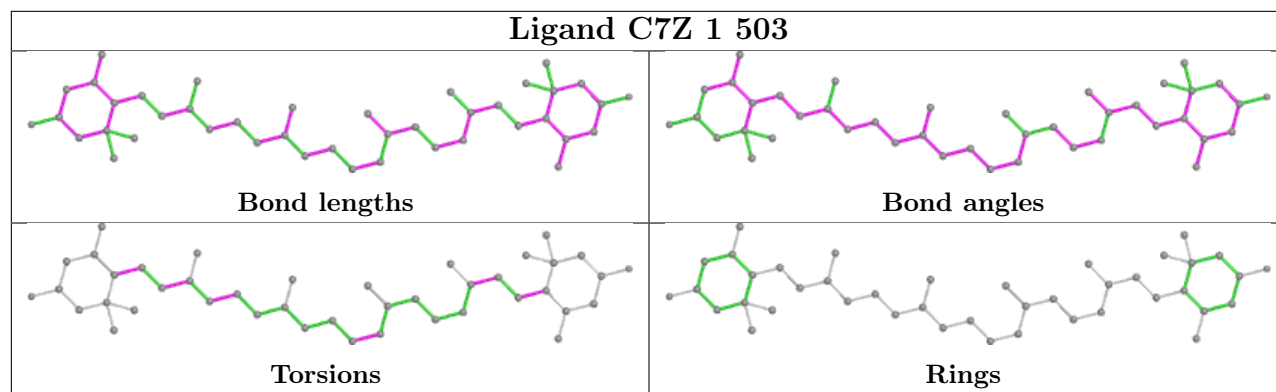


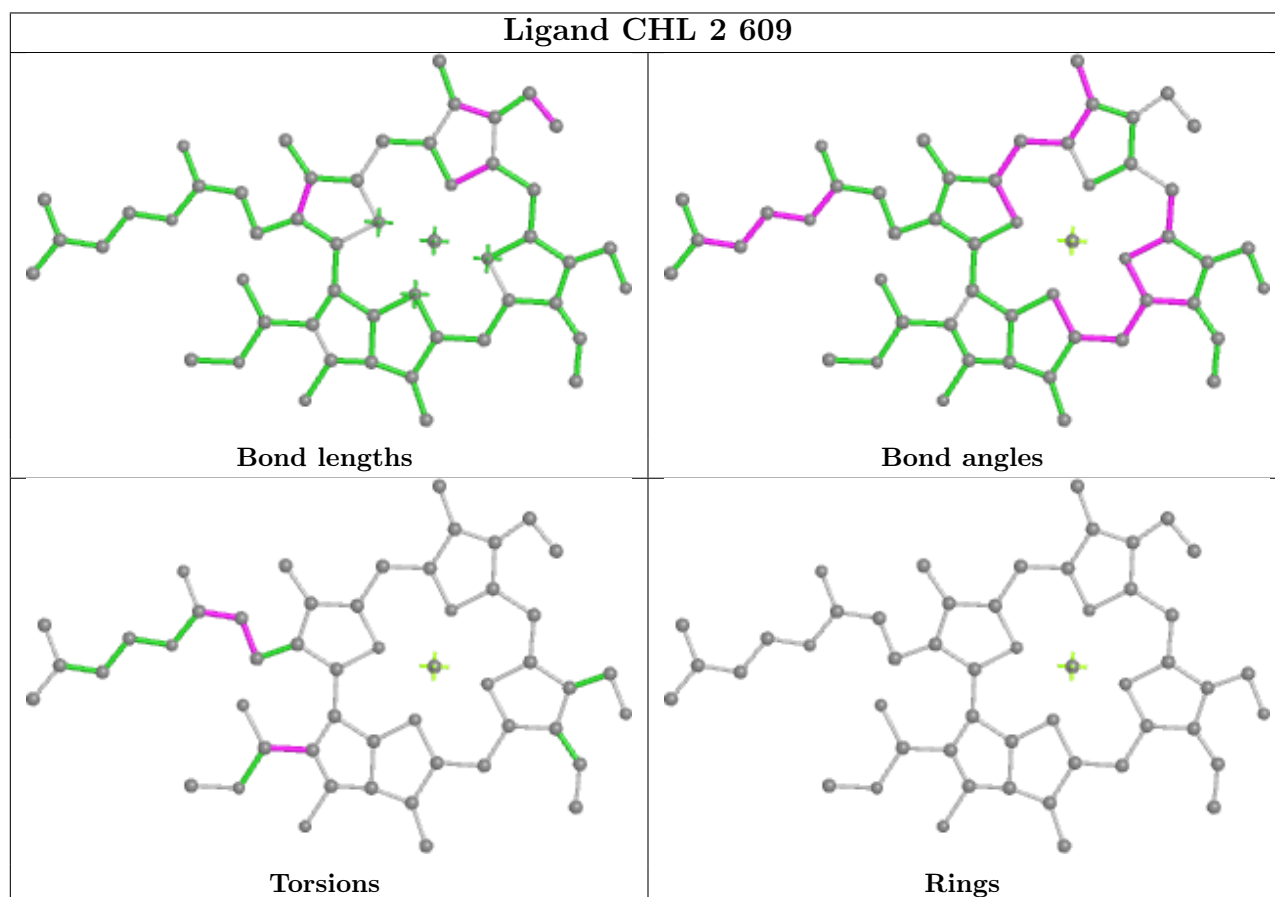
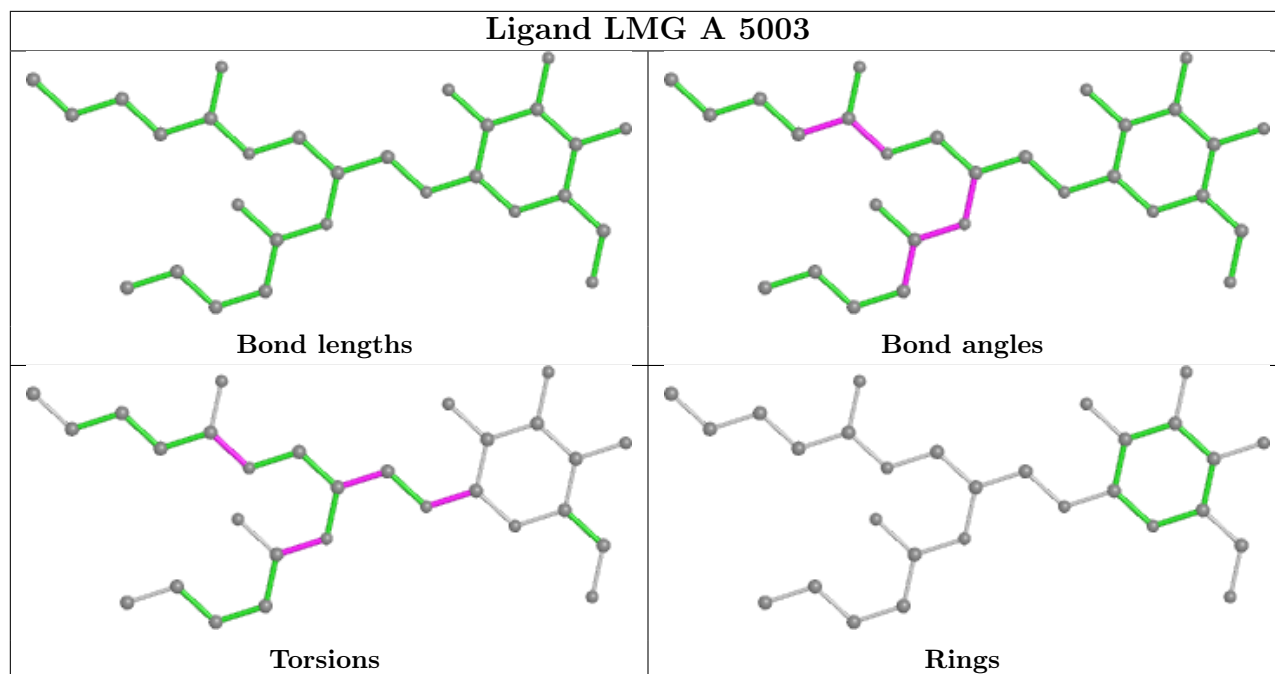




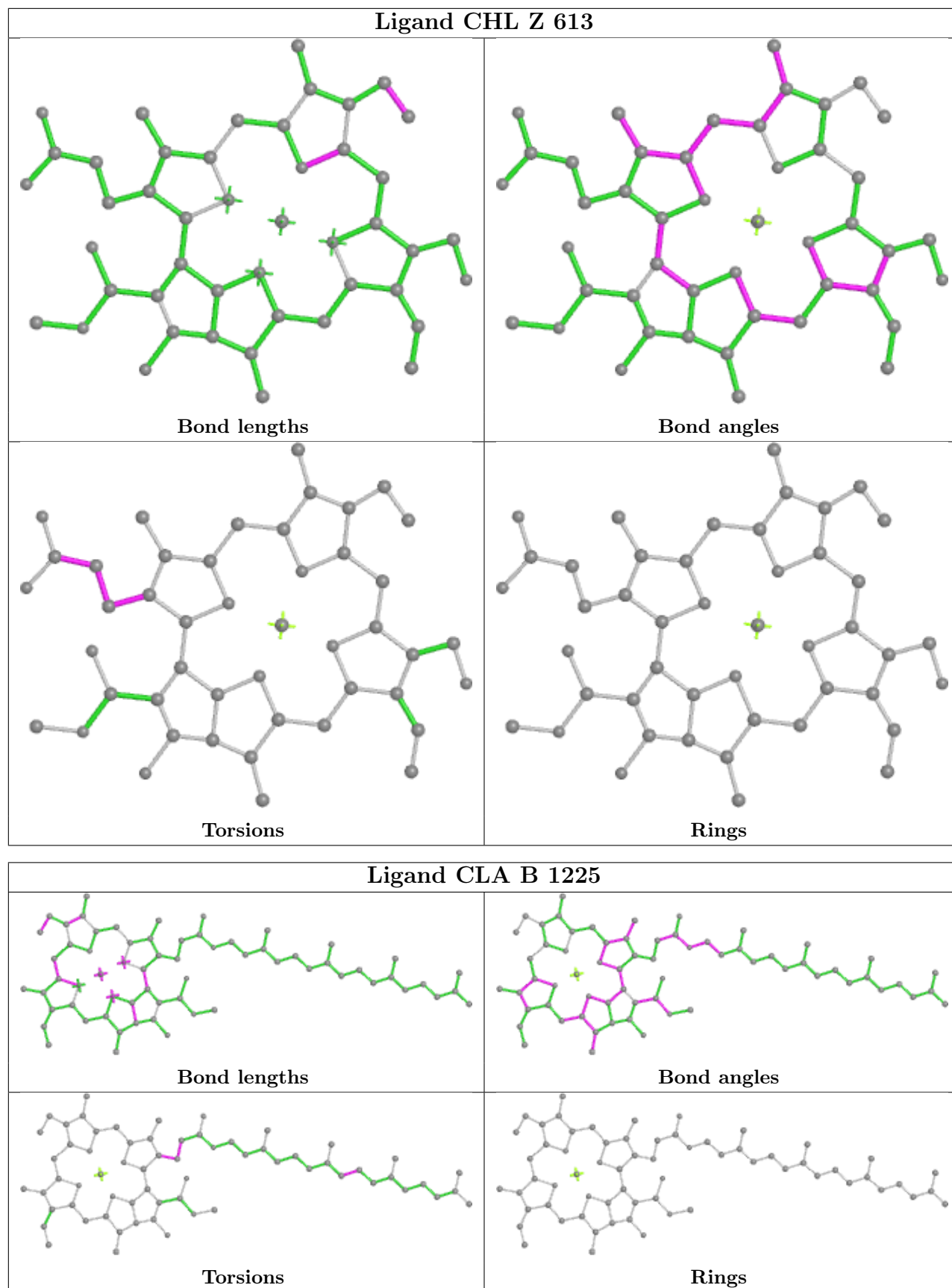


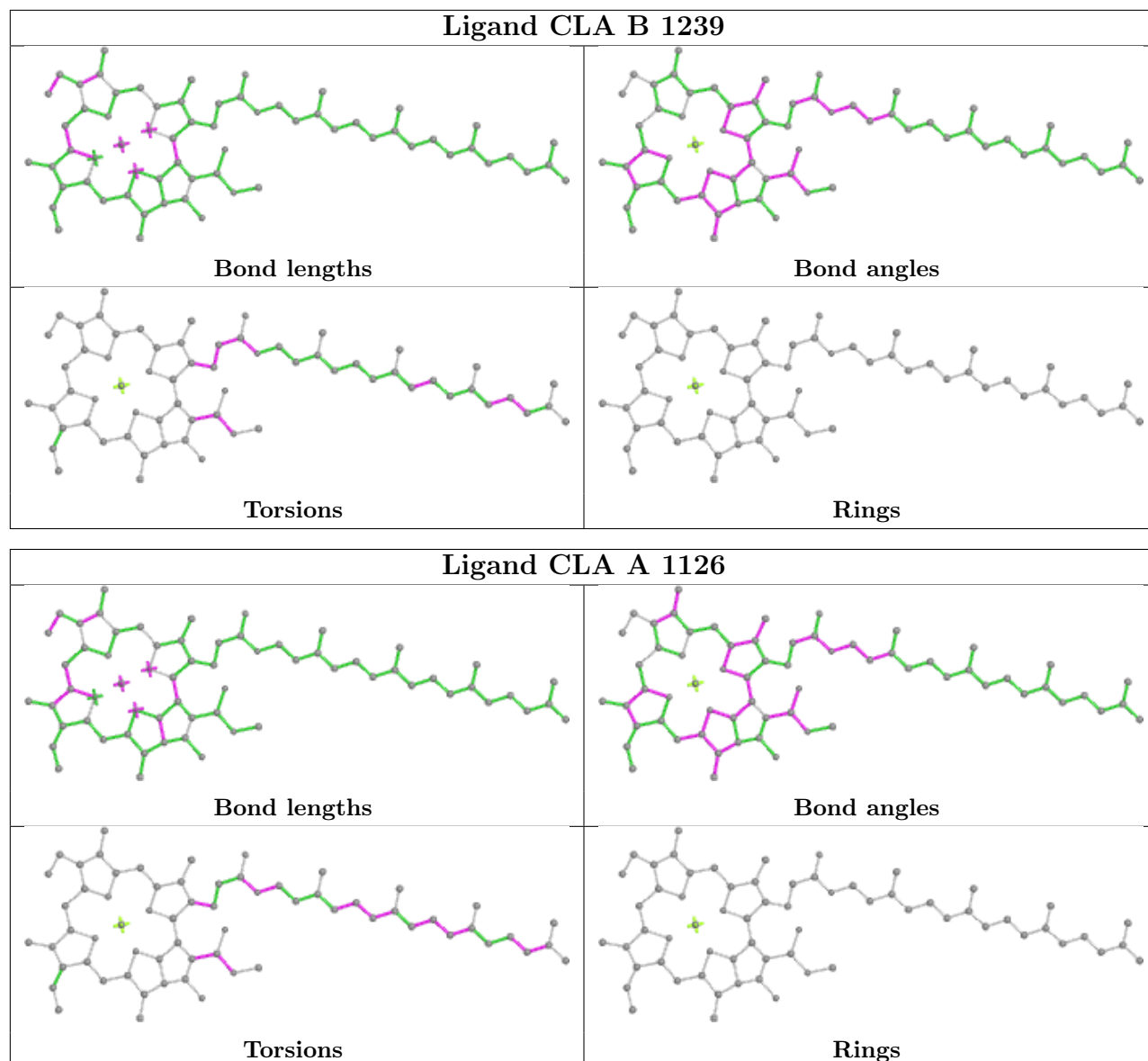


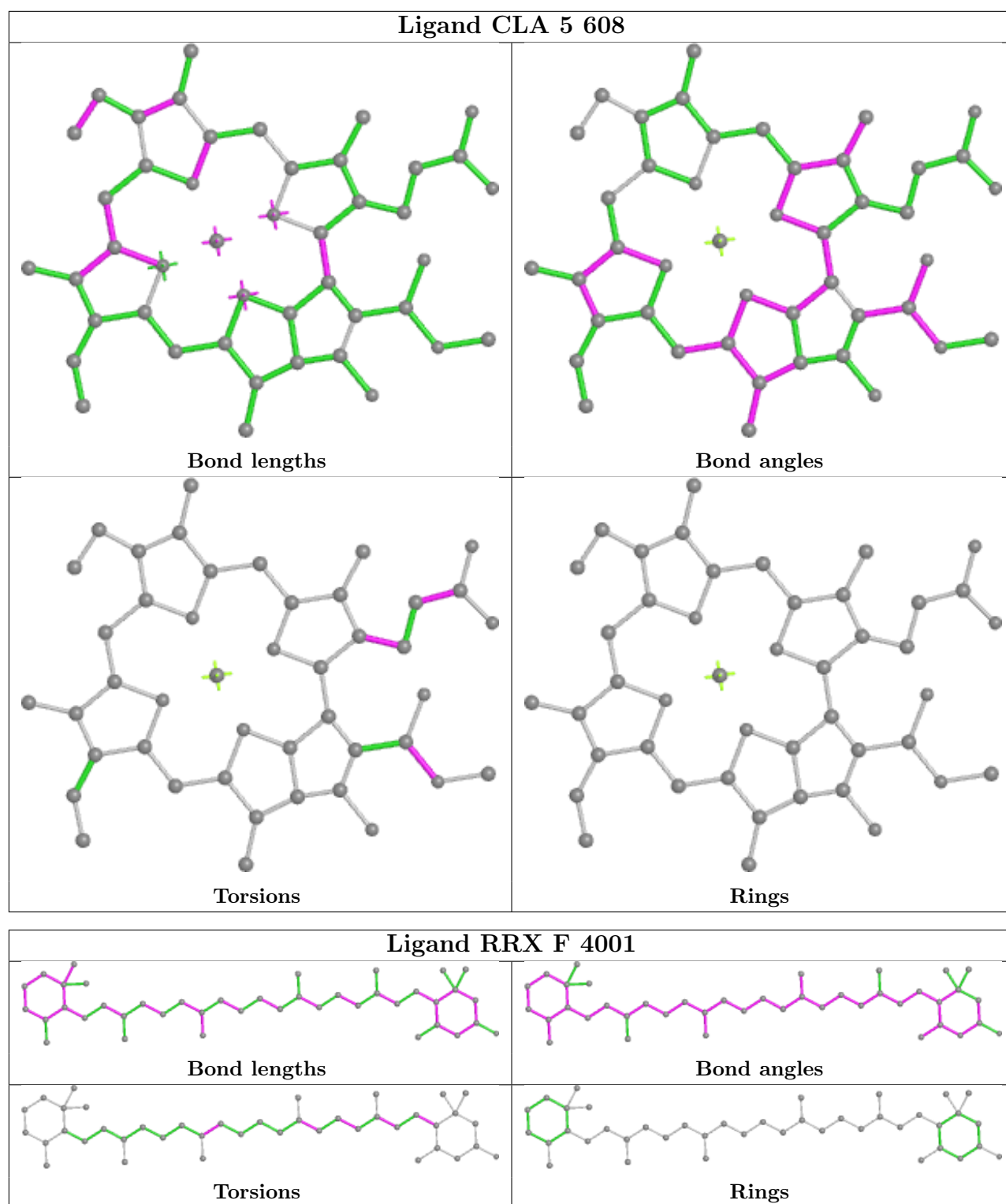


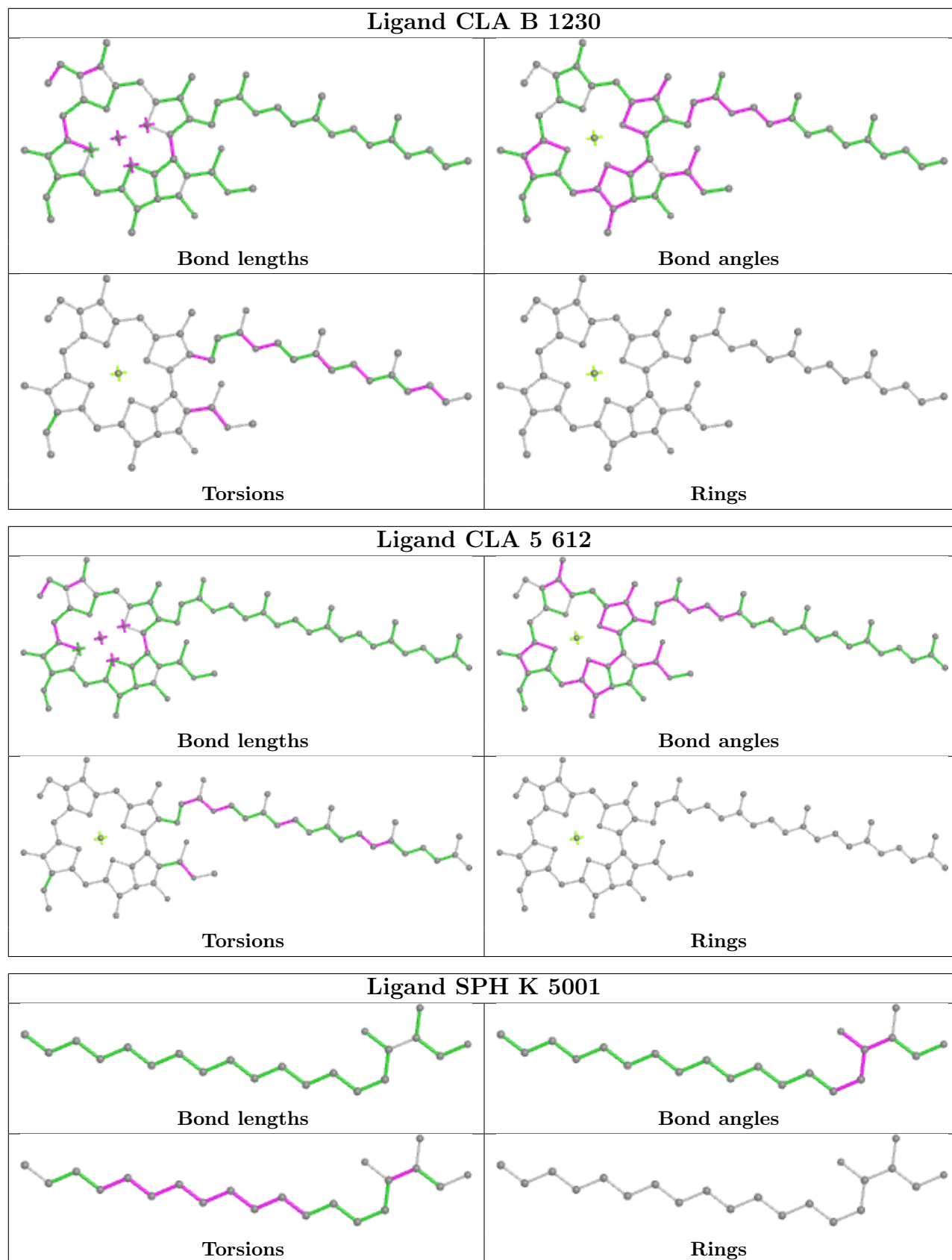


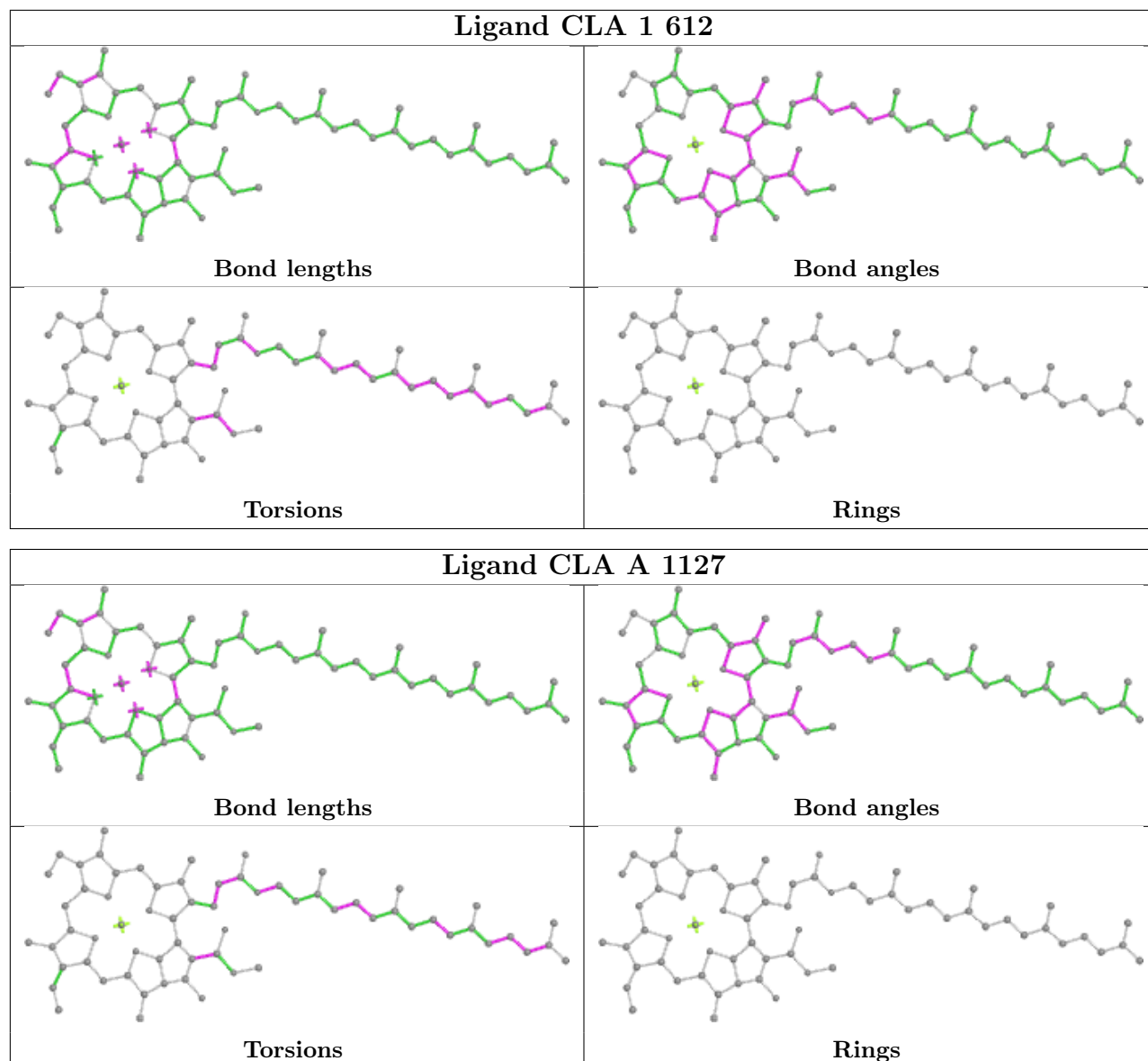




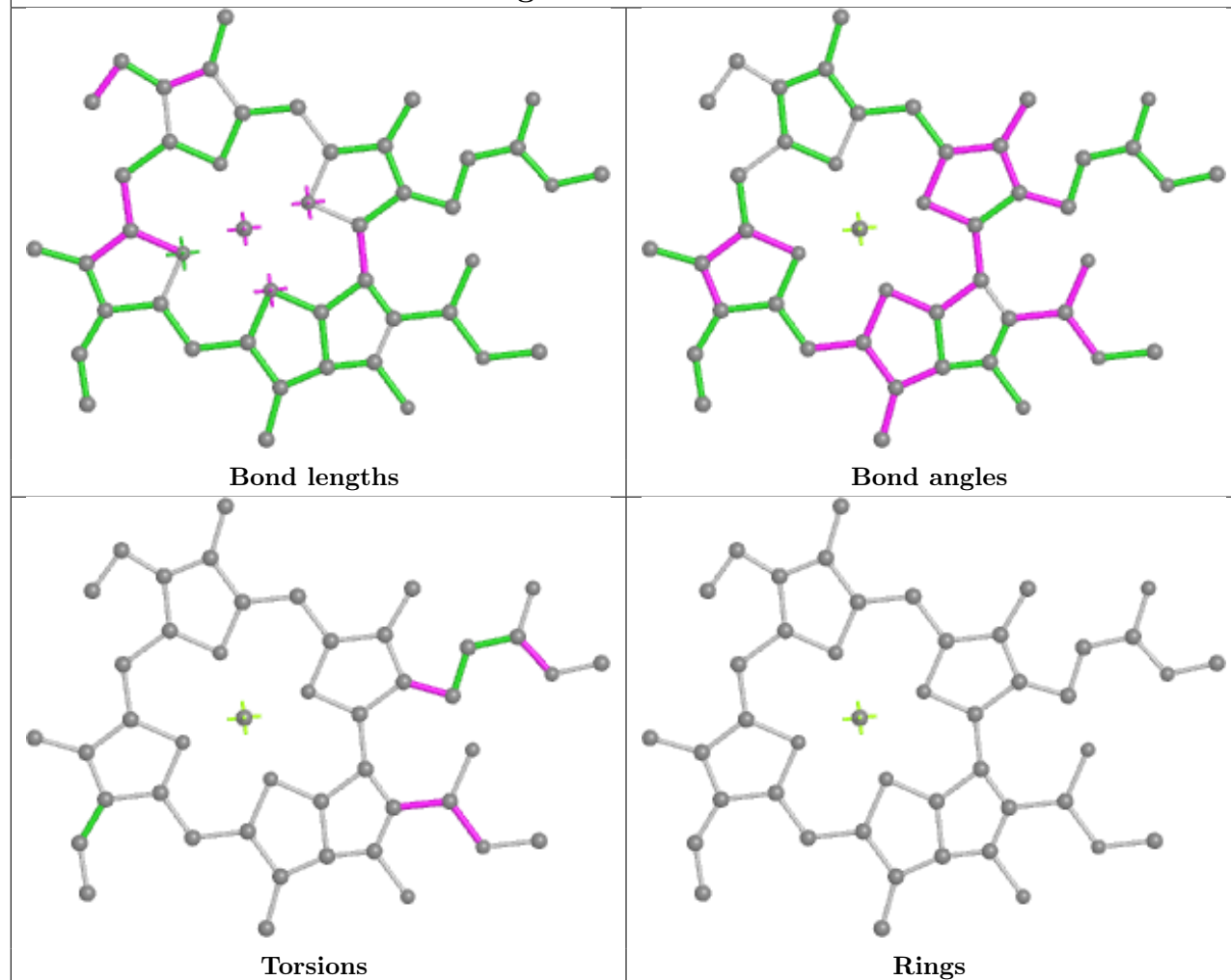




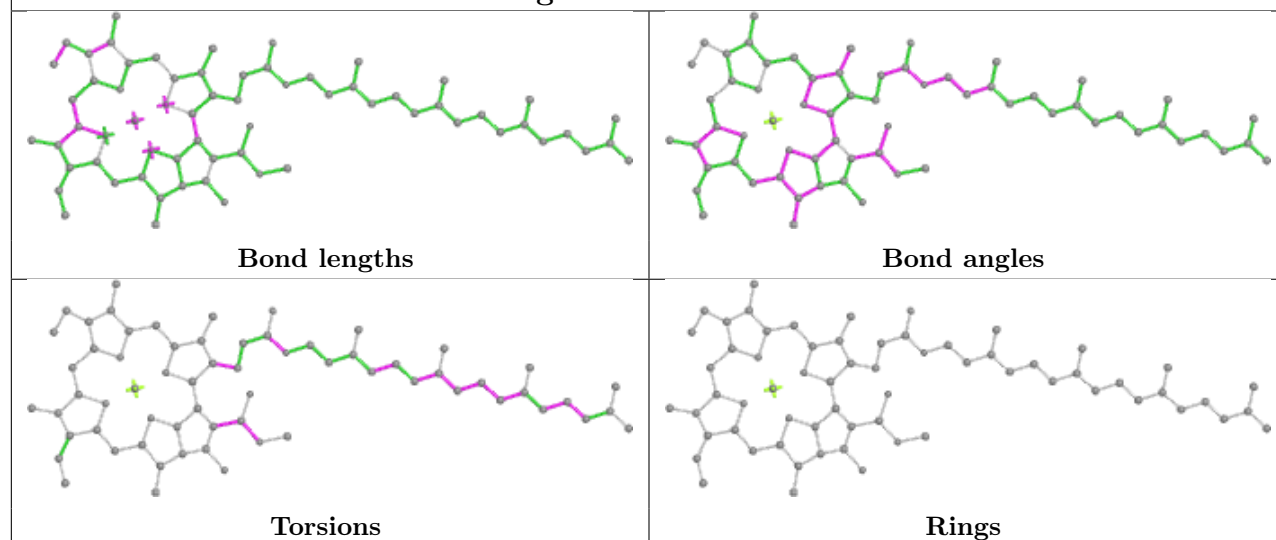


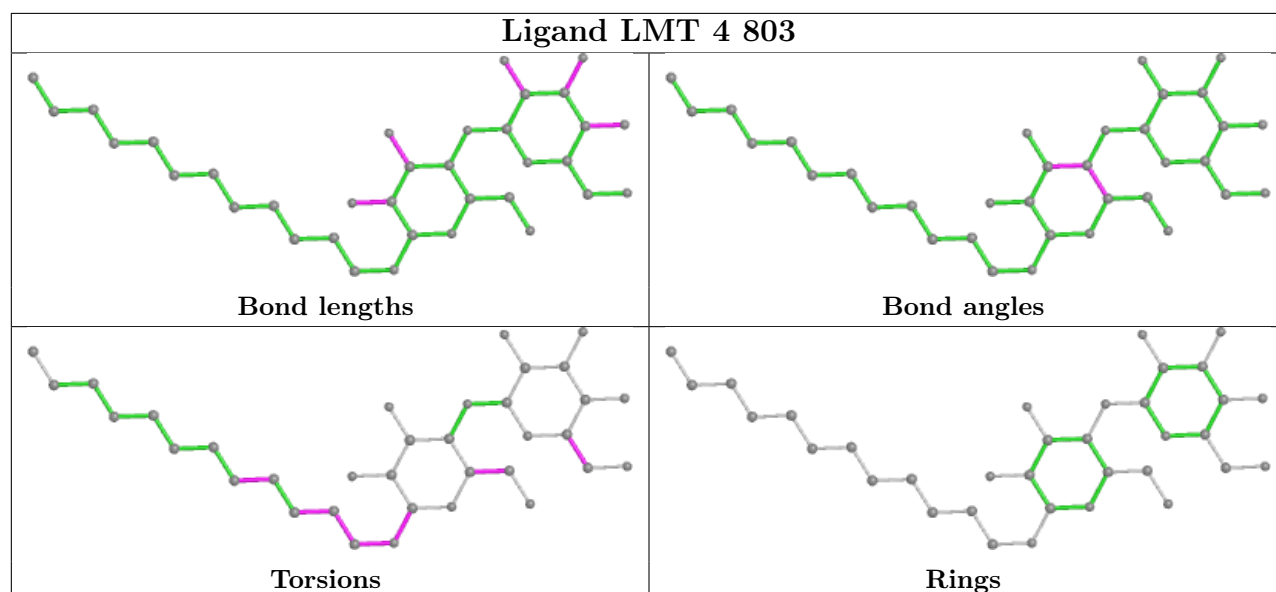
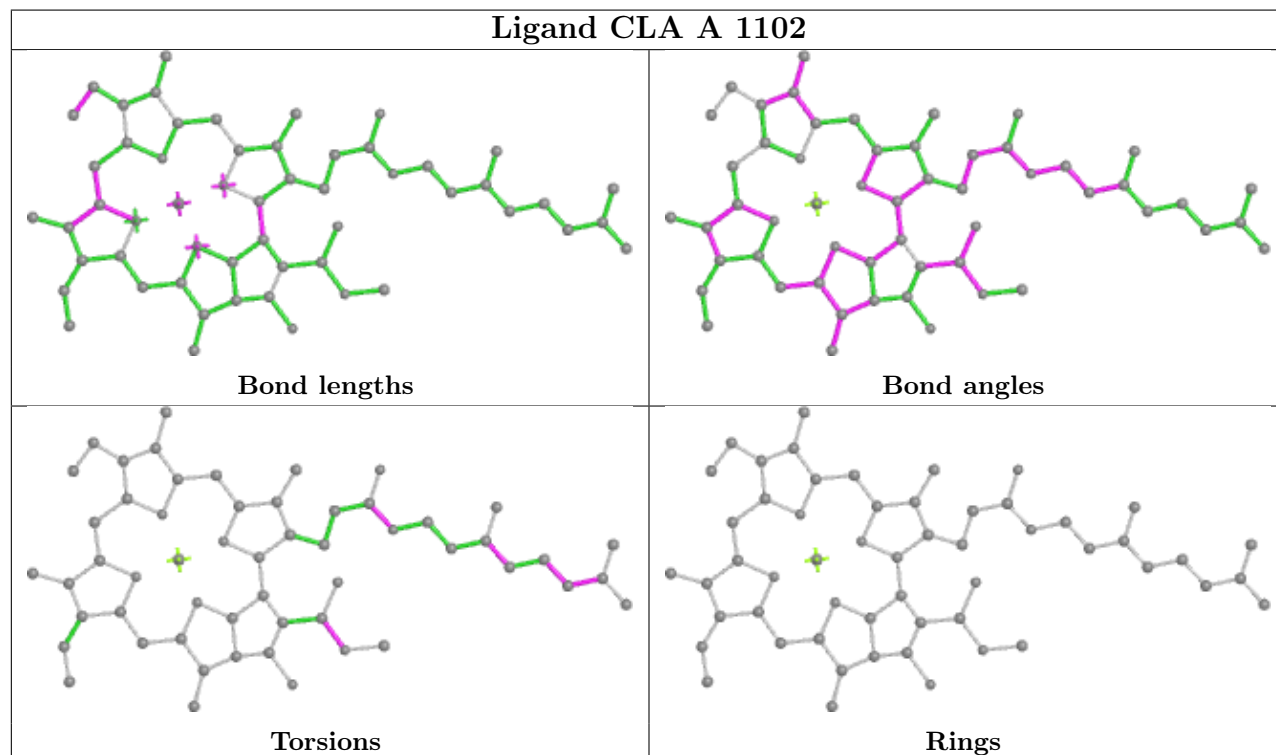
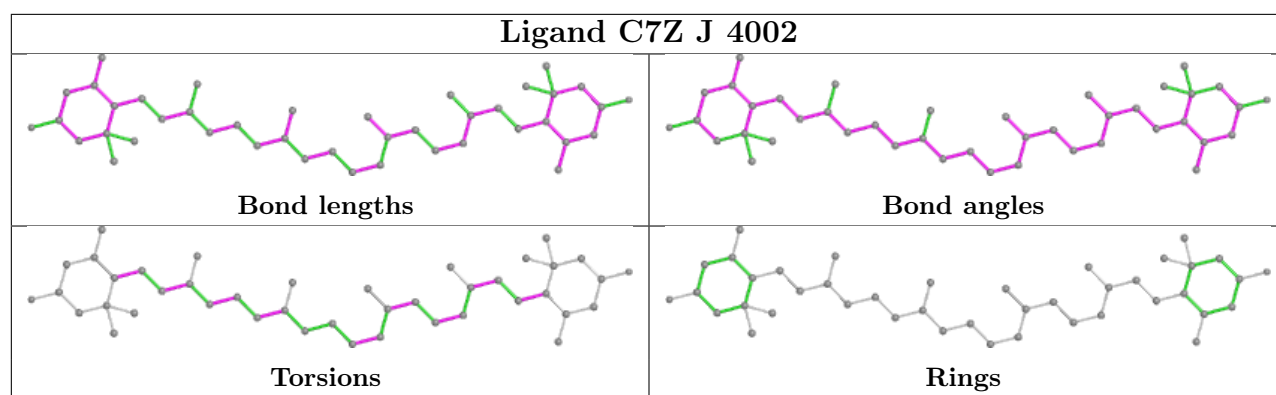


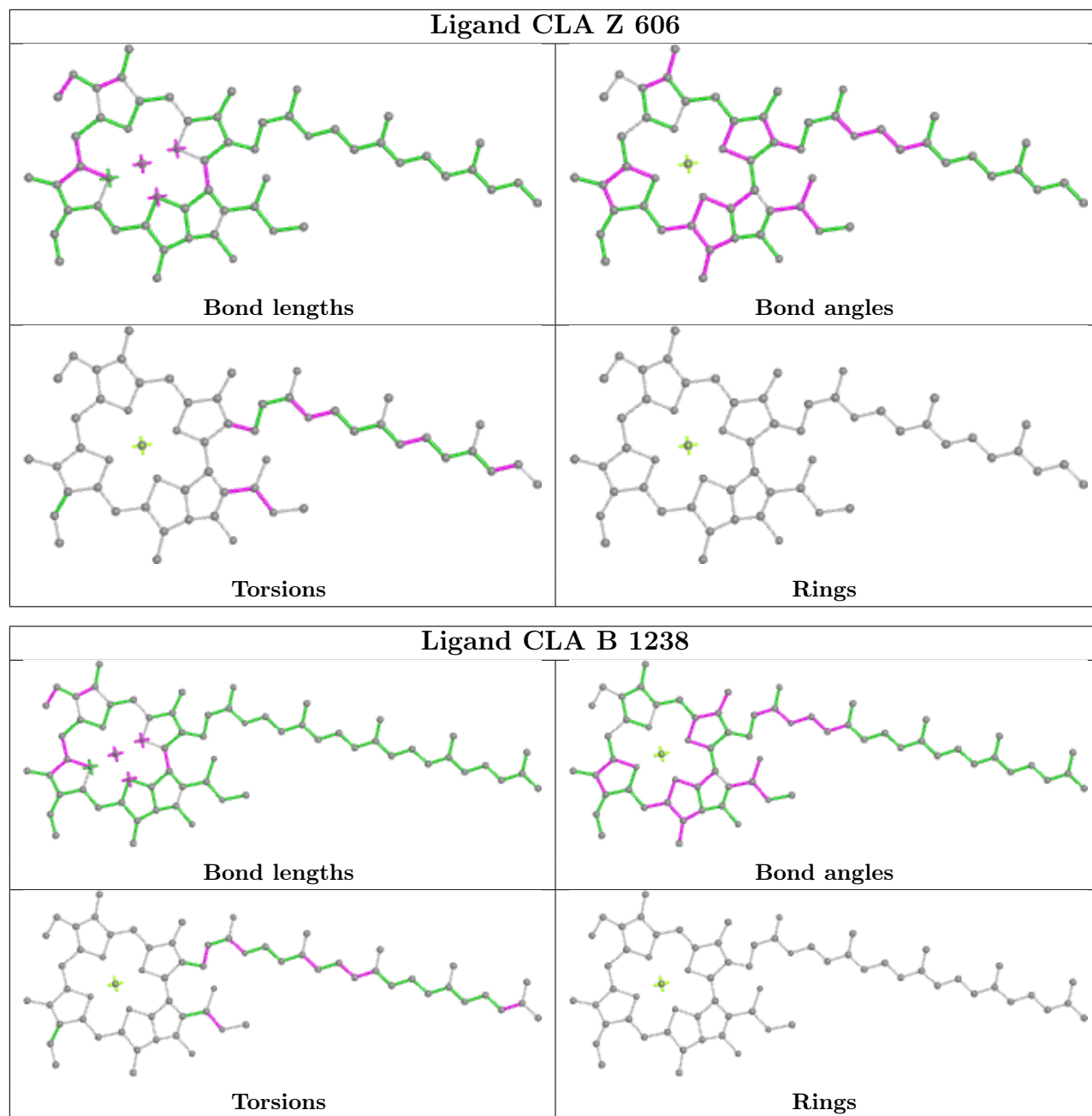
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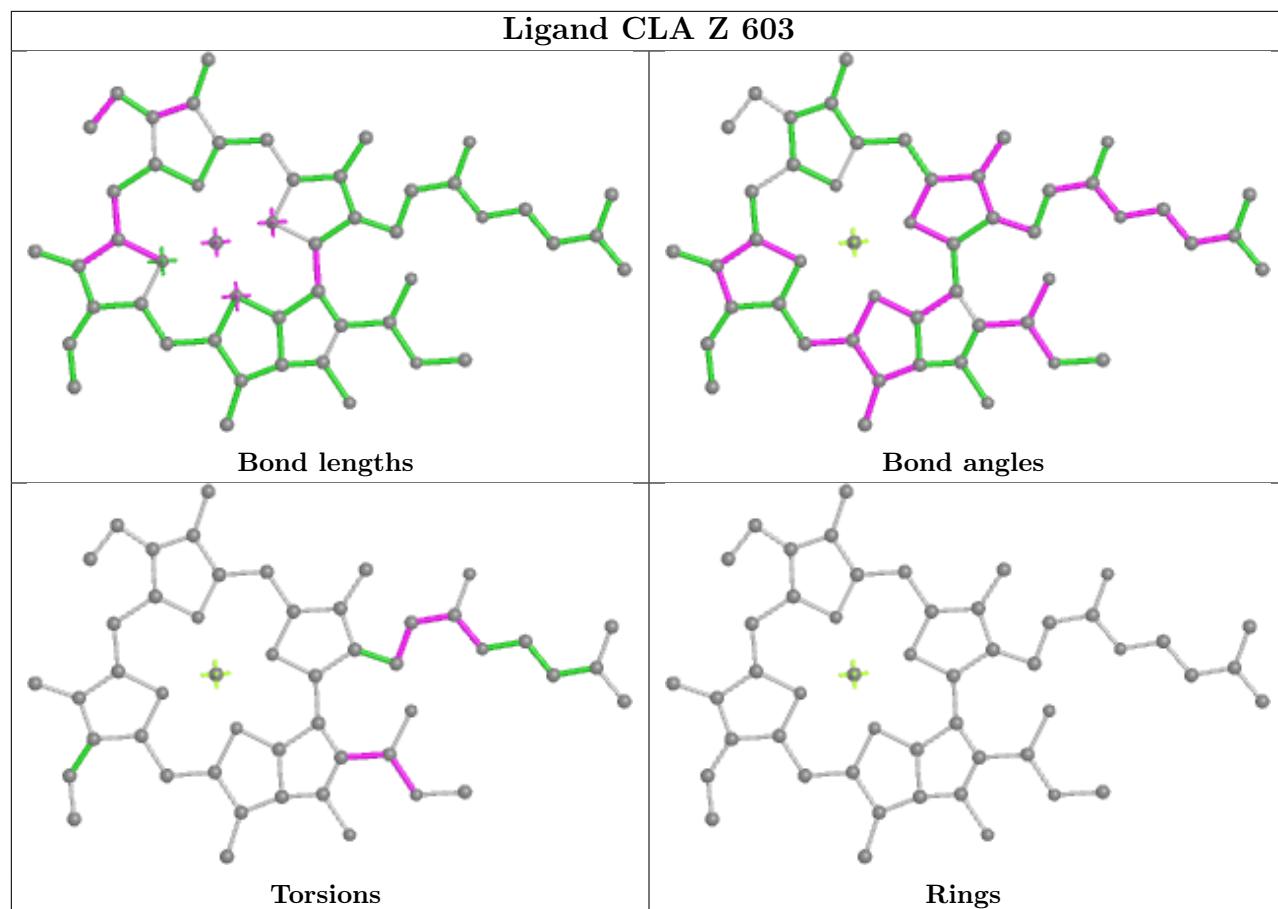
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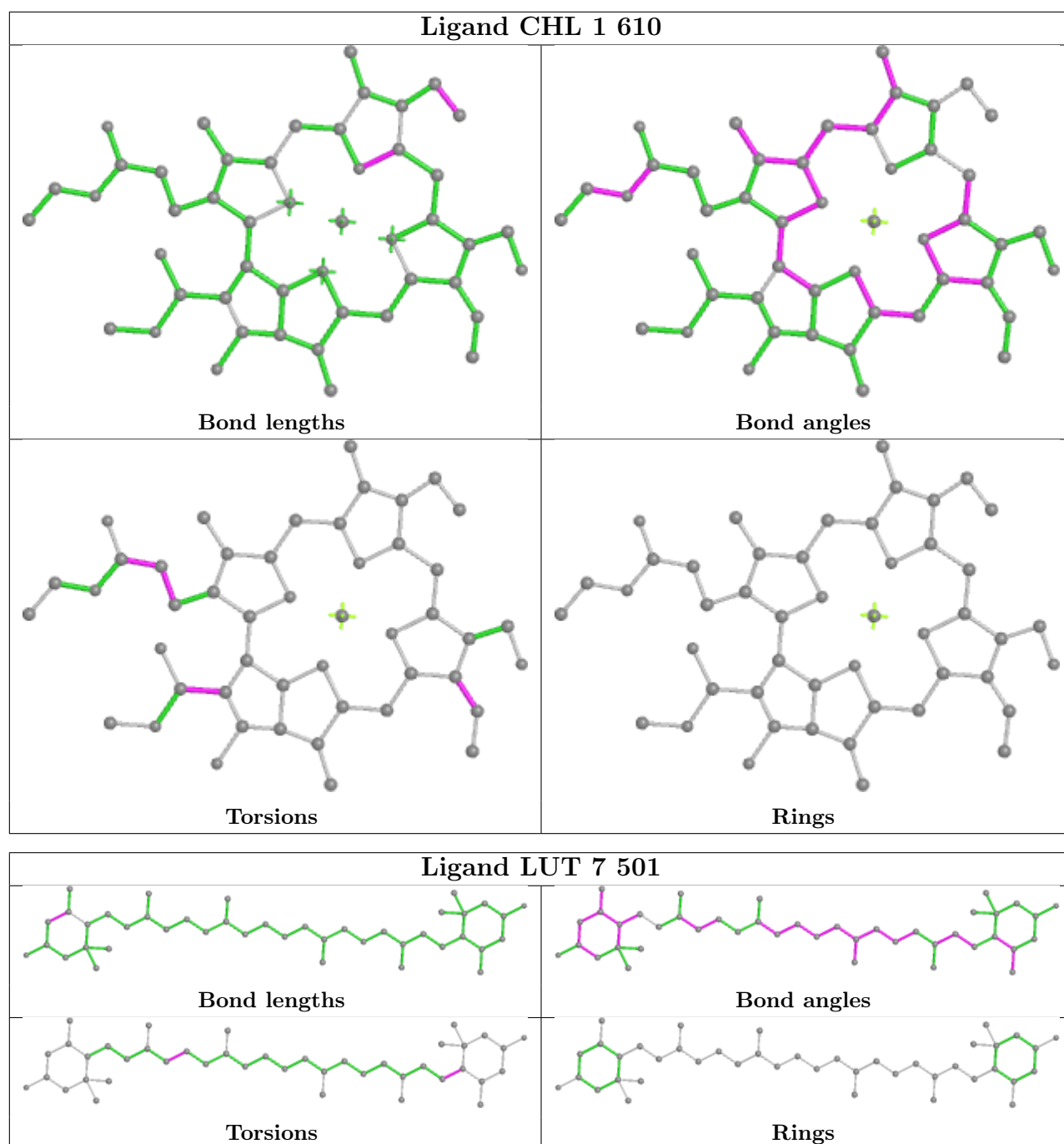


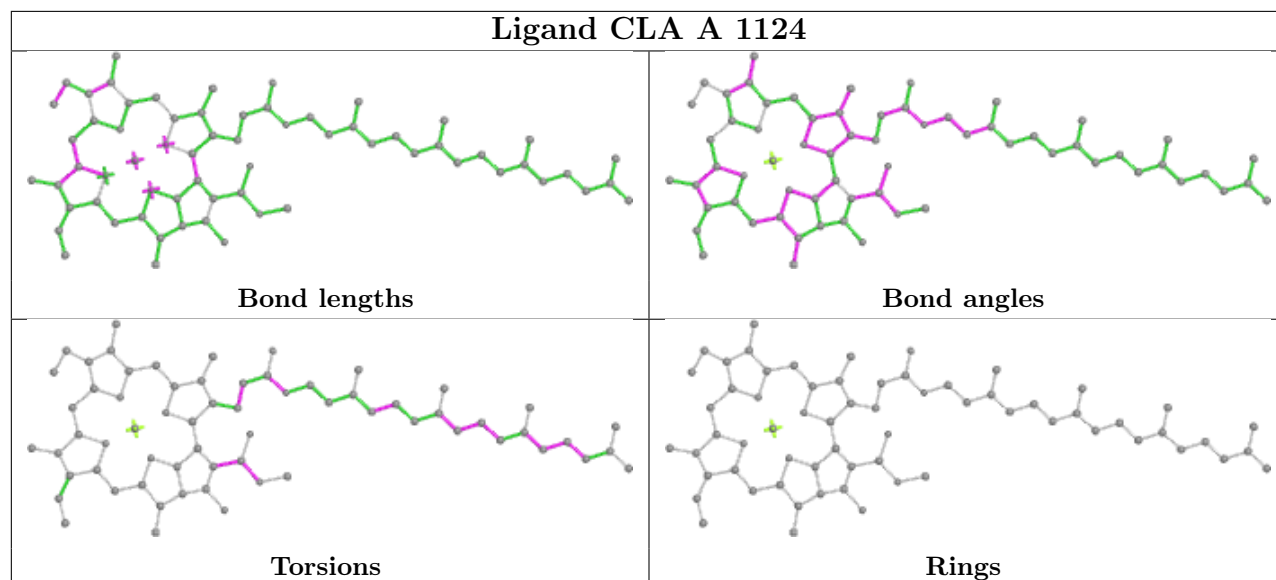
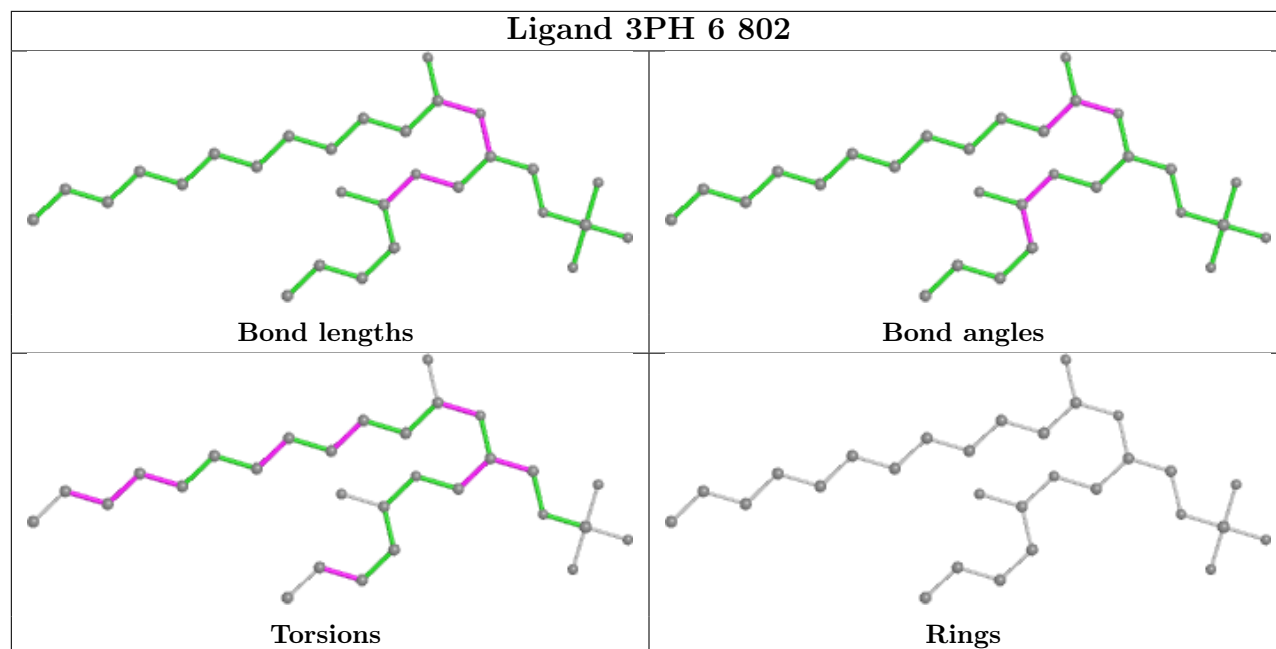


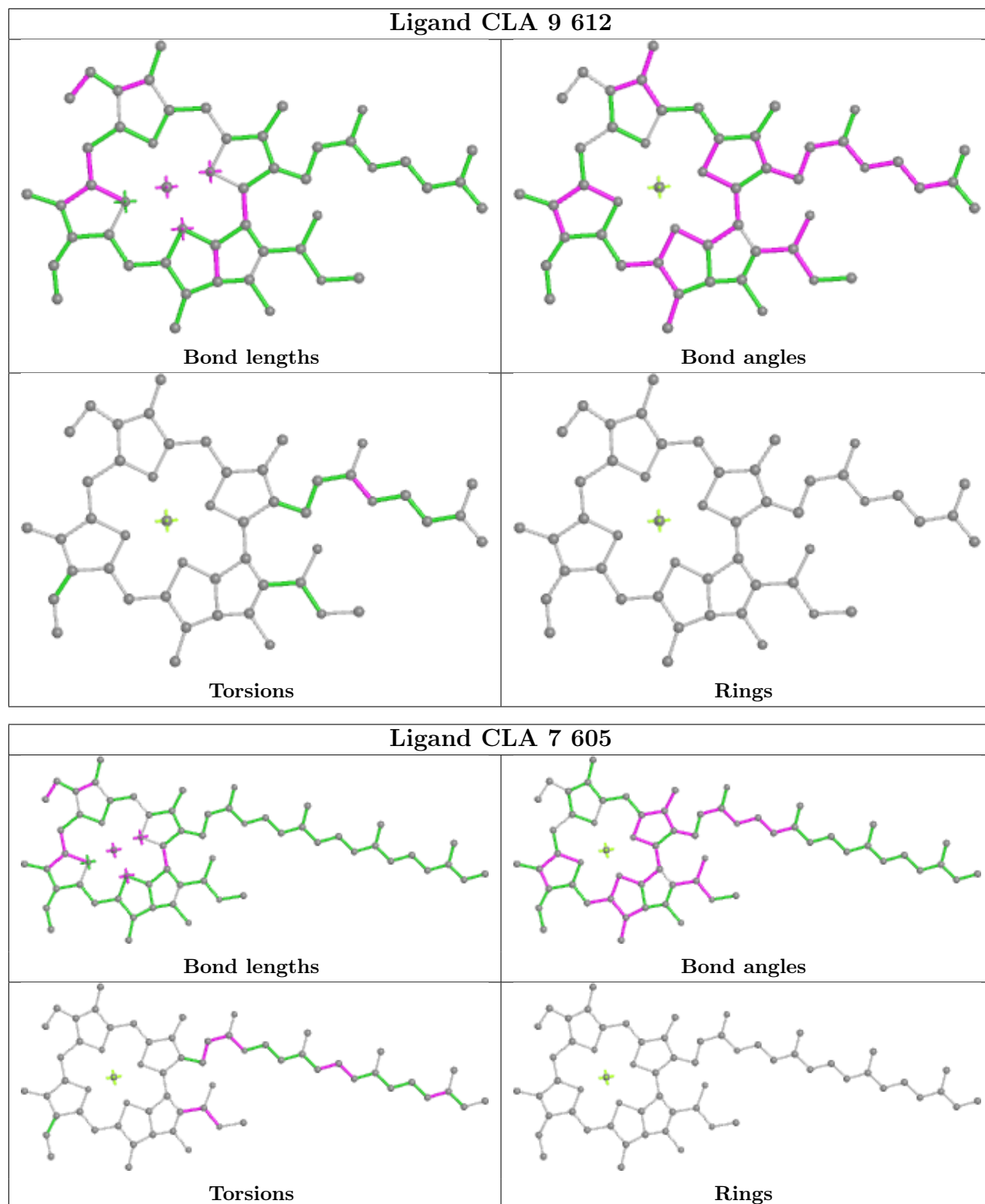


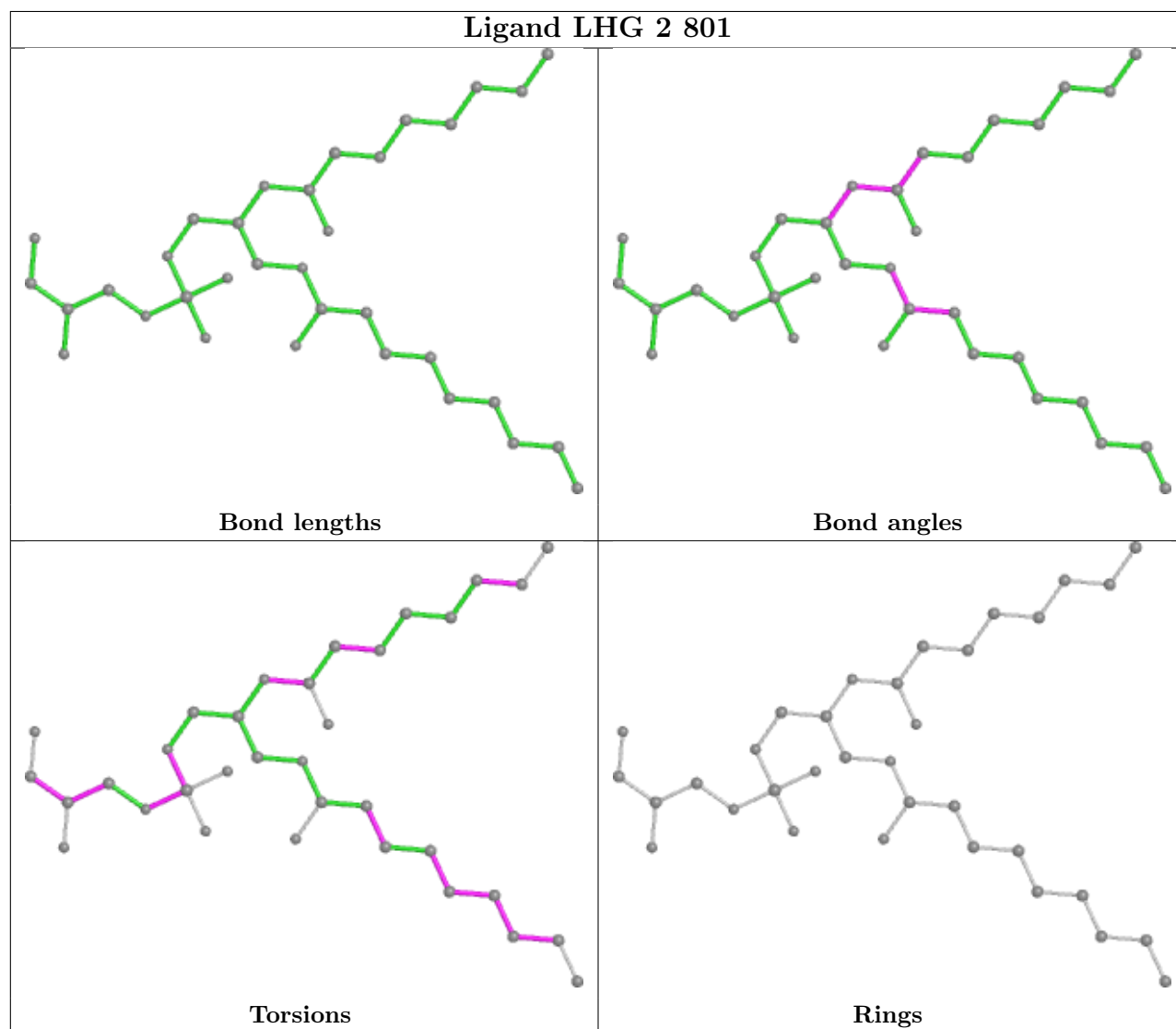
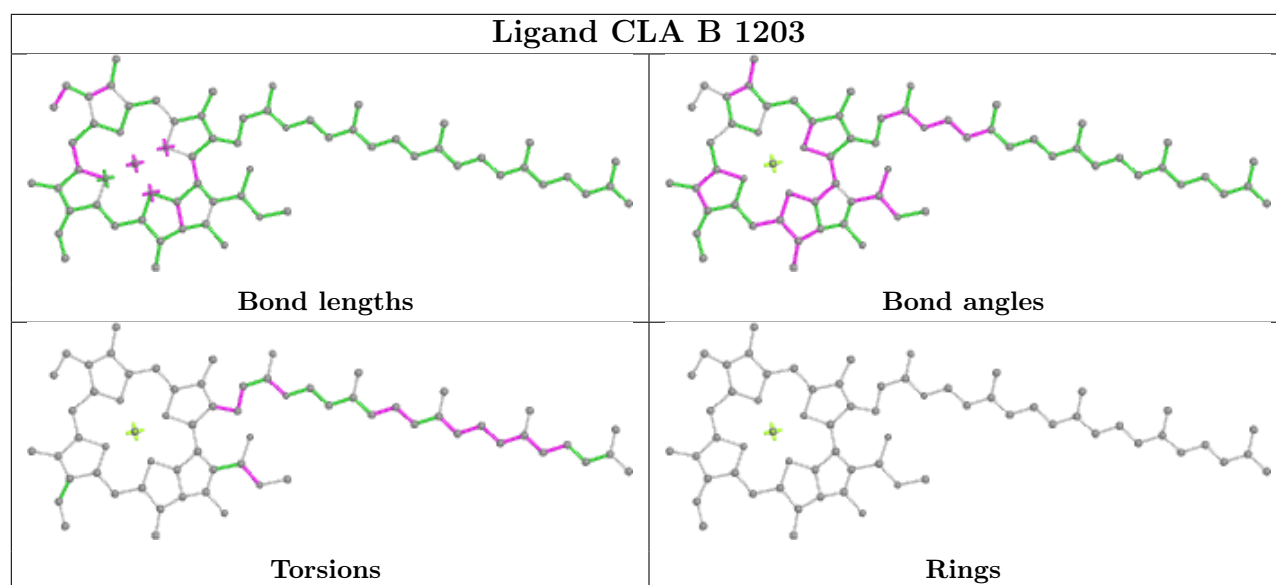


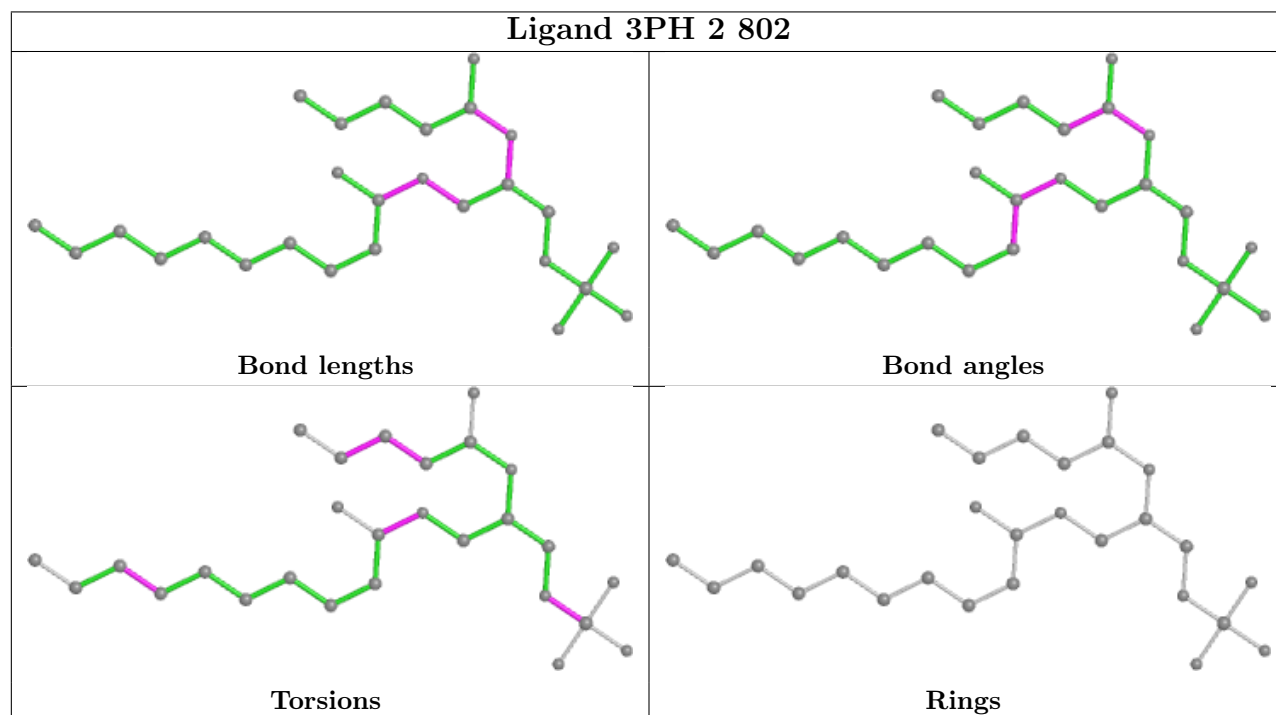
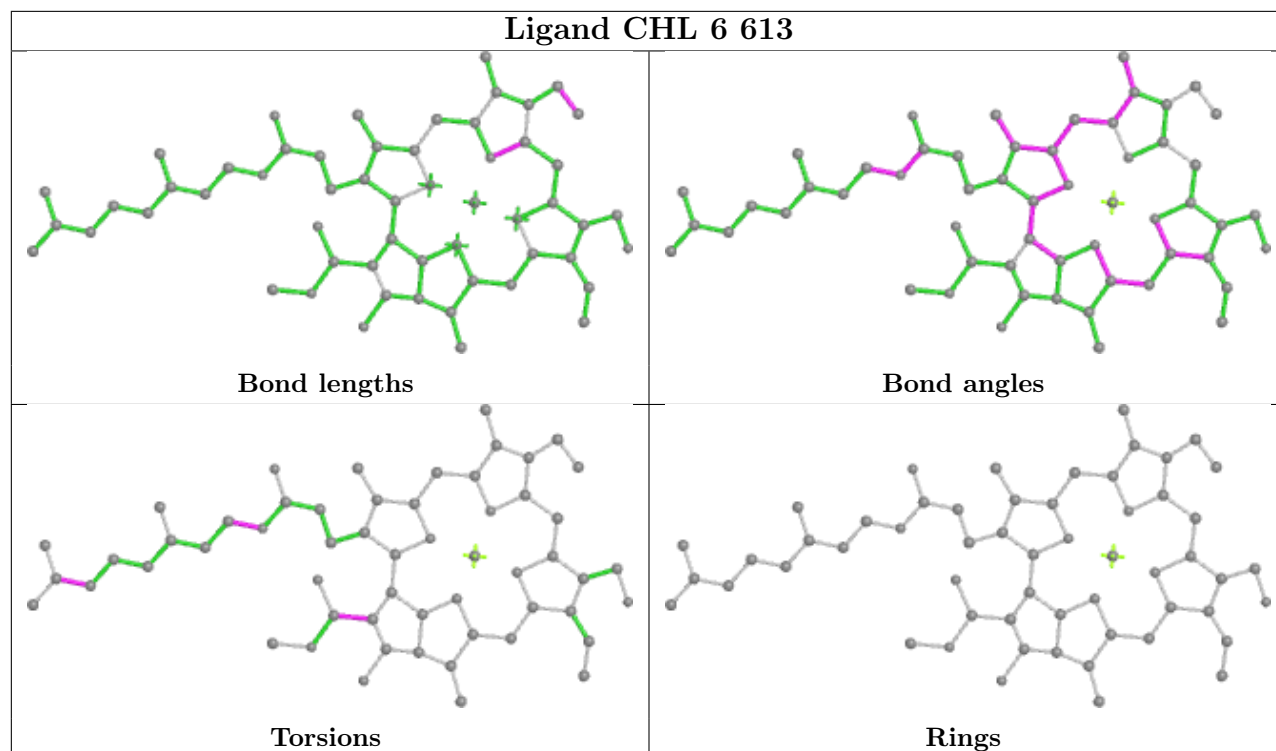


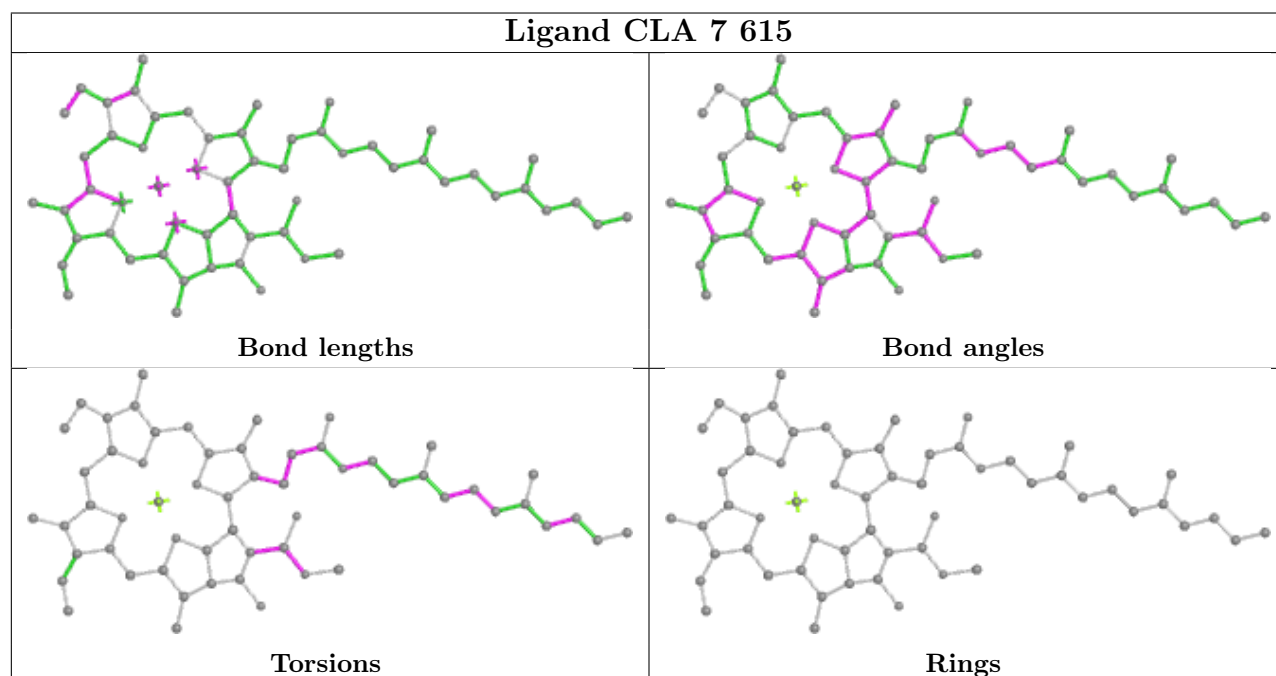
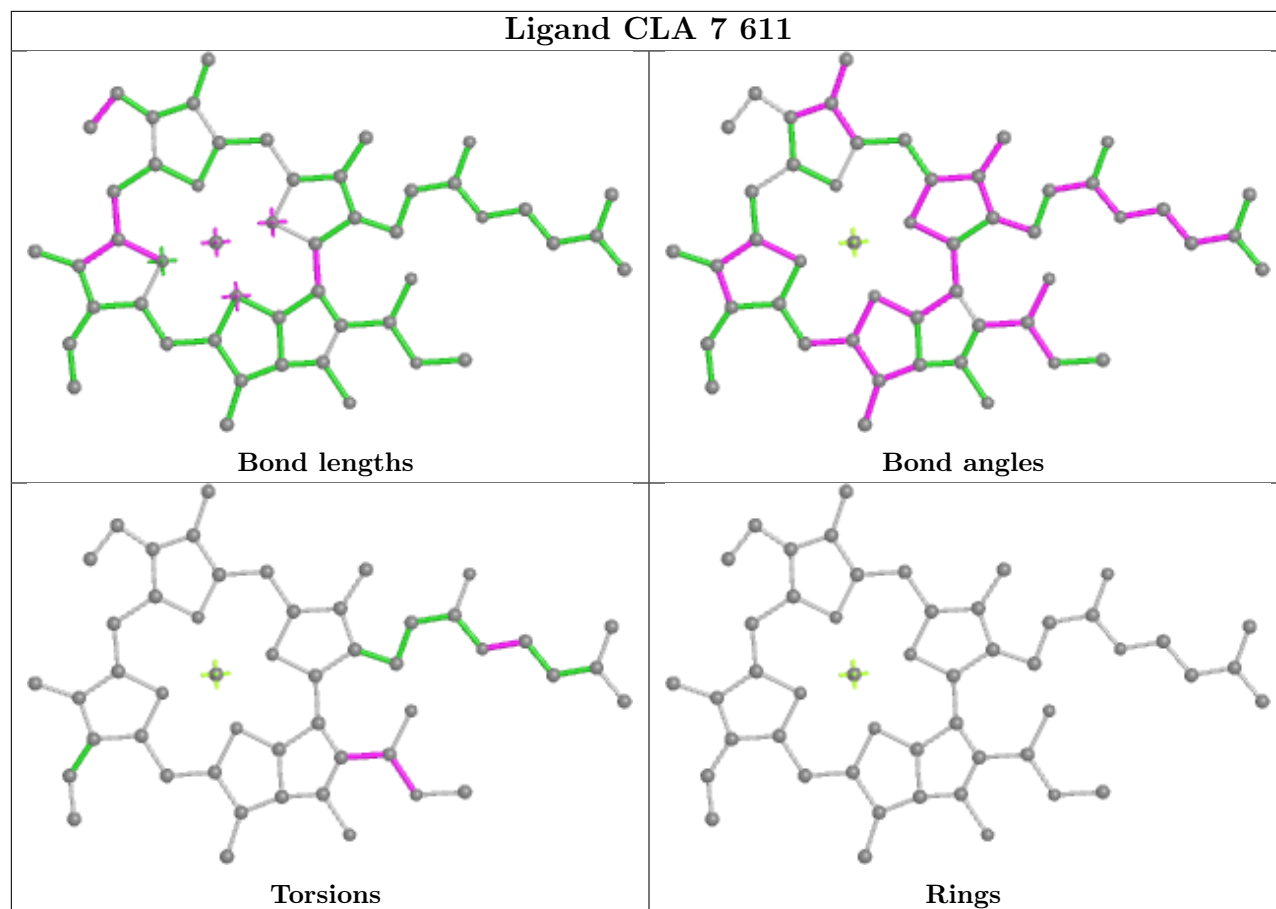


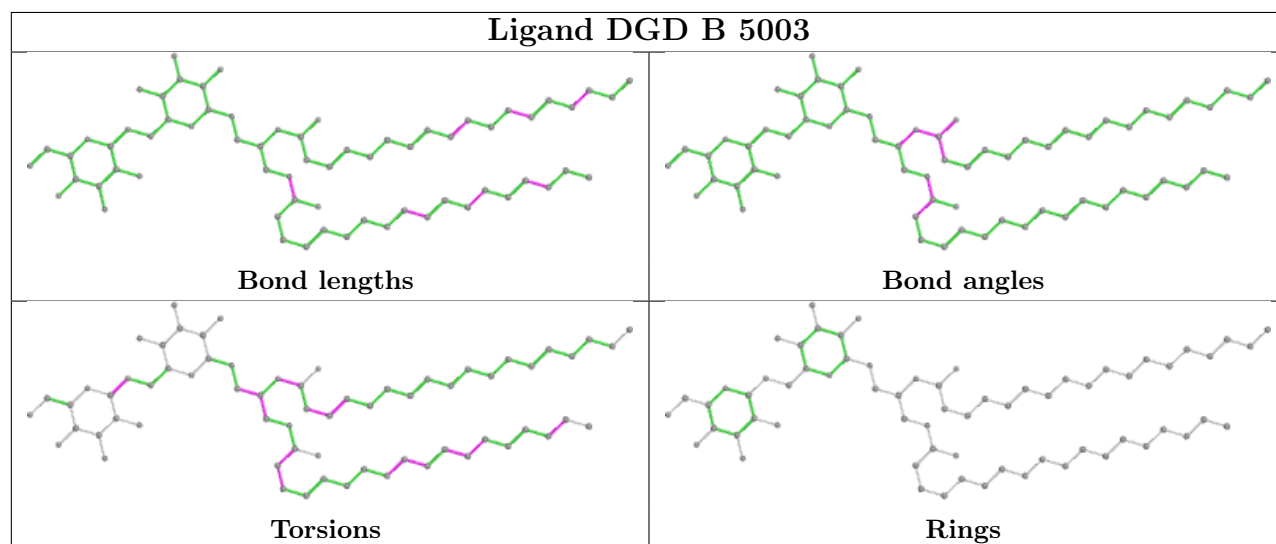
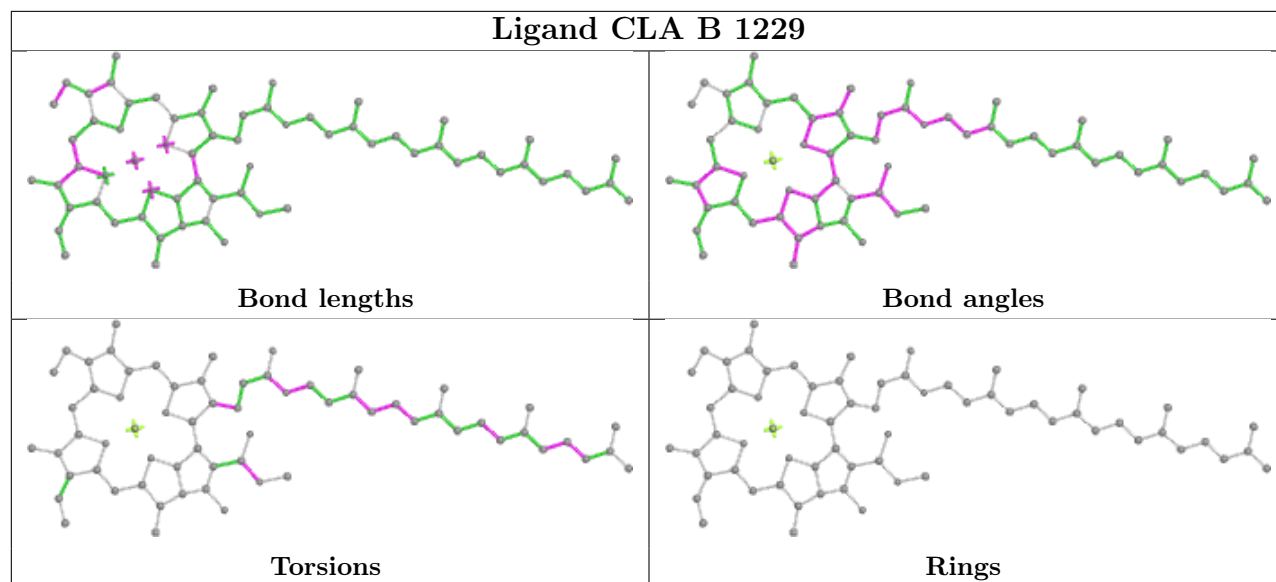




