



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:30 PM UTC

PDB ID : 6ZZY / pdb_00006zzy
EMDB ID : EMD-11589
Title : Structure of high-light grown *Chlorella ohadii* photosystem I
Authors : Caspy, I.; Nelson, N.; Nechushtai, R.; Shkolnisky, Y.; Neumann, E.
Deposited on : 2020-08-05
Resolution : 3.16 Å (reported)
Based on initial model : 6IJO

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

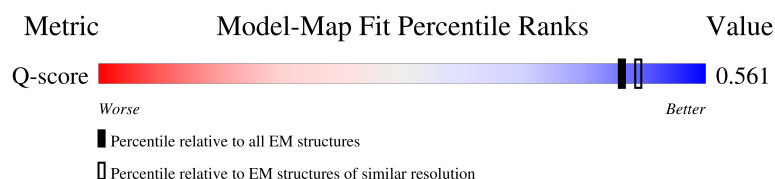
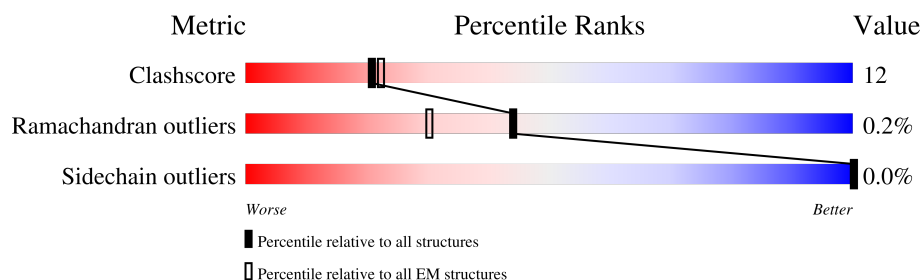
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.16 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14474 (2.66 - 3.66)

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

Mol	Chain	Length	Quality of chain
1	A	741	78% 22%
2	B	731	77% 23%
3	C	80	81% 19%
4	D	143	73% 27%

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Mol	Chain	Length	Quality of chain
5	E	64	
6	F	165	
7	G	99	
8	J	41	
9	K	86	
10	M	31	
11	I	35	
12	H	94	
13	L	157	
14	1	192	
14	a	192	
15	3	241	
16	4	207	
17	5	227	
18	6	231	
19	7	221	
20	8	219	
21	2	215	
22	9	182	

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
23	CL0	A	1011	X	-	-	-
24	CLA	1	601	X	-	-	-
24	CLA	1	602	X	-	-	-
24	CLA	1	603	X	-	-	-
24	CLA	1	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	1	605	X	-	-	-
24	CLA	1	606	X	-	-	-
24	CLA	1	607	X	-	-	-
24	CLA	1	608	X	-	-	-
24	CLA	1	610	X	-	-	-
24	CLA	1	611	X	-	-	-
24	CLA	1	612	X	-	-	-
24	CLA	1	615	X	-	-	-
24	CLA	2	601	X	-	-	-
24	CLA	2	602	X	-	-	-
24	CLA	2	603	X	-	-	-
24	CLA	2	604	X	-	-	-
24	CLA	2	605	X	-	-	-
24	CLA	2	606	X	-	-	-
24	CLA	2	607	X	-	-	-
24	CLA	2	608	X	-	-	-
24	CLA	2	609	X	-	-	-
24	CLA	2	610	X	-	-	-
24	CLA	2	612	X	-	-	-
24	CLA	2	613	X	-	-	-
24	CLA	2	615	X	-	-	-
24	CLA	2	621	X	-	-	-
24	CLA	3	601	X	-	-	-
24	CLA	3	602	X	-	-	-
24	CLA	3	603	X	-	-	-
24	CLA	3	604	X	-	-	-
24	CLA	3	605	X	-	-	-
24	CLA	3	606	X	-	-	-
24	CLA	3	607	X	-	-	-
24	CLA	3	610	X	-	-	-
24	CLA	3	612	X	-	-	-
24	CLA	3	613	X	-	-	-
24	CLA	3	616	X	-	-	-
24	CLA	3	618	X	-	-	-
24	CLA	4	601	X	-	-	-
24	CLA	4	602	X	-	-	-
24	CLA	4	603	X	-	-	-
24	CLA	4	604	X	-	-	-
24	CLA	4	605	X	-	-	-
24	CLA	4	606	X	-	-	-
24	CLA	4	607	X	-	-	-
24	CLA	4	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	4	610	X	-	-	-
24	CLA	4	611	X	-	-	-
24	CLA	4	612	X	-	-	-
24	CLA	4	615	X	-	-	-
24	CLA	4	616	X	-	-	-
24	CLA	4	617	X	-	-	-
24	CLA	5	601	X	-	-	-
24	CLA	5	602	X	-	-	-
24	CLA	5	603	X	-	-	-
24	CLA	5	604	X	-	-	-
24	CLA	5	605	X	-	-	-
24	CLA	5	606	X	-	-	-
24	CLA	5	607	X	-	-	-
24	CLA	5	608	X	-	-	-
24	CLA	5	609	X	-	-	-
24	CLA	5	612	X	-	-	-
24	CLA	5	614	X	-	-	-
24	CLA	5	616	X	-	-	-
24	CLA	5	617	X	-	-	-
24	CLA	5	618	X	-	-	-
24	CLA	6	601	X	-	-	-
24	CLA	6	602	X	-	-	-
24	CLA	6	603	X	-	-	-
24	CLA	6	604	X	-	-	-
24	CLA	6	605	X	-	-	-
24	CLA	6	606	X	-	-	-
24	CLA	6	607	X	-	-	-
24	CLA	6	608	X	-	-	-
24	CLA	6	609	X	-	-	-
24	CLA	6	612	X	-	-	-
24	CLA	6	615	X	-	-	-
24	CLA	6	617	X	-	-	-
24	CLA	6	618	X	-	-	-
24	CLA	7	601	X	-	-	-
24	CLA	7	602	X	-	-	-
24	CLA	7	603	X	-	-	-
24	CLA	7	604	X	-	-	-
24	CLA	7	605	X	-	-	-
24	CLA	7	606	X	-	-	-
24	CLA	7	607	X	-	-	-
24	CLA	7	608	X	-	-	-
24	CLA	7	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	7	610	X	-	-	-
24	CLA	7	611	X	-	-	-
24	CLA	7	612	X	-	-	-
24	CLA	7	615	X	-	-	-
24	CLA	7	617	X	-	-	-
24	CLA	8	602	X	-	-	-
24	CLA	8	603	X	-	-	-
24	CLA	8	605	X	-	-	-
24	CLA	8	606	X	-	-	-
24	CLA	8	607	X	-	-	-
24	CLA	8	608	X	-	-	-
24	CLA	8	609	X	-	-	-
24	CLA	8	610	X	-	-	-
24	CLA	8	611	X	-	-	-
24	CLA	8	612	X	-	-	-
24	CLA	8	615	X	-	-	-
24	CLA	8	618	X	-	-	-
24	CLA	8	620	X	-	-	-
24	CLA	9	601	X	-	-	-
24	CLA	9	602	X	-	-	-
24	CLA	9	603	X	-	-	-
24	CLA	9	604	X	-	-	-
24	CLA	9	605	X	-	-	-
24	CLA	9	606	X	-	-	-
24	CLA	9	607	X	-	-	-
24	CLA	9	608	X	-	-	-
24	CLA	9	609	X	-	-	-
24	CLA	9	612	X	-	-	-
24	CLA	A	1012	X	-	-	-
24	CLA	A	1013	X	-	-	-
24	CLA	A	1101	X	-	-	-
24	CLA	A	1102	X	-	-	-
24	CLA	A	1103	X	-	-	-
24	CLA	A	1104	X	-	-	-
24	CLA	A	1105	X	-	-	-
24	CLA	A	1106	X	-	-	-
24	CLA	A	1107	X	-	-	-
24	CLA	A	1108	X	-	-	-
24	CLA	A	1109	X	-	-	-
24	CLA	A	1110	X	-	-	-
24	CLA	A	1111	X	-	-	-
24	CLA	A	1112	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	A	1113	X	-	-	-
24	CLA	A	1114	X	-	-	-
24	CLA	A	1115	X	-	-	-
24	CLA	A	1116	X	-	-	-
24	CLA	A	1117	X	-	-	-
24	CLA	A	1118	X	-	-	-
24	CLA	A	1119	X	-	-	-
24	CLA	A	1120	X	-	-	-
24	CLA	A	1121	X	-	-	-
24	CLA	A	1122	X	-	-	-
24	CLA	A	1123	X	-	-	-
24	CLA	A	1124	X	-	-	-
24	CLA	A	1125	X	-	-	-
24	CLA	A	1126	X	-	-	-
24	CLA	A	1127	X	-	-	-
24	CLA	A	1128	X	-	-	-
24	CLA	A	1129	X	-	-	-
24	CLA	A	1130	X	-	-	-
24	CLA	A	1131	X	-	-	-
24	CLA	A	1132	X	-	-	-
24	CLA	A	1133	X	-	-	-
24	CLA	A	1134	X	-	-	-
24	CLA	A	1135	X	-	-	-
24	CLA	A	1136	X	-	-	-
24	CLA	A	1137	X	-	-	-
24	CLA	A	1138	X	-	-	-
24	CLA	A	1139	X	-	-	-
24	CLA	A	1140	X	-	-	-
24	CLA	A	1141	X	-	-	-
24	CLA	B	1021	X	-	-	-
24	CLA	B	1022	X	-	-	-
24	CLA	B	1023	X	-	-	-
24	CLA	B	1201	X	-	-	-
24	CLA	B	1202	X	-	-	-
24	CLA	B	1203	X	-	-	-
24	CLA	B	1204	X	-	-	-
24	CLA	B	1205	X	-	-	-
24	CLA	B	1206	X	-	-	-
24	CLA	B	1207	X	-	-	-
24	CLA	B	1208	X	-	-	-
24	CLA	B	1209	X	-	-	-
24	CLA	B	1210	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	B	1211	X	-	-	-
24	CLA	B	1212	X	-	-	-
24	CLA	B	1213	X	-	-	-
24	CLA	B	1214	X	-	-	-
24	CLA	B	1215	X	-	-	-
24	CLA	B	1216	X	-	-	-
24	CLA	B	1217	X	-	-	-
24	CLA	B	1218	X	-	-	-
24	CLA	B	1219	X	-	-	-
24	CLA	B	1220	X	-	-	-
24	CLA	B	1221	X	-	-	-
24	CLA	B	1222	X	-	-	-
24	CLA	B	1223	X	-	-	-
24	CLA	B	1224	X	-	-	-
24	CLA	B	1225	X	-	-	-
24	CLA	B	1226	X	-	-	-
24	CLA	B	1227	X	-	-	-
24	CLA	B	1228	X	-	-	-
24	CLA	B	1229	X	-	-	-
24	CLA	B	1230	X	-	-	-
24	CLA	B	1231	X	-	-	-
24	CLA	B	1232	X	-	-	-
24	CLA	B	1234	X	-	-	-
24	CLA	B	1235	X	-	-	-
24	CLA	B	1236	X	-	-	-
24	CLA	B	1237	X	-	-	-
24	CLA	B	1238	X	-	-	-
24	CLA	B	1239	X	-	-	-
24	CLA	B	1240	X	-	-	-
24	CLA	F	1301	X	-	-	-
24	CLA	F	1302	X	-	-	-
24	CLA	G	1601	X	-	-	-
24	CLA	G	1602	X	-	-	-
24	CLA	G	1603	X	-	-	-
24	CLA	H	1701	X	-	-	-
24	CLA	H	1702	X	-	-	-
24	CLA	H	1703	X	-	-	-
24	CLA	J	1901	X	-	-	-
24	CLA	K	1401	X	-	-	-
24	CLA	K	1402	X	-	-	-
24	CLA	K	1403	X	-	-	-
24	CLA	K	1404	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	L	1501	X	-	-	-
24	CLA	L	1502	X	-	-	-
24	CLA	L	1503	X	-	-	-
24	CLA	a	601	X	-	-	-
24	CLA	a	602	X	-	-	-
24	CLA	a	603	X	-	-	-
24	CLA	a	604	X	-	-	-
24	CLA	a	605	X	-	-	-
24	CLA	a	607	X	-	-	-
24	CLA	a	608	X	-	-	-
24	CLA	a	611	X	-	-	-
24	CLA	a	612	X	-	-	-
24	CLA	a	615	X	-	-	-
36	ERG	G	5002	X	-	-	-
37	RRX	J	4002	X	-	-	-
40	LUT	1	503	X	-	-	-
40	LUT	6	501	X	-	-	-
40	LUT	6	502	X	-	-	-
40	LUT	7	501	X	-	-	-
40	LUT	9	502	X	-	-	-
41	CHL	1	609	X	-	-	-
41	CHL	1	613	X	-	-	-
41	CHL	3	608	X	-	-	-
41	CHL	3	611	X	-	-	-
41	CHL	4	609	X	-	-	-
41	CHL	4	613	X	-	-	-
41	CHL	4	618	X	-	-	-
41	CHL	5	610	X	-	-	-
41	CHL	5	611	X	-	-	-
41	CHL	5	613	X	-	-	-
41	CHL	6	610	X	-	-	-
41	CHL	6	611	X	-	-	-
41	CHL	6	613	X	-	-	-
41	CHL	6	619	X	-	-	-
41	CHL	7	613	X	-	-	-
41	CHL	8	601	X	-	-	-
41	CHL	8	604	X	-	-	-
41	CHL	8	613	X	-	-	-
41	CHL	9	610	X	-	-	-
41	CHL	9	613	X	-	-	-
41	CHL	a	606	X	-	-	-
41	CHL	a	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
41	CHL	a	610	X	-	-	-
41	CHL	a	613	X	-	-	-
43	QTB	3	506	X	-	-	-
43	QTB	a	504	X	-	-	-
48	XAT	7	502	X	-	-	-
49	C7Z	7	504	X	-	-	-

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 54609 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	741	Total	C	N	O	S	0	0
			5824	3815	988	1001	20		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	368	ALA	SER	variant	UNP W8SY74
A	437	ILE	MET	variant	UNP W8SY74

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	731	Total	C	N	O	S	0	0
			5796	3807	980	994	15		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	5	LEU	-	insertion	UNP W8SUA3
B	241	ALA	VAL	conflict	UNP W8SUA3
B	402	ALA	GLU	conflict	UNP W8SUA3
B	403	GLN	ALA	conflict	UNP W8SUA3

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			601	367	104	119	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	143	Total	C	N	O	S	0	0
			1124	716	196	208	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	188	ALA	VAL	variant	UNP A0A2P6TKF8
D	320	ILE	VAL	variant	UNP A0A2P6TKF8

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	64	Total	C	N	O	S	0	0
			509	323	91	95			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	44	GLN	THR	variant	UNP A0A2P6U4S6
E	48	LEU	MET	variant	UNP A0A2P6U4S6
E	96	VAL	GLU	variant	UNP A0A2P6U4S6
E	97	ALA	GLU	variant	UNP A0A2P6U4S6
E	98	ALA	VAL	variant	UNP A0A2P6U4S6

- Molecule 6 is a protein called PSI-F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	165	Total	C	N	O	S	0	0
			1277	830	216	228	3		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	346	LEU	MET	variant	UNP A0A2P6TPV8
F	348	ASN	LYS	variant	UNP A0A2P6TPV8
F	351	ALA	GLU	variant	UNP A0A2P6TPV8
F	352	ASP	GLY	variant	UNP A0A2P6TPV8
F	360	LYS	GLN	variant	UNP A0A2P6TPV8
F	364	ALA	ASP	variant	UNP A0A2P6TPV8
F	367	GLU	ASN	variant	UNP A0A2P6TPV8
F	430	ALA	SER	variant	UNP A0A2P6TPV8
F	431	ALA	SER	variant	UNP A0A2P6TPV8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	432	THR	MET	variant	UNP A0A2P6TPV8
F	433	ALA	THR	variant	UNP A0A2P6TPV8

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	99	Total	C	N	O	S	0	0
			727	466	127	130	4		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	1229	ALA	SER	variant	UNP A0A2P6TZI8
G	1272	LEU	MET	variant	UNP A0A2P6TZI8
G	1285	ILE	VAL	variant	UNP A0A2P6TZI8
G	1313	ILE	LEU	variant	UNP A0A2P6TZI8
G	1317	SER	HIS	variant	UNP A0A2P6TZI8
G	1320	GLY	GLN	variant	UNP A0A2P6TZI8
G	1321	LEU	VAL	variant	UNP A0A2P6TZI8
G	1324	ASN	VAL	variant	UNP A0A2P6TZI8

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	41	Total	C	N	O	S	0	0
			316	212	46	57	1		

- Molecule 9 is a protein called PSI-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	86	Total	C	N	O	S	0	0
			613	390	106	115	2		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	74	ALA	GLU	variant	UNP A0A2P6U0J1
K	103	LEU	ILE	variant	UNP A0A2P6U0J1
K	105	CYS	VAL	variant	UNP A0A2P6U0J1
K	107	ILE	VAL	variant	UNP A0A2P6U0J1
K	108	VAL	ILE	variant	UNP A0A2P6U0J1

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Chain	Residue	Modelled	Actual	Comment	Reference
K	112	LYS	ARG	variant	UNP A0A2P6U0J1
K	113	SER	GLY	variant	UNP A0A2P6U0J1

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	31	Total	C	N	O	S	0	0
			239	163	36	39	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	35	Total	C	N	O	S	0	0
			270	183	37	47	3		

- Molecule 12 is a protein called Photosystem I reaction center subunit VI-chloroplastic-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	94	Total	C	N	O	S	0	0
			729	457	132	139	1		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	92	ILE	VAL	conflict	UNP A0A2P6TPU7
H	102	GLY	LEU	conflict	UNP A0A2P6TPU7
H	105	ALA	SER	conflict	UNP A0A2P6TPU7
H	106	ALA	SER	conflict	UNP A0A2P6TPU7
H	109	ARG	SER	conflict	UNP A0A2P6TPU7
H	?	-	ILE	deletion	UNP A0A2P6TPU7
H	113	VAL	LYS	conflict	UNP A0A2P6TPU7

- Molecule 13 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	157	Total	C	N	O	S	0	0
			1165	758	192	211	4		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	350	TYR	PHE	conflict	UNP A0A2P6TC44
L	364	ASP	ASN	conflict	UNP A0A2P6TC44
L	?	-	ALA	deletion	UNP A0A2P6TC44
L	421	ASP	GLU	conflict	UNP A0A2P6TC44
L	443	LEU	ILE	conflict	UNP A0A2P6TC44

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	1	192	Total	C	N	O	S	0	0
			1405	900	237	261	7		
14	a	192	Total	C	N	O	S	0	0
			1405	900	237	261	7		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	166	SER	LEU	conflict	UNP A0A2P6TT36
1	167	LYS	GLU	conflict	UNP A0A2P6TT36
1	171	THR	VAL	conflict	UNP A0A2P6TT36
1	194	THR	ASN	conflict	UNP A0A2P6TT36
1	196	ALA	GLN	conflict	UNP A0A2P6TT36
1	204	SER	ALA	conflict	UNP A0A2P6TT36
1	210	MET	LEU	conflict	UNP A0A2P6TT36
a	166	SER	LEU	conflict	UNP A0A2P6TT36
a	167	LYS	GLU	conflict	UNP A0A2P6TT36
a	171	THR	VAL	conflict	UNP A0A2P6TT36
a	194	THR	ASN	conflict	UNP A0A2P6TT36
a	196	ALA	GLN	conflict	UNP A0A2P6TT36
a	204	SER	ALA	conflict	UNP A0A2P6TT36
a	210	MET	LEU	conflict	UNP A0A2P6TT36

- Molecule 15 is a protein called Glutathione reductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	3	241	Total	C	N	O	S	0	0
			1844	1194	302	337	11		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	314	CYS	GLY	conflict	UNP A0A2P6TMT4
3	329	ILE	VAL	conflict	UNP A0A2P6TMT4

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Chain	Residue	Modelled	Actual	Comment	Reference
3	339	THR	SER	conflict	UNP A0A2P6TMT4
3	359	LYS	ASN	conflict	UNP A0A2P6TMT4
3	405	GLY	ALA	conflict	UNP A0A2P6TMT4
3	429	GLU	ALA	conflict	UNP A0A2P6TMT4
3	484	THR	ARG	conflict	UNP A0A2P6TMT4
3	485	ILE	ARG	conflict	UNP A0A2P6TMT4
3	486	LEU	ARG	conflict	UNP A0A2P6TMT4
3	487	LYS	ALA	conflict	UNP A0A2P6TMT4

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	4	207	Total	C	N	O	S	0	0
			1631	1056	277	294	4		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	37	GLU	ASP	conflict	UNP A0A2P6TQ14
4	109	ASP	ASN	conflict	UNP A0A2P6TQ14
4	112	ASN	ASP	conflict	UNP A0A2P6TQ14
4	213	GLY	SER	conflict	UNP A0A2P6TQ14
4	218	ASN	ASP	conflict	UNP A0A2P6TQ14
4	?	-	LEU	deletion	UNP A0A2P6TQ14
4	236	ASN	ARG	variant	UNP A0A2P6TQ14

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	5	227	Total	C	N	O	S	0	0
			1769	1136	307	314	12		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	32	LYS	ASP	conflict	UNP A0A2P6U4K1
5	38	VAL	ALA	conflict	UNP A0A2P6U4K1
5	40	ALA	SER	conflict	UNP A0A2P6U4K1
5	42	GLY	ALA	conflict	UNP A0A2P6U4K1
5	113	SER	GLY	conflict	UNP A0A2P6U4K1
5	127	ILE	LEU	conflict	UNP A0A2P6U4K1
5	195	VAL	ILE	conflict	UNP A0A2P6U4K1

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	6	231	Total	C	N	O	S	0	0
			1787	1168	295	314	10		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	83	CYS	ALA	conflict	UNP A0A2P6TPR7
6	94	LEU	MET	conflict	UNP A0A2P6TPR7
6	196	ILE	VAL	conflict	UNP A0A2P6TPR7
6	201	ALA	GLY	conflict	UNP A0A2P6TPR7
6	250	GLN	ASN	conflict	UNP A0A2P6TPR7

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	7	221	Total	C	N	O	S	0	0
			1698	1090	294	308	6		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7	6	VAL	ASP	conflict	UNP A0A2P6TS63
7	8	GLU	PRO	conflict	UNP A0A2P6TS63
7	17	VAL	ALA	conflict	UNP A0A2P6TS63
7	82	PHE	TYR	conflict	UNP A0A2P6TS63
7	96	ASP	SER	conflict	UNP A0A2P6TS63
7	107	MET	LEU	conflict	UNP A0A2P6TS63
7	154	TYR	PHE	conflict	UNP A0A2P6TS63
7	205	VAL	ILE	conflict	UNP A0A2P6TS63
7	209	ALA	SER	conflict	UNP A0A2P6TS63
7	218	HIS	TYR	conflict	UNP A0A2P6TS63

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	8	219	Total	C	N	O	S	0	0
			1669	1073	285	305	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
8	103	GLU	ASP	conflict	UNP A0A2P6TZ50

- Molecule 21 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	2	215	Total	C	N	O	S	0	0
			1666	1074	277	309	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	64	ASP	GLU	conflict	UNP A0A2P6TMX4
2	97	PRO	ASN	conflict	UNP A0A2P6TMX4

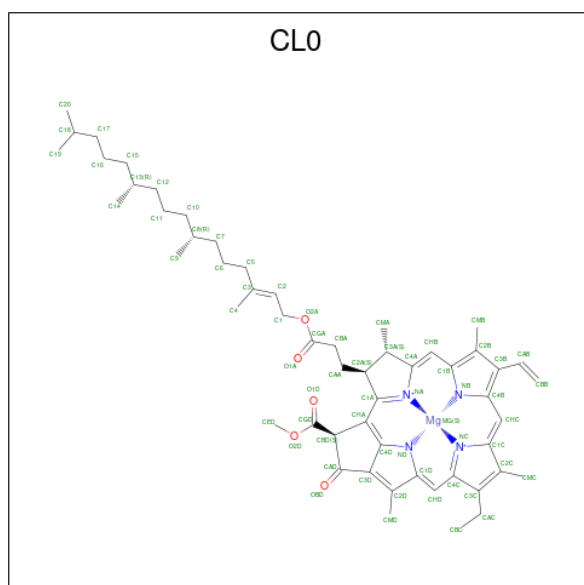
- Molecule 22 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	9	182	Total	C	N	O	S	0	0
			1397	906	231	254	6		

There is a discrepancy between the modelled and reference sequences:

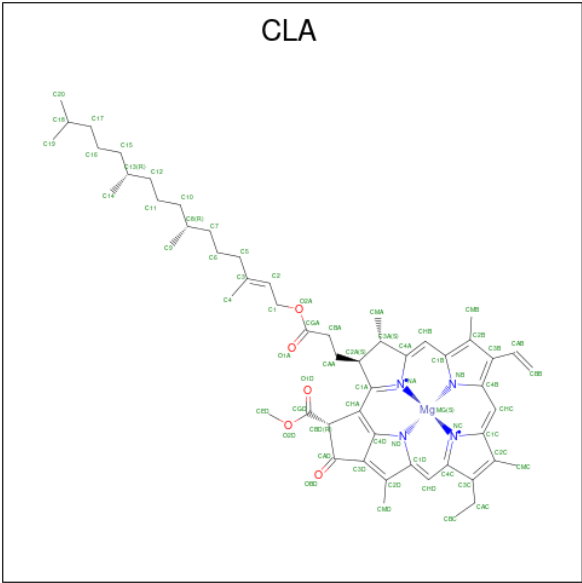
Chain	Residue	Modelled	Actual	Comment	Reference
9	257	TYR	HIS	conflict	UNP A0A2P6TMI2

- Molecule 23 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



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

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	B	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	B	1	Total 62	C 52	Mg 1	N 4	O 5	0
24	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	B	1	Total 61	C 51	Mg 1	N 4	O 5	0
24	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
24	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
24	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 53	C 43	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	F	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	F	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
24	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	K	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	K	1	Total 52	C 42	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	H	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	H	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	H	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	1	1	Total 57	C 47	Mg 1	N 4	O 5	0
24	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	a	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
24	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	a	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
24	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	3	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
24	3	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
24	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	4	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
24	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	4	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
24	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
24	4	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
24	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	5	1	Total 52	C 42	Mg 1	N 4	O 5	0
24	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	6	1	Total 52	C 42	Mg 1	N 4	O 5	0
24	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	6	1	Total 52	C 42	Mg 1	N 4	O 5	0
24	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	7	1	Total 44	C 35	Mg 1	N 4	O 4	0
24	7	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	7	1	Total 44	C 34	Mg 1	N 4	O 5	0
24	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	7	1	Total 59	C 49	Mg 1	N 4	O 5	0
24	7	1	Total 42	C 34	Mg 1	N 4	O 3	0
24	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	7	1	Total 54	C 44	Mg 1	N 4	O 5	0
24	8	1	Total 52	C 42	Mg 1	N 4	O 5	0
24	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	8	1	Total 57	C 47	Mg 1	N 4	O 5	0
24	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	8	1	Total 52	C 42	Mg 1	N 4	O 5	0
24	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	8	1	Total 46	C 36	Mg 1	N 4	O 5	0

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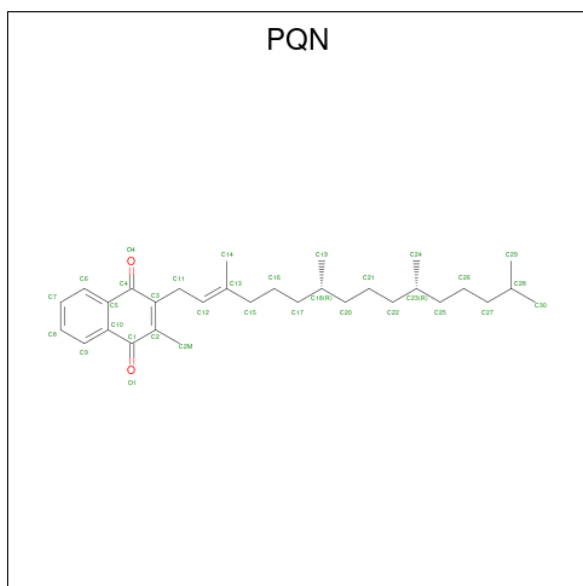
Mol	Chain	Residues	Atoms					AltConf
24	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
24	2	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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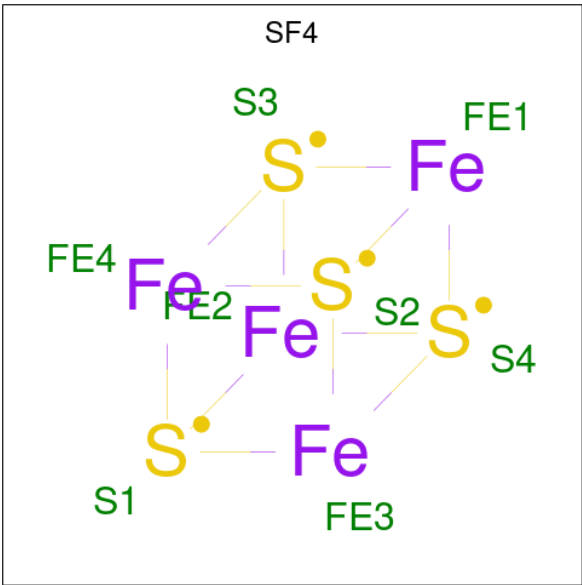
Mol	Chain	Residues	Atoms					AltConf
24	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	9	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
24	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 25 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



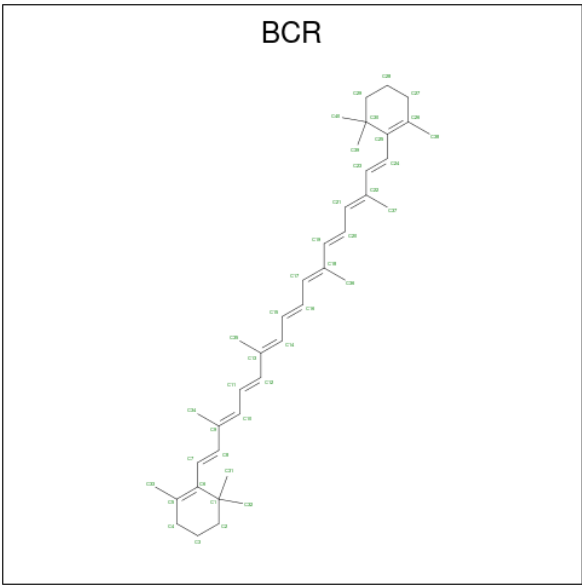
Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	C	O	0
			33	31	2	
25	B	1	Total	C	O	0
			33	31	2	

- Molecule 26 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 27 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		AltConf
27	A	1	Total	C	0
			40	40	

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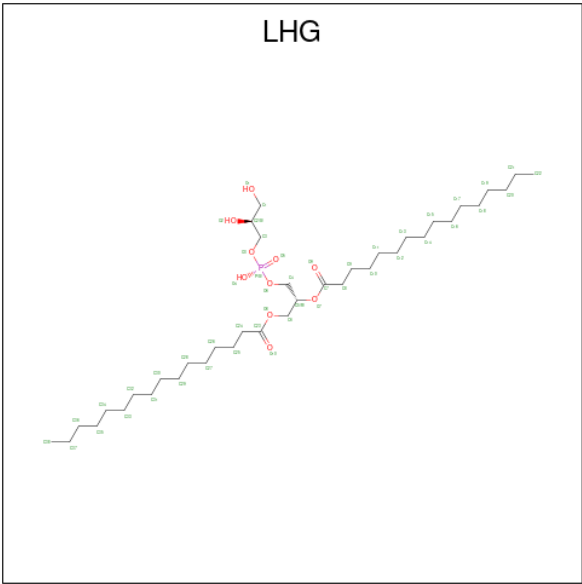
Mol	Chain	Residues	Atoms	AltConf
27	A	1	Total C 40 40	0
27	A	1	Total C 40 40	0
27	A	1	Total C 40 40	0
27	A	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	F	1	Total C 40 40	0
27	G	1	Total C 40 40	0
27	J	1	Total C 40 40	0
27	K	1	Total C 40 40	0
27	K	1	Total C 40 40	0
27	I	1	Total C 40 40	0
27	H	1	Total C 40 40	0
27	L	1	Total C 40 40	0
27	L	1	Total C 40 40	0
27	L	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms		AltConf
27	3	1	Total	C	0
			40	40	
27	3	1	Total	C	0
			40	40	
27	3	1	Total	C	0
			40	40	
27	4	1	Total	C	0
			40	40	
27	5	1	Total	C	0
			40	40	
27	5	1	Total	C	0
			40	40	
27	6	1	Total	C	0
			40	40	
27	6	1	Total	C	0
			40	40	
27	7	1	Total	C	0
			40	40	
27	8	1	Total	C	0
			40	40	

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	O	P	0
			29	18	10	1	

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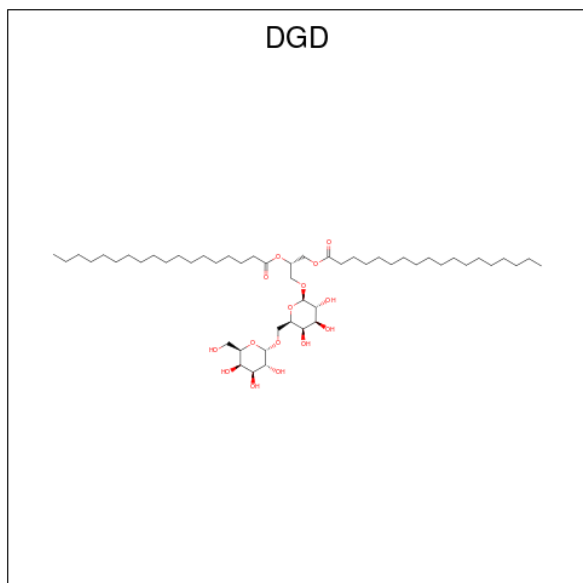
Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	O	P	0
			49	38	10	1	
28	A	1	Total	C	O	P	0
			42	31	10	1	
28	B	1	Total	C	O	P	0
			46	35	10	1	
28	B	1	Total	C	O	P	0
			49	38	10	1	
28	F	1	Total	C	O	P	0
			43	32	10	1	
28	F	1	Total	C	O	P	0
			36	25	10	1	
28	1	1	Total	C	O	P	0
			35	24	10	1	
28	1	1	Total	C	O	P	0
			42	31	10	1	
28	a	1	Total	C	O	P	0
			35	24	10	1	
28	3	1	Total	C	O	P	0
			49	38	10	1	
28	4	1	Total	C	O	P	0
			49	38	10	1	
28	4	1	Total	C	O	P	0
			32	21	10	1	
28	5	1	Total	C	O	P	0
			49	38	10	1	
28	6	1	Total	C	O	P	0
			49	38	10	1	
28	6	1	Total	C	O	P	0
			37	26	10	1	
28	7	1	Total	C	O	P	0
			49	38	10	1	
28	7	1	Total	C	O	P	0
			36	25	10	1	
28	7	1	Total	C	O	P	0
			43	32	10	1	
28	8	1	Total	C	O	P	0
			37	26	10	1	
28	2	1	Total	C	O	P	0
			49	38	10	1	
28	2	1	Total	C	O	P	0
			49	38	10	1	

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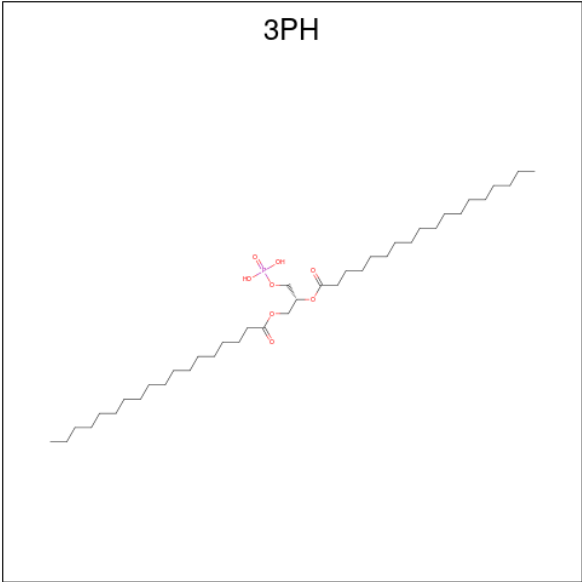
Mol	Chain	Residues	Atoms				AltConf
28	9	1	Total	C	O	P	0
			33	22	10	1	
28	9	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



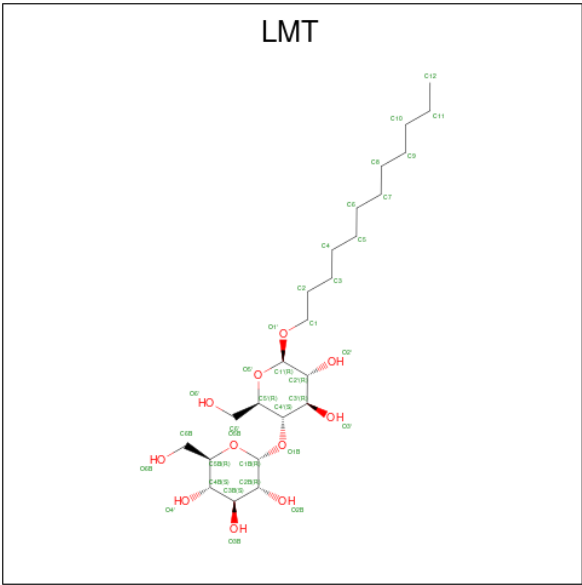
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			51	36	15	
29	B	1	Total	C	O	0
			66	51	15	
29	8	1	Total	C	O	0
			66	51	15	

- Molecule 30 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$).



Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O	P	0
			33	24	8	1	

- Molecule 31 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



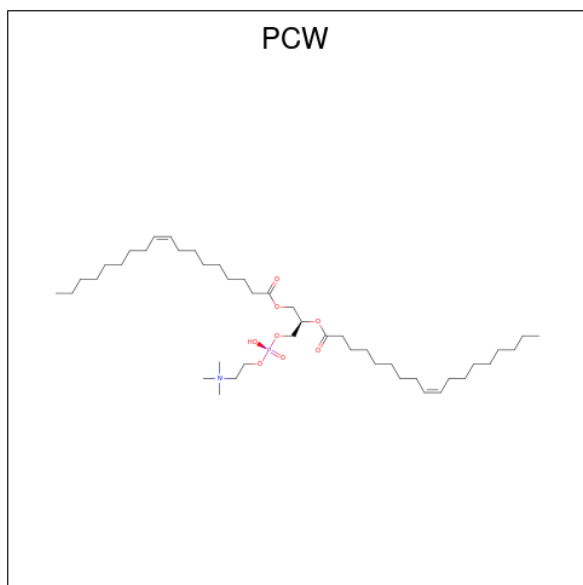
Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			35	24	11	
31	B	1	Total	C	O	0
			35	24	11	
31	1	1	Total	C	O	0
			35	24	11	

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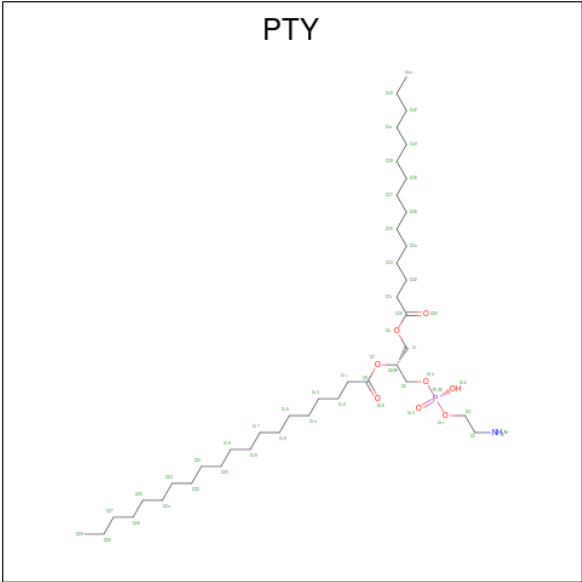
Mol	Chain	Residues	Atoms			AltConf
31	2	1	Total	C	O	0
			35	24	11	

- Molecule 32 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: $C_{44}H_{85}NO_8P$).