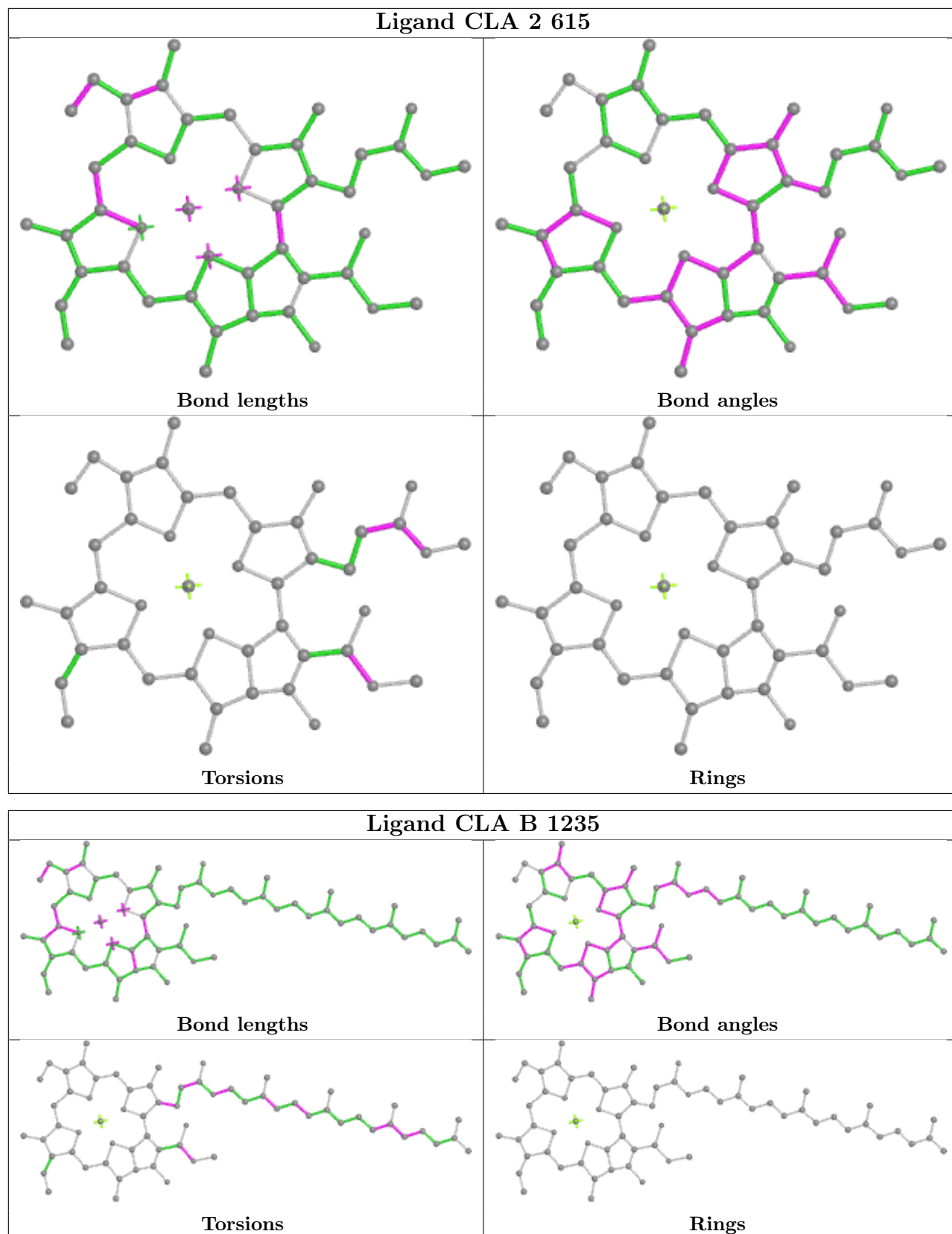


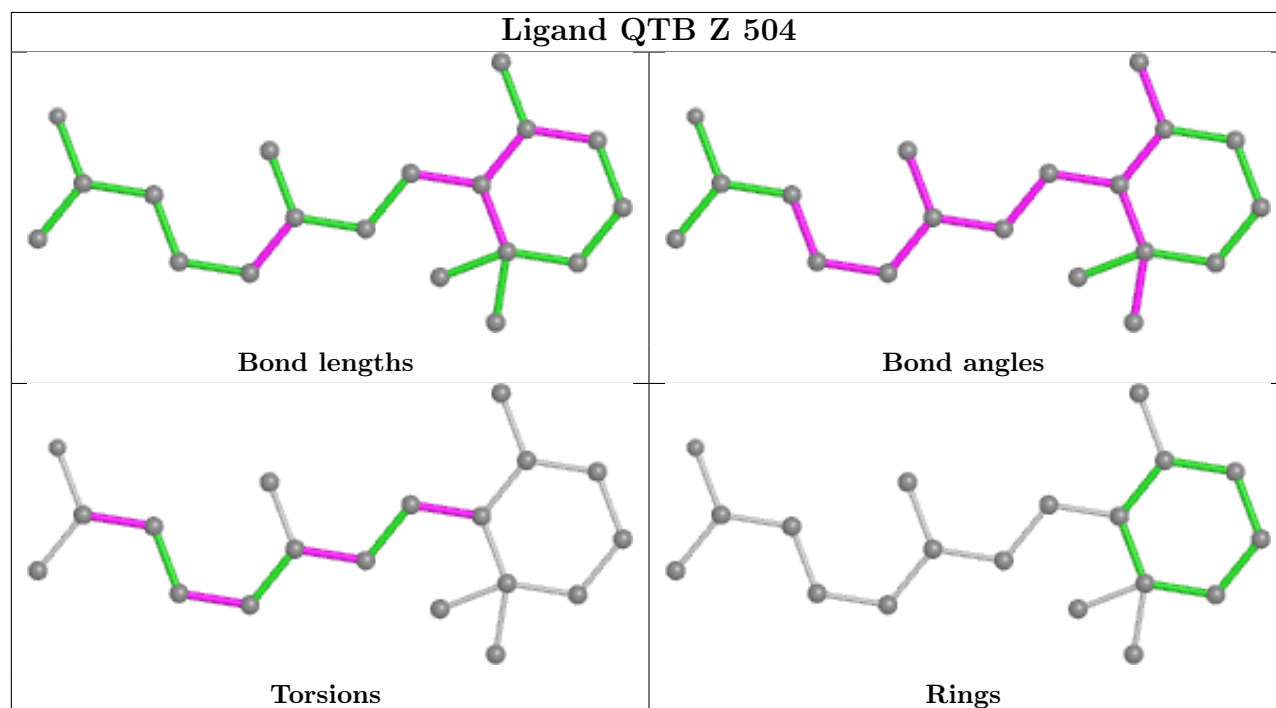
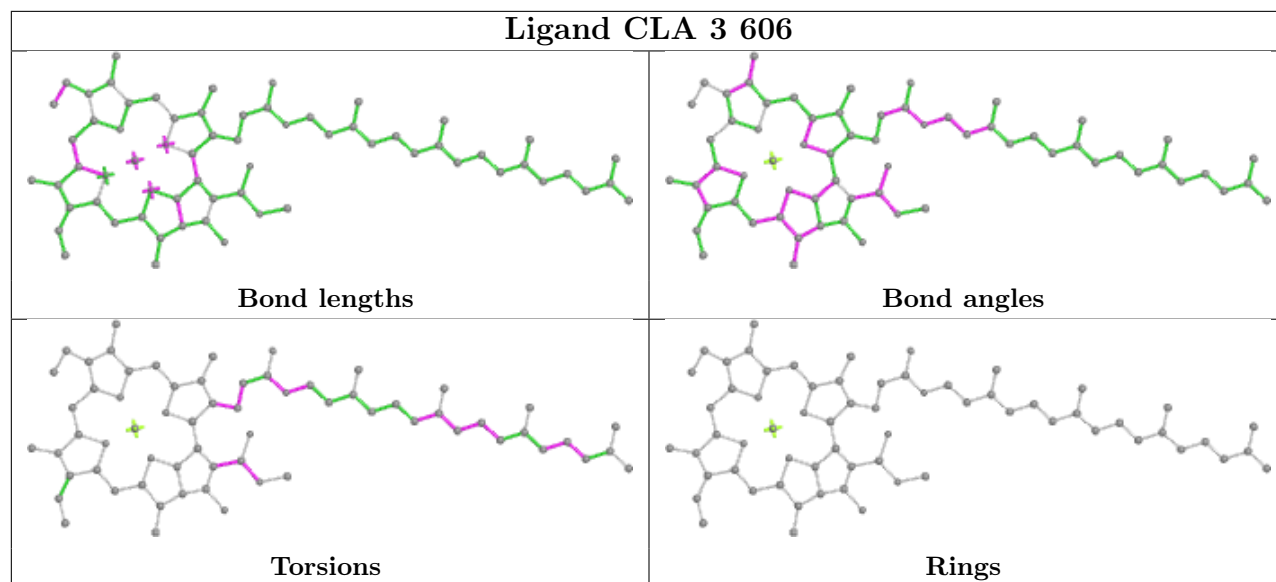


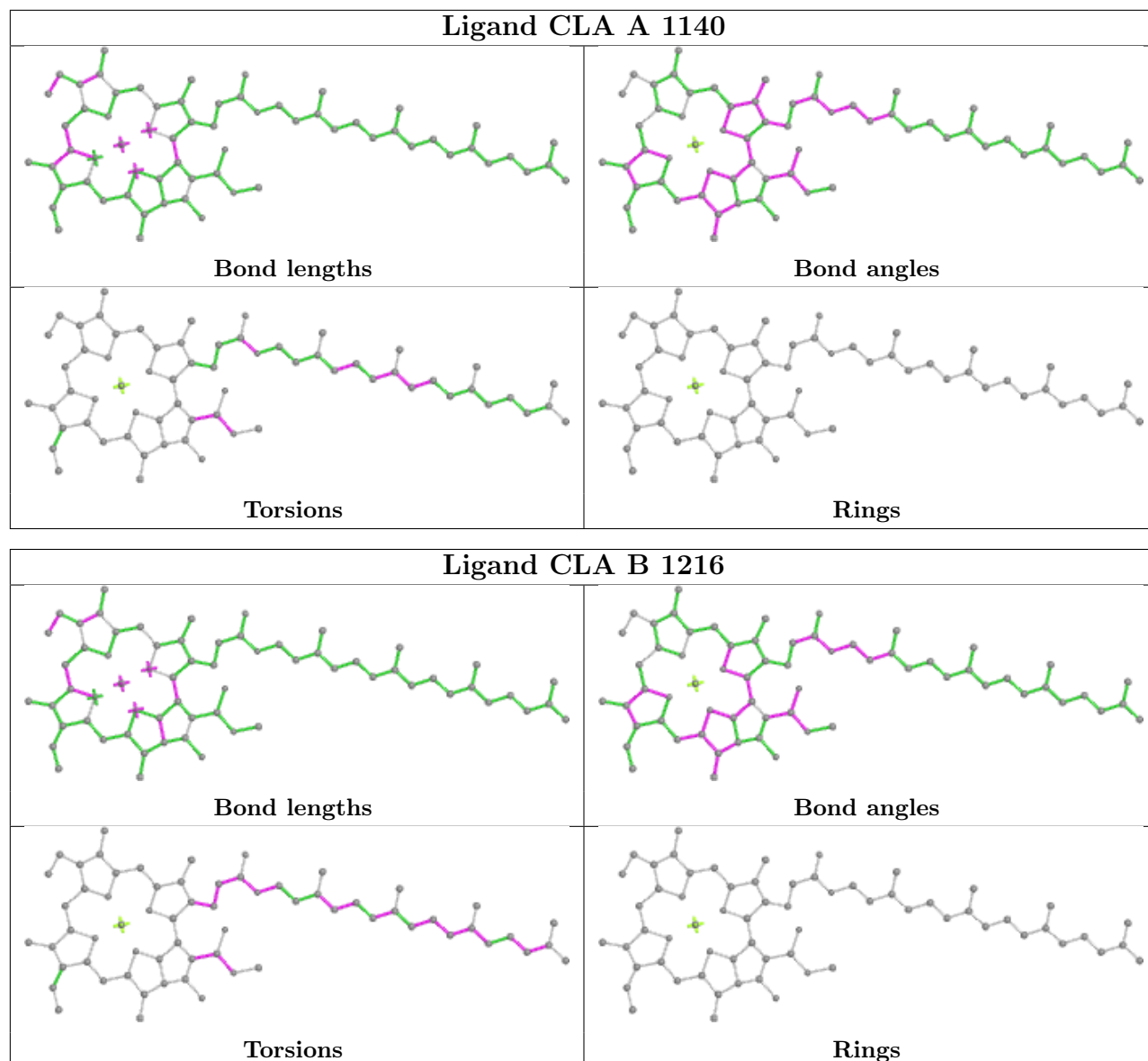


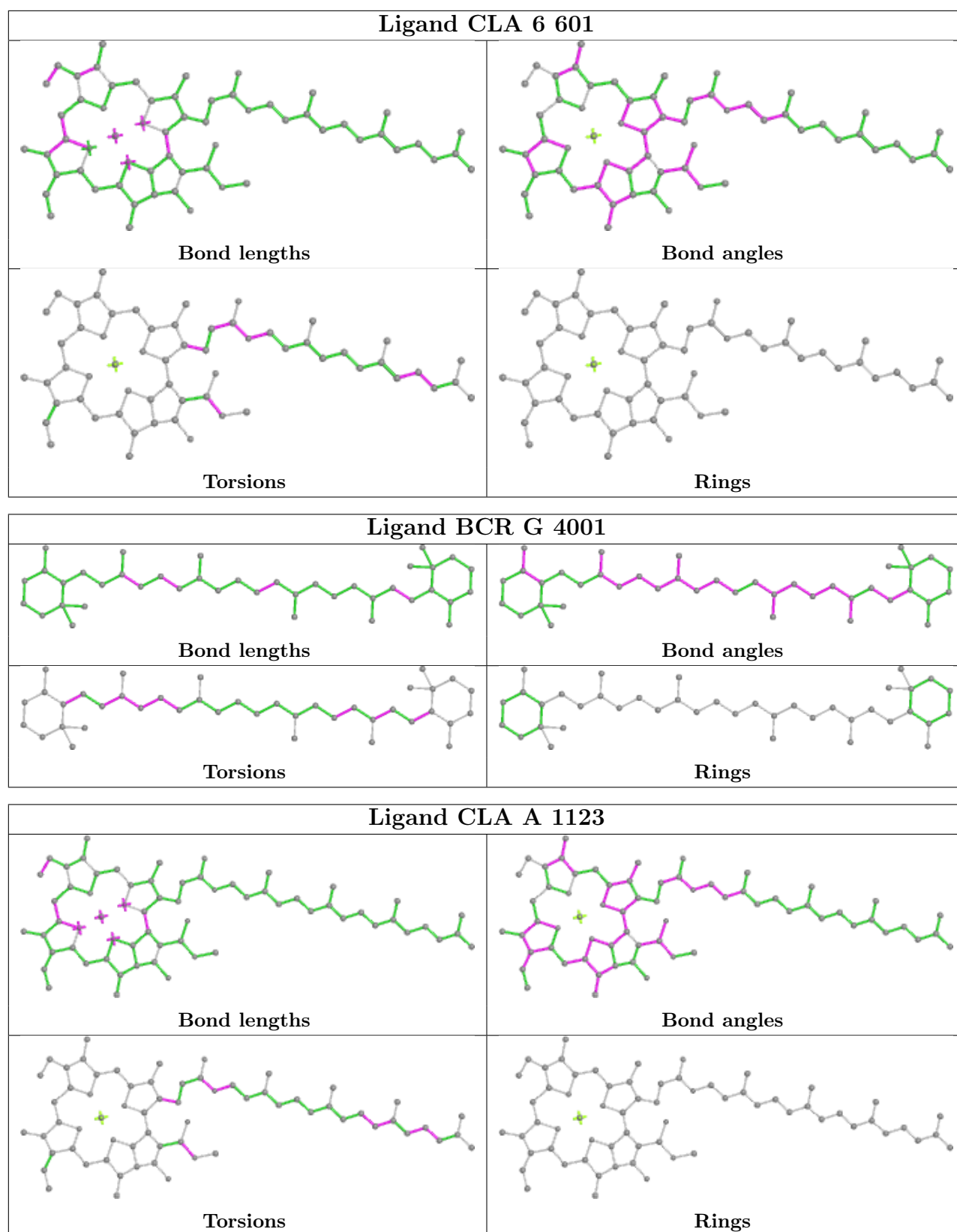


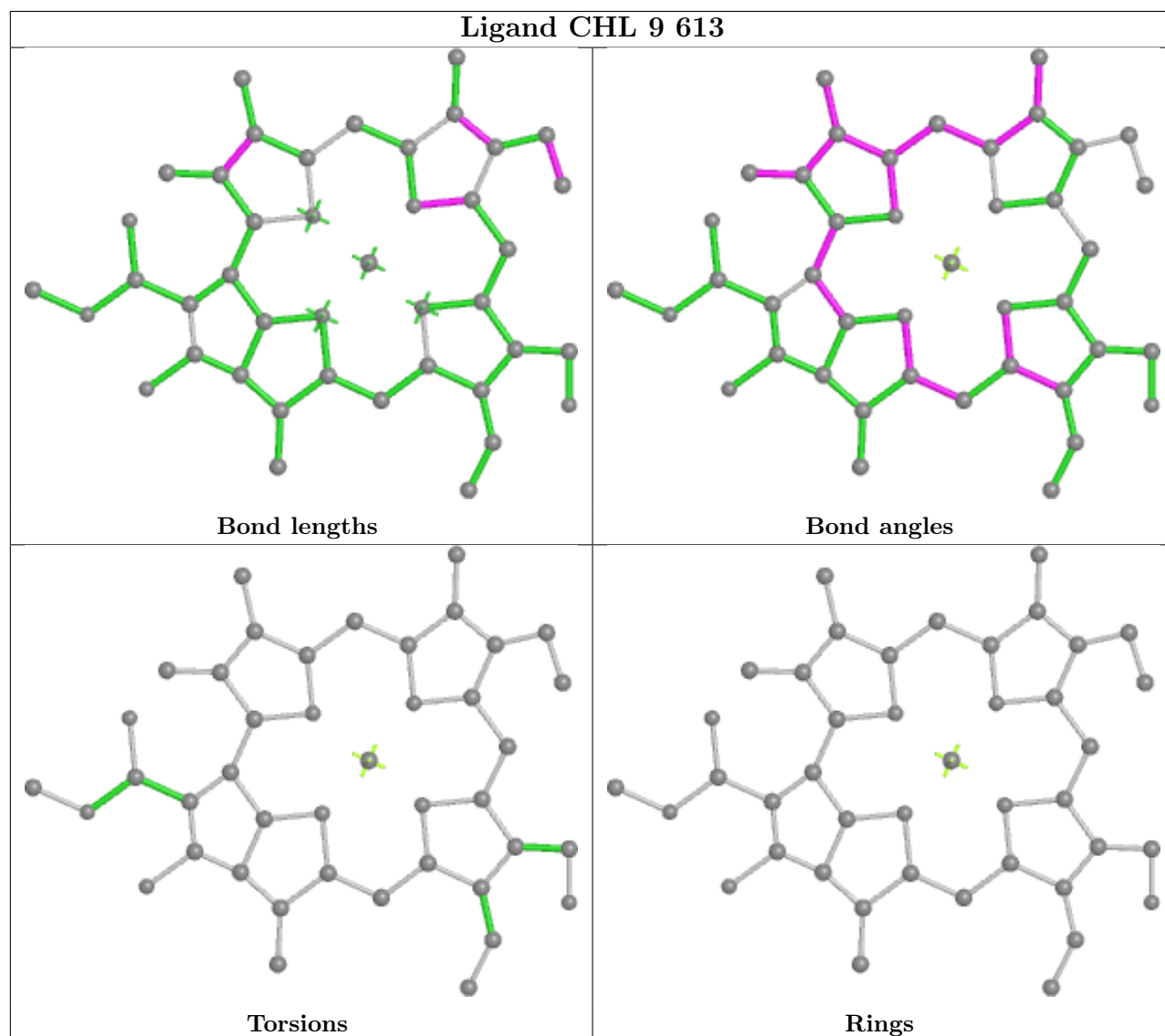
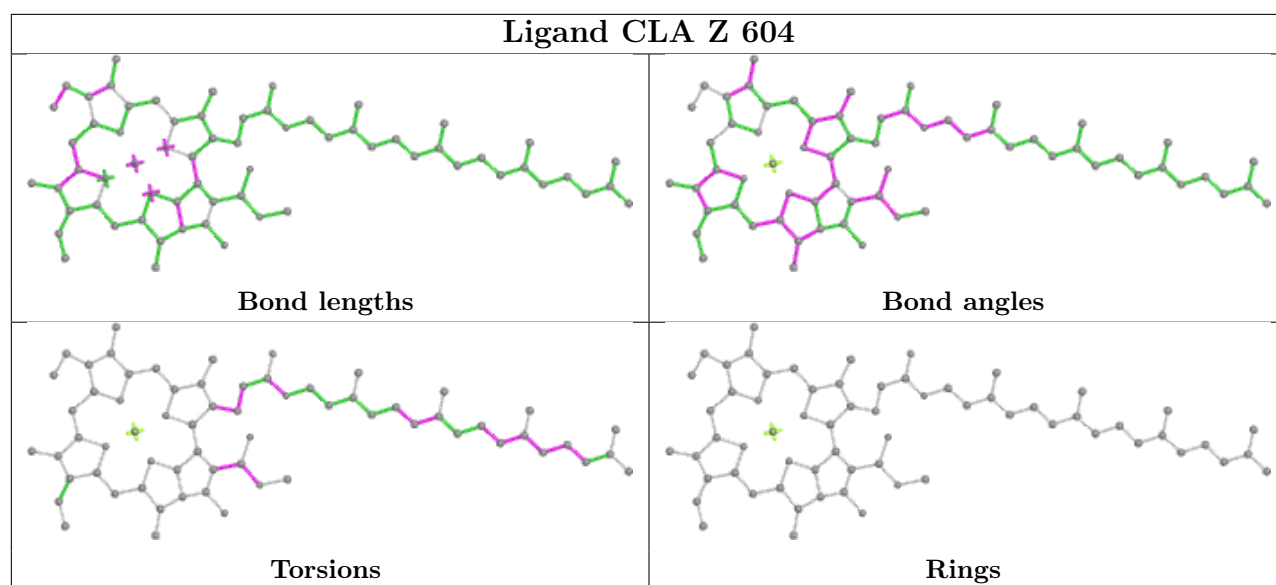


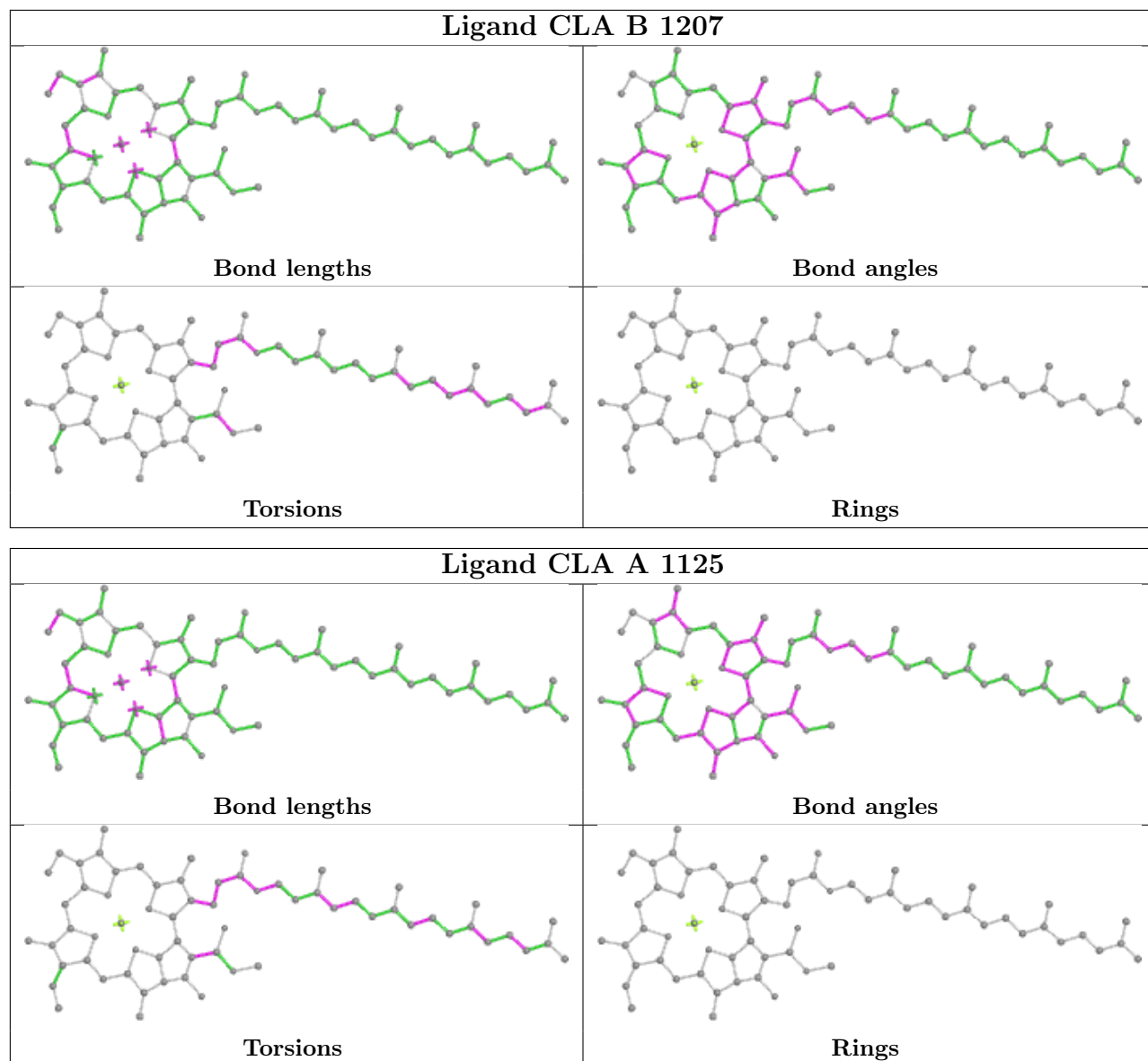


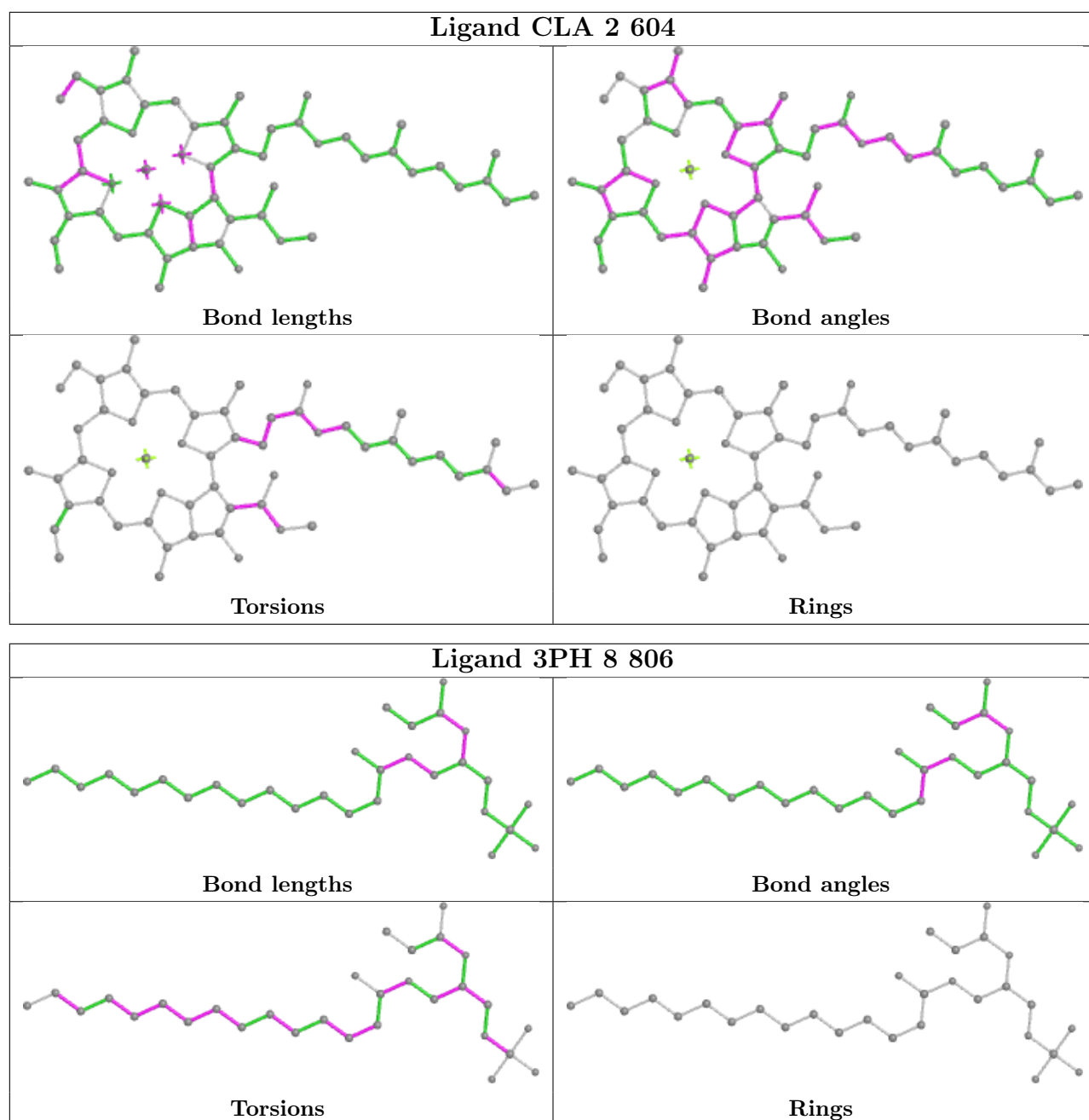


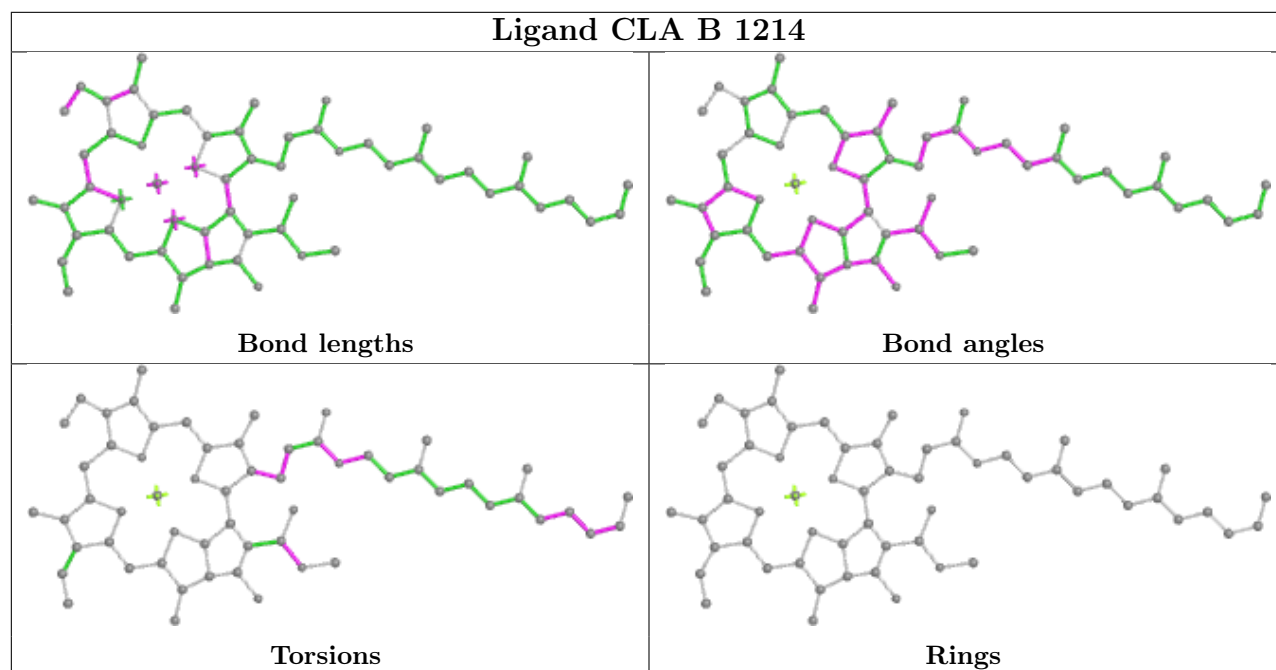
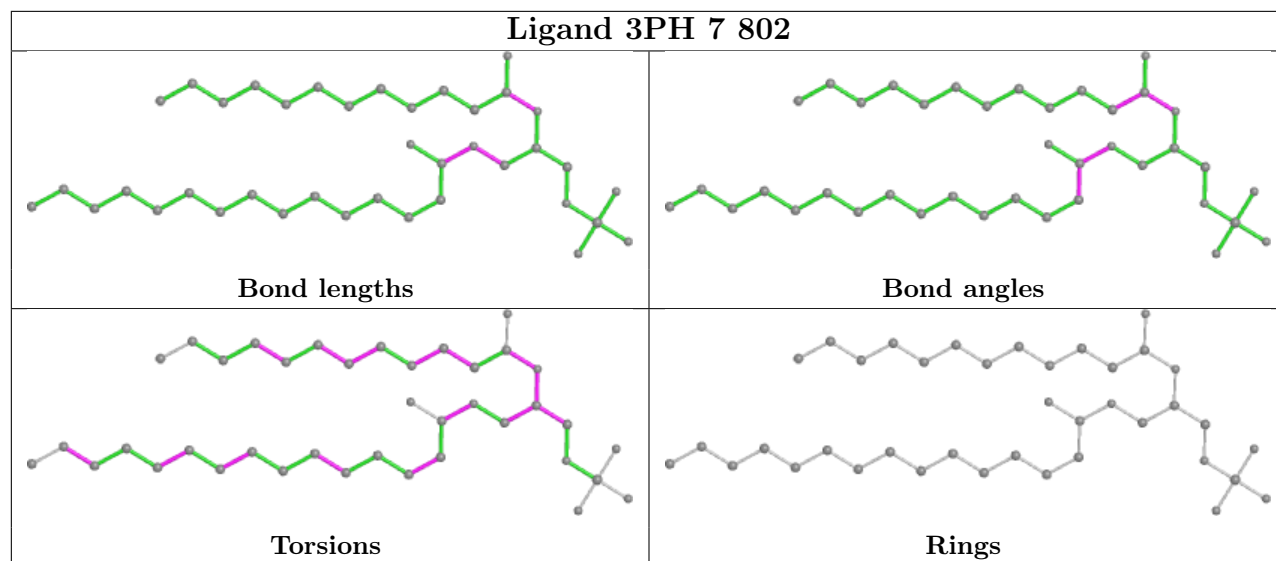




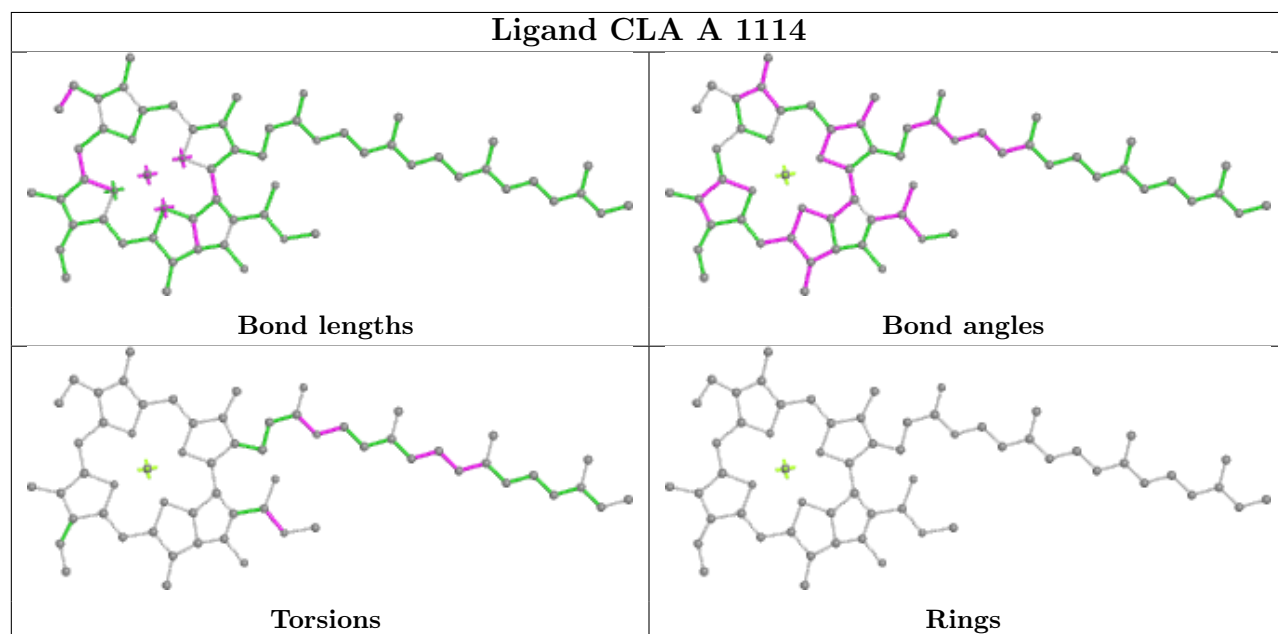
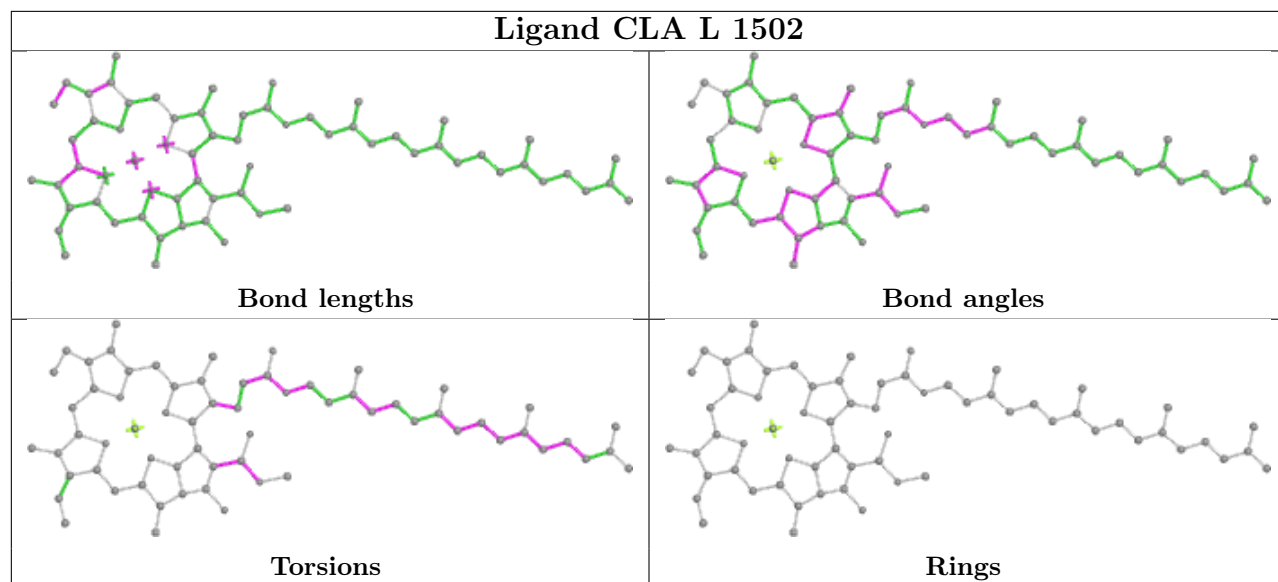


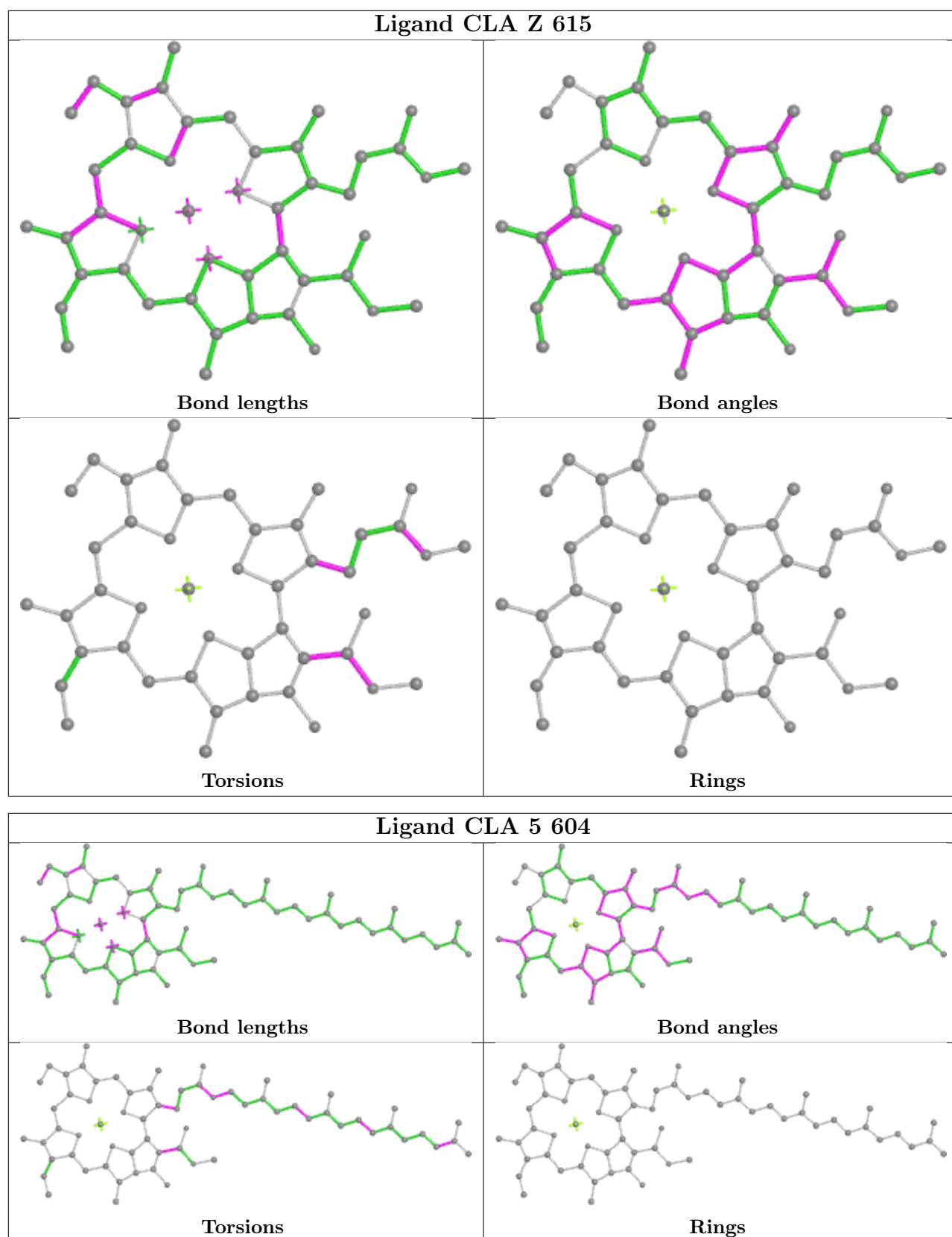


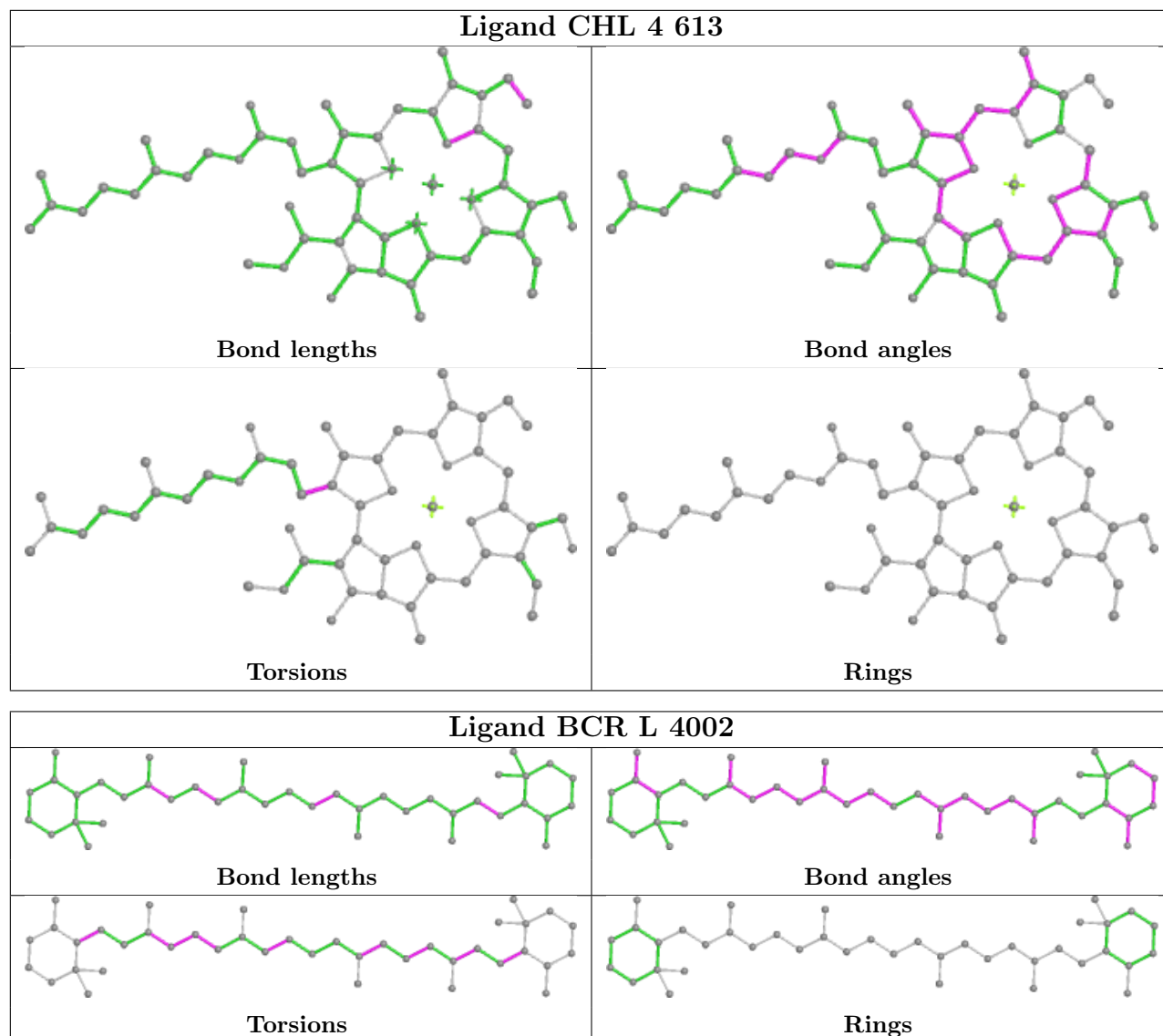


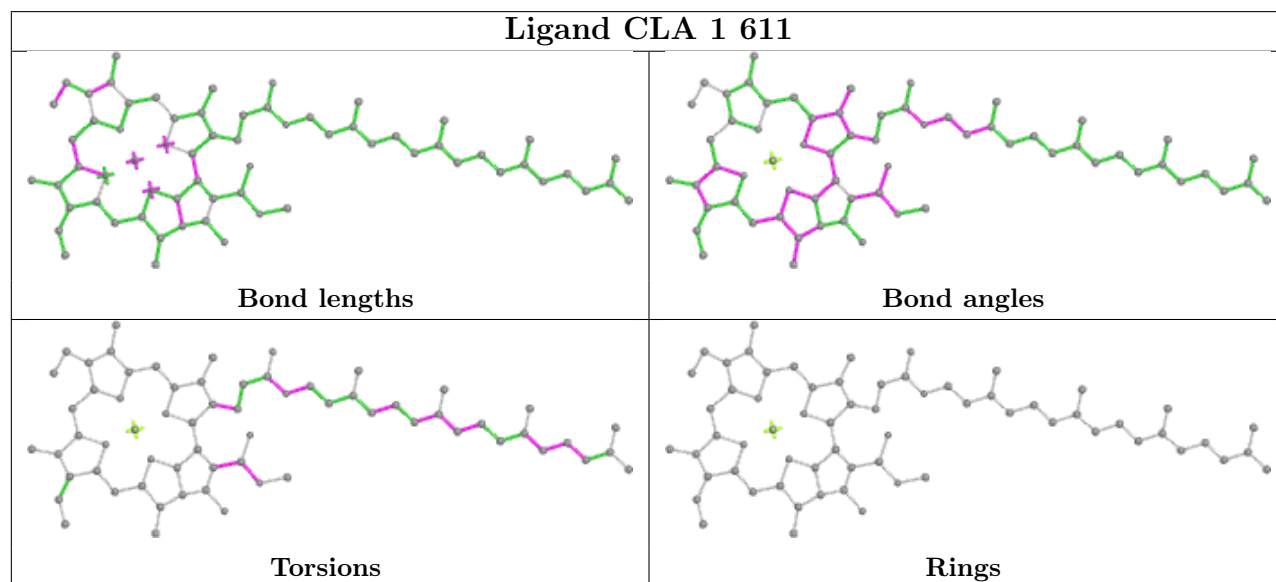
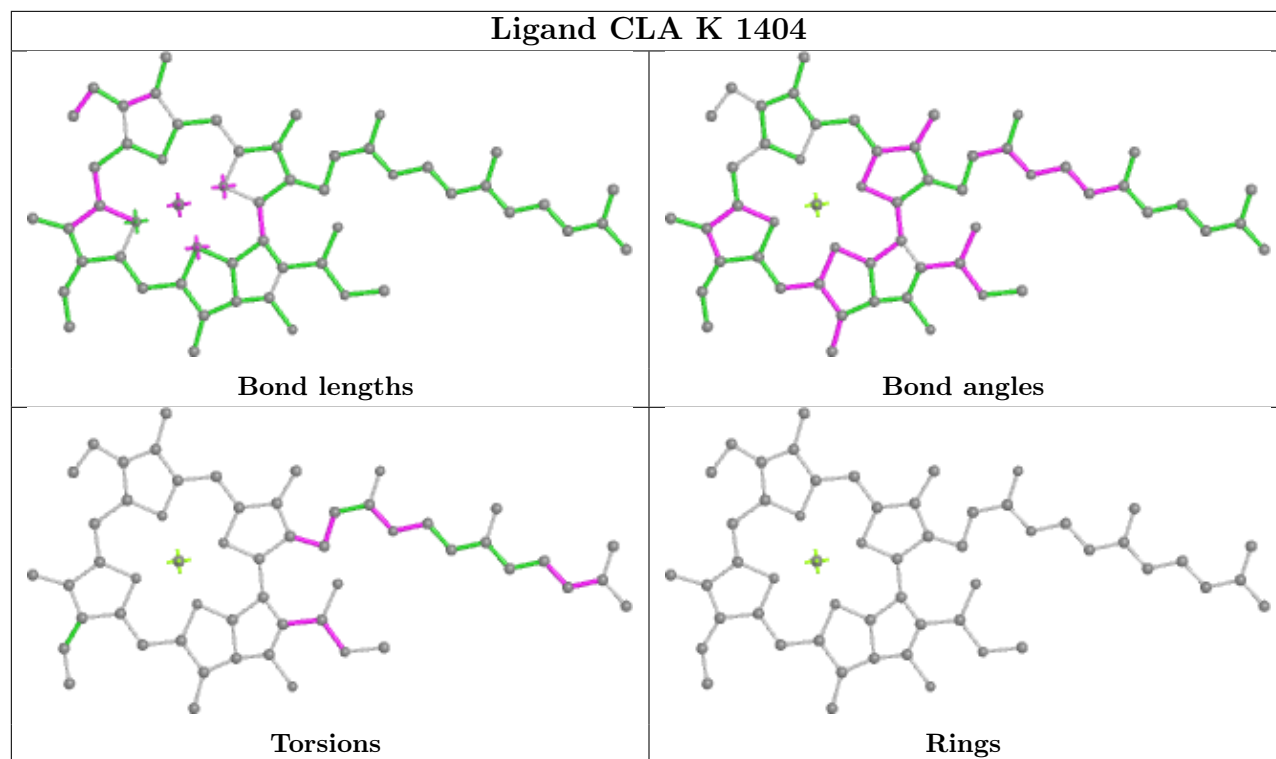


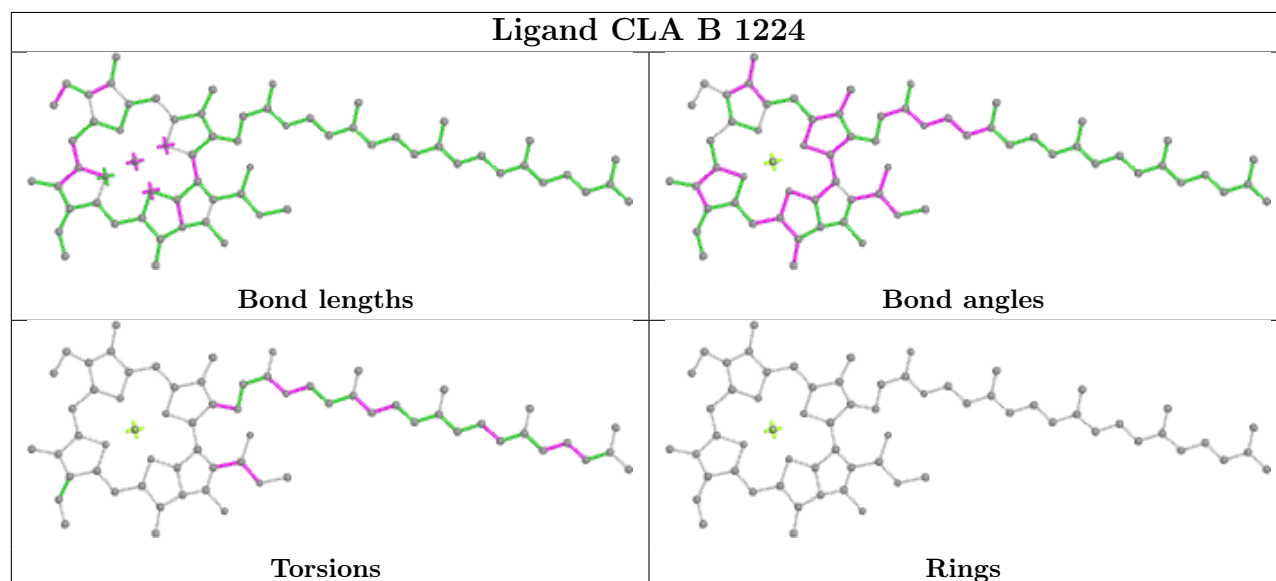
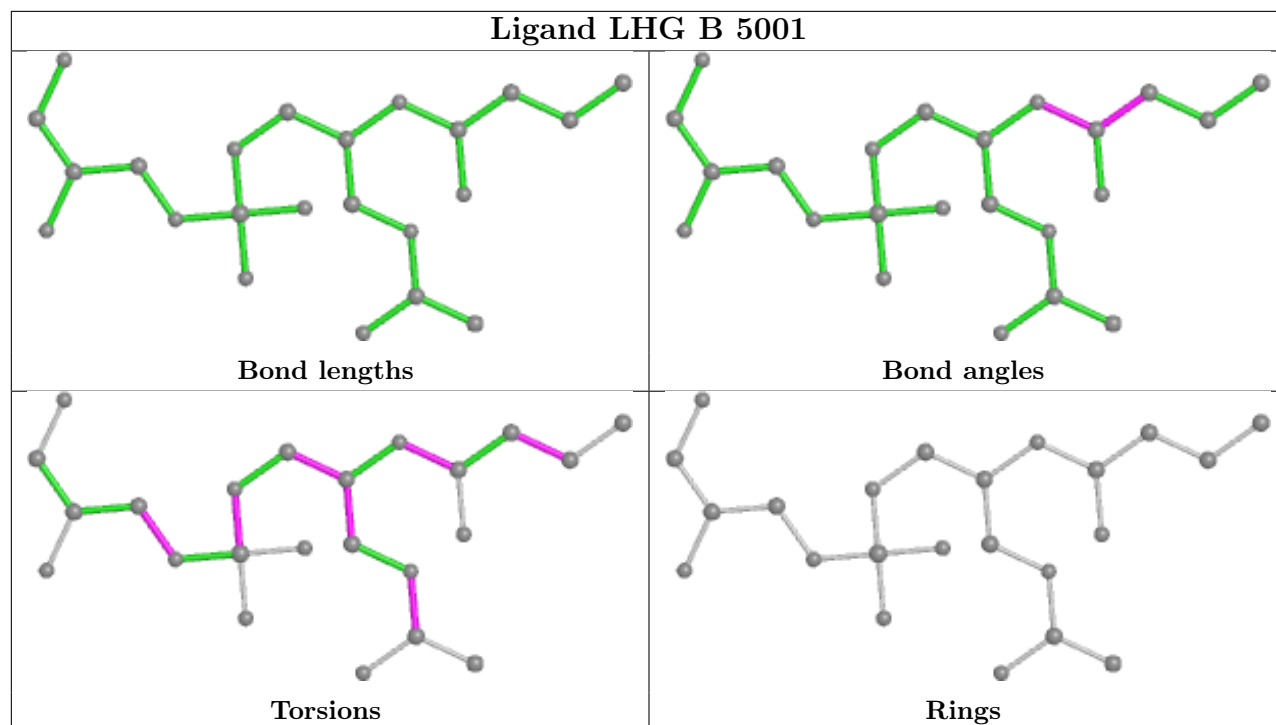


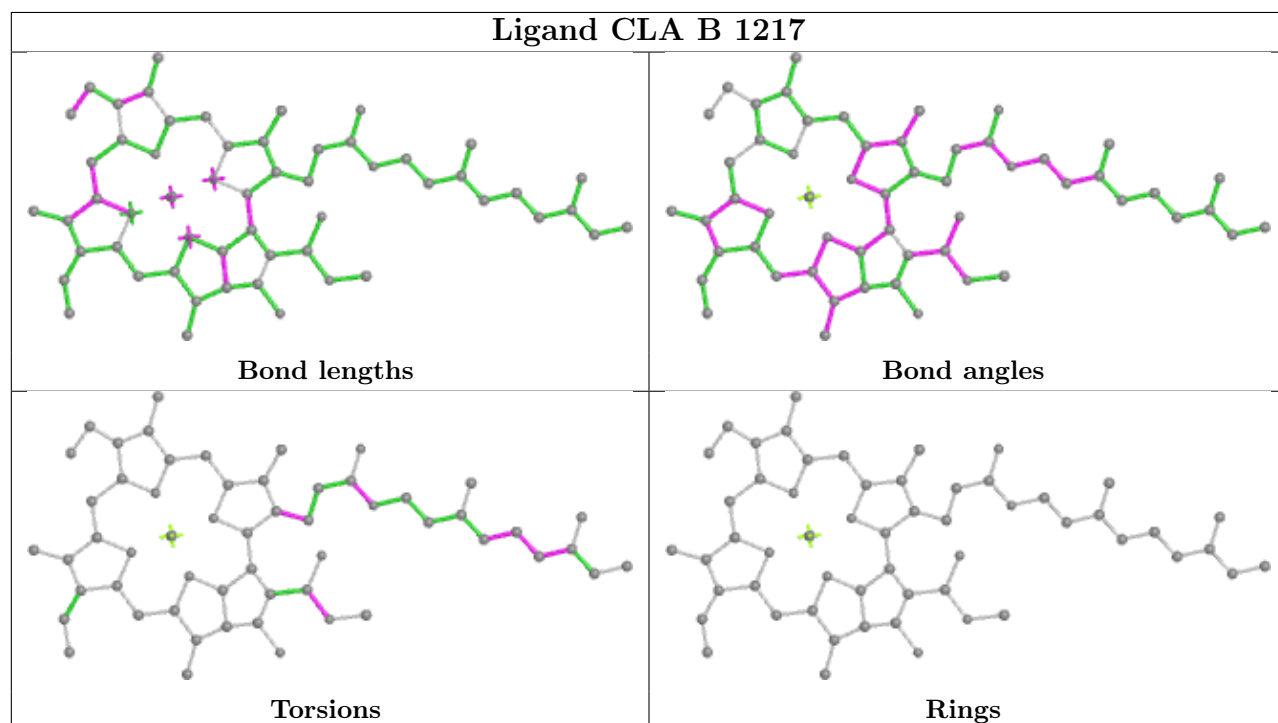
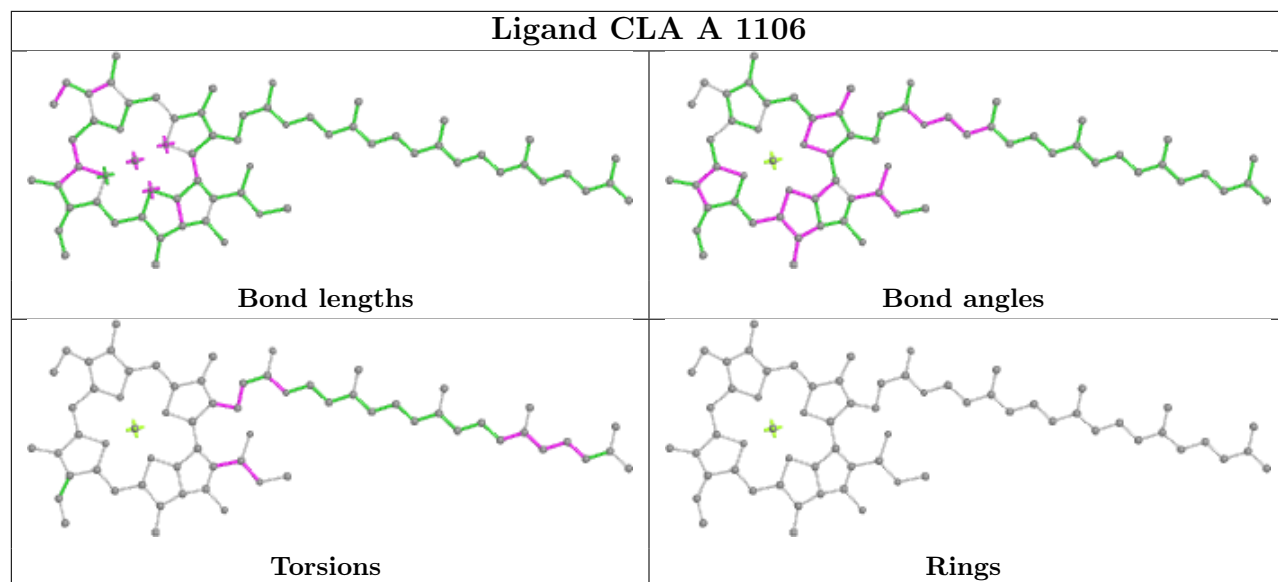


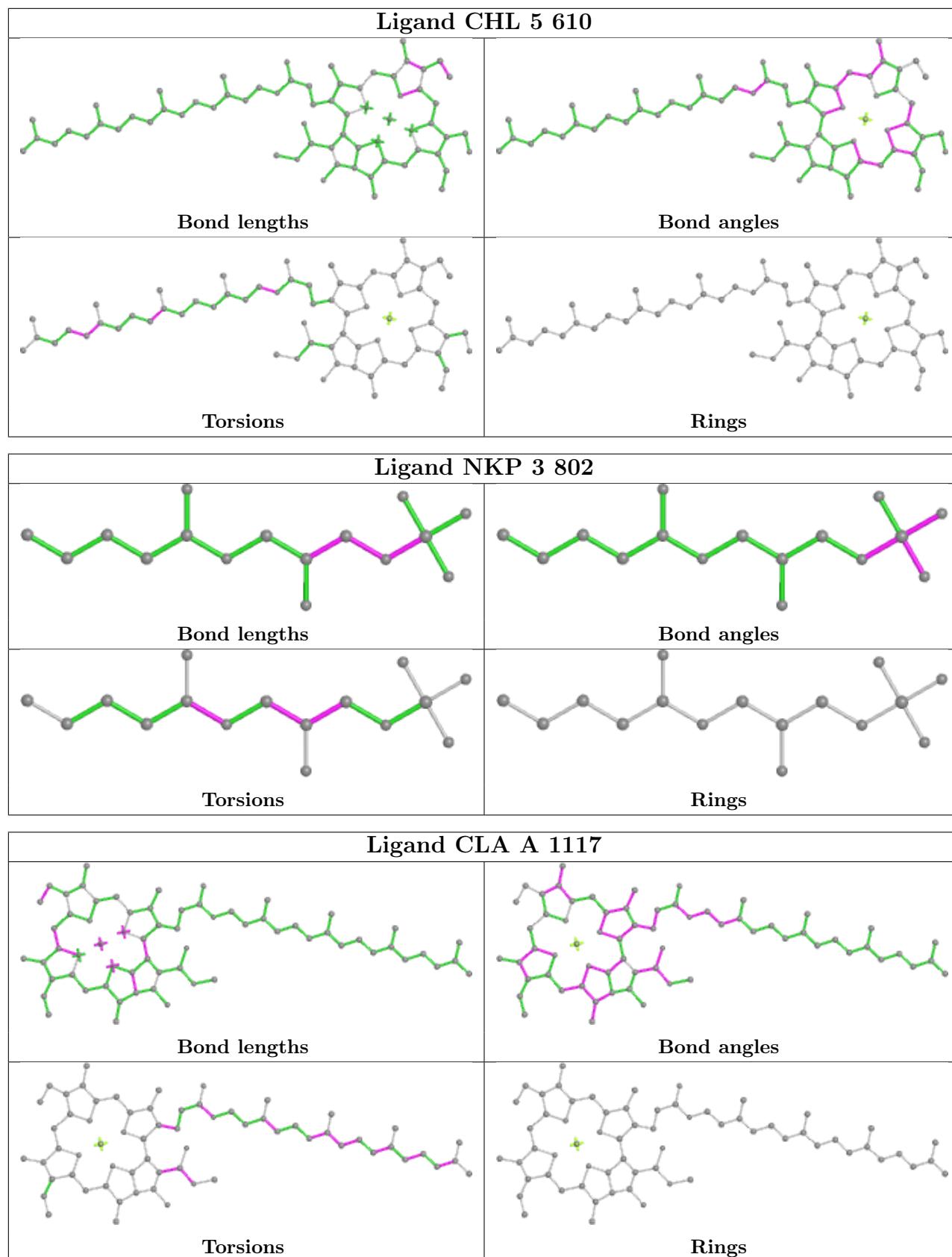


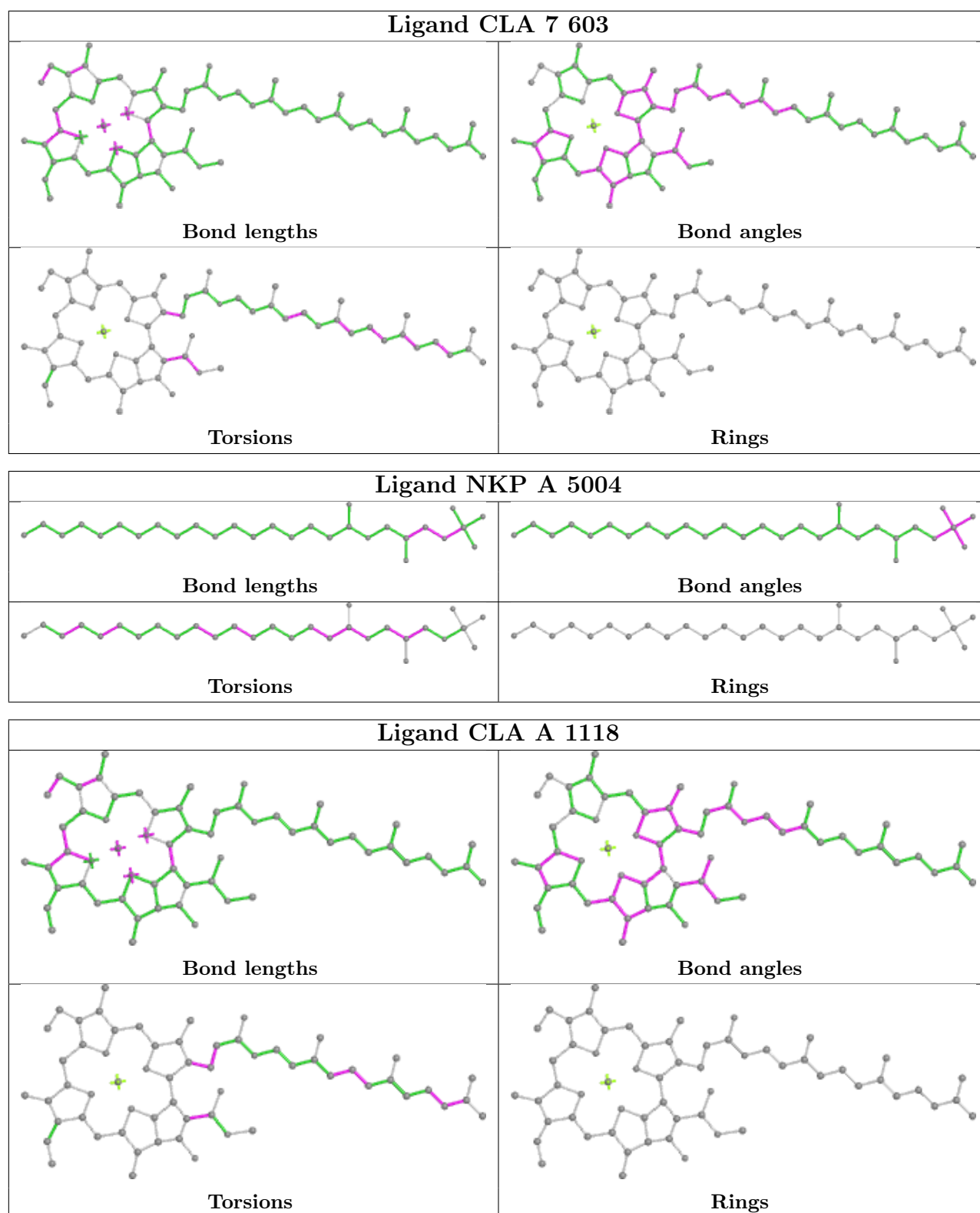




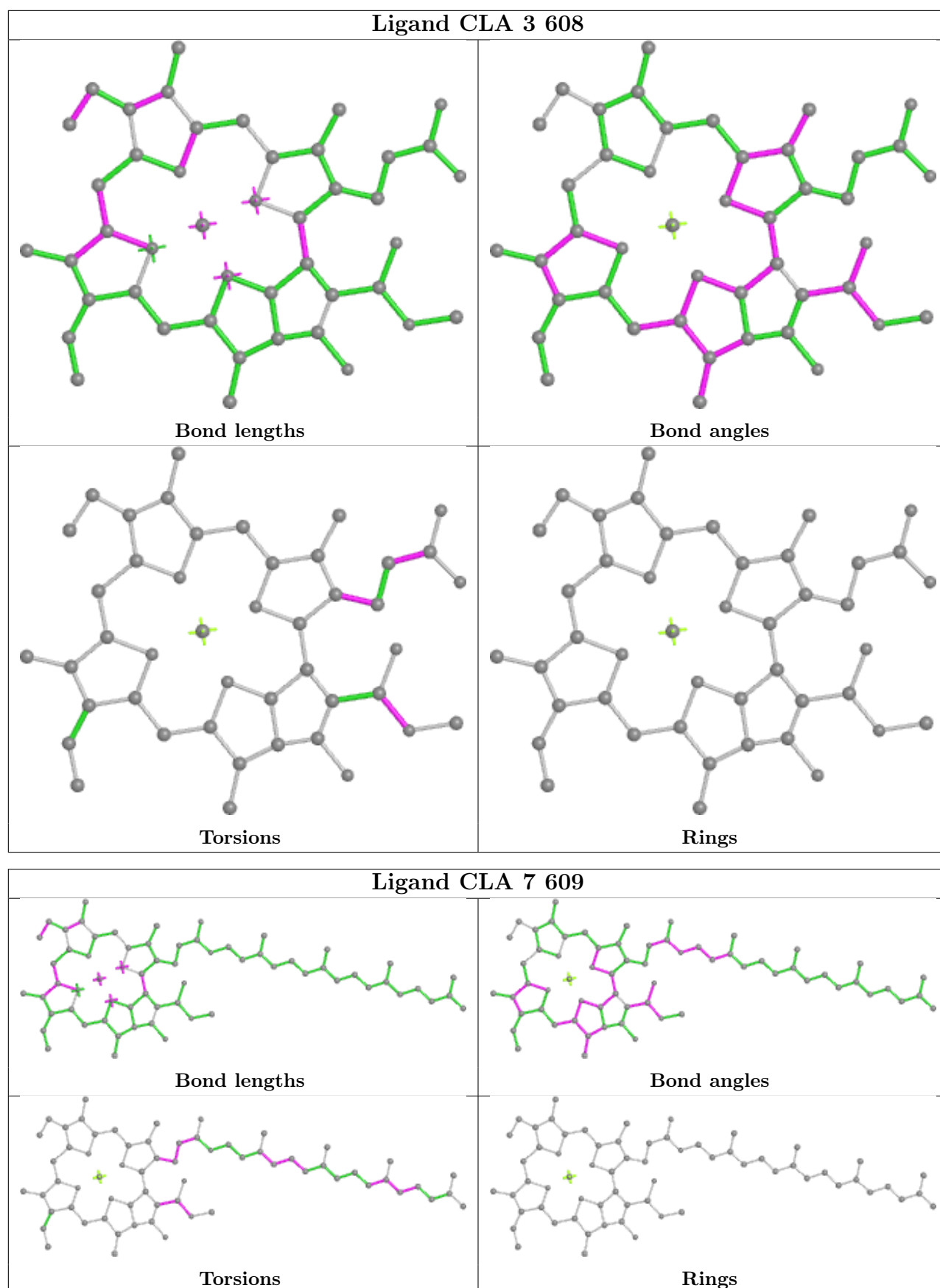


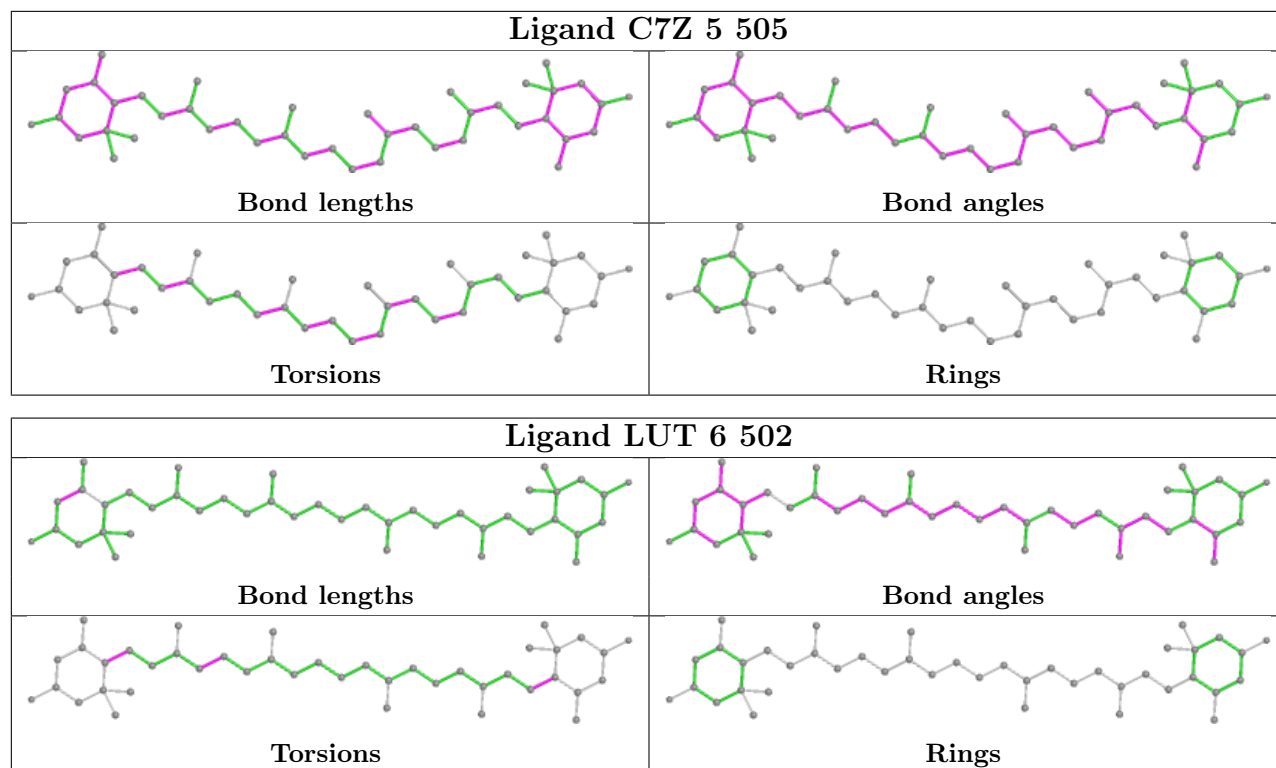


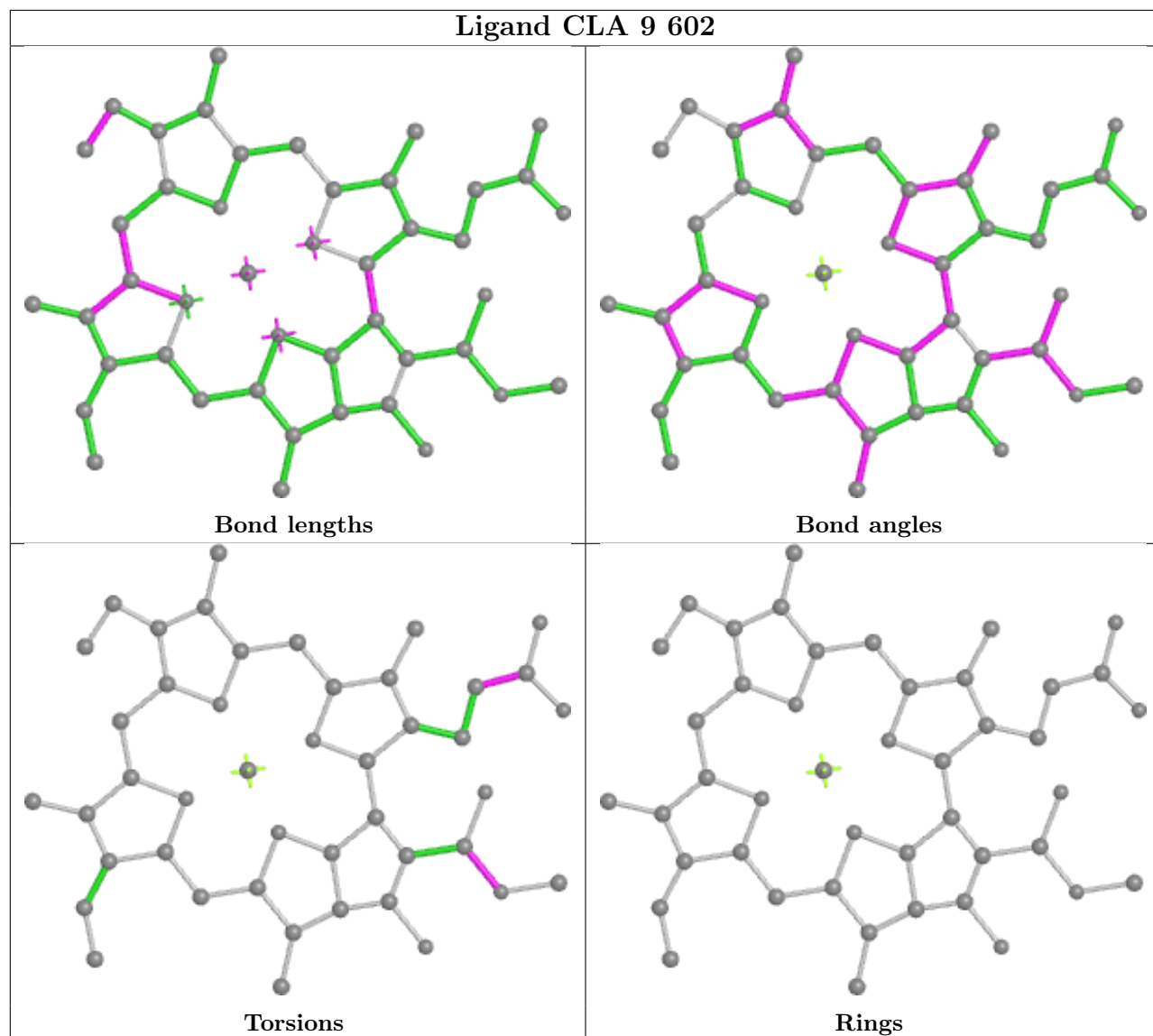


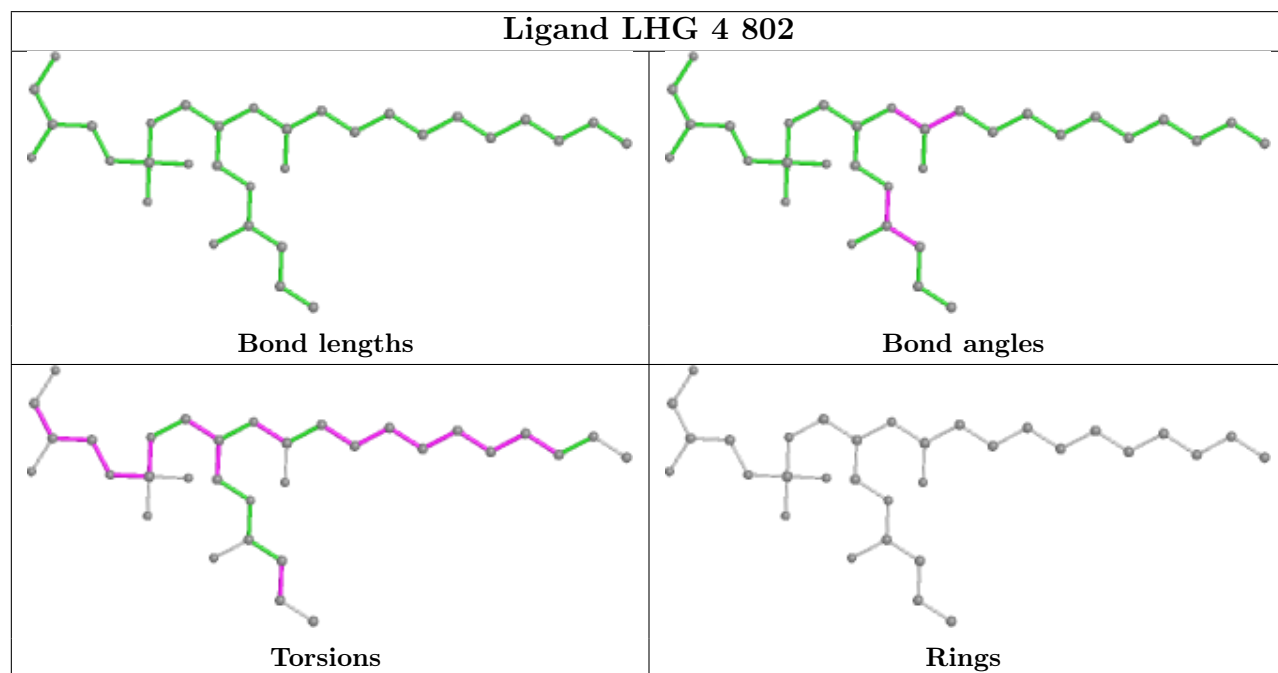
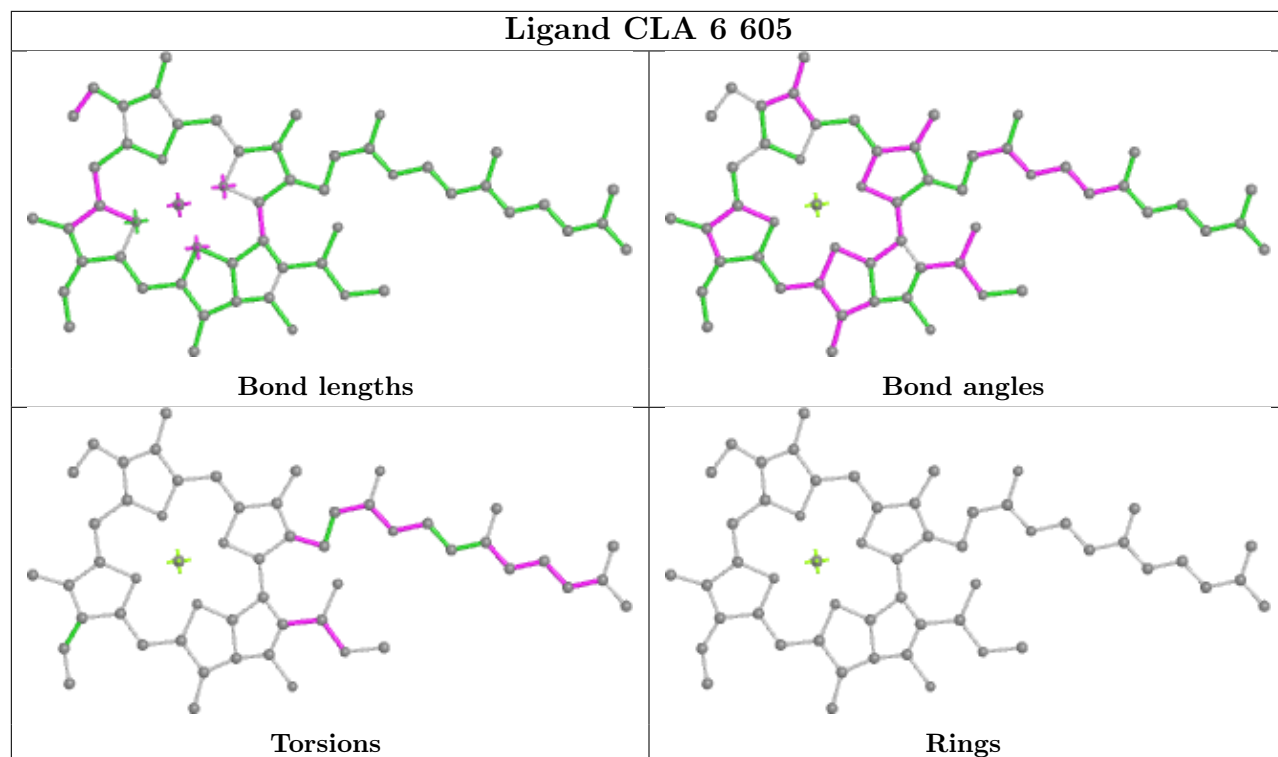