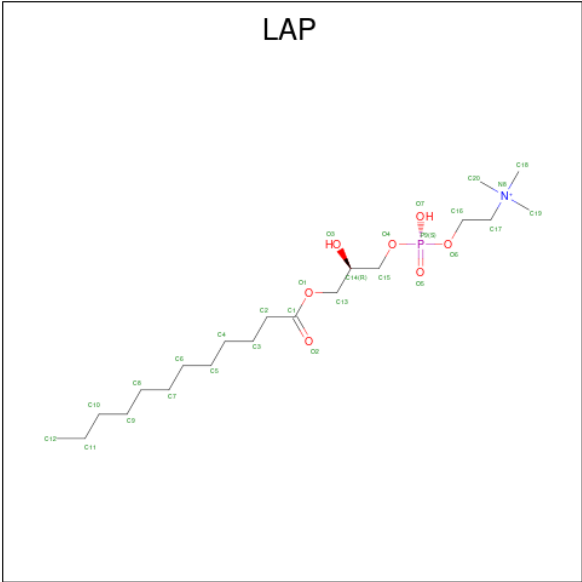
Mol	Chain	Residues	Atoms					AltConf
32	B	1	Total	C	N	O	P	0
			30	20	1	8	1	
32	6	1	Total	C	N	O	P	0
			36	26	1	8	1	

- Molecule 33 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$).



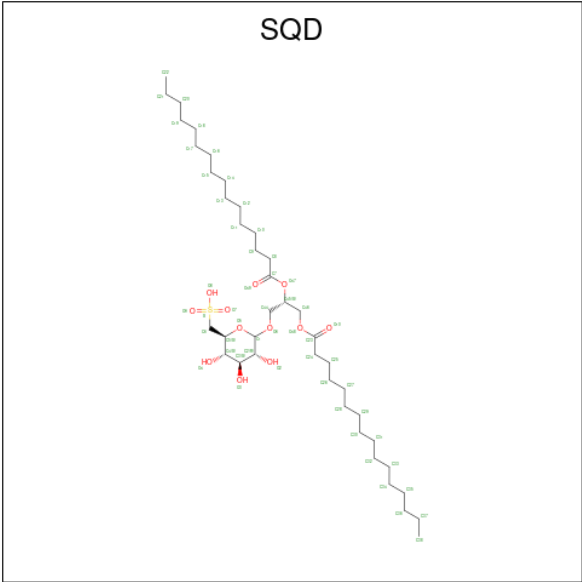
Mol	Chain	Residues	Atoms					AltConf
33	B	1	Total	C	N	O	P	0
			41	31	1	8	1	
33	3	1	Total	C	N	O	P	0
			38	28	1	8	1	
33	5	1	Total	C	N	O	P	0
			38	28	1	8	1	
33	7	1	Total	C	N	O	P	0
			33	23	1	8	1	
33	8	1	Total	C	N	O	P	0
			35	25	1	8	1	
33	9	1	Total	C	N	O	P	0
			48	38	1	8	1	

- Molecule 34 is [2-(((1-oxododecanoxy-(2-hydroxy-3-propanyl))-phosphonate-oxy)-ethyl)-trimethylammonium (CCD ID: LAP) (formula: C₂₀H₄₃NO₇P).



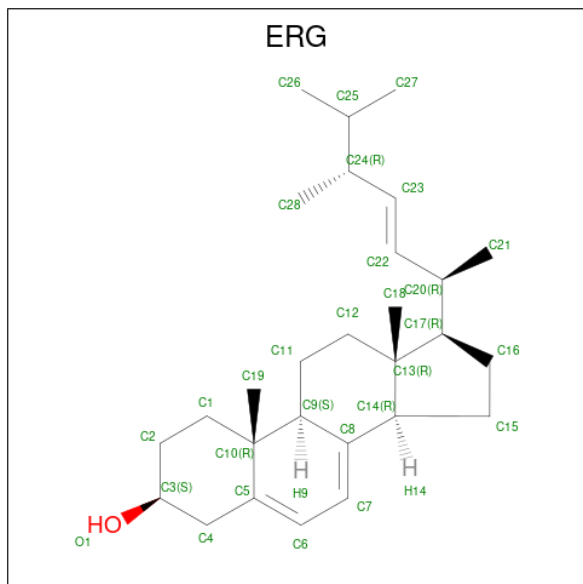
Mol	Chain	Residues	Atoms					AltConf
34	B	1	Total	C	N	O	P	0
			29	20	1	7	1	
34	F	1	Total	C	N	O	P	0
			29	20	1	7	1	
34	K	1	Total	C	N	O	P	0
			29	20	1	7	1	

- Molecule 35 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



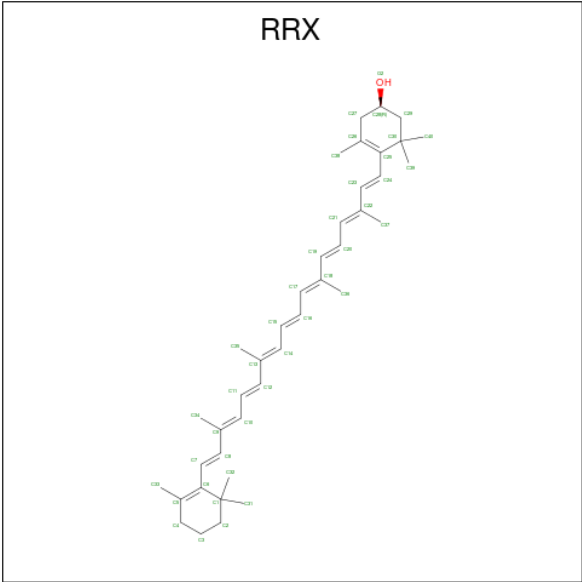
Mol	Chain	Residues	Atoms				AltConf
35	G	1	Total	C	O	S	0
			46	33	12	1	
35	H	1	Total	C	O	S	0
			45	32	12	1	
35	7	1	Total	C	O	S	0
			39	26	12	1	

- Molecule 36 is ERGOSTEROL (CCD ID: ERG) (formula: $C_{28}H_{44}O$).



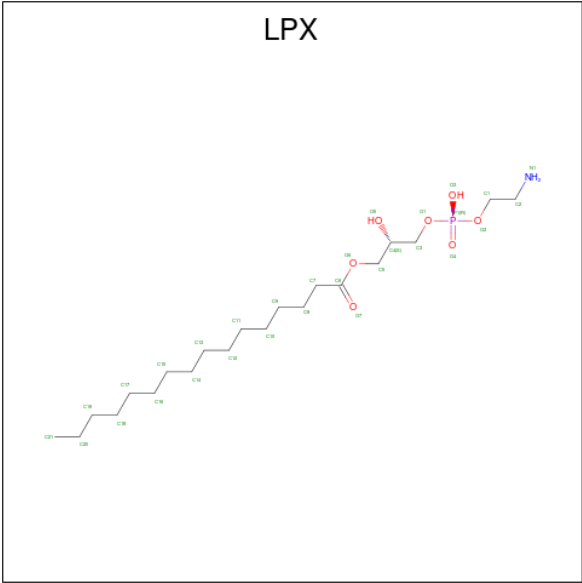
Mol	Chain	Residues	Atoms				AltConf
36	G	1	Total	C	O		0
			29	28	1		

- Molecule 37 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: $C_{40}H_{56}O$).



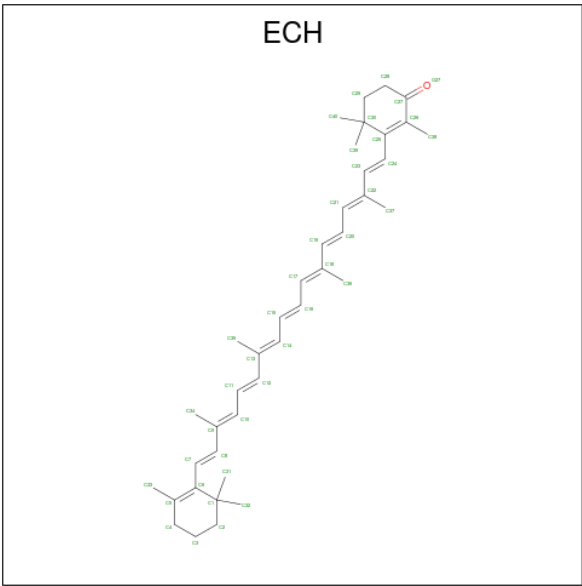
Mol	Chain	Residues	Atoms			AltConf
37	J	1	Total	C	O	0
			41	40	1	

- Molecule 38 is (2S)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (CCD ID: LPX) (formula: C₂₁H₄₄NO₇P).



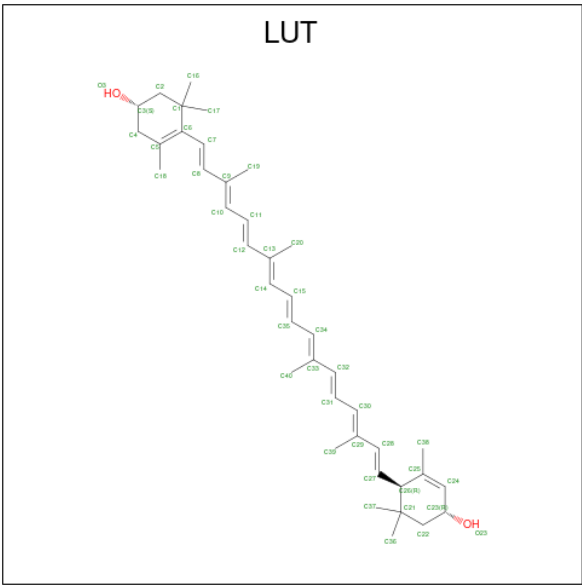
Mol	Chain	Residues	Atoms					AltConf
38	J	1	Total	C	N	O	P	0
			17	8	1	7	1	
38	a	1	Total	C	N	O	P	0
			30	21	1	7	1	

- Molecule 39 is beta,beta-caroten-4-one (CCD ID: ECH) (formula: C₄₀H₅₄O).



Mol	Chain	Residues	Atoms			AltConf
39	M	1	Total	C	O	0
			41	40	1	

- Molecule 40 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



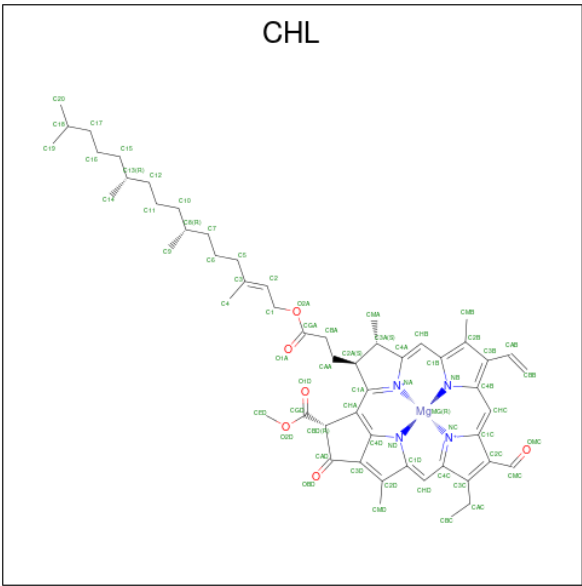
Mol	Chain	Residues	Atoms			AltConf
40	1	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
40	1	1	Total 42	C 40	O 2	0
40	1	1	Total 42	C 40	O 2	0
40	a	1	Total 42	C 40	O 2	0
40	a	1	Total 42	C 40	O 2	0
40	a	1	Total 42	C 40	O 2	0
40	3	1	Total 42	C 40	O 2	0
40	3	1	Total 42	C 40	O 2	0
40	4	1	Total 42	C 40	O 2	0
40	4	1	Total 42	C 40	O 2	0
40	5	1	Total 42	C 40	O 2	0
40	5	1	Total 42	C 40	O 2	0
40	5	1	Total 42	C 40	O 2	0
40	6	1	Total 42	C 40	O 2	0
40	6	1	Total 42	C 40	O 2	0
40	7	1	Total 42	C 40	O 2	0
40	8	1	Total 42	C 40	O 2	0
40	8	1	Total 42	C 40	O 2	0
40	2	1	Total 42	C 40	O 2	0
40	2	1	Total 42	C 40	O 2	0
40	9	1	Total 42	C 40	O 2	0
40	9	1	Total 42	C 40	O 2	0

- Molecule 41 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆).



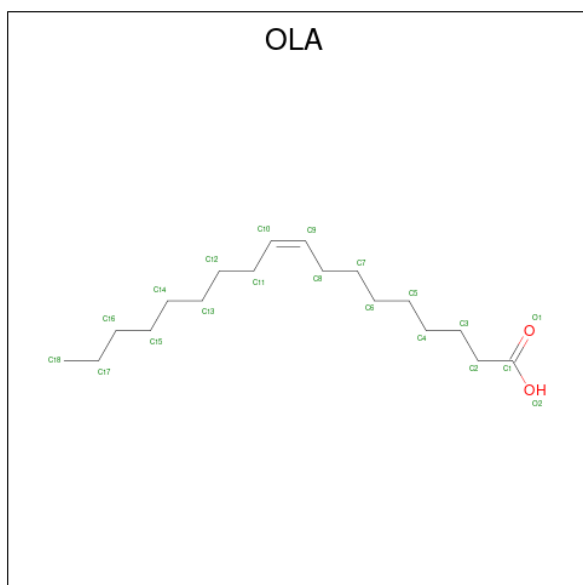
Mol	Chain	Residues	Atoms					AltConf
41	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
41	1	1	Total 48	C 37	Mg 1	N 4	O 6	0
41	a	1	Total 56	C 45	Mg 1	N 4	O 6	0
41	a	1	Total 53	C 42	Mg 1	N 4	O 6	0
41	a	1	Total 48	C 37	Mg 1	N 4	O 6	0
41	a	1	Total 46	C 35	Mg 1	N 4	O 6	0
41	3	1	Total 43	C 34	Mg 1	N 4	O 4	0
41	3	1	Total 55	C 44	Mg 1	N 4	O 6	0
41	4	1	Total 66	C 55	Mg 1	N 4	O 6	0
41	4	1	Total 52	C 41	Mg 1	N 4	O 6	0
41	4	1	Total 56	C 45	Mg 1	N 4	O 6	0
41	5	1	Total 66	C 55	Mg 1	N 4	O 6	0
41	5	1	Total 51	C 40	Mg 1	N 4	O 6	0

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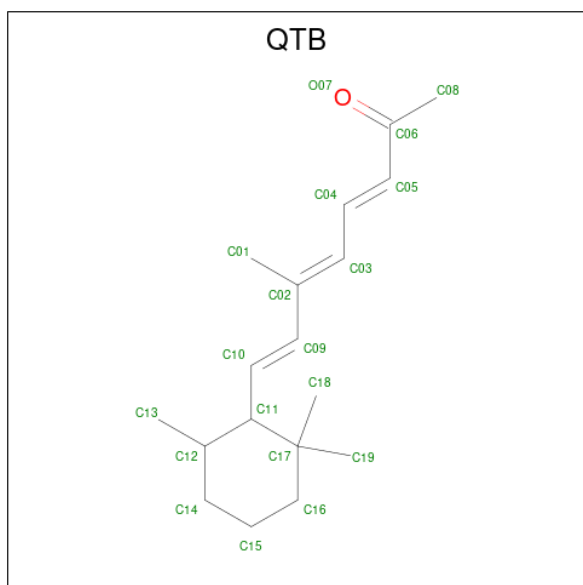
Mol	Chain	Residues	Atoms					AltConf
41	5	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
41	6	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
41	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
41	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
41	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
41	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
41	8	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
41	8	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
41	8	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
41	9	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
41	9	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

- Molecule 42 is OLEIC ACID (CCD ID: OLA) (formula: $C_{18}H_{34}O_2$).



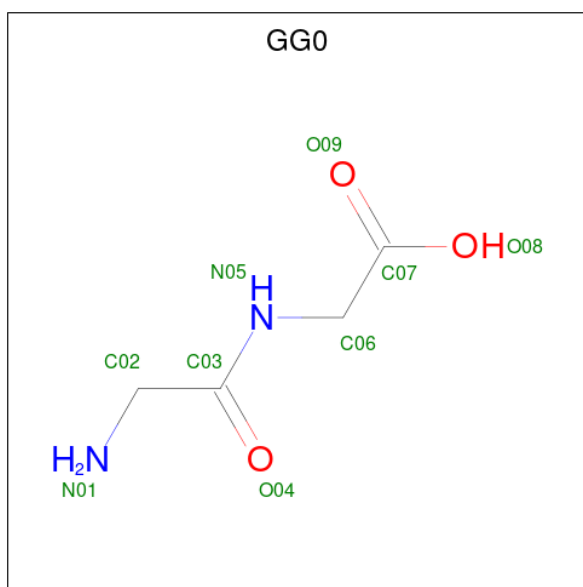
Mol	Chain	Residues	Atoms			AltConf
42	1	1	Total	C	O	0
			20	18	2	
42	8	1	Total	C	O	0
			20	18	2	

- Molecule 43 is (3 {E},5 {E},7 {E})-6-methyl-8-[(6 {R})-2,2,6-trimethylcyclohexyl]octa-3,5,7-trien-2-one (CCD ID: QTB) (formula: C₁₈H₂₈O).



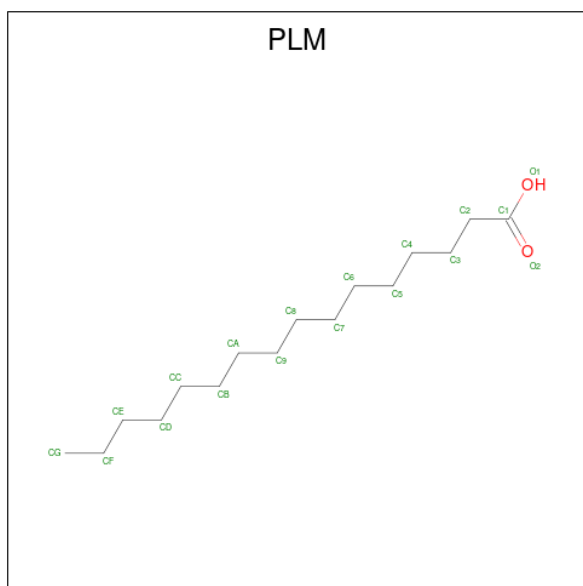
Mol	Chain	Residues	Atoms			AltConf
43	a	1	Total	C	O	0
			19	18	1	
43	3	1	Total	C	O	0
			19	18	1	

- Molecule 44 is 2-(2-azanylethanoylamino)ethanoic acid (CCD ID: GG0) (formula: C₄H₈N₂O₃).