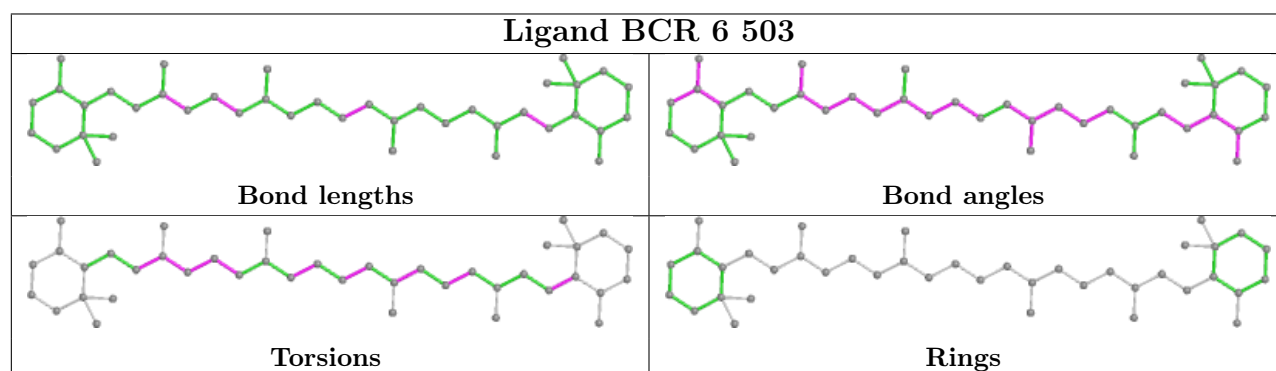
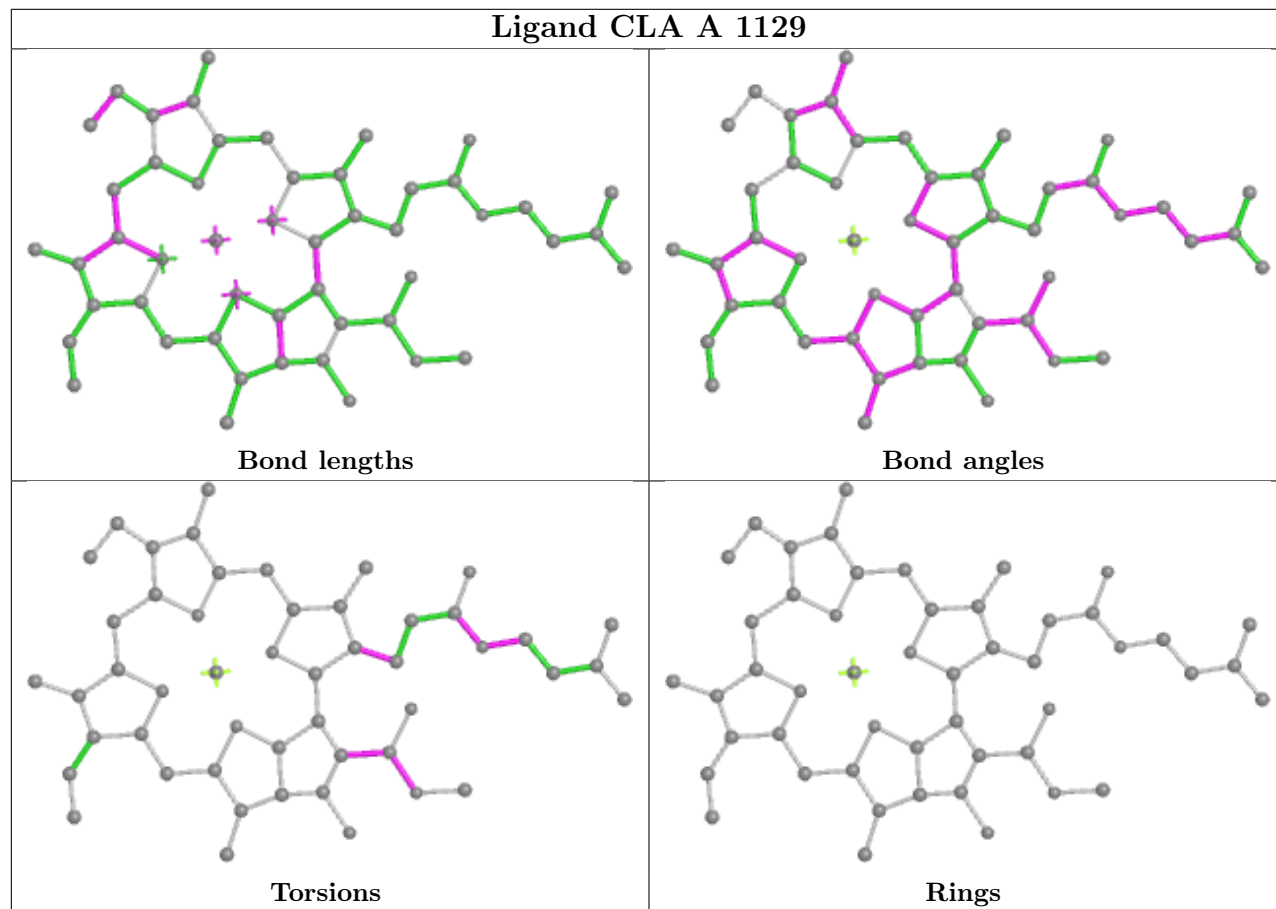
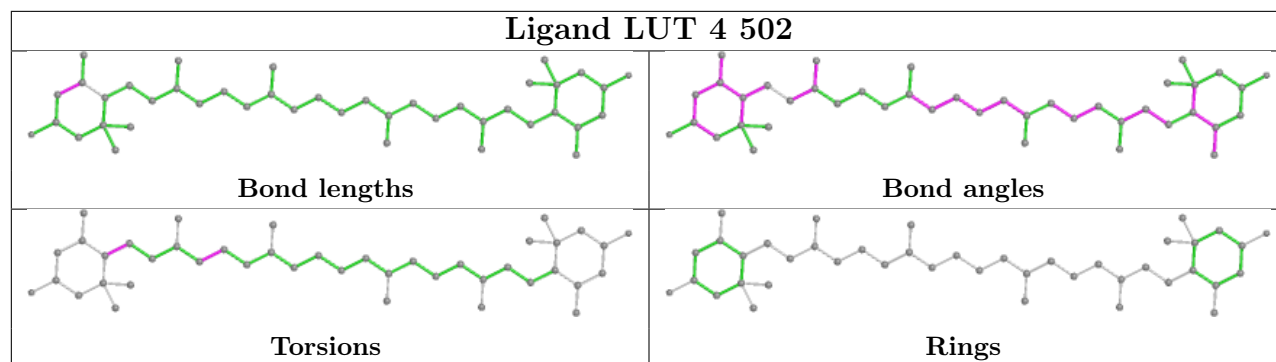


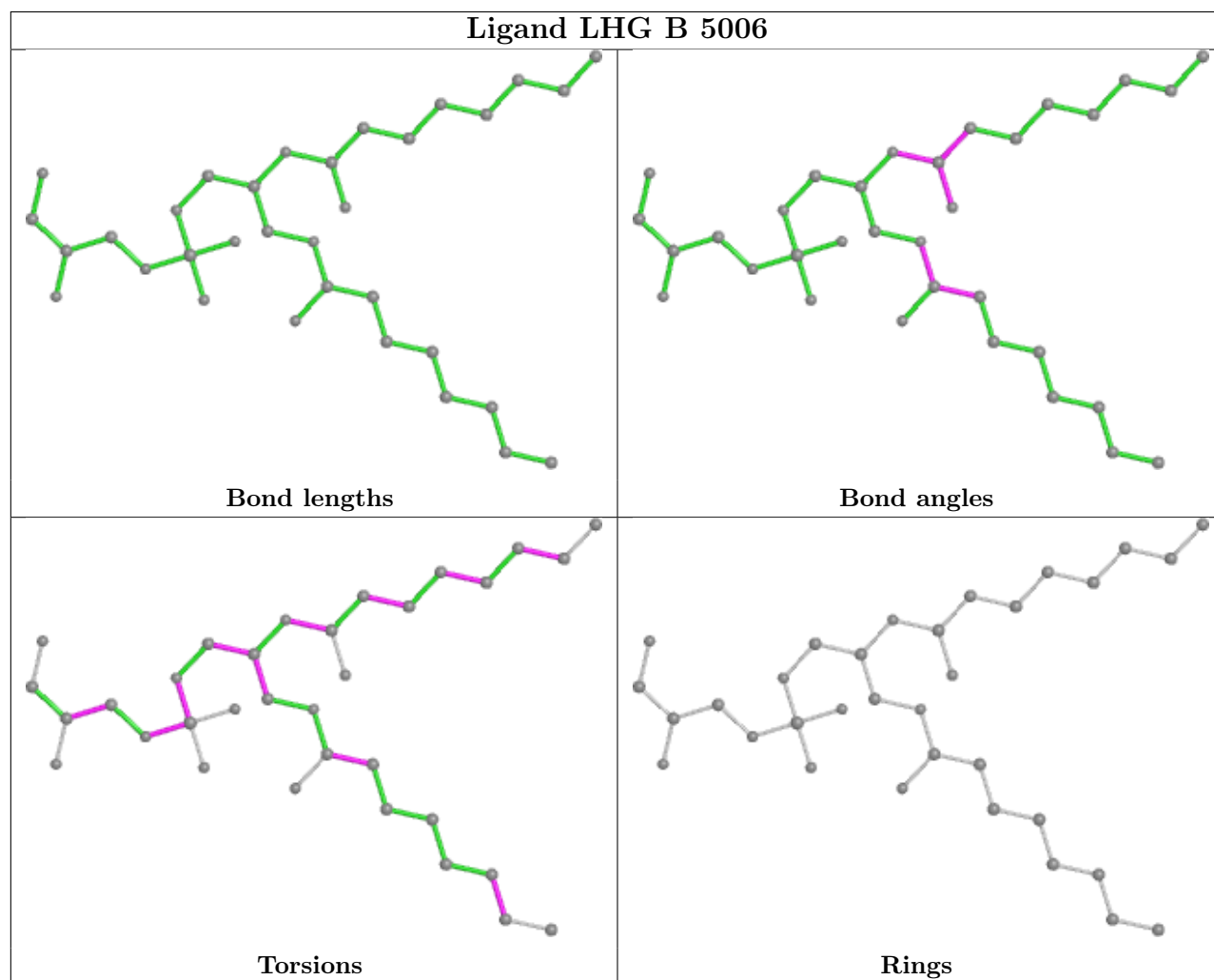
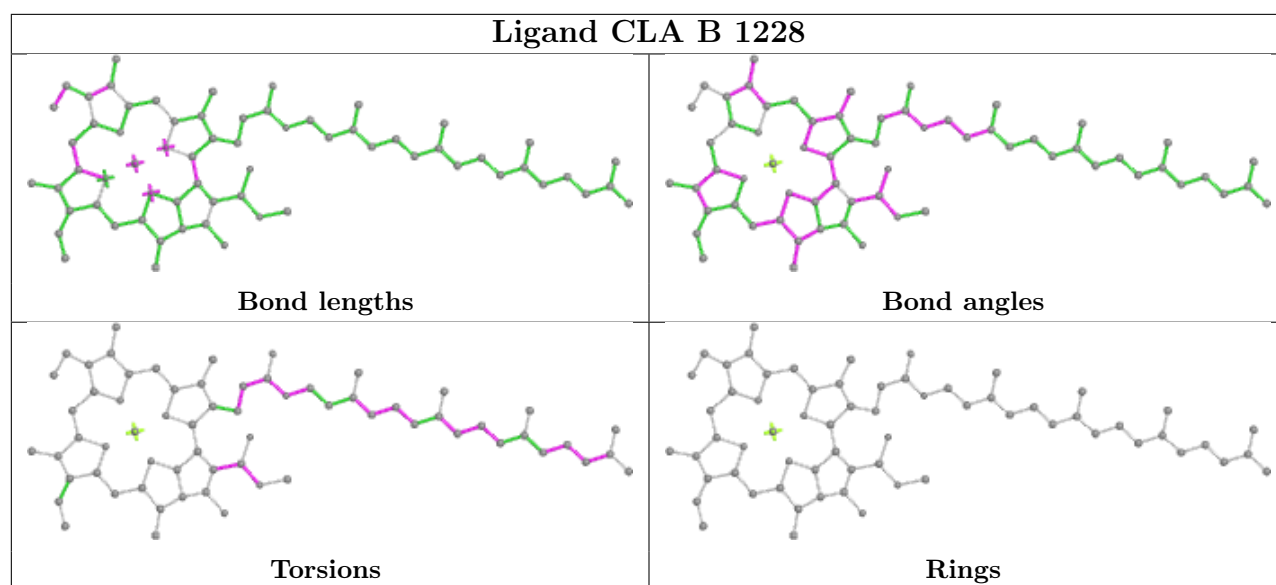


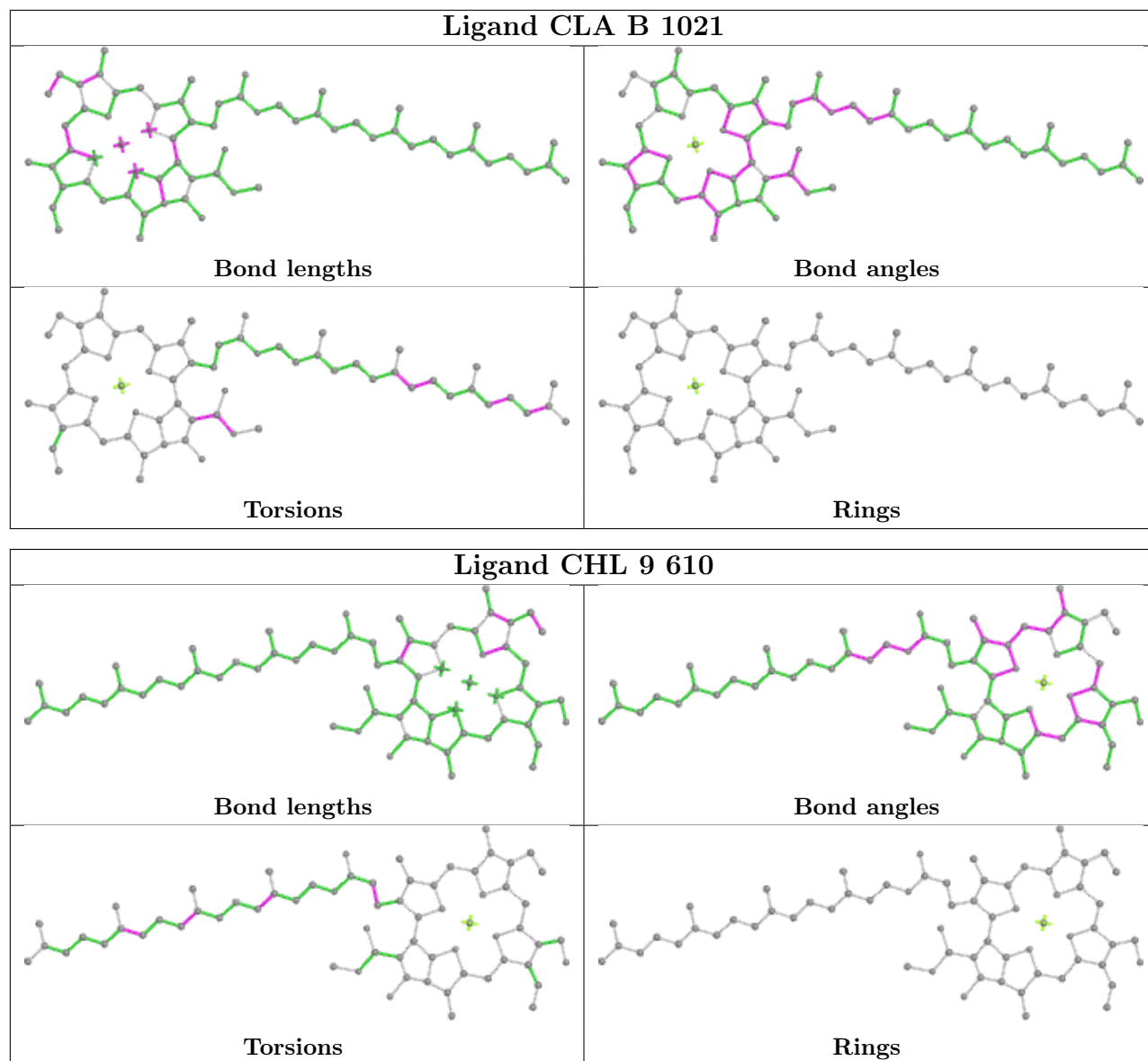


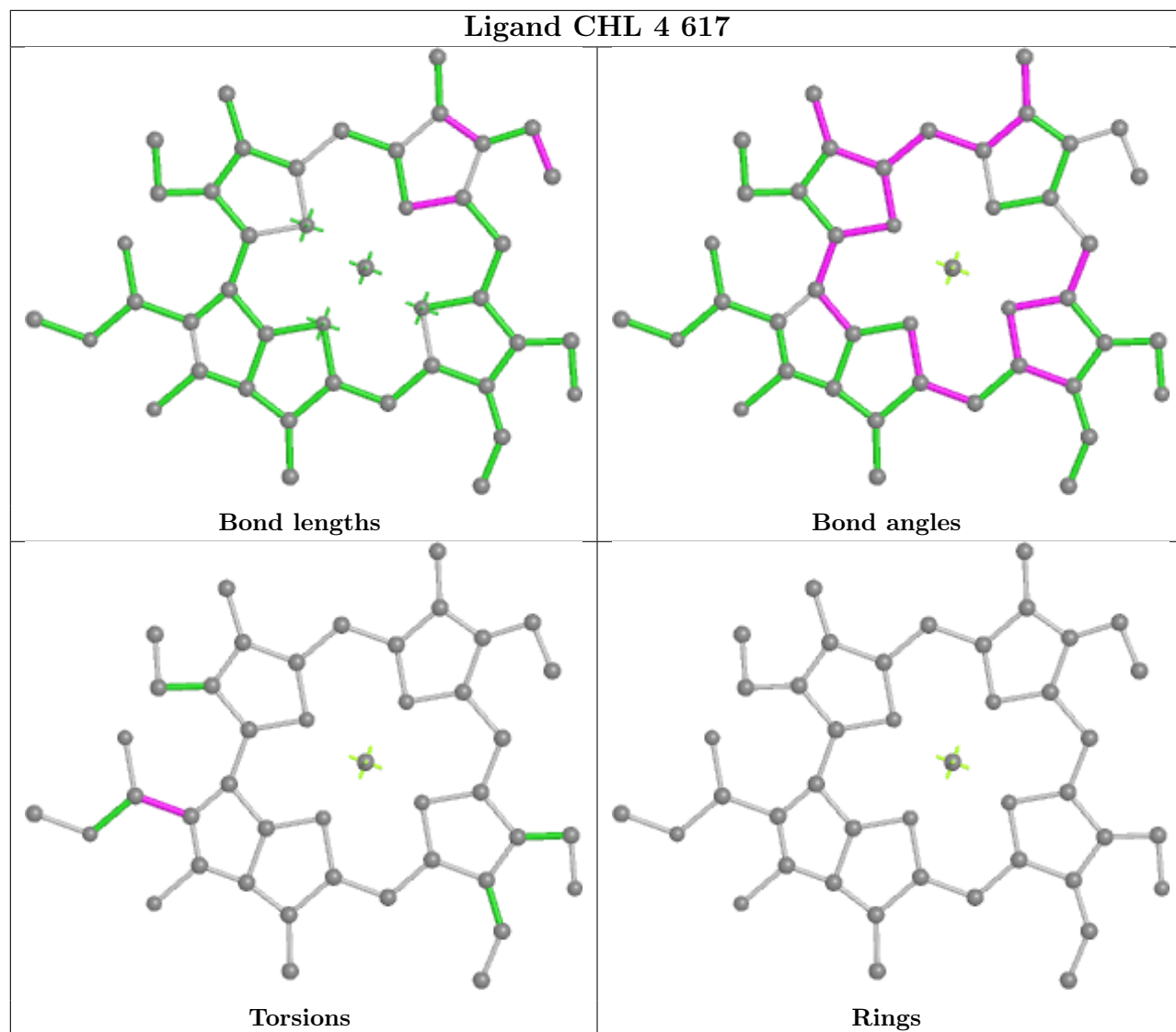




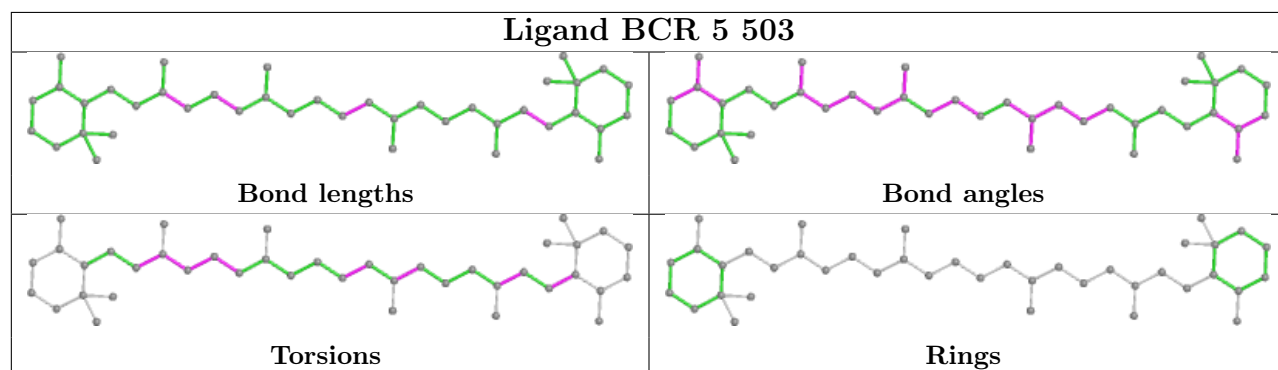
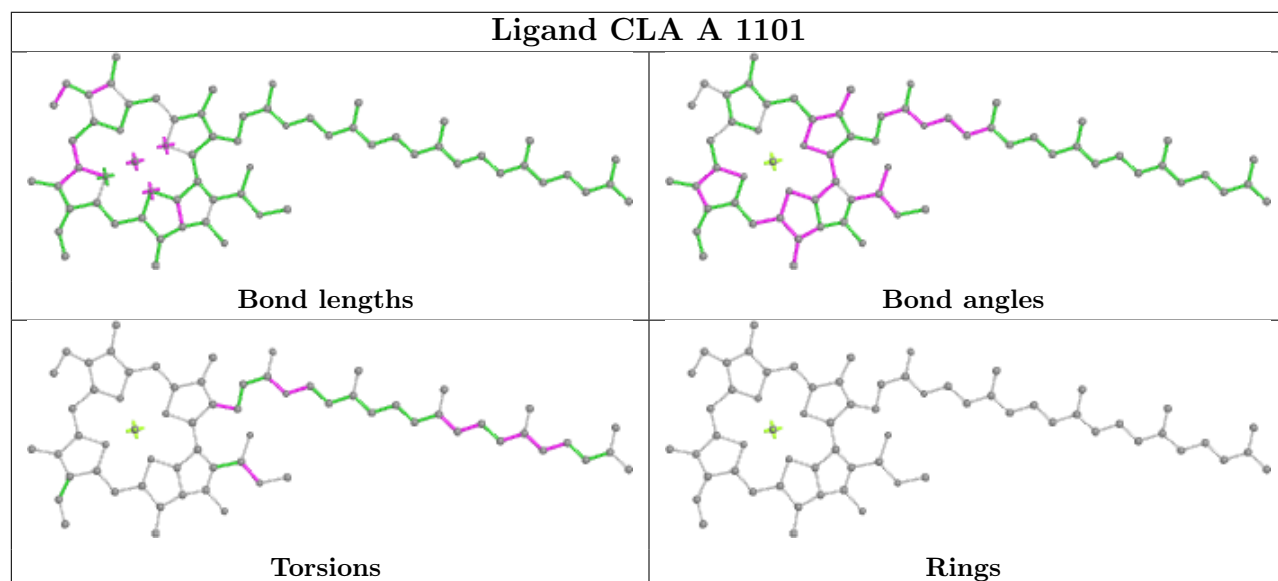
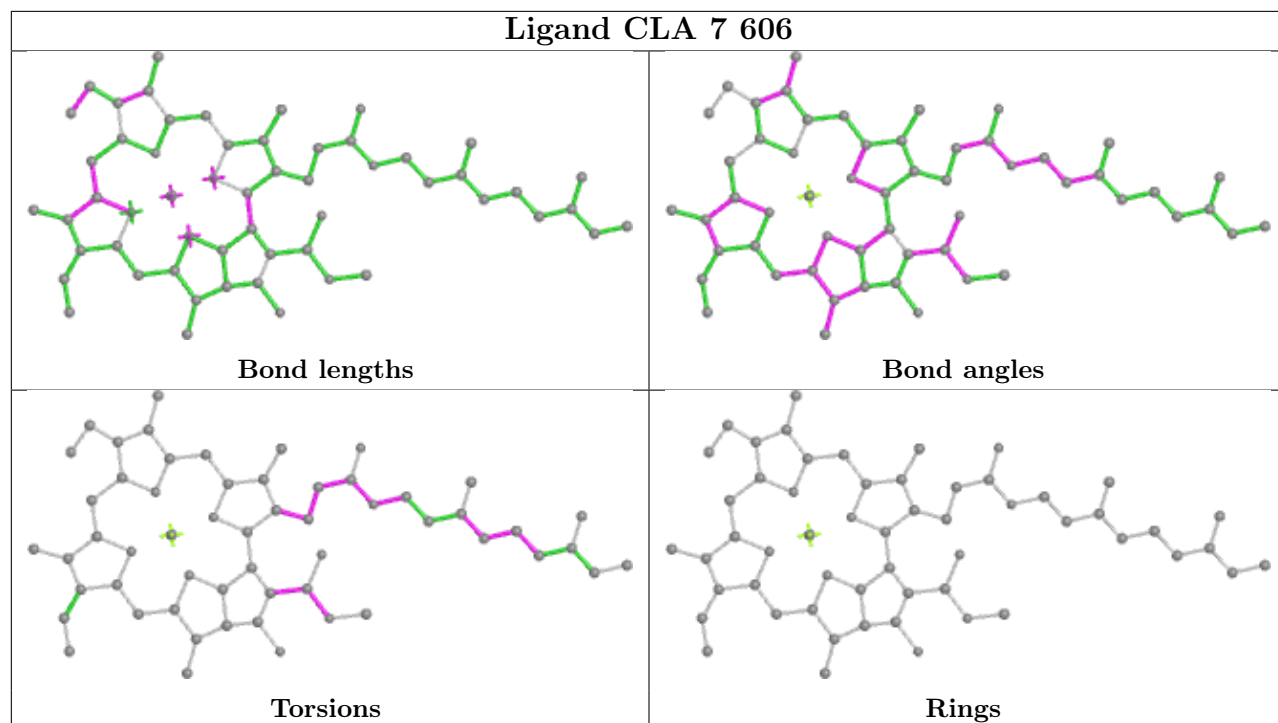


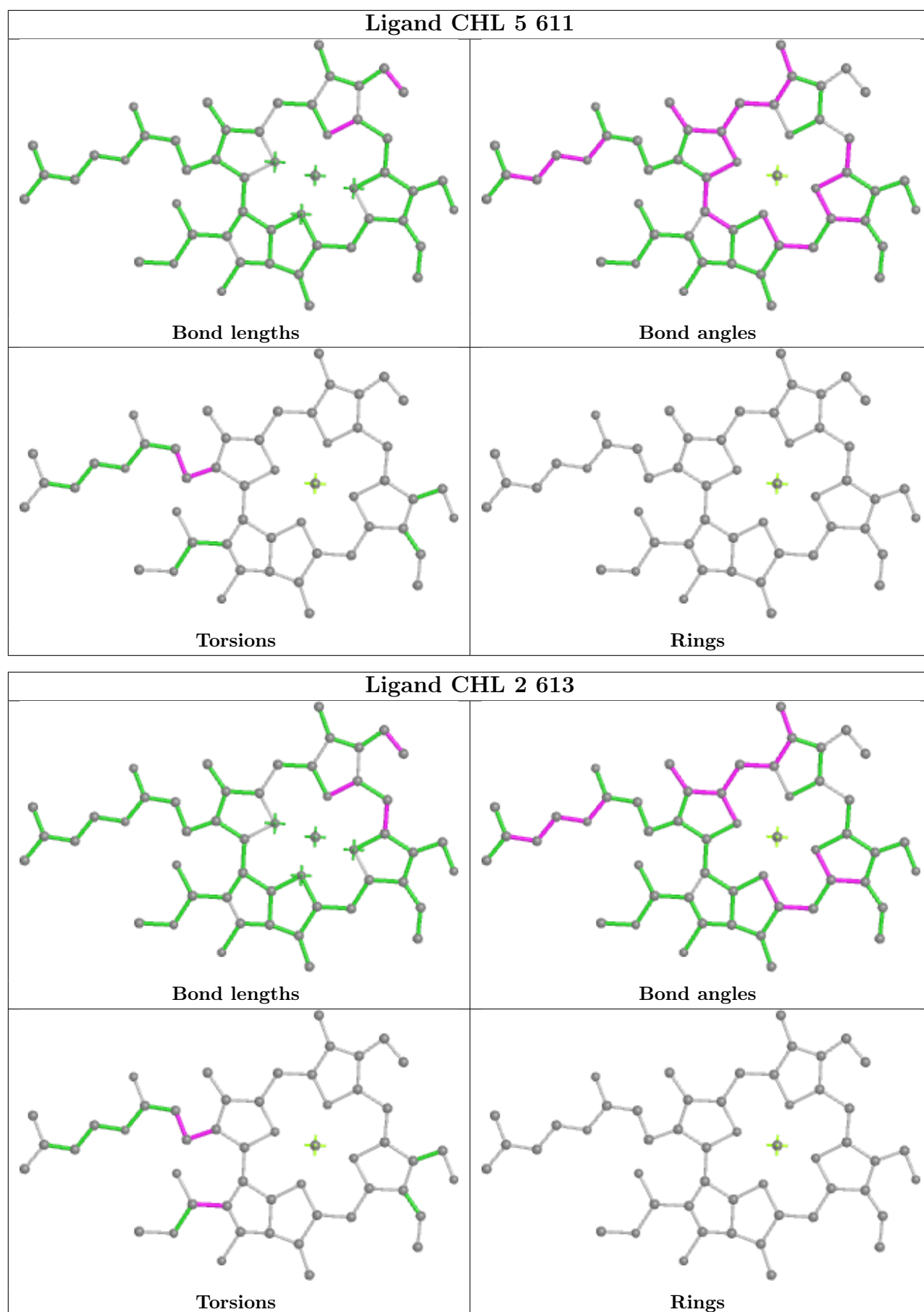


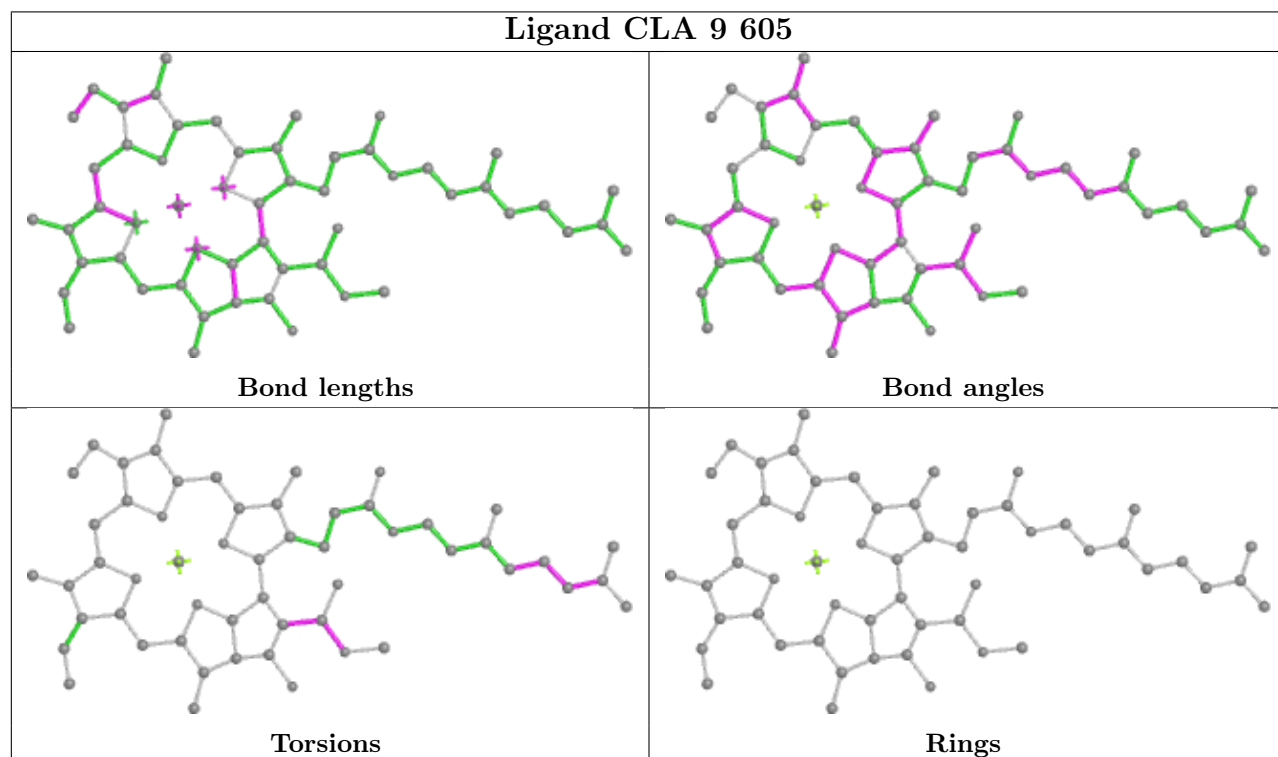
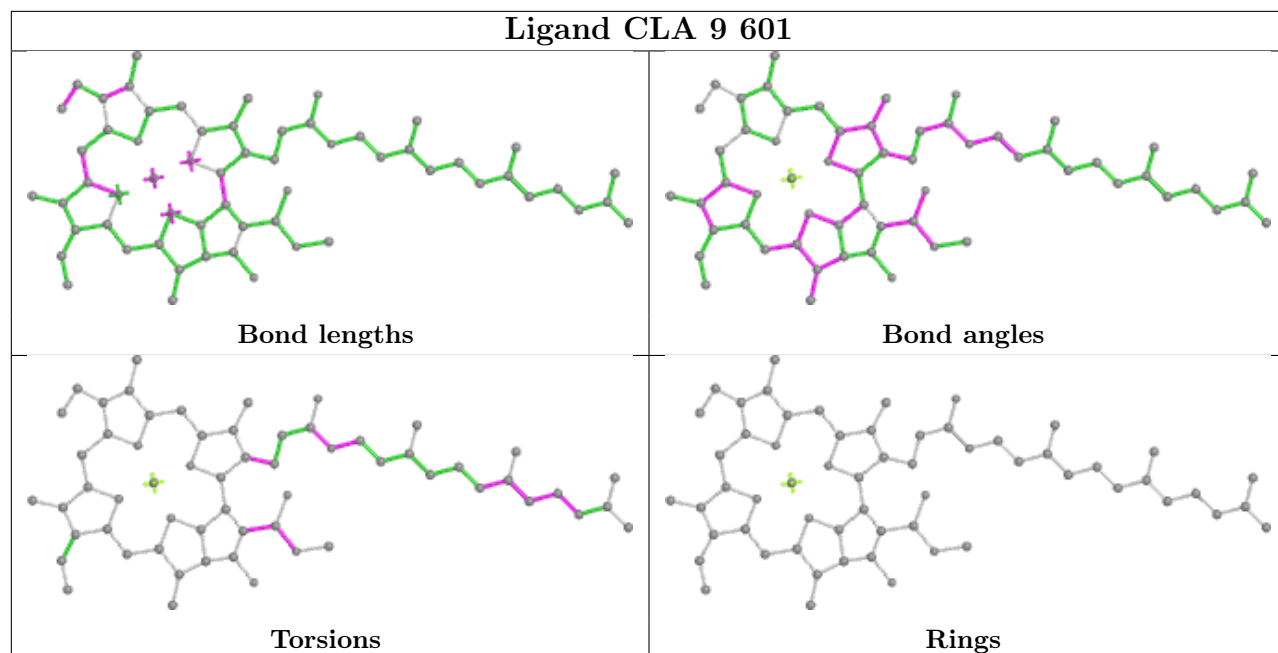


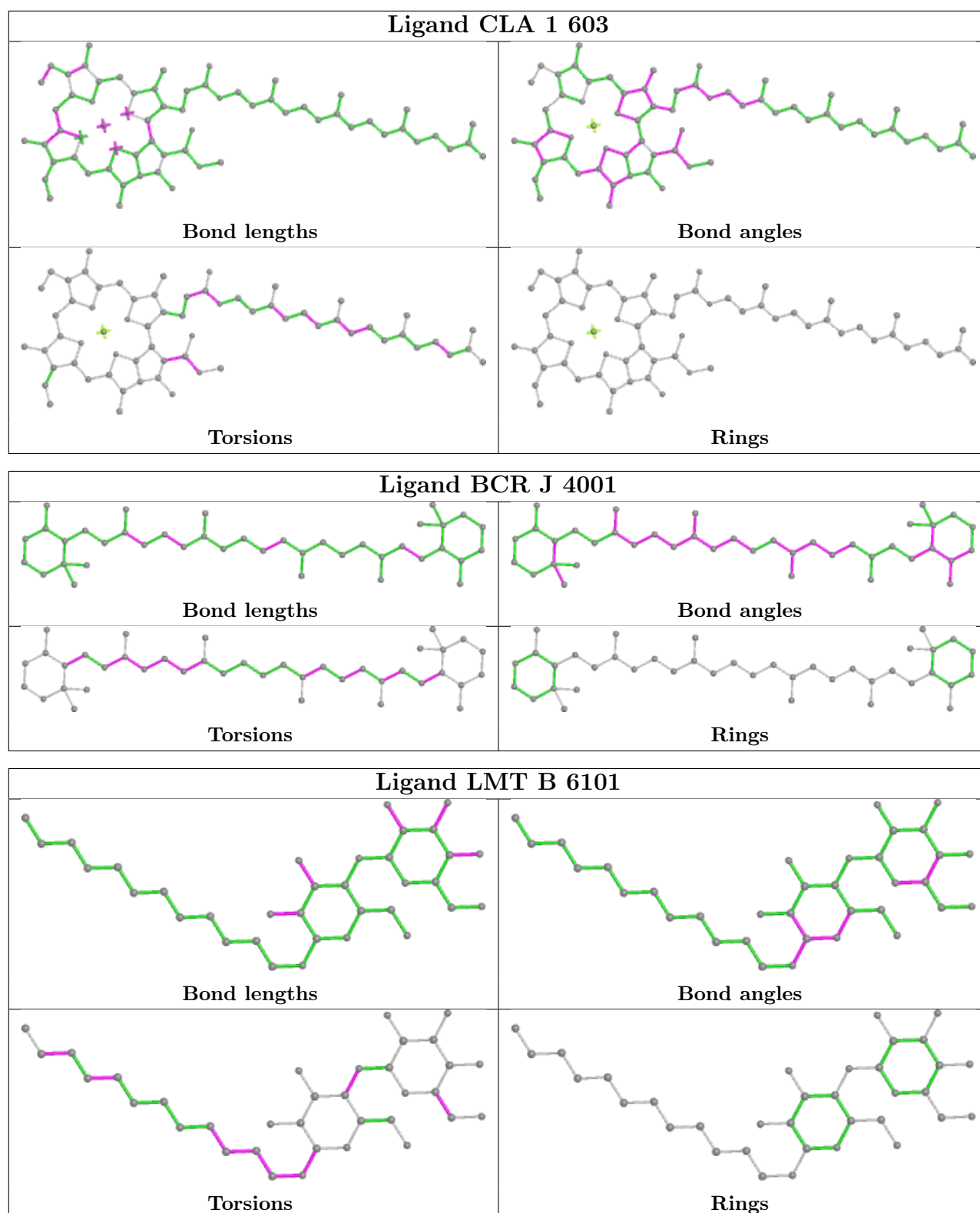


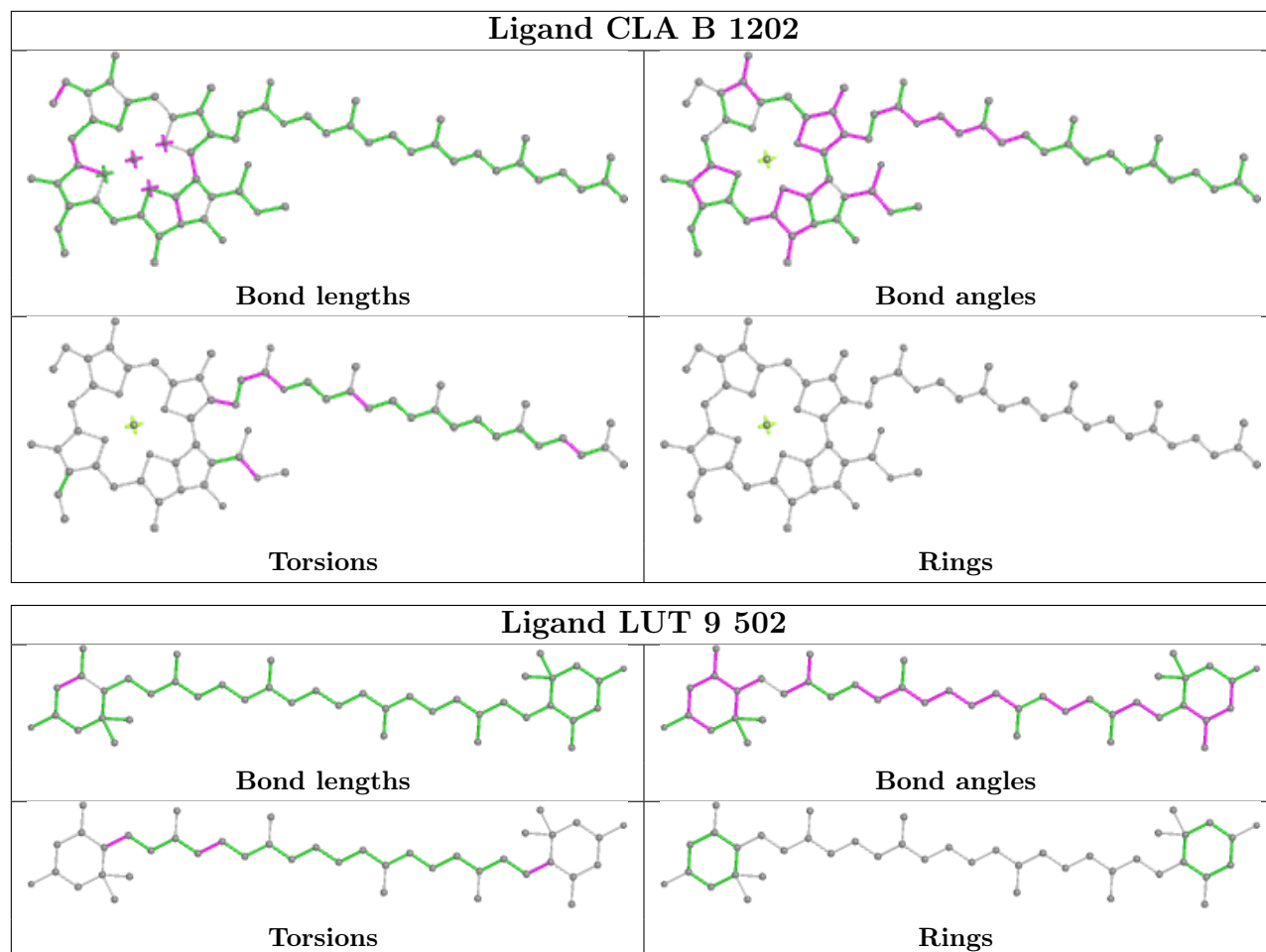


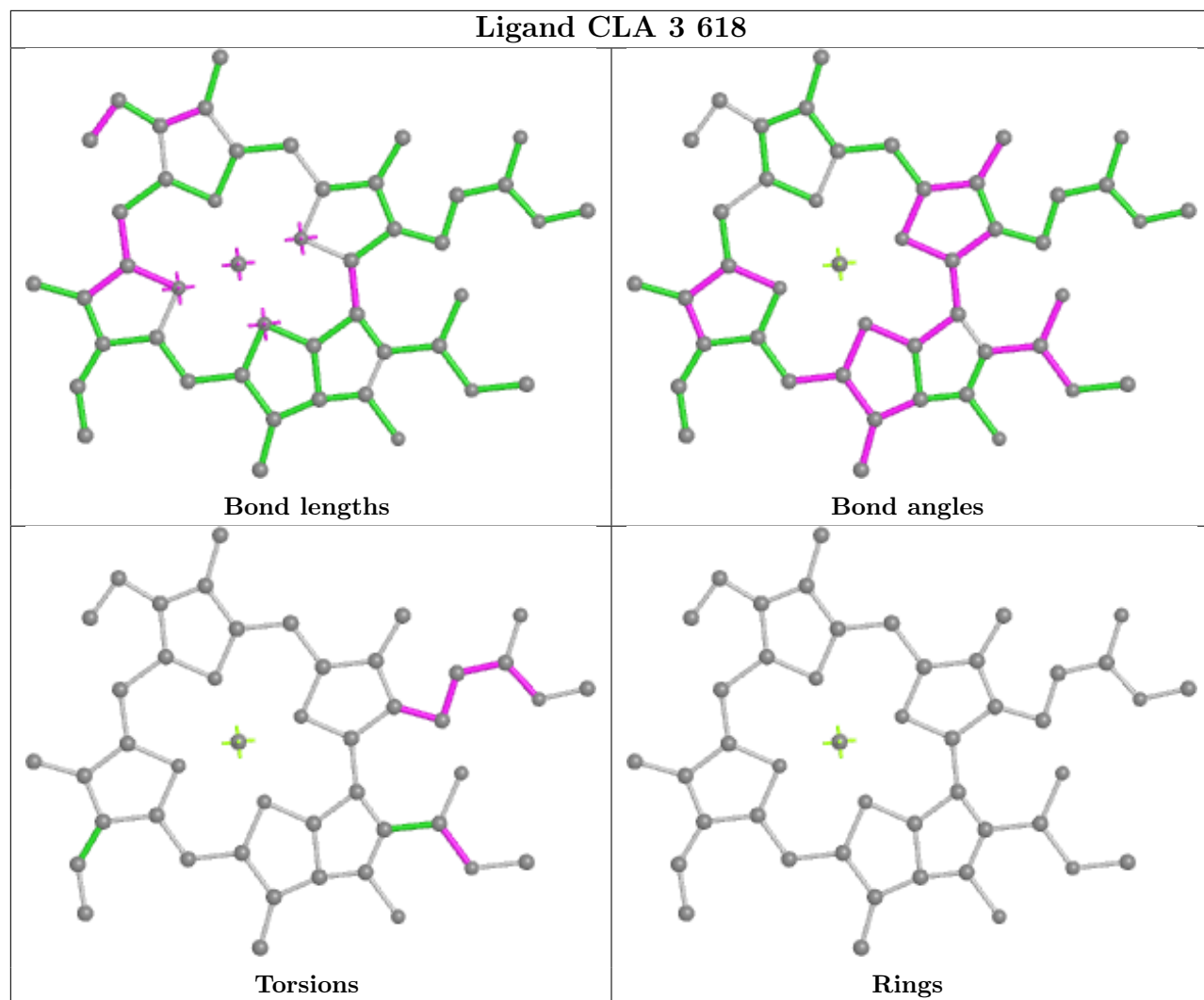


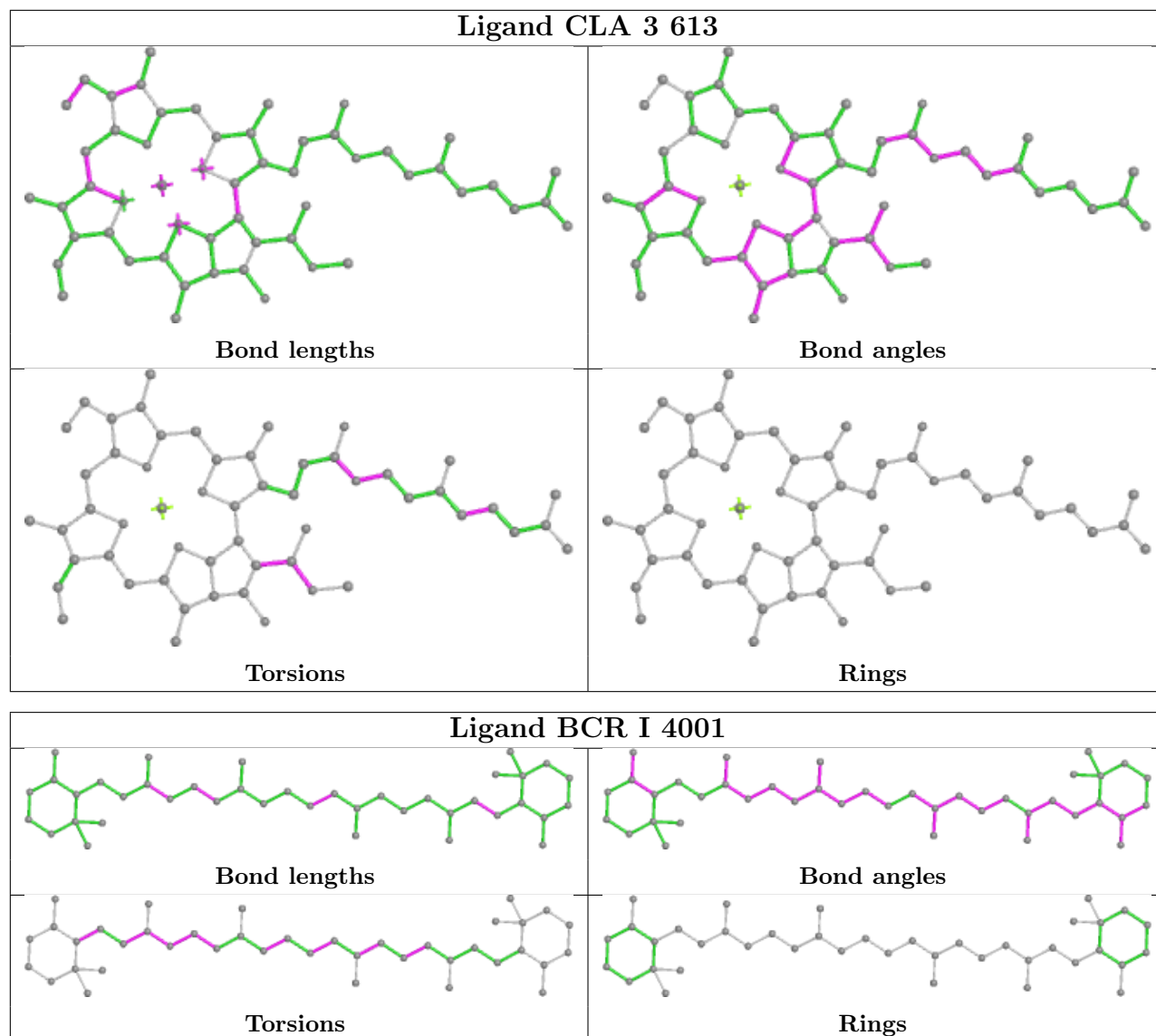




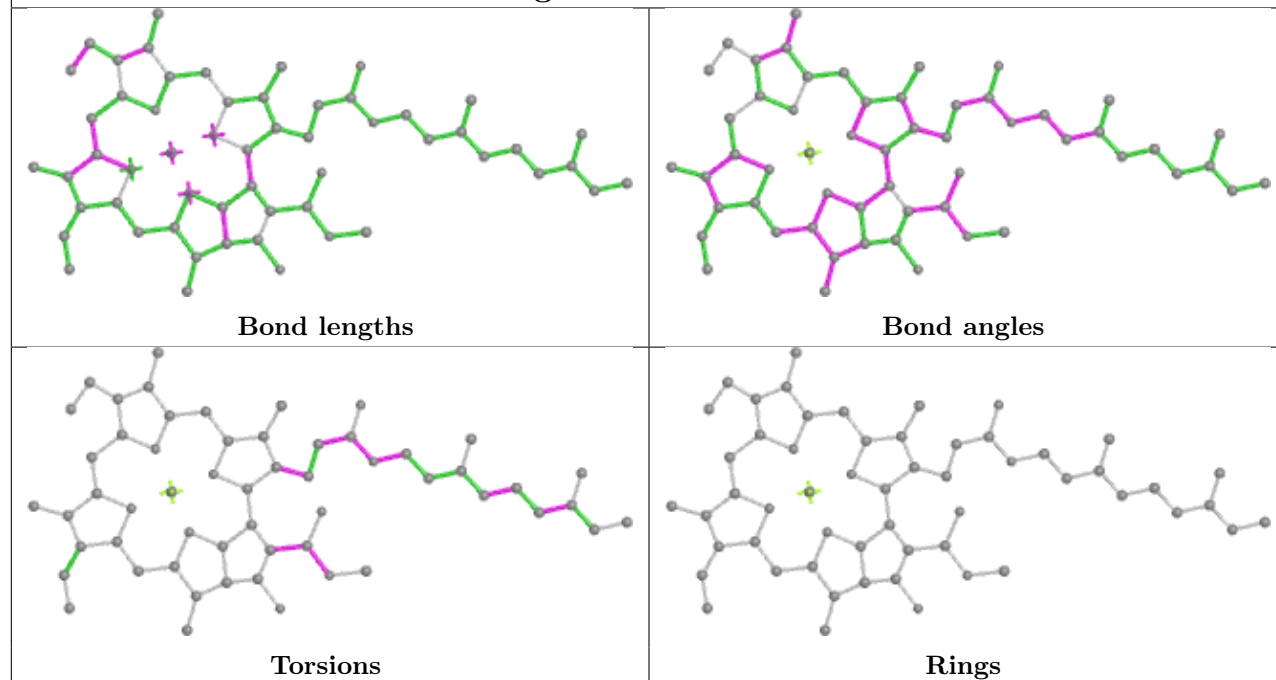




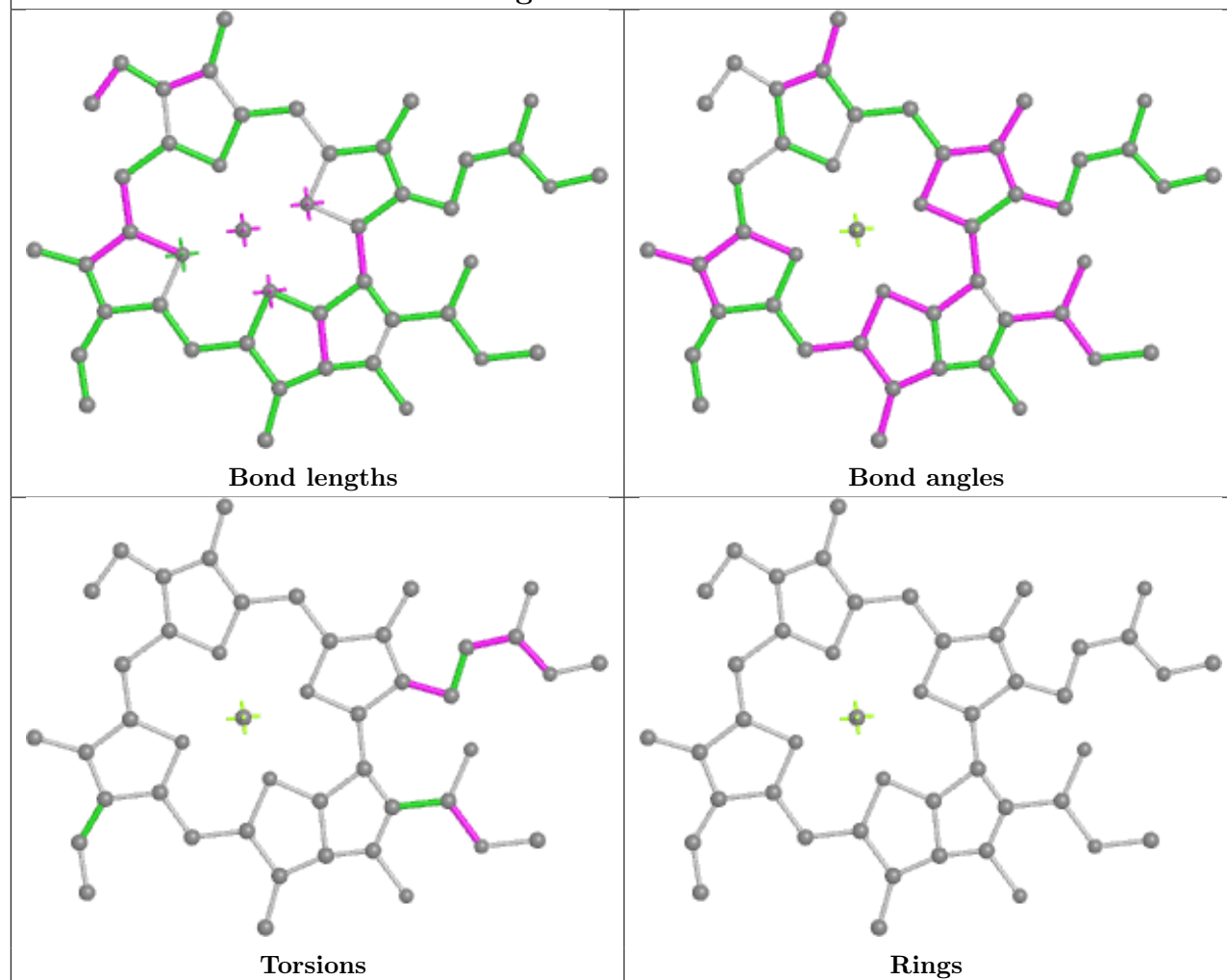




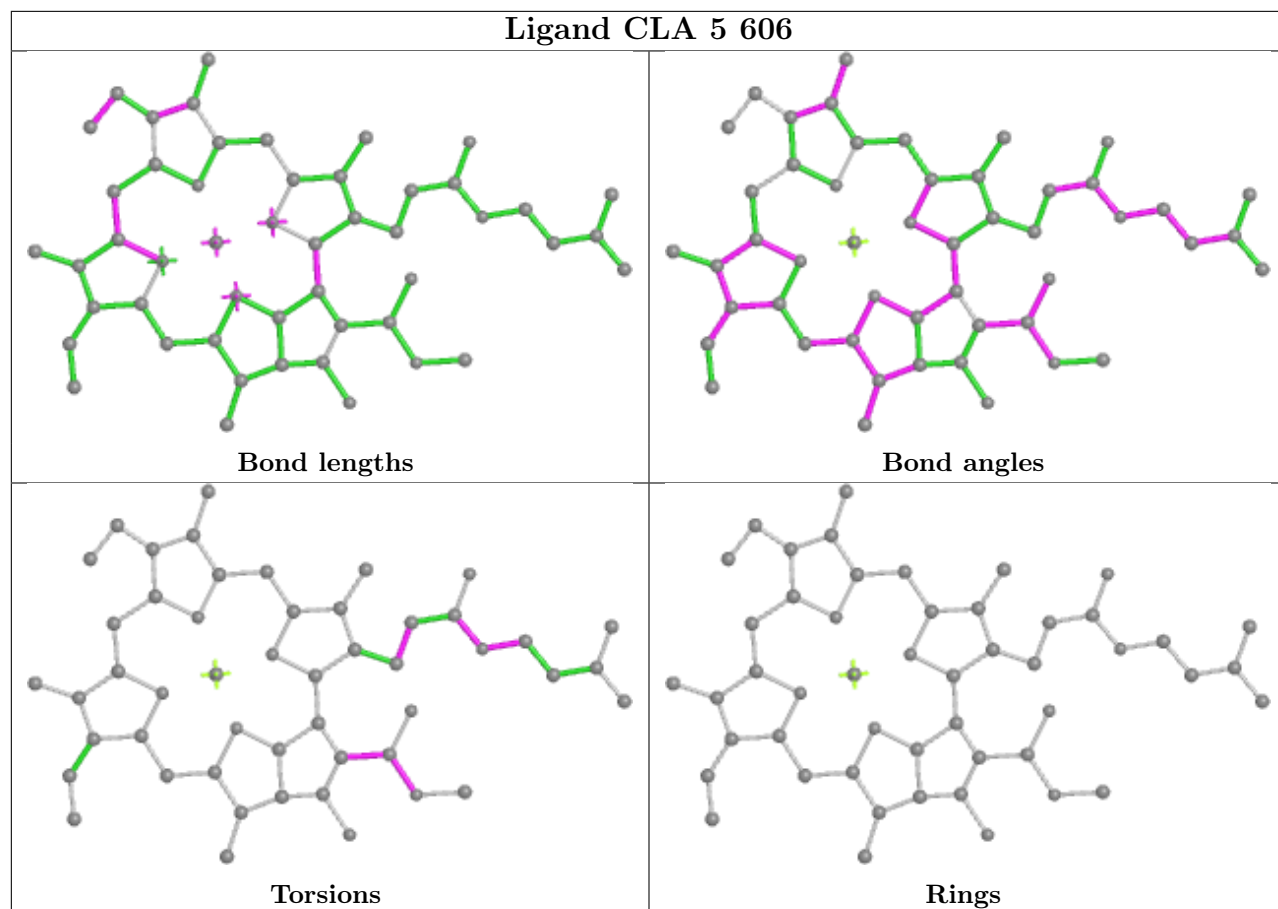
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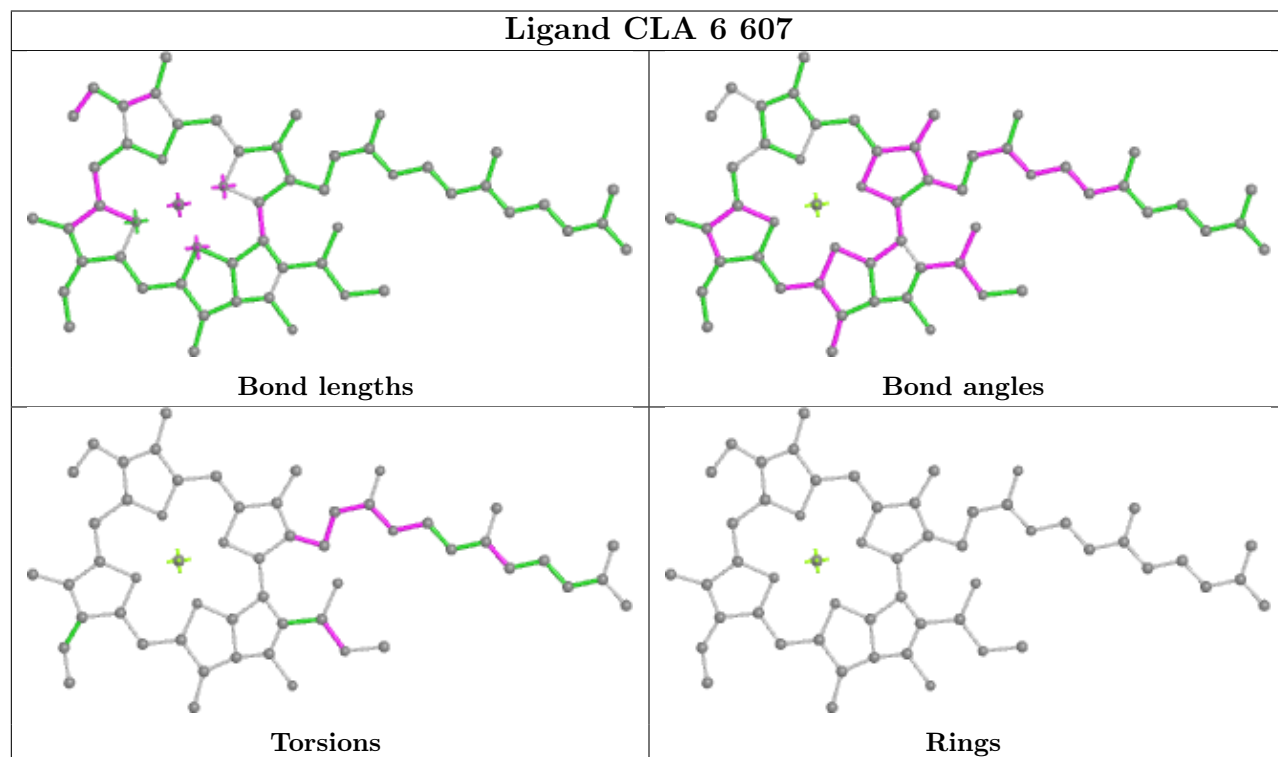
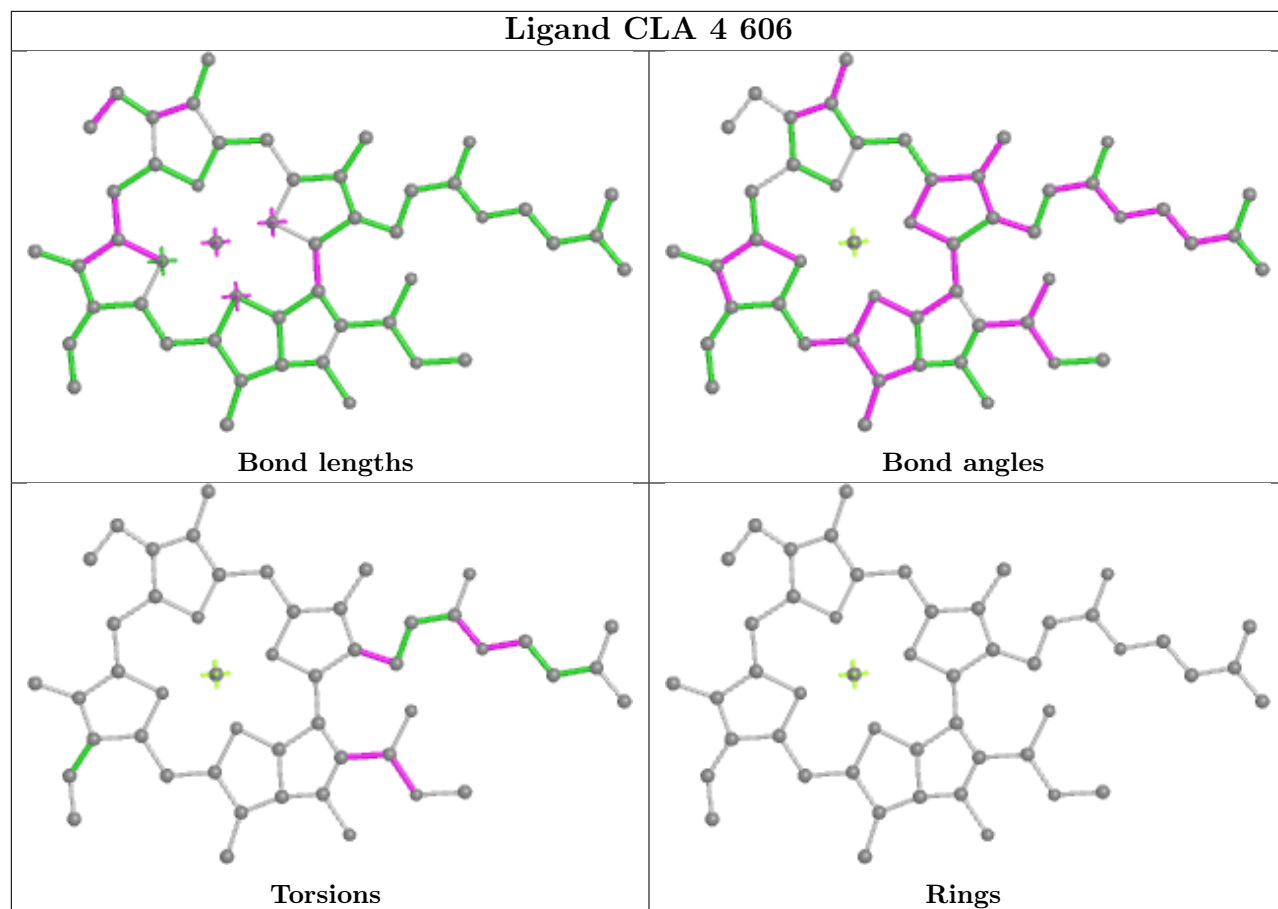


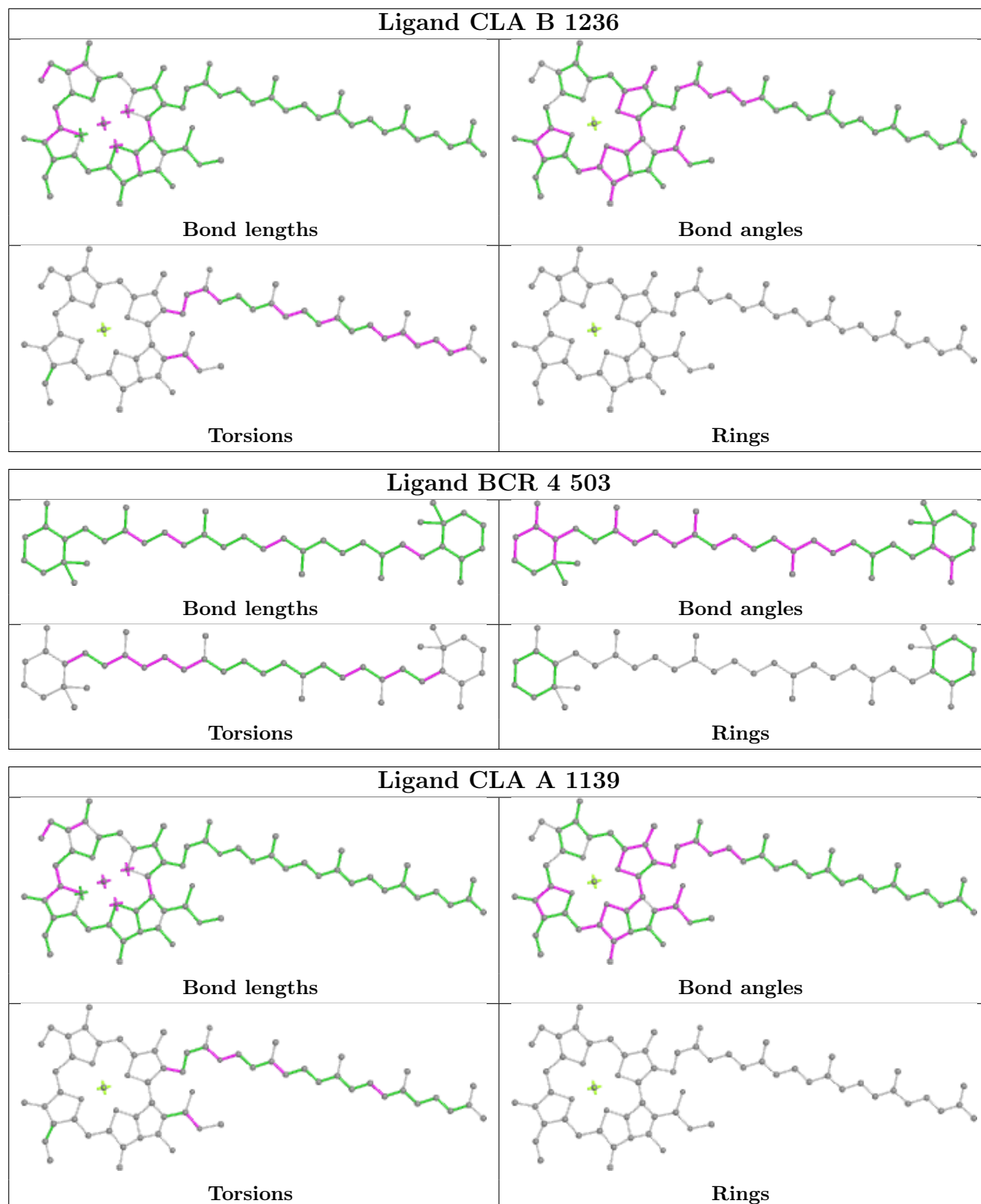
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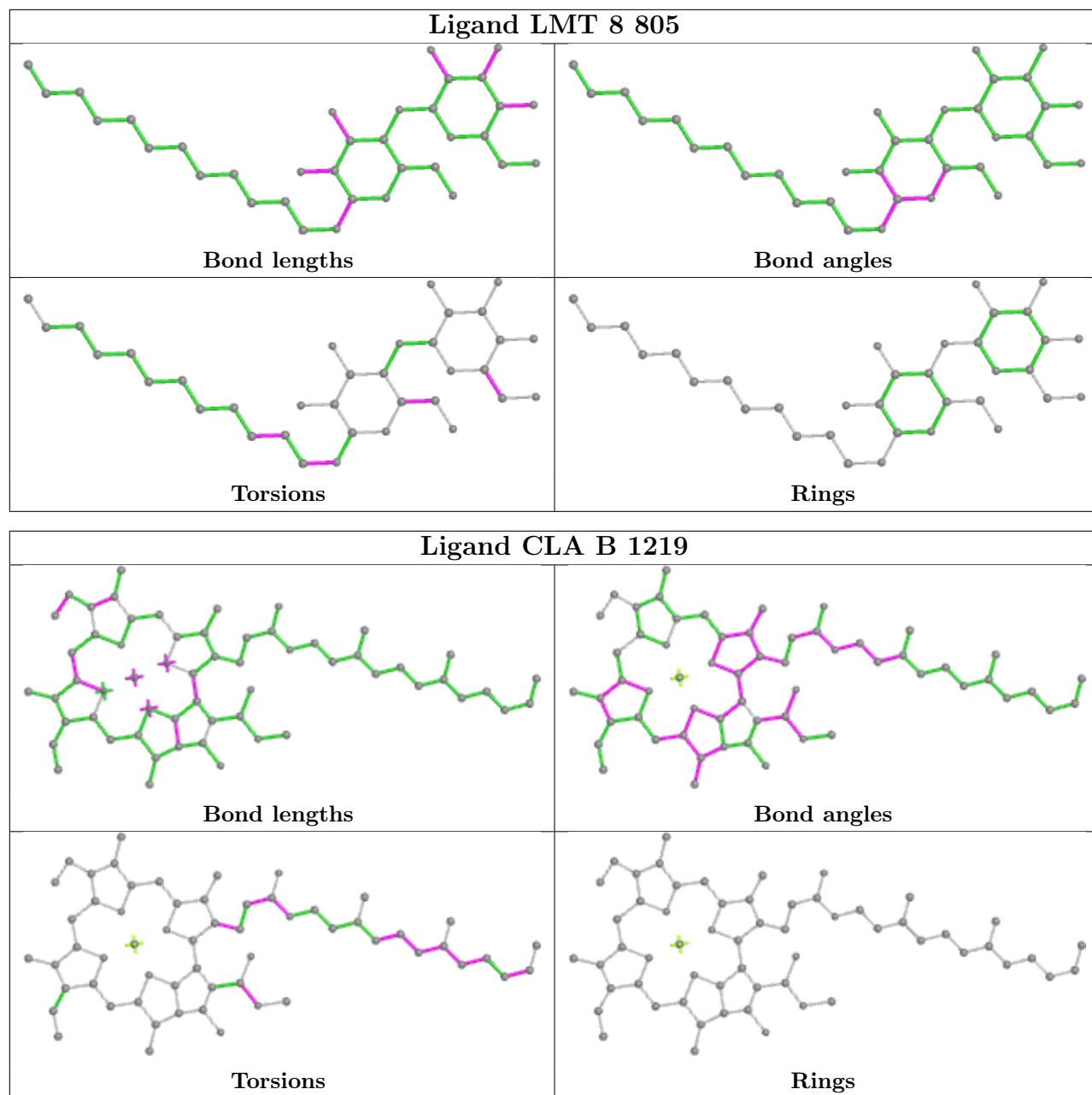


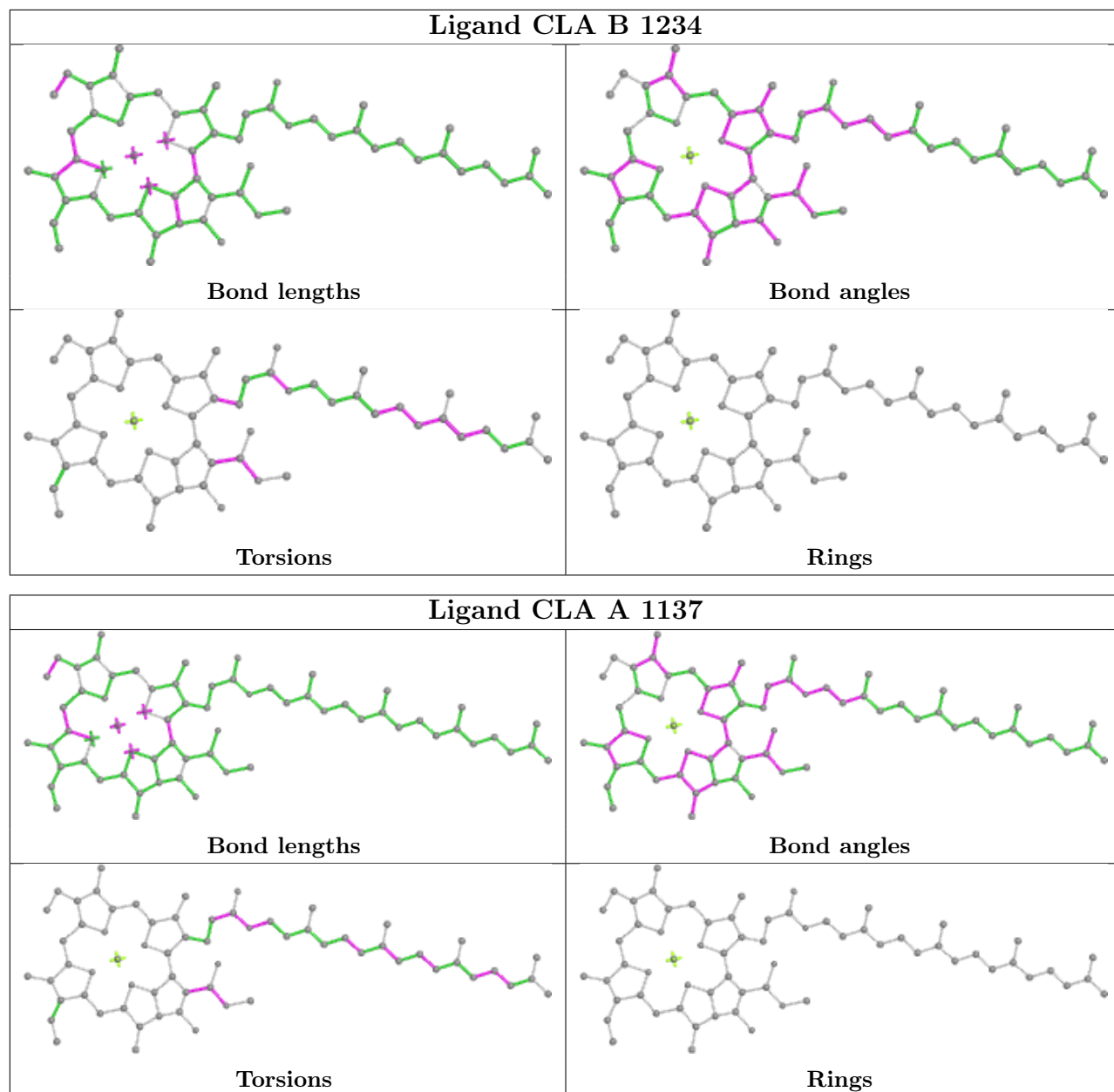


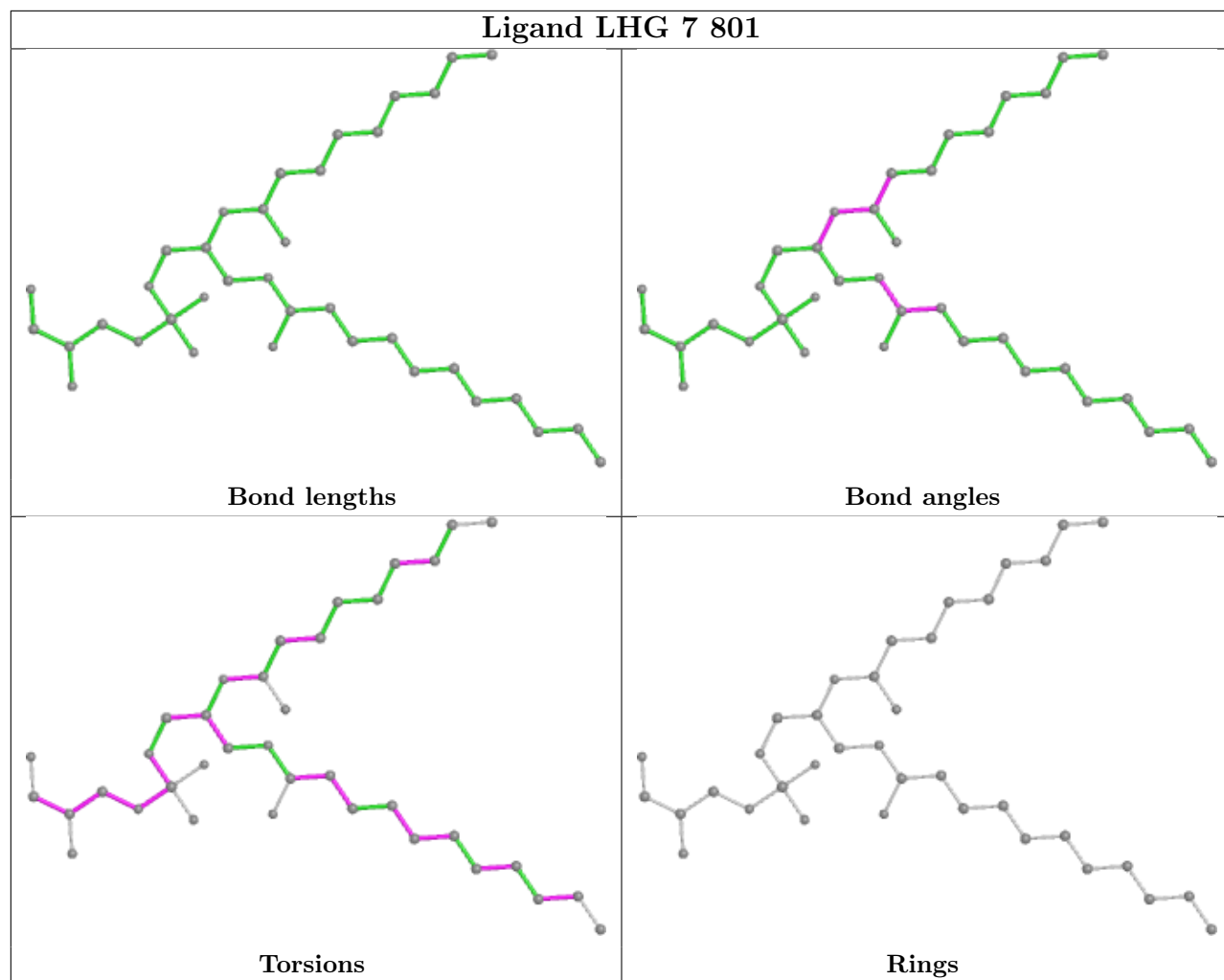


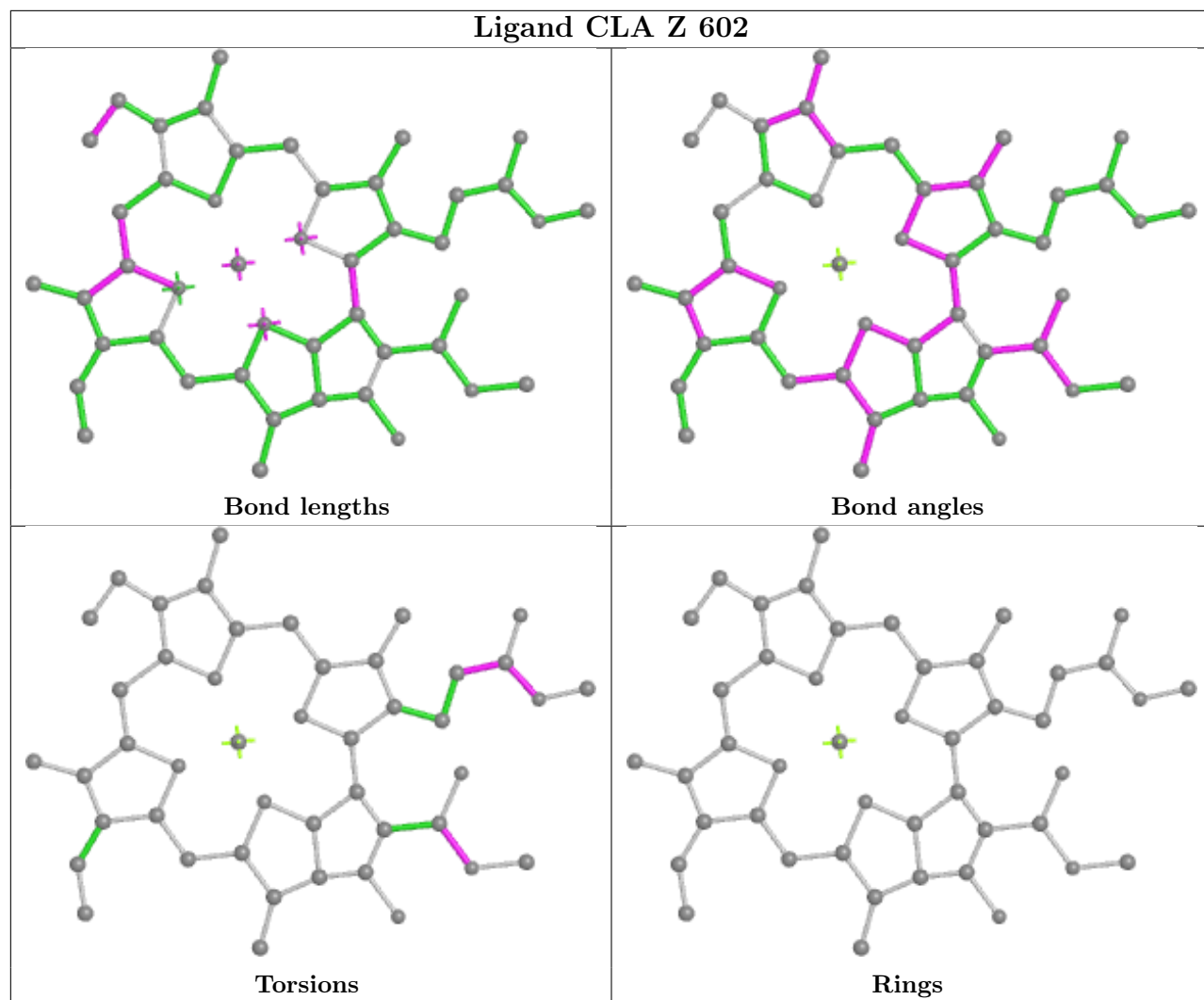


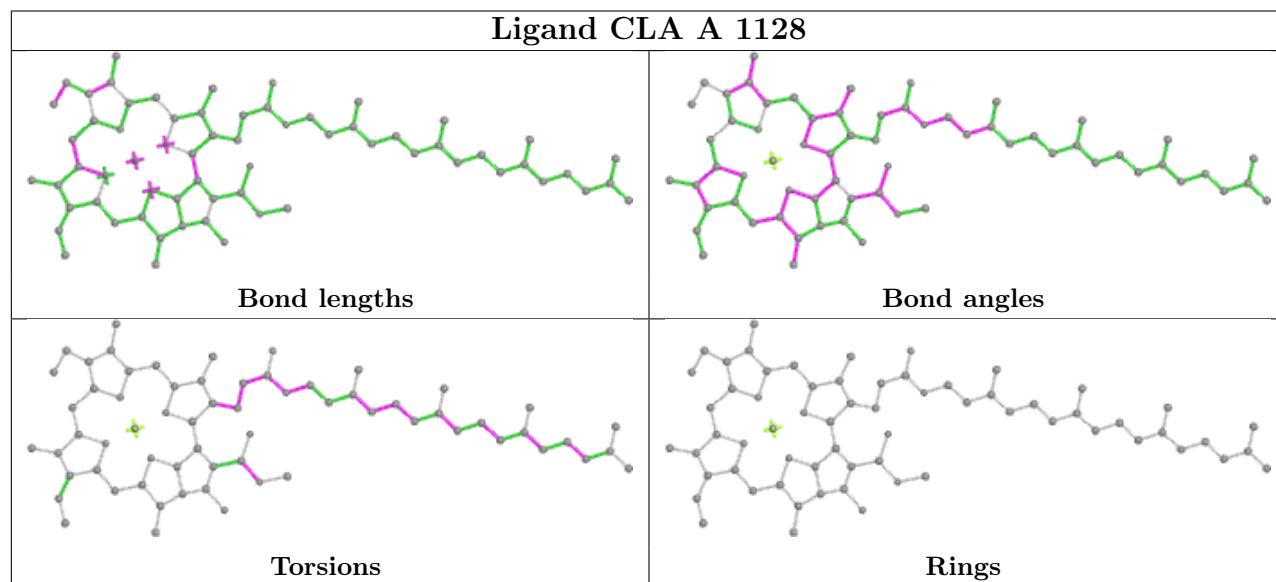
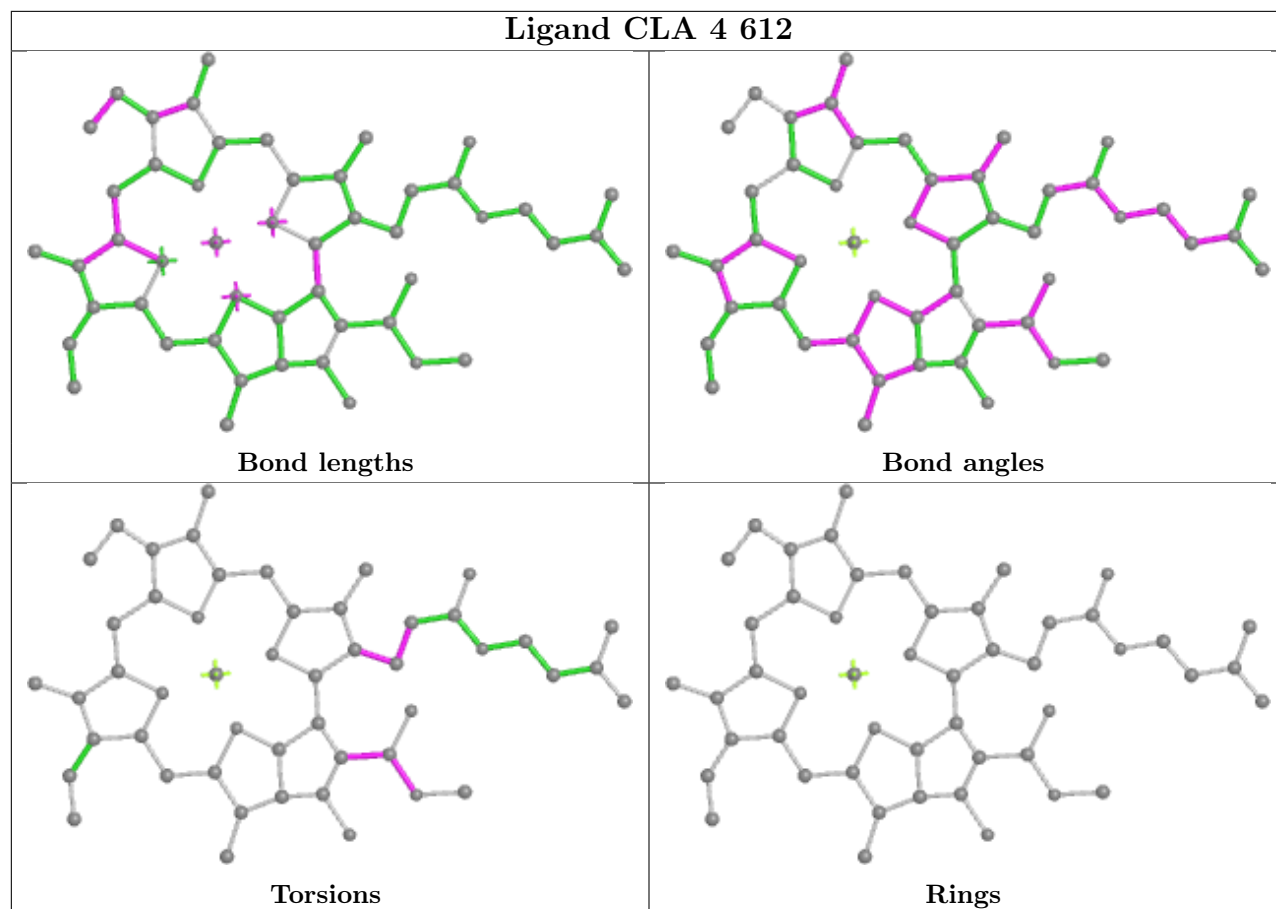




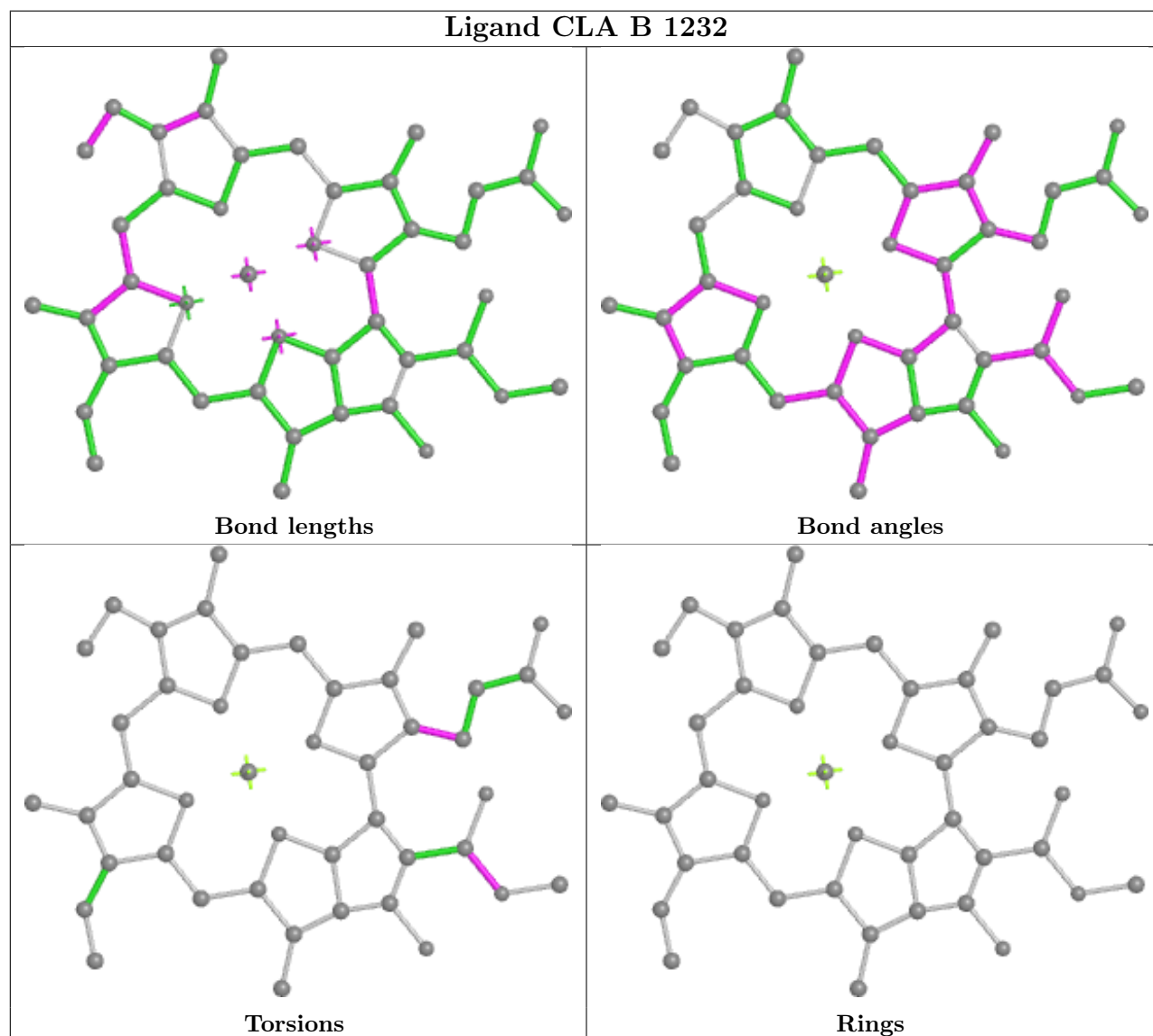
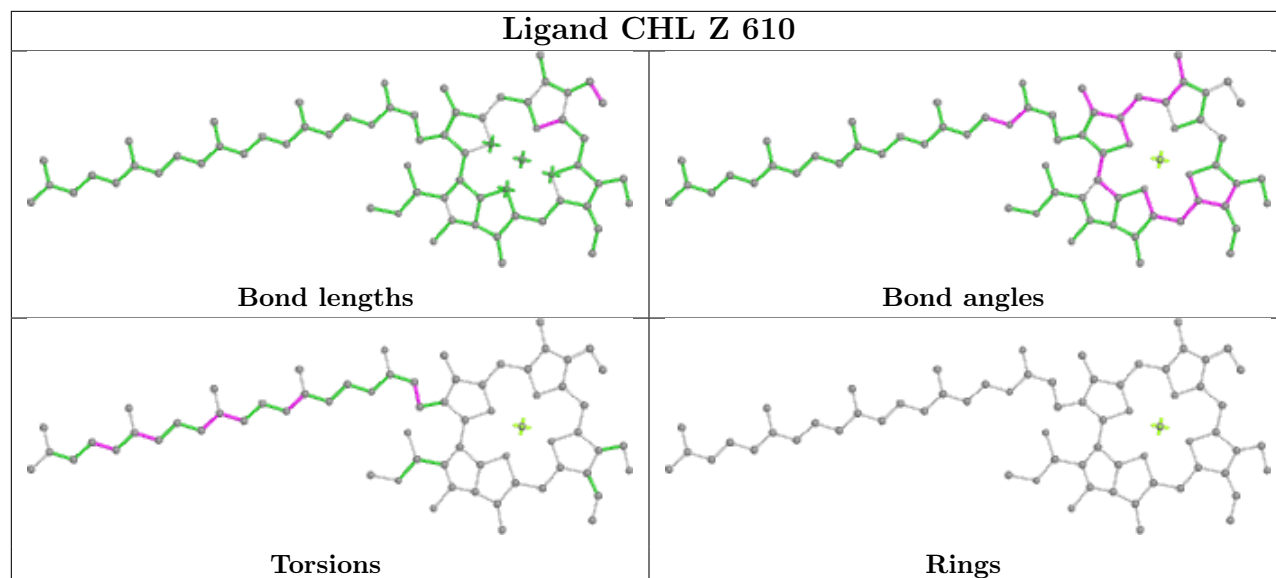


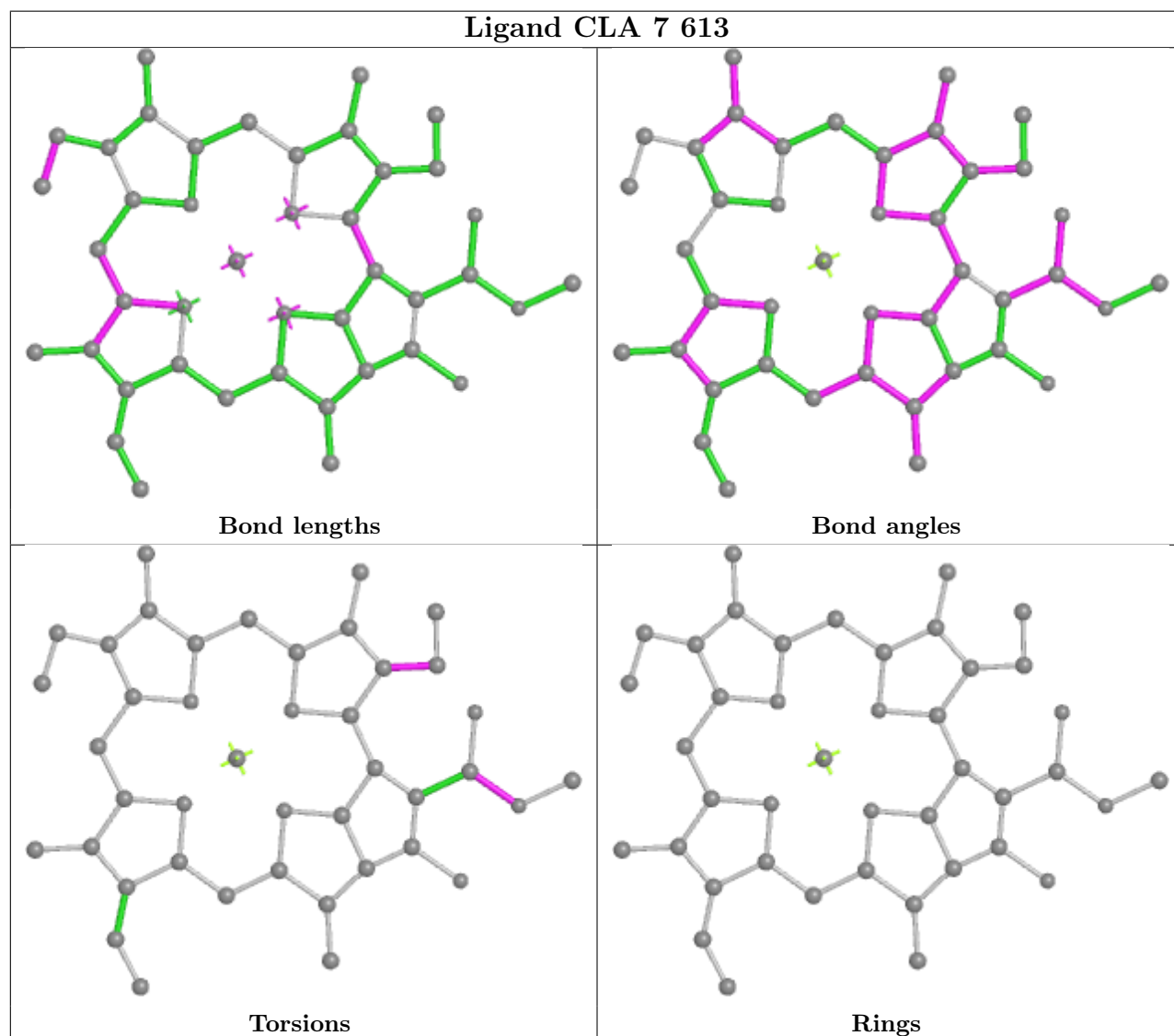
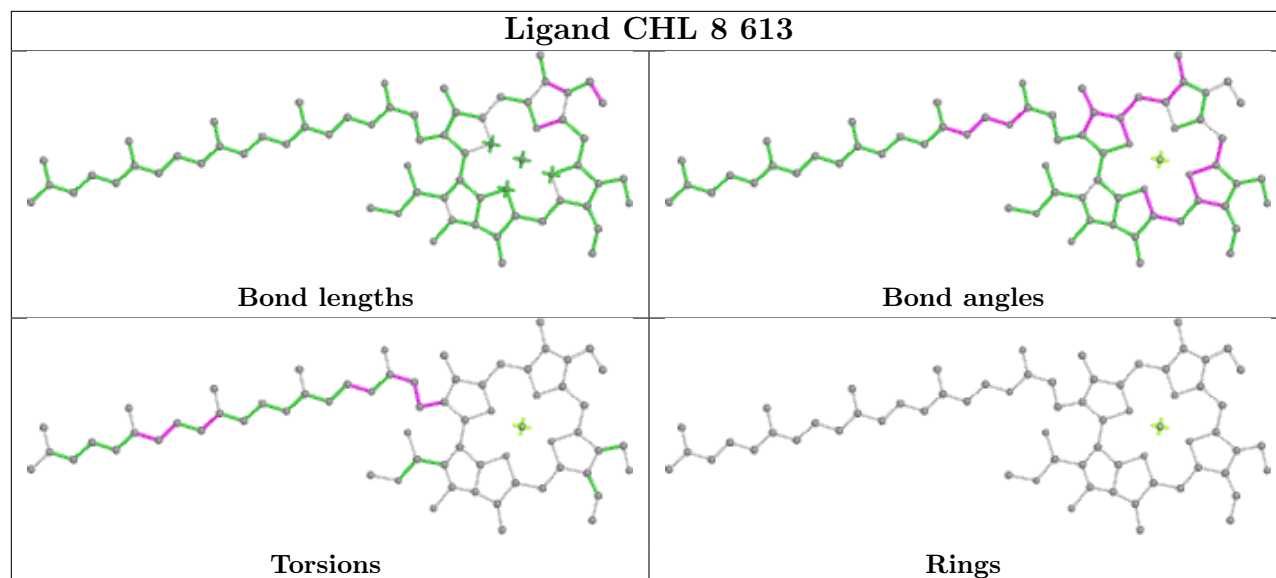


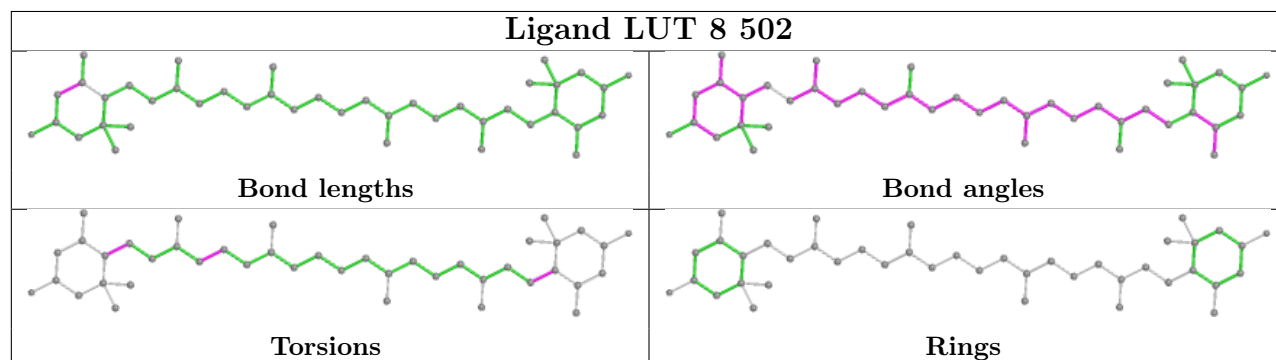
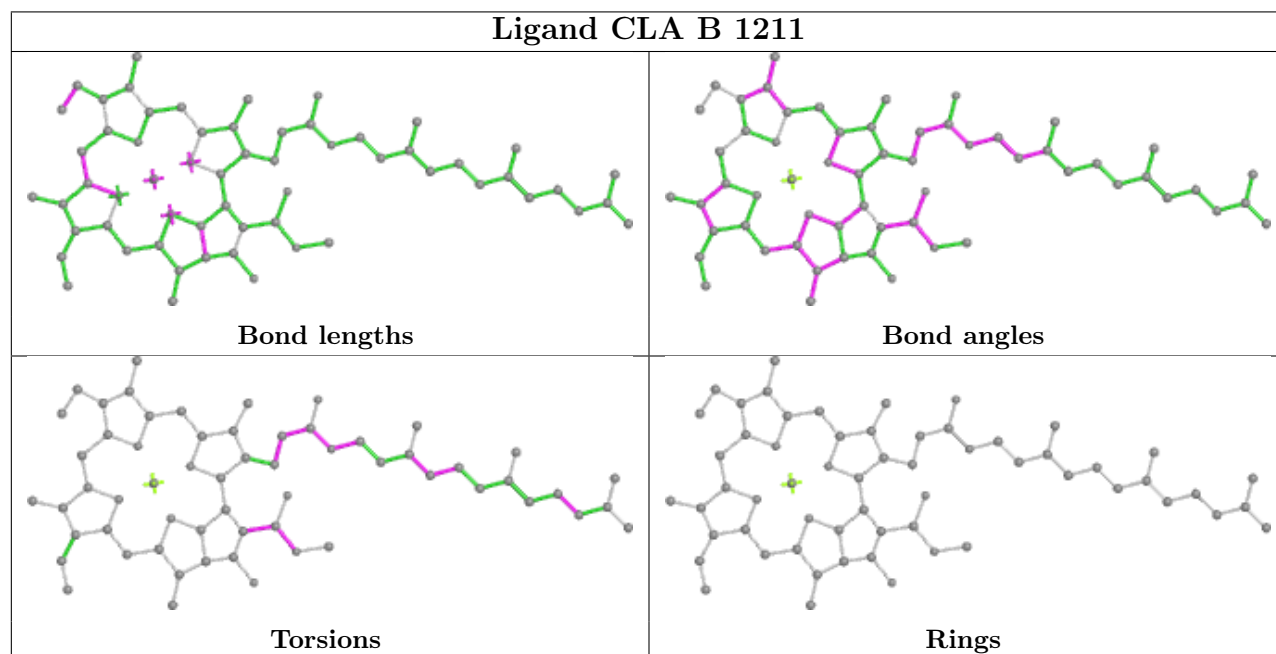
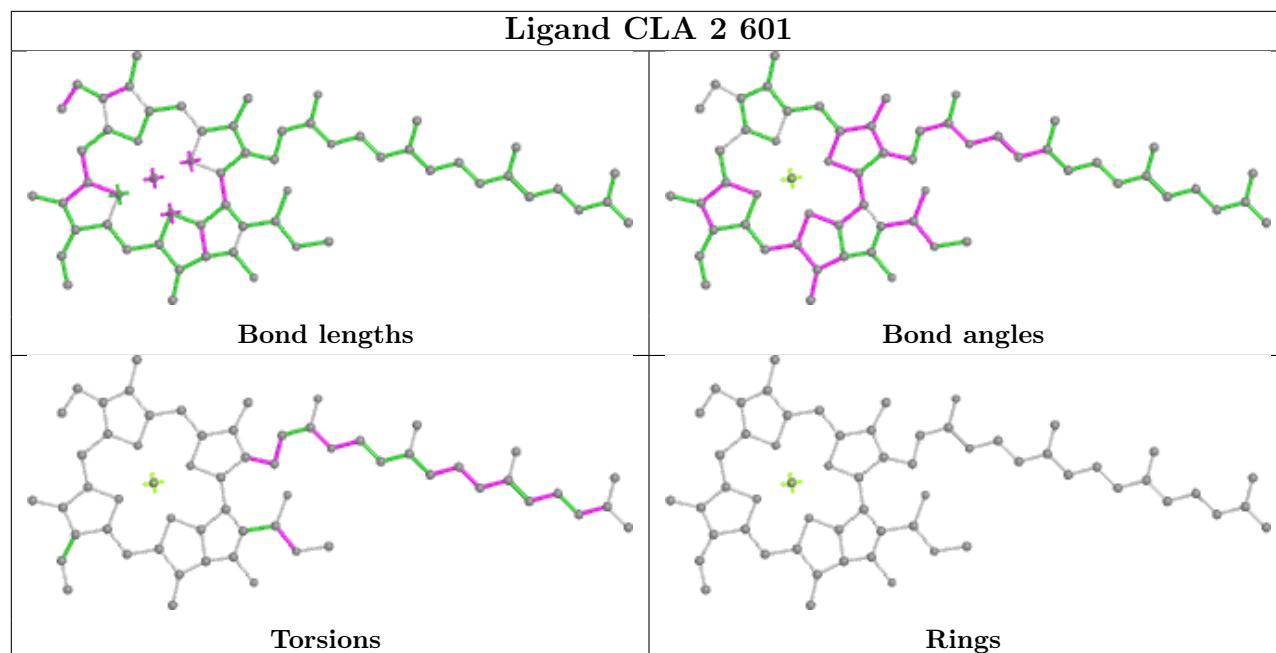


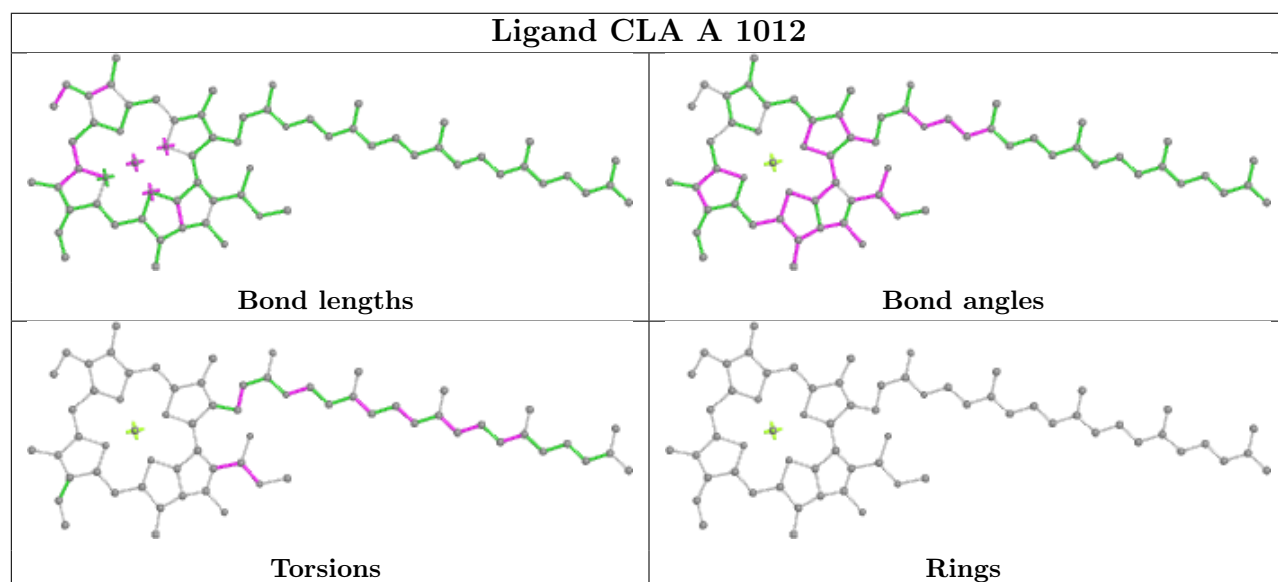
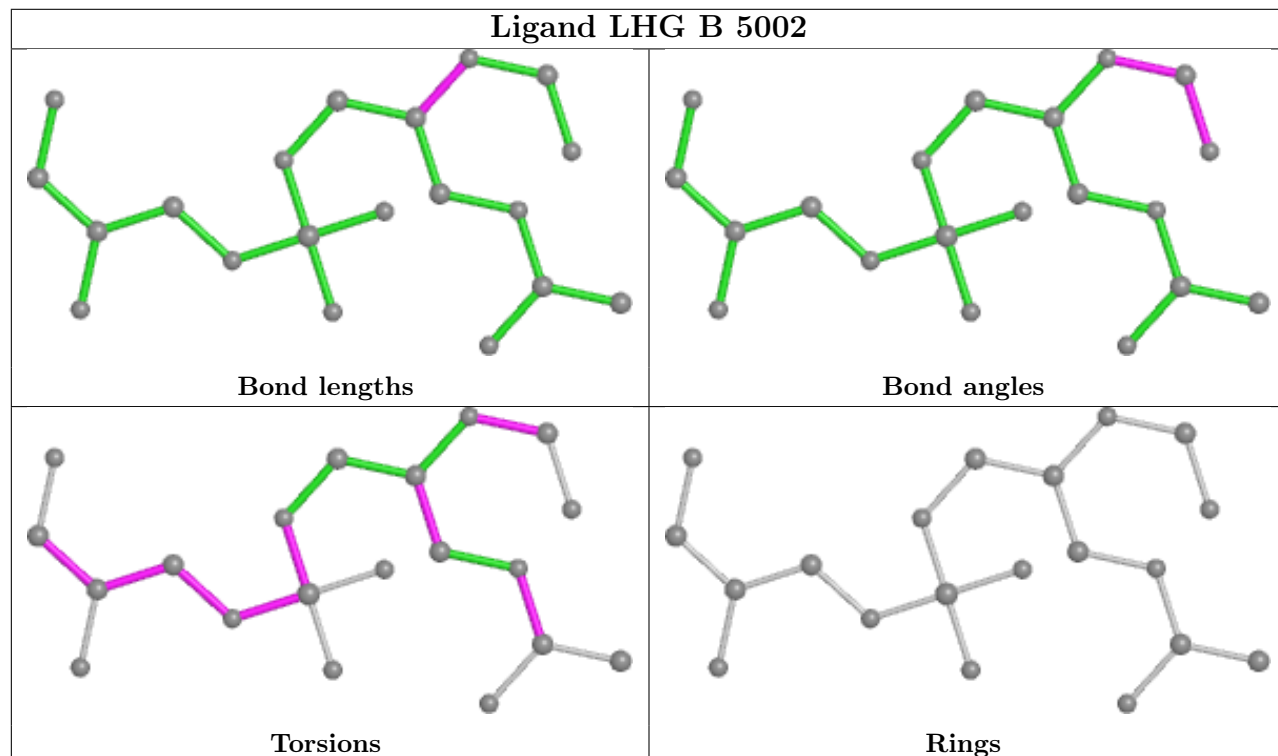
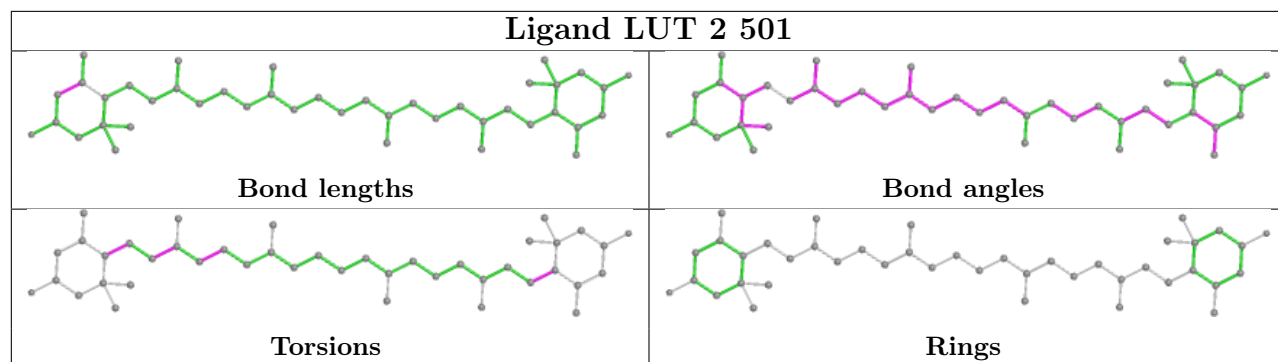


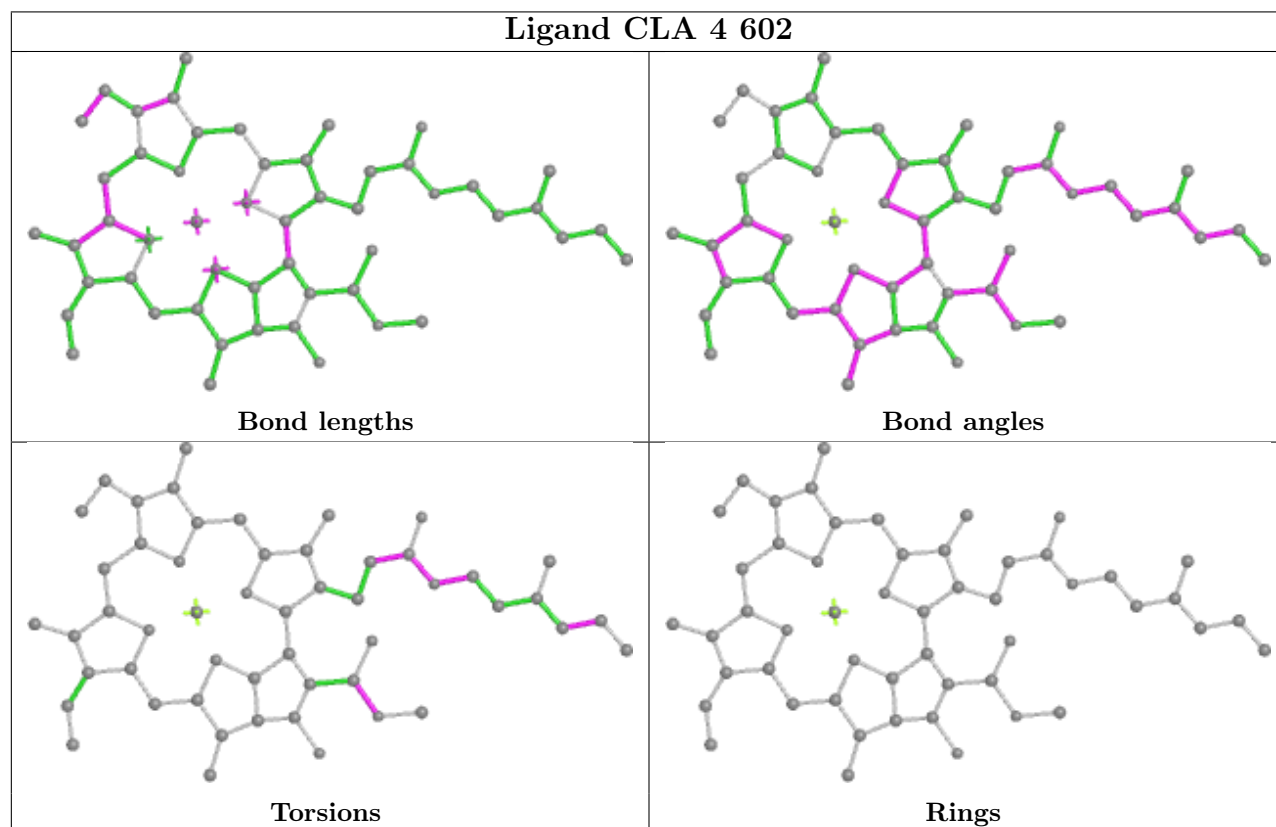
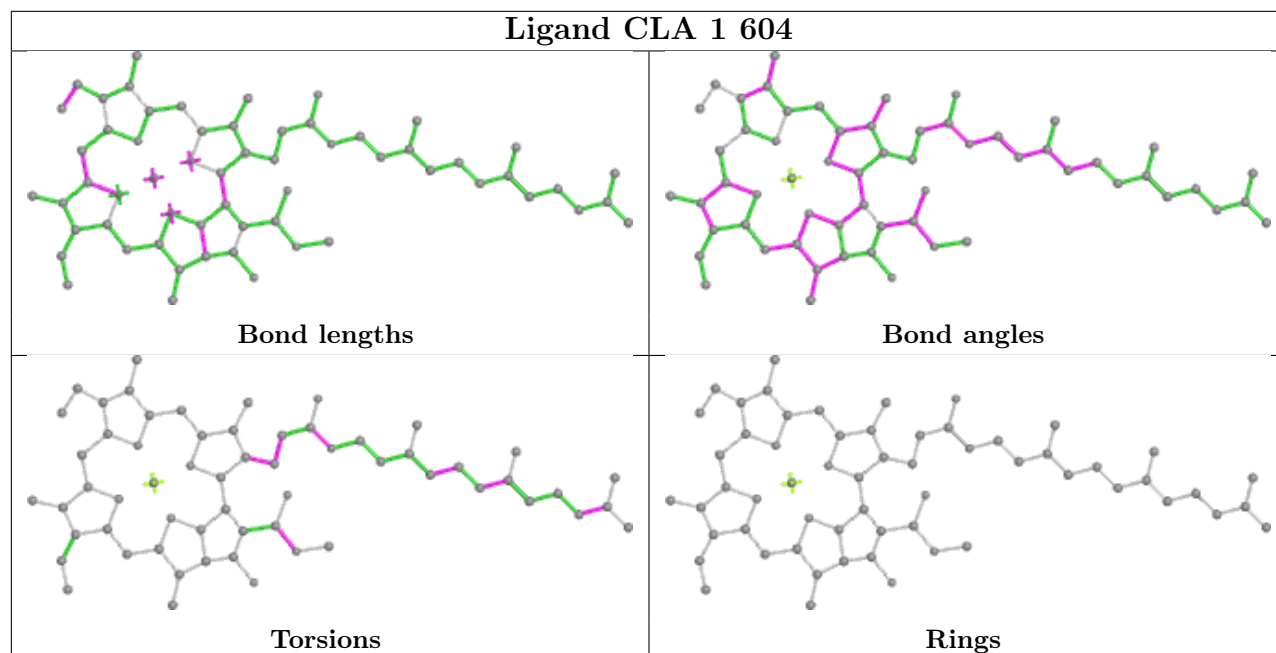


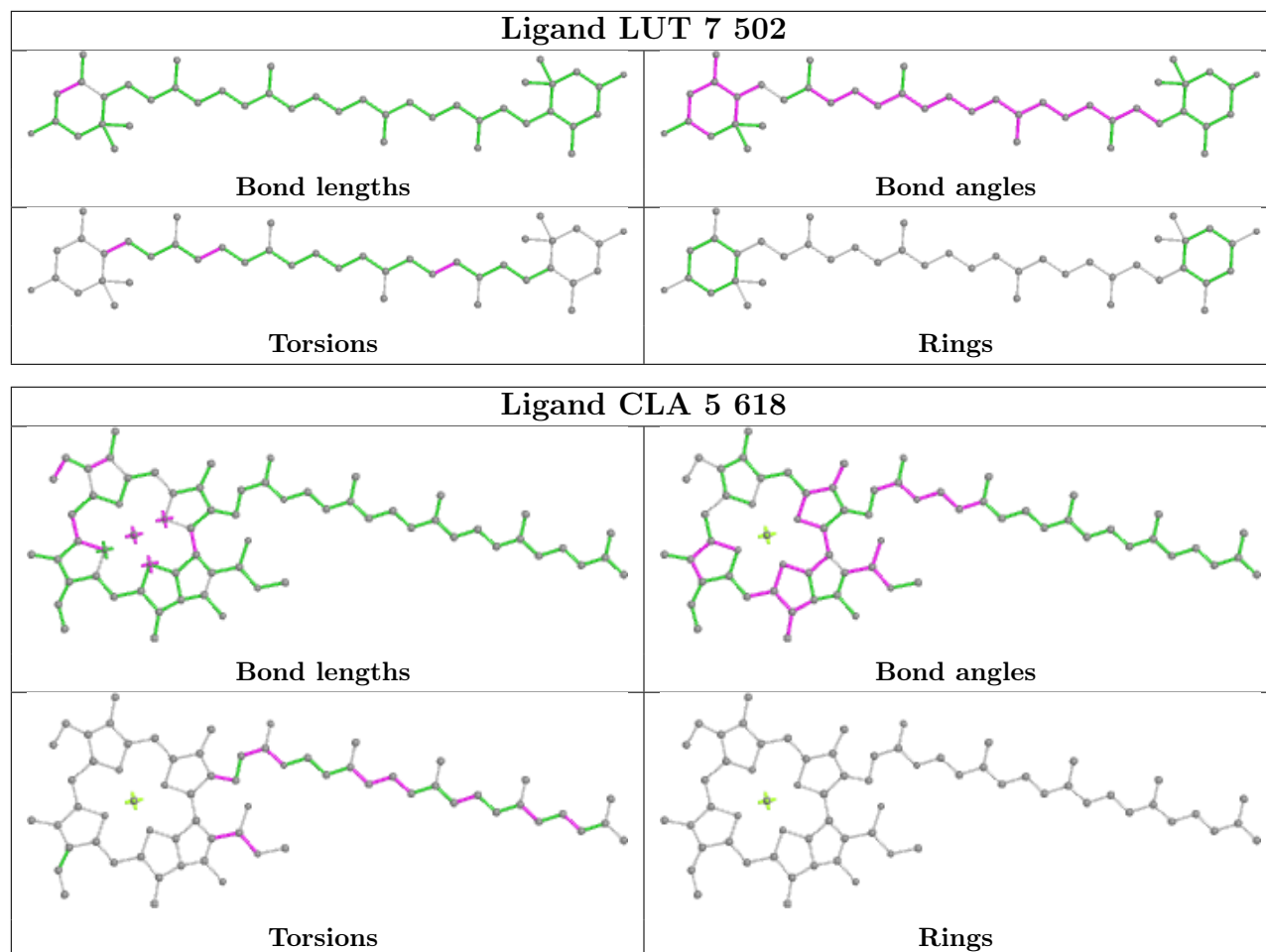


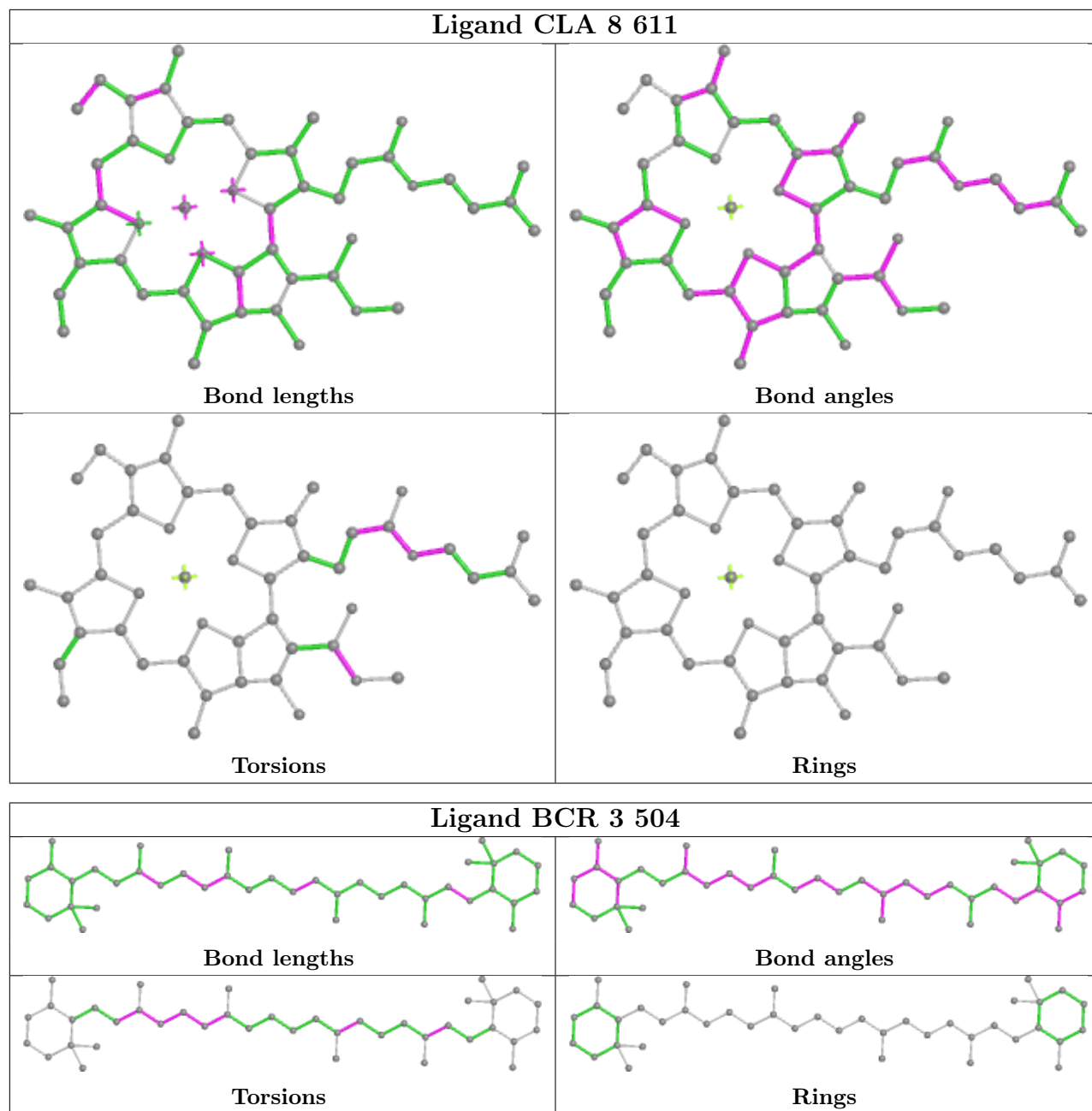


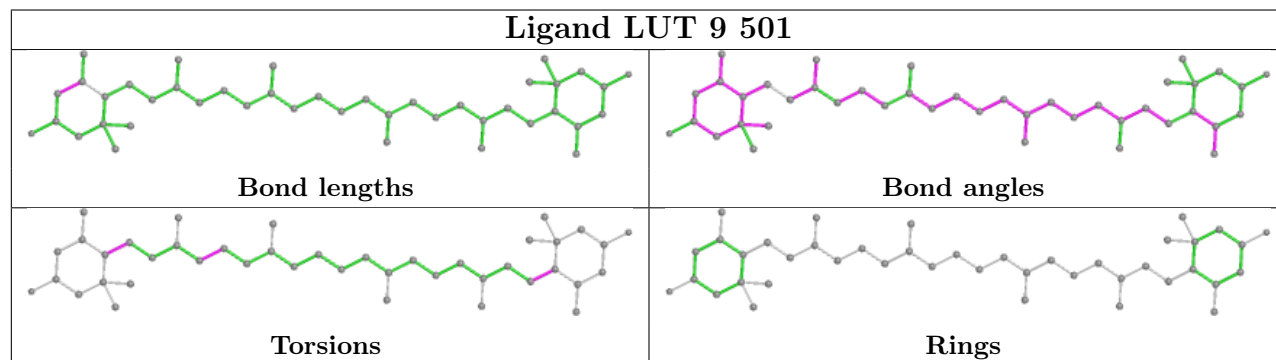
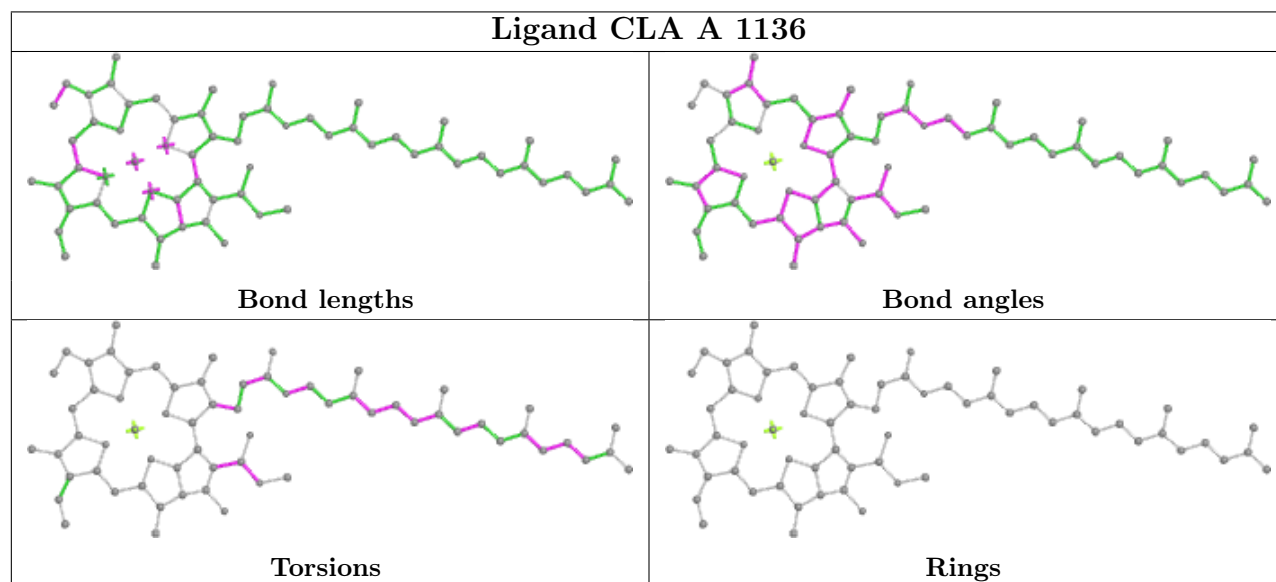
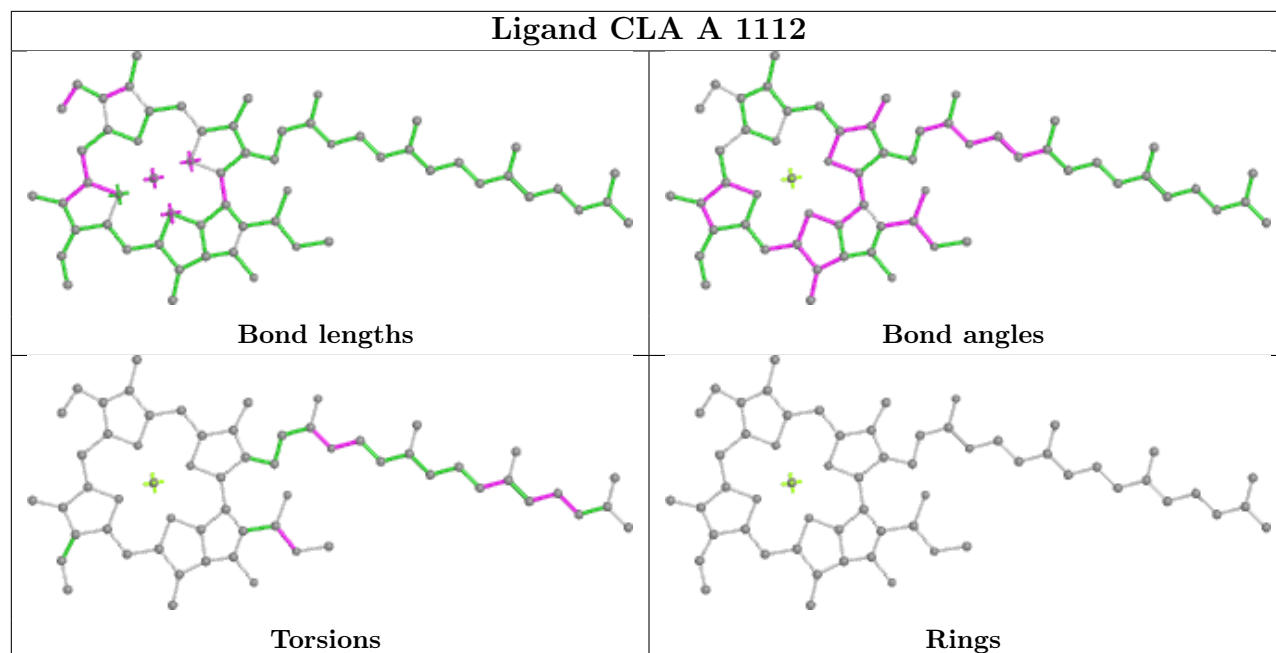




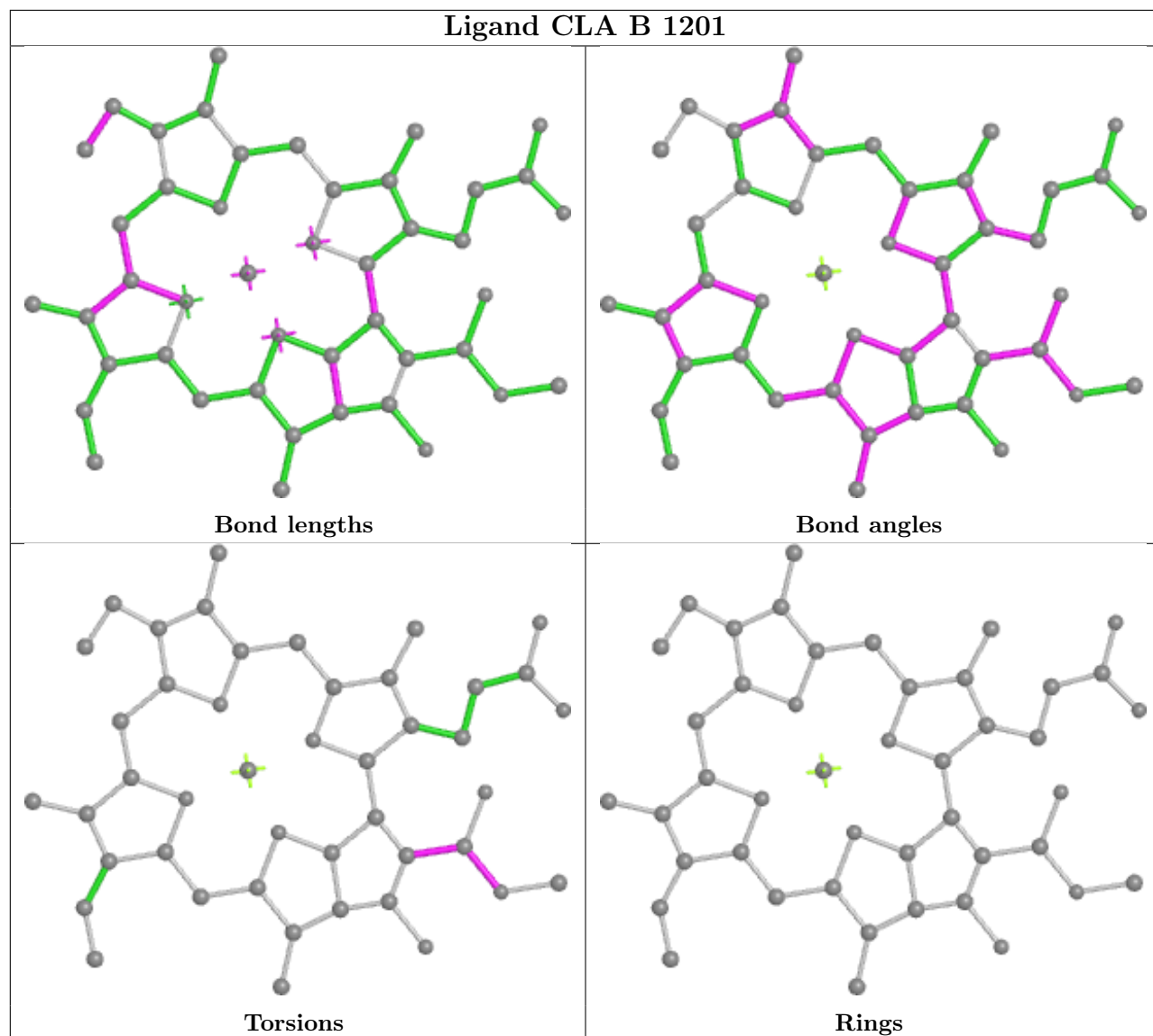


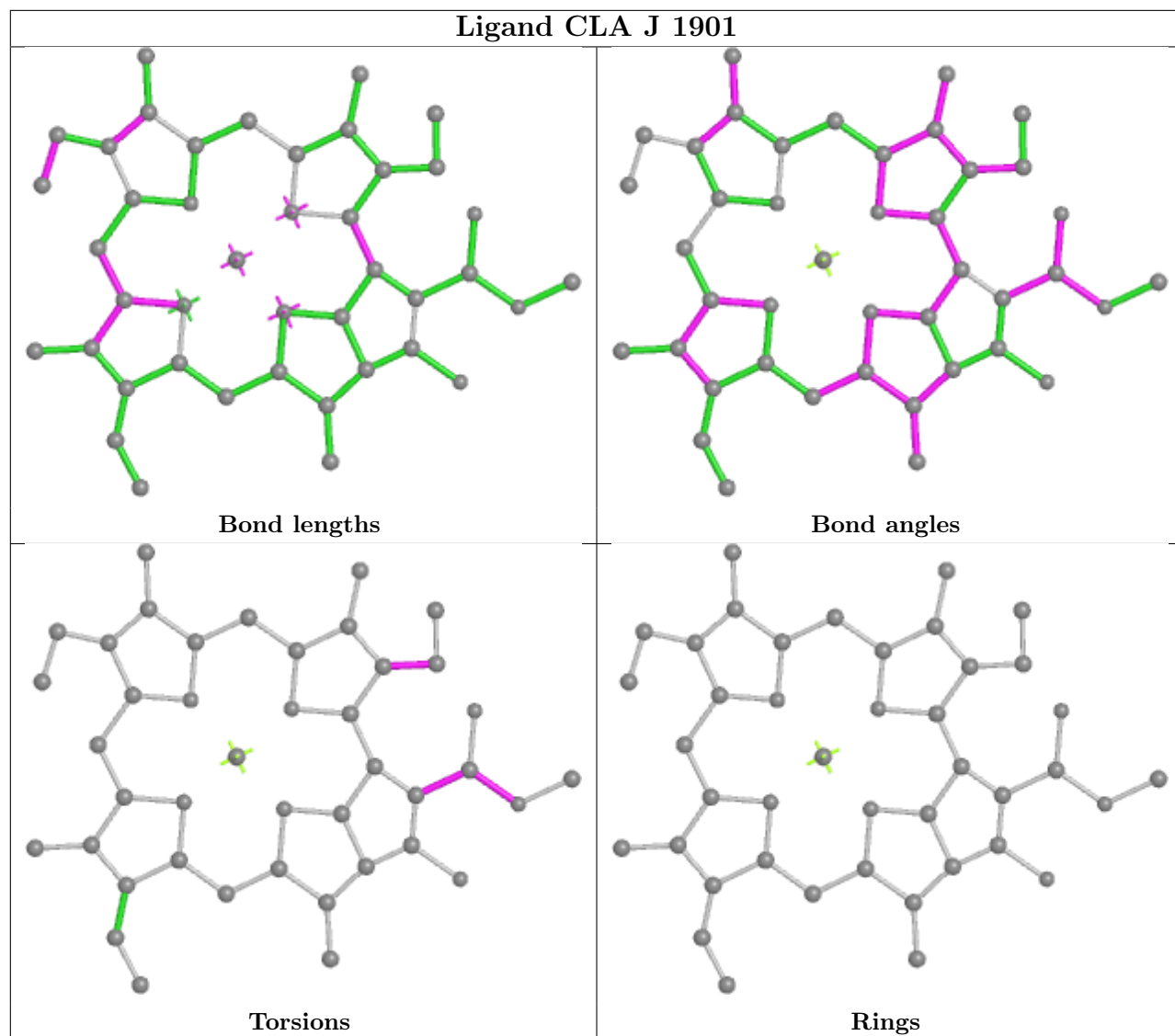


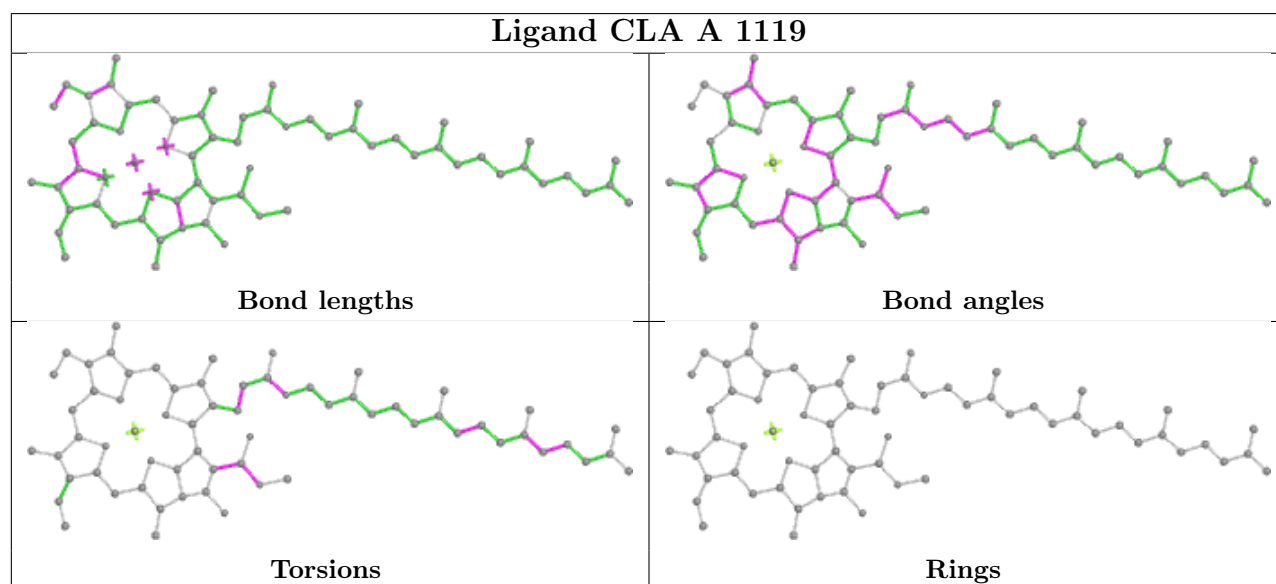
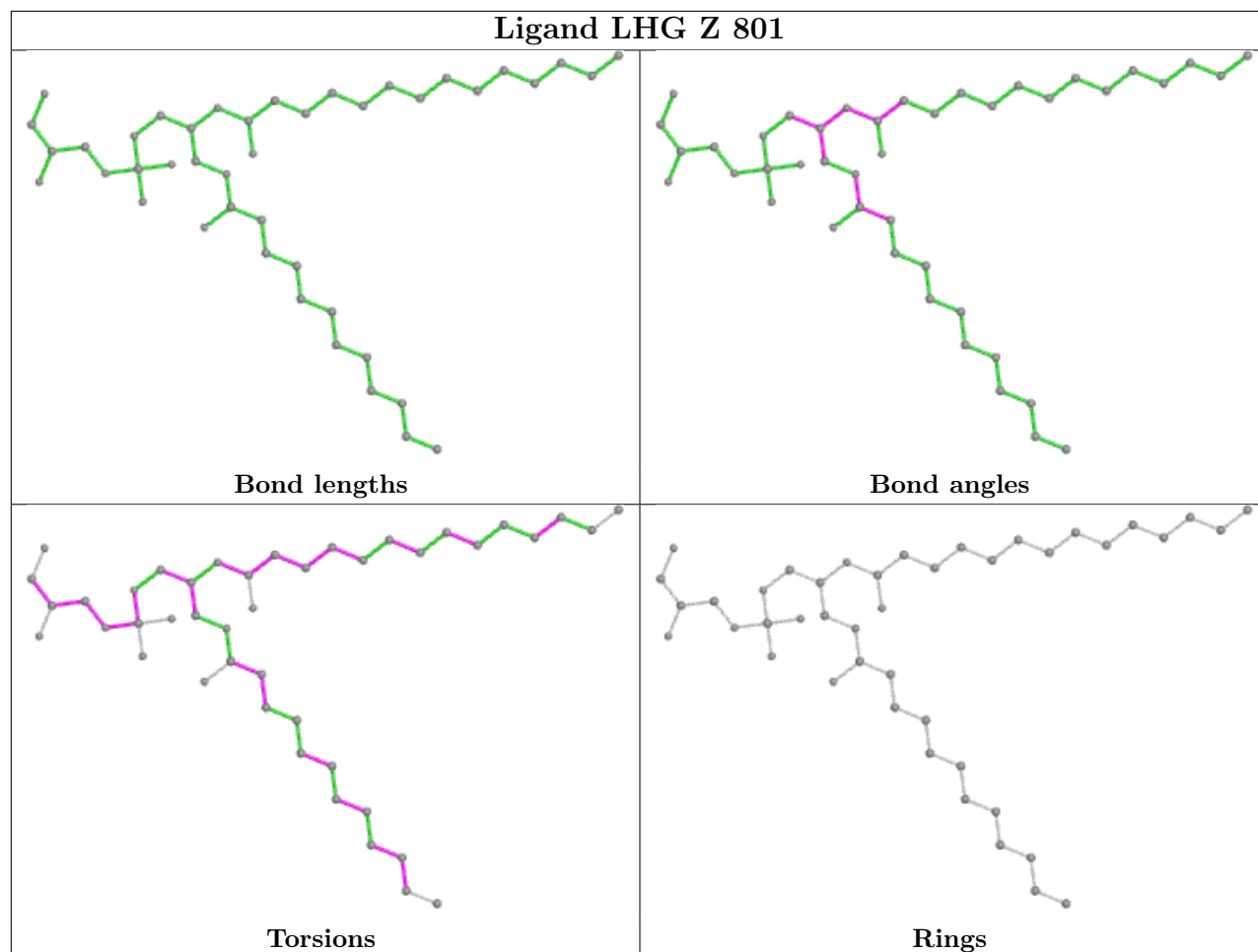


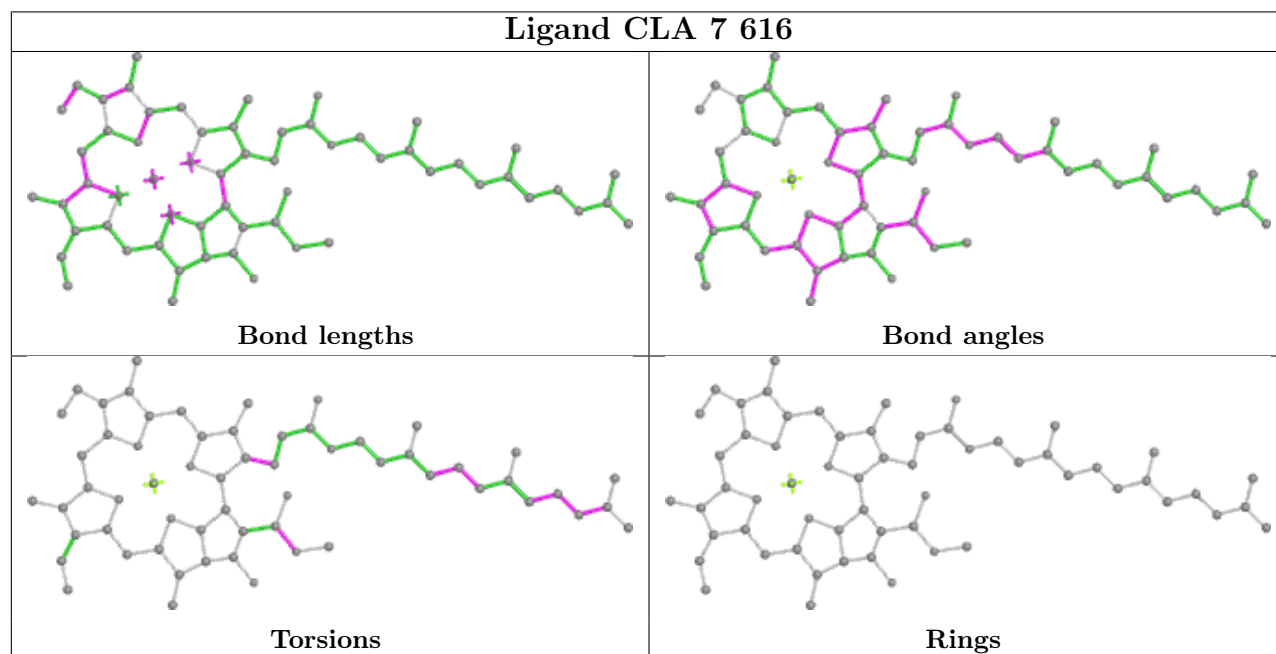
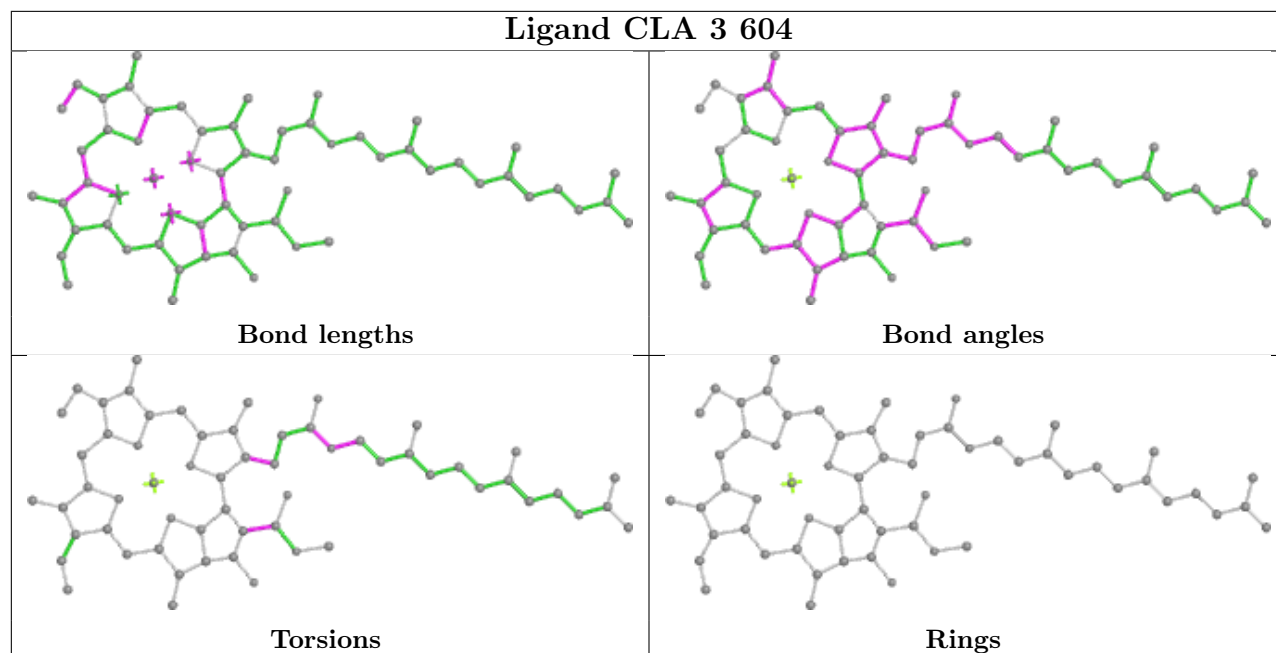


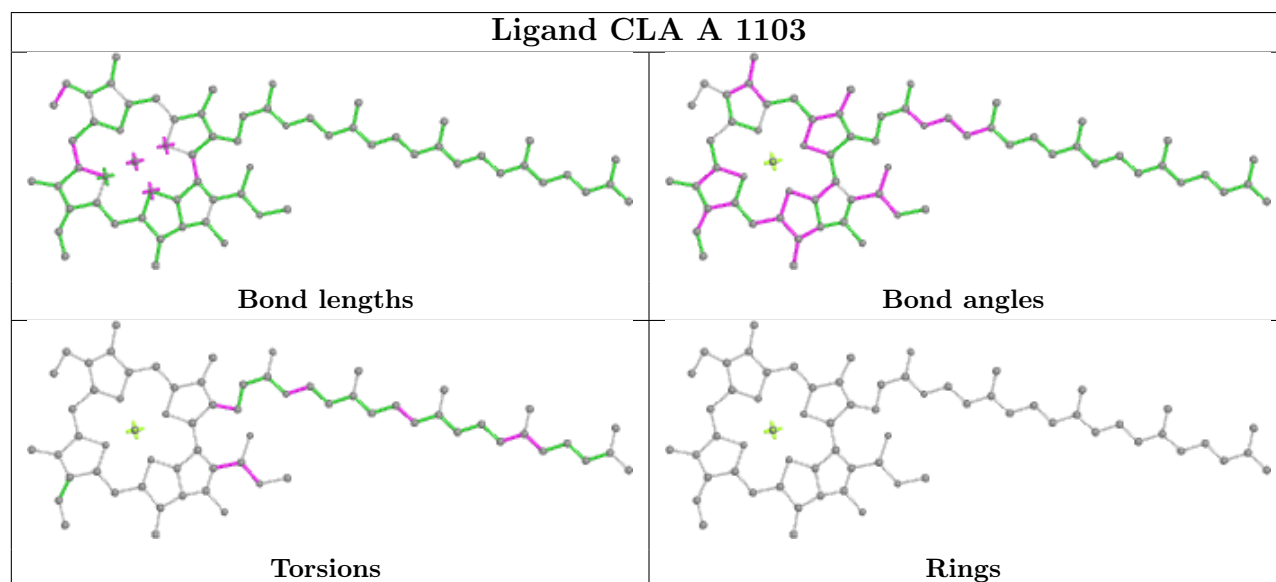
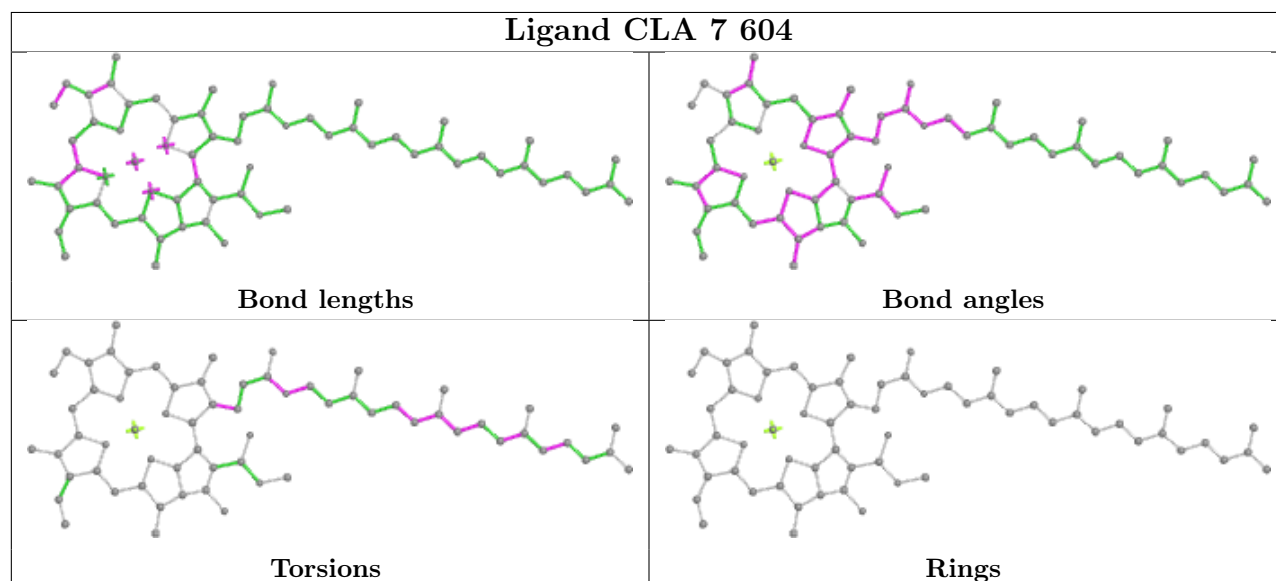
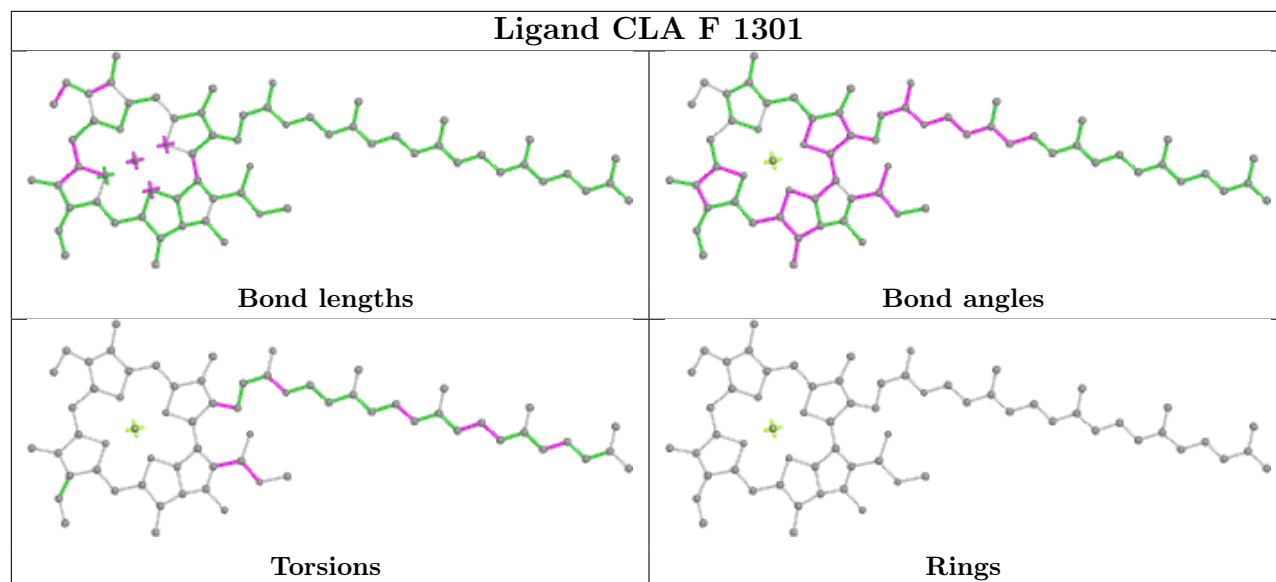


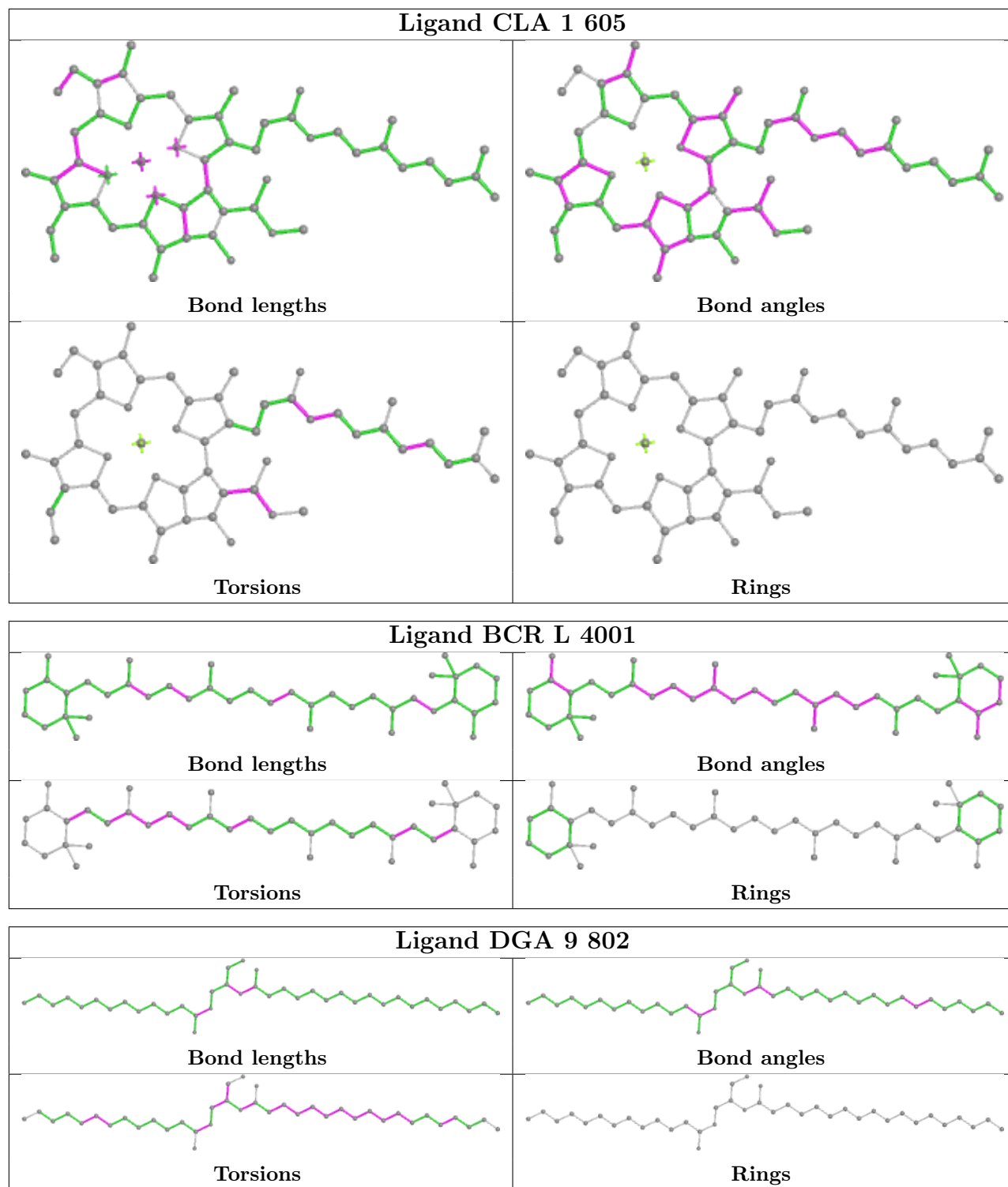


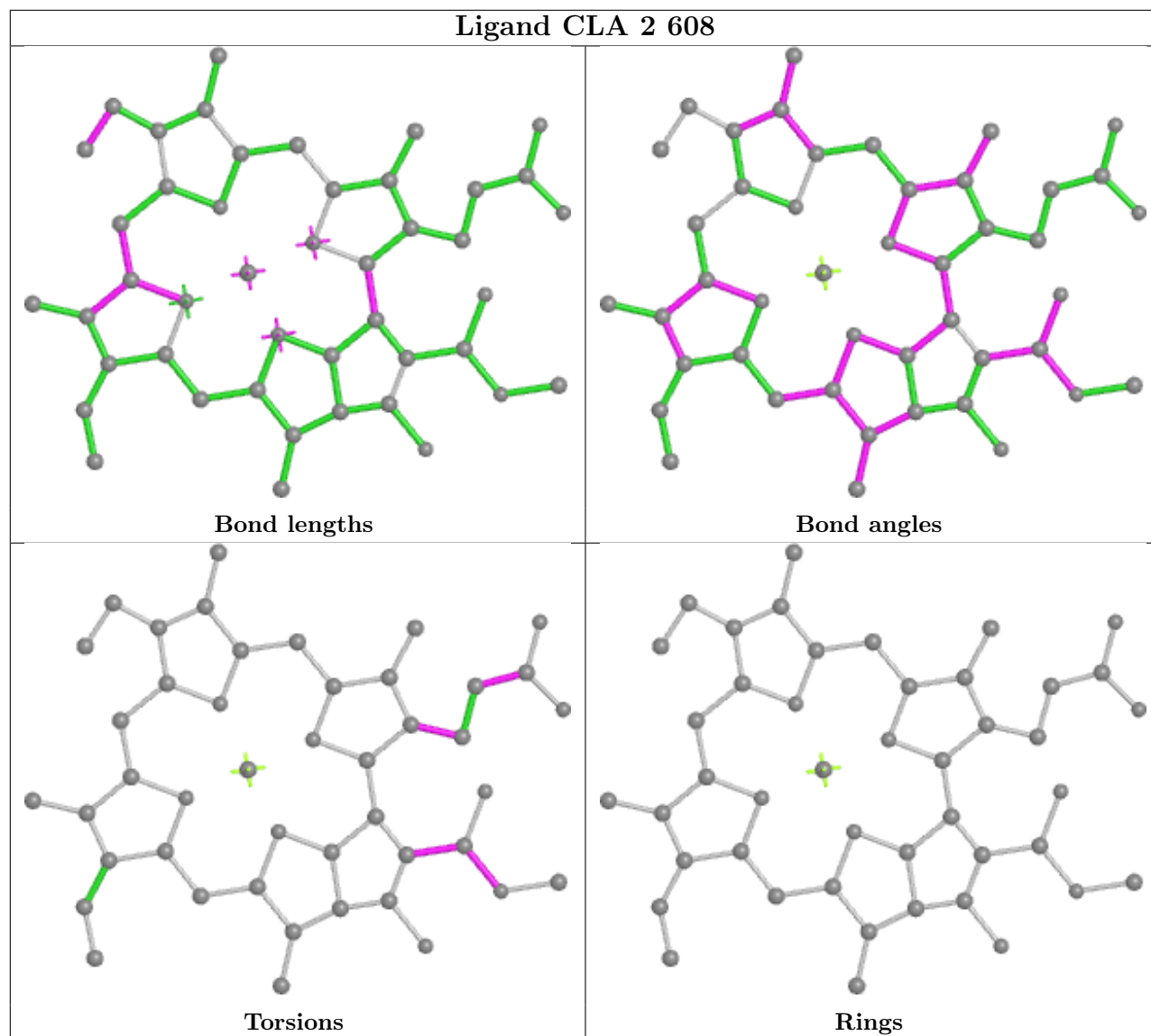
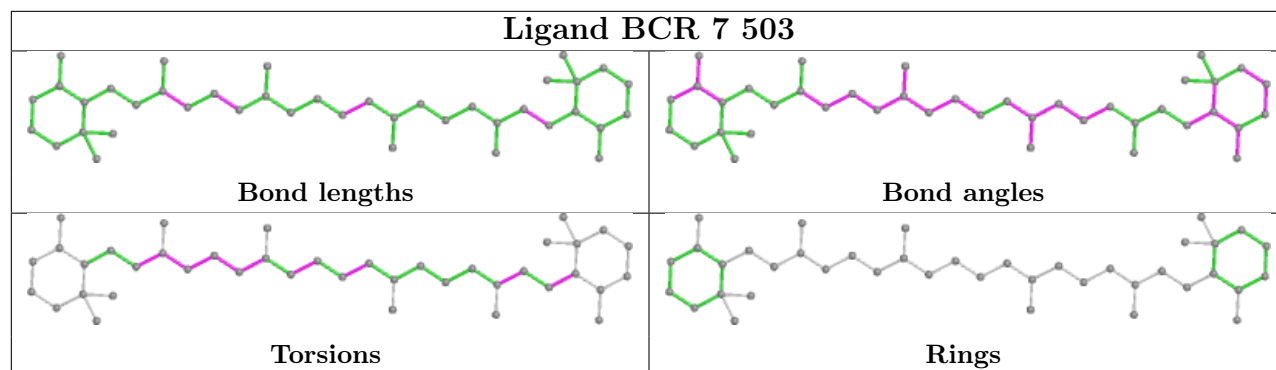