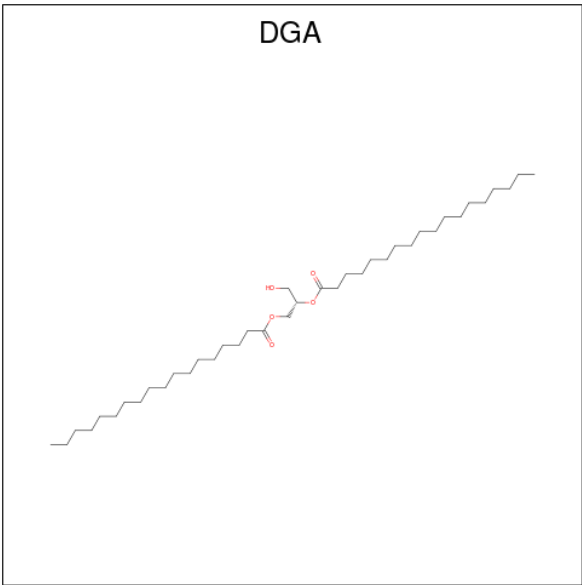
Mol	Chain	Residues	Atoms				AltConf
44	a	1	Total	C	N	O	0
			9	4	2	3	

- Molecule 45 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



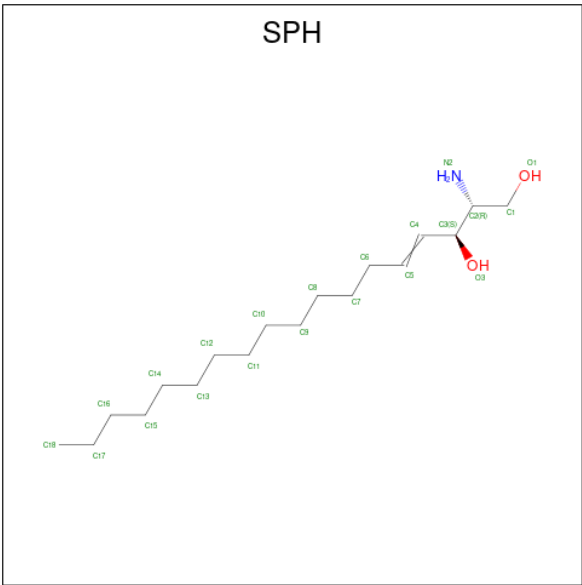
Mol	Chain	Residues	Atoms			AltConf
45	4	1	Total	C	O	0
			17	16	1	
45	6	1	Total	C	O	0
			18	16	2	

- Molecule 46 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$).



Mol	Chain	Residues	Atoms			AltConf
46	5	1	Total	C	O	0
			23	18	5	
46	8	1	Total	C	O	0
			30	25	5	

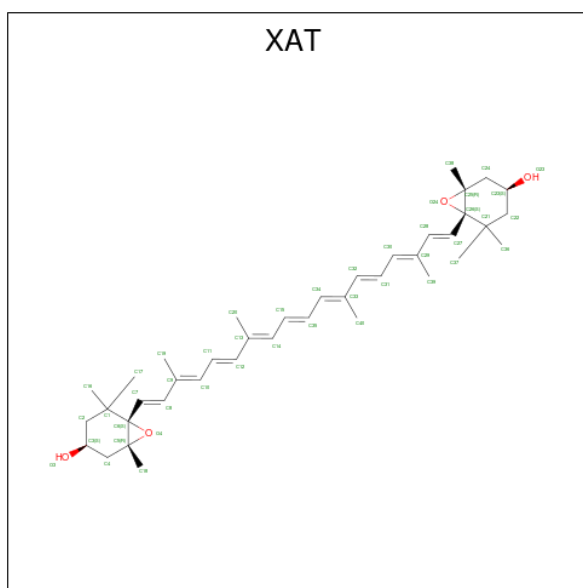
- Molecule 47 is SPHINGOSINE (CCD ID: SPH) (formula: C₁₈H₃₇NO₂).



Mol	Chain	Residues	Atoms				AltConf
47	6	1	Total	C	N	O	0
			21	18	1	2	

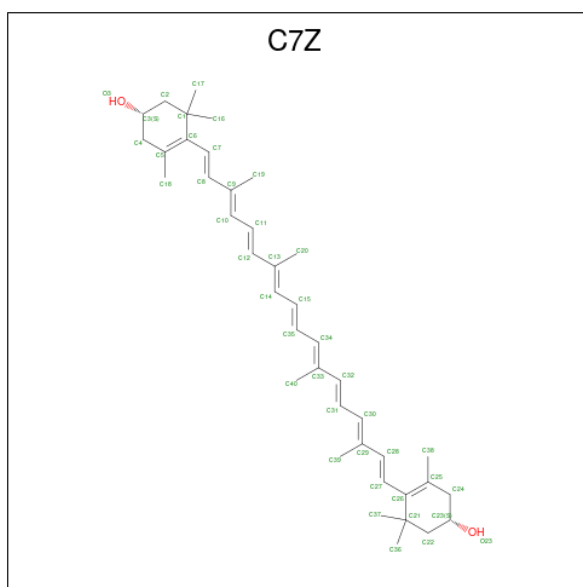
- Molecule 48 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA

,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$).



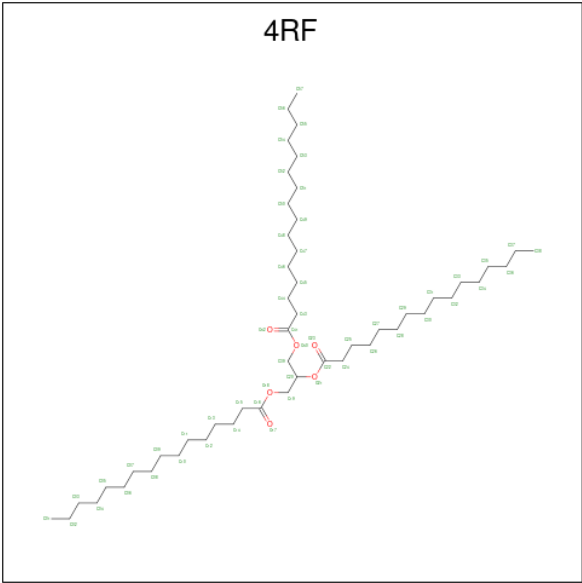
Mol	Chain	Residues	Atoms		AltConf
48	7	1	Total	C	O
			44	40	4
					0

- Molecule 49 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 (CCD ID: C7Z) (formula: $C_{40}H_{56}O_2$).



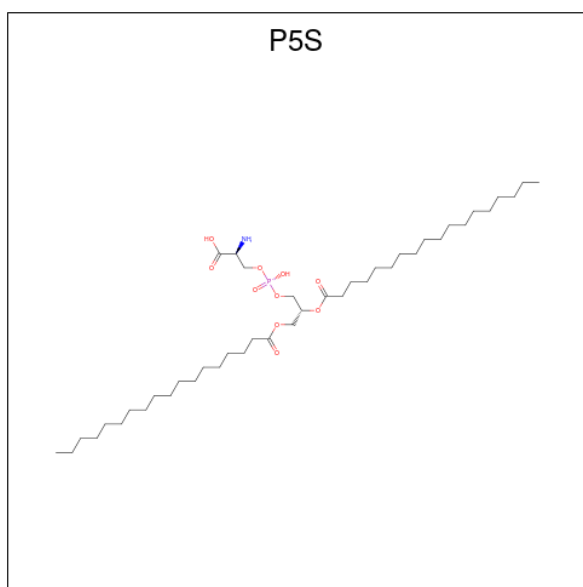
Mol	Chain	Residues	Atoms			AltConf
49	7	1	Total	C	O	0
			42	40	2	

- Molecule 50 is Tripalmitoylglycerol (CCD ID: 4RF) (formula: C₅₁H₉₈O₆).



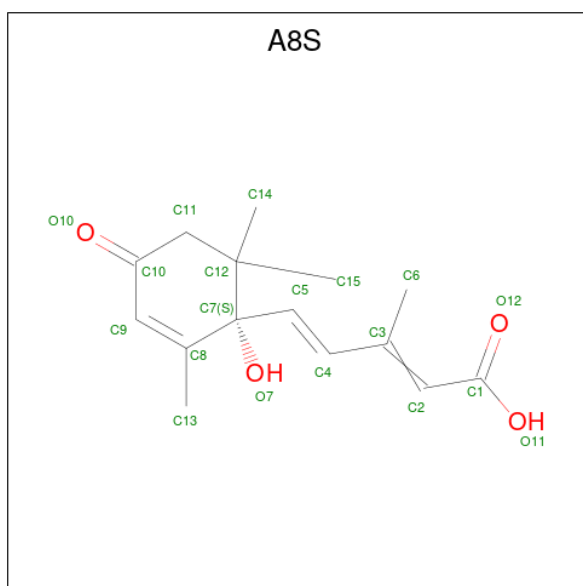
Mol	Chain	Residues	Atoms			AltConf
50	7	1	Total	C	O	0
			32	26	6	
50	8	1	Total	C	O	0
			42	36	6	
50	8	1	Total	C	O	0
			54	48	6	

- Molecule 51 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (CCD ID: P5S) (formula: C₄₂H₈₂NO₁₀P).



Mol	Chain	Residues	Atoms					AltConf
51	8	1	Total	C	N	O	P	0
			37	25	1	10	1	

- Molecule 52 is (2Z,4E)-5-[(1S)-1-hydroxy-2,6,6-trimethyl-4-oxocyclohex-2-en-1-yl]-3-methyl penta-2,4-dienoic acid (CCD ID: A8S) (formula: $C_{15}H_{20}O_4$).

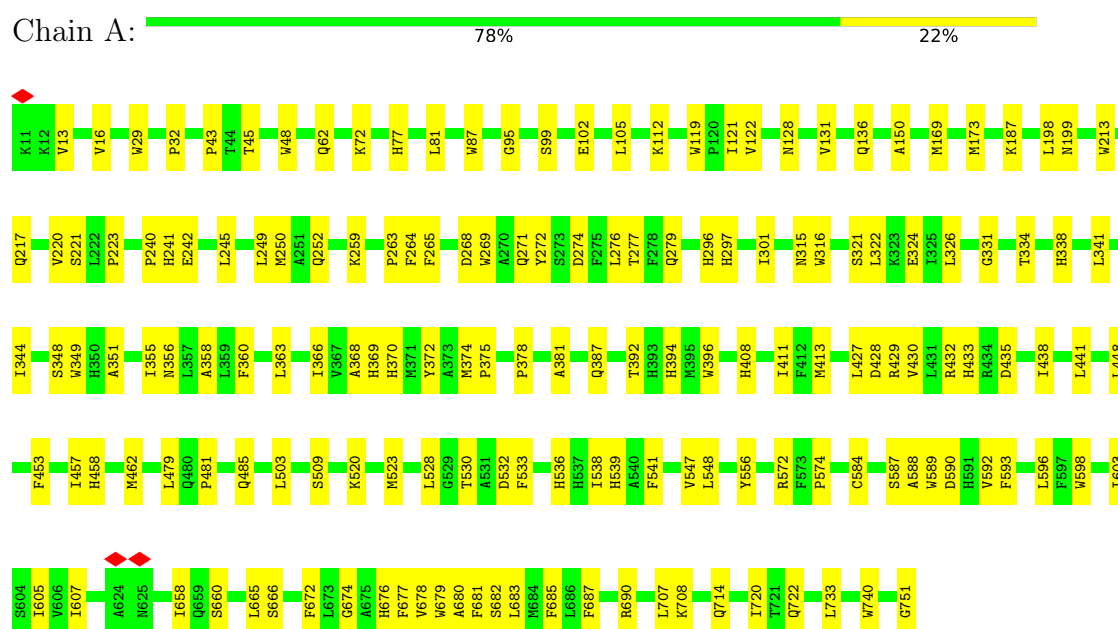


Mol	Chain	Residues	Atoms				AltConf
52	9	1	Total	C	O		0
			19	15	4		

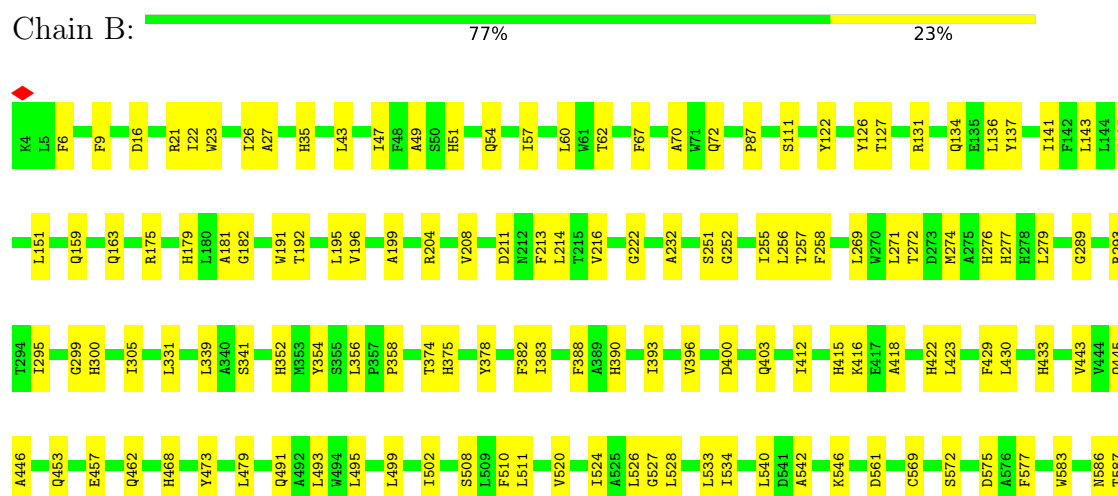
3 Residue-property plots

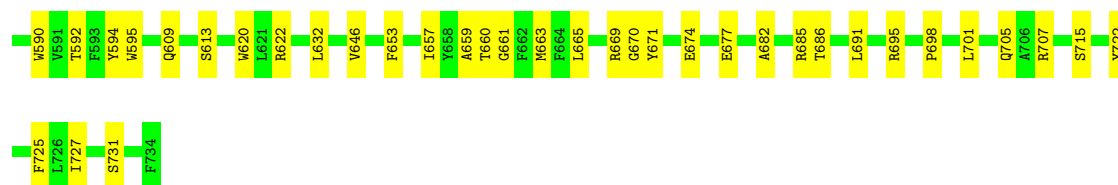
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2





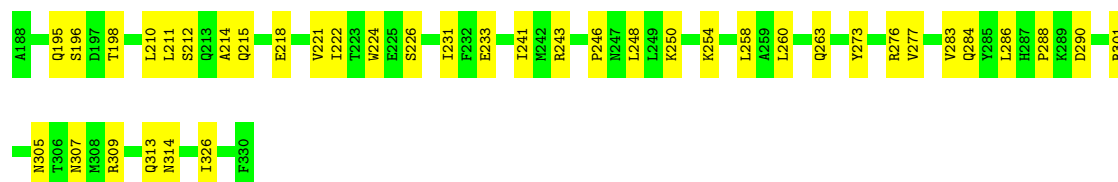
• Molecule 3: Photosystem I iron-sulfur center

Chain C: 81% 19%



• Molecule 4: Photosystem I reaction center subunit chloroplastic

Chain D: 73% 27%



• Molecule 5: Photosystem I reaction center subunit IV

Chain E: 83% 17%



• Molecule 6: PSI-F

Chain F: 87% 13%



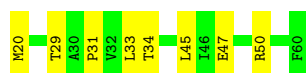
• Molecule 7: Photosystem I reaction center subunit chloroplastic

Chain G: 79% 21%



• Molecule 8: Photosystem I reaction center subunit IX

Chain J: 80% 20%



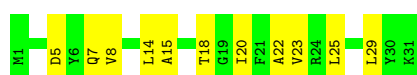
- Molecule 9: PSI-K

Chain K: 85% 15%



- Molecule 10: Photosystem I reaction center subunit XII

Chain M: 65% 35%



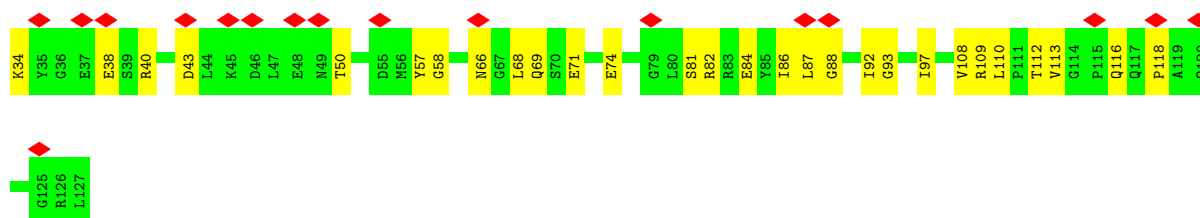
- Molecule 11: Photosystem I reaction center subunit VIII

Chain I: 66% 34%



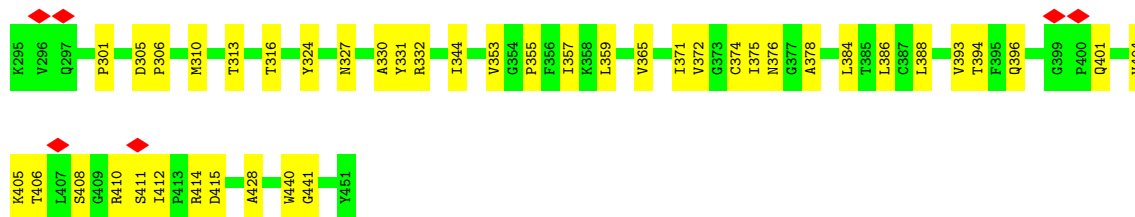
- Molecule 12: Photosystem I reaction center subunit VI-chloroplastic-like

Chain H: 18% 70% 30%



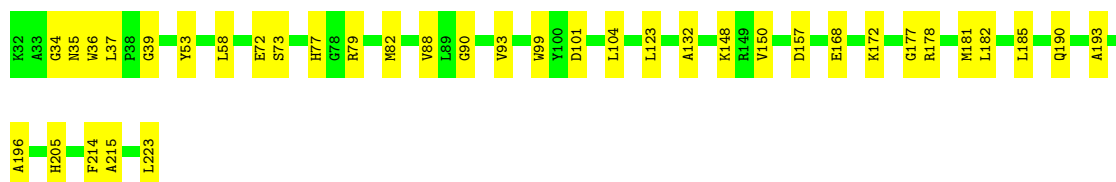
- Molecule 13: PSI subunit V

Chain L: 73% 27%



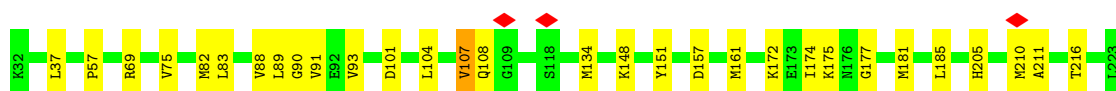
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain 1: 81% 19%



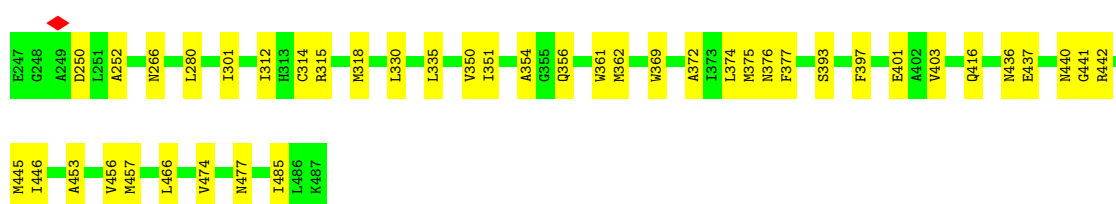
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain a: 84% 15%



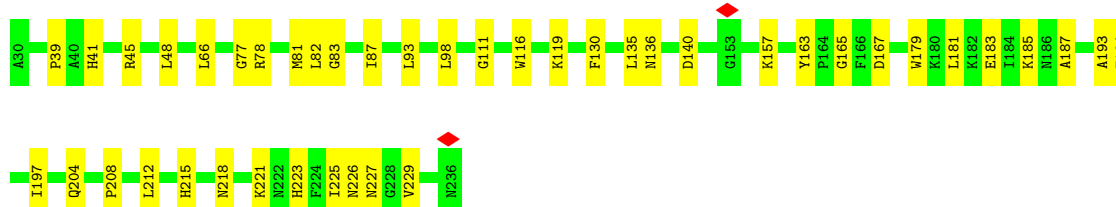
- Molecule 15: Glutathione reductase

Chain 3: 83% 17%



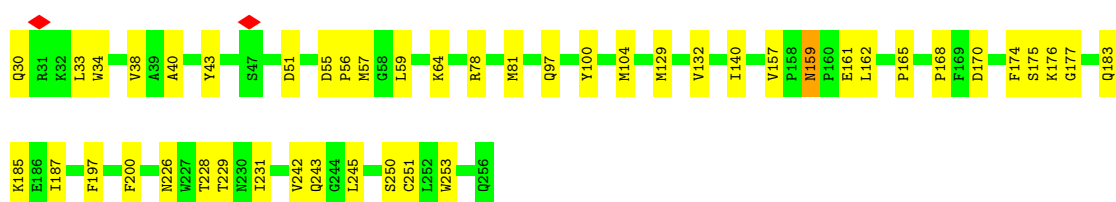
- Molecule 16: Chlorophyll a-b binding protein, chloroplastic

Chain 4: 79% 21%



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

Chain 5: 79% 20%

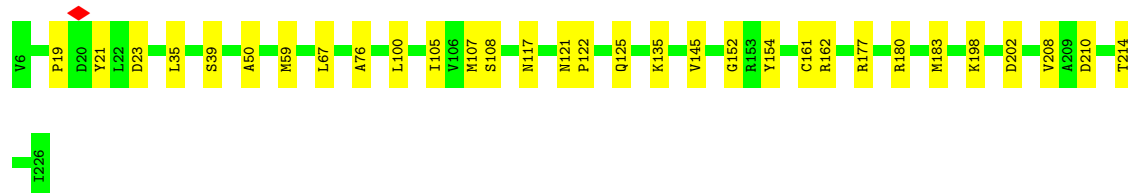


- Molecule 18: Chlorophyll a-b binding protein, chloroplastic

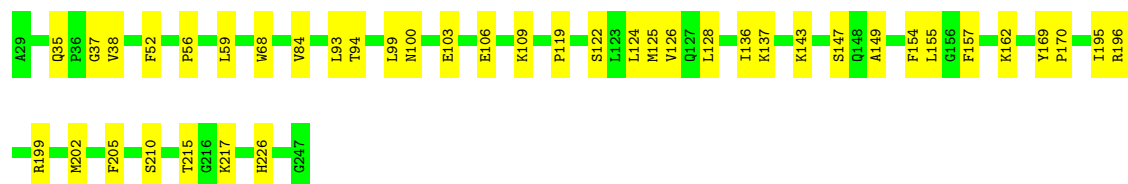
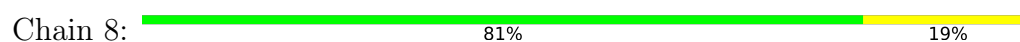
Chain 6: 77% 23%



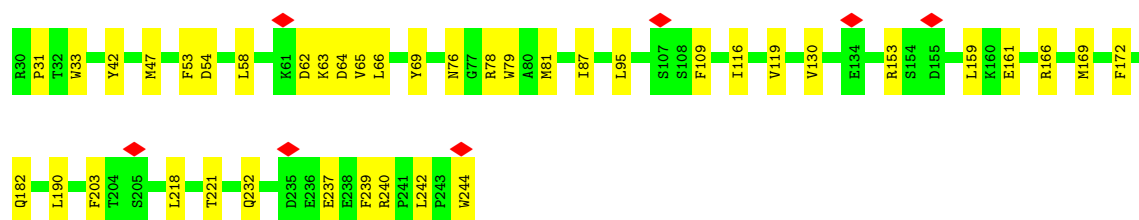
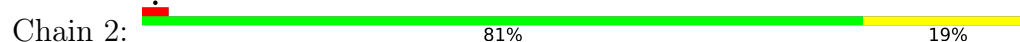
- Molecule 19: Chlorophyll a-b binding protein, chloroplastic



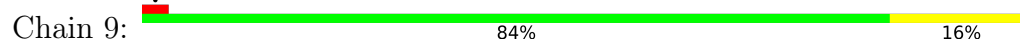
- Molecule 20: Chlorophyll a-b binding protein, chloroplastic



- Molecule 21: Chlorophyll a-b binding protein, chloroplastic



- Molecule 22: Chlorophyll a-b binding protein, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	75049	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 ($e^-/\text{\AA}^2$)	46.04	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.082	Depositor
Minimum map value	-0.041	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.007	Depositor
Map size ($\text{\AA}$)	414.72, 414.72, 414.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.81, 0.81, 0.81	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ERG, ECH, BCR, RRX, DGA, SQD, CLA, 4RF, PTY, SPH, 3PH, SF4, LMT, PCW, XAT, PLM, CL0, GG0, DGD, LAP, LUT, OLA, LHG, A8S, QTB, P5S, C7Z, PQN, LPX, CHL

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	0.15	0/6022	0.35	0/8215
2	B	0.17	0/6006	0.35	0/8205
3	C	0.11	0/611	0.34	0/828
4	D	0.14	0/1150	0.36	0/1551
5	E	0.12	0/520	0.34	0/705
6	F	0.15	0/1309	0.33	0/1771
7	G	0.16	0/743	0.42	0/1007
8	J	0.15	0/322	0.39	0/439
9	K	0.14	0/622	0.35	0/844
10	M	0.16	0/244	0.32	0/330
11	I	0.19	0/276	0.41	0/373
12	H	0.16	0/744	0.43	0/1000
13	L	0.16	0/1195	0.41	0/1635
14	1	0.18	0/1443	0.41	0/1960
14	a	0.19	0/1443	0.49	0/1960
15	3	0.17	0/1896	0.40	0/2573
16	4	0.16	0/1681	0.43	2/2285 (0.1%)
17	5	0.16	0/1825	0.38	0/2483
18	6	0.17	0/1845	0.37	0/2515
19	7	0.14	0/1748	0.34	0/2372
20	8	0.15	0/1717	0.33	0/2330
21	2	0.18	0/1708	0.44	0/2318
22	9	0.19	0/1435	0.46	1/1946 (0.1%)
All	All	0.16	0/36505	0.38	3/49645 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	9	355	LEU	CB-CA-C	-5.41	110.32	116.54
16	4	218	ASN	CA-C-N	5.21	139.49	127.00
16	4	218	ASN	C-N-CA	5.21	139.49	127.00

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	5824	0	5675	125	0
2	B	5796	0	5576	148	0
3	C	601	0	576	16	0
4	D	1124	0	1129	27	0
5	E	509	0	507	8	0
6	F	1277	0	1296	20	0
7	G	727	0	724	20	0
8	J	316	0	332	8	0
9	K	613	0	639	11	0
10	M	239	0	255	14	0
11	I	270	0	287	14	0
12	H	729	0	705	26	0
13	L	1165	0	1181	37	0
14	1	1405	0	1370	29	0
14	a	1405	0	1370	27	0
15	3	1844	0	1805	33	0
16	4	1631	0	1575	40	0
17	5	1769	0	1719	39	0
18	6	1787	0	1762	42	0
19	7	1698	0	1640	28	0
20	8	1669	0	1619	40	0
21	2	1666	0	1657	34	0
22	9	1397	0	1374	26	0
23	A	65	0	72	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	1	693	0	673	39	0
24	2	724	0	608	38	0
24	3	719	0	724	32	0
24	4	768	0	683	32	0
24	5	739	0	635	23	0
24	6	711	0	648	32	0
24	7	778	0	716	35	0
24	8	699	0	619	25	0
24	9	549	0	499	25	0
24	A	2621	0	2693	157	0
24	B	2583	0	2673	153	0
24	F	105	0	87	6	0
24	G	141	0	104	3	0
24	H	156	0	129	8	0
24	J	42	0	30	1	0
24	K	204	0	165	7	0
24	L	155	0	130	5	0
24	a	571	0	538	25	0
25	A	33	0	46	5	0
25	B	33	0	46	7	0
26	A	8	0	0	0	0
26	C	16	0	0	1	0
27	3	120	0	159	10	0
27	4	40	0	51	1	0
27	5	80	0	106	6	0
27	6	80	0	105	4	0
27	7	40	0	52	2	0
27	8	40	0	53	1	0
27	A	200	0	264	26	0
27	B	280	0	369	29	0
27	F	40	0	53	7	0
27	G	40	0	53	3	0
27	H	40	0	52	2	0
27	I	40	0	53	6	0
27	J	40	0	53	4	0
27	K	80	0	106	8	0
27	L	120	0	159	10	0
28	1	77	0	97	6	0
28	2	98	0	148	6	0
28	3	49	0	74	5	0
28	4	81	0	108	3	0
28	5	49	0	74	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	6	86	0	118	7	0
28	7	128	0	175	4	0
28	8	37	0	44	1	0
28	9	82	0	110	6	0
28	A	120	0	159	10	0
28	B	95	0	139	5	0
28	F	79	0	101	5	0
28	a	35	0	40	2	0
29	8	66	0	96	8	0
29	A	51	0	60	3	0
29	B	66	0	96	10	0
30	A	33	0	39	0	0
31	1	35	0	45	0	0
31	2	35	0	46	1	0
31	A	35	0	45	3	0
31	B	35	0	45	5	0
32	6	36	0	44	2	0
32	B	30	0	34	2	0
33	3	38	0	49	1	0
33	5	38	0	49	3	0
33	7	33	0	39	1	0
33	8	35	0	43	2	0
33	9	48	0	72	2	0
33	B	41	0	55	2	0
34	B	29	0	42	0	0
34	F	29	0	42	3	0
34	K	29	0	42	2	0
35	7	39	0	41	1	0
35	G	46	0	55	2	0
35	H	45	0	53	6	0
36	G	29	0	38	6	0
37	J	41	0	56	6	0
38	J	17	0	14	1	0
38	a	30	0	43	0	0
39	M	41	0	54	4	0
40	1	126	0	165	12	0
40	2	84	0	110	13	0
40	3	84	0	110	10	0
40	4	84	0	110	13	0
40	5	126	0	165	15	0
40	6	84	0	110	12	0
40	7	42	0	55	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	8	84	0	110	15	0
40	9	84	0	110	11	0
40	a	126	0	165	10	0
41	1	114	0	101	8	0
41	3	98	0	73	7	0
41	4	174	0	156	10	0
41	5	173	0	152	13	0
41	6	224	0	188	7	0
41	7	66	0	69	4	0
41	8	174	0	150	12	0
41	9	93	0	62	2	0
41	a	203	0	148	11	0
42	1	20	0	33	2	0
42	8	20	0	33	3	0
43	3	19	0	0	0	0
43	a	19	0	0	0	0
44	a	9	0	0	0	0
45	4	17	0	31	1	0
45	6	18	0	31	2	0
46	5	23	0	28	1	0
46	8	30	0	42	2	0
47	6	21	0	37	1	0
48	7	44	0	56	3	0
49	7	42	0	0	0	0
50	7	32	0	39	1	0
50	8	96	0	142	3	0
51	8	37	0	40	0	0
52	9	19	0	19	1	0
All	All	54609	0	54543	1313	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 12.