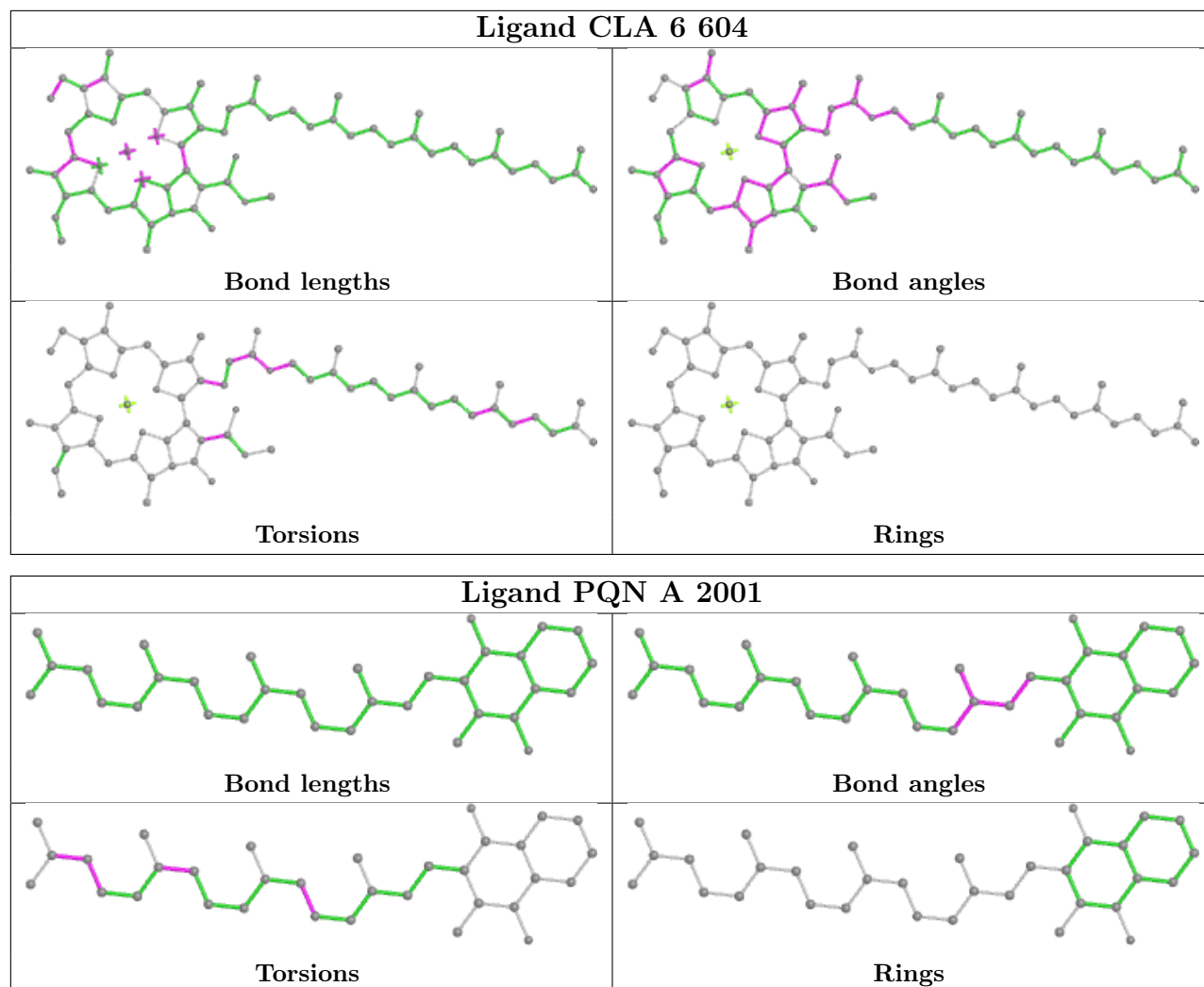




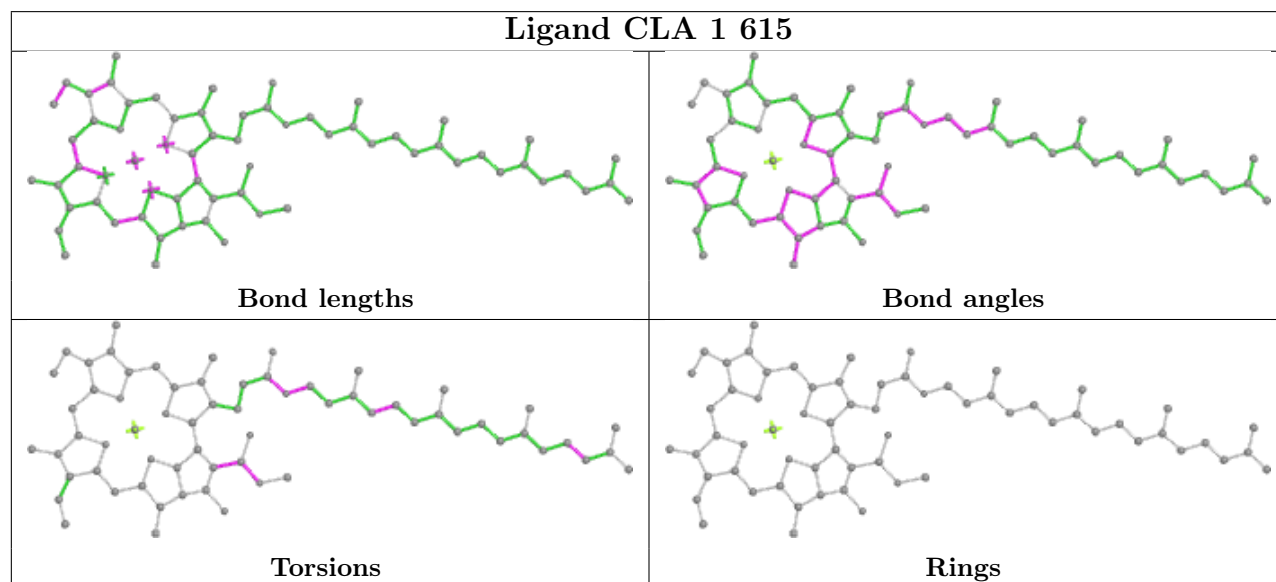
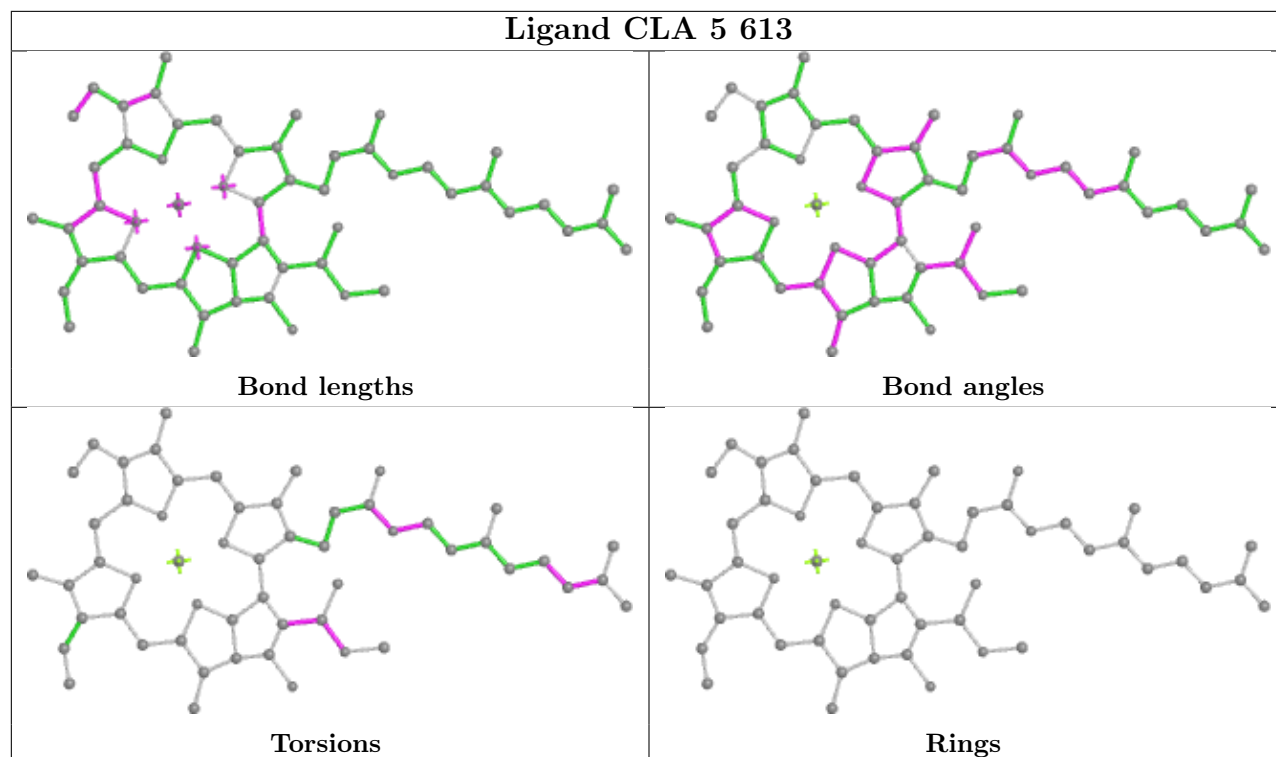


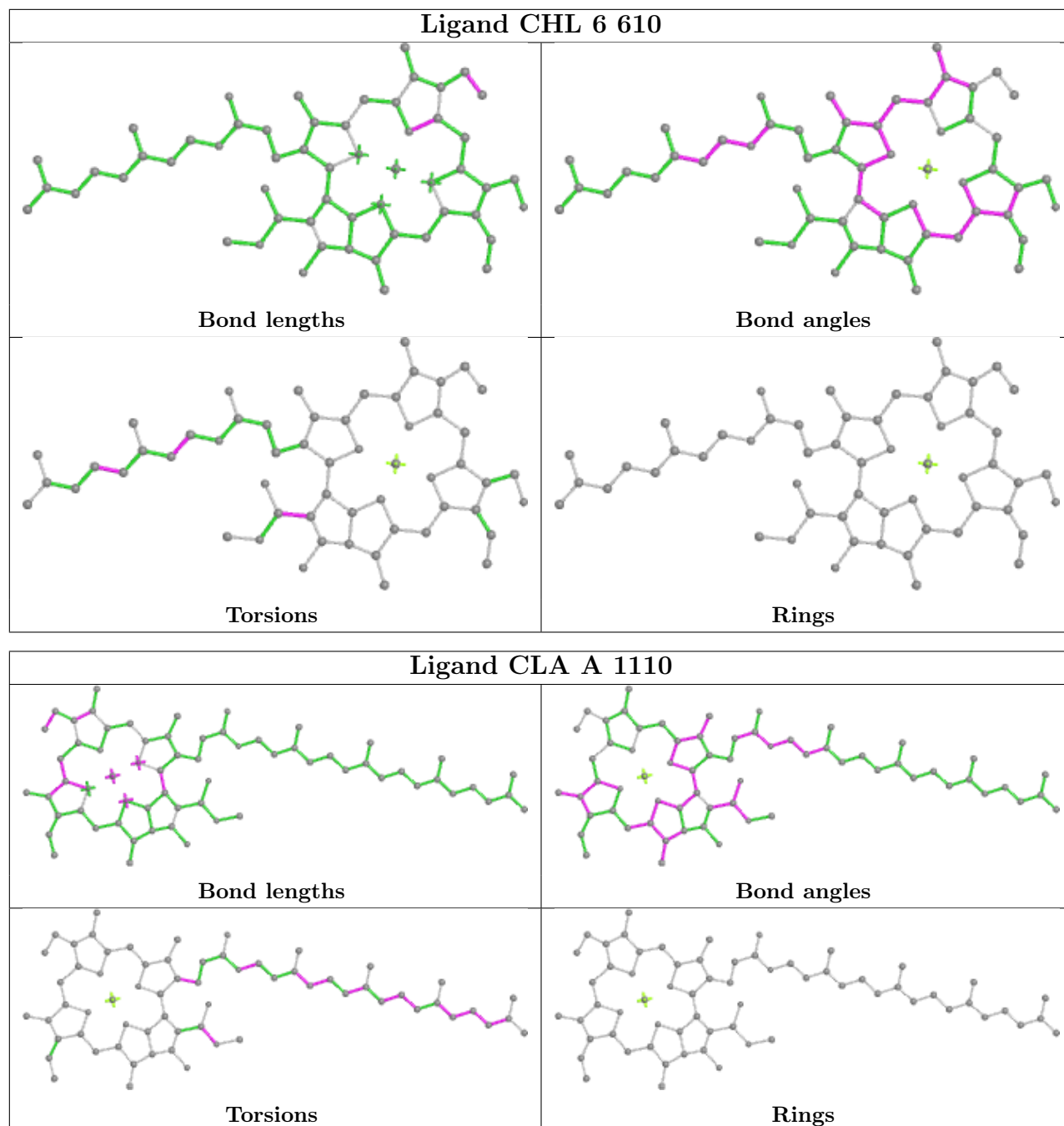


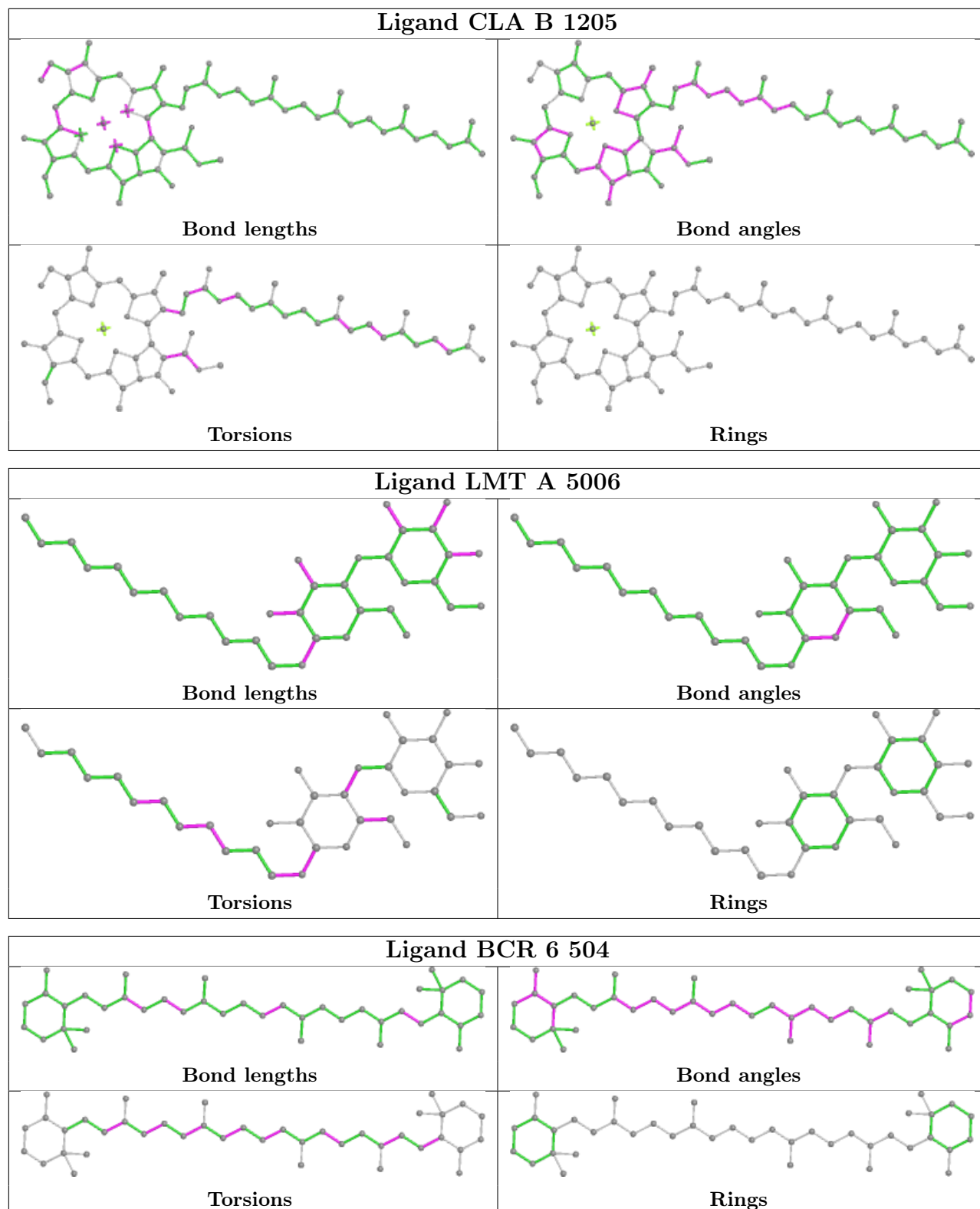


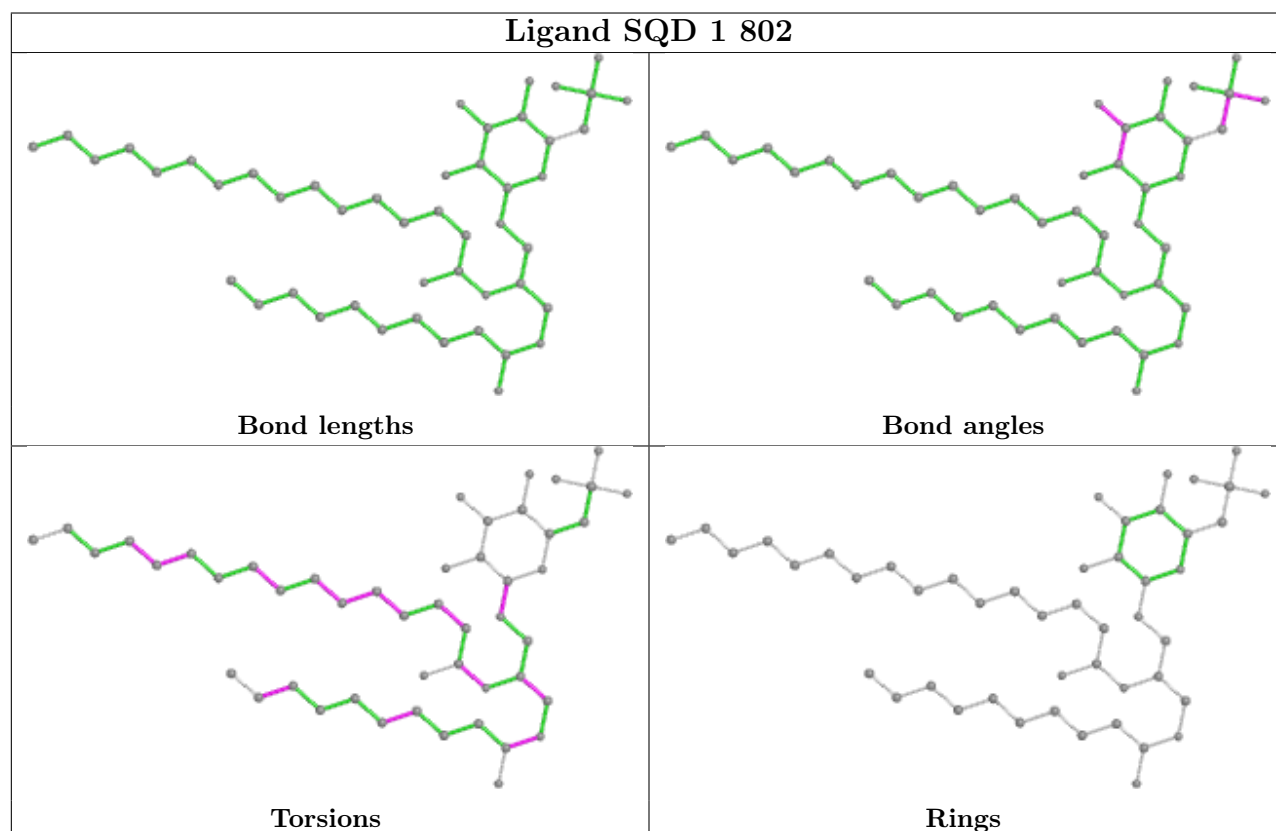
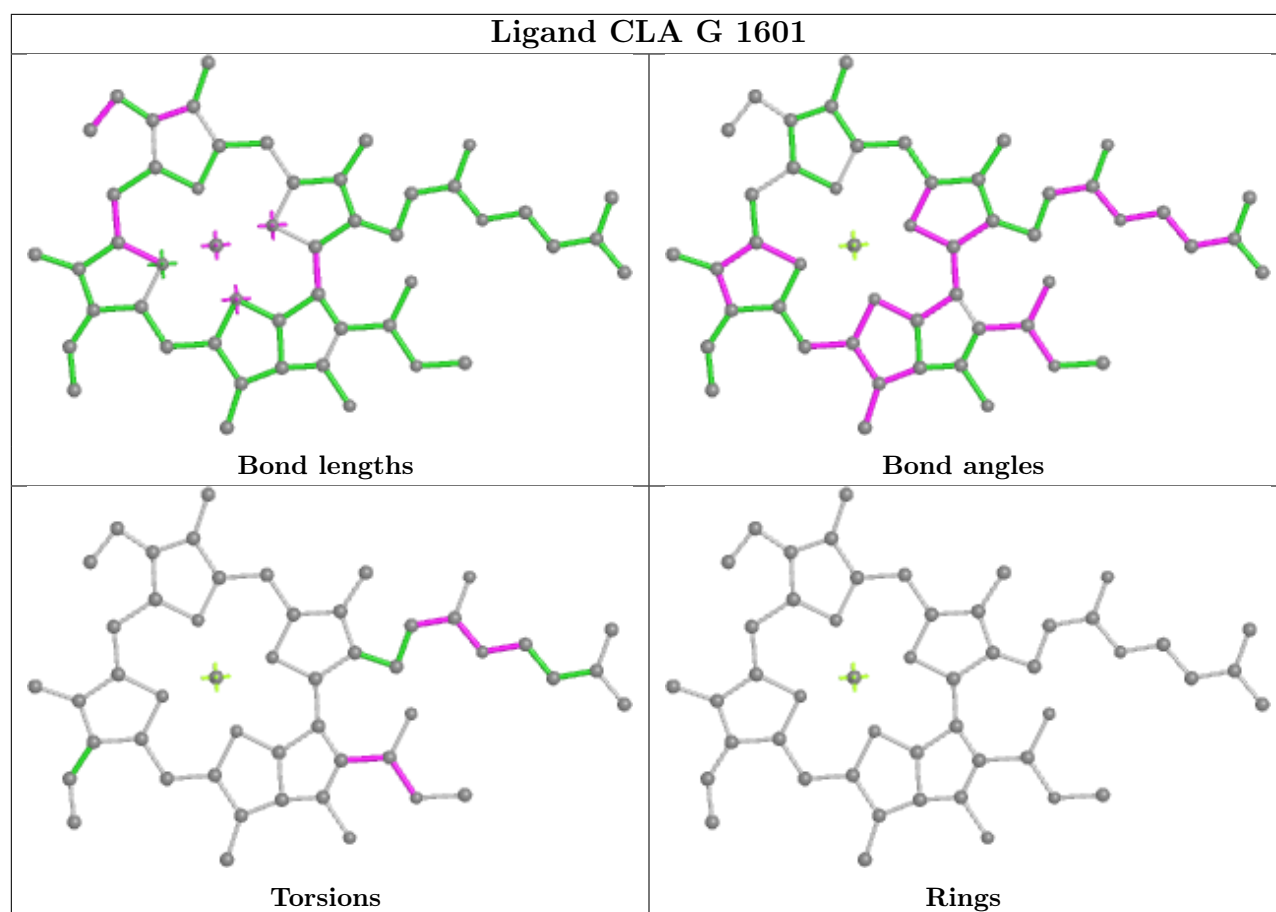


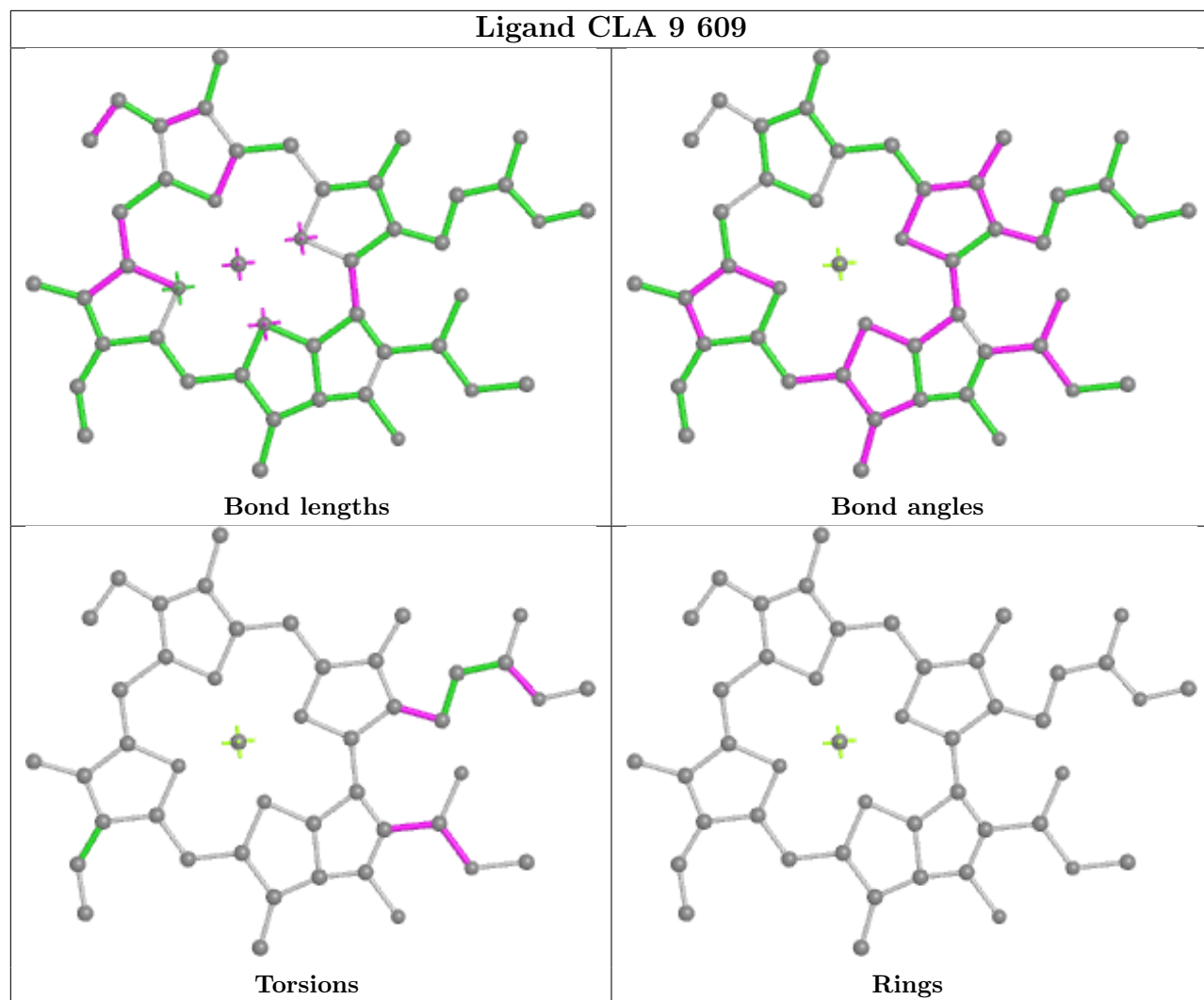


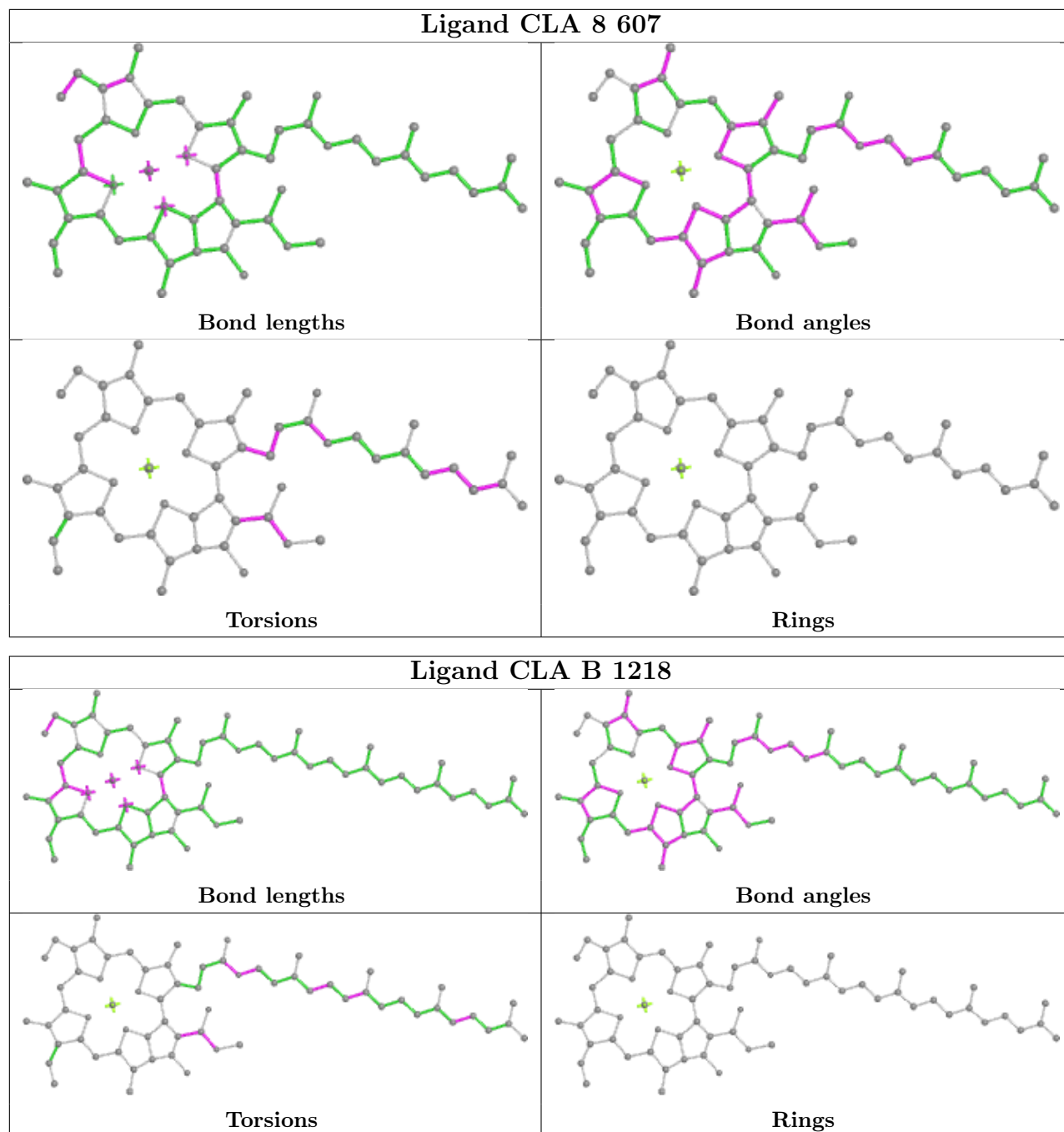


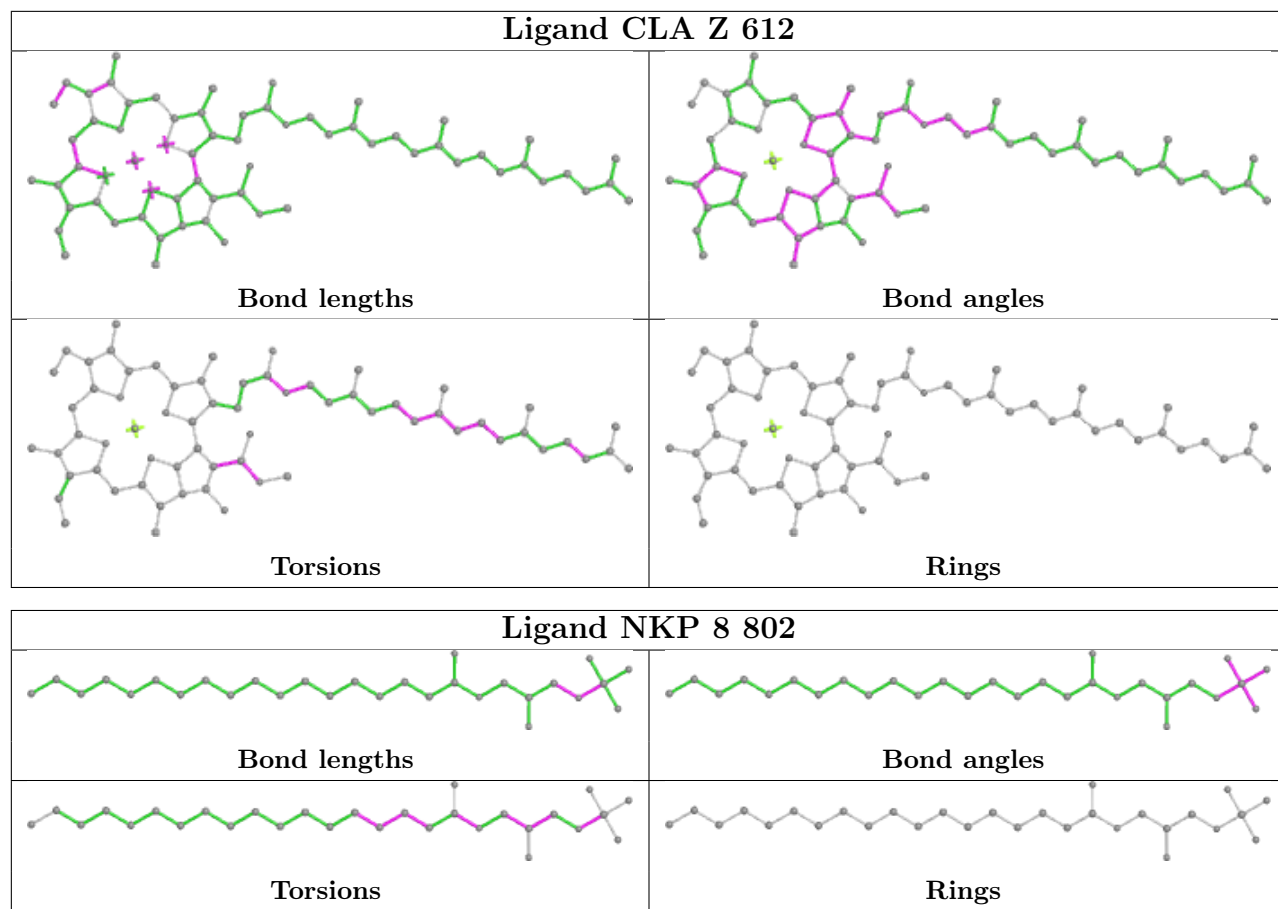


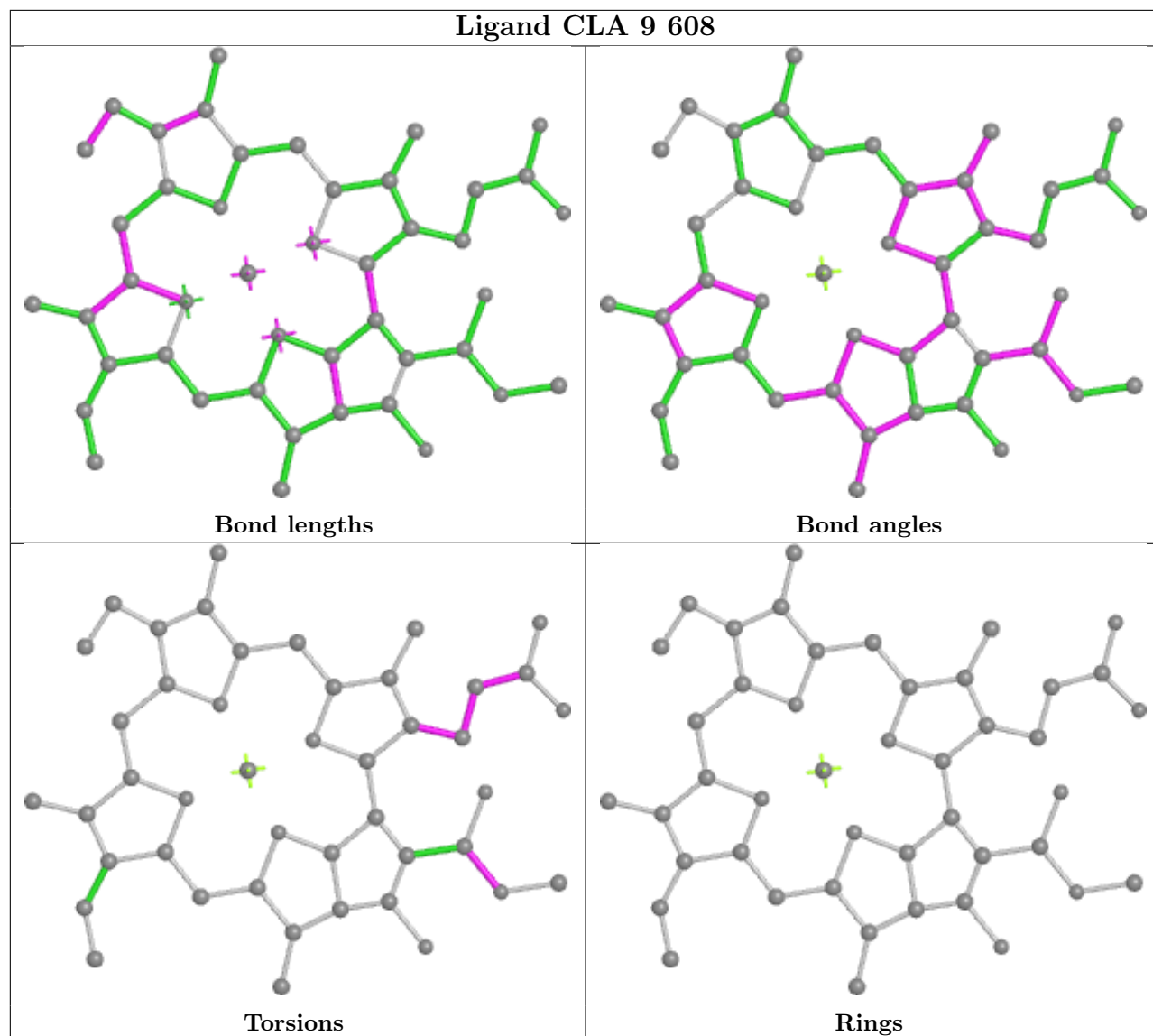




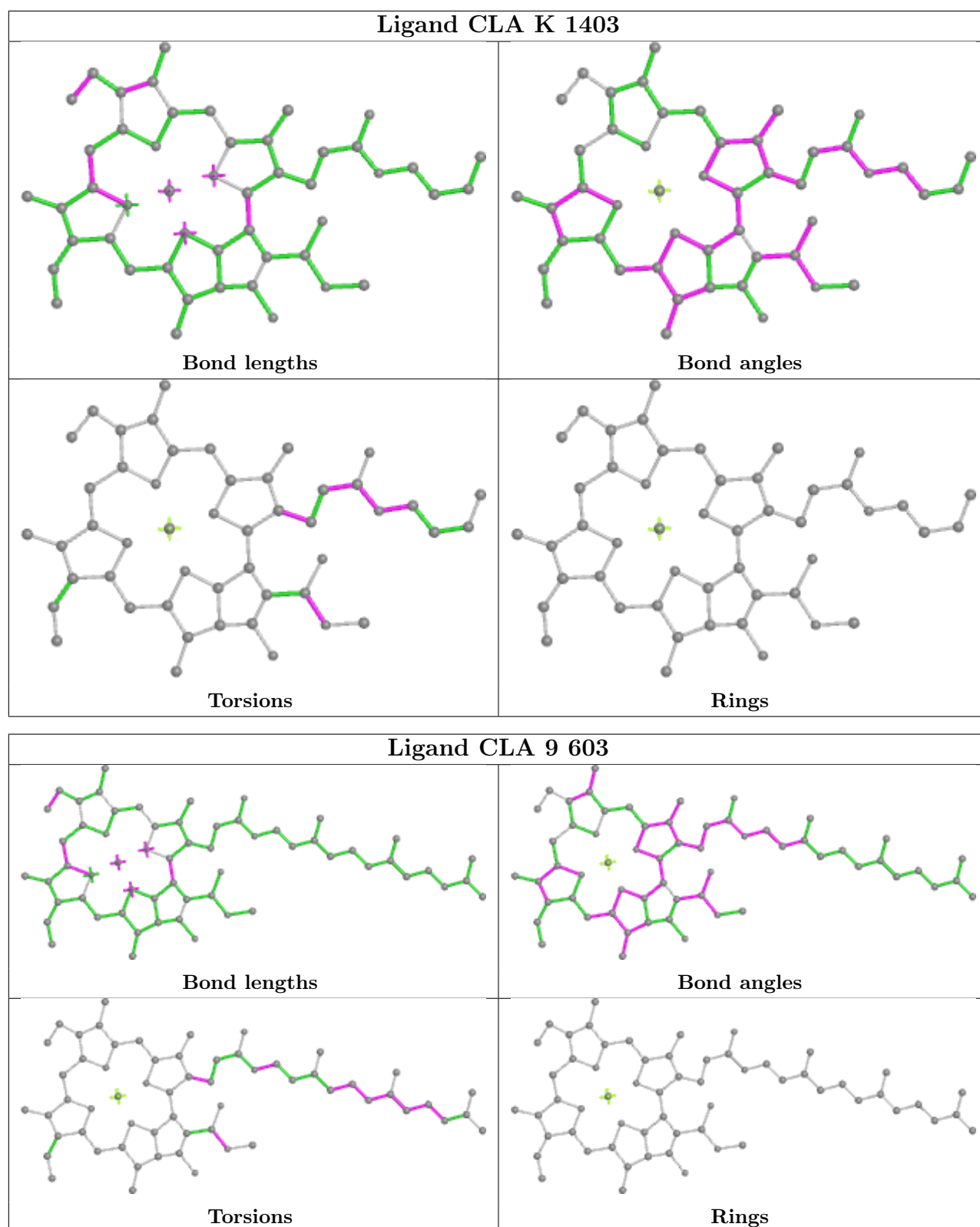


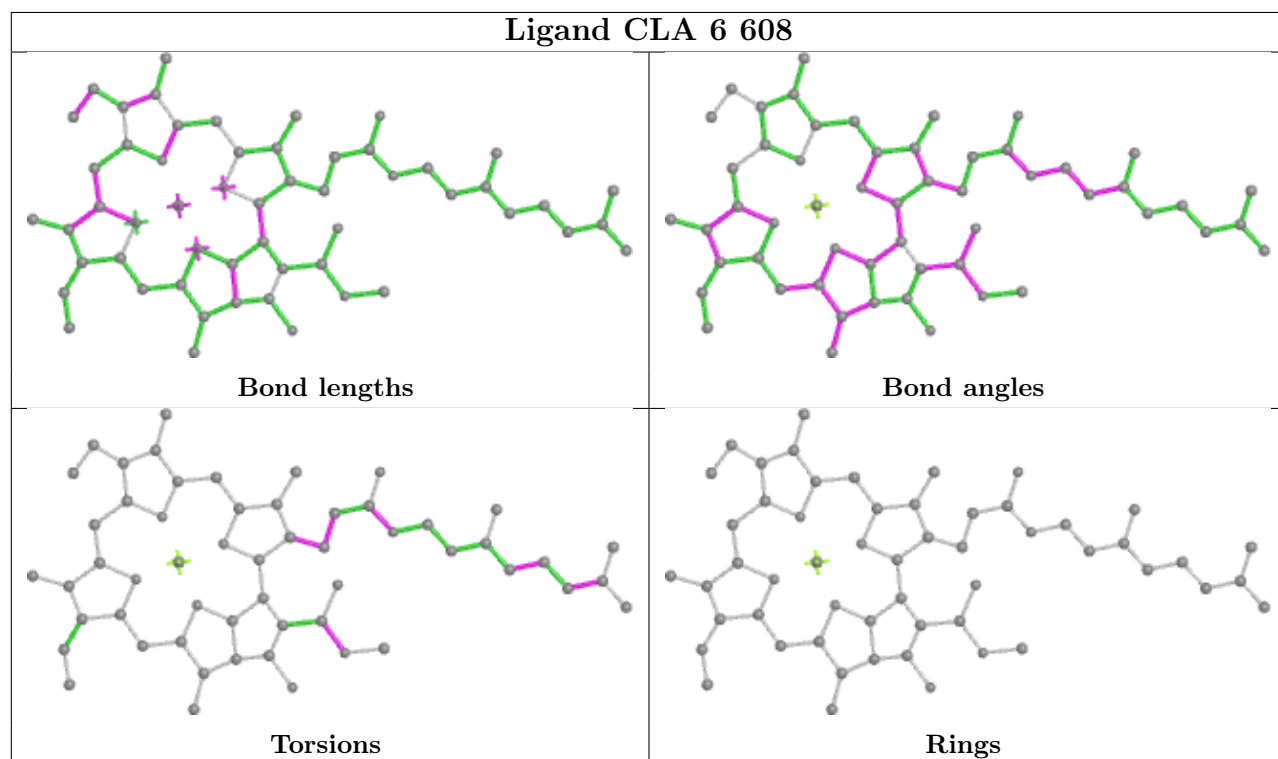
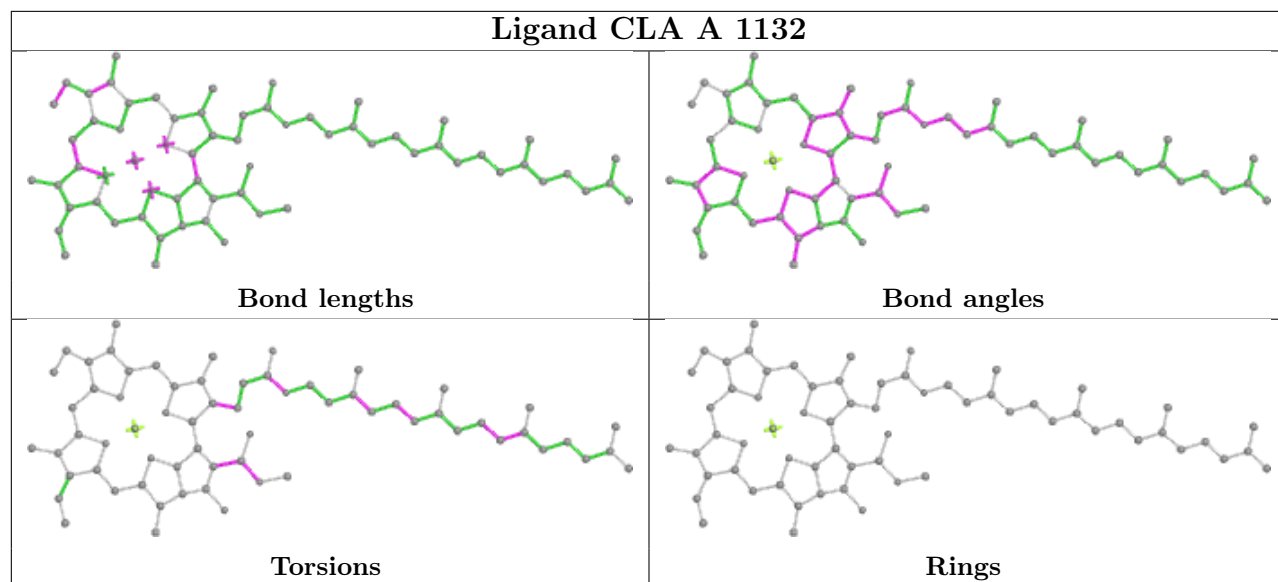


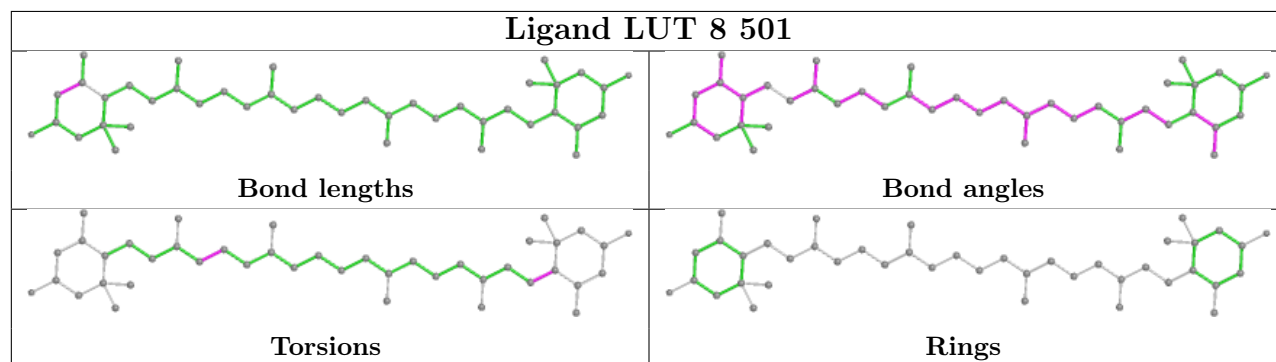
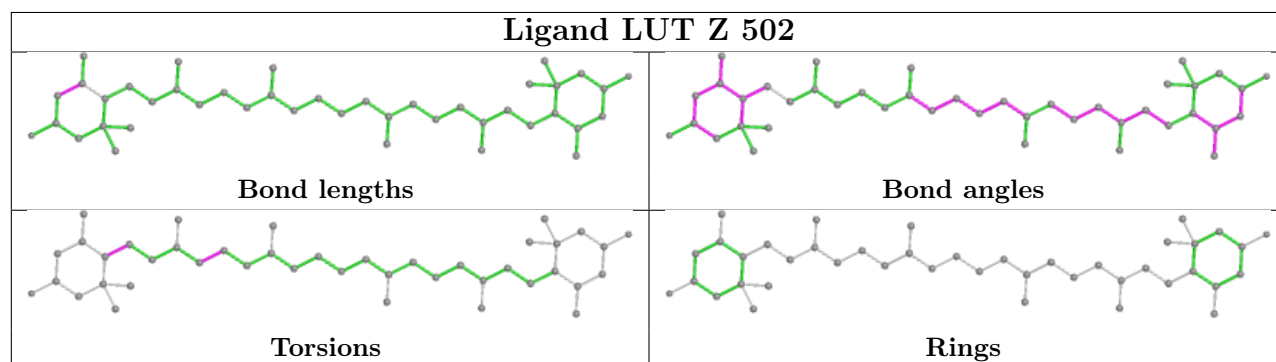
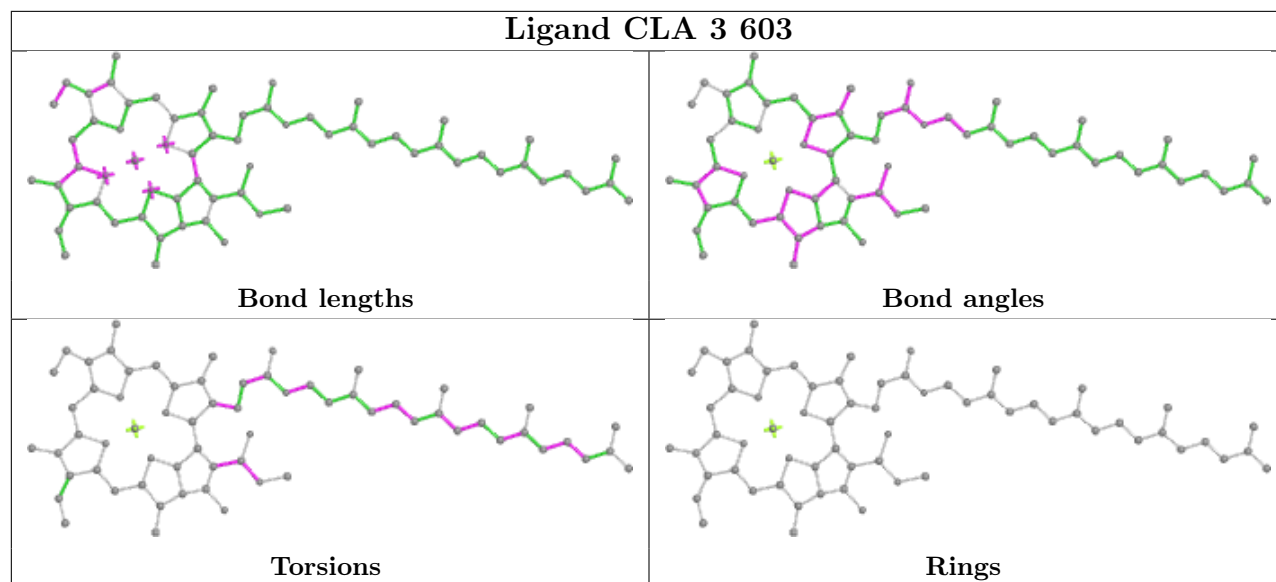


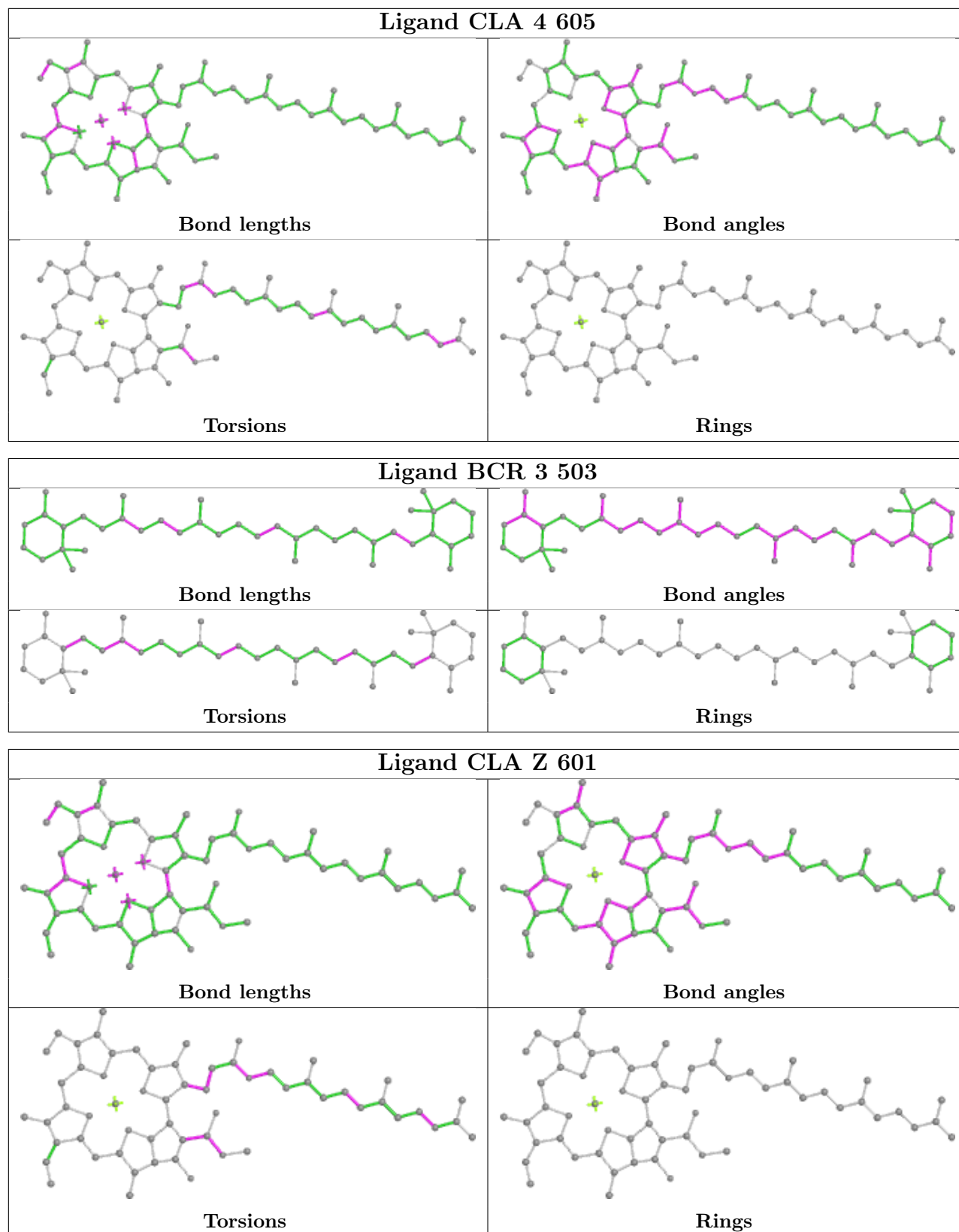


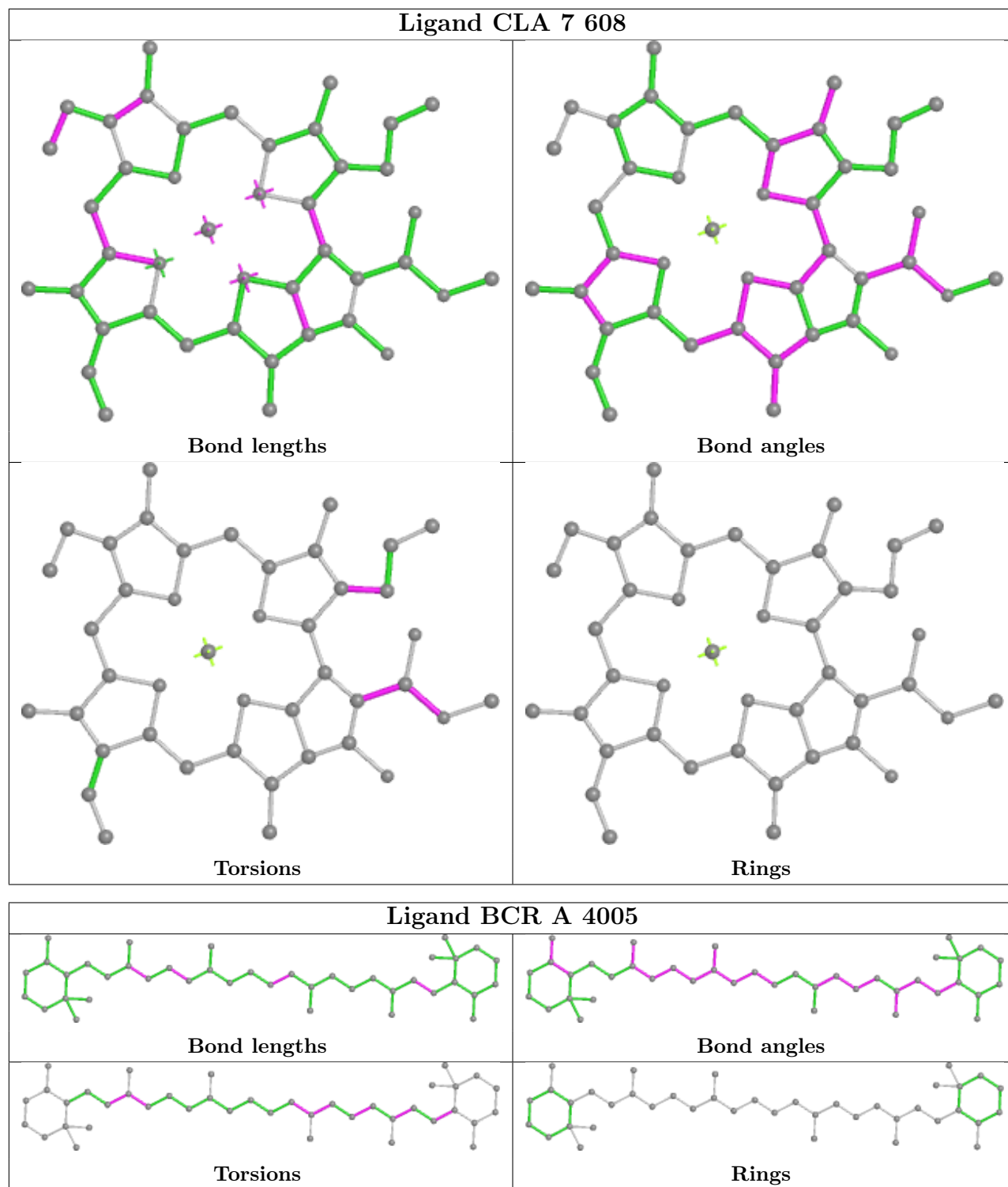


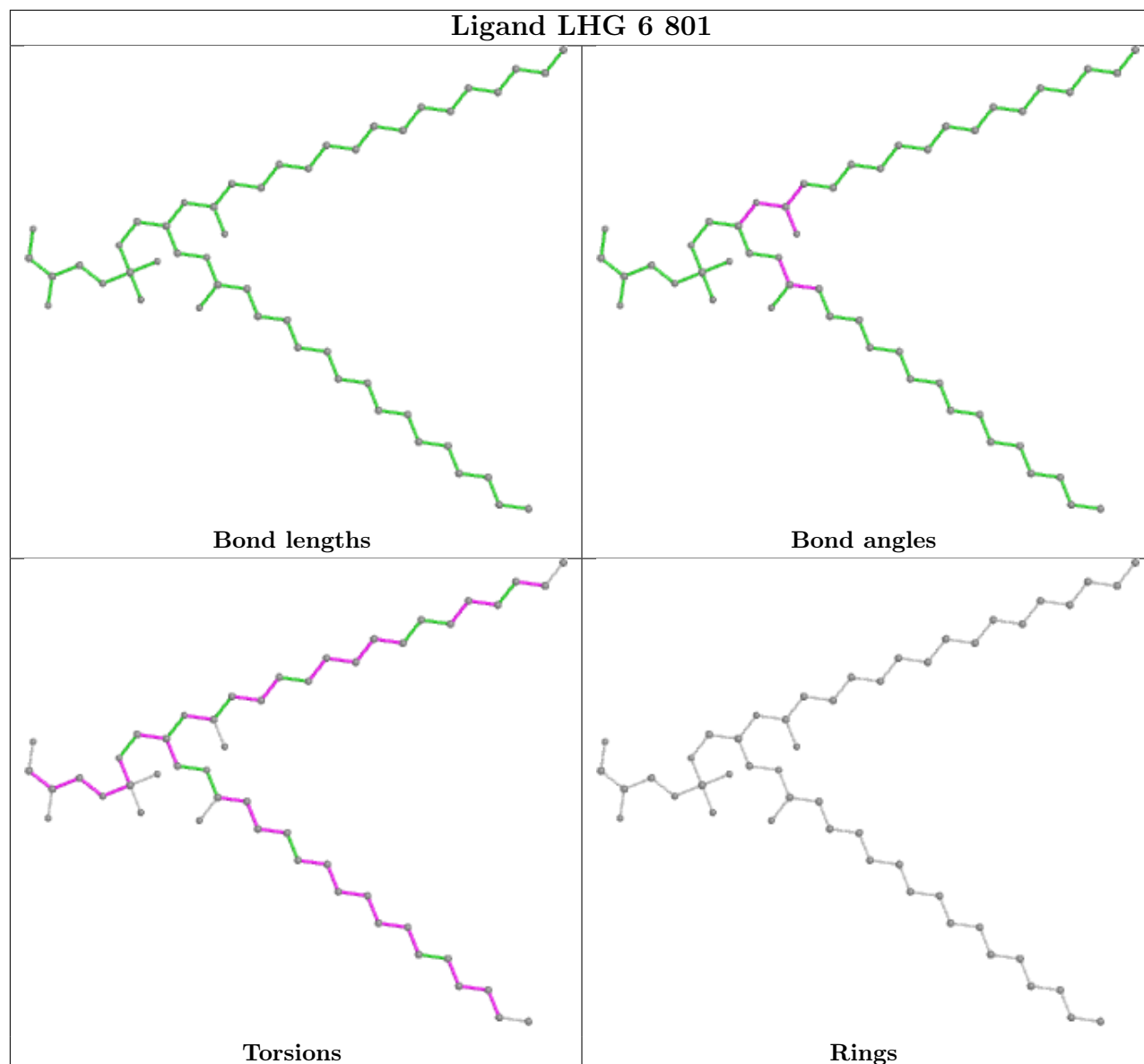
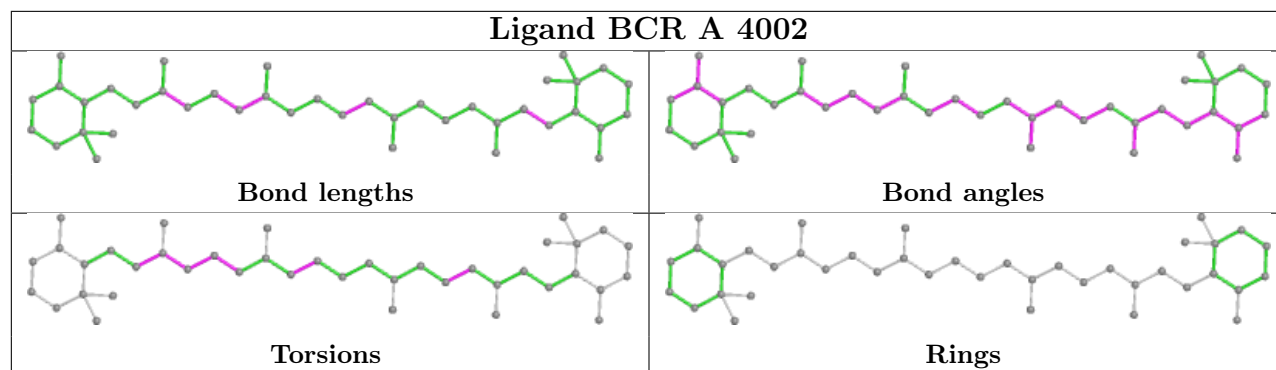


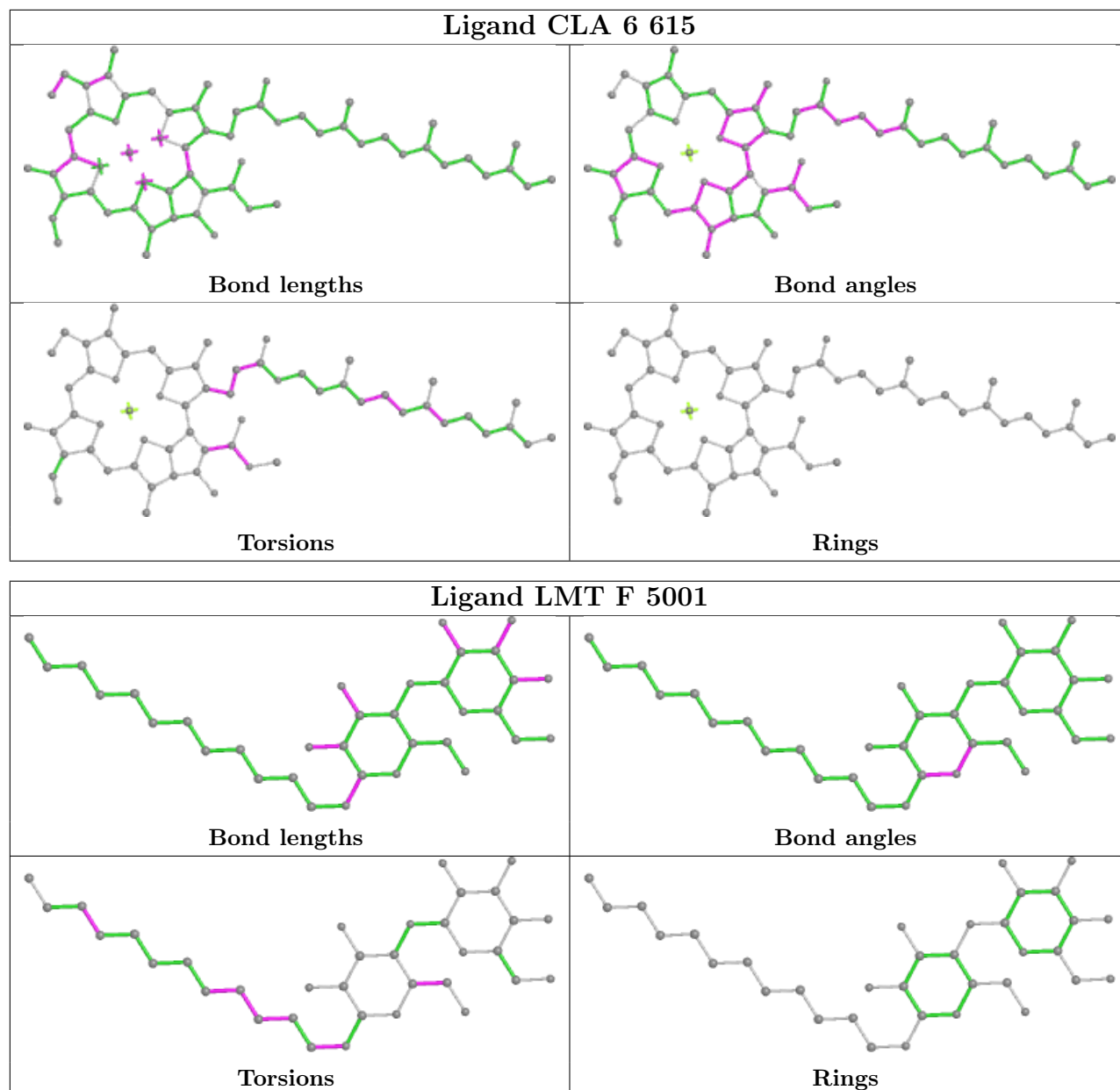


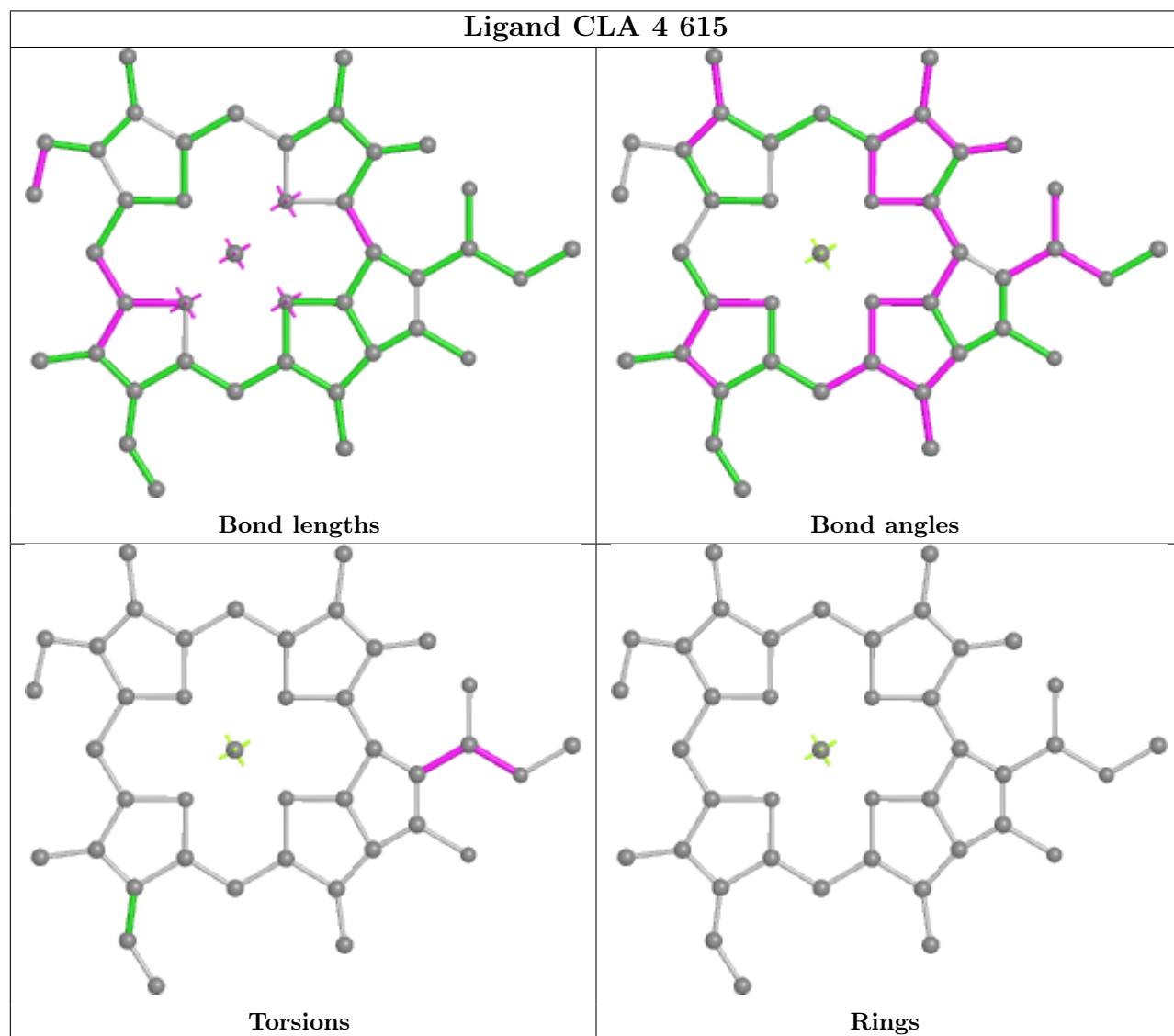
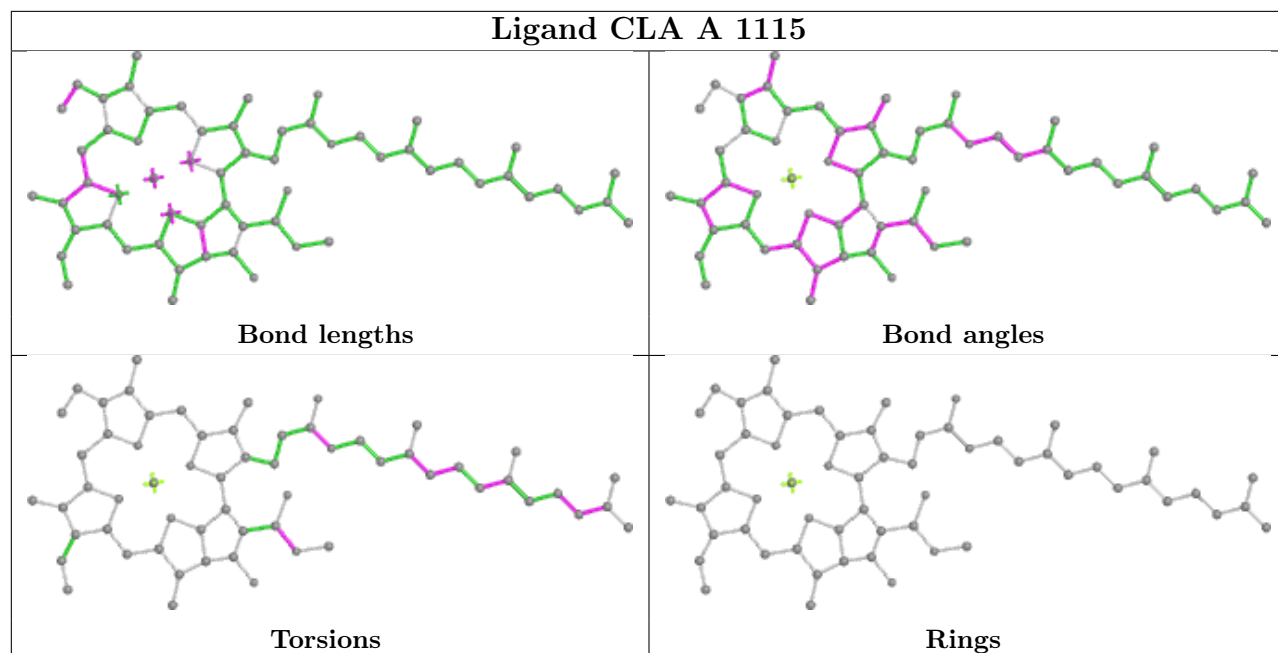




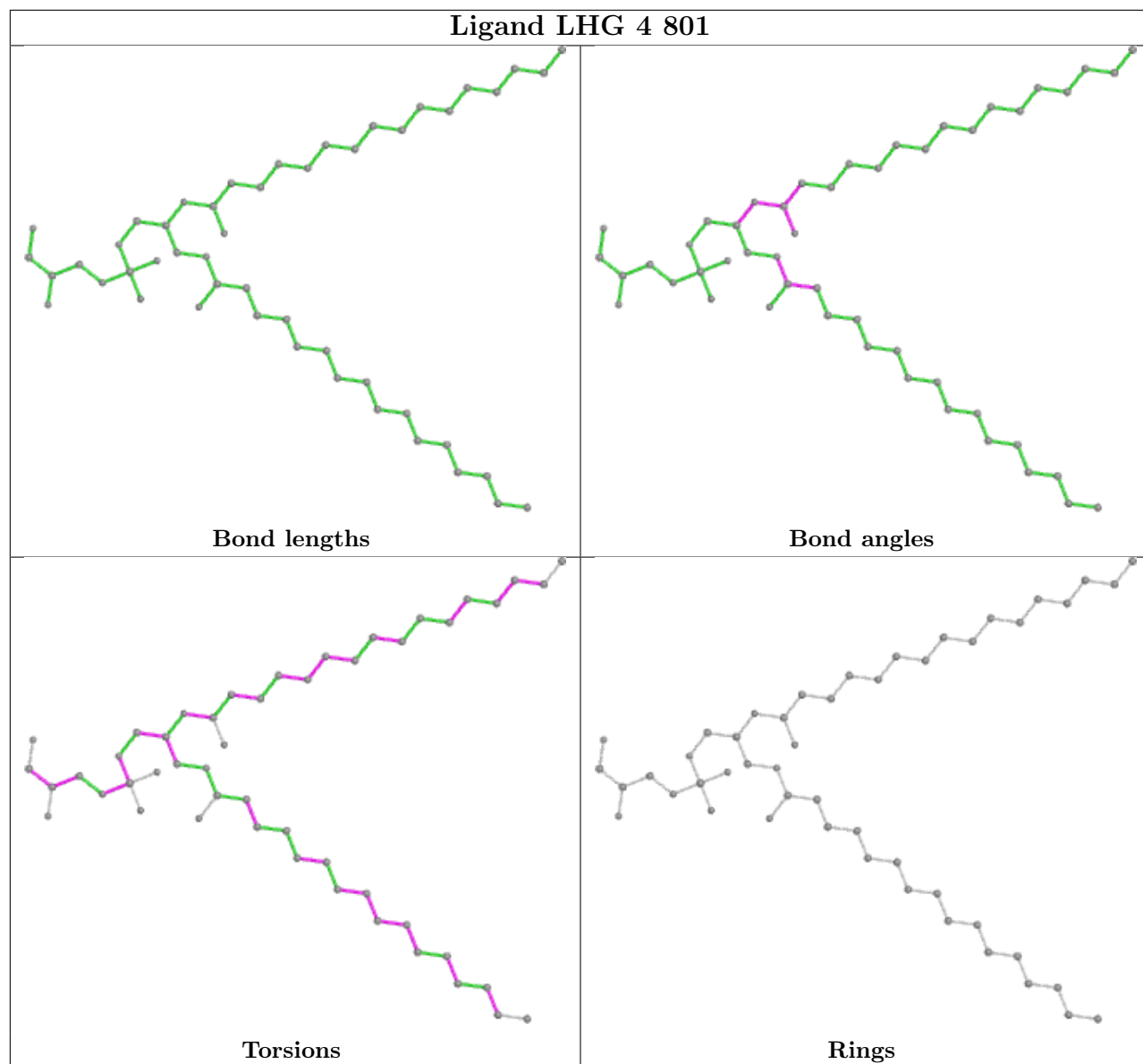


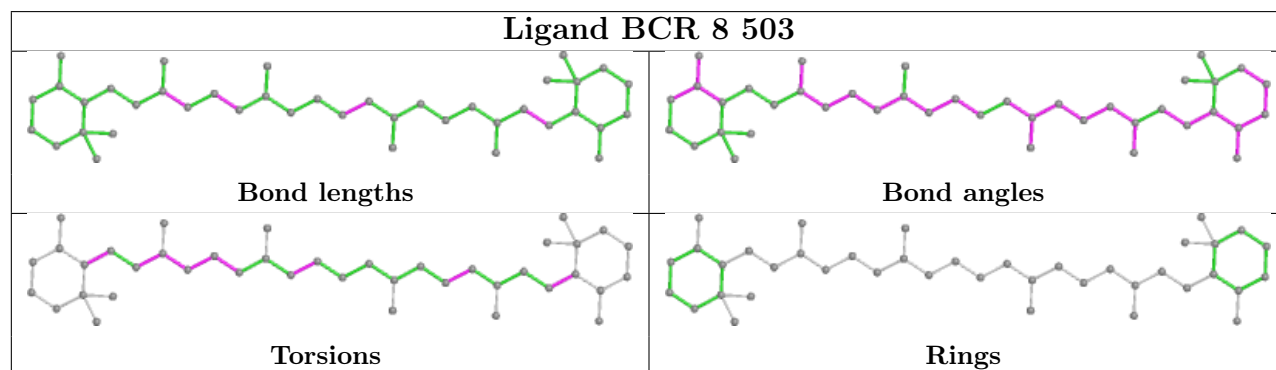
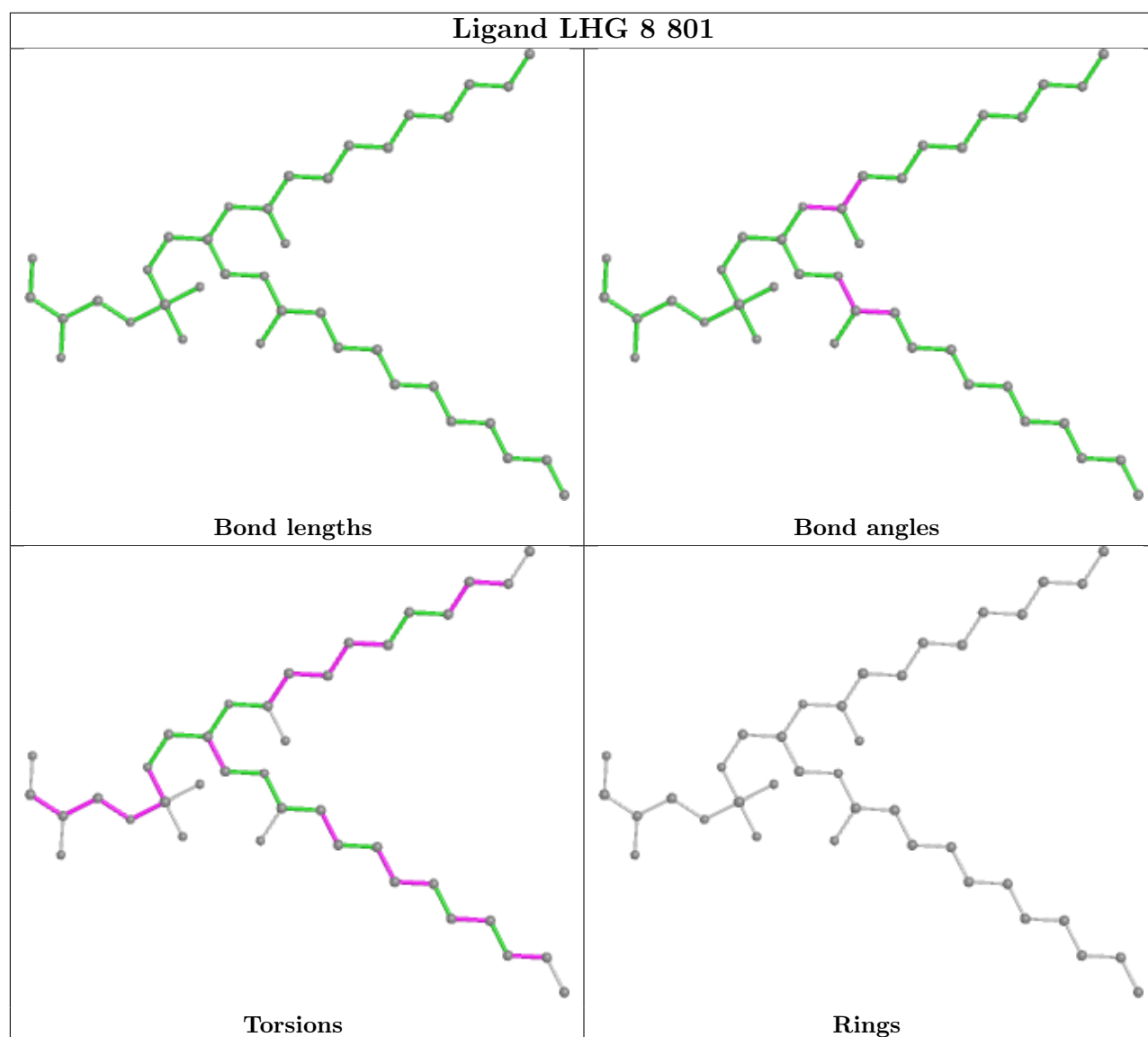