All (1313) 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)
36:G:5002:ERG:O1	36:G:5002:ERG:C3	1.70	1.38
24:A:1131:CLA:HBB1	24:A:1132:CLA:H2	1.44	0.97
40:4:502:LUT:H32	24:4:604:CLA:HAB	1.49	0.95
1:A:396:TRP:CD1	24:A:1126:CLA:HAB	2.13	0.84
21:2:169:MET:HE1	24:2:604:CLA:HAB	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:20:MET:N	19:7:39:SER:HG	1.77	0.81
27:3:503:BCR:H311	24:7:607:CLA:HAB	1.66	0.78
2:B:609:GLN:O	2:B:613:SER:HB2	1.85	0.76
24:A:1117:CLA:HAB	24:A:1117:CLA:H8	1.66	0.76
24:5:612:CLA:H121	24:5:617:CLA:HAB	1.68	0.75
7:G:1228:LEU:N	7:G:1317:SER:HG	1.85	0.75
2:B:685:ARG:HH21	4:D:211:LEU:HD23	1.52	0.74
48:7:502:XAT:H28	24:7:604:CLA:H61	1.70	0.73
24:B:1220:CLA:HBA1	27:B:4004:BCR:H16C	1.69	0.73
14:a:83:LEU:HB3	41:a:606:CHL:HBB2	1.71	0.73
2:B:143:LEU:HD21	27:B:4003:BCR:H23C	1.71	0.73
24:7:617:CLA:HBA2	29:8:802:DGD:HAH1	1.71	0.72
24:B:1205:CLA:HAB	24:B:1206:CLA:HBA1	1.69	0.72
21:2:78:ARG:HA	21:2:81:MET:HE3	1.70	0.72
41:a:609:CHL:HMA2	16:4:135:LEU:HD13	1.70	0.72
1:A:375:PRO:HG2	1:A:381:ALA:HB2	1.71	0.71
24:B:1211:CLA:HMB1	27:B:4003:BCR:H24C	1.73	0.70
40:5:505:LUT:H35	41:5:610:CHL:H151	1.71	0.70
24:B:1235:CLA:H151	27:F:4001:BCR:H24C	1.73	0.69
1:A:533:PHE:HA	24:A:1136:CLA:HED1	1.75	0.68
24:B:1228:CLA:H151	6:F:458:PRO:HB3	1.76	0.68
40:9:502:LUT:H32	24:9:604:CLA:HAB	1.75	0.68
24:A:1101:CLA:HED1	8:J:34:THR:HG21	1.75	0.68
24:F:1301:CLA:HBB1	27:F:4001:BCR:H392	1.75	0.68
11:I:23:MET:HG2	27:L:4001:BCR:H10C	1.75	0.68
14:a:148:LYS:HG3	24:a:611:CLA:HBC1	1.76	0.68
17:5:161:GLU:OE2	17:5:183:GLN:NE2	2.27	0.68
24:2:604:CLA:HMD1	24:2:609:CLA:HAB	1.73	0.68
12:H:68:LEU:HD22	24:H:1701:CLA:HAC2	1.75	0.68
24:A:1101:CLA:HBB1	37:J:4002:RRX:H58	1.76	0.67
24:F:1301:CLA:H2	34:F:5003:LAP:H131	1.77	0.67
21:2:119:VAL:HG23	24:2:612:CLA:HBB2	1.75	0.67
14:1:82:MET:SD	24:1:601:CLA:HAB	2.35	0.67
24:B:1207:CLA:H101	12:H:97:ILE:HD13	1.76	0.67
36:G:5002:ERG:H122	14:1:123:LEU:HD23	1.77	0.67
2:B:722:TYR:HB2	24:B:1021:CLA:HED3	1.78	0.66
1:A:358:ALA:HB1	27:A:4004:BCR:H10C	1.77	0.66
24:B:1228:CLA:H2	27:F:4001:BCR:H353	1.75	0.66
19:7:59:MET:SD	24:7:601:CLA:HAB	2.35	0.66
19:7:107:MET:HE1	41:7:613:CHL:HED3	1.78	0.66
19:7:105:ILE:HG23	24:7:612:CLA:HBB2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:327:ASN:HB3	24:L:1501:CLA:HAC1	1.77	0.66
2:B:388:PHE:HZ	24:B:1222:CLA:HAB	1.61	0.66
24:B:1222:CLA:H72	24:B:1231:CLA:HAB	1.78	0.66
24:9:601:CLA:HBB1	24:9:601:CLA:H62	1.76	0.66
7:G:1245:LEU:HD21	14:1:132:ALA:HA	1.77	0.66
1:A:121:ILE:HG13	1:A:122:VAL:HG13	1.78	0.66
24:A:1126:CLA:H191	27:J:4001:BCR:H19C	1.77	0.66
29:8:802:DGD:HG31	29:8:802:DGD:HA41	1.78	0.66
1:A:370:HIS:ND1	24:A:1116:CLA:OBD	2.29	0.65
10:M:5:ASP:OD1	11:I:2:SER:OG	2.14	0.65
24:A:1102:CLA:HAB	24:A:1104:CLA:CAD	2.27	0.65
24:2:615:CLA:HED1	31:2:804:LMT:H3'	1.79	0.65
13:L:353:VAL:HA	13:L:376:ASN:HD21	1.62	0.65
24:3:616:CLA:H51	24:5:616:CLA:HAA2	1.78	0.65
2:B:16:ASP:HB3	2:B:21:ARG:HB2	1.78	0.65
36:G:5002:ERG:O1	36:G:5002:ERG:C2	2.40	0.65
1:A:223:PRO:HD3	1:A:250:MET:HE1	1.79	0.64
24:A:1106:CLA:HBB2	24:A:1126:CLA:H202	1.79	0.64
24:A:1117:CLA:H193	24:A:1117:CLA:H122	1.80	0.64
1:A:678:VAL:HG11	1:A:733:LEU:HD23	1.78	0.64
41:a:606:CHL:HMA2	41:a:613:CHL:HBC3	1.79	0.64
12:H:109:ARG:HH22	13:L:365:VAL:HG11	1.62	0.64
14:a:90:GLY:HA3	41:a:606:CHL:HBC3	1.80	0.63
18:6:77:GLU:HG2	18:6:140:ILE:HG13	1.80	0.63
24:B:1201:CLA:H93	11:I:26:MET:HE1	1.80	0.63
1:A:690:ARG:H	2:B:569:CYS:HB2	1.63	0.63
24:B:1204:CLA:H18	27:I:4001:BCR:HC7	1.80	0.63
16:4:116:TRP:NE1	41:4:613:CHL:OBD	2.28	0.63
24:A:1124:CLA:H72	24:A:1133:CLA:HAB	1.78	0.63
9:K:41:MET:HG3	24:K:1401:CLA:HMD2	1.80	0.63
24:B:1212:CLA:H2	27:B:4001:BCR:H292	1.79	0.63
27:B:4006:BCR:H10C	6:F:411:PHE:CE1	2.33	0.63
24:A:1120:CLA:H12	24:K:1403:CLA:HHB	1.80	0.62
24:B:1209:CLA:H203	24:9:609:CLA:HBB2	1.81	0.62
8:J:20:MET:N	19:7:39:SER:OG	2.31	0.62
27:H:4001:BCR:H372	27:L:4003:BCR:H341	1.81	0.62
14:1:101:ASP:HA	14:1:104:LEU:HD23	1.81	0.62
24:1:603:CLA:H102	41:1:609:CHL:H72	1.81	0.62
41:a:609:CHL:HED3	16:4:136:ASN:HA	1.79	0.62
14:a:134:MET:HB3	24:a:612:CLA:HAB	1.82	0.62
40:a:502:LUT:H382	24:a:604:CLA:H2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:ARG:HB2	24:B:1210:CLA:HBC2	1.82	0.62
2:B:691:LEU:HD11	13:L:330:ALA:HB1	1.81	0.62
13:L:406:THR:HG23	13:L:408:SER:H	1.65	0.62
24:5:617:CLA:HED3	28:6:801:LHG:H132	1.82	0.62
20:8:103:GLU:HB3	20:8:106:GLU:HG2	1.82	0.62
2:B:685:ARG:HH11	13:L:310:MET:HG2	1.65	0.61
24:A:1122:CLA:HMD2	24:A:1123:CLA:HAB	1.83	0.61
21:2:203:PHE:HB2	22:9:326:PRO:HG3	1.82	0.61
24:B:1207:CLA:H112	13:L:378:ALA:HB2	1.81	0.61
13:L:357:ILE:HG12	13:L:372:VAL:HG11	1.82	0.61
15:3:376:ASN:ND2	24:7:609:CLA:O1A	2.33	0.61
3:C:63:LEU:HD11	3:C:66:ARG:HD3	1.82	0.61
18:6:164:TYR:HB3	24:6:601:CLA:HED3	1.81	0.61
3:C:61:ASP:O	5:E:88:ASN:ND2	2.33	0.61
2:B:257:THR:H	2:B:272:THR:HB	1.65	0.60
4:D:309:ARG:NH1	4:D:314:ASN:OD1	2.35	0.60
8:J:29:THR:HG22	8:J:31:PRO:HD2	1.82	0.60
14:1:35:ASN:O	14:1:37:LEU:N	2.33	0.60
1:A:596:LEU:HD21	24:A:1128:CLA:HBC1	1.83	0.60
9:K:38:ASN:ND2	24:K:1401:CLA:OBD	2.34	0.60
16:4:45:ARG:HH21	16:4:66:LEU:HD13	1.65	0.60
45:6:804:PLM:H81	19:7:208:VAL:HG11	1.84	0.60
24:7:601:CLA:HBC1	41:7:613:CHL:H122	1.84	0.60
2:B:701:LEU:HG	25:B:2002:PQN:H12	1.82	0.60
17:5:157:VAL:HG12	17:5:168:PRO:HD2	1.84	0.60
1:A:374:MET:HE3	24:A:1116:CLA:HBD	1.83	0.60
1:A:321:SER:HB3	1:A:324:GLU:HG3	1.84	0.60
2:B:388:PHE:CZ	24:B:1222:CLA:HAB	2.36	0.60
24:B:1224:CLA:HBC3	29:B:5003:DGD:HBG3	1.84	0.59
6:F:444:VAL:HG11	38:J:5001:LPX:H7	1.84	0.59
27:I:4001:BCR:H331	27:I:4001:BCR:H10C	1.83	0.59
24:4:605:CLA:HBB1	24:4:610:CLA:H191	1.84	0.59
18:6:87:MET:SD	24:6:601:CLA:HAB	2.42	0.59
27:7:503:BCR:H333	24:8:607:CLA:HAB	1.84	0.59
2:B:429:PHE:CE2	24:B:1235:CLA:HAB	2.36	0.59
40:5:501:LUT:H30	24:5:601:CLA:H61	1.83	0.59
40:6:501:LUT:H28	24:6:601:CLA:H72	1.84	0.59
1:A:707:LEU:HD13	27:F:4001:BCR:H321	1.83	0.59
24:B:1207:CLA:H41	24:B:1207:CLA:H92	1.84	0.59
16:4:163:TYR:HB3	24:4:601:CLA:HED3	1.84	0.59
18:6:245:ASP:HA	18:6:257:GLY:HA2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:6:265:PRO:HD2	24:6:615:CLA:HED2	1.85	0.59
24:B:1220:CLA:HAB	24:B:1227:CLA:HMD1	1.84	0.59
5:E:48:LEU:HD11	5:E:96:VAL:HG13	1.84	0.59
27:A:4001:BCR:H282	34:K:5001:LAP:H112	1.85	0.59
24:2:603:CLA:H101	24:2:603:CLA:HAB	1.85	0.59
27:B:4004:BCR:H10C	28:B:5001:LHG:H172	1.83	0.59
40:1:502:LUT:H28	24:1:604:CLA:H51	1.85	0.59
11:I:30:ILE:HG13	11:I:31:GLU:HG3	1.84	0.59
41:4:609:CHL:O1A	18:6:130:HIS:ND1	2.31	0.59
4:D:231:ILE:HG12	4:D:241:ILE:HG12	1.84	0.58
40:1:501:LUT:H162	24:1:608:CLA:HBC1	1.85	0.58
1:A:369:HIS:HA	1:A:372:TYR:CE1	2.39	0.58
27:3:504:BCR:HC7	41:3:611:CHL:HMB2	1.85	0.58
24:B:1217:CLA:HBB1	27:B:4001:BCR:H17C	1.85	0.58
24:B:1231:CLA:HBC1	28:1:802:LHG:H211	1.85	0.58
7:G:1316:THR:OG1	24:G:1603:CLA:OBD	2.20	0.58
9:K:58:PRO:HG2	27:K:4001:BCR:H291	1.85	0.58
17:5:159:ASN:O	17:5:159:ASN:ND2	2.37	0.58
2:B:416:LYS:HB2	2:B:540:LEU:HD13	1.86	0.58
12:H:57:TYR:OH	13:L:316:THR:O	2.19	0.58
18:6:250:GLN:HB2	27:6:504:BCR:H343	1.84	0.58
21:2:81:MET:SD	24:2:601:CLA:HAB	2.44	0.58
24:A:1118:CLA:HBB1	27:K:4001:BCR:H16C	1.86	0.58
40:8:502:LUT:H32	41:8:604:CHL:HBB1	1.85	0.58
24:8:605:CLA:HBB1	50:8:807:4RF:H49	1.84	0.58
24:B:1238:CLA:HAB	25:B:2002:PQN:H162	1.85	0.58
24:B:1240:CLA:H61	28:B:5001:LHG:H282	1.85	0.58
41:1:609:CHL:HED1	20:8:136:ILE:HG22	1.86	0.58
16:4:204:GLN:NE2	16:4:227:ASN:OD1	2.37	0.58
17:5:243:GLN:HB2	27:5:504:BCR:H342	1.86	0.58
19:7:67:LEU:HD13	24:7:606:CLA:HAC2	1.84	0.58
22:9:399:PRO:O	40:9:501:LUT:O3	2.22	0.58
2:B:659:ALA:C	24:B:1023:CLA:HAB	2.29	0.58
21:2:239:PHE:O	21:2:240:ARG:NE	2.36	0.58
19:7:35:LEU:HD13	48:7:502:XAT:H221	1.86	0.58
22:9:264:GLY:H	22:9:372:THR:HG22	1.69	0.58
24:B:1207:CLA:HED1	27:L:4002:BCR:H23C	1.84	0.57
15:3:314:CYS:HB2	15:3:441:GLY:HA3	1.85	0.57
19:7:76:ALA:HB2	35:7:805:SQD:H172	1.85	0.57
1:A:296:HIS:HB3	24:A:1116:CLA:HMB2	1.86	0.57
2:B:429:PHE:CD2	24:B:1235:CLA:HAB	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:TRP:NE1	24:A:1117:CLA:O1D	2.31	0.57
24:A:1108:CLA:HAA1	15:3:301:ILE:HG13	1.85	0.57
24:B:1222:CLA:H71	24:B:1234:CLA:H52	1.85	0.57
4:D:198:THR:HB	4:D:248:LEU:HD22	1.87	0.57
15:3:397:PHE:CE2	41:3:611:CHL:HBB2	2.39	0.57
24:B:1239:CLA:H8	11:I:23:MET:HE1	1.87	0.57
24:B:1237:CLA:HHD	27:B:4007:BCR:H383	1.87	0.57
24:A:1103:CLA:H51	24:A:1111:CLA:H12	1.87	0.57
40:5:505:LUT:H182	33:5:802:PTY:H131	1.86	0.57
16:4:48:LEU:HD21	16:4:66:LEU:HD21	1.87	0.56
24:7:604:CLA:HHD	24:7:609:CLA:HBB2	1.87	0.56
2:B:546:LYS:NZ	5:E:52:SER:O	2.38	0.56
24:B:1207:CLA:HAB	11:I:15:GLY:HA3	1.87	0.56
15:3:377:PHE:HD2	27:3:503:BCR:H14C	1.70	0.56
1:A:396:TRP:HD1	24:A:1126:CLA:HAB	1.65	0.56
7:G:1255:ARG:NH2	7:G:1293:GLY:O	2.37	0.56
24:K:1401:CLA:HAC2	27:K:4002:BCR:HC41	1.87	0.56
15:3:474:VAL:O	15:3:477:ASN:ND2	2.38	0.56
1:A:539:HIS:HB3	24:A:1135:CLA:HAB	1.88	0.56
35:G:5001:SQD:H111	35:G:5001:SQD:H272	1.88	0.56
13:L:393:VAL:O	13:L:396:GLN:NE2	2.38	0.56
40:1:501:LUT:H30	24:1:601:CLA:H52	1.86	0.56
17:5:78:ARG:NH1	41:5:611:CHL:OBD	2.37	0.56
27:B:4001:BCR:H372	27:G:4001:BCR:HC42	1.86	0.56
1:A:334:THR:OG1	28:A:5001:LHG:O2	2.23	0.56
1:A:356:ASN:O	1:A:360:PHE:HB2	2.06	0.56
13:L:406:THR:HG22	13:L:410:ARG:H	1.70	0.56
17:5:165:PRO:HB3	41:5:611:CHL:HBC2	1.88	0.56
18:6:122:LEU:HD13	41:6:610:CHL:HAC2	1.88	0.56
20:8:128:LEU:HD13	24:8:618:CLA:HAB	1.87	0.56
1:A:112:LYS:HE3	1:A:131:VAL:HA	1.88	0.56
1:A:366:ILE:HG21	24:A:1117:CLA:H201	1.88	0.56
1:A:392:THR:HB	24:A:1126:CLA:HMB2	1.88	0.56
24:3:603:CLA:H172	28:3:801:LHG:H322	1.88	0.56
2:B:127:THR:HG22	2:B:271:LEU:HD21	1.88	0.56
15:3:315:ARG:NE	15:3:437:GLU:OE2	2.35	0.56
17:5:64:LYS:NZ	46:5:803:DGA:OA1	2.39	0.56
1:A:605:ILE:HG13	23:A:1011:CL0:H64	1.88	0.56
27:B:4006:BCR:H10C	6:F:411:PHE:CD1	2.41	0.56
22:9:378:GLY:O	22:9:382:MET:HG3	2.06	0.56
2:B:493:LEU:HD11	7:G:1323:ARG:HG3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:a:606:CHL:H43	41:a:613:CHL:HAA2	1.87	0.55
9:K:59:THR:HG22	9:K:61:THR:H	1.71	0.55
14:1:185:LEU:HD13	24:1:605:CLA:HBB2	1.88	0.55
24:9:603:CLA:HBA1	24:9:603:CLA:HBD	1.88	0.55
2:B:416:LYS:HD2	2:B:540:LEU:HB3	1.89	0.55
3:C:24:ASP:HB2	4:D:258:LEU:HD21	1.89	0.55
4:D:196:SER:HB2	12:H:43:ASP:HA	1.88	0.55
36:G:5002:ERG:O1	36:G:5002:ERG:C4	2.42	0.55
14:a:107:VAL:HG12	14:a:108:GLN:H	1.71	0.55
16:4:212:LEU:HD13	40:4:501:LUT:H163	1.89	0.55
1:A:680:ALA:HB3	24:A:1013:CLA:HBB2	1.87	0.55
27:A:4005:BCR:H291	27:B:4006:BCR:H14C	1.88	0.55
2:B:479:LEU:HD22	2:B:495:LEU:HD11	1.89	0.55
28:a:801:LHG:H302	41:4:618:CHL:HED1	1.89	0.55
17:5:228:THR:HG22	17:5:229:THR:HG23	1.89	0.55
24:9:603:CLA:H143	28:9:801:LHG:H121	1.89	0.55
1:A:448:LEU:HB3	1:A:541:PHE:HB2	1.88	0.55
1:A:199:ASN:HB3	24:A:1118:CLA:HMD2	1.88	0.55
24:A:1012:CLA:HAB	2:B:583:TRP:CH2	2.42	0.55
2:B:192:THR:HG21	2:B:279:LEU:HB2	1.87	0.55
16:4:111:GLY:HA3	24:4:610:CLA:HBC1	1.89	0.55
40:9:502:LUT:H32	24:9:604:CLA:CAB	2.37	0.55
1:A:259:LYS:NZ	1:A:271:GLN:OE1	2.40	0.55
2:B:418:ALA:O	2:B:422:HIS:ND1	2.33	0.55
24:B:1023:CLA:H122	27:I:4001:BCR:H281	1.88	0.55
41:a:606:CHL:HHC	41:a:606:CHL:HBB1	1.89	0.55
28:4:801:LHG:HC92	27:6:503:BCR:HC22	1.88	0.55
24:8:610:CLA:HBA2	50:8:808:4RF:H72	1.88	0.55
31:A:5008:LMT:O3B	15:3:356:GLN:NE2	2.38	0.55
2:B:255:ILE:HG13	2:B:256:LEU:HG	1.89	0.55
18:6:68:ASN:HB3	18:6:71:ARG:HB2	1.89	0.55
24:A:1117:CLA:H203	24:A:1125:CLA:HBA2	1.88	0.55
40:4:502:LUT:H32	24:4:604:CLA:CAB	2.31	0.55
40:8:501:LUT:H32	41:8:601:CHL:HBB1	1.88	0.55
12:H:84:GLU:HG3	21:2:65:VAL:HG21	1.89	0.54
40:6:502:LUT:H32	24:6:604:CLA:CAB	2.37	0.54
41:6:610:CHL:HBB2	41:6:613:CHL:HBB2	1.89	0.54
1:A:672:PHE:O	1:A:676:HIS:ND1	2.39	0.54
2:B:269:LEU:HB2	2:B:274:MET:HE3	1.90	0.54
24:F:1302:CLA:H51	50:7:807:4RF:H4	1.89	0.54
40:8:502:LUT:H171	24:8:610:CLA:HBB1	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:8:606:CLA:HMA2	41:8:613:CHL:HBC3	1.89	0.54
40:2:502:LUT:H41	24:2:604:CLA:H11	1.89	0.54
1:A:268:ASP:OD2	1:A:271:GLN:NE2	2.41	0.54
2:B:524:ILE:HG21	24:B:1234:CLA:HAB	1.89	0.54
4:D:226:SER:OG	4:D:243:ARG:O	2.24	0.54
40:3:502:LUT:H393	28:3:801:LHG:H321	1.90	0.54
17:5:97:GLN:HG2	24:5:606:CLA:HED3	1.87	0.54
18:6:261:HIS:O	18:6:263:LEU:N	2.40	0.54
40:2:501:LUT:H32	24:2:601:CLA:CAB	2.37	0.54
1:A:77:HIS:ND1	24:A:1111:CLA:OBD	2.33	0.54
14:a:75:VAL:HG22	14:a:174:ILE:HD11	1.89	0.54
24:A:1101:CLA:HBB2	24:A:1109:CLA:H102	1.88	0.54
24:B:1225:CLA:H112	27:B:4003:BCR:H372	1.88	0.54