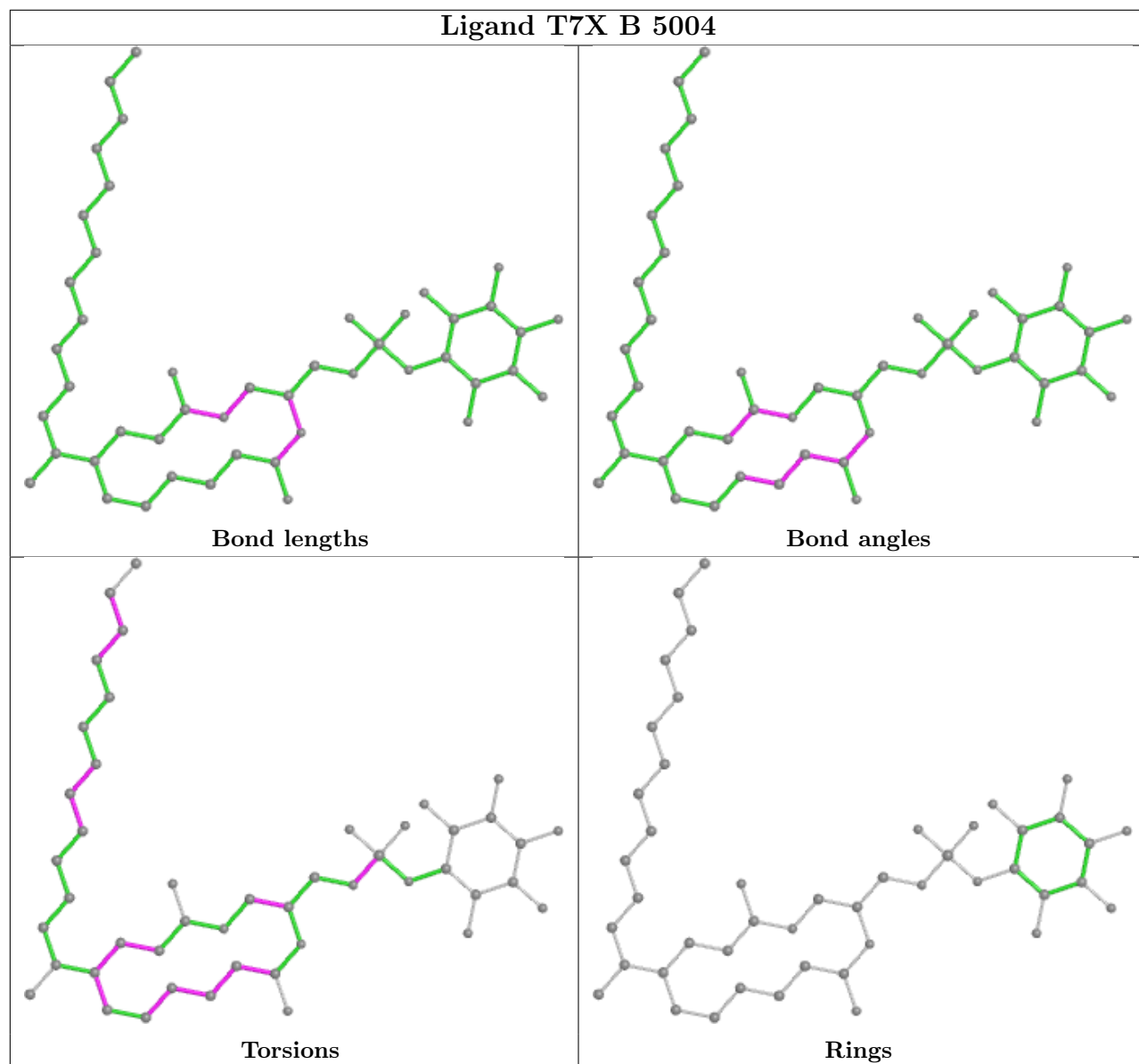


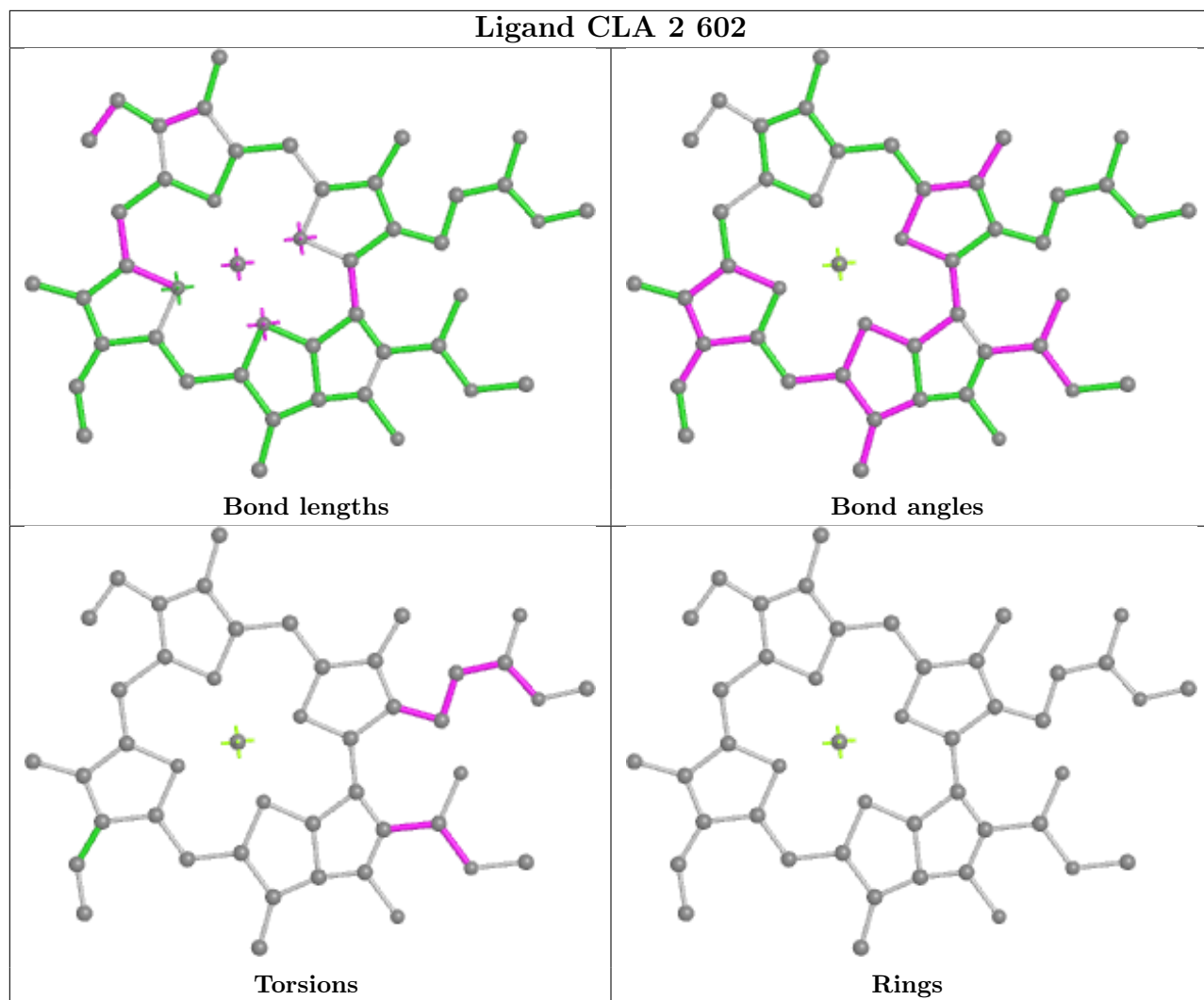


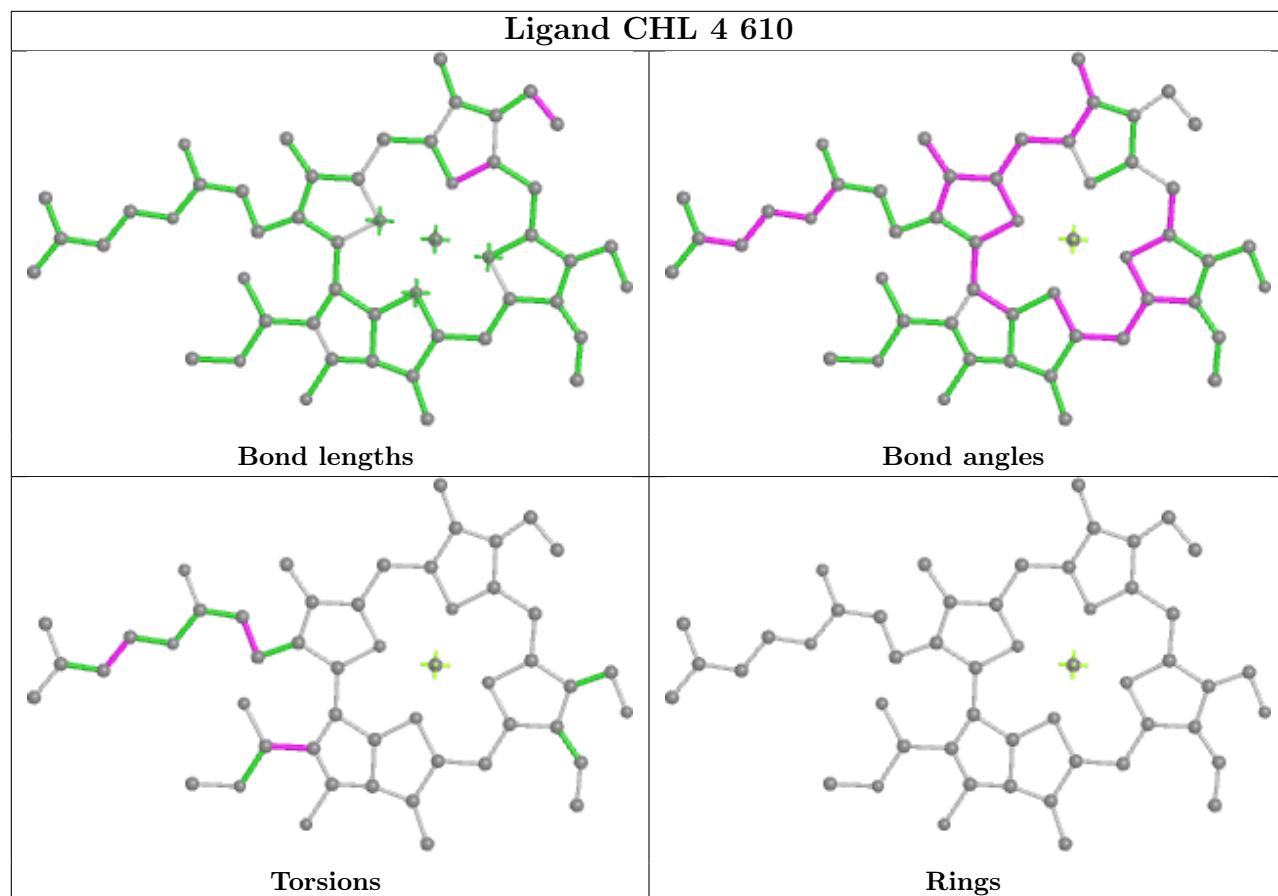


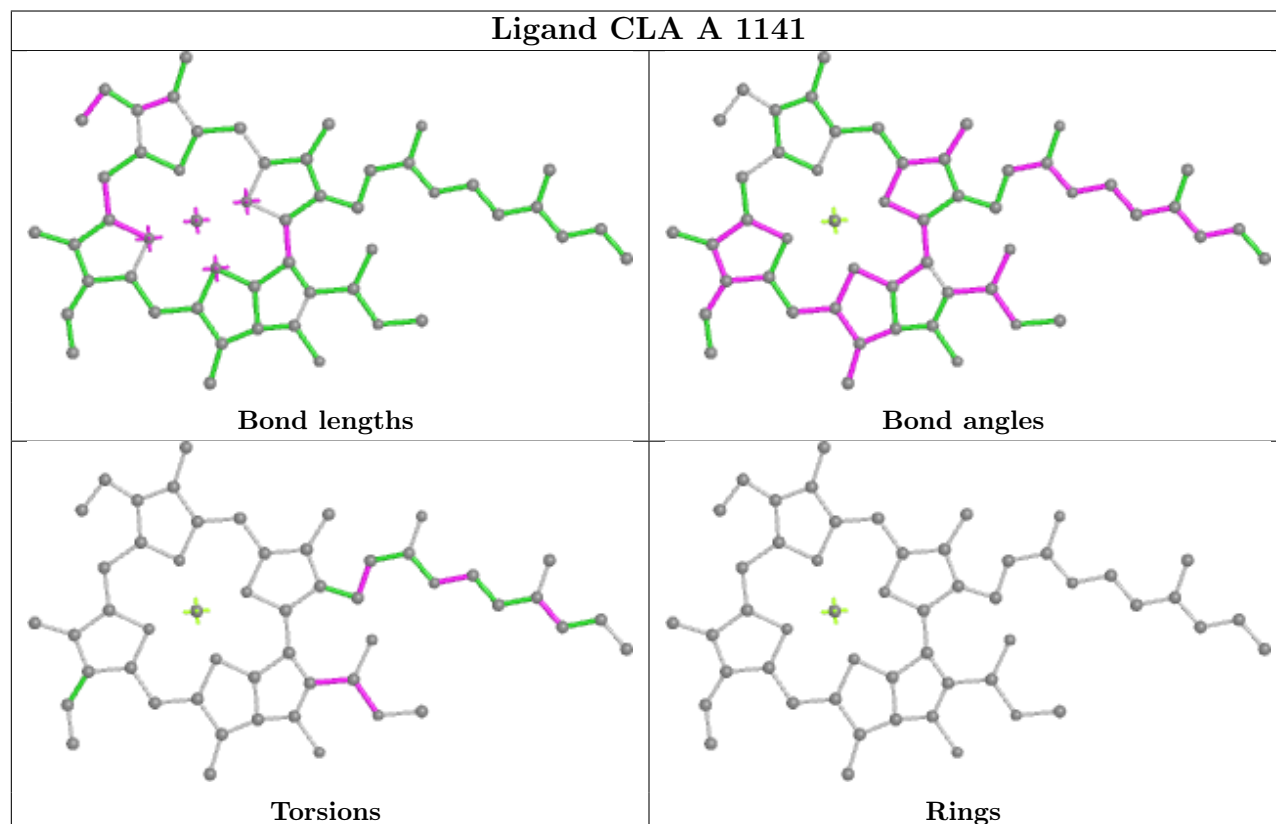
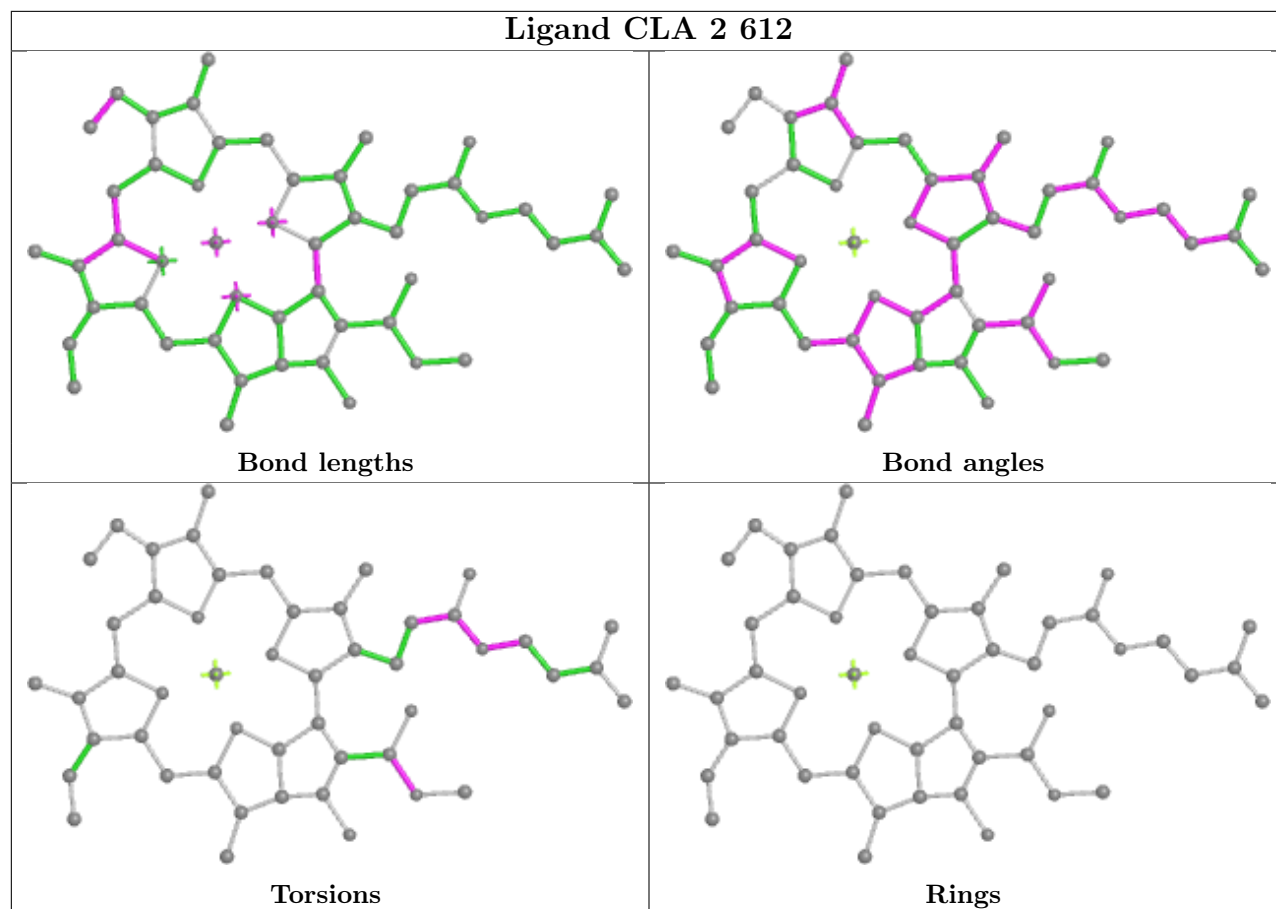


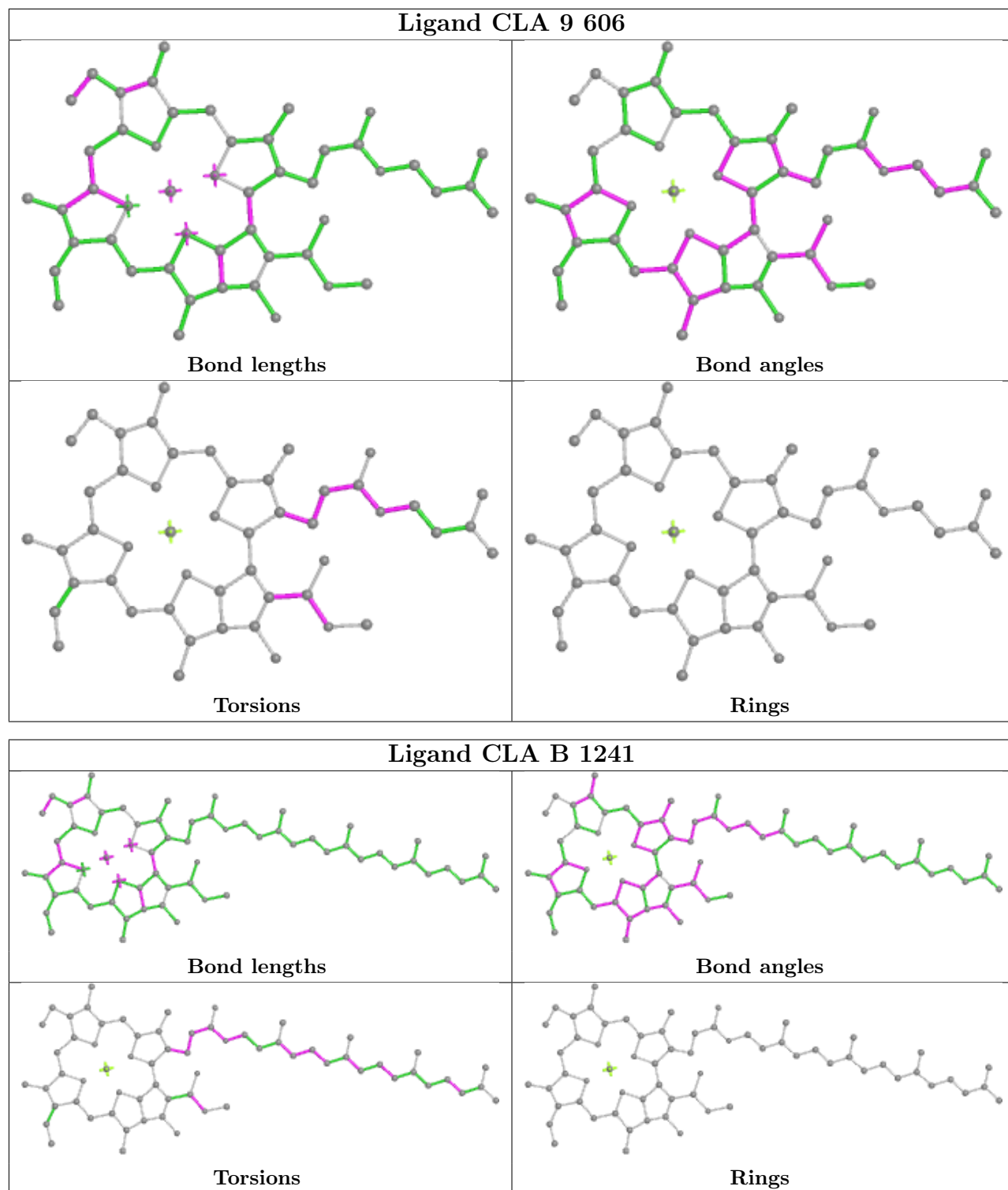


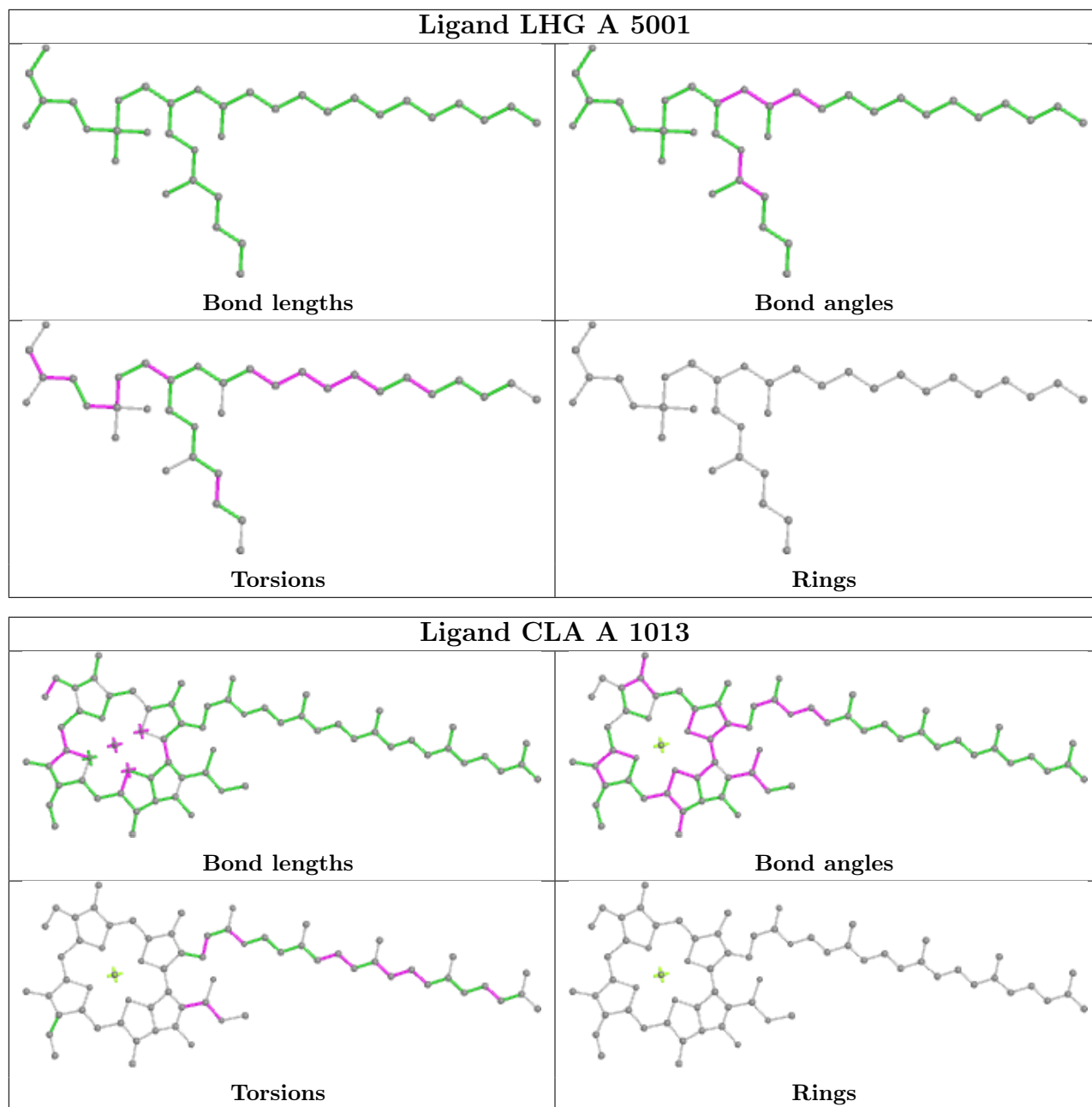




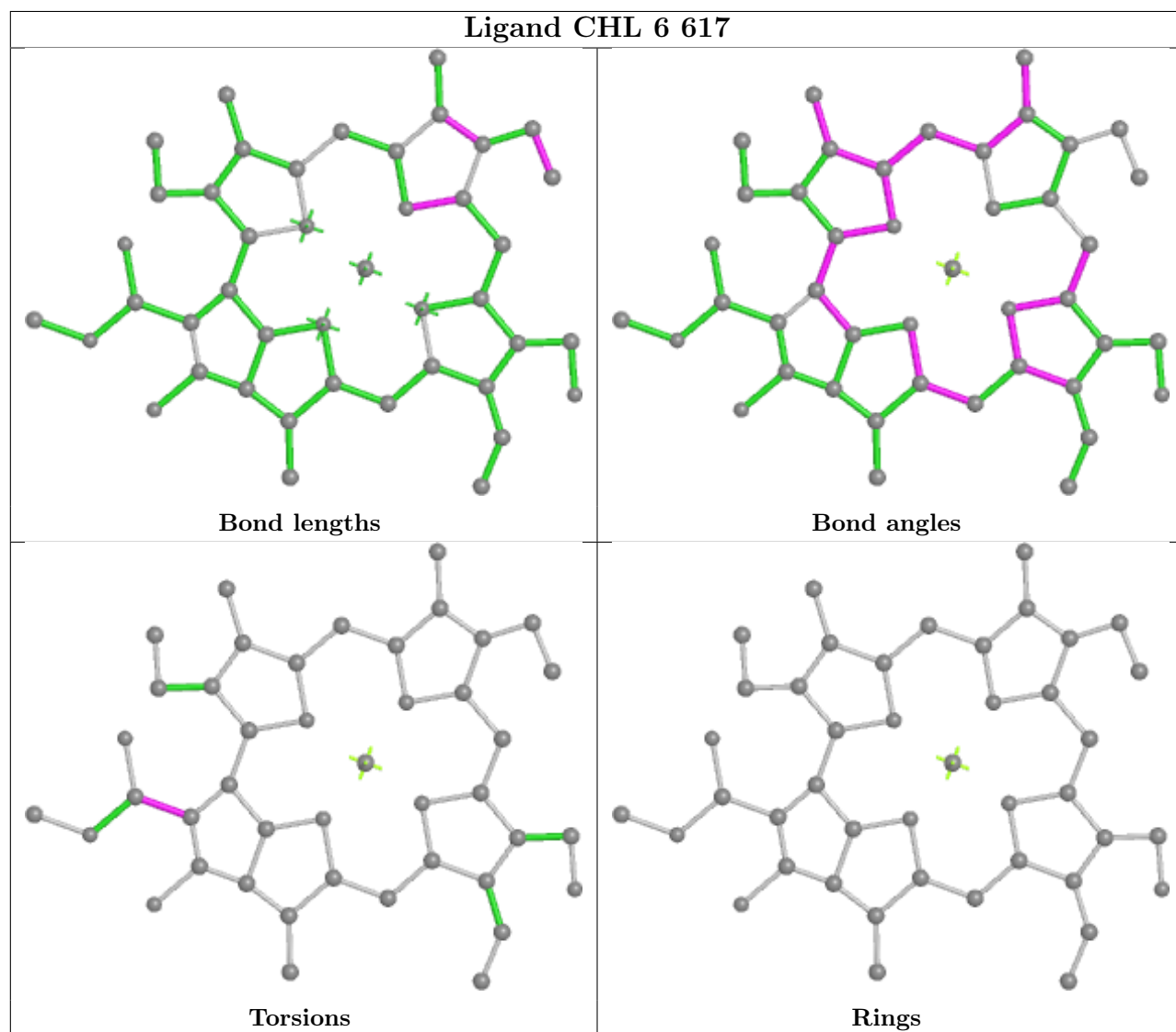
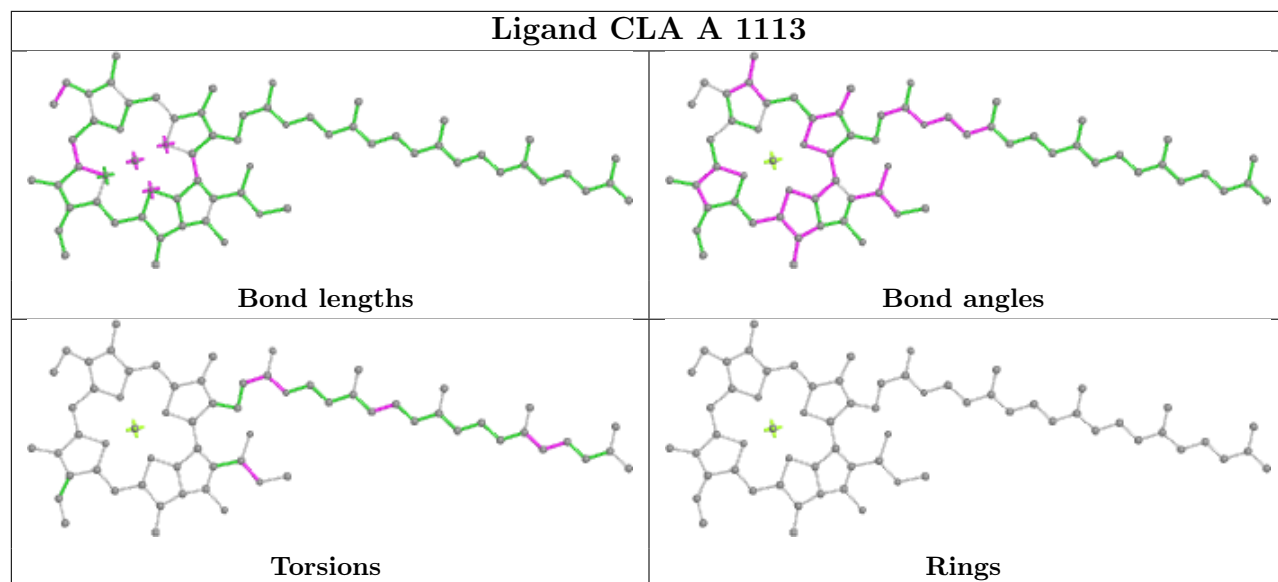


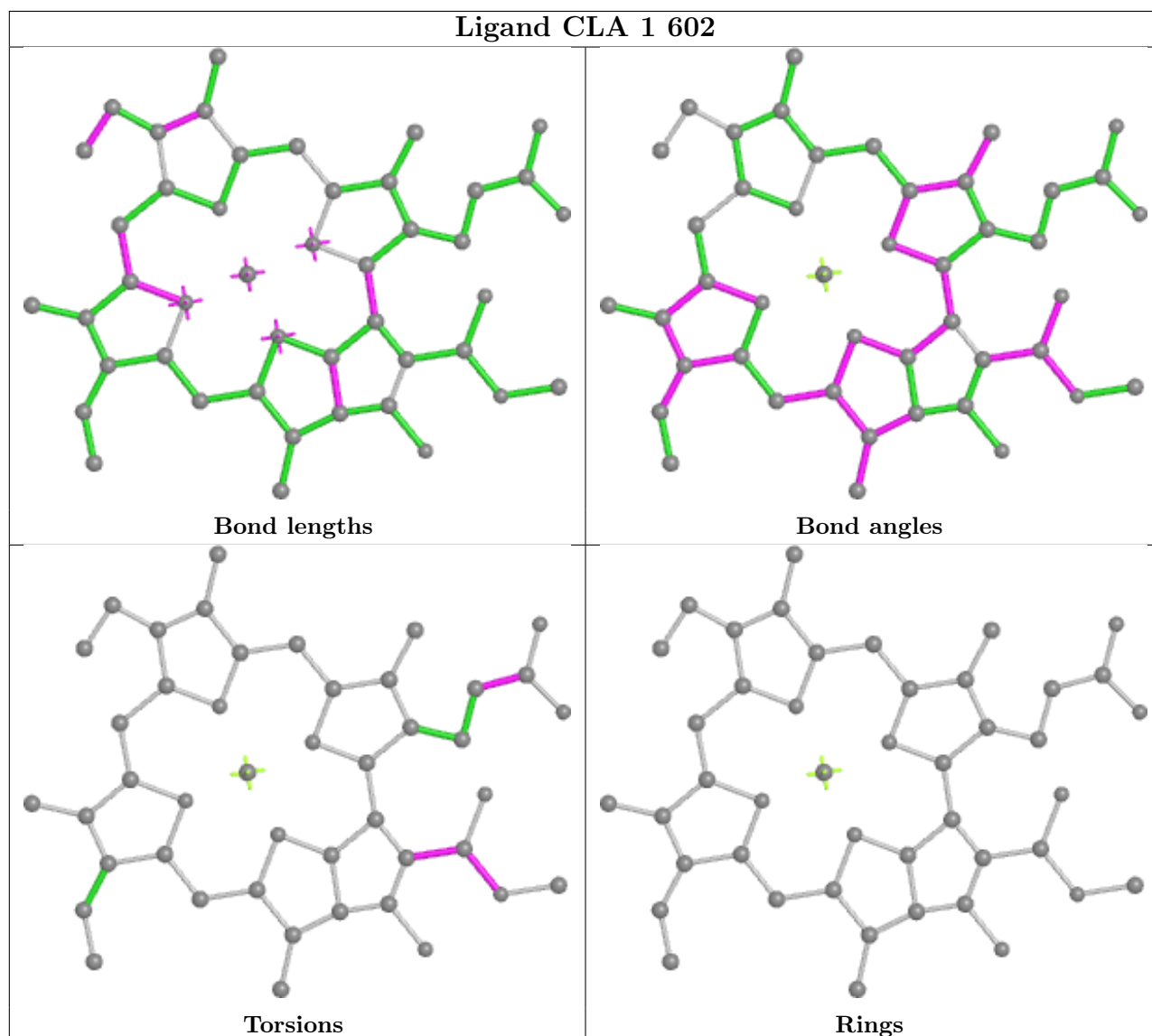
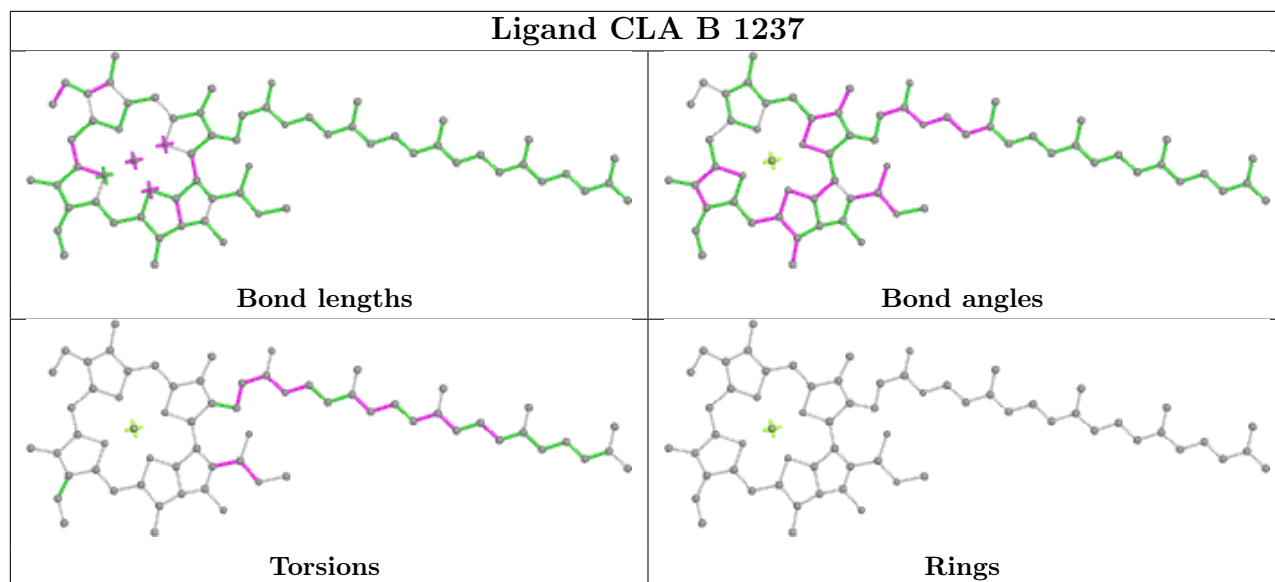


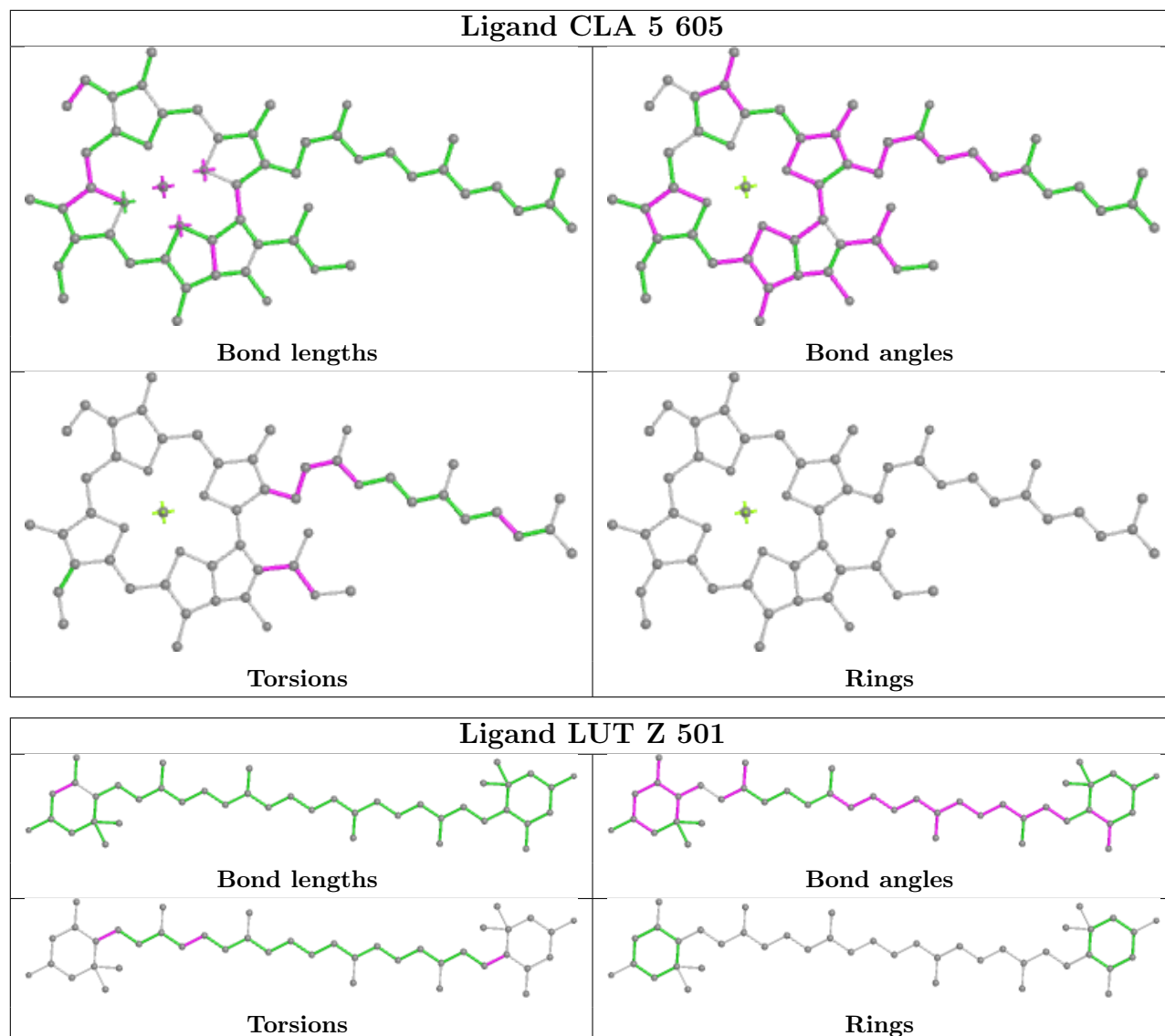


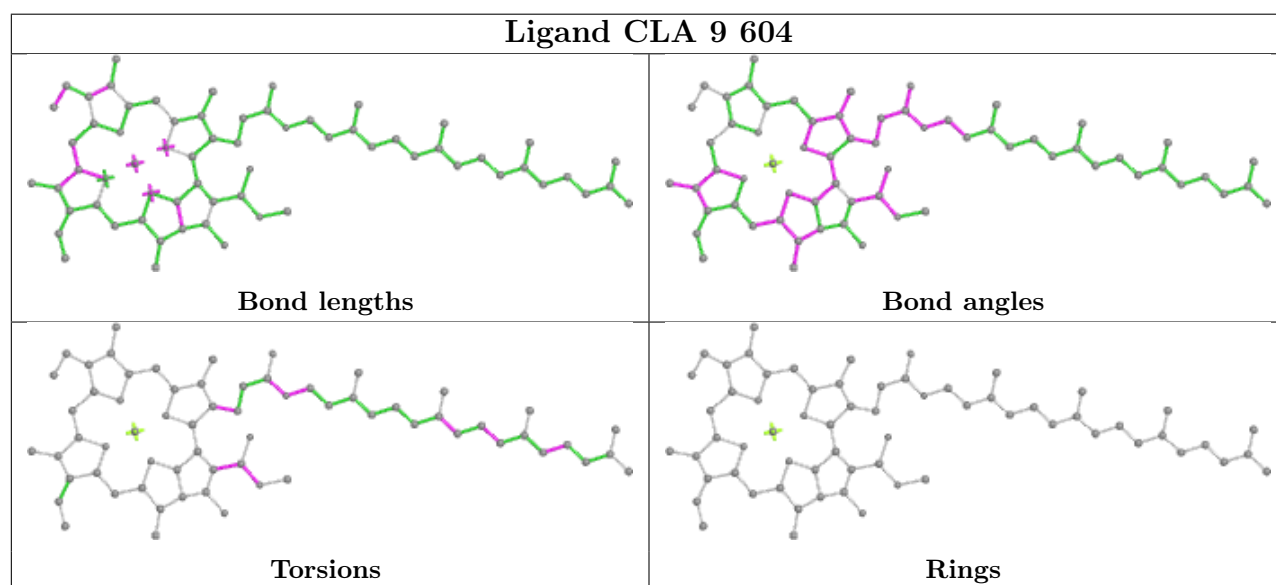
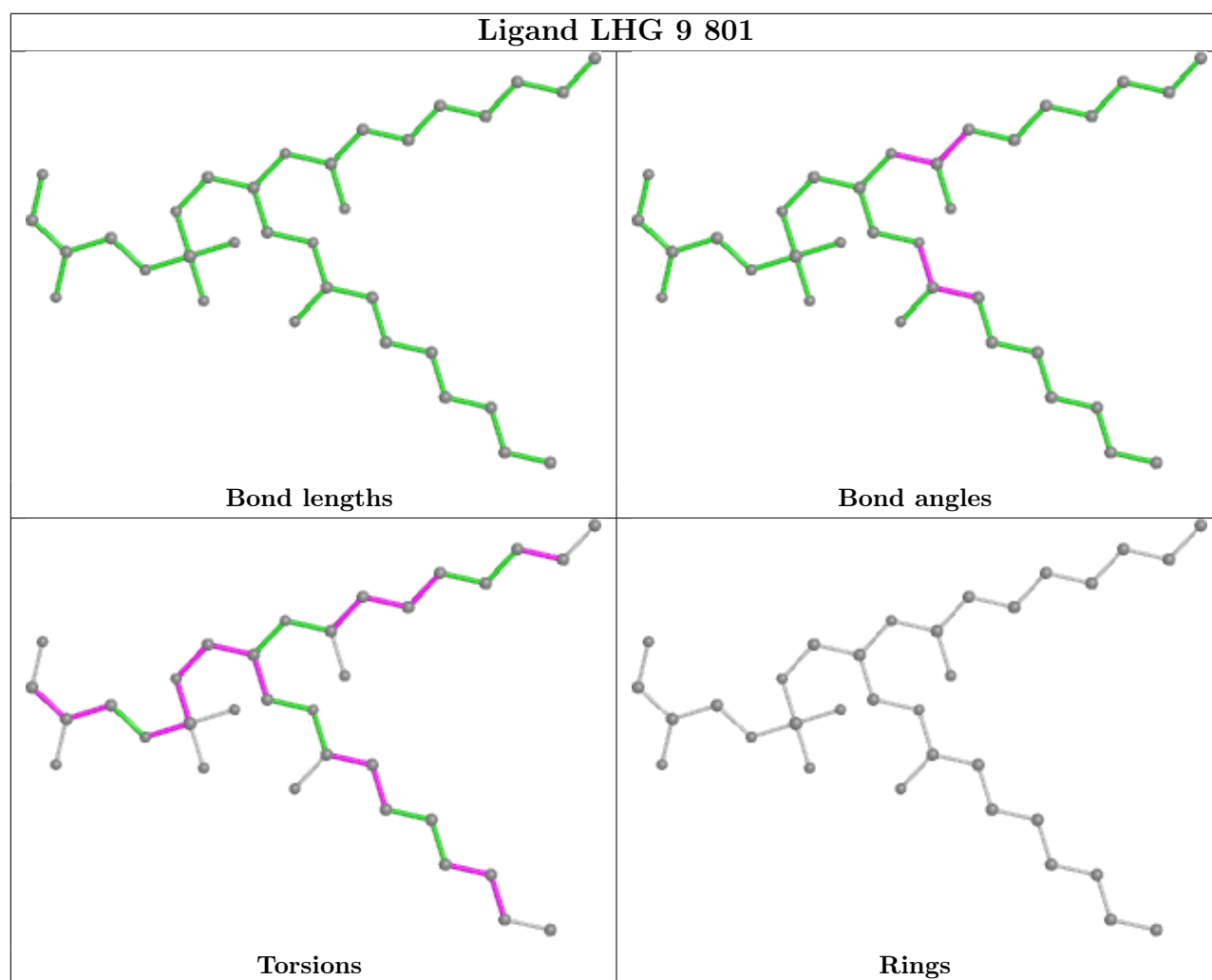


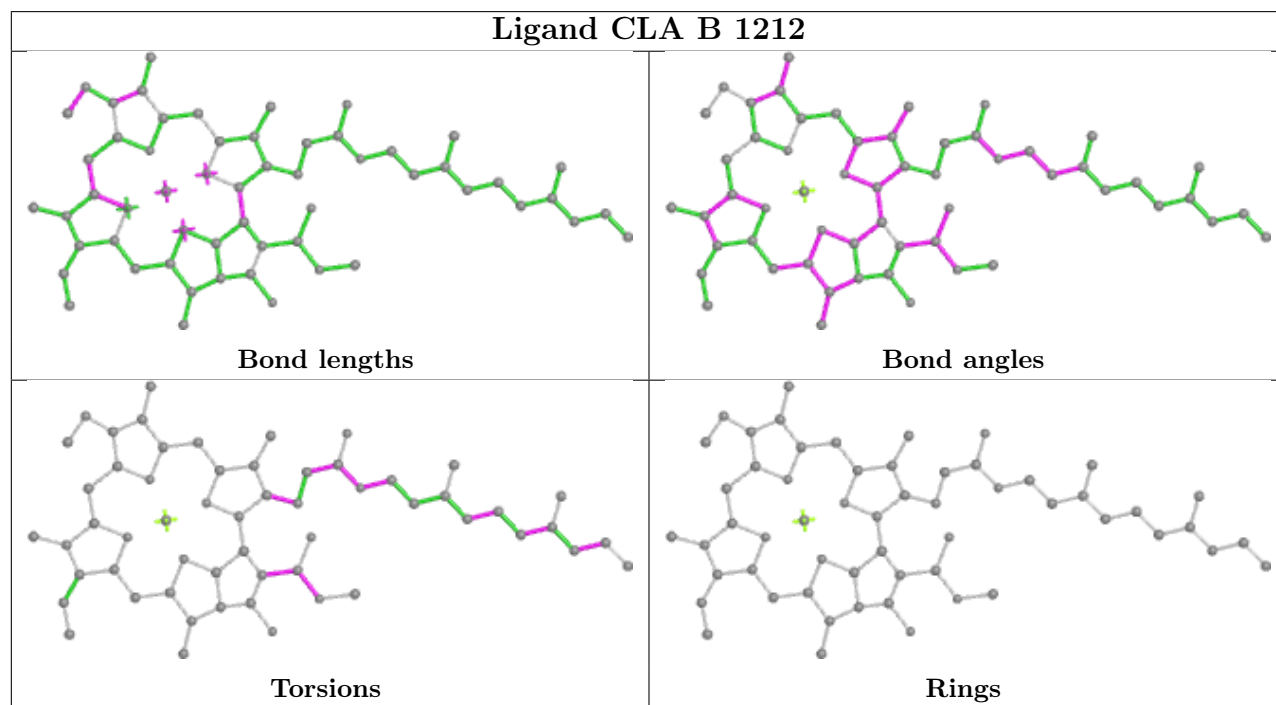
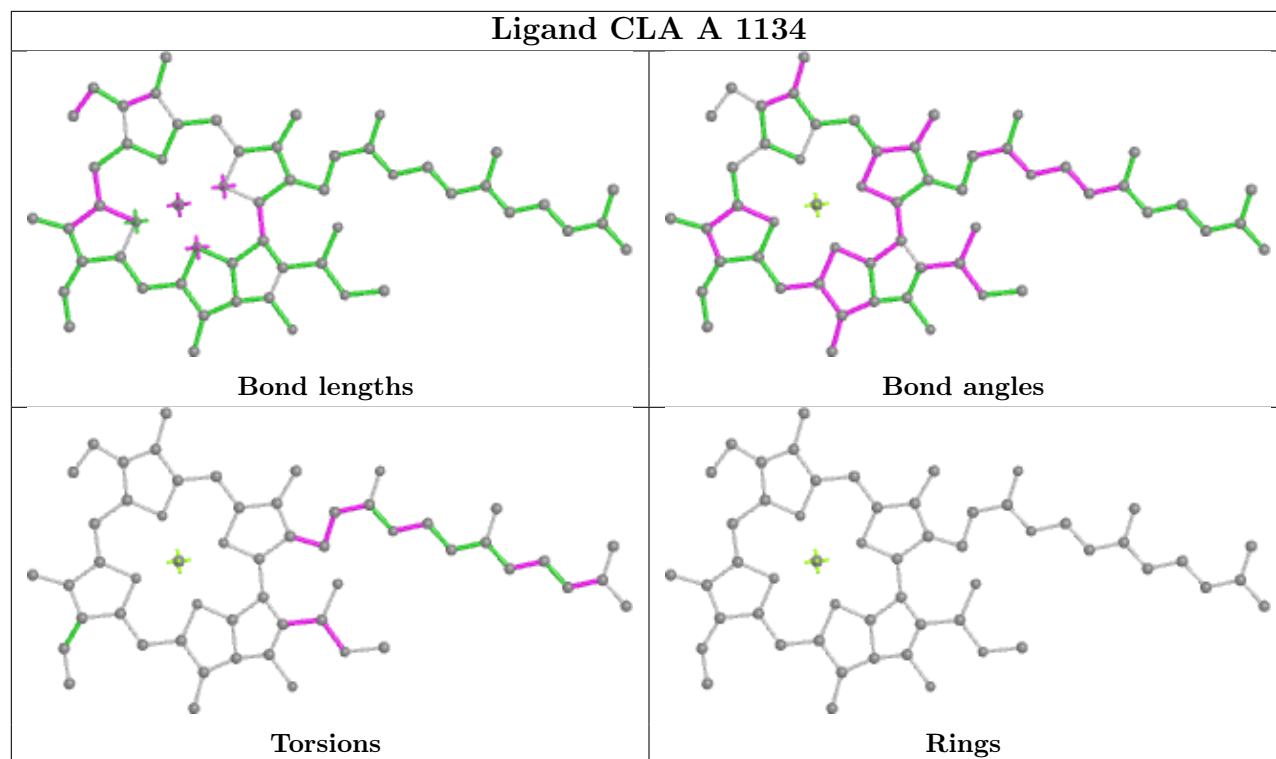


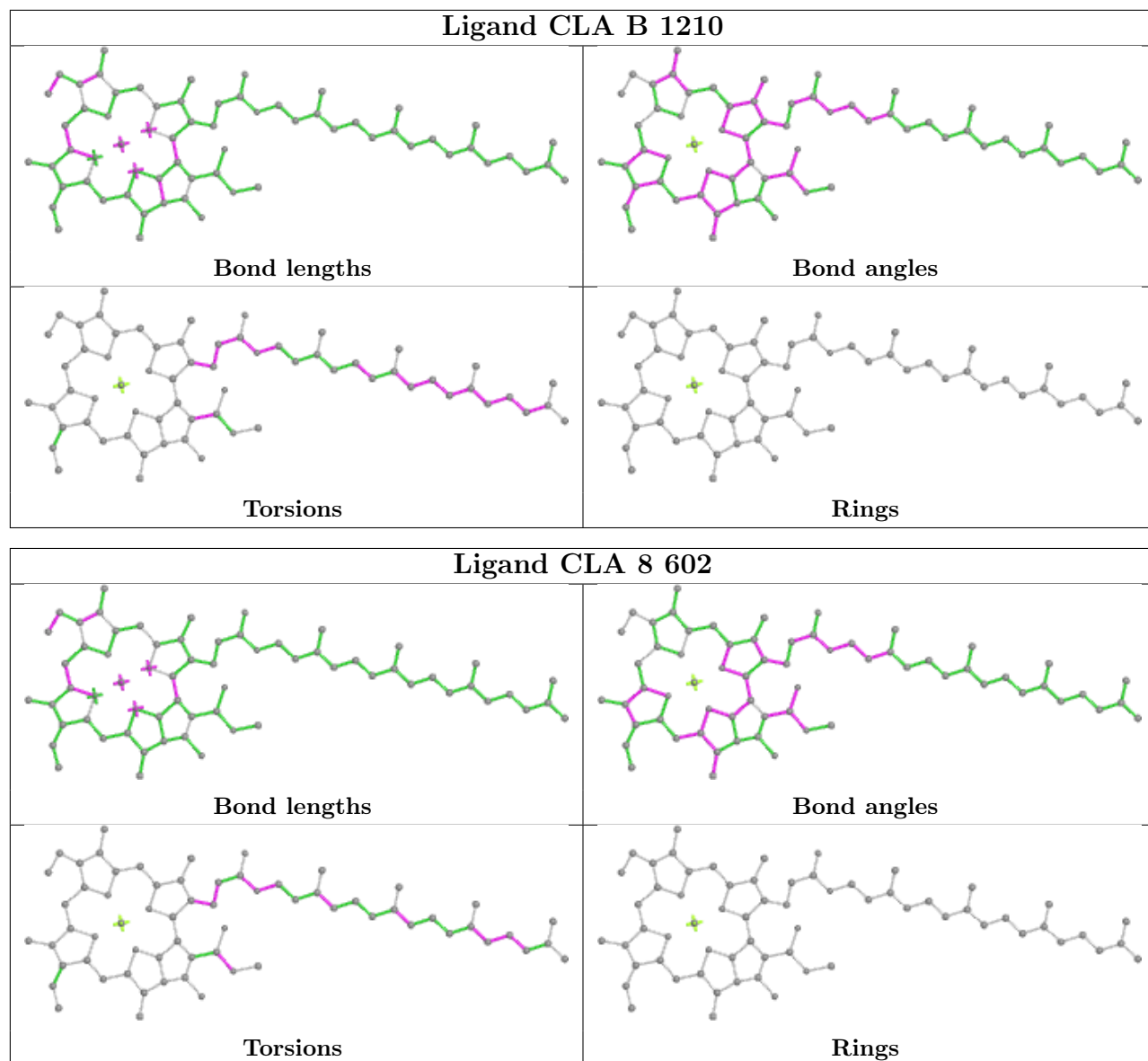


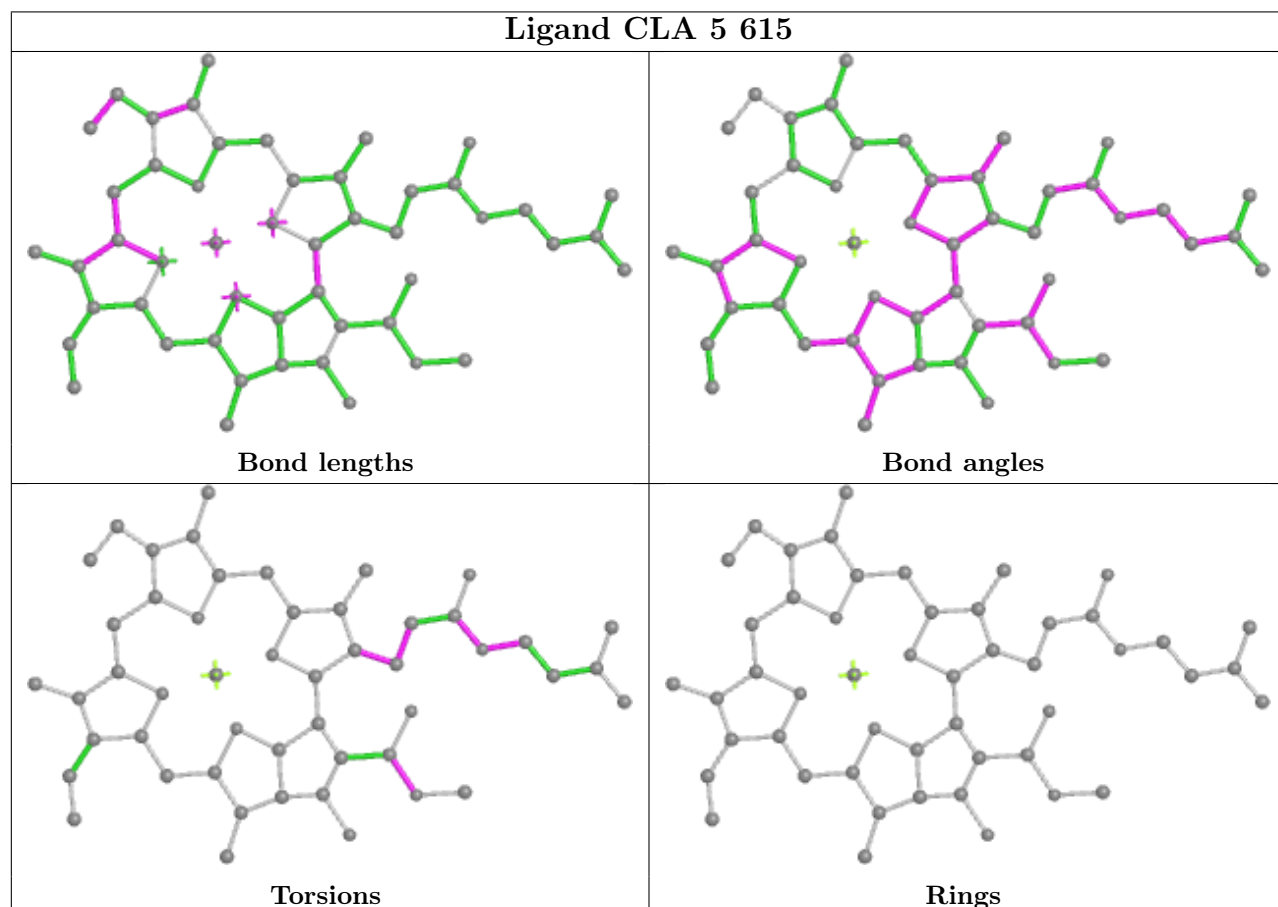
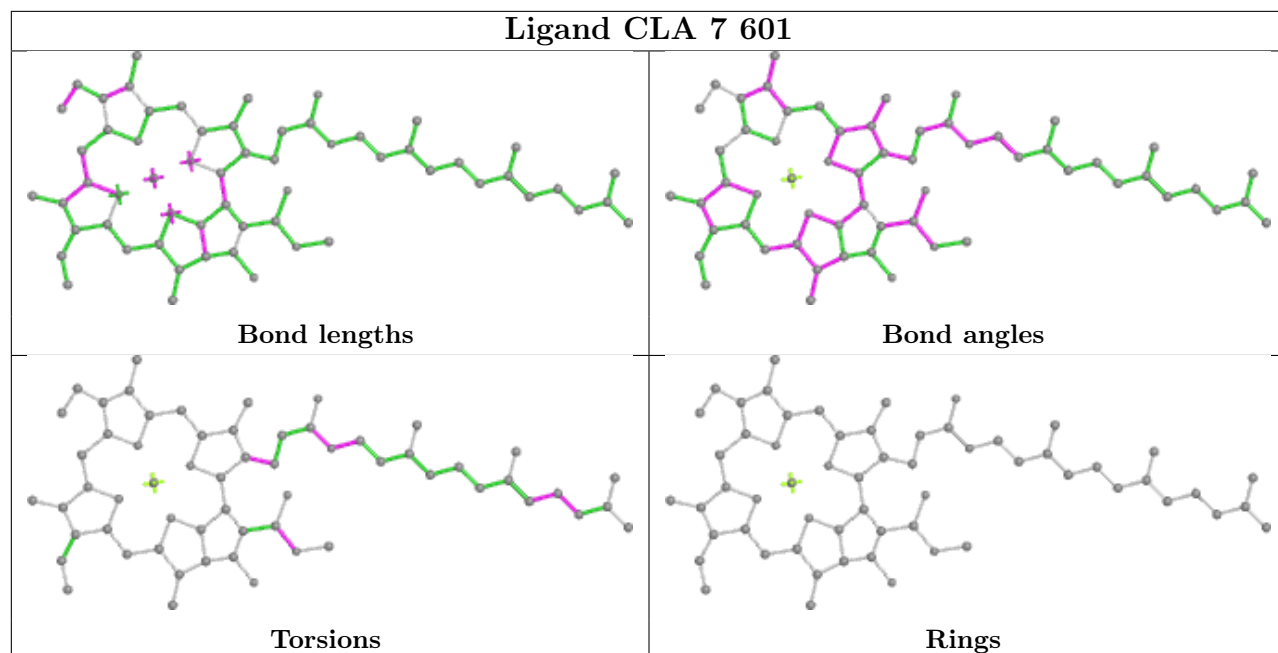


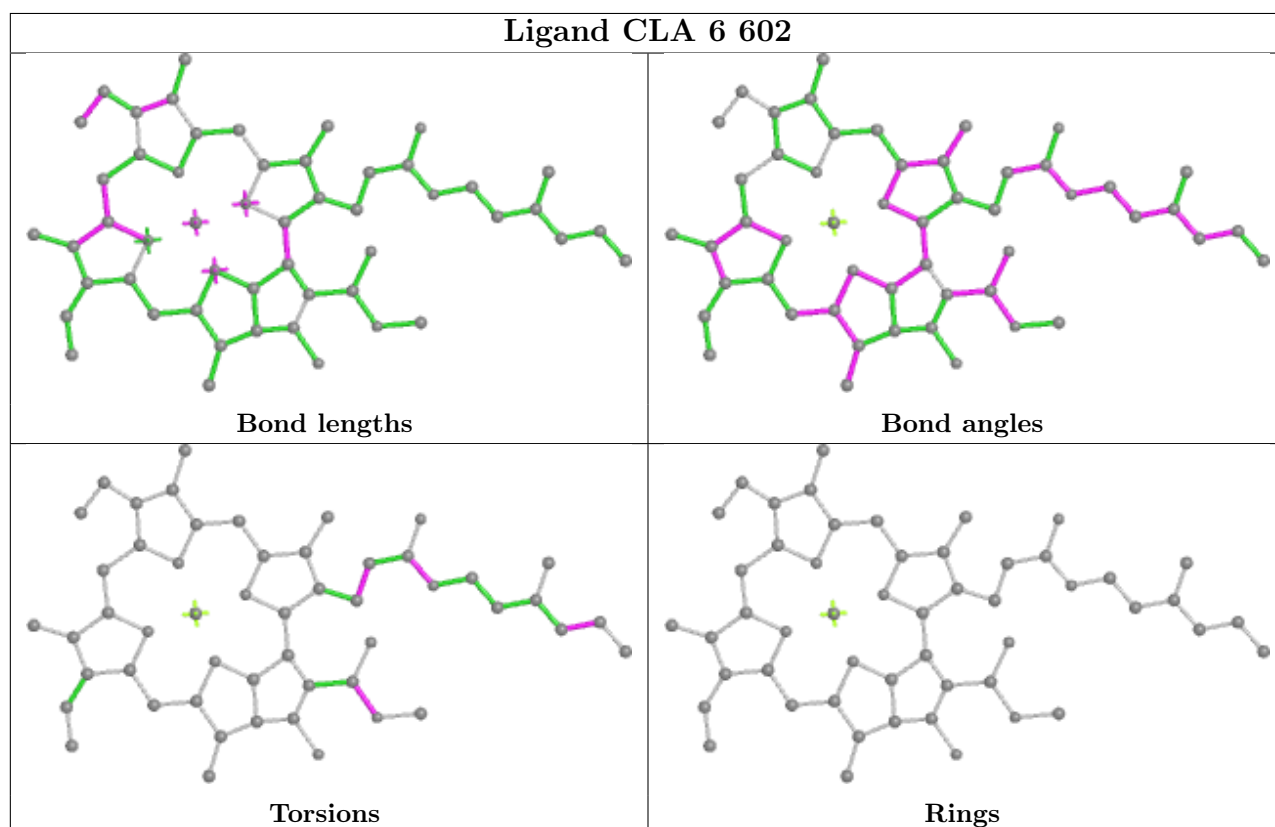
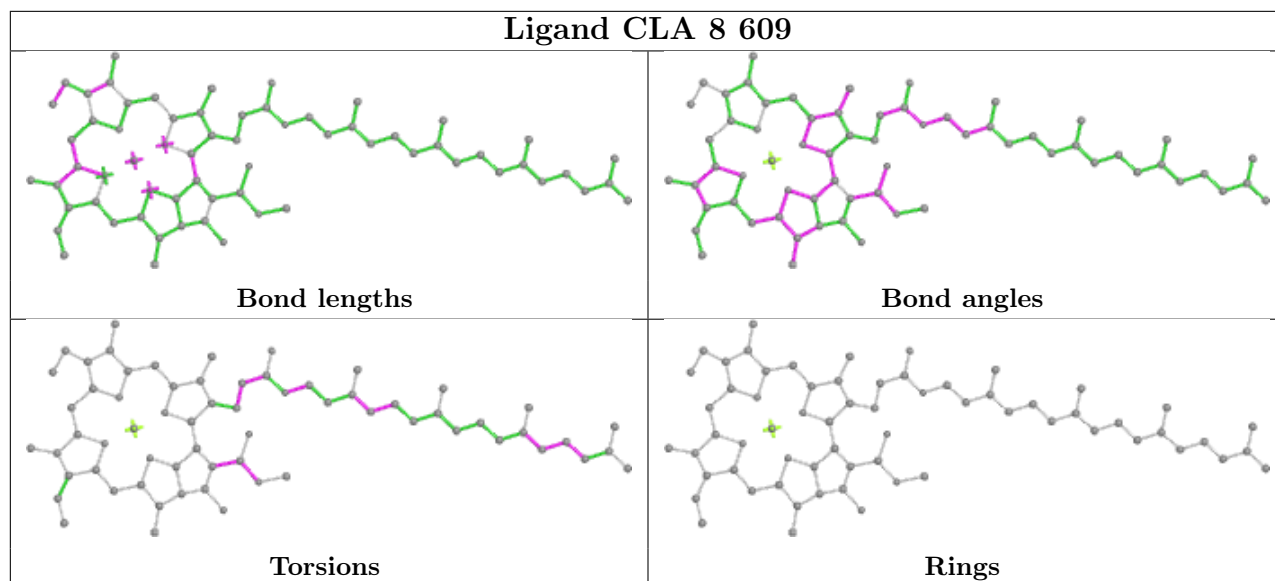
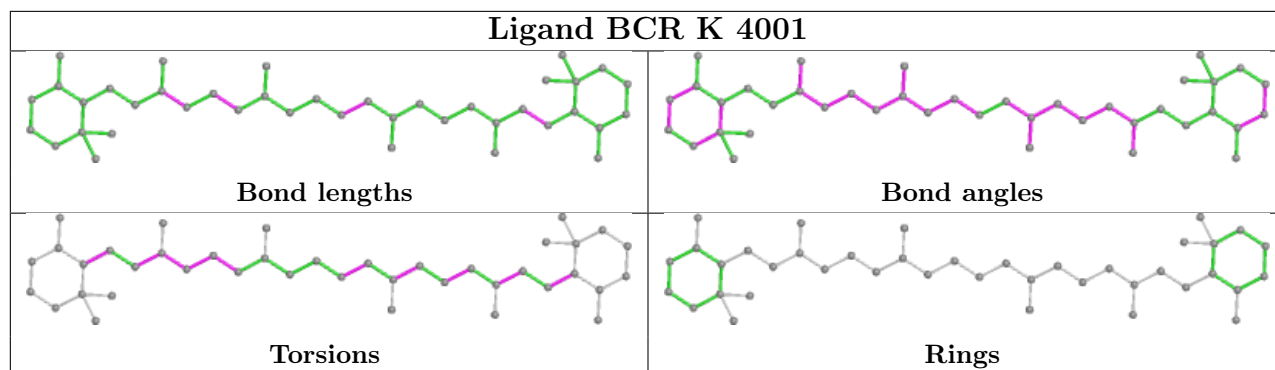




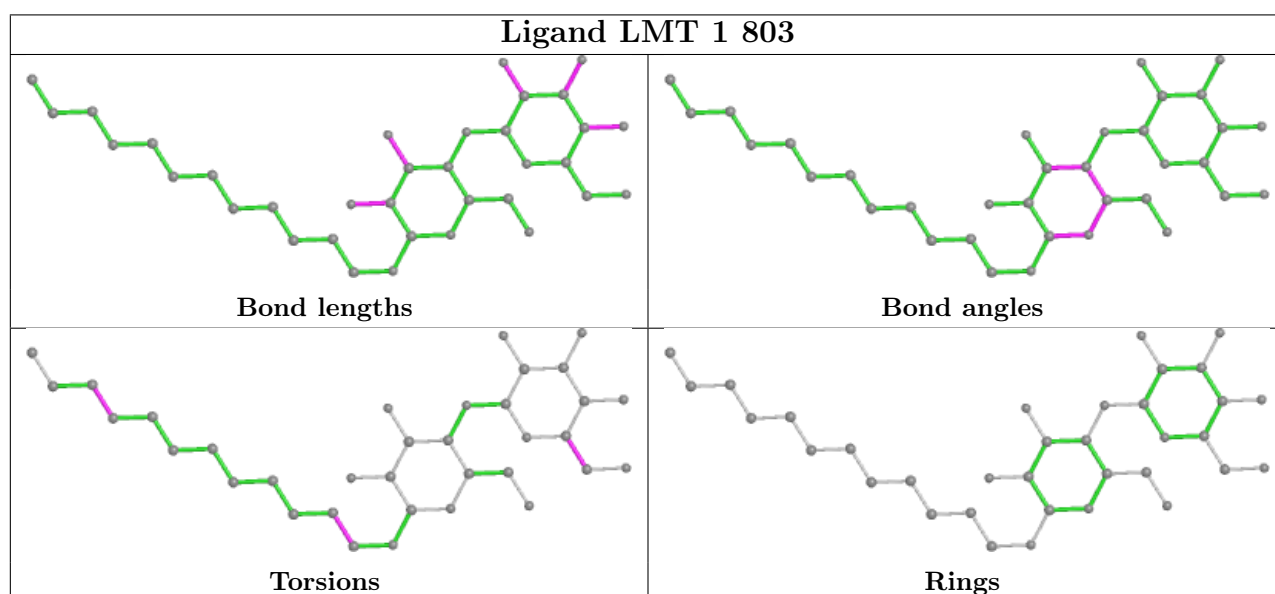
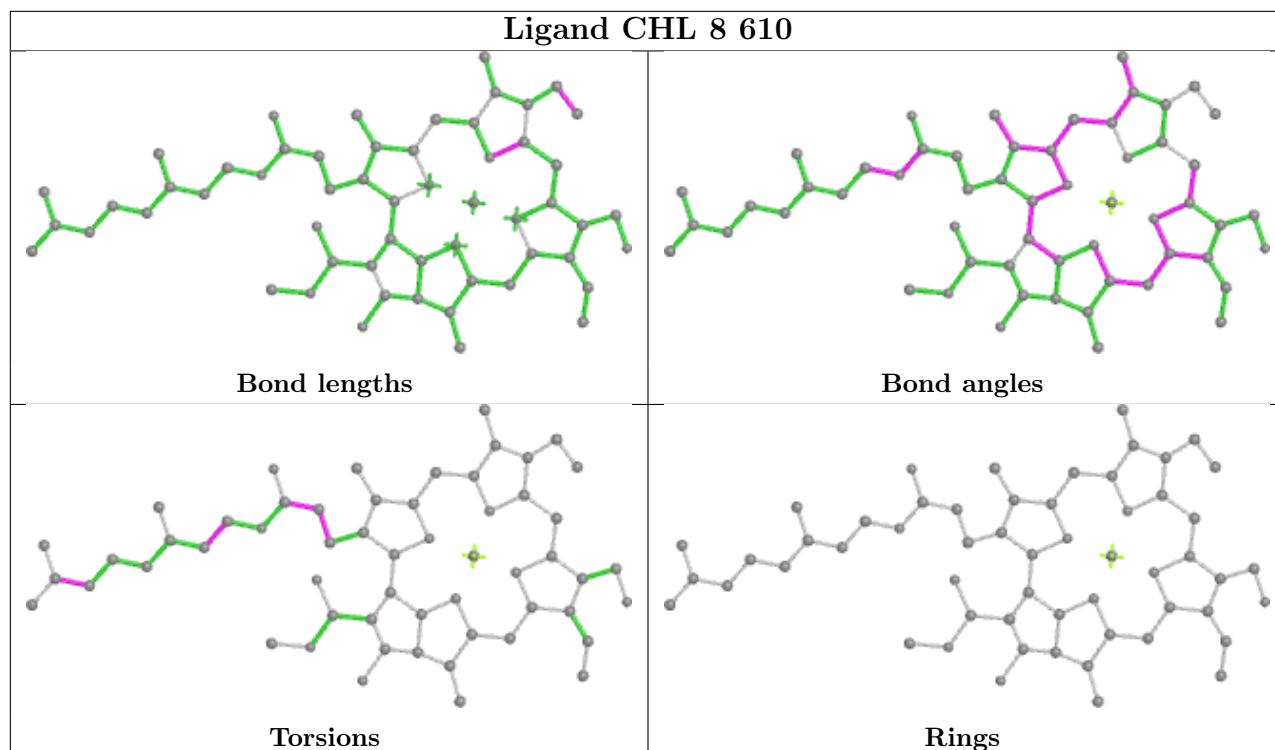
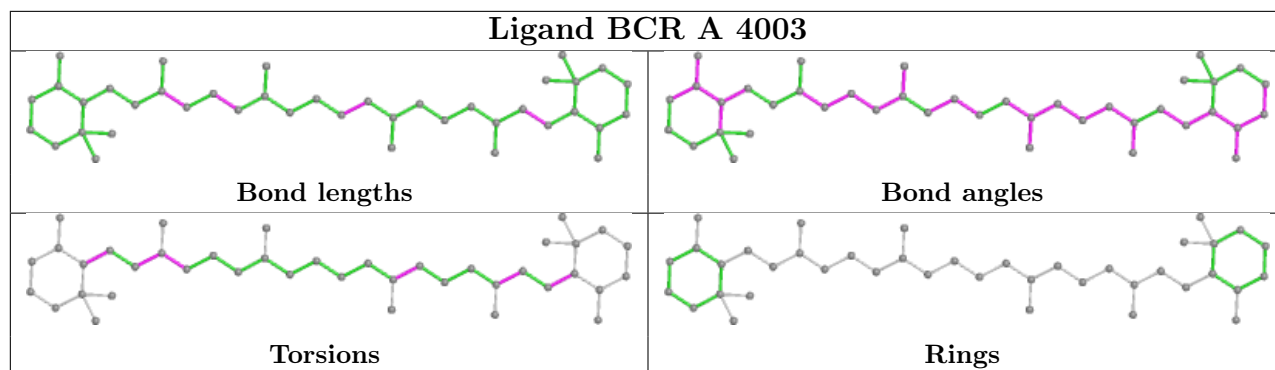


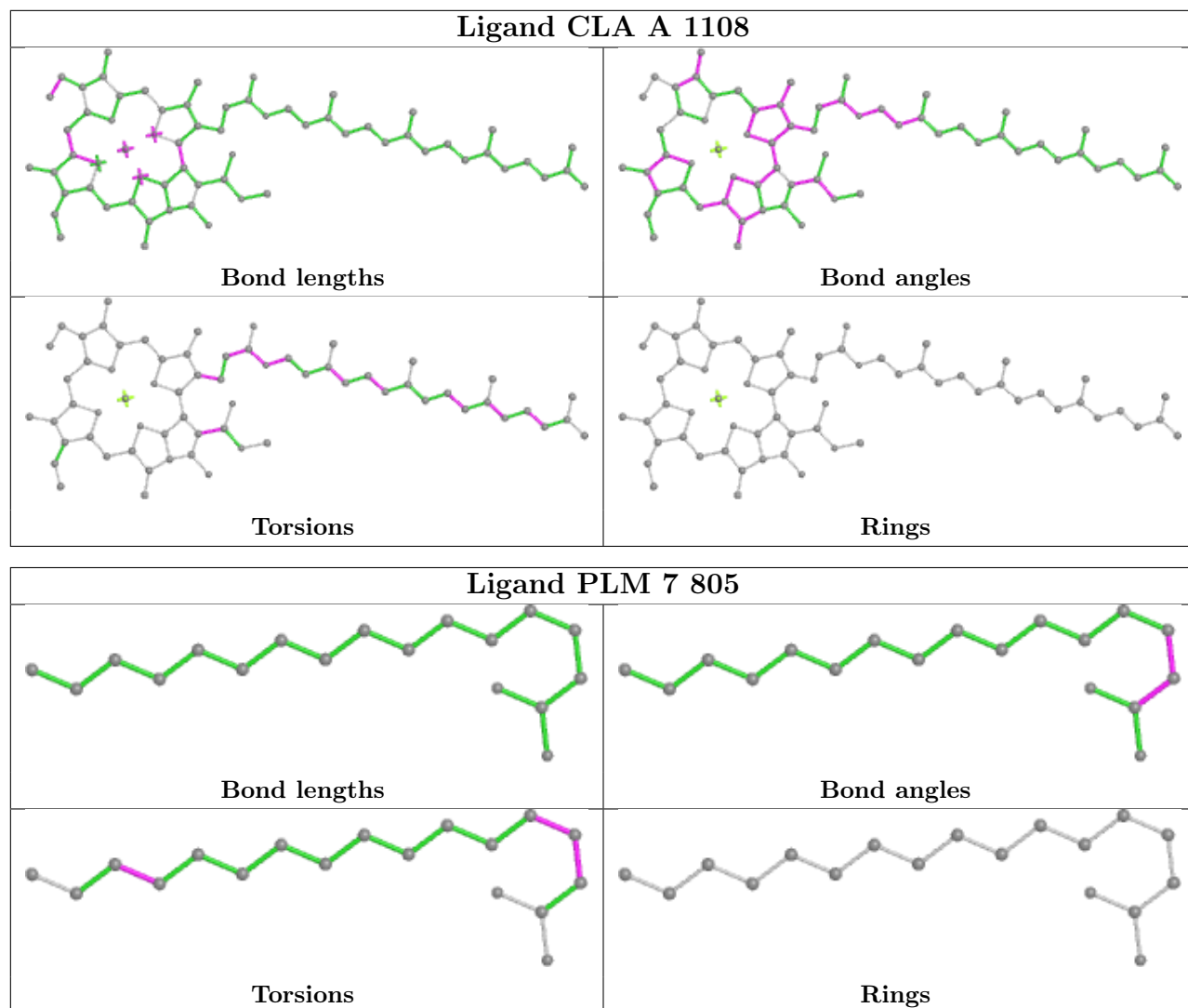


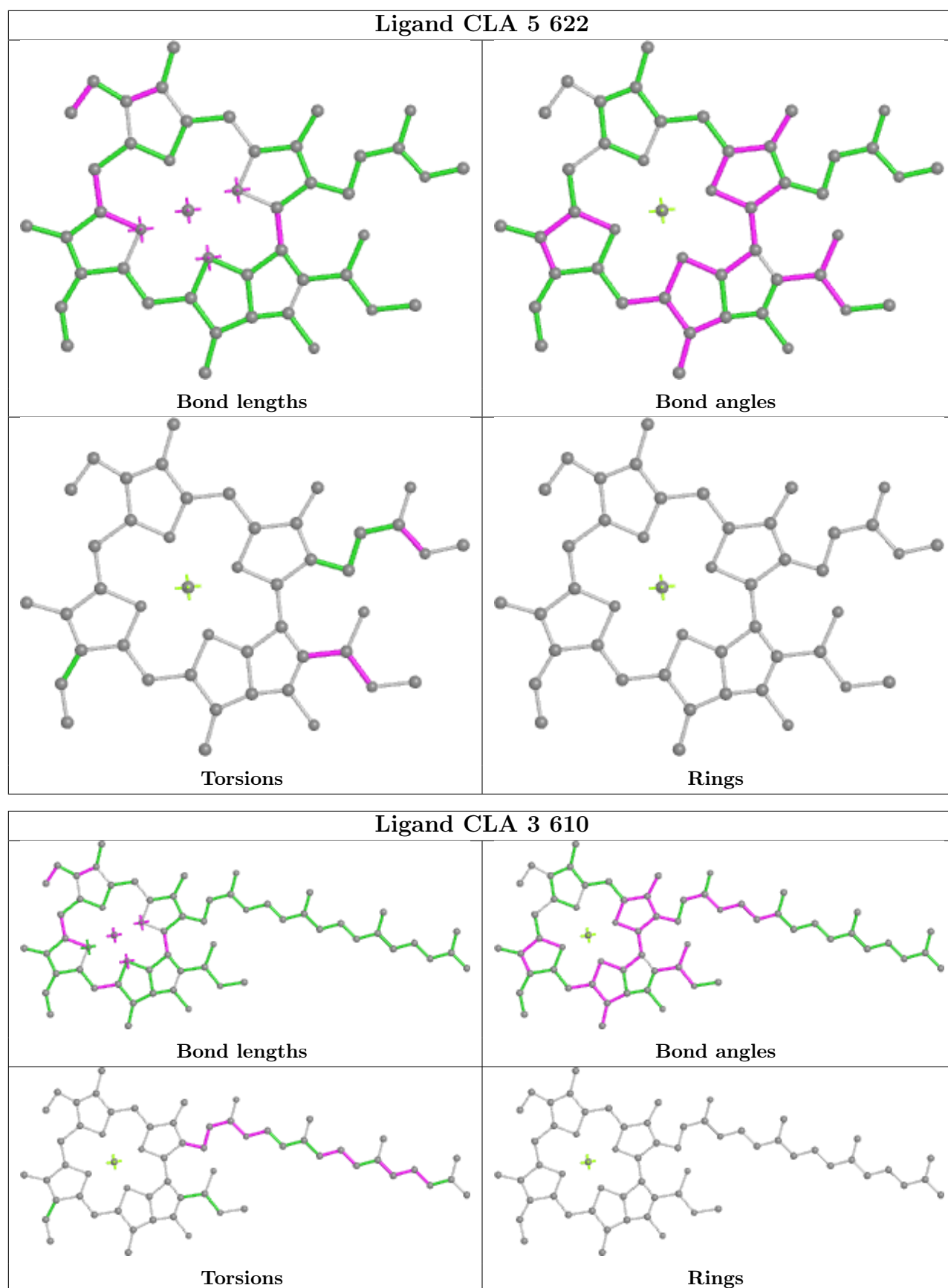


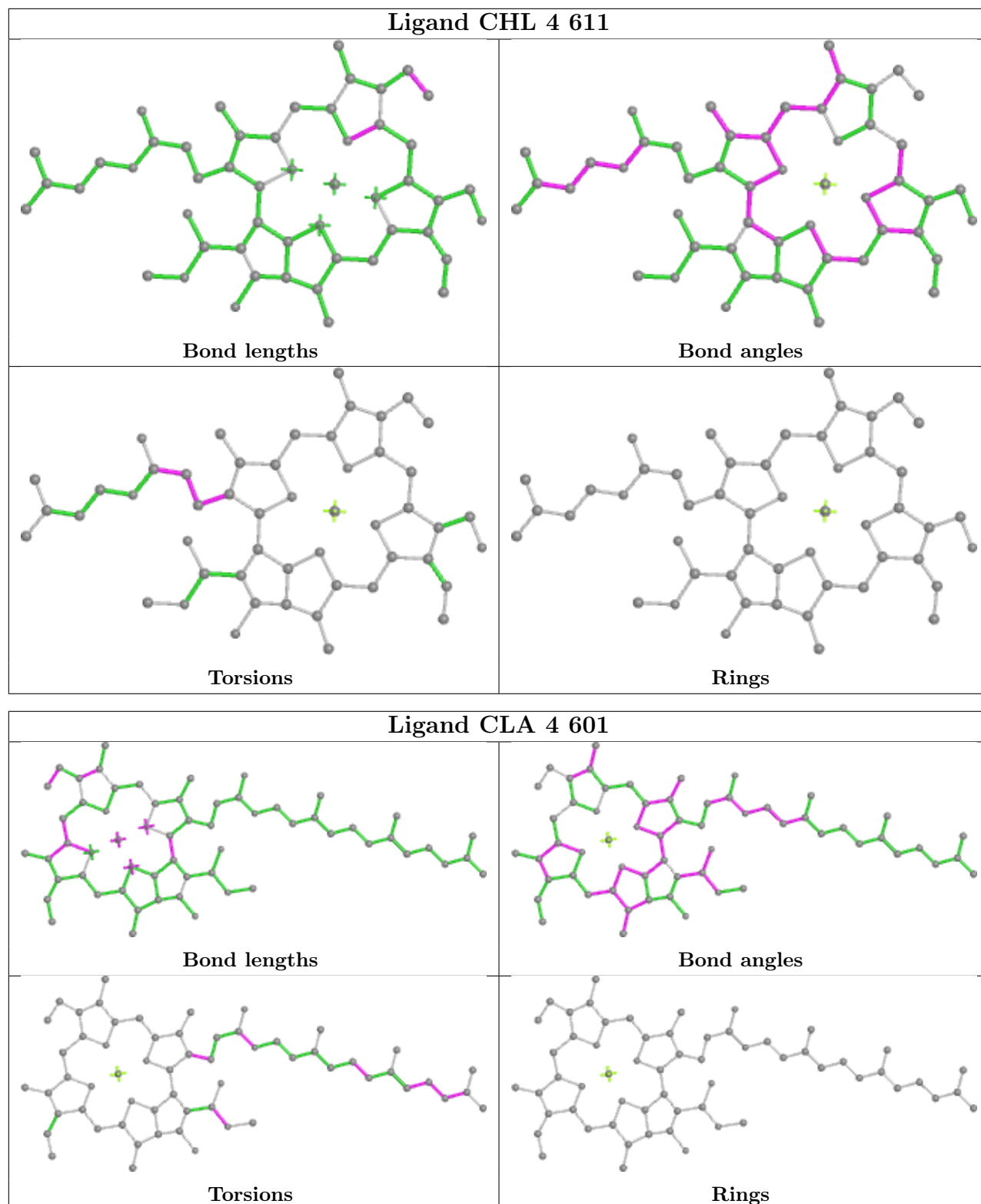


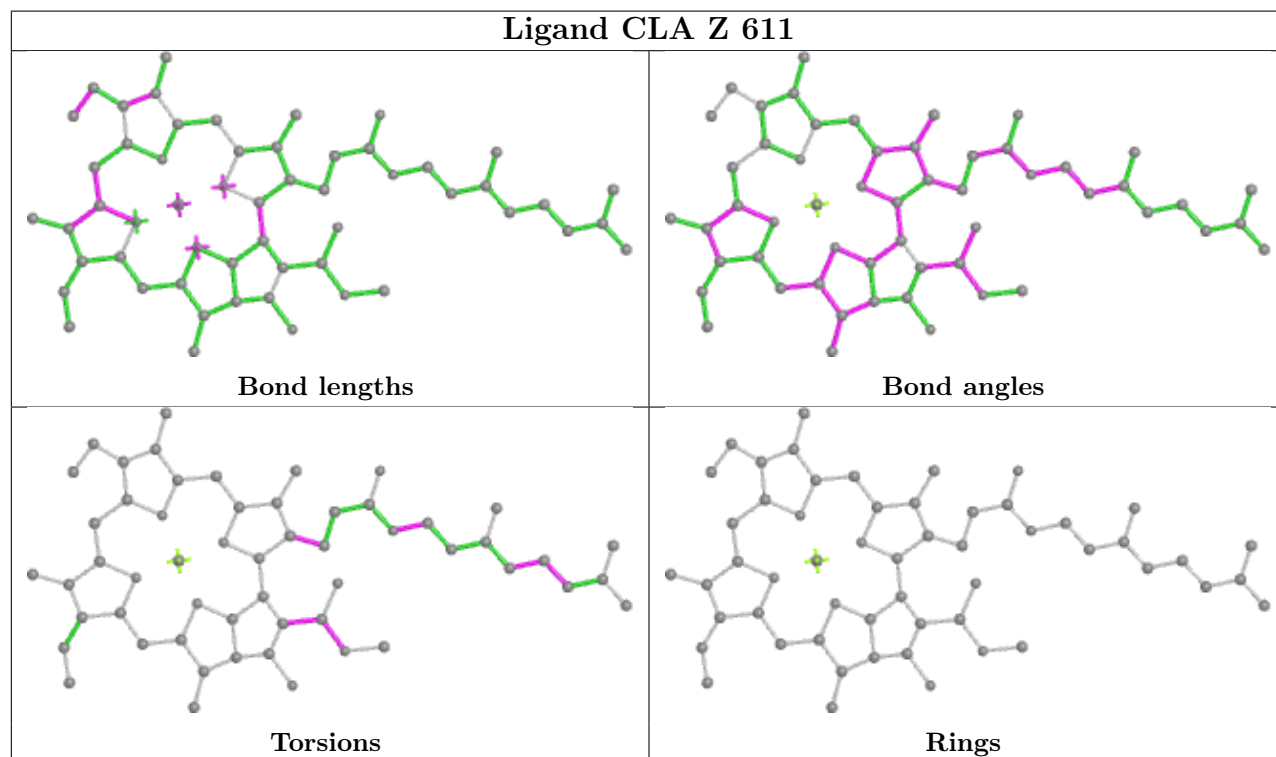
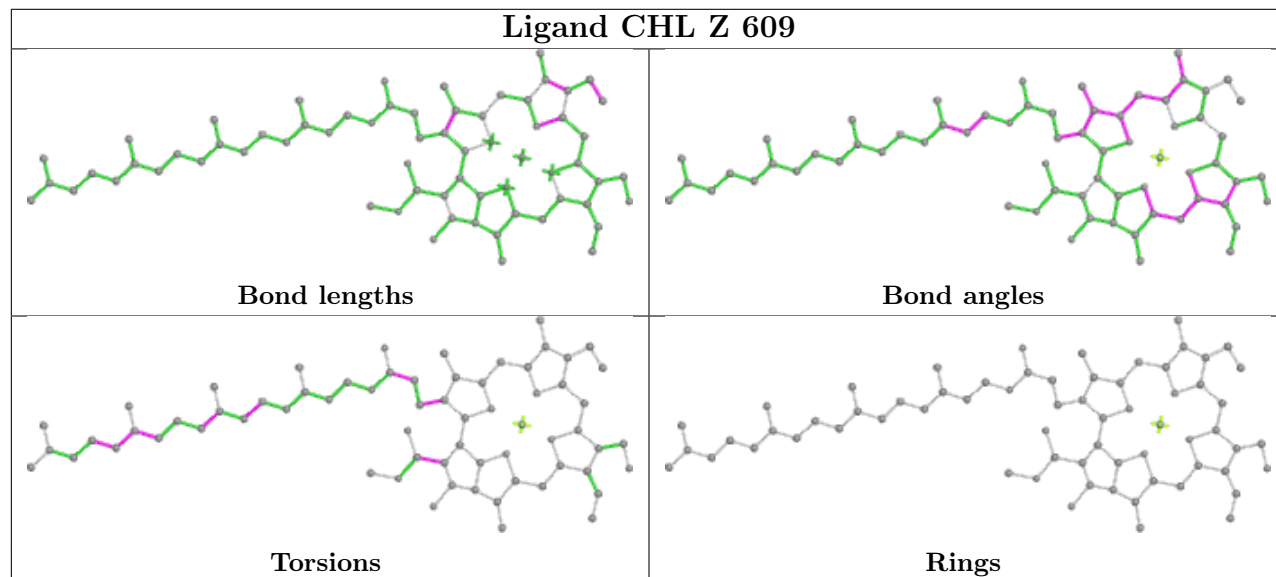
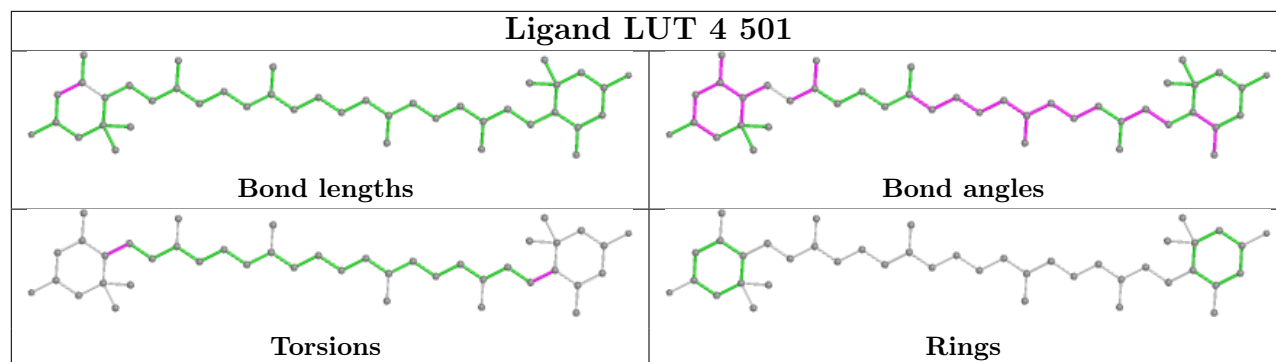