24:B:1225:CLA:H121	27:B:4002:BCR:H19C	1.89	0.54
24:2:615:CLA:HBC1	28:2:801:LHG:H221	1.88	0.54
2:B:26:ILE:HD12	27:L:4001:BCR:HC41	1.88	0.54
2:B:43:LEU:O	2:B:47:ILE:HG12	2.08	0.54
14:1:182:LEU:HD11	28:1:801:LHG:H281	1.89	0.54
40:3:501:LUT:H28	24:3:601:CLA:H43	1.89	0.54
17:5:245:LEU:HD23	27:5:504:BCR:H352	1.90	0.54
18:6:87:MET:O	40:6:501:LUT:H34	2.08	0.54
22:9:276:ASP:HB2	22:9:279:ARG:HB2	1.89	0.54
24:A:1120:CLA:HMD2	27:K:4001:BCR:H23C	1.90	0.54
2:B:111:SER:O	12:H:116:GLN:NE2	2.41	0.54
29:8:802:DGD:HE1	29:8:802:DGD:HA21	1.89	0.54
1:A:587:SER:OG	1:A:590:ASP:OD2	2.25	0.53
6:F:408:THR:HG21	27:F:4001:BCR:H272	1.90	0.53
21:2:172:PHE:CE2	40:2:502:LUT:H32	2.42	0.53
14:a:37:LEU:HD21	41:a:609:CHL:HMA3	1.88	0.53
24:A:1120:CLA:HMA2	24:A:1121:CLA:HBD	1.91	0.53
2:B:51:HIS:ND1	24:B:1210:CLA:OBD	2.35	0.53
41:6:611:CHL:HHC	41:6:611:CHL:HBB1	1.90	0.53
2:B:57:ILE:HG23	24:B:1204:CLA:H141	1.89	0.53
2:B:412:ILE:HD13	27:B:4004:BCR:H402	1.90	0.53
24:B:1022:CLA:H151	24:B:1207:CLA:HBC3	1.90	0.53
24:3:616:CLA:HBB1	24:3:616:CLA:H71	1.90	0.53
19:7:19:PRO:O	19:7:21:TYR:N	2.37	0.53
24:A:1101:CLA:HED2	24:A:1101:CLA:HBA2	1.90	0.53
16:4:77:GLY:HA3	16:4:187:ALA:HB1	1.91	0.53
19:7:198:LYS:HE2	19:7:202:ASP:HB3	1.91	0.53
1:A:45:THR:HG22	1:A:714:GLN:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:1132:CLA:HMC2	24:B:1023:CLA:H101	1.89	0.53
2:B:151:LEU:HD23	10:M:25:LEU:HD13	1.91	0.53
2:B:695:ARG:NH2	11:I:33:GLU:OE2	2.41	0.53
24:B:1224:CLA:H162	29:B:5003:DGD:HAG2	1.91	0.53
1:A:441:LEU:HD21	1:A:547:VAL:HG12	1.90	0.53
2:B:179:HIS:HE1	24:B:1202:CLA:H142	1.73	0.53
1:A:722:GLN:HE22	28:A:5002:LHG:HC81	1.72	0.53
24:A:1131:CLA:H51	27:B:4007:BCR:H372	1.89	0.53
41:9:610:CHL:HHC	41:9:610:CHL:HBB1	1.90	0.53
1:A:708:LYS:O	6:F:427:GLN:NE2	2.35	0.53
24:A:1122:CLA:HHB	24:A:1141:CLA:HAB	1.90	0.53
17:5:129:MET:HA	17:5:132:VAL:HG22	1.90	0.53
24:A:1108:CLA:H12	24:A:1110:CLA:H2	1.91	0.53
24:B:1219:CLA:HBB2	27:B:4004:BCR:H343	1.90	0.53
24:F:1302:CLA:HBB1	20:8:56:PRO:HB2	1.90	0.53
16:4:181:LEU:HD11	16:4:185:LYS:HE3	1.90	0.53
24:A:1114:CLA:H203	28:A:5003:LHG:H242	1.90	0.52
40:5:505:LUT:H173	24:7:608:CLA:HAB	1.90	0.52
24:A:1012:CLA:HBC2	2:B:586:ASN:HB2	1.90	0.52
24:B:1220:CLA:H71	28:B:5001:LHG:H171	1.90	0.52
4:D:222:ILE:HG21	4:D:260:LEU:HD23	1.90	0.52
41:4:609:CHL:HHC	41:4:609:CHL:HBB1	1.91	0.52
17:5:159:ASN:HB3	17:5:165:PRO:HA	1.90	0.52
21:2:190:LEU:HB2	40:2:501:LUT:H22	1.92	0.52
24:A:1106:CLA:HBB1	24:A:1126:CLA:H101	1.91	0.52
27:A:4001:BCR:H272	24:K:1401:CLA:HMC3	1.91	0.52
27:B:4001:BCR:H362	27:G:4001:BCR:H312	1.91	0.52
2:B:499:LEU:HA	2:B:502:ILE:HG22	1.92	0.52
24:A:1132:CLA:H162	24:A:1136:CLA:H193	1.92	0.52
2:B:390:HIS:HA	2:B:393:ILE:HD12	1.91	0.52
2:B:423:LEU:HD13	2:B:533:LEU:HA	1.91	0.52
7:G:1232:ASN:ND2	35:G:5001:SQD:O49	2.41	0.52
40:8:502:LUT:H32	41:8:604:CHL:CBB	2.39	0.52
27:A:4003:BCR:H341	28:A:5001:LHG:H252	1.91	0.52
14:1:90:GLY:HA3	24:1:606:CLA:HBC3	1.92	0.52
21:2:218:LEU:HA	21:2:221:THR:HG22	1.92	0.52
24:A:1013:CLA:H143	25:A:2001:PQN:H241	1.92	0.52
18:6:97:GLU:OE2	18:6:209:PRO:HD2	2.09	0.52
24:A:1119:CLA:HMB2	24:A:1123:CLA:HED2	1.92	0.52
2:B:214:LEU:HB3	22:9:396:ARG:NH2	2.24	0.52
4:D:290:ASP:OD2	4:D:301:ARG:NE	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:a:610:CHL:HHC	41:a:610:CHL:HBB1	1.92	0.52
18:6:195:PHE:CD2	40:6:502:LUT:H12	2.44	0.52
20:8:170:PRO:HB3	24:8:611:CLA:HBC2	1.91	0.52
25:A:2001:PQN:H162	27:B:4006:BCR:H382	1.92	0.52
2:B:400:ASP:HB3	2:B:403:GLN:HG2	1.91	0.52
18:6:129:MET:HA	18:6:132:VAL:HG22	1.92	0.52
1:A:532:ASP:O	1:A:536:HIS:ND1	2.38	0.51
2:B:151:LEU:HD22	10:M:22:ALA:HA	1.92	0.51
14:a:134:MET:HG3	24:a:612:CLA:HMC2	1.91	0.51
15:3:318:MET:HG3	15:3:441:GLY:HA2	1.92	0.51
15:3:456:VAL:HB	27:3:505:BCR:H341	1.92	0.51
21:2:31:PRO:HG3	28:2:801:LHG:HC31	1.93	0.51
1:A:128:ASN:HB3	1:A:136:GLN:HB3	1.92	0.51
24:B:1215:CLA:HAB	24:B:1215:CLA:H8	1.93	0.51
7:G:1248:PHE:HB3	40:1:503:LUT:H373	1.91	0.51
41:4:609:CHL:HMA2	24:6:618:CLA:HMA1	1.92	0.51
13:L:401:GLN:H	13:L:414:ARG:HH12	1.58	0.51
41:5:610:CHL:HHC	41:5:610:CHL:HBB1	1.92	0.51
24:2:609:CLA:HAC2	28:2:801:LHG:HC5	1.91	0.51
24:A:1127:CLA:HHC	24:A:1127:CLA:HBB1	1.91	0.51
2:B:698:PRO:O	3:C:81:TYR:OH	2.21	0.51
41:4:618:CHL:HHC	41:4:618:CHL:HBB1	1.91	0.51
17:5:170:ASP:OD1	40:5:501:LUT:O23	2.27	0.51
41:6:610:CHL:CBB	41:6:613:CHL:HBB2	2.40	0.51
23:A:1011:CL0:H12	24:A:1012:CLA:CAD	2.41	0.51
2:B:179:HIS:ND1	24:B:1221:CLA:O1D	2.41	0.51
24:B:1201:CLA:HMA2	10:M:29:LEU:HD22	1.92	0.51
18:6:170:ALA:HB2	24:6:601:CLA:HBD	1.93	0.51
24:6:603:CLA:H72	28:6:801:LHG:H172	1.92	0.51
20:8:126:VAL:HG11	41:8:613:CHL:HED2	1.93	0.51
1:A:150:ALA:HB2	1:A:378:PRO:HD2	1.93	0.51
24:A:1105:CLA:OBD	29:A:5005:DGD:O2D	2.29	0.51
9:K:99:LEU:HB2	27:K:4001:BCR:H24C	1.93	0.51
15:3:372:ALA:O	15:3:376:ASN:HB2	2.11	0.51
17:5:100:TYR:CD1	41:5:610:CHL:HMA2	2.46	0.51
24:6:604:CLA:HBC1	28:6:801:LHG:H302	1.93	0.51
2:B:182:GLY:HA3	24:B:1210:CLA:HBB1	1.92	0.51
13:L:344:ILE:HG21	27:L:4001:BCR:H282	1.93	0.51
14:1:177:GLY:O	14:1:181:MET:HG3	2.11	0.51
17:5:185:LYS:HG3	24:5:607:CLA:HED2	1.93	0.51
24:2:604:CLA:HBC1	28:2:801:LHG:H101	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:9:406:HIS:CG	24:9:603:CLA:HAA1	2.46	0.51
14:1:72:GLU:HG3	14:1:150:VAL:HB	1.92	0.51
14:1:73:SER:O	14:1:77:HIS:ND1	2.39	0.51
15:3:453:ALA:O	15:3:457:MET:HB2	2.10	0.51
41:3:611:CHL:HHC	41:3:611:CHL:HBB1	1.92	0.51
17:5:56:PRO:HD2	40:5:502:LUT:H23	1.91	0.51
40:7:501:LUT:H30	24:7:601:CLA:H72	1.92	0.51
20:8:124:LEU:HD13	24:8:610:CLA:HBC3	1.93	0.51
1:A:272:TYR:HB3	1:A:276:LEU:HD12	1.93	0.50
2:B:671:TYR:OH	24:B:1023:CLA:OBD	2.28	0.50
41:5:610:CHL:HBB2	24:5:612:CLA:HBC3	1.93	0.50
24:A:1112:CLA:C2B	27:A:4001:BCR:H10C	2.41	0.50
19:7:180:ARG:HA	19:7:183:MET:HE3	1.92	0.50
24:8:609:CLA:H141	29:8:802:DGD:HBN2	1.92	0.50
21:2:79:TRP:CZ2	24:2:612:CLA:HBC1	2.47	0.50
24:A:1126:CLA:O1D	24:A:1127:CLA:HHB	2.11	0.50
40:9:501:LUT:H221	24:9:601:CLA:H12	1.93	0.50
1:A:363:LEU:HD11	24:A:1117:CLA:H72	1.93	0.50
2:B:660:THR:N	24:B:1023:CLA:HAB	2.26	0.50
17:5:140:ILE:HA	17:5:162:LEU:HD11	1.93	0.50
12:H:34:LYS:NZ	13:L:305:ASP:OD2	2.42	0.50
16:4:78:ARG:NH1	24:4:611:CLA:OBD	2.42	0.50
24:4:608:CLA:HBA1	18:6:124:PHE:HD1	1.77	0.50
1:A:392:THR:HG23	1:A:607:ILE:HG21	1.93	0.50
24:A:1107:CLA:H62	37:J:4002:RRX:H38	1.94	0.50
2:B:145:VAL:HG11	28:B:5002:LHG:H191	1.94	0.50
36:G:5002:ERG:C3	36:G:5002:ERG:HO1	2.13	0.50
21:2:182:GLN:HE22	24:2:603:CLA:HED2	1.75	0.50
24:A:1013:CLA:H101	27:A:4005:BCR:H23C	1.93	0.50
2:B:277:HIS:HB2	24:B:1214:CLA:C1B	2.42	0.50
18:6:176:SER:OG	18:6:179:GLU:OE1	2.28	0.50
50:8:808:4RF:H43	42:8:809:OLA:H112	1.94	0.50
1:A:242:GLU:HA	1:A:245:LEU:HB2	1.93	0.50
31:B:5006:LMT:H6'2	7:G:1260:LYS:HD2	1.94	0.50
7:G:1265:LYS:HA	7:G:1270:THR:HA	1.93	0.50
2:B:695:ARG:HD3	13:L:394:THR:HA	1.94	0.50
24:B:1216:CLA:H12	24:B:1221:CLA:HBB1	1.94	0.50
24:B:1226:CLA:H52	29:B:5003:DGD:HB51	1.94	0.50
31:B:5006:LMT:H32	24:1:612:CLA:H11	1.93	0.50
2:B:62:THR:HG23	2:B:143:LEU:HD13	1.93	0.49
24:B:1203:CLA:H91	29:B:5003:DGD:HBF2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:a:172:LYS:HD3	24:a:602:CLA:HBA1	1.93	0.49
24:A:1013:CLA:HMD3	2:B:534:ILE:HG12	1.94	0.49
24:A:1136:CLA:HBB1	24:A:1136:CLA:H101	1.93	0.49
2:B:352:HIS:HB3	24:B:1214:CLA:HED2	1.93	0.49
24:B:1204:CLA:HED2	11:I:7:PRO:HB3	1.93	0.49
15:3:403:VAL:HG12	15:3:416:GLN:HB2	1.93	0.49
24:3:605:CLA:H122	24:3:612:CLA:H11	1.94	0.49
19:7:183:MET:SD	24:7:604:CLA:HAB	2.51	0.49
24:A:1102:CLA:HBA2	24:A:1109:CLA:H61	1.95	0.49
2:B:222:GLY:H	22:9:423:PRO:HG3	1.77	0.49
2:B:396:VAL:HG23	2:B:542:ALA:HB1	1.94	0.49
2:B:572:SER:OG	2:B:575:ASP:OD2	2.28	0.49
5:E:64:VAL:O	5:E:66:GLN:NE2	2.44	0.49
12:H:38:GLU:OE1	12:H:40:ARG:NH1	2.45	0.49
14:1:39:GLY:HA3	20:8:147:SER:HB3	1.95	0.49
16:4:130:PHE:CB	24:4:612:CLA:HAB	2.42	0.49
2:B:378:TYR:CD1	24:B:1224:CLA:HAB	2.47	0.49
6:F:413:TYR:HA	6:F:457:TRP:HE1	1.78	0.49
15:3:466:LEU:HB2	40:3:501:LUT:H22	1.93	0.49
27:3:504:BCR:H281	24:3:607:CLA:H18	1.94	0.49
16:4:39:PRO:O	16:4:41:HIS:ND1	2.45	0.49
41:9:610:CHL:HBC2	33:9:803:PTY:H221	1.94	0.49
24:A:1119:CLA:H152	27:A:4003:BCR:H21C	1.94	0.49
14:a:82:MET:SD	24:a:601:CLA:HAB	2.52	0.49
16:4:221:LYS:O	16:4:226:ASN:ND2	2.35	0.49
21:2:79:TRP:HD1	40:2:502:LUT:H402	1.76	0.49
24:A:1138:CLA:HBB2	6:F:422:GLY:HA3	1.94	0.49
2:B:374:THR:HG23	2:B:592:THR:HG21	1.94	0.49
2:B:670:GLY:O	2:B:674:GLU:HG3	2.12	0.49
24:B:1228:CLA:H41	24:B:1228:CLA:H92	1.95	0.49
24:B:1228:CLA:HBC2	24:B:1236:CLA:HMC2	1.93	0.49
14:1:90:GLY:HA2	14:1:93:VAL:HG12	1.94	0.49
24:a:604:CLA:HBC1	28:a:801:LHG:H292	1.95	0.49
28:4:801:LHG:O2	18:6:150:PRO:O	2.29	0.49
17:5:59:LEU:HD13	24:5:604:CLA:H42	1.94	0.49
3:C:4:THR:HB	3:C:68:TYR:HB2	1.95	0.49
14:a:185:LEU:HD23	24:a:603:CLA:HAC1	1.94	0.49
14:a:205:HIS:CG	24:a:603:CLA:HAA2	2.48	0.49
40:5:505:LUT:H27	24:5:617:CLA:HBC3	1.93	0.49
18:6:195:PHE:CE1	40:6:502:LUT:H10	2.47	0.49
20:8:119:PRO:HG2	20:8:122:SER:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:9:385:PHE:CD2	40:9:502:LUT:H12	2.47	0.49
2:B:9:PHE:HB2	2:B:35:HIS:CG	2.47	0.49
20:8:68:TRP:CD1	46:8:803:DGA:HB62	2.48	0.49
20:8:226:HIS:CG	24:8:603:CLA:HAA2	2.48	0.49
15:3:436:ASN:O	15:3:440:ASN:ND2	2.39	0.49
16:4:167:ASP:OD1	40:4:501:LUT:O23	2.29	0.49
19:7:23:ASP:OD1	19:7:23:ASP:N	2.46	0.49
22:9:305:GLU:HB3	22:9:400:ILE:HD13	1.94	0.49
1:A:87:TRP:HZ3	27:A:4002:BCR:H322	1.76	0.48
3:C:42:ALA:O	4:D:305:ASN:ND2	2.39	0.48
40:1:503:LUT:H10	41:1:613:CHL:HAA1	1.95	0.48
24:1:610:CLA:CBB	41:1:613:CHL:HBB2	2.43	0.48
14:a:83:LEU:HB3	41:a:606:CHL:CBB	2.41	0.48
17:5:33:LEU:HD21	17:5:40:ALA:HB2	1.94	0.48
2:B:527:GLY:HA2	2:B:583:TRP:HZ3	1.78	0.48
24:B:1231:CLA:HBB2	24:B:1234:CLA:HBA1	1.95	0.48
11:I:27:PHE:HB2	27:L:4001:BCR:H14C	1.95	0.48
14:1:223:LEU:HD22	42:8:809:OLA:H82	1.96	0.48
16:4:212:LEU:HB2	40:4:501:LUT:H22	1.94	0.48
24:a:601:CLA:H51	24:a:601:CLA:HBB1	1.94	0.48
24:5:608:CLA:HBA2	24:5:608:CLA:H3A	1.61	0.48
20:8:35:GLN:HB3	20:8:38:VAL:HB	1.95	0.48
1:A:241:HIS:O	1:A:245:LEU:N	2.46	0.48
2:B:6:PHE:HB2	11:I:30:ILE:HA	1.96	0.48
2:B:577:PHE:CE1	24:B:1226:CLA:HAC2	2.48	0.48
4:D:195:GLN:O	4:D:198:THR:OG1	2.31	0.48
19:7:108:SER:OG	24:7:612:CLA:HAB	2.13	0.48
2:B:251:SER:OG	2:B:252:GLY:N	2.41	0.48
2:B:527:GLY:HA2	2:B:583:TRP:CZ3	2.49	0.48
24:3:606:CLA:H51	24:3:613:CLA:HBD	1.95	0.48
40:8:501:LUT:H34	41:8:601:CHL:CBB	2.43	0.48
27:B:4002:BCR:H15C	27:B:4002:BCR:H351	1.57	0.48
14:1:157:ASP:OD1	40:1:501:LUT:O23	2.28	0.48
22:9:282:TRP:HZ2	24:9:612:CLA:HAA1	1.77	0.48
24:A:1119:CLA:H52	24:A:1122:CLA:H51	1.94	0.48
6:F:326:SER:OG	6:F:374:ALA:O	2.31	0.48
16:4:227:ASN:HB3	16:4:229:VAL:HG12	1.95	0.48
27:5:504:BCR:H16C	41:5:610:CHL:HBC2	1.95	0.48
20:8:205:PHE:CE1	40:8:502:LUT:H10	2.49	0.48
1:A:438:ILE:HG13	1:A:556:TYR:HE2	1.77	0.48
1:A:479:LEU:HB2	1:A:530:THR:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:SER:HB2	2:B:446:ALA:HB1	1.95	0.48
2:B:62:THR:HG21	24:B:1225:CLA:H42	1.95	0.48
2:B:141:ILE:HD12	10:M:14:LEU:HD12	1.96	0.48
2:B:276:HIS:HB3	24:B:1214:CLA:HMB2	1.95	0.48
24:3:603:CLA:H151	28:3:801:LHG:H281	1.96	0.48
2:B:258:PHE:HE2	2:B:493:LEU:HB3	1.79	0.48
24:B:1220:CLA:HBB2	24:B:1240:CLA:H51	1.94	0.48
12:H:112:THR:HG23	12:H:113:VAL:HG13	1.96	0.48
13:L:305:ASP:OD1	13:L:305:ASP:N	2.47	0.48
24:L:1501:CLA:H3A	24:L:1501:CLA:HBA2	1.39	0.48
18:6:78:SER:HB3	24:6:612:CLA:HED2	1.96	0.48
1:A:265:PHE:HD2	34:K:5001:LAP:H71	1.78	0.48
1:A:341:LEU:HD23	1:A:344:ILE:HD11	1.96	0.48
1:A:485:GLN:NE2	1:A:528:LEU:O	2.45	0.48
12:H:34:LYS:HA	12:H:50:THR:HG22	1.94	0.48
14:a:157:ASP:OD1	40:a:501:LUT:O23	2.29	0.48
14:a:177:GLY:O	14:a:181:MET:HG3	2.14	0.48
15:3:446:ILE:HG22	24:3:603:CLA:HAB	1.95	0.48
24:7:609:CLA:H2	28:7:801:LHG:H282	1.96	0.48
2:B:60:LEU:HD12	39:M:4001:ECH:H37A	1.96	0.47
4:D:218:GLU:OE2	4:D:277:VAL:N	2.46	0.47
40:a:502:LUT:H28	24:a:604:CLA:H72	1.96	0.47
19:7:135:LYS:HG2	19:7:145:VAL:HG23	1.95	0.47
22:9:257:TYR:OH	22:9:269:ASP:OD2	2.32	0.47
1:A:590:ASP:HA	1:A:593:PHE:HB3	1.96	0.47
24:A:1128:CLA:H192	27:A:4005:BCR:H10C	1.96	0.47
2:B:211:ASP:OD1	2:B:211:ASP:N	2.47	0.47
24:B:1227:CLA:HBC1	27:B:4004:BCR:H21C	1.95	0.47
24:1:611:CLA:HBC3	42:1:803:OLA:H31	1.96	0.47
28:1:801:LHG:HC81	28:1:801:LHG:H111	1.73	0.47
24:7:604:CLA:H72	24:7:605:CLA:HMB1	1.97	0.47
1:A:605:ILE:HD12	23:A:1011:CL0:H53	1.96	0.47
24:B:1207:CLA:H2	24:B:1207:CLA:HMA3	1.96	0.47
27:B:4002:BCR:HC32	24:9:612:CLA:H161	1.95	0.47
9:K:112:LYS:HG2	9:K:117:LEU:HD22	1.96	0.47