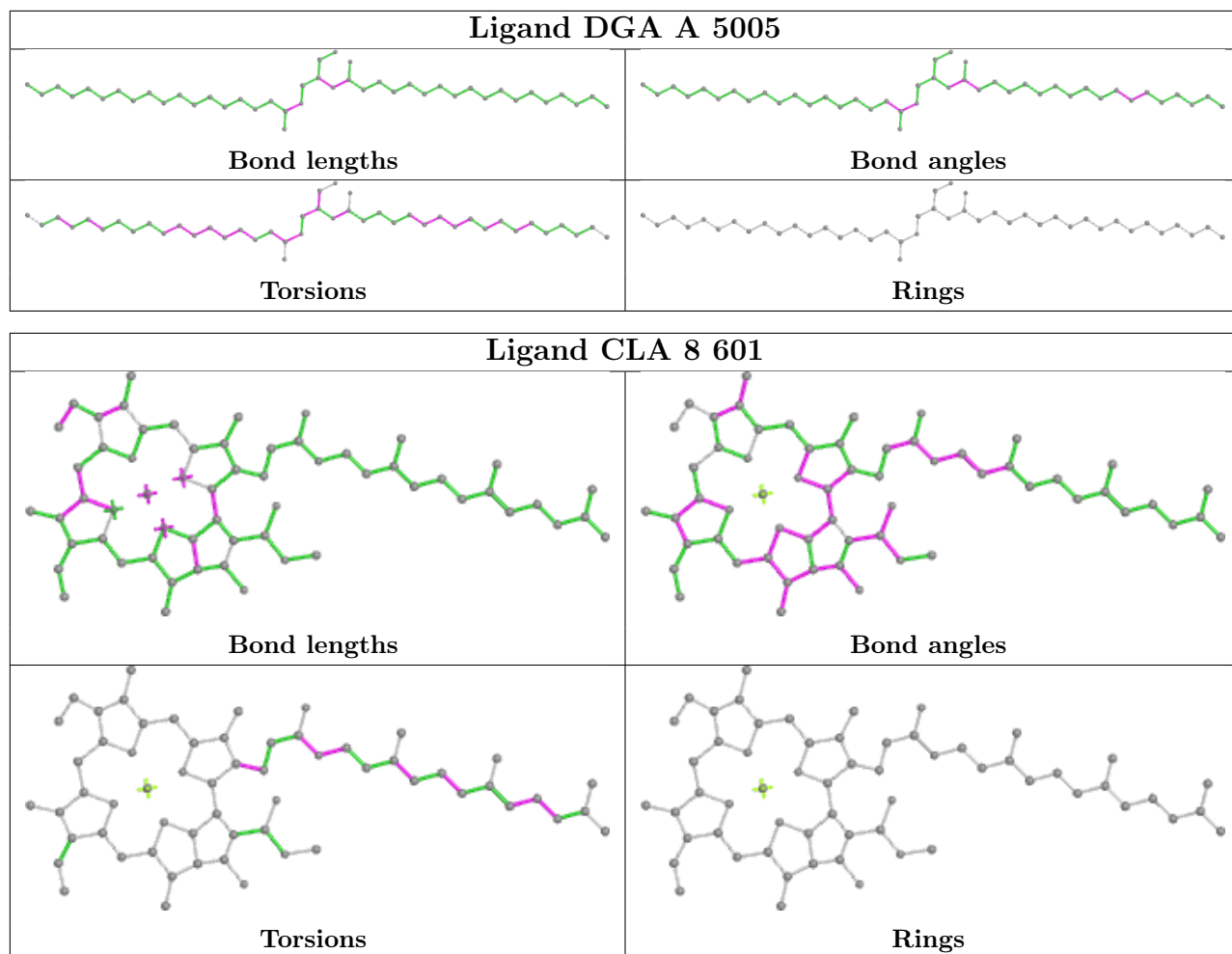


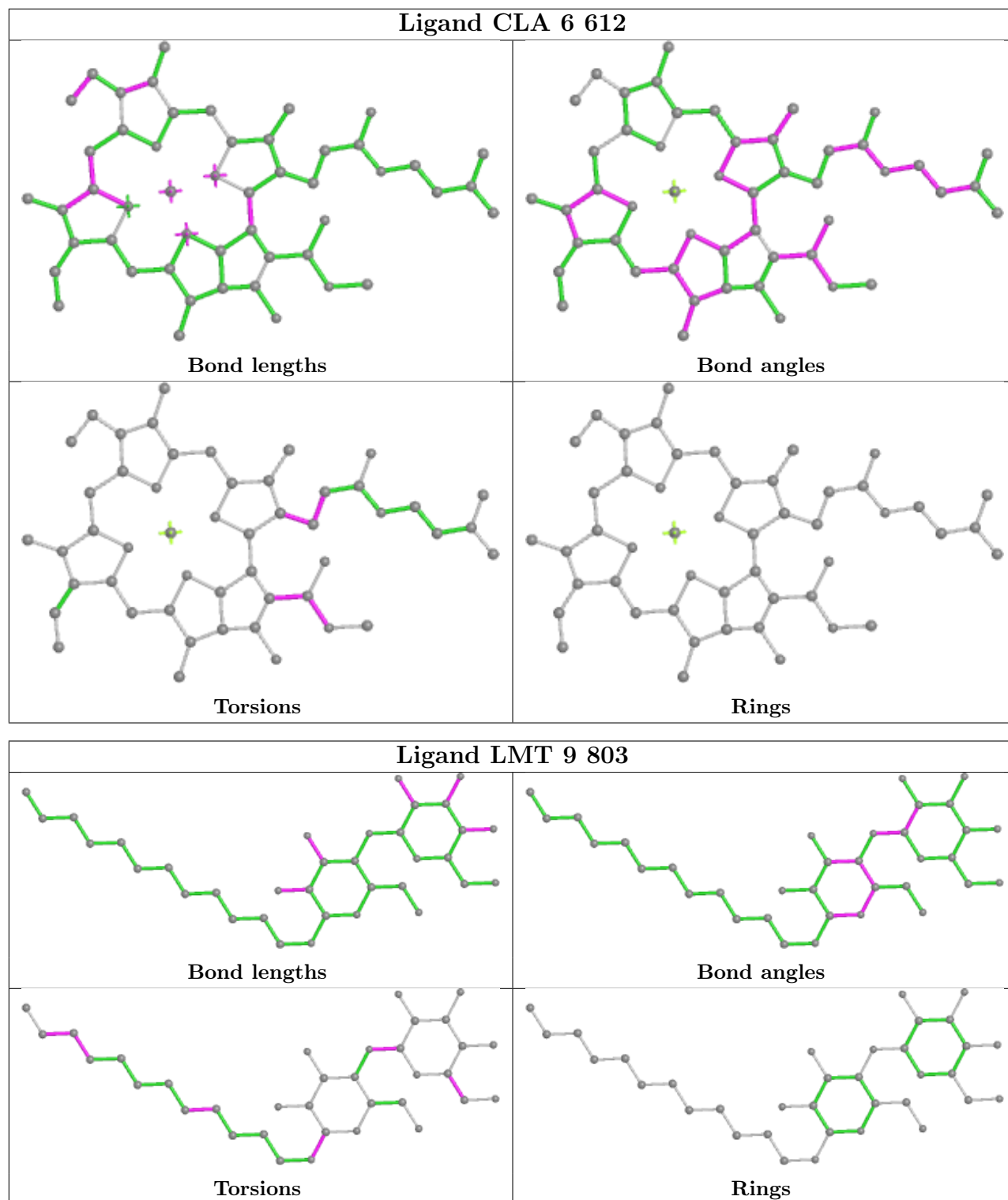


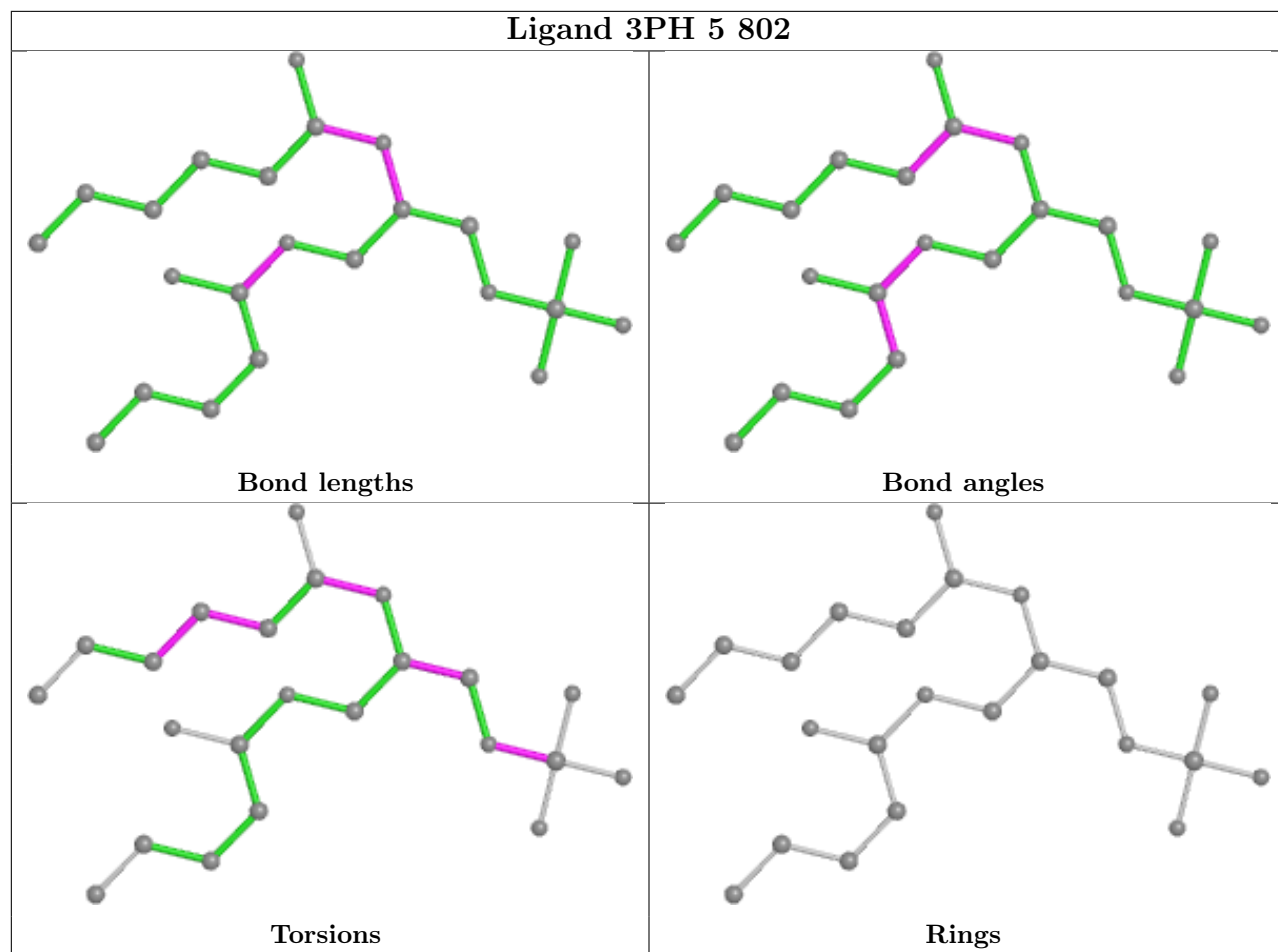




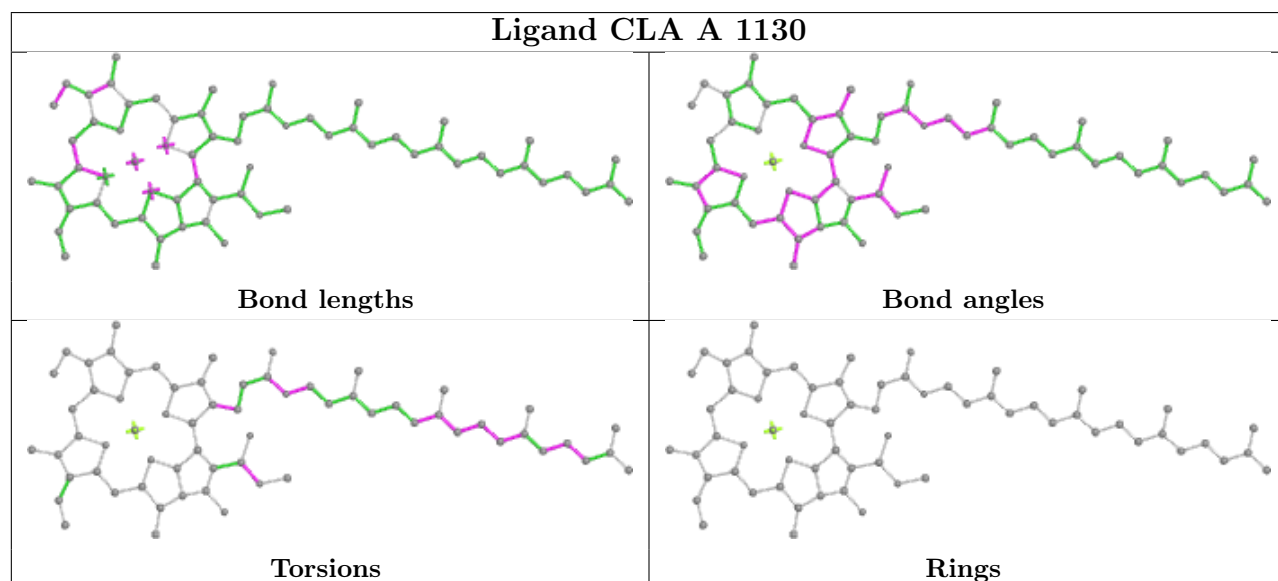
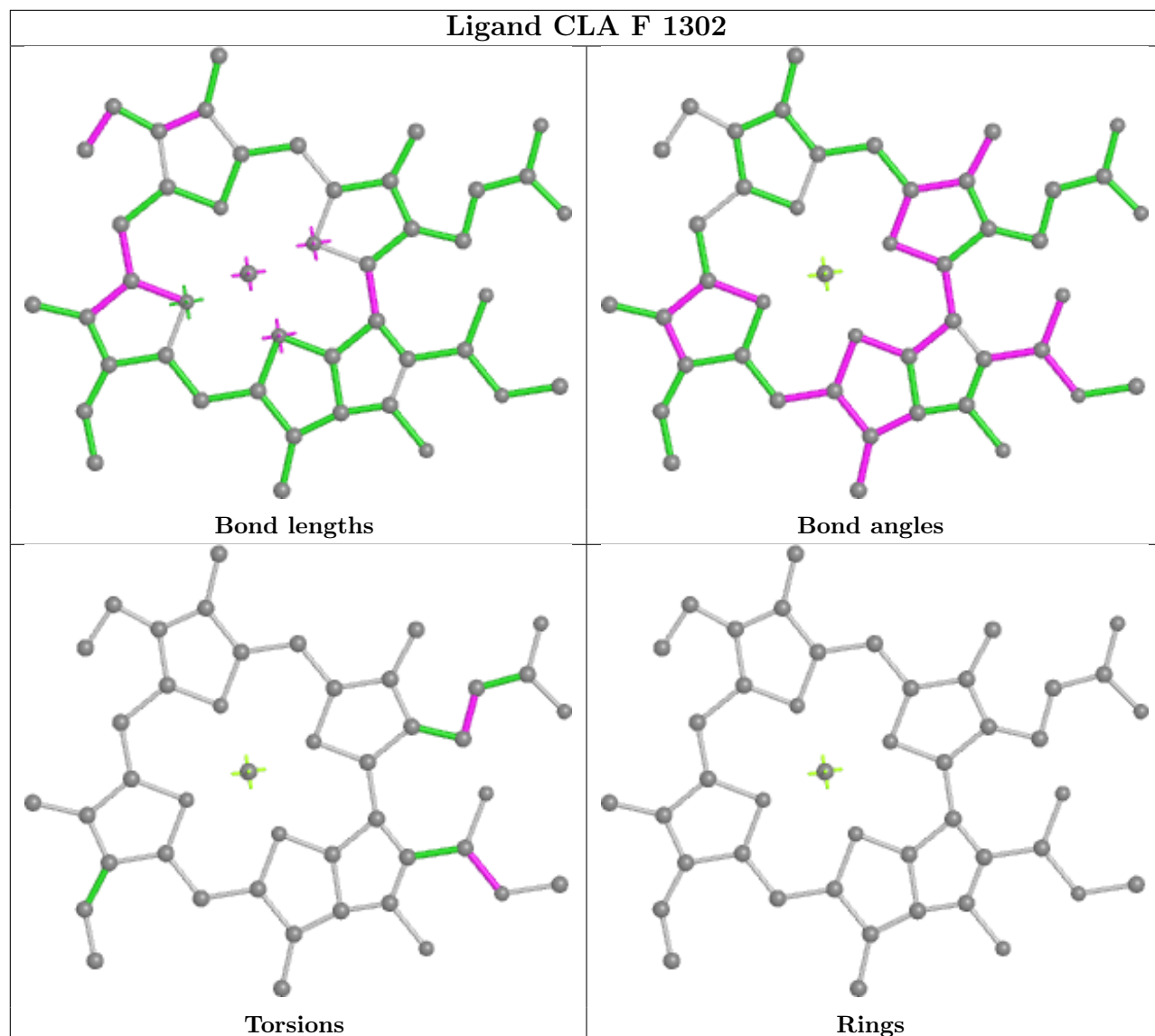


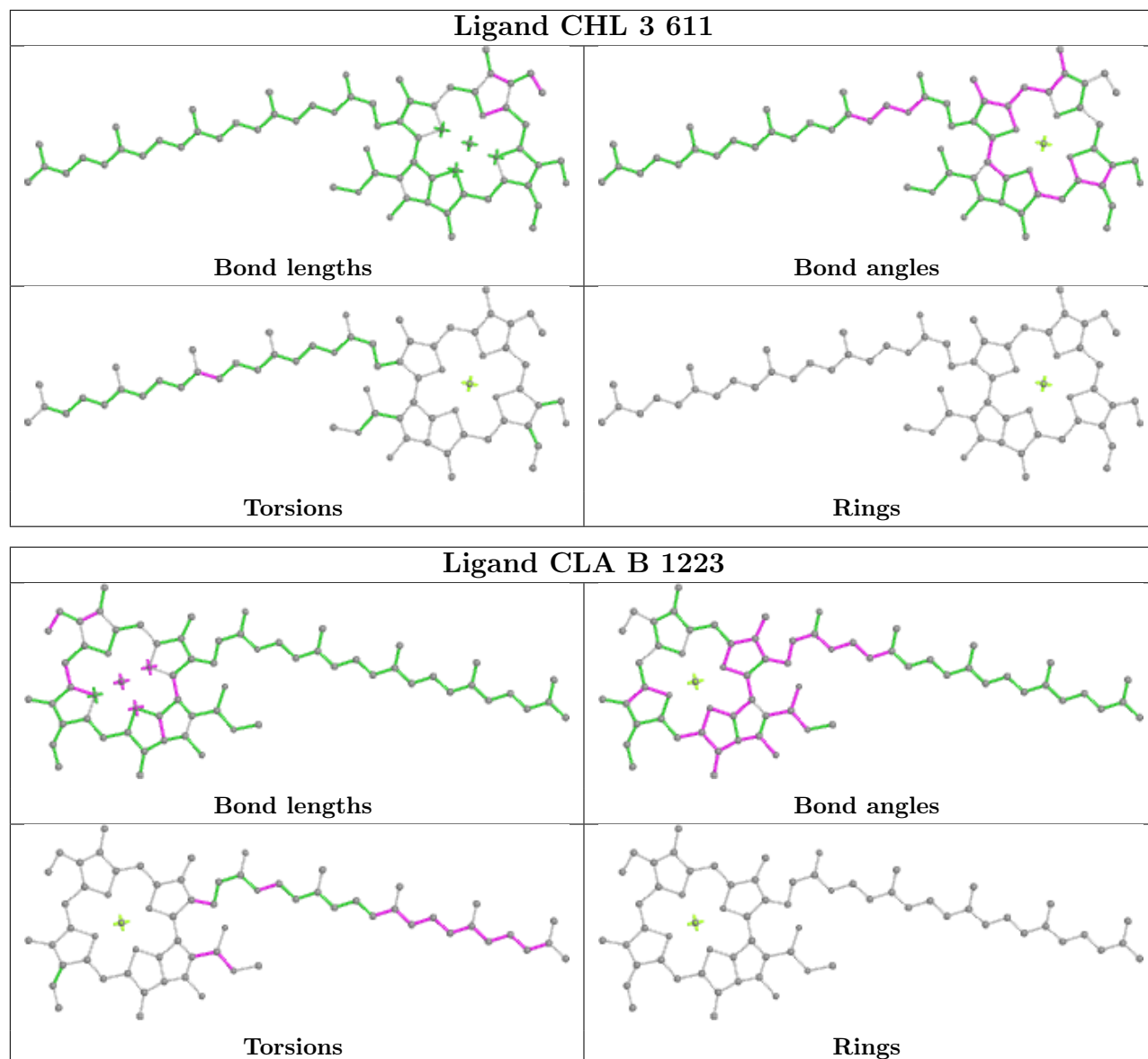


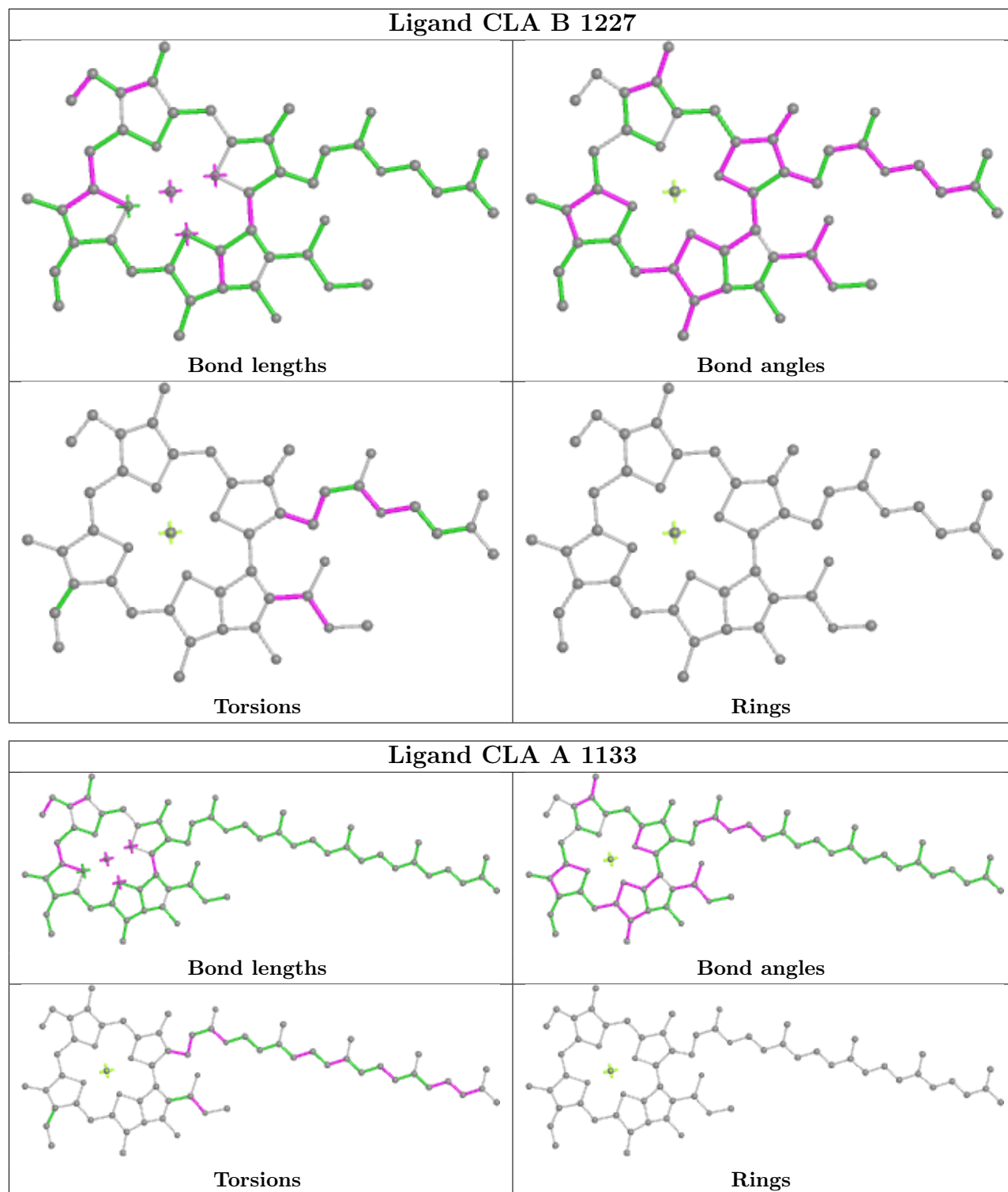


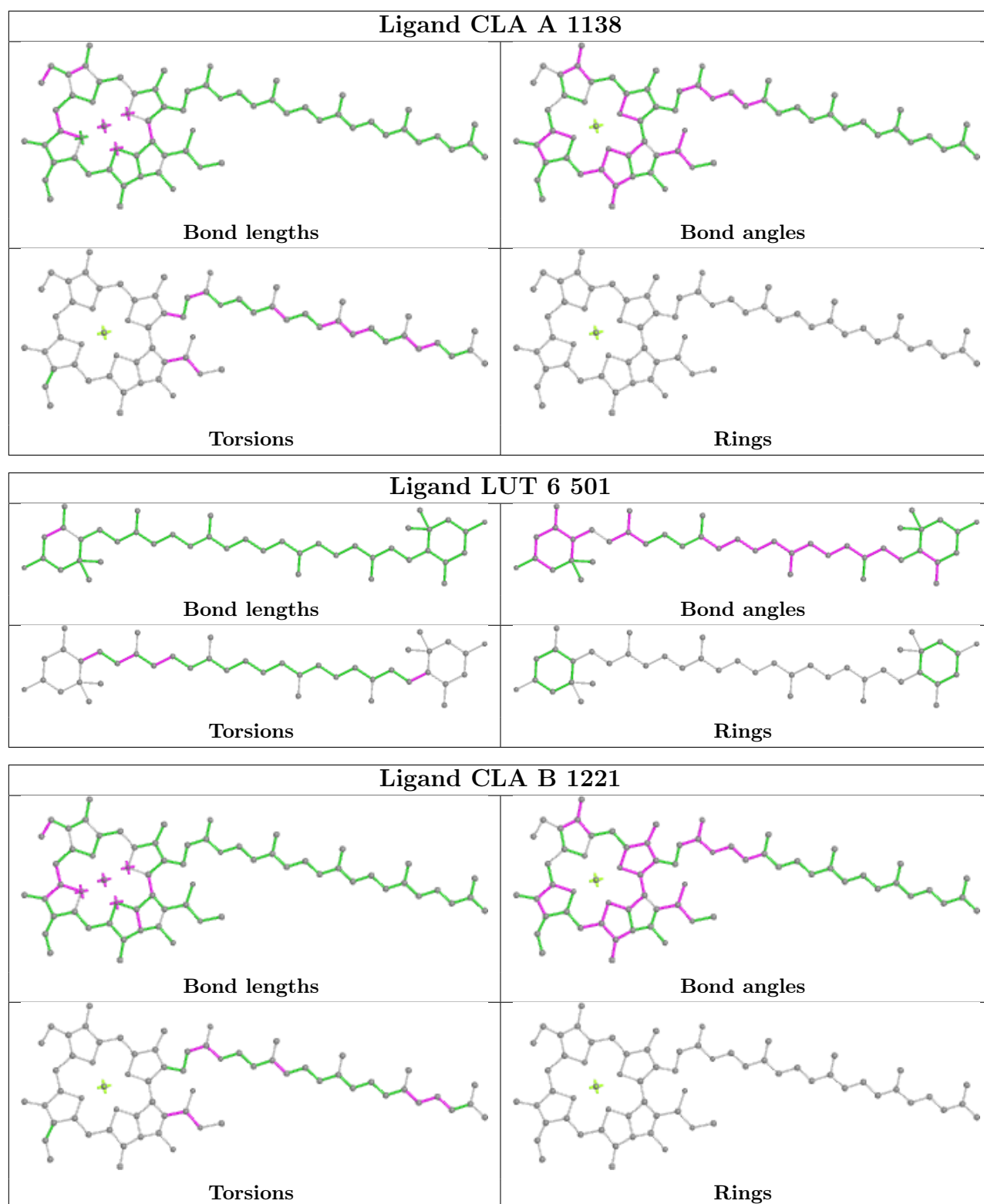


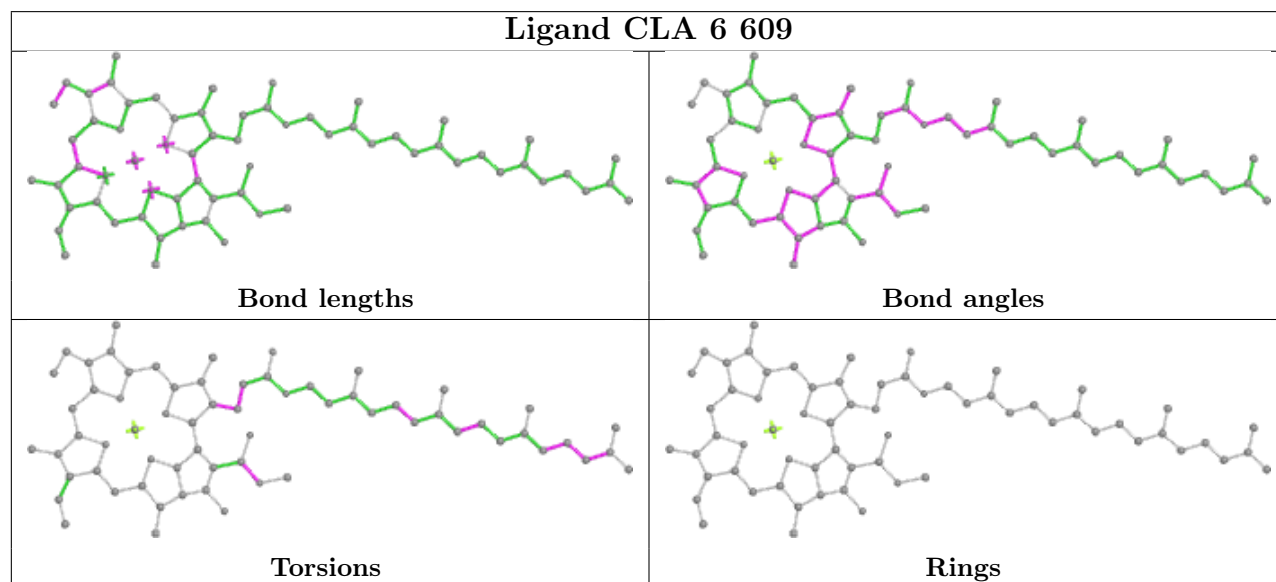
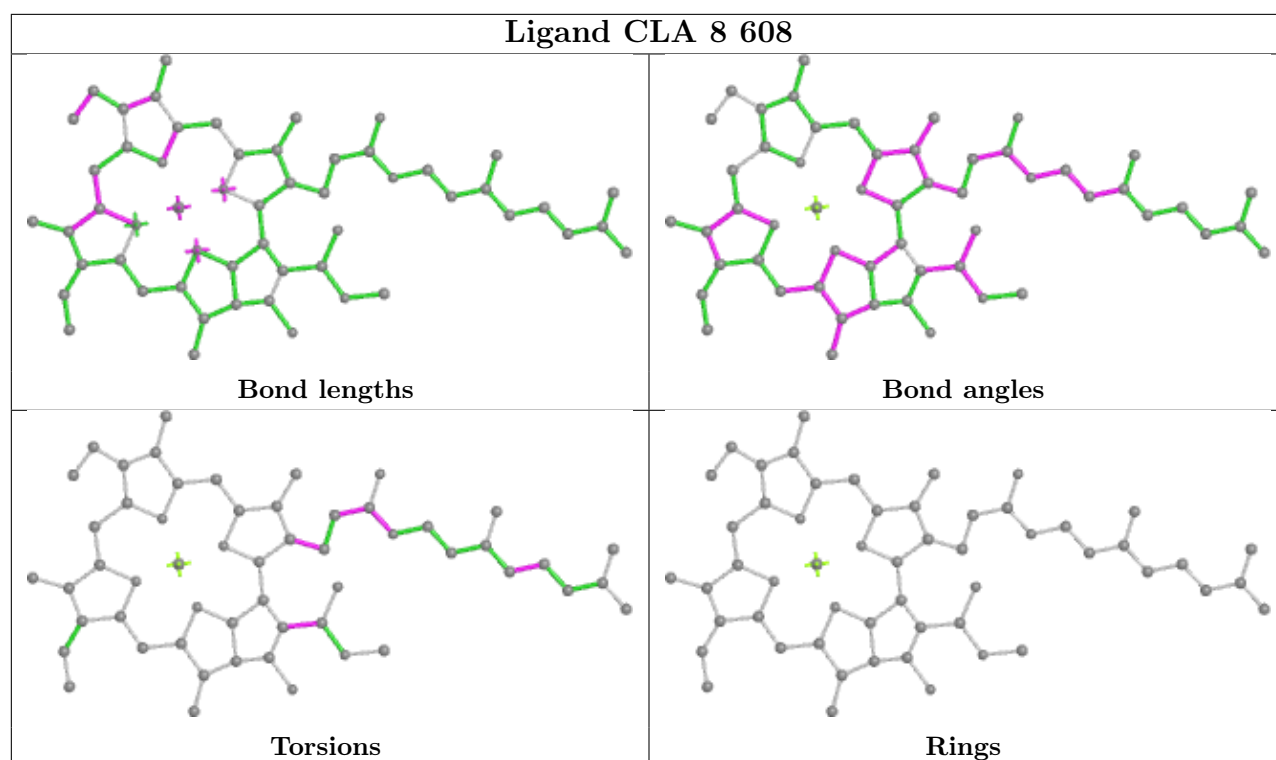


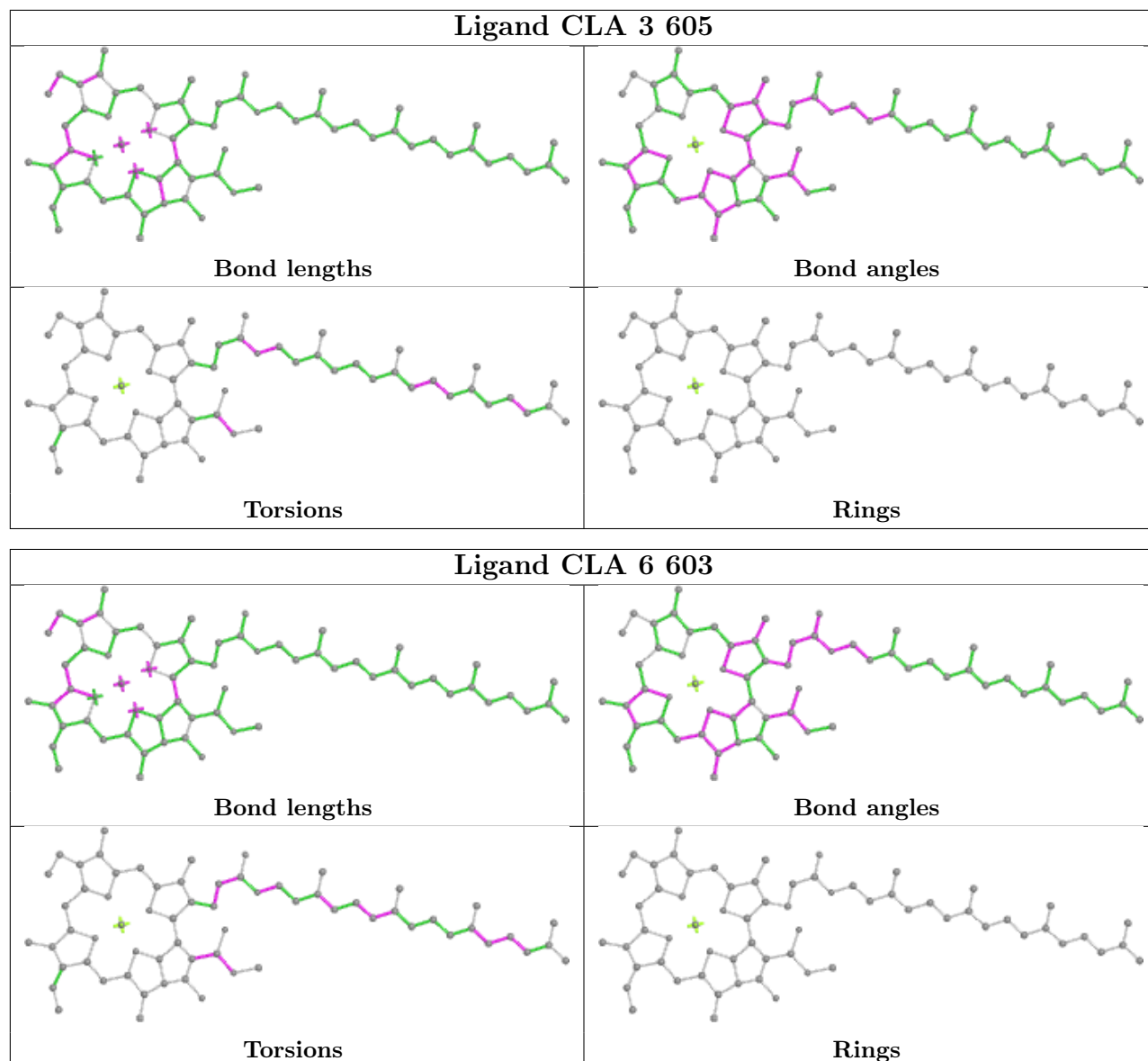


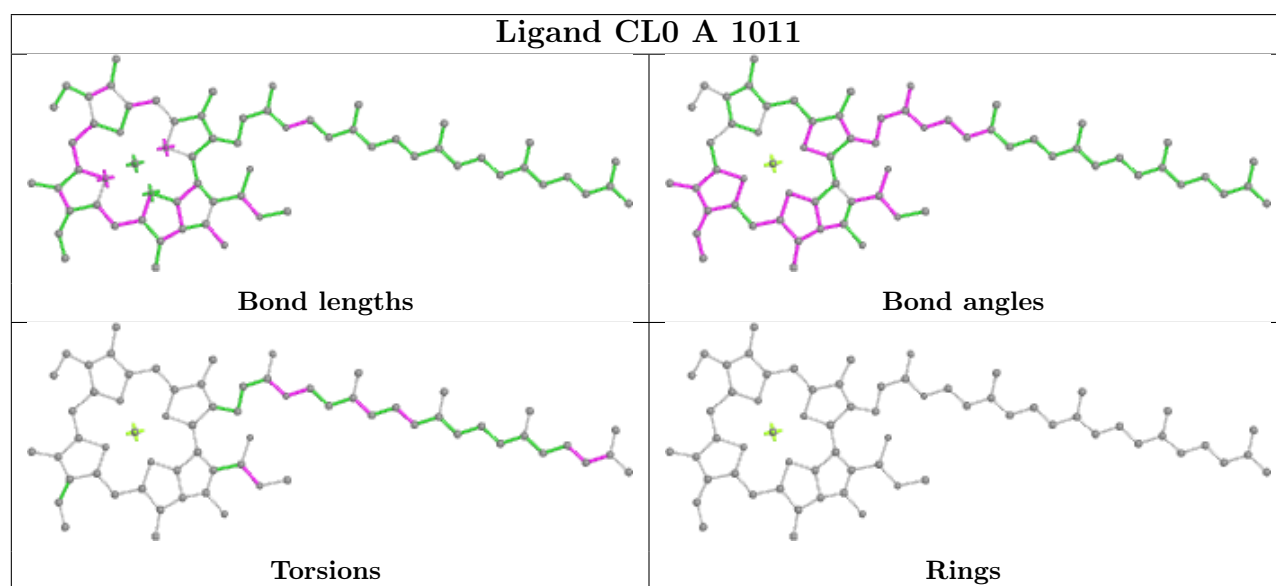
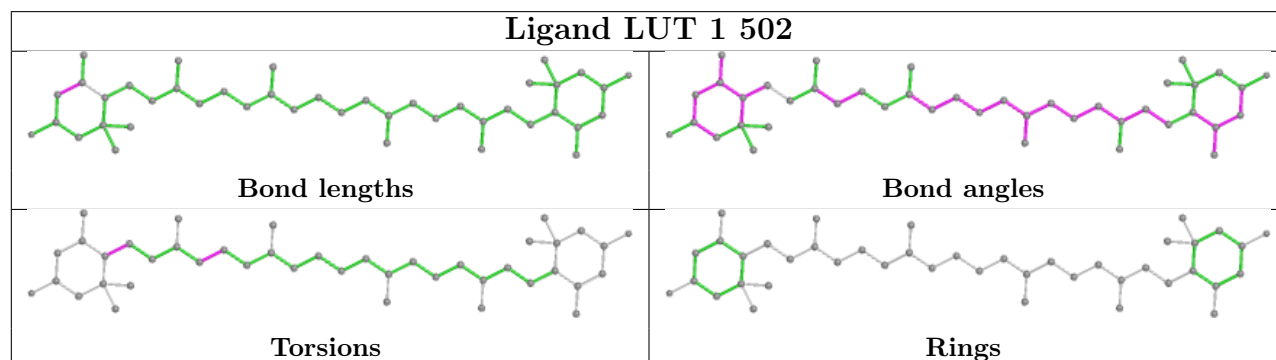
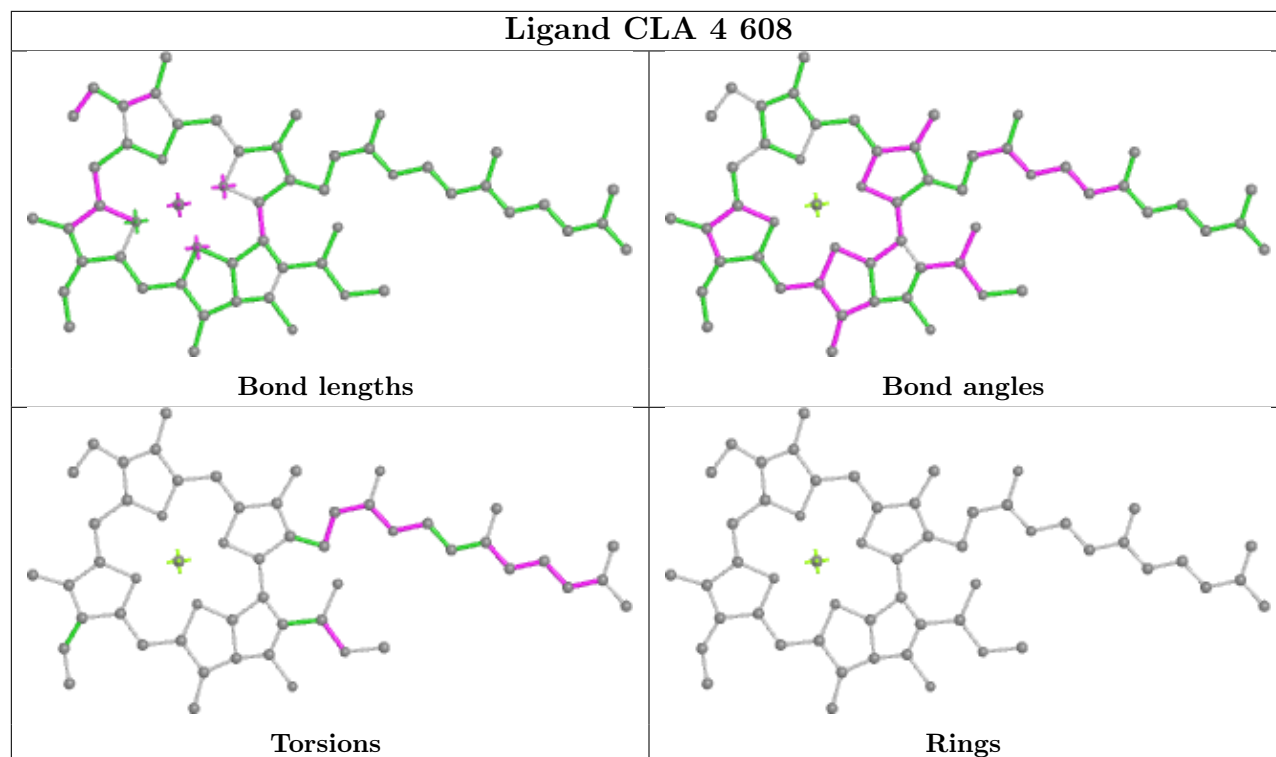


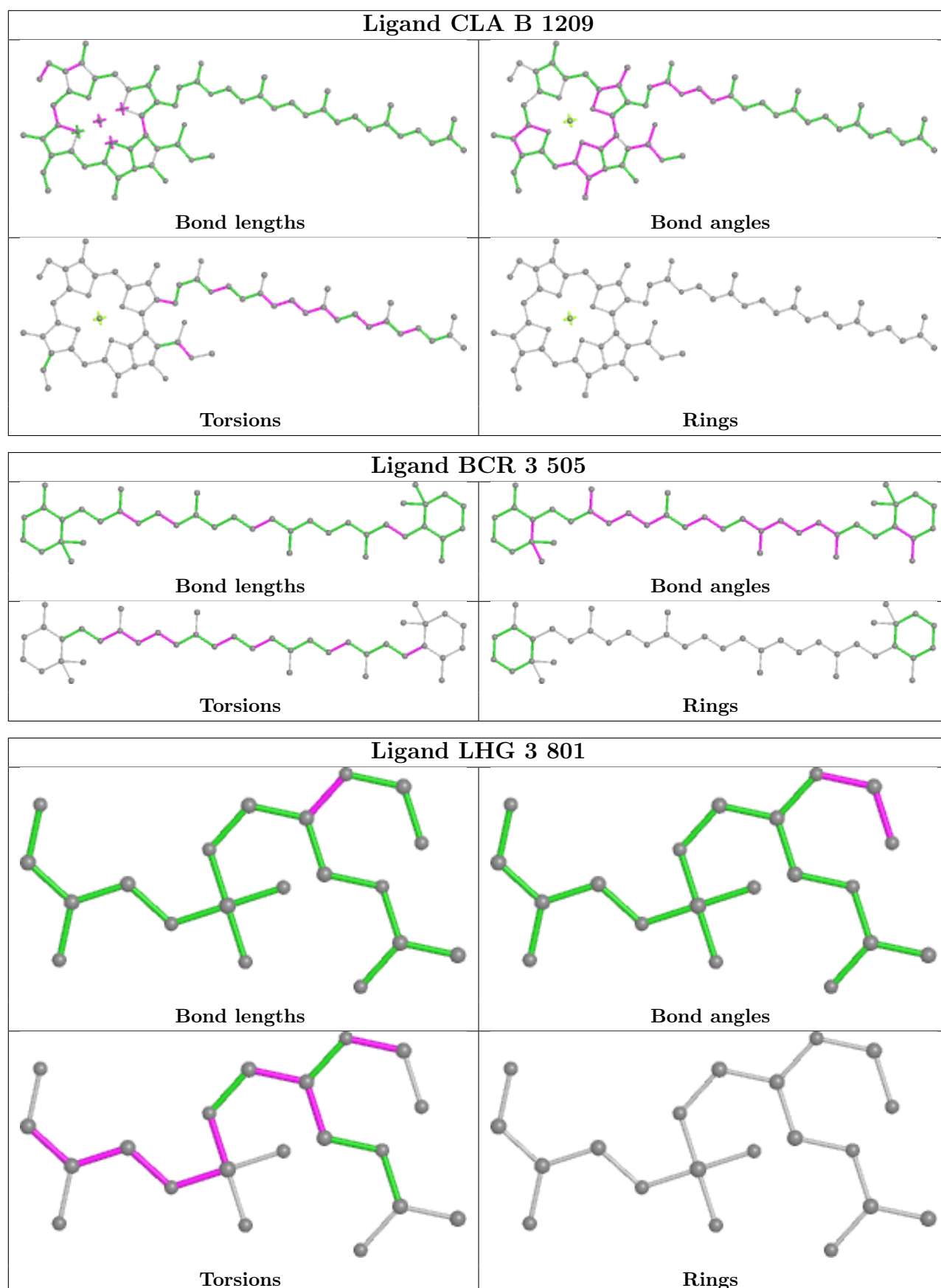




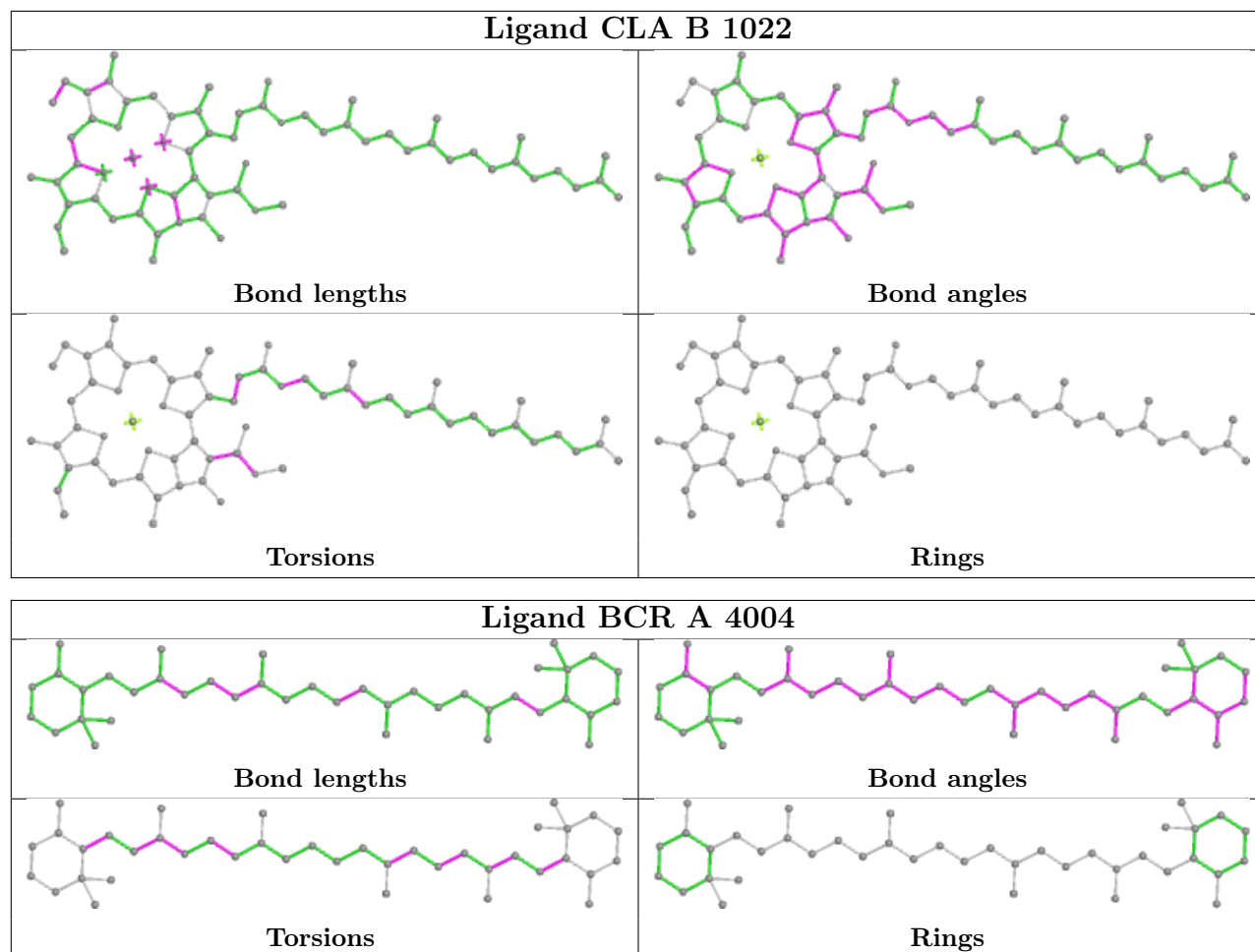


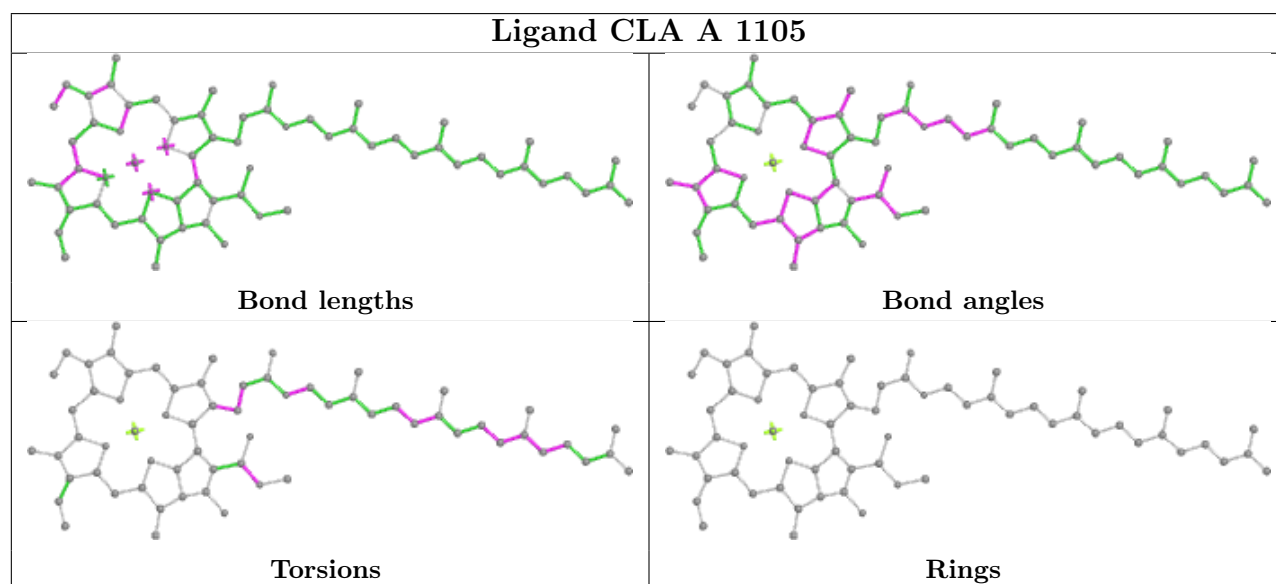
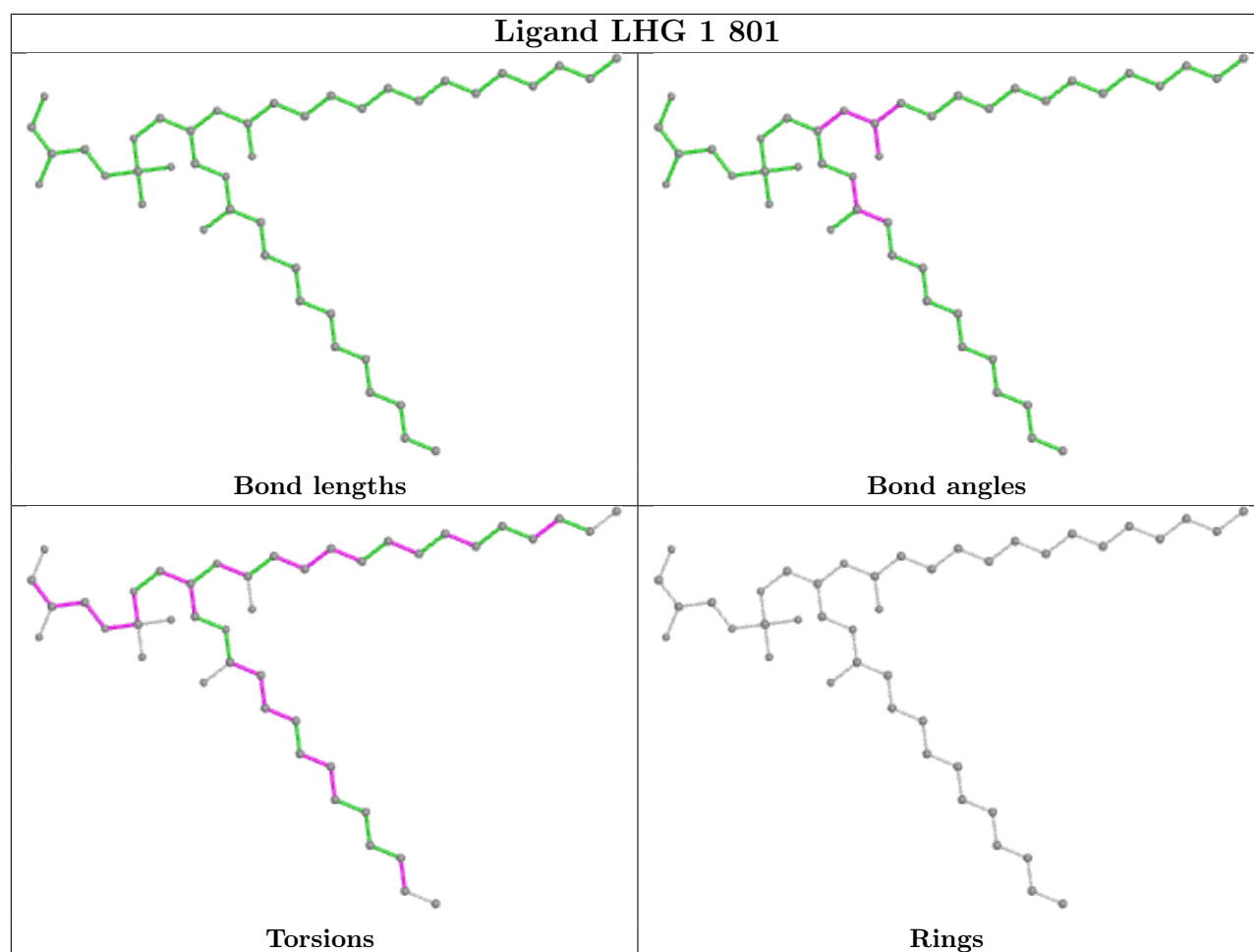


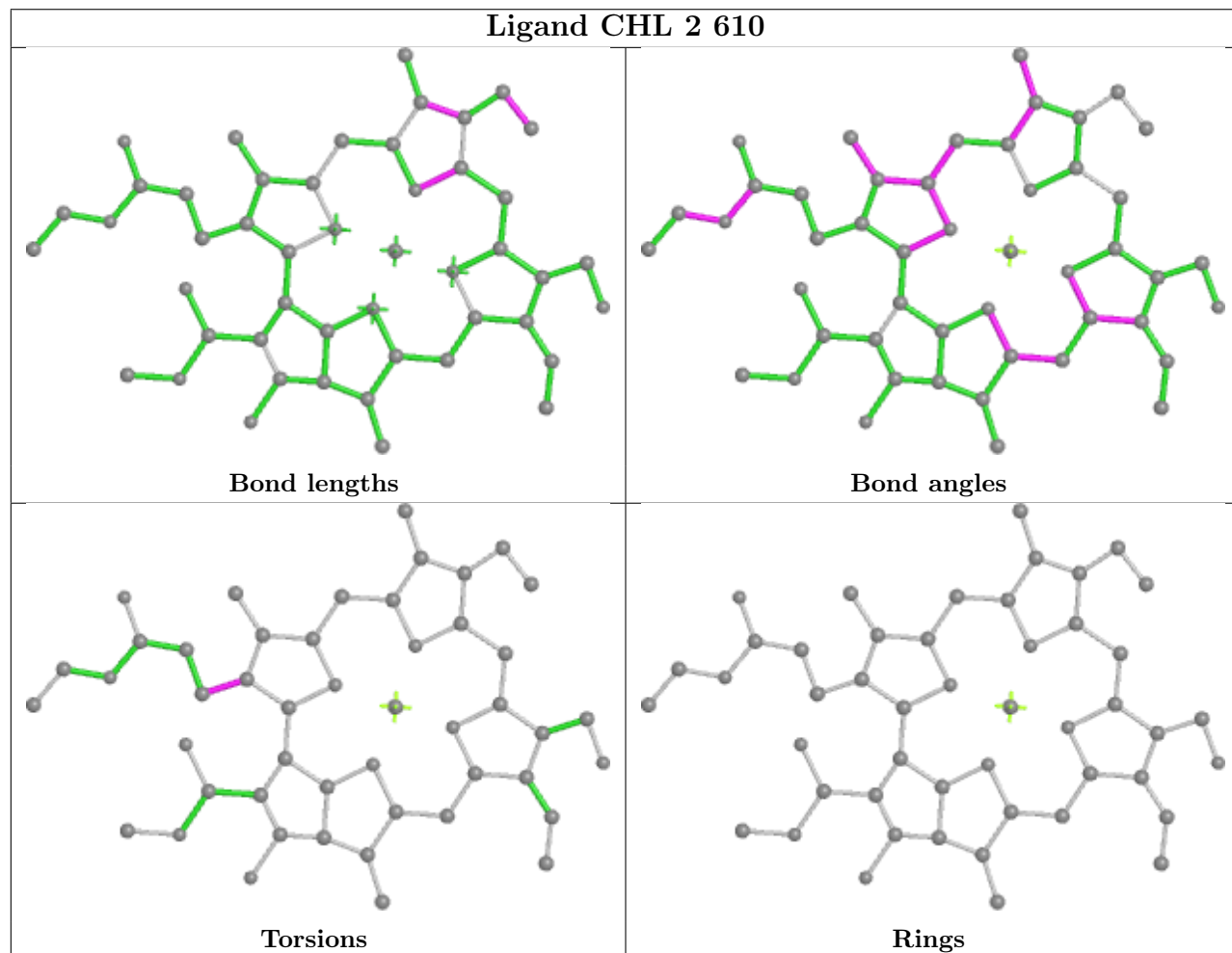
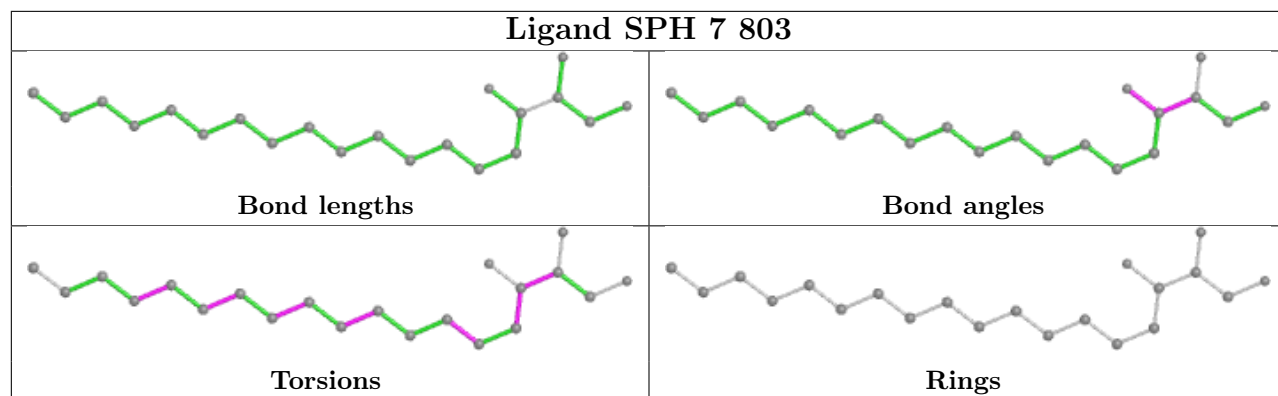


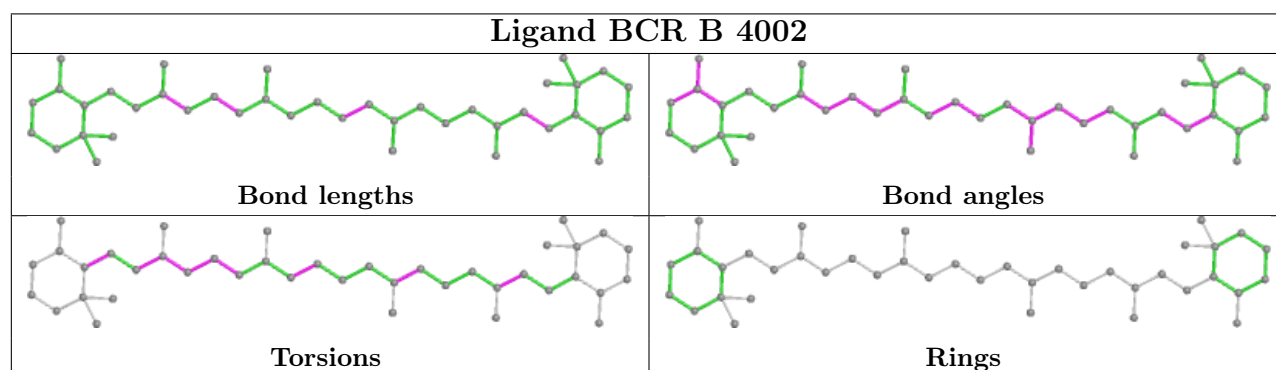
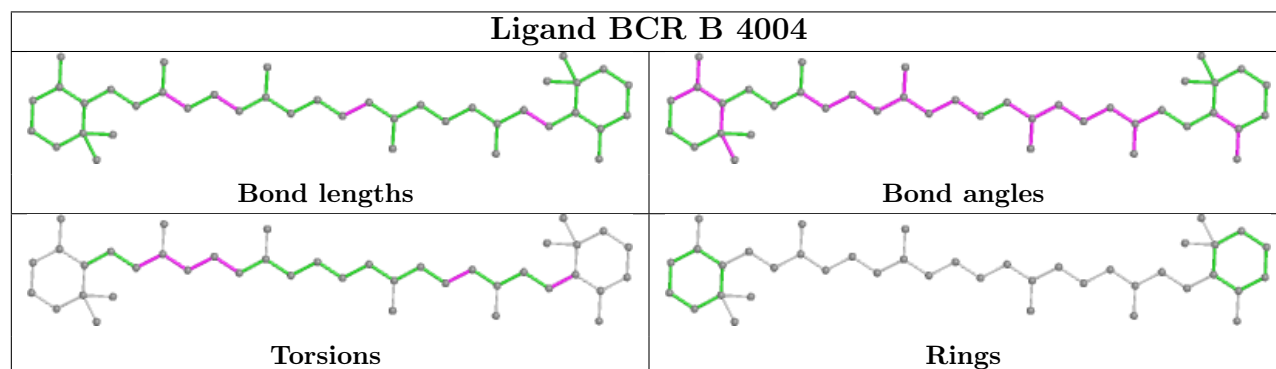
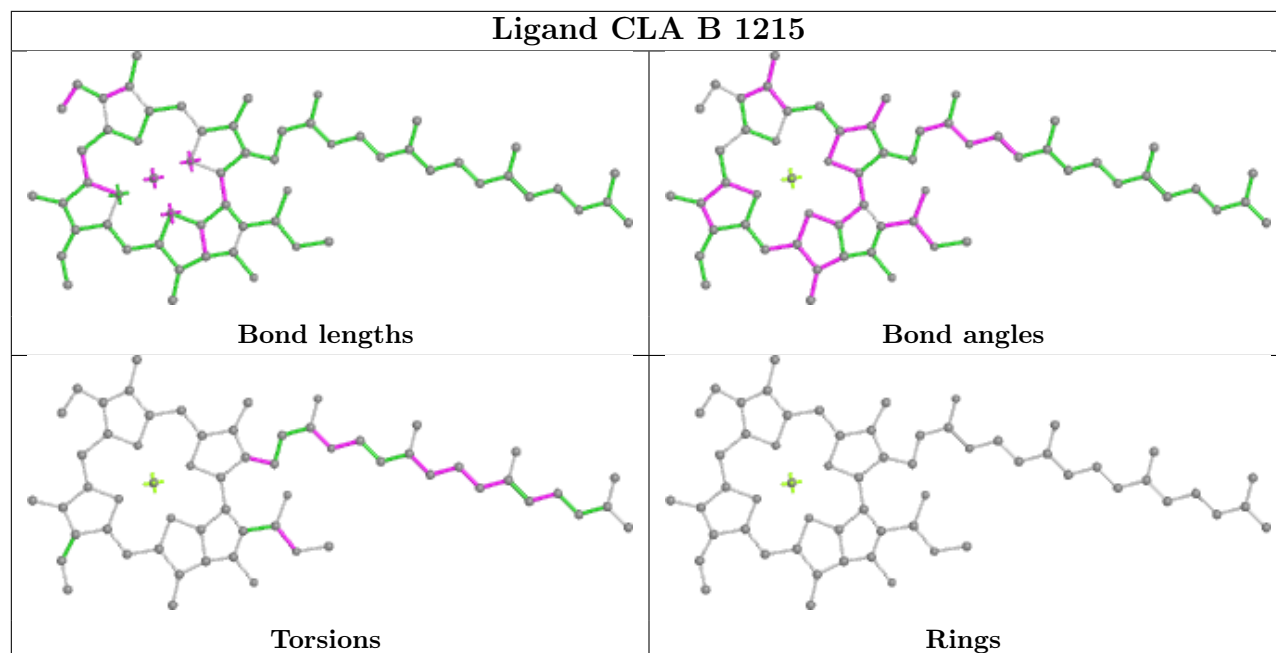


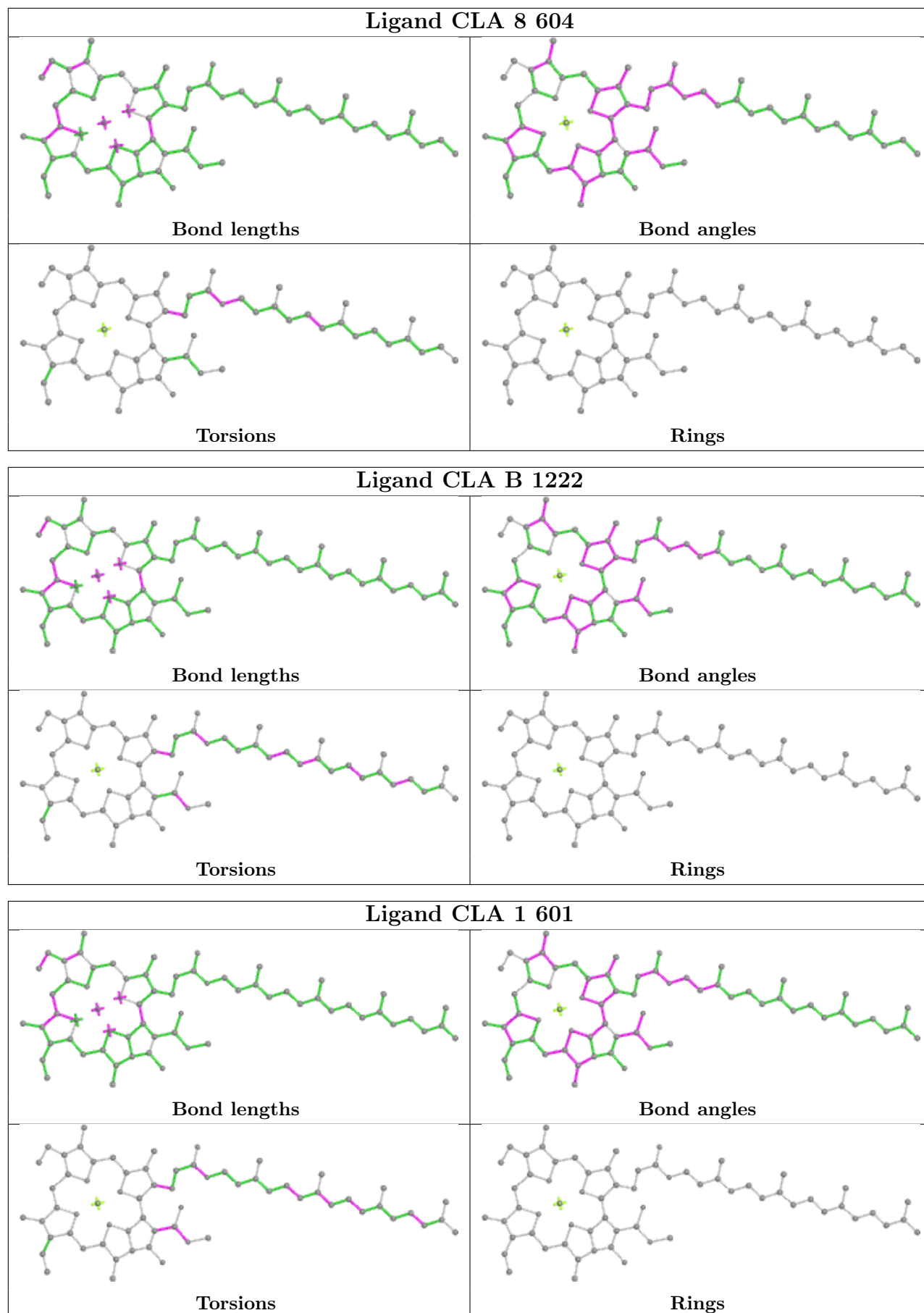


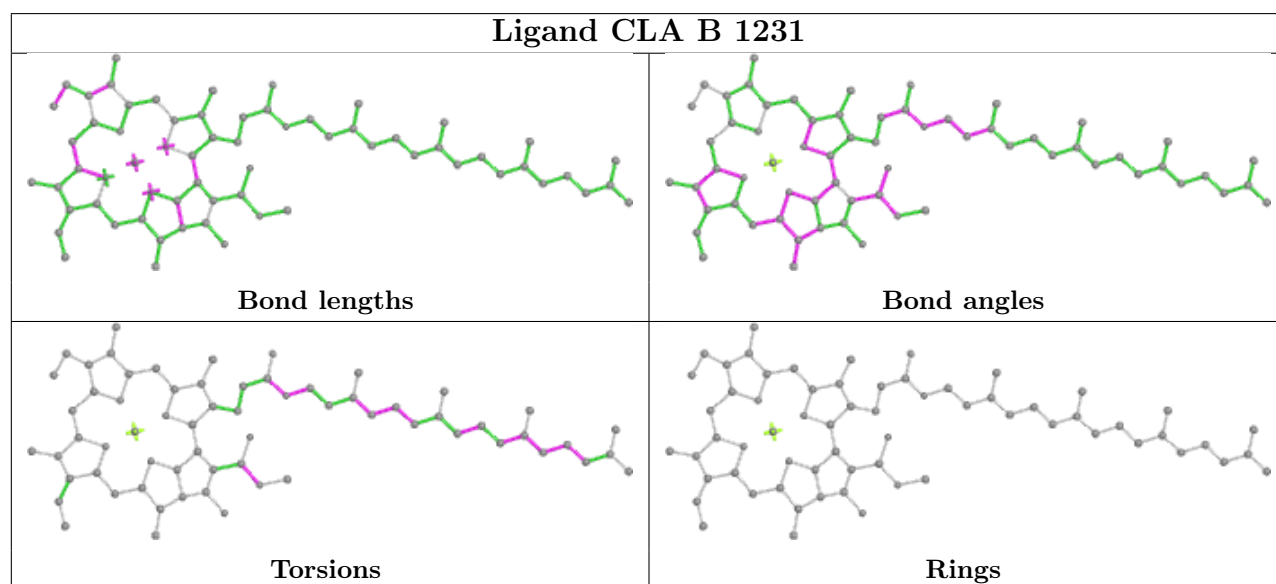
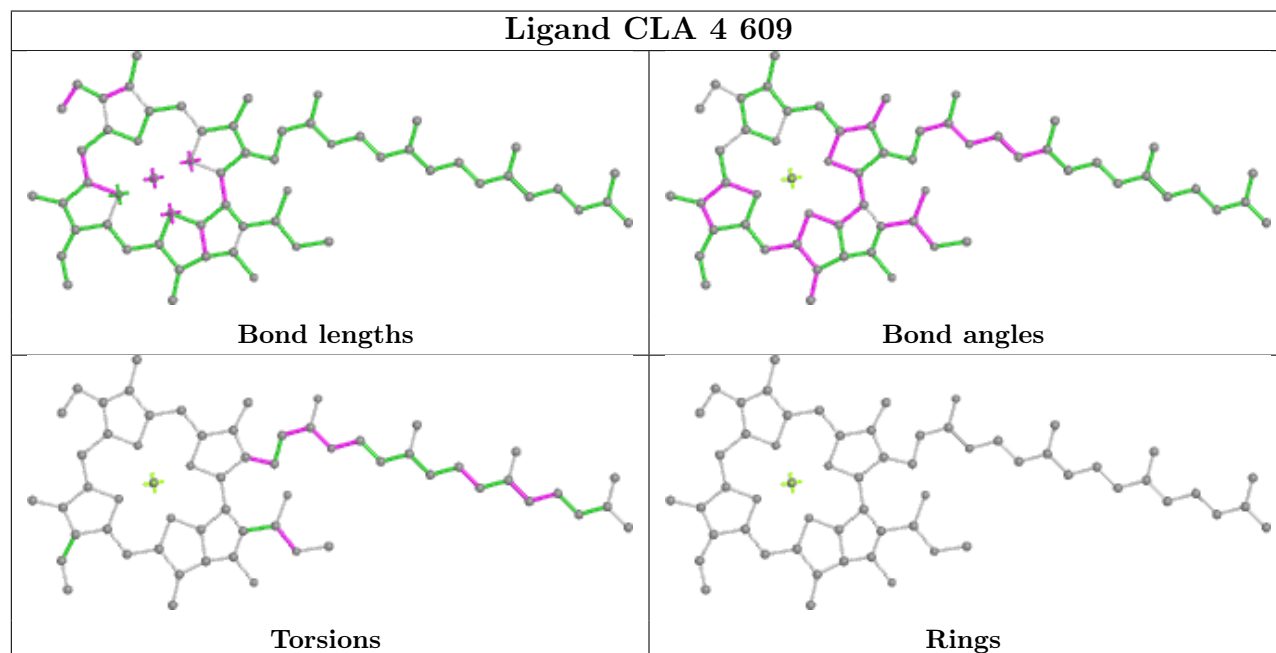
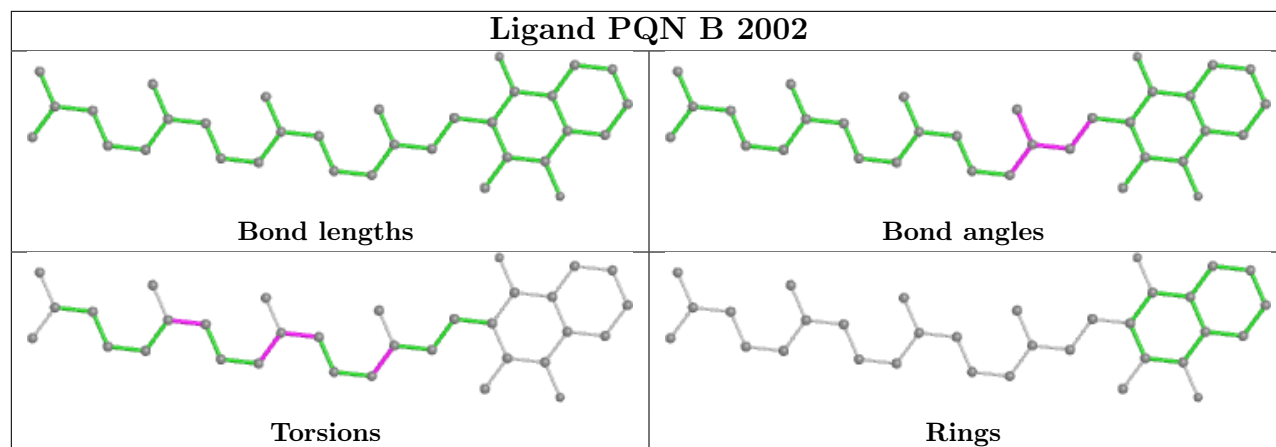


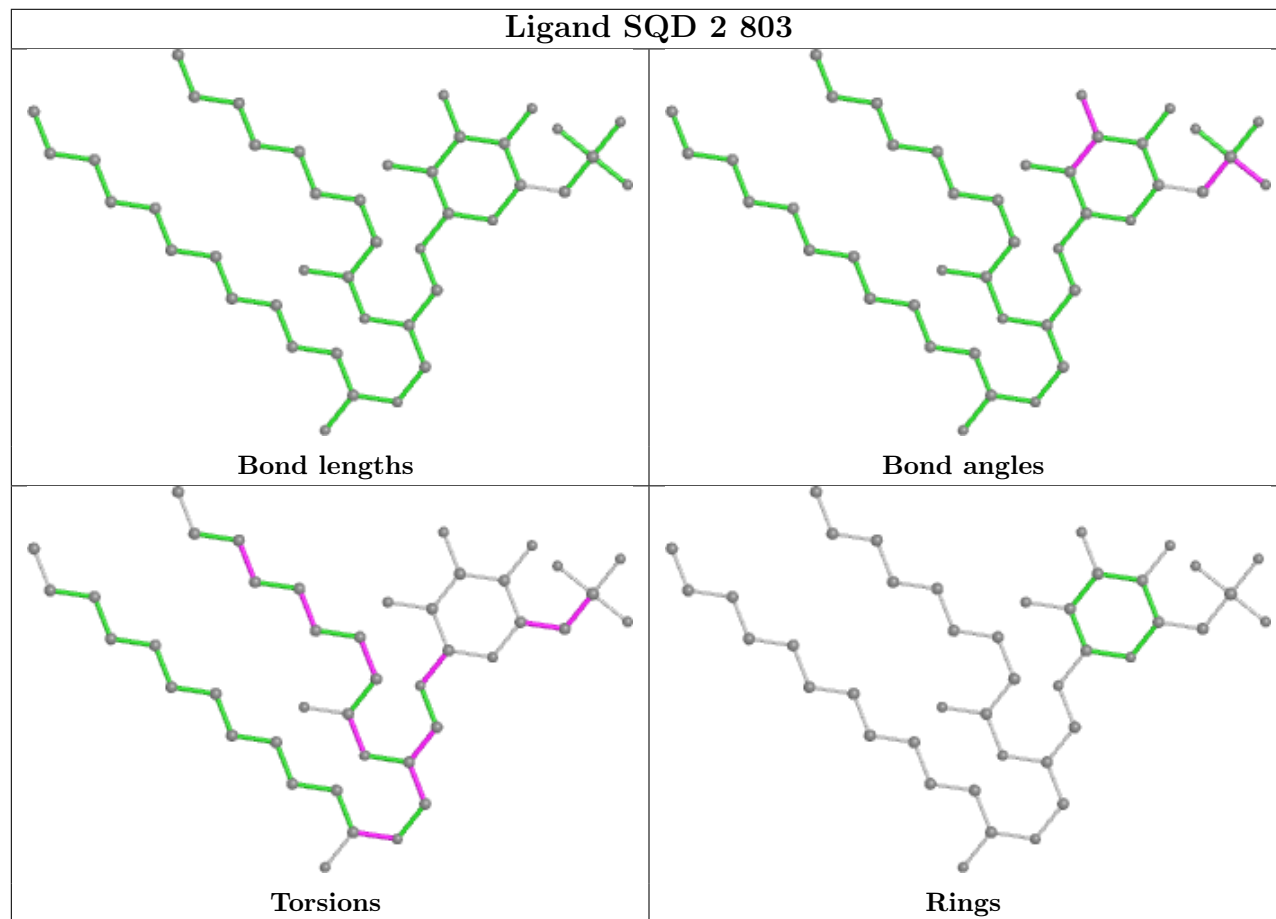
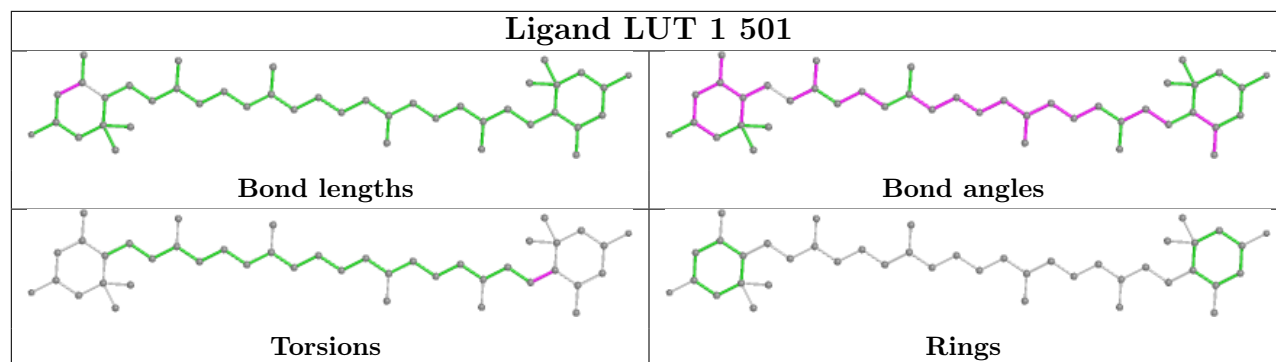


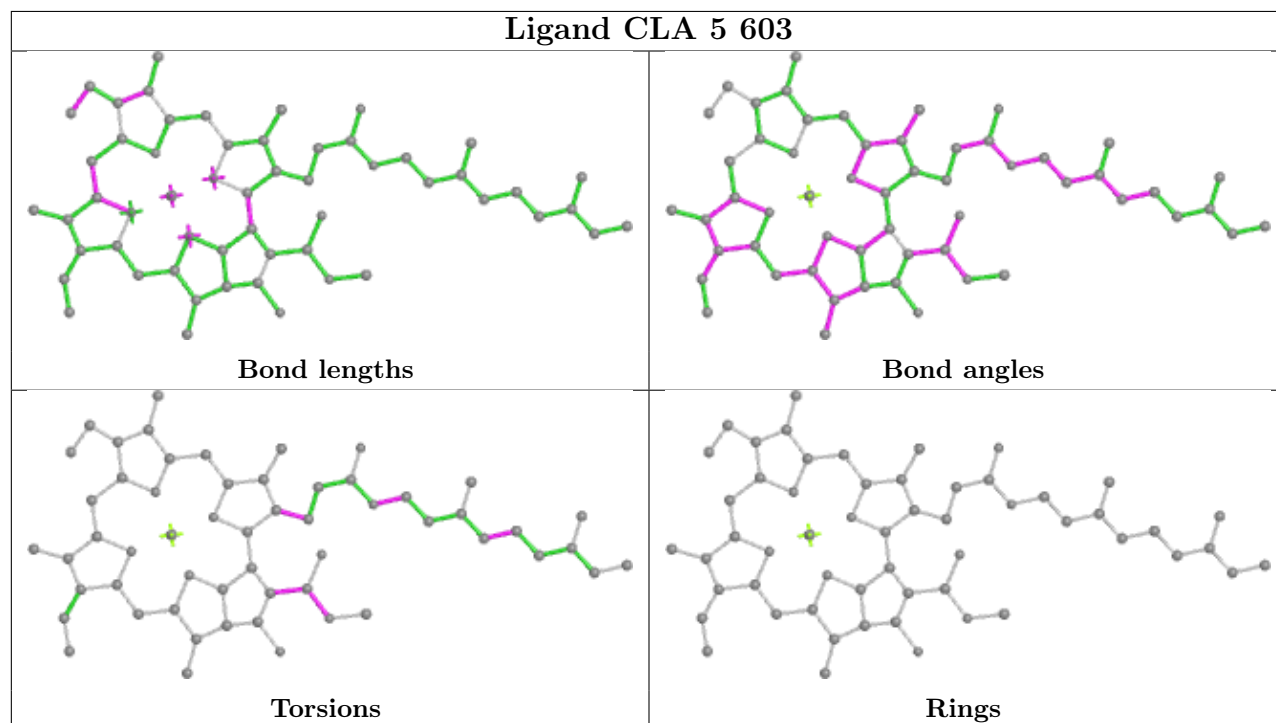
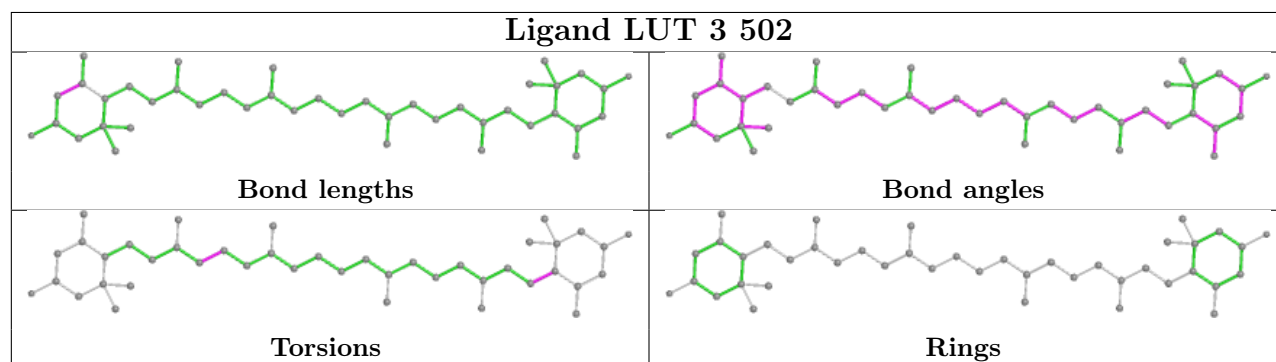
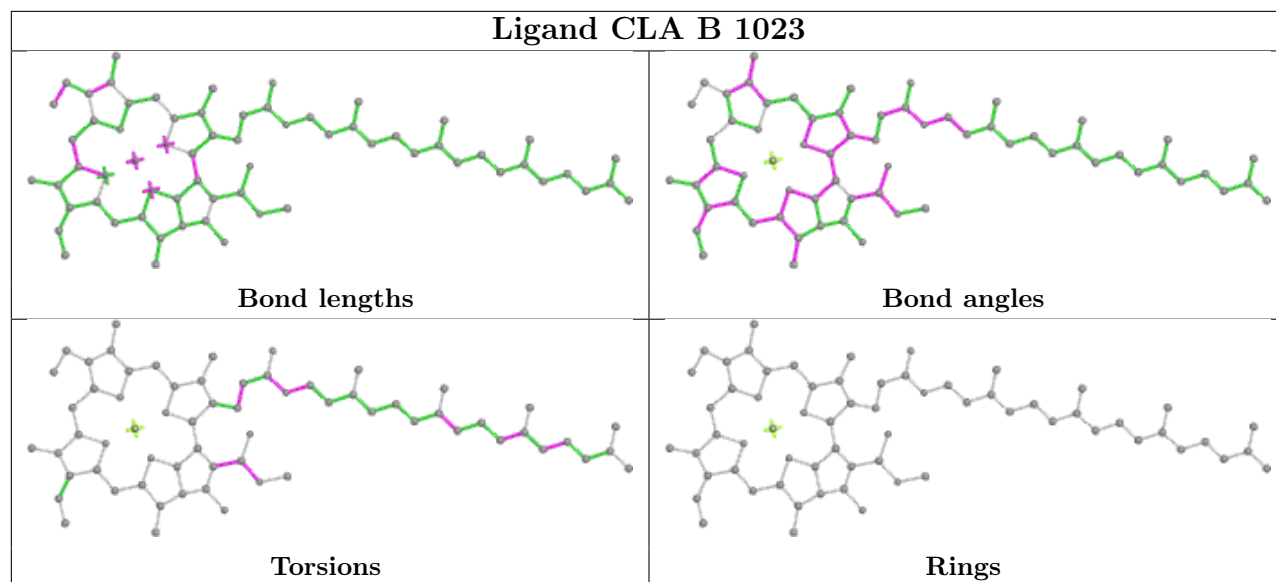




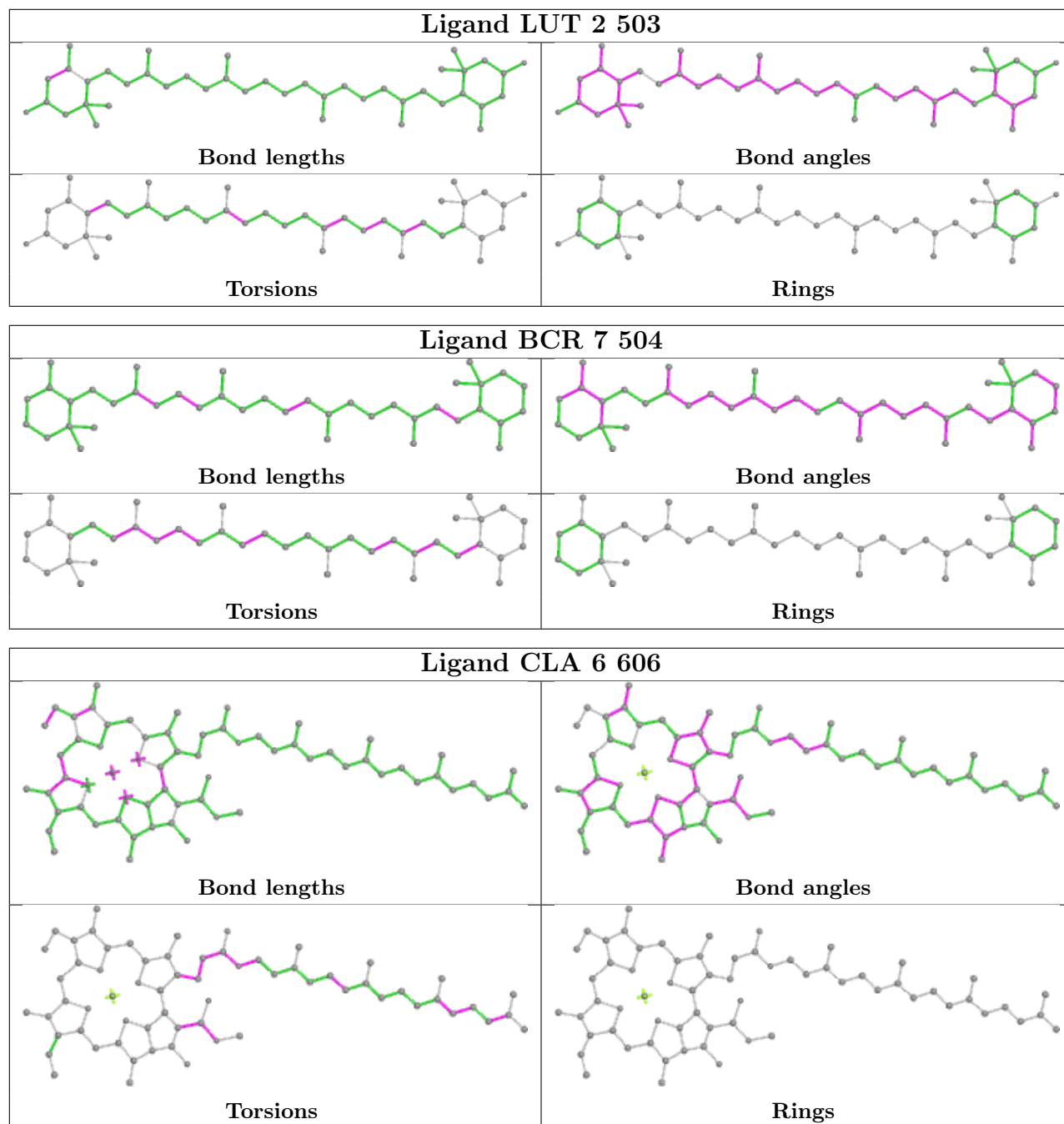


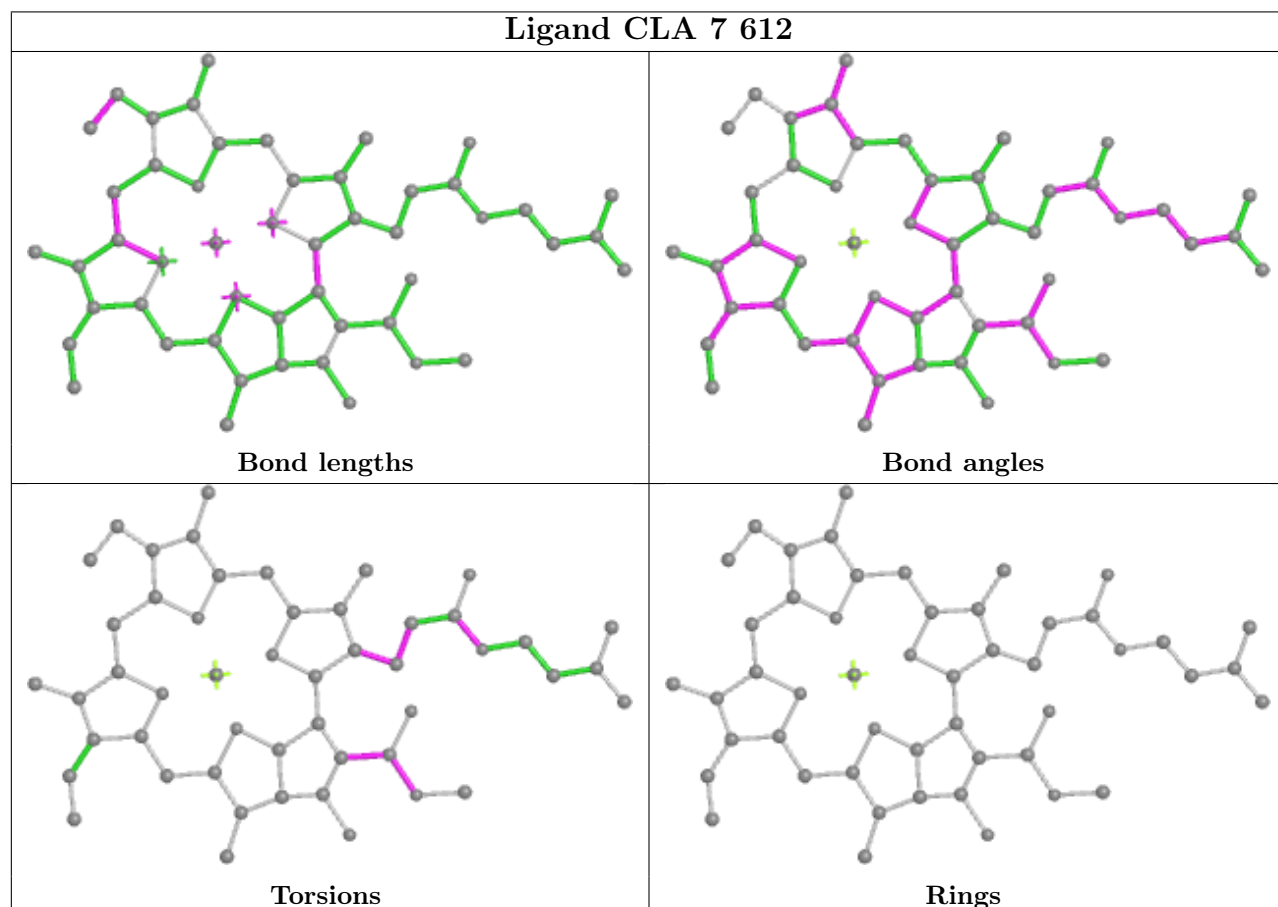
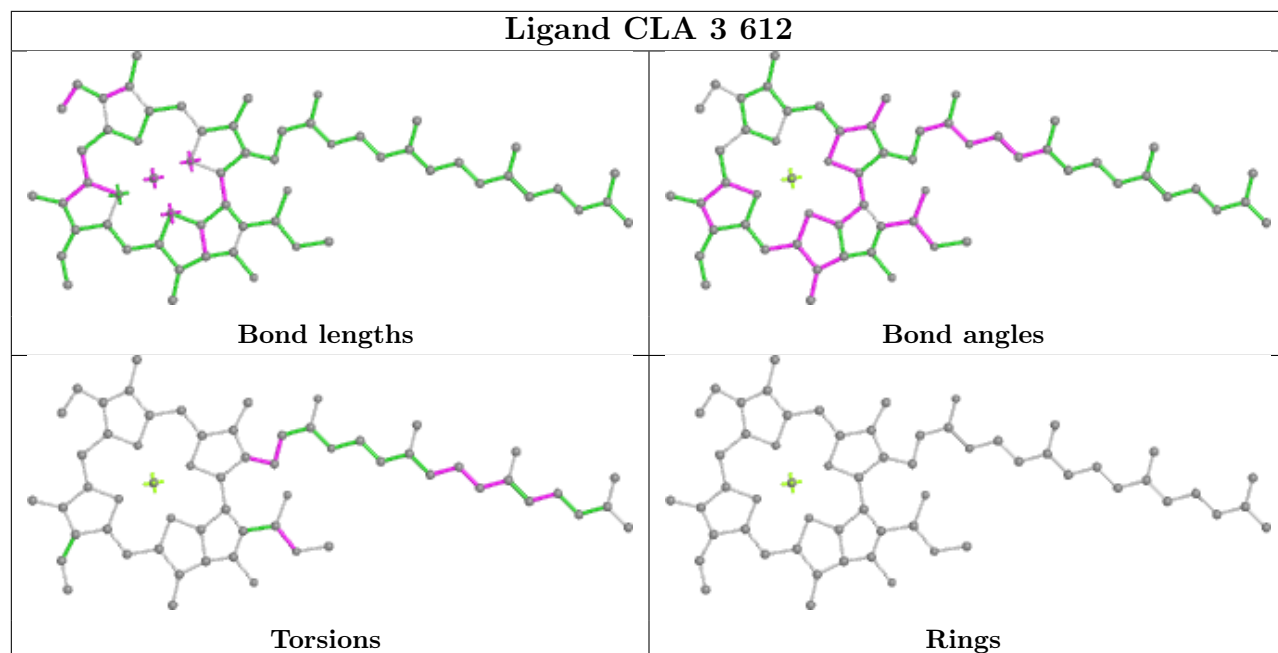


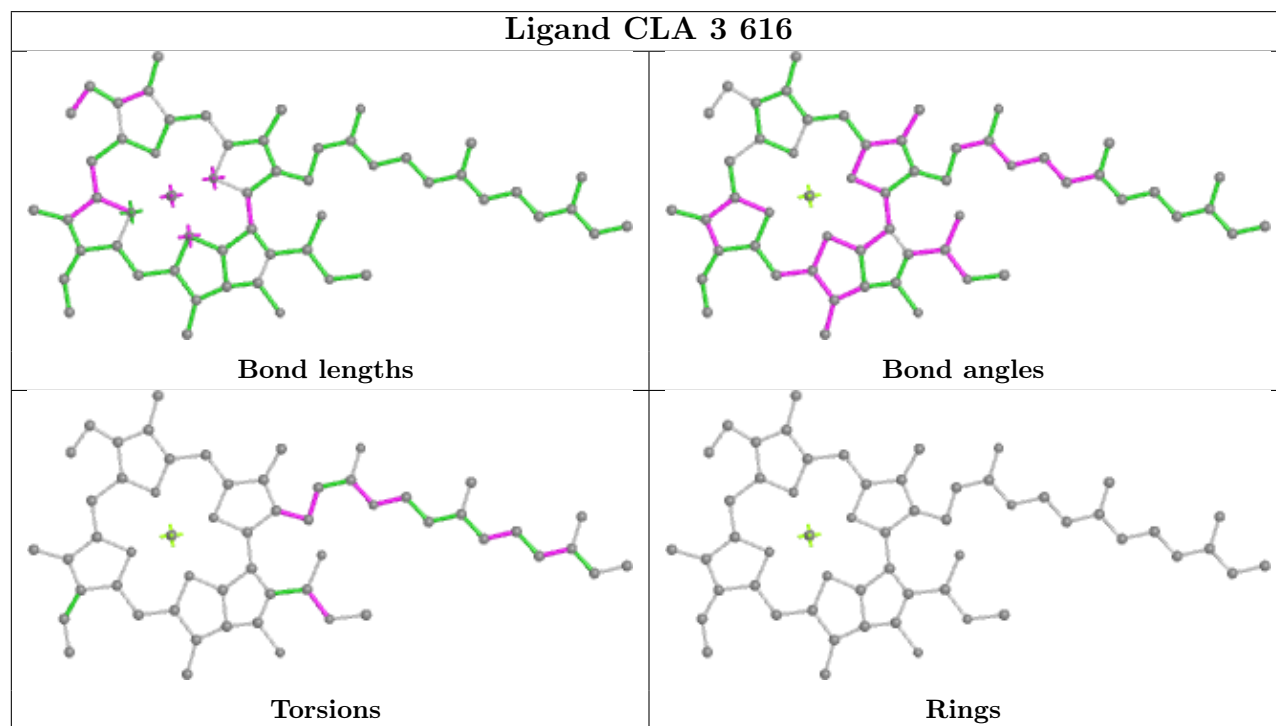
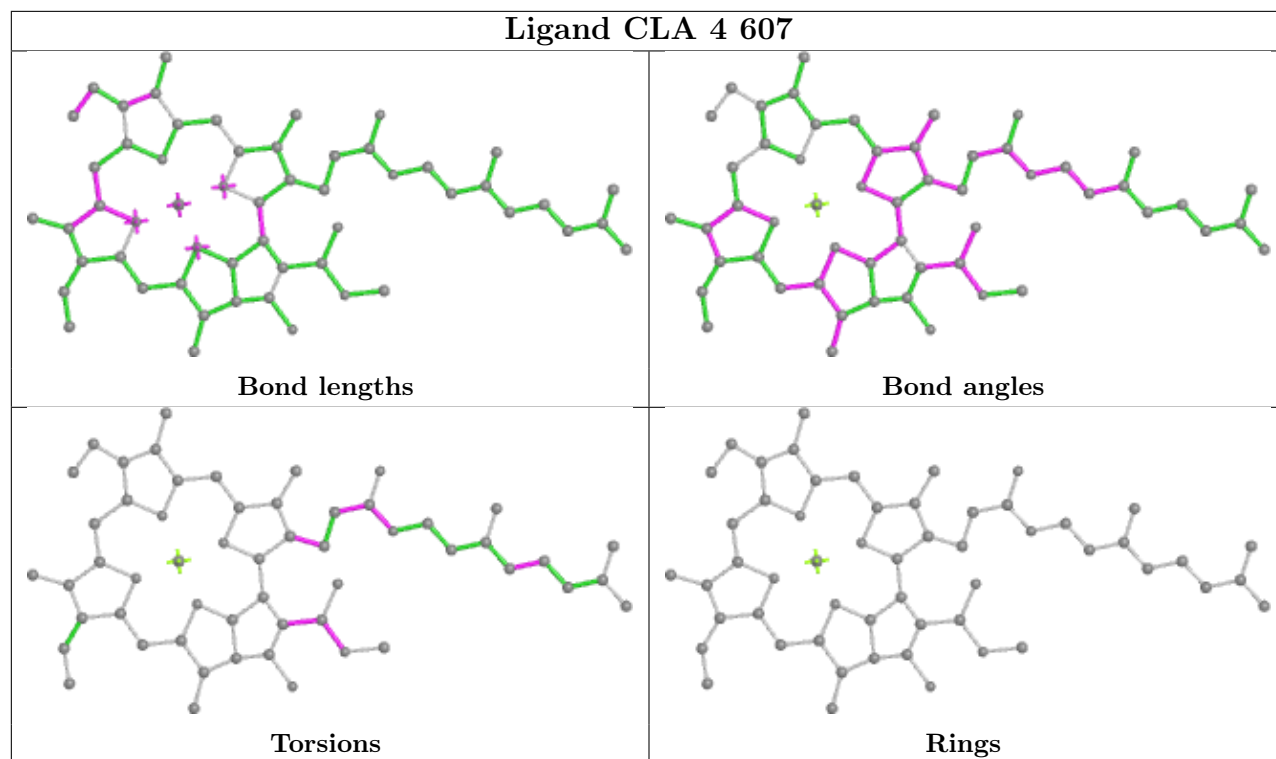


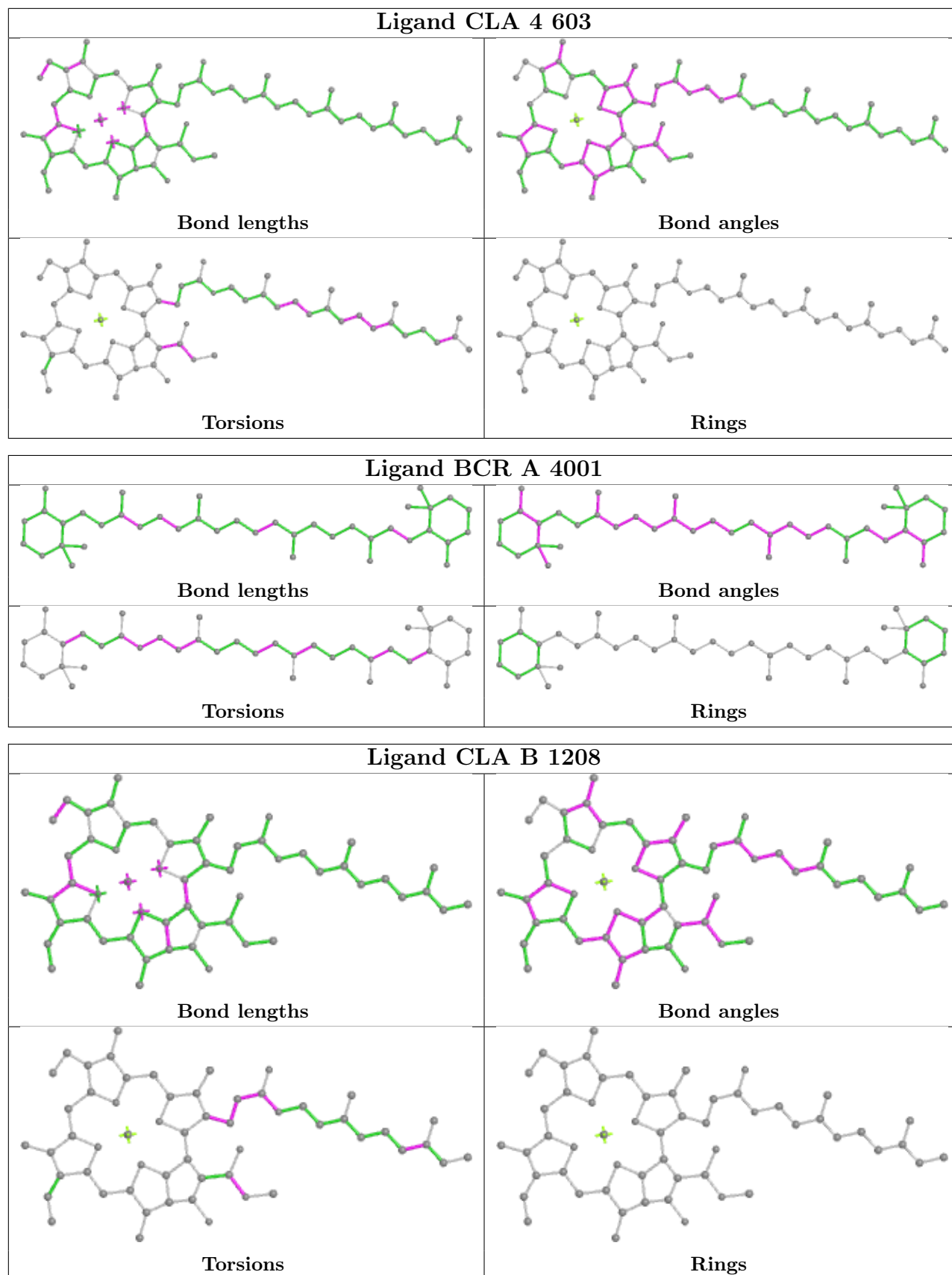


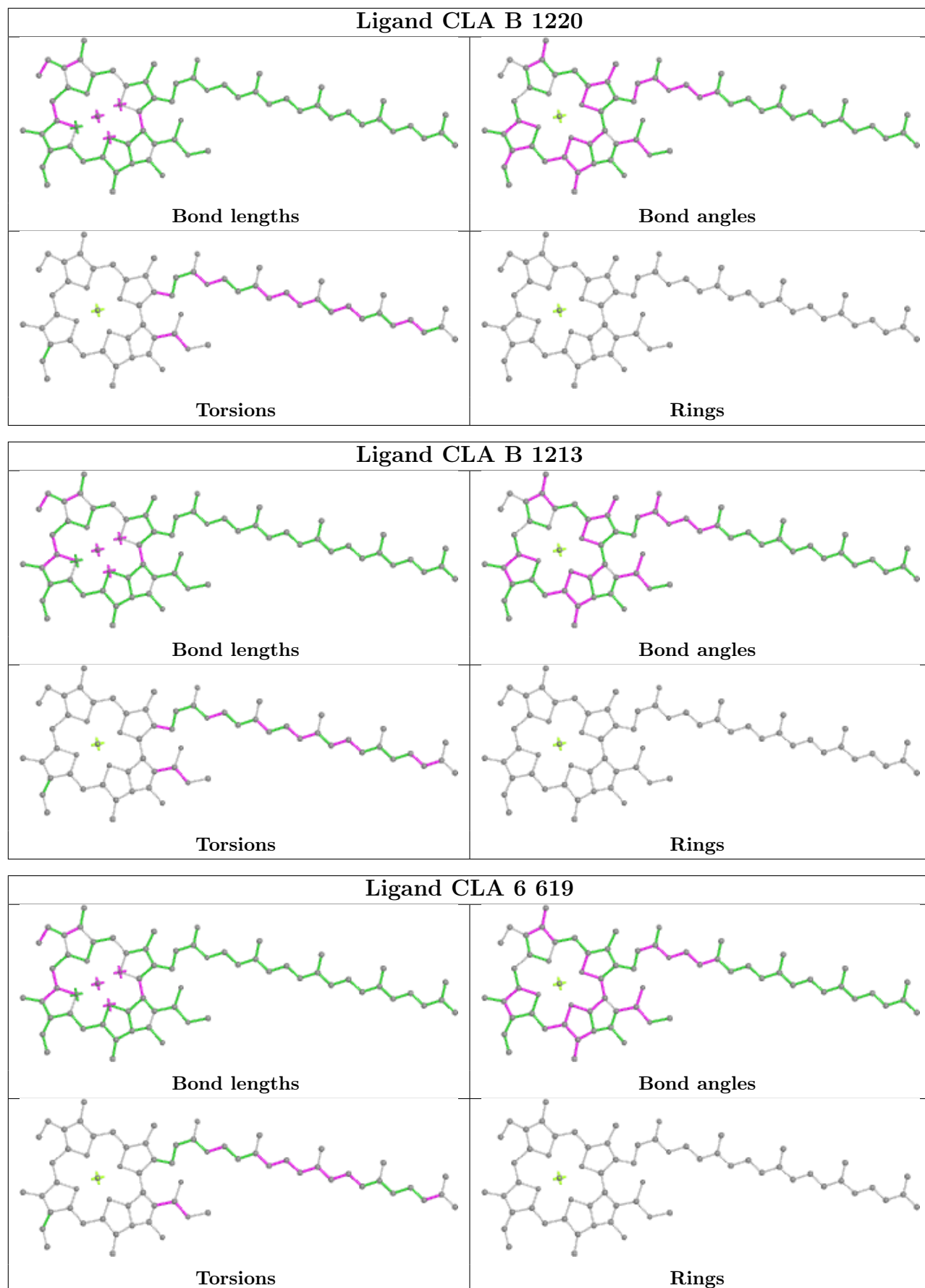


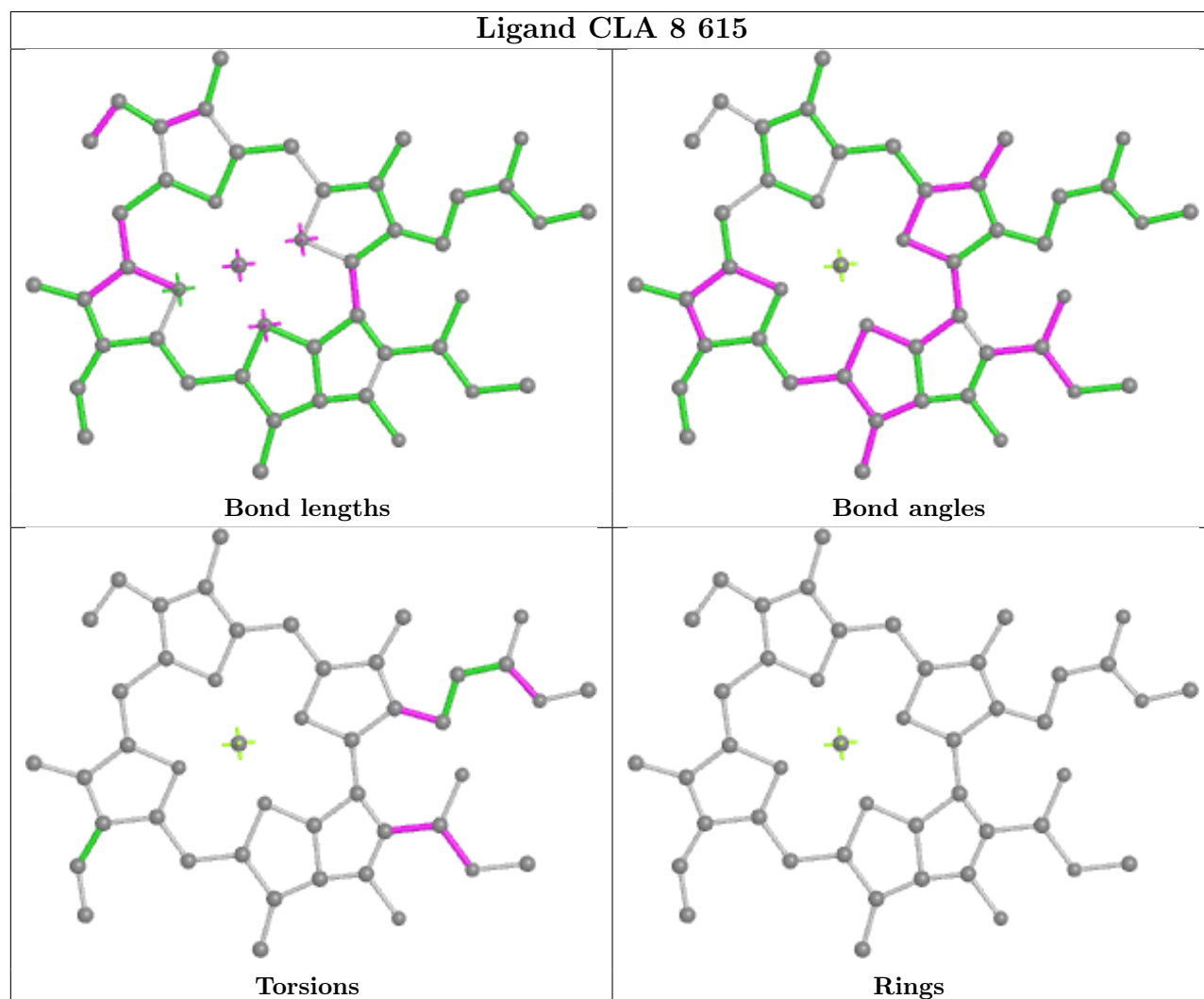
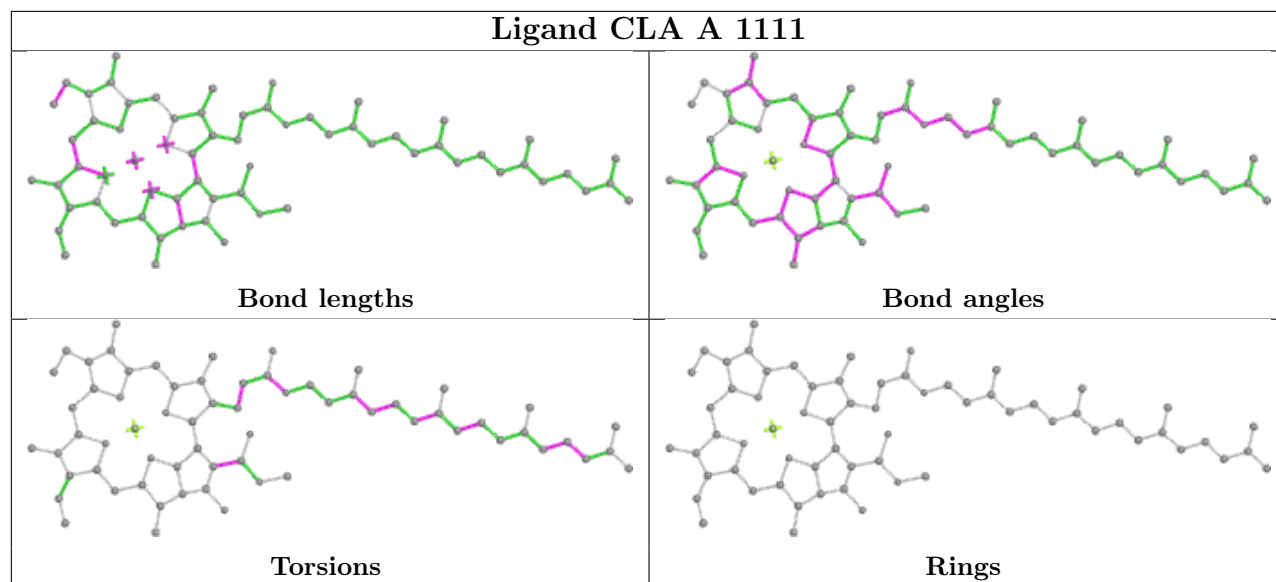


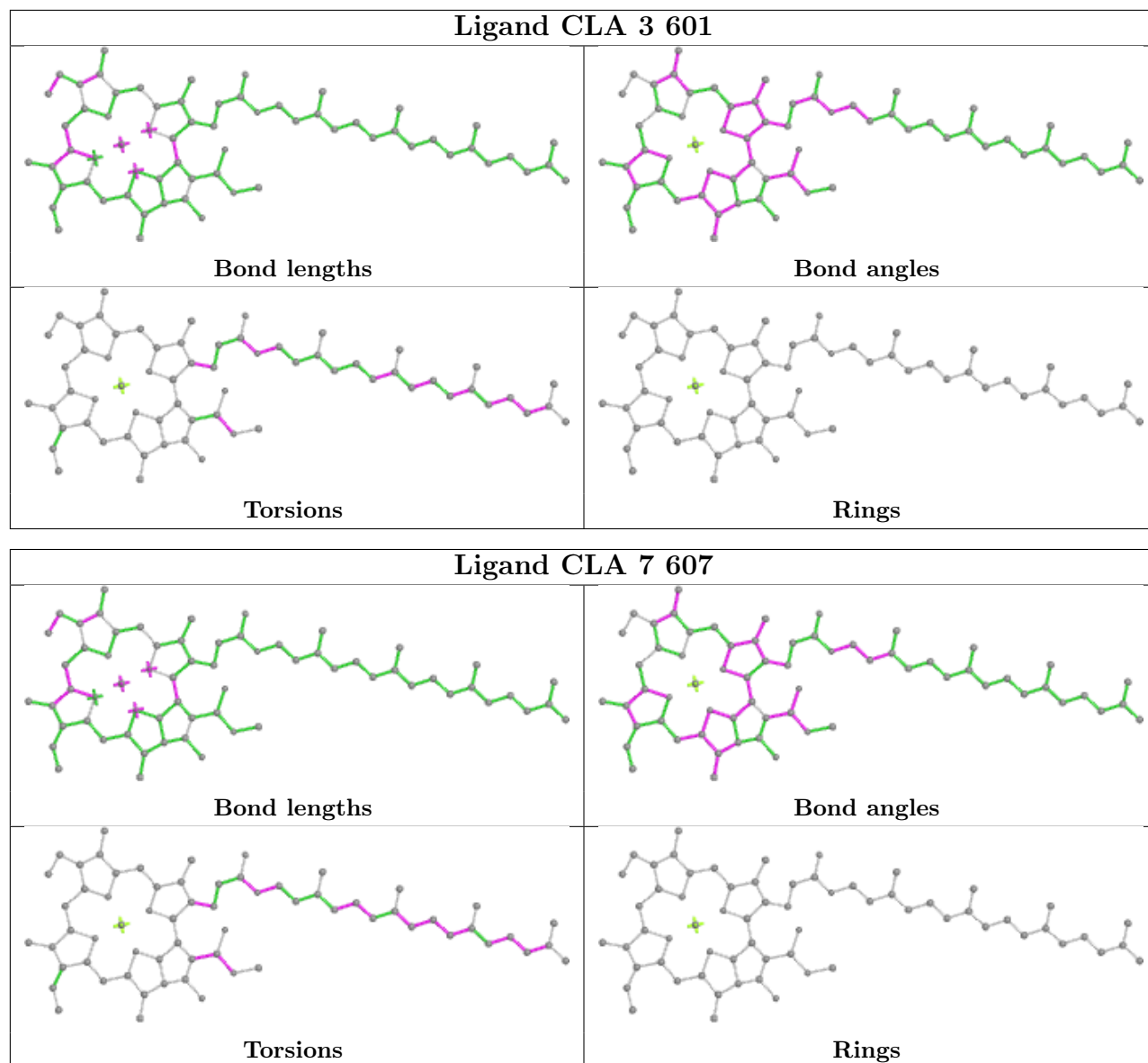












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

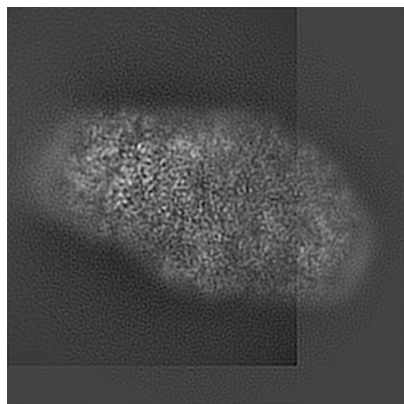
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12180. These allow visual inspection of the internal detail of the map and identification of artifacts.

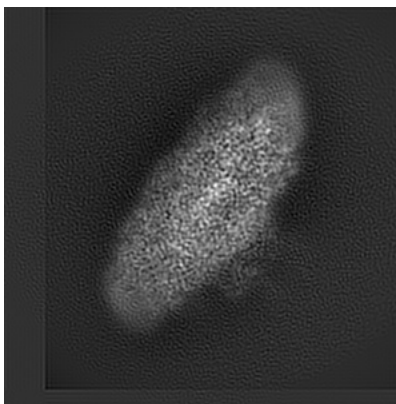
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

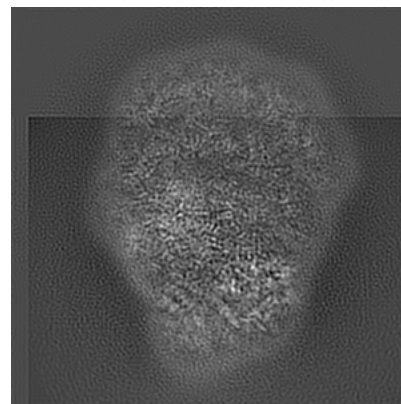
#### 6.1.1 Primary map



X

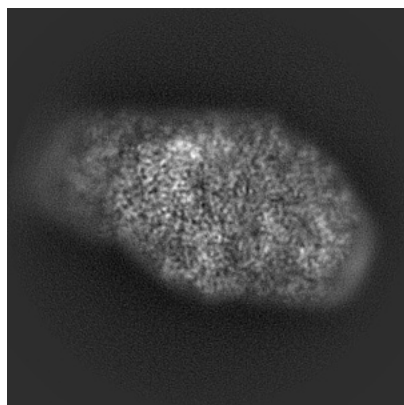


Y

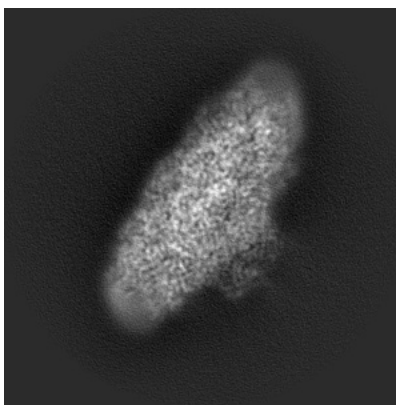


Z

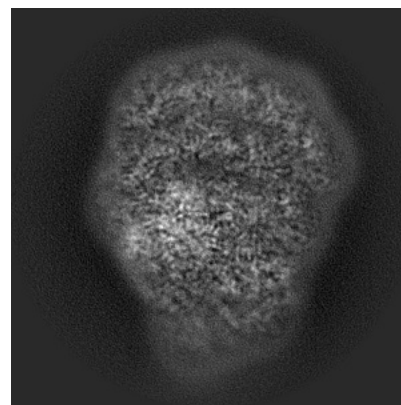
#### 6.1.2 Raw map



X



Y



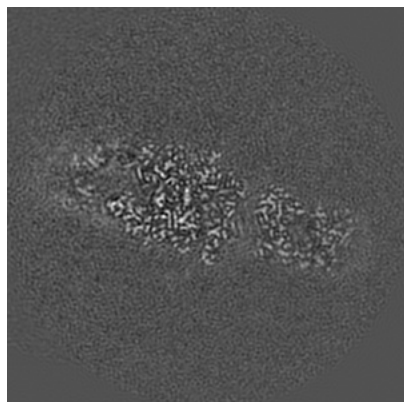
Z

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

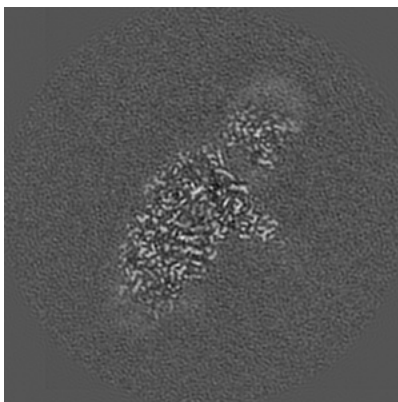


## 6.2 Central slices [i](#)

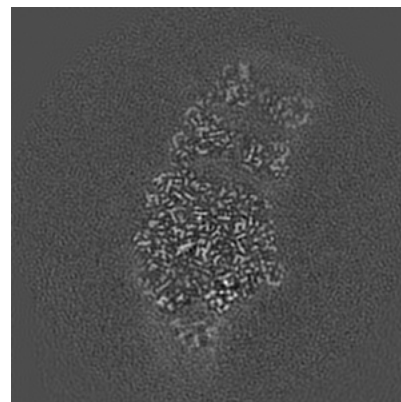
### 6.2.1 Primary map



X Index: 160

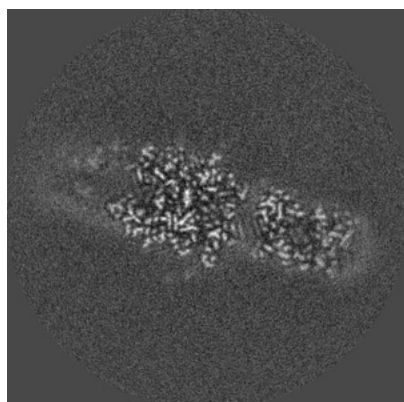


Y Index: 160

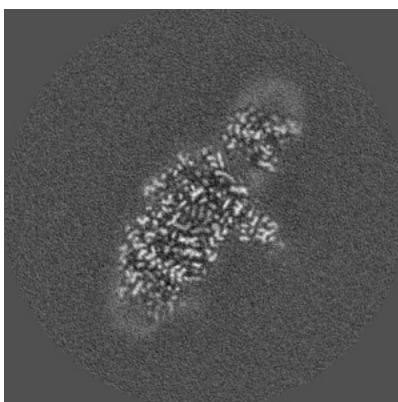


Z Index: 160

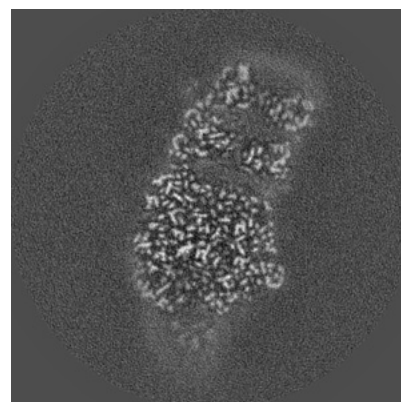
### 6.2.2 Raw map



X Index: 160



Y Index: 160

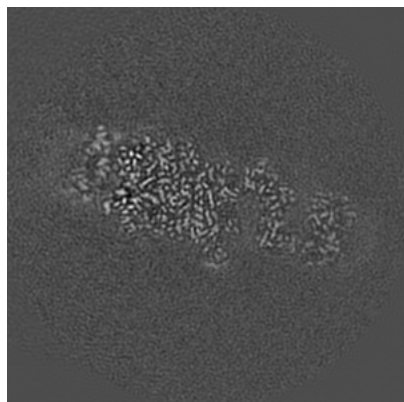


Z Index: 160

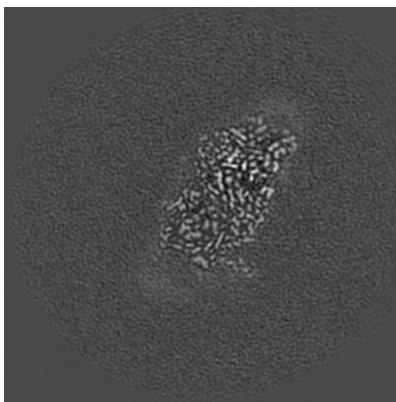
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

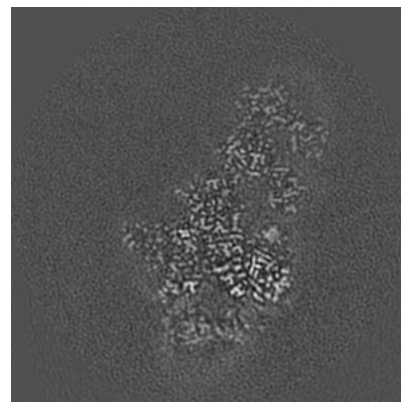
### 6.3.1 Primary map



X Index: 172

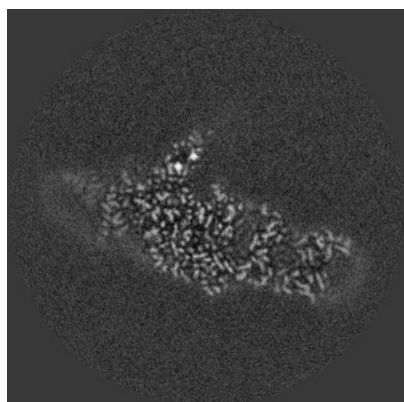


Y Index: 112

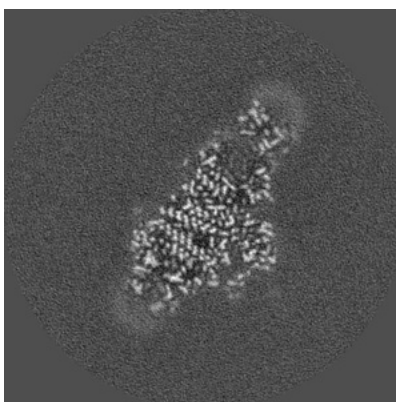


Z Index: 180

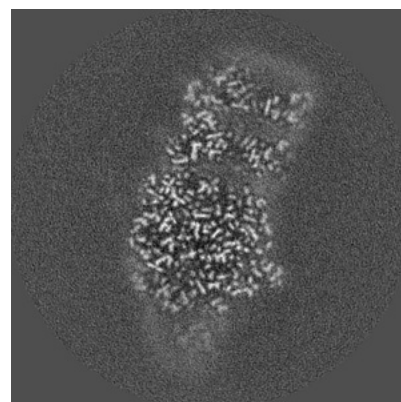
### 6.3.2 Raw map



X Index: 127



Y Index: 145

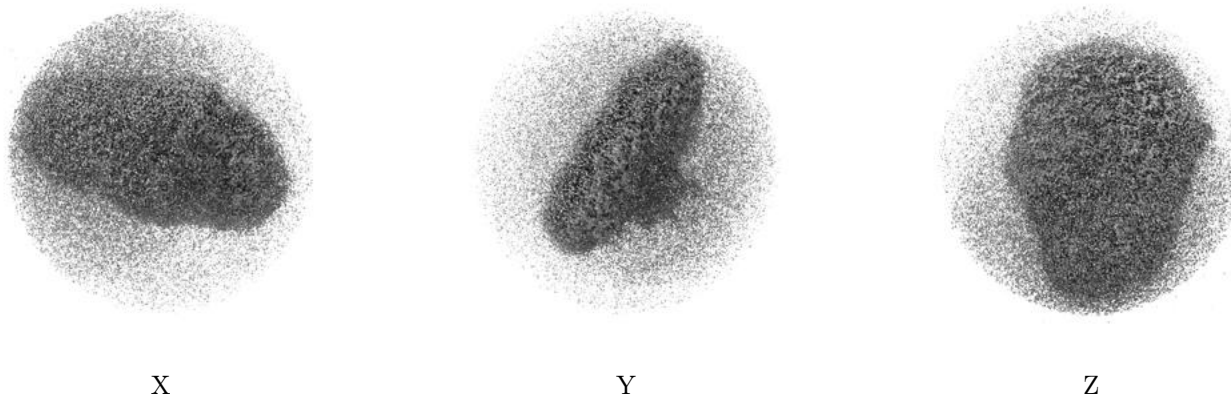


Z Index: 157

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

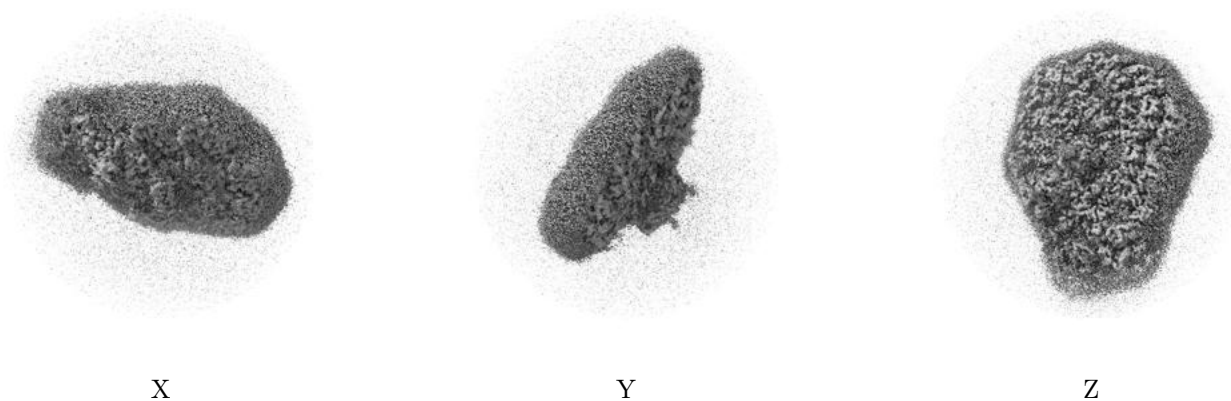
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

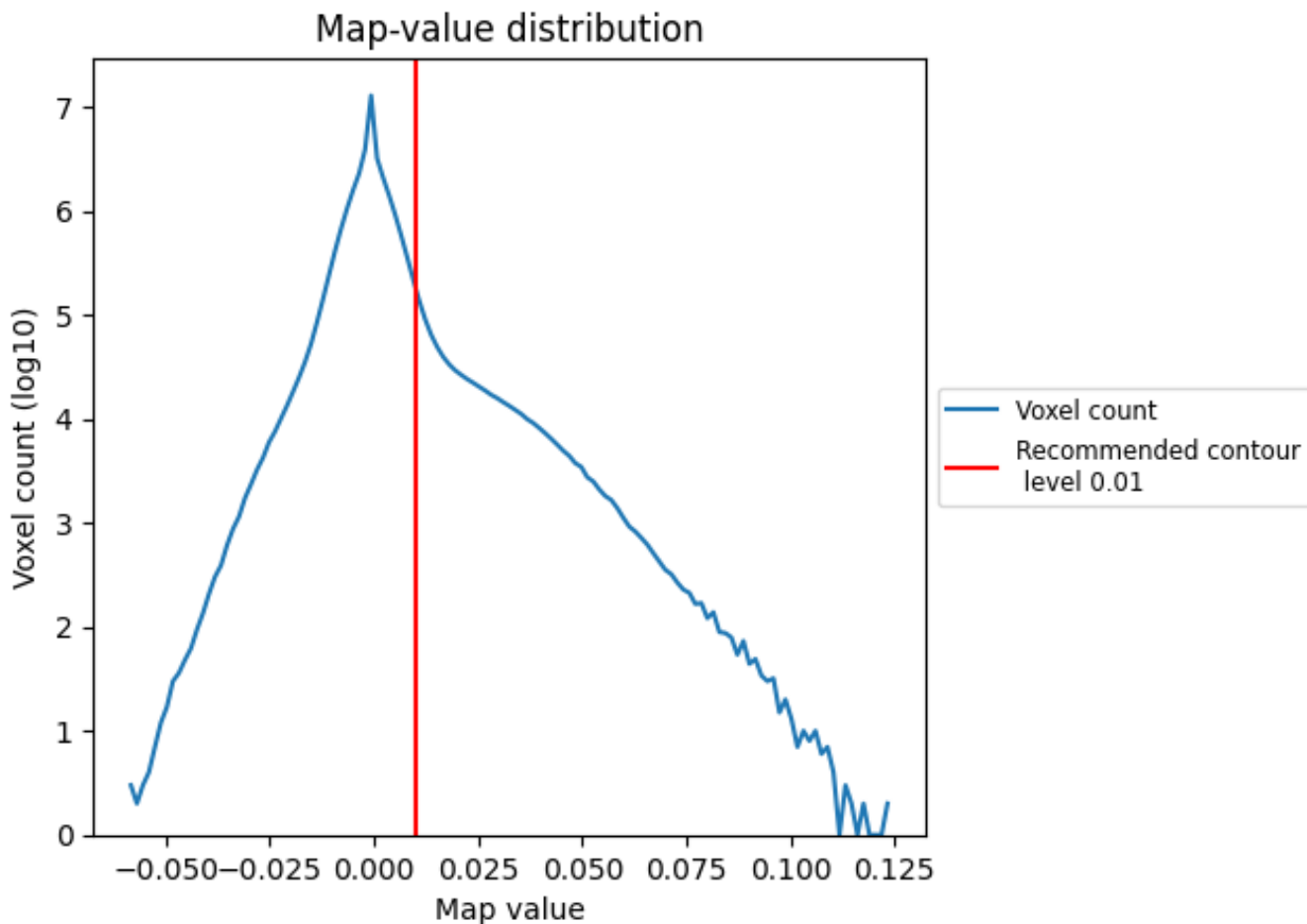
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

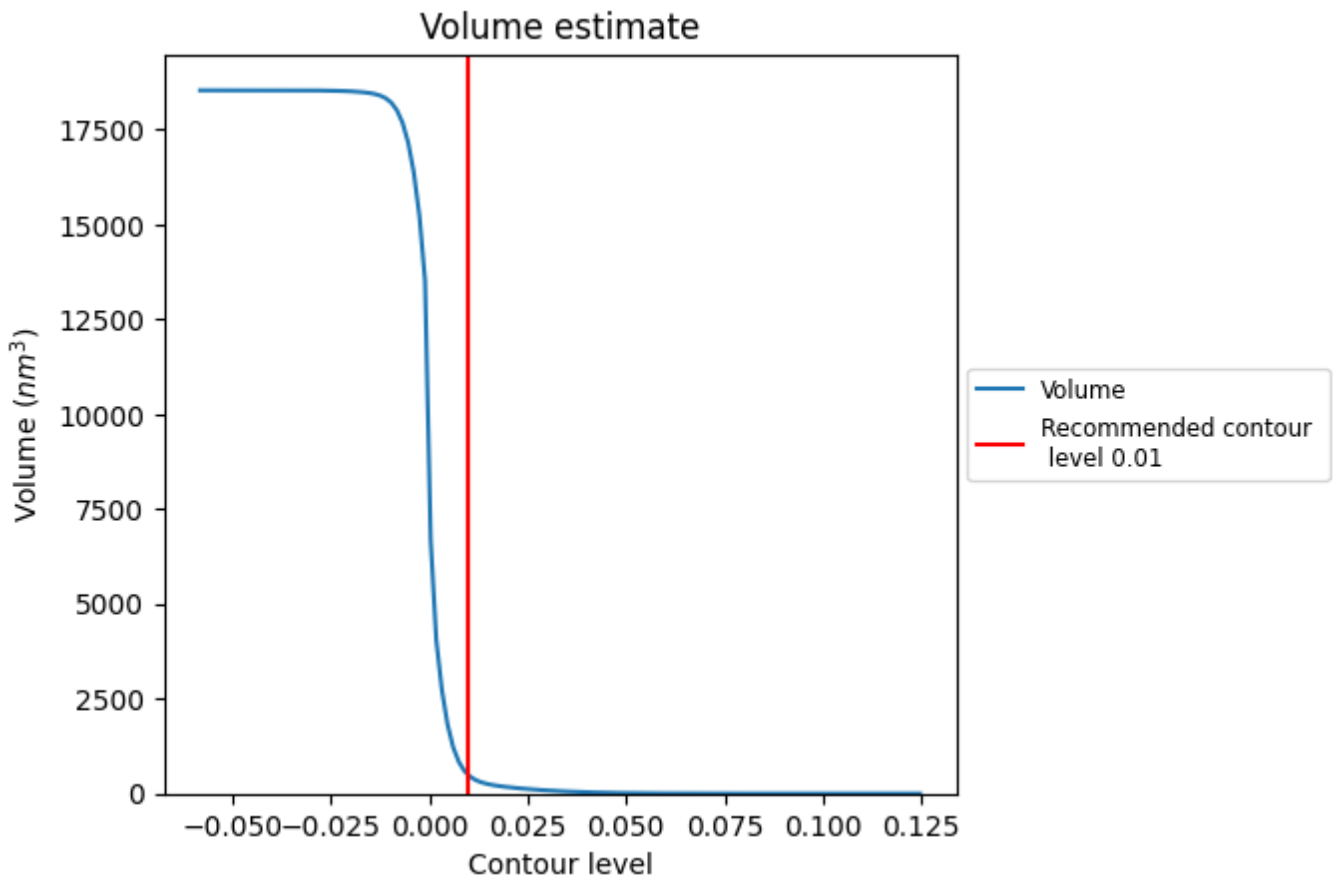
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

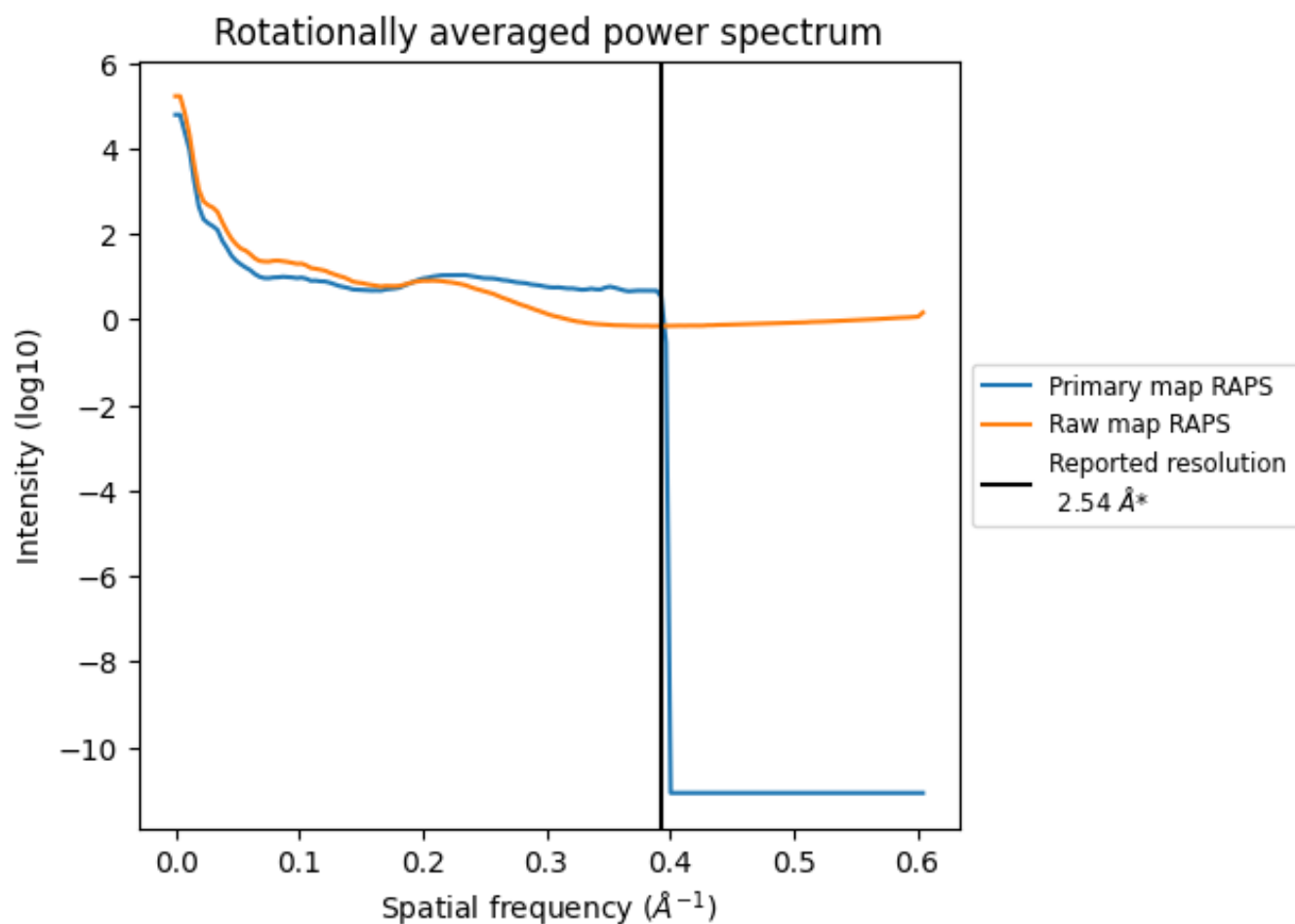
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 483  $\text{nm}^3$ ; this corresponds to an approximate mass of 436 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](#)

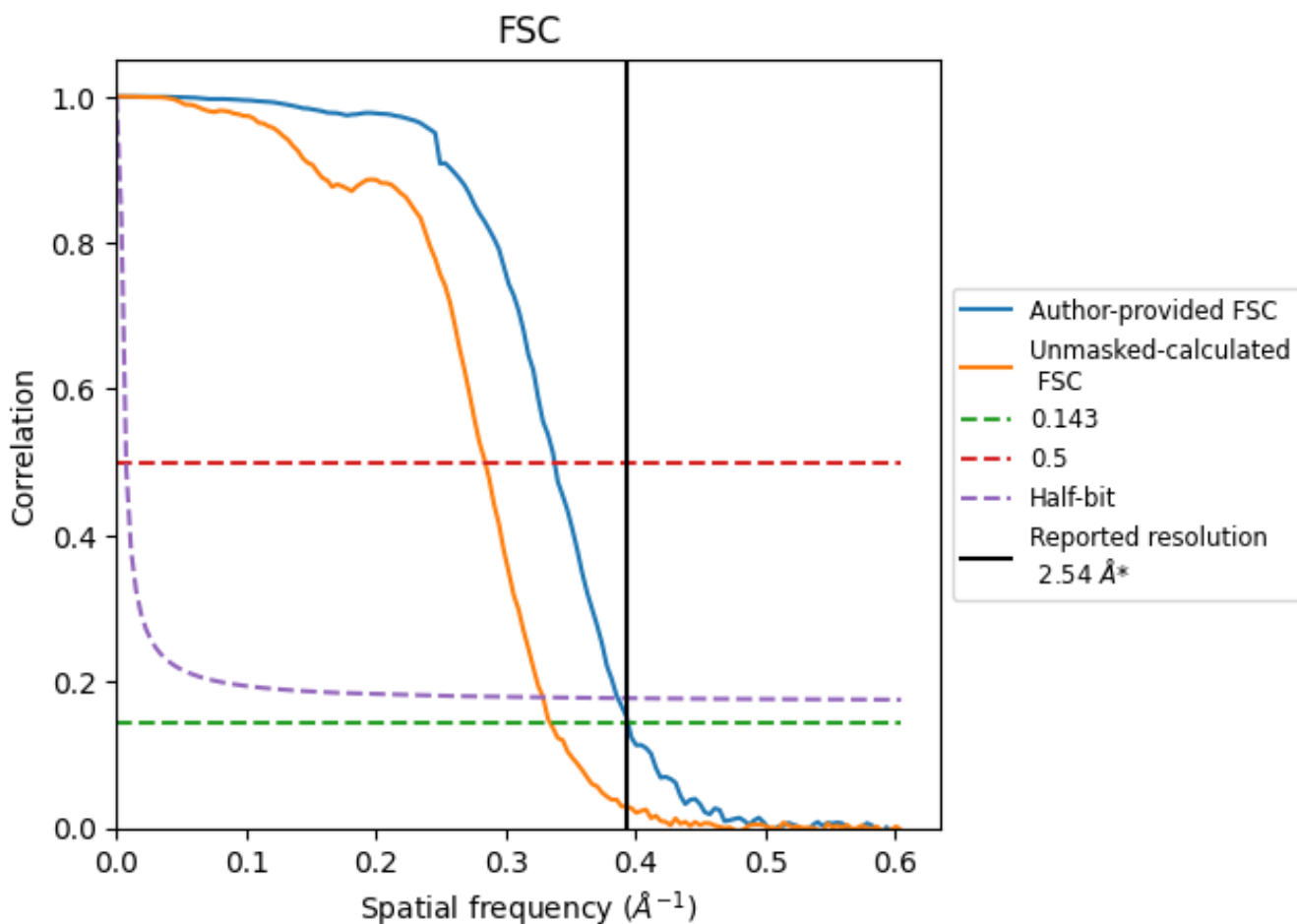


\*Reported resolution corresponds to spatial frequency of 0.394 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [\(i\)](#)

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

### 8.1 FSC [\(i\)](#)



\*Reported resolution corresponds to spatial frequency of 0.394 Å<sup>-1</sup>

## 8.2 Resolution estimates

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.54	-	-
Author-provided FSC curve	2.54	2.96	2.59
Unmasked-calculated*	2.99	3.52	3.04

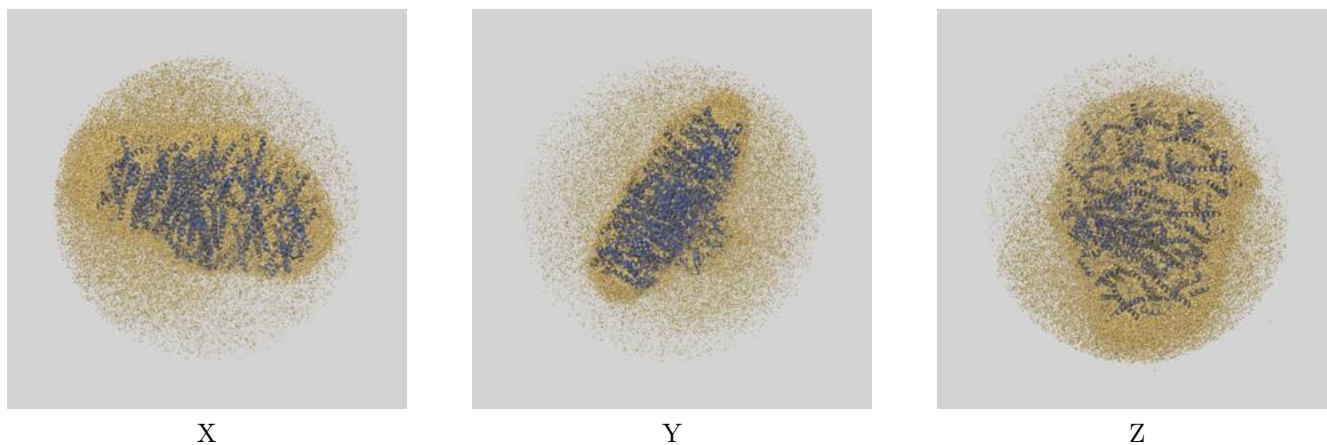
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.99 differs from the reported value 2.54 by more than 10 %



## 9 Map-model fit [i](#)

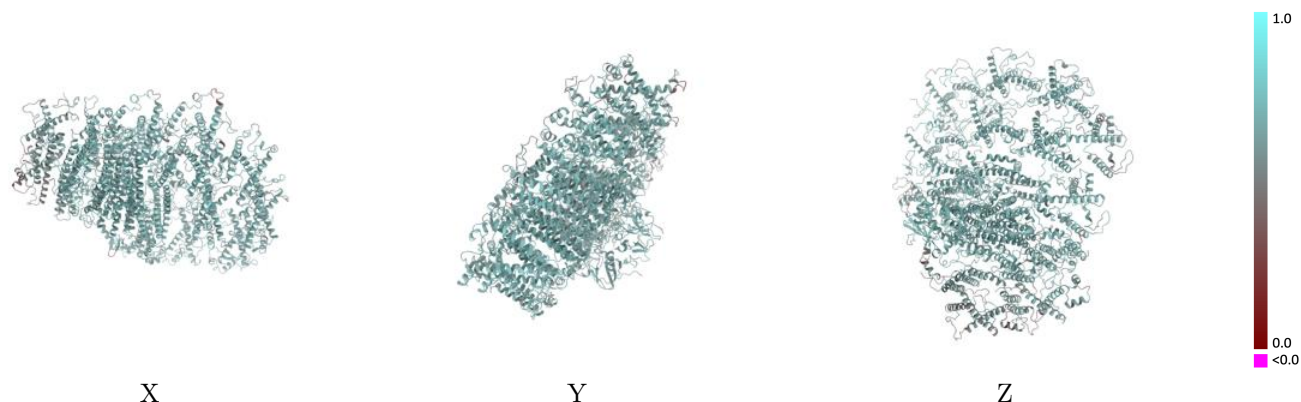
This section contains information regarding the fit between EMDB map EMD-12180 and PDB model 7BGI. Per-residue inclusion information can be found in section [3](#) on page [47](#).

### 9.1 Map-model overlay [i](#)



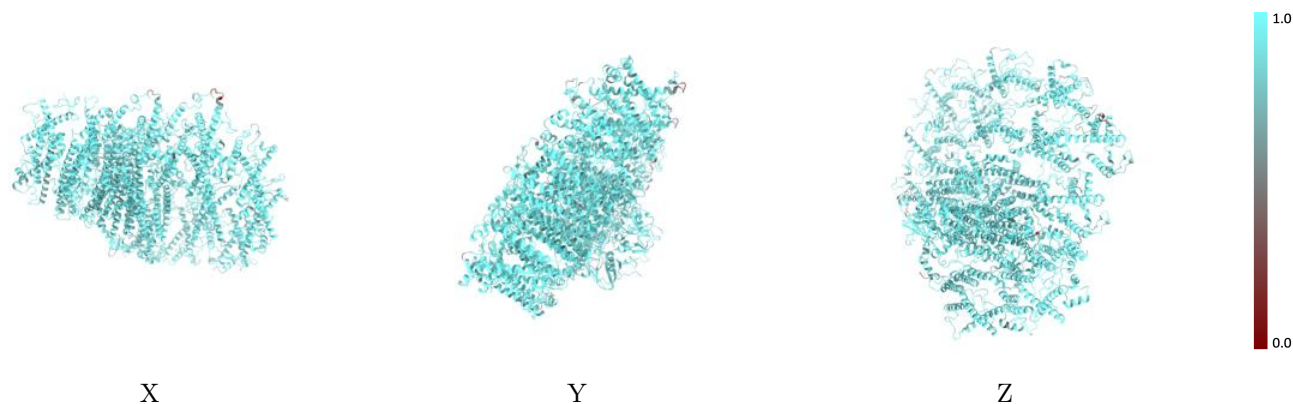
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



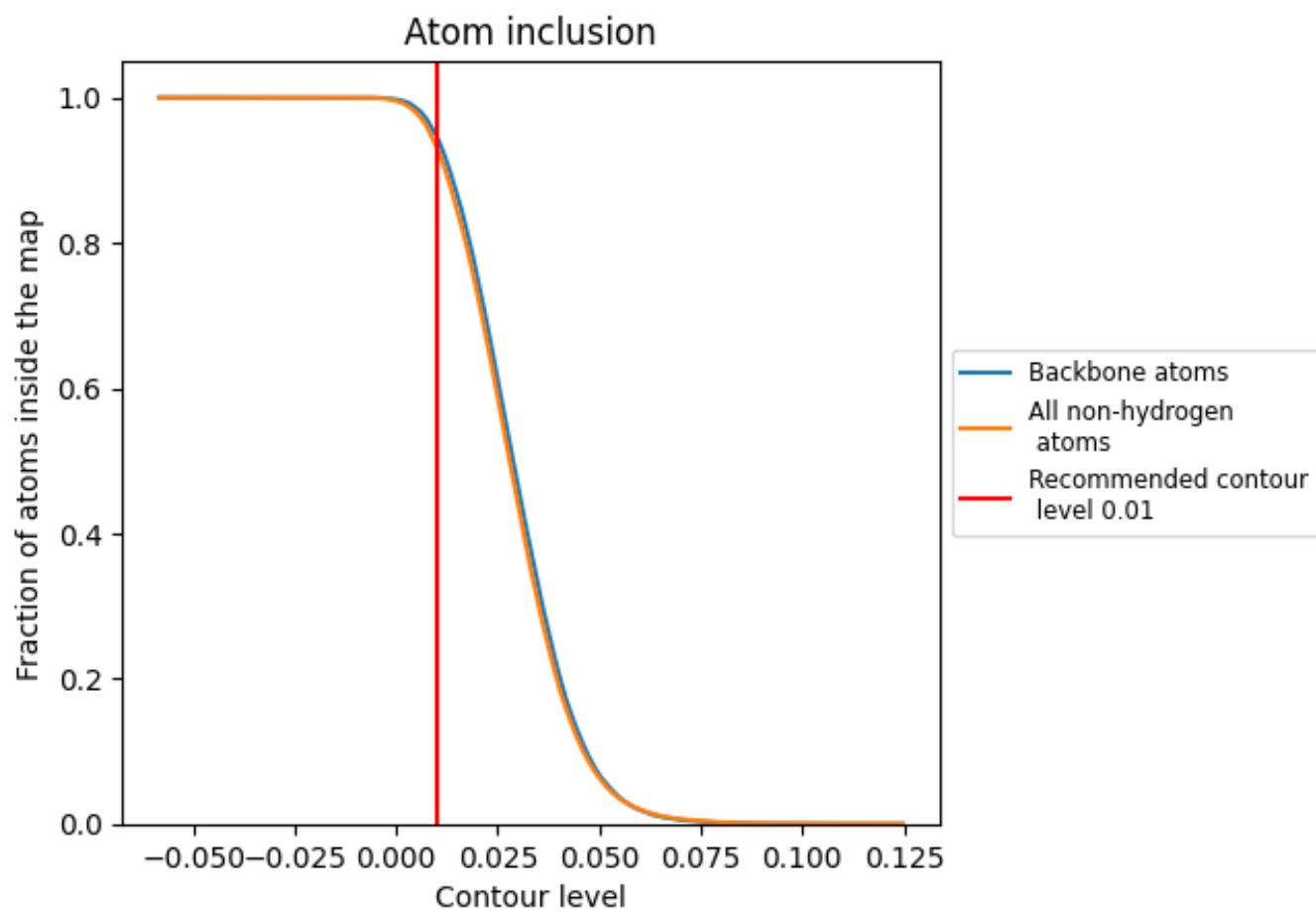
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).













































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 93% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9315	 0.6290
1	 0.9111	 0.6250
2	 0.8945	 0.5190
3	 0.9241	 0.6360
4	 0.8848	 0.6060
5	 0.8946	 0.6180
6	 0.9014	 0.6180
7	 0.9309	 0.6430
8	 0.9371	 0.6450
9	 0.9381	 0.5690
A	 0.9594	 0.6640
B	 0.9706	 0.6600
C	 0.9701	 0.6640
D	 0.9407	 0.6380
E	 0.9525	 0.6430
F	 0.9409	 0.6430
G	 0.9104	 0.5900
I	 0.9750	 0.6150
J	 0.9597	 0.6600
K	 0.8510	 0.5850
L	 0.9034	 0.5770
Z	 0.8490	 0.5870