14:1:214:PHE:HE1	24:1:608:CLA:HED3	1.79	0.47
16:4:119:LYS:HZ1	24:4:610:CLA:HBC3	1.78	0.47
2:B:508:SER:HA	2:B:511:LEU:HD21	1.95	0.47
24:B:1229:CLA:HBB2	27:B:4006:BCR:HC41	1.97	0.47
21:2:242:LEU:O	21:2:244:TRP:N	2.46	0.47
24:A:1118:CLA:HBA1	9:K:91:VAL:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:1231:CLA:H2	24:B:1232:CLA:HMB1	1.96	0.47
14:1:168:GLU:OE2	14:1:172:LYS:HE3	2.15	0.47
14:1:190:GLN:NE2	14:1:196:ALA:O	2.47	0.47
16:4:39:PRO:O	16:4:41:HIS:N	2.45	0.47
21:2:47:MET:HE1	21:2:66:LEU:HG	1.97	0.47
2:B:51:HIS:HE1	24:B:1202:CLA:H171	1.79	0.47
24:B:1222:CLA:H52	24:B:1231:CLA:HBB2	1.96	0.47
14:a:161:MET:HE3	24:a:601:CLA:H11	1.97	0.47
40:5:505:LUT:H11	40:5:505:LUT:H191	1.62	0.47
24:8:609:CLA:H143	29:8:802:DGD:HBW1	1.97	0.47
1:A:660:SER:HB2	1:A:665:LEU:HB2	1.97	0.47
1:A:681:PHE:HZ	24:A:1139:CLA:HBC2	1.79	0.47
24:A:1102:CLA:H61	24:A:1102:CLA:H93	1.75	0.47
24:A:1127:CLA:H2	27:A:4002:BCR:HC7	1.96	0.47
24:A:1139:CLA:HBA2	24:A:1139:CLA:H3A	1.42	0.47
24:A:1140:CLA:HMC2	27:B:4006:BCR:H381	1.97	0.47
27:I:4001:BCR:H311	27:I:4001:BCR:H342	1.97	0.47
12:H:108:VAL:CG1	24:H:1702:CLA:HAB	2.45	0.47
13:L:327:ASN:OD1	13:L:332:ARG:NH2	2.48	0.47
40:1:503:LUT:H41	24:1:606:CLA:H62	1.96	0.47
16:4:193:ALA:O	16:4:197:ILE:HG12	2.15	0.47
17:5:226:ASN:ND2	17:5:228:THR:H	2.13	0.47
40:5:505:LUT:H21	24:7:608:CLA:HMB1	1.96	0.47
28:5:801:LHG:H262	28:5:801:LHG:H291	1.69	0.47
19:7:122:PRO:HB2	19:7:145:VAL:HG13	1.97	0.47
20:8:94:THR:HG23	20:8:100:ASN:HA	1.97	0.47
22:9:352:SER:OG	24:9:601:CLA:O1D	2.33	0.47
24:A:1110:CLA:H112	24:3:604:CLA:H121	1.96	0.47
2:B:433:HIS:HD2	33:B:5005:PTY:H242	1.79	0.47
14:a:69:ARG:NH1	20:8:155:LEU:O	2.48	0.47
24:3:616:CLA:H41	24:3:616:CLA:H61	1.64	0.47
24:4:615:CLA:H92	24:4:615:CLA:H62	1.81	0.47
24:6:609:CLA:H2	28:6:801:LHG:H141	1.96	0.47
19:7:100:LEU:HG	24:7:610:CLA:HBC1	1.97	0.47
24:7:617:CLA:HBA2	29:8:802:DGD:HAT2	1.97	0.47
24:A:1113:CLA:HBD	15:3:485:ILE:HD11	1.96	0.47
24:A:1136:CLA:H171	24:A:1136:CLA:H13	1.73	0.47
2:B:67:PHE:HZ	10:M:8:VAL:HG13	1.79	0.47
3:C:15:THR:HG22	3:C:28:MET:HE2	1.96	0.47
17:5:174:PHE:HD2	24:5:601:CLA:H11	1.80	0.47
21:2:232:GLN:NE2	21:2:237:GLU:OE2	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:1214:CLA:H102	24:B:1214:CLA:H61	1.63	0.47
24:B:1240:CLA:H2A	24:B:1240:CLA:HED2	1.96	0.47
25:B:2002:PQN:H292	27:L:4001:BCR:HC7	1.97	0.47
7:G:1313:ILE:HA	7:G:1316:THR:HG22	1.96	0.47
33:7:804:PTY:H162	33:7:804:PTY:HC11	1.97	0.47
24:2:615:CLA:H3A	24:2:615:CLA:HBA2	1.47	0.47
1:A:316:TRP:CD1	9:K:91:VAL:HG21	2.51	0.46
24:A:1124:CLA:HAB	27:A:4004:BCR:C8	2.44	0.46
28:A:5003:LHG:H162	24:3:610:CLA:HAC2	1.97	0.46
2:B:126:TYR:O	2:B:131:ARG:NH1	2.48	0.46
4:D:210:LEU:HD22	4:D:214:ALA:HB2	1.97	0.46
10:M:23:VAL:HG12	24:2:621:CLA:H2	1.97	0.46
11:I:14:VAL:HB	27:I:4001:BCR:H333	1.96	0.46
14:1:58:LEU:HD13	40:1:502:LUT:H222	1.96	0.46
24:1:604:CLA:H192	24:1:604:CLA:H161	1.77	0.46
27:3:505:BCR:H331	24:3:603:CLA:HMD1	1.97	0.46
17:5:184:THR:HA	17:5:187:ILE:HG22	1.96	0.46
24:8:603:CLA:H143	24:8:609:CLA:H92	1.97	0.46
24:8:608:CLA:H43	24:8:609:CLA:H41	1.97	0.46
1:A:520:LYS:NZ	1:A:751:GLY:OXT	2.42	0.46
1:A:740:TRP:HB2	24:A:1126:CLA:HBB1	1.97	0.46
29:A:5005:DGD:HG11	29:A:5005:DGD:HA21	1.72	0.46
2:B:22:ILE:O	2:B:26:ILE:HG12	2.15	0.46
3:C:4:THR:HG21	4:D:326:ILE:HD11	1.98	0.46
41:4:618:CHL:HBD	41:4:618:CHL:HBA1	1.97	0.46
24:8:606:CLA:H41	24:8:606:CLA:H62	1.65	0.46
2:B:620:TRP:HB3	24:B:1021:CLA:H102	1.98	0.46
24:1:604:CLA:HBA2	24:1:604:CLA:H3A	1.61	0.46
24:2:605:CLA:HBA1	24:2:605:CLA:H3A	1.64	0.46
22:9:394:LEU:HD12	24:9:603:CLA:HMD3	1.98	0.46
1:A:217:GLN:HA	1:A:221:SER:HB2	1.97	0.46
24:A:1013:CLA:H92	24:A:1013:CLA:H61	1.76	0.46
24:A:1103:CLA:H2	24:A:1103:CLA:H62	1.77	0.46
2:B:134:GLN:OE1	10:M:7:GLN:NE2	2.47	0.46
24:1:605:CLA:H43	24:1:605:CLA:HED3	1.97	0.46
16:4:82:LEU:HB3	24:4:606:CLA:HAB	1.97	0.46
16:4:215:HIS:CG	24:4:603:CLA:HAA2	2.50	0.46
24:8:620:CLA:HBA2	24:8:620:CLA:H3A	1.74	0.46
21:2:58:LEU:HB2	24:2:604:CLA:H12	1.96	0.46
24:A:1102:CLA:H8	37:J:4002:RRX:H54	1.96	0.46
24:A:1115:CLA:H51	24:A:1115:CLA:H11	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:5008:LMT:H71	24:7:615:CLA:HBB2	1.96	0.46
2:B:457:GLU:OE1	6:F:387:HIS:ND1	2.47	0.46
3:C:17:CYS:HB3	26:C:3003:SF4:S4	2.55	0.46
4:D:309:ARG:HB2	4:D:313:GLN:HB2	1.97	0.46
24:1:608:CLA:H142	24:a:612:CLA:H112	1.97	0.46
27:3:504:BCR:H351	27:3:504:BCR:H15C	1.72	0.46
17:5:175:SER:OG	17:5:176:LYS:N	2.49	0.46
24:5:617:CLA:HED2	24:6:609:CLA:HMB1	1.96	0.46
20:8:210:SER:OG	24:8:615:CLA:OBD	2.25	0.46
24:8:612:CLA:HBA2	24:8:612:CLA:H3A	1.49	0.46
24:A:1013:CLA:H151	24:A:1013:CLA:H112	1.61	0.46
24:A:1103:CLA:H191	24:A:1108:CLA:H151	1.98	0.46
2:B:528:LEU:HD23	2:B:587:THR:HG21	1.98	0.46
4:D:273:TYR:HD2	4:D:288:PRO:HG2	1.80	0.46
24:3:610:CLA:H62	24:3:610:CLA:H41	1.72	0.46
1:A:264:PHE:HB2	1:A:272:TYR:HE2	1.81	0.46
24:A:1126:CLA:H3A	24:A:1126:CLA:HBA2	1.54	0.46
2:B:23:TRP:CG	2:B:705:GLN:HE22	2.33	0.46
2:B:595:TRP:HB2	24:B:1234:CLA:HMC1	1.98	0.46
24:B:1215:CLA:H41	24:B:1215:CLA:H62	1.60	0.46
7:G:1307:HIS:CE1	27:G:4001:BCR:H14C	2.50	0.46
10:M:20:ILE:HD11	24:2:621:CLA:HBC2	1.97	0.46
24:a:605:CLA:H202	24:a:605:CLA:H161	1.85	0.46
21:2:33:TRP:HB3	21:2:53:PHE:HB2	1.98	0.46
21:2:153:ARG:HH11	24:2:601:CLA:HED1	1.79	0.46
24:A:1133:CLA:C1D	24:A:1134:CLA:HAB	2.45	0.46
2:B:181:ALA:HB2	2:B:289:GLY:HA3	1.98	0.46
24:B:1021:CLA:H122	24:B:1021:CLA:H161	1.72	0.46
24:B:1204:CLA:HBC3	10:M:15:ALA:HB2	1.97	0.46
27:B:4006:BCR:H10C	6:F:411:PHE:HE1	1.80	0.46
4:D:198:THR:HG23	4:D:246:PRO:HB2	1.97	0.46
5:E:57:GLU:OE2	6:F:478:THR:OG1	2.29	0.46
28:F:5001:LHG:H302	28:F:5001:LHG:H251	1.98	0.46
24:a:612:CLA:H92	24:a:612:CLA:H61	1.76	0.46
1:A:43:PRO:HB3	1:A:48:TRP:CE3	2.51	0.46
1:A:297:HIS:HB2	24:A:1116:CLA:C1B	2.46	0.46
1:A:538:ILE:HG21	23:A:1011:CL0:H60	1.97	0.46
24:A:1106:CLA:HBA2	24:A:1106:CLA:H3A	1.39	0.46
24:A:1118:CLA:H3A	24:A:1118:CLA:HBA2	1.44	0.46
24:A:1125:CLA:H2	24:A:1125:CLA:H61	1.75	0.46
24:B:1204:CLA:H61	27:I:4001:BCR:HC31	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:B:5004:PCW:H322	27:F:4001:BCR:H351	1.97	0.46
24:1:603:CLA:HMA1	24:1:608:CLA:HBC3	1.96	0.46
24:a:605:CLA:H101	24:a:605:CLA:H41	1.98	0.46
17:5:242:VAL:HG11	41:5:610:CHL:HMD3	1.97	0.46
19:7:117:ASN:HD21	20:8:38:VAL:HG23	1.80	0.46
28:7:801:LHG:H291	28:7:801:LHG:H262	1.63	0.46
21:2:76:ASN:HB3	21:2:169:MET:HE3	1.98	0.46
22:9:383:THR:HG21	28:9:801:LHG:H122	1.97	0.46
24:A:1117:CLA:H2	24:A:1127:CLA:H92	1.98	0.46
2:B:468:HIS:CE1	2:B:510:PHE:CZ	3.05	0.46
24:L:1502:CLA:H91	24:L:1502:CLA:H111	1.65	0.46
40:a:503:LUT:H35	40:a:503:LUT:H401	1.66	0.46
18:6:201:ALA:O	18:6:205:THR:OG1	2.26	0.46
40:2:501:LUT:H11	40:2:501:LUT:H191	1.81	0.46
1:A:102:GLU:HA	1:A:105:LEU:HD12	1.97	0.45
1:A:572:ARG:HG3	1:A:589:TRP:CD1	2.51	0.45
24:A:1130:CLA:HBC2	24:A:1137:CLA:HMC2	1.97	0.45
2:B:204:ARG:HG2	2:B:251:SER:HB2	1.98	0.45
24:B:1021:CLA:HBA2	24:B:1021:CLA:H3A	1.74	0.45
16:4:208:PRO:O	40:4:501:LUT:O3	2.33	0.45
40:4:501:LUT:H32	24:4:601:CLA:CAB	2.46	0.45
24:6:609:CLA:HBA2	28:6:801:LHG:H131	1.99	0.45
19:7:50:ALA:HB2	24:7:612:CLA:HED2	1.98	0.45
19:7:121:ASN:ND2	20:8:37:GLY:O	2.49	0.45
24:A:1133:CLA:H51	24:A:1133:CLA:H11	1.73	0.45
24:B:1217:CLA:H61	24:B:1217:CLA:H41	1.77	0.45
6:F:460:ARG:HD3	20:8:59:LEU:HA	1.97	0.45
14:1:193:ALA:HB2	24:1:615:CLA:HED3	1.98	0.45
24:9:612:CLA:H3A	28:9:802:LHG:H251	1.98	0.45
27:A:4001:BCR:H292	27:3:505:BCR:HC31	1.98	0.45
2:B:412:ILE:HA	2:B:415:HIS:CE1	2.51	0.45
24:B:1207:CLA:H93	13:L:374:CYS:HB3	1.98	0.45
24:B:1208:CLA:HMD2	28:9:802:LHG:HC82	1.99	0.45
35:H:5001:SQD:H272	24:2:605:CLA:HED3	1.98	0.45
14:a:57:PRO:HB3	45:4:803:PLM:H41	1.98	0.45
1:A:217:GLN:NE2	24:A:1117:CLA:O1D	2.49	0.45
1:A:269:TRP:CE3	9:K:109:LEU:HD21	2.52	0.45
24:A:1106:CLA:H71	24:A:1128:CLA:H171	1.99	0.45
2:B:175:ARG:HH12	24:B:1202:CLA:H193	1.81	0.45
24:B:1230:CLA:H12	27:B:4006:BCR:HC32	1.98	0.45
12:H:66:ASN:H	12:H:69:GLN:HE21	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:4:165:GLY:HA2	24:4:601:CLA:HED2	1.97	0.45
24:5:606:CLA:HMA2	41:5:613:CHL:HAC2	1.98	0.45
18:6:122:LEU:HD22	27:6:504:BCR:H14C	1.99	0.45
21:2:62:ASP:OD1	21:2:63:LYS:N	2.49	0.45
1:A:677:PHE:CG	27:A:4005:BCR:H363	2.52	0.45
24:A:1133:CLA:H193	24:A:1133:CLA:H162	1.77	0.45
2:B:213:PHE:HA	2:B:216:VAL:HG12	1.98	0.45
2:B:299:GLY:HA2	24:B:1218:CLA:HMD2	1.98	0.45
2:B:339:LEU:HD22	2:B:383:ILE:HG23	1.98	0.45
2:B:443:VAL:HG21	24:B:1230:CLA:HAC2	1.99	0.45
24:B:1225:CLA:H3A	24:B:1225:CLA:HBA2	1.44	0.45
40:5:502:LUT:H35	40:5:502:LUT:H401	1.83	0.45
19:7:152:GLY:O	19:7:162:ARG:NH1	2.49	0.45
41:8:613:CHL:HHC	41:8:613:CHL:HBB1	1.99	0.45
21:2:78:ARG:NE	21:2:161:GLU:OE2	2.49	0.45
1:A:331:GLY:N	28:A:5001:LHG:O2	2.48	0.45
24:A:1126:CLA:H41	27:A:4005:BCR:HC7	1.97	0.45
2:B:293:ARG:HD3	7:G:1264:PRO:HD3	1.98	0.45
14:a:175:LYS:NZ	24:a:607:CLA:O2D	2.47	0.45
24:3:612:CLA:HMC3	24:3:613:CLA:HBB1	1.98	0.45
17:5:251:CYS:O	17:5:253:TRP:N	2.44	0.45
48:7:502:XAT:H201	48:7:502:XAT:H15	1.80	0.45
1:A:277:THR:HB	1:A:279:GLN:HE22	1.81	0.45
24:A:1117:CLA:HAB	24:A:1117:CLA:H111	1.98	0.45
2:B:256:LEU:HD11	24:B:1212:CLA:HBC1	1.98	0.45
24:B:1202:CLA:HBA1	24:B:1202:CLA:H3A	1.53	0.45
4:D:211:LEU:HB3	4:D:212:SER:H	1.68	0.45
12:H:86:ILE:HG23	13:L:388:LEU:HD12	1.98	0.45
14:1:79:ARG:HA	14:1:82:MET:HE3	1.99	0.45
18:6:190:LEU:HG	40:6:501:LUT:H191	1.99	0.45
24:6:612:CLA:HBA1	24:6:612:CLA:H3A	1.80	0.45
21:2:79:TRP:NE1	40:2:502:LUT:H391	2.31	0.45
40:9:501:LUT:H373	24:9:601:CLA:H52	1.98	0.45
24:A:1123:CLA:HBA2	24:A:1127:CLA:H192	1.99	0.45
2:B:27:ALA:HB2	29:B:5003:DGD:HA51	1.99	0.45
2:B:375:HIS:HB2	24:B:1224:CLA:C1B	2.47	0.45
3:C:34:CYS:HA	5:E:69:ILE:HG23	1.97	0.45
41:1:609:CHL:O1D	20:8:137:LYS:NZ	2.49	0.45
40:a:503:LUT:H15	40:a:503:LUT:H201	1.74	0.45
16:4:183:GLU:HG3	24:4:601:CLA:C1B	2.46	0.45
24:5:612:CLA:H2	24:5:612:CLA:H62	1.66	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:5:612:CLA:H72	24:5:612:CLA:H112	1.74	0.45
24:6:617:CLA:H3A	24:6:617:CLA:HBA2	1.72	0.45
19:7:161:CYS:SG	24:7:601:CLA:HAA2	2.56	0.45
41:7:613:CHL:HHC	41:7:613:CHL:HBB1	1.99	0.45
20:8:149:ALA:HB1	20:8:162:LYS:HD2	1.99	0.45
24:2:603:CLA:H11	24:2:603:CLA:H51	1.73	0.45
1:A:349:TRP:HB3	24:A:1103:CLA:HAC1	1.99	0.45
2:B:214:LEU:HB3	22:9:396:ARG:HH22	1.81	0.45
24:B:1225:CLA:H171	27:B:4002:BCR:H352	1.99	0.45
10:M:20:ILE:HD12	24:2:621:CLA:HMD1	1.98	0.45
24:H:1703:CLA:HAA2	21:2:130:VAL:HG21	1.99	0.45
14:1:34:GLY:HA3	14:1:53:TYR:HD1	1.82	0.45
14:a:151:TYR:HB3	24:a:601:CLA:HED3	1.98	0.45
40:3:502:LUT:H35	40:3:502:LUT:H401	1.86	0.45
16:4:130:PHE:HB2	24:4:612:CLA:HAB	1.99	0.45
1:A:29:TRP:NE1	24:A:1109:CLA:O1A	2.50	0.45
1:A:119:TRP:HE1	29:A:5005:DGD:HD3	1.80	0.45
24:A:1119:CLA:HED2	24:A:1122:CLA:HED3	2.00	0.45
24:A:1137:CLA:H43	27:A:4004:BCR:H19C	1.99	0.45
2:B:677:GLU:HG2	3:C:81:TYR:HE1	1.82	0.45
24:B:1220:CLA:H62	24:B:1220:CLA:H41	1.69	0.45
7:G:1272:LEU:HD13	7:G:1280:GLU:HB2	1.99	0.45
24:1:602:CLA:HAC2	24:1:603:CLA:H191	1.99	0.45
24:a:605:CLA:H2	24:a:605:CLA:HED2	1.99	0.45
27:5:504:BCR:H21C	41:5:610:CHL:CGA	2.46	0.45
24:7:604:CLA:H192	24:7:604:CLA:H162	1.82	0.45
1:A:62:GLN:OE1	1:A:72:LYS:NZ	2.45	0.44
1:A:344:ILE:O	1:A:348:SER:OG	2.31	0.44
24:A:1114:CLA:H172	28:A:5003:LHG:H262	1.98	0.44
24:A:1124:CLA:HBA2	24:A:1124:CLA:H3A	1.58	0.44
24:A:1140:CLA:H2	6:F:442:ILE:HD13	1.99	0.44
3:C:61:ASP:HA	3:C:62:PHE:HA	1.75	0.44
40:1:502:LUT:H35	40:1:502:LUT:H401	1.82	0.44
16:4:194:PHE:CE1	40:4:502:LUT:H10	2.52	0.44
24:6:615:CLA:H3A	24:6:615:CLA:HBA2	1.68	0.44
22:9:385:PHE:CZ	40:9:502:LUT:H10	2.51	0.44
24:A:1119:CLA:H171	27:A:4003:BCR:H23C	1.99	0.44
24:B:1202:CLA:HBC2	24:B:1226:CLA:HMA1	1.98	0.44
5:E:93:ASP:OD1	5:E:93:ASP:N	2.50	0.44
10:M:15:ALA:HA	10:M:18:THR:HG22	1.99	0.44
24:a:605:CLA:H101	24:a:605:CLA:H61	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:4:193:ALA:HA	24:4:603:CLA:HBB1	1.99	0.44
27:5:503:BCR:H351	27:5:503:BCR:H15C	1.63	0.44
40:8:502:LUT:H35	40:8:502:LUT:H401	1.81	0.44
24:2:604:CLA:H93	24:2:604:CLA:H61	1.77	0.44
1:A:32:PRO:HB3	24:A:1101:CLA:HAC1	1.99	0.44
24:A:1125:CLA:HBA1	24:A:1125:CLA:H3A	1.60	0.44
2:B:663:MET:HE2	25:B:2002:PQN:H2M3	2.00	0.44
3:C:7:ILE:O	4:D:307:ASN:N	2.50	0.44
24:1:611:CLA:H8	24:1:611:CLA:H52	1.66	0.44
40:a:501:LUT:H15	40:a:501:LUT:H201	1.84	0.44
17:5:197:PHE:CE1	40:5:502:LUT:H10	2.52	0.44
1:A:358:ALA:HB1	27:A:4004:BCR:C10	2.45	0.44
24:A:1116:CLA:O1D	24:A:1117:CLA:HHB	2.17	0.44
24:A:1133:CLA:H93	24:A:1133:CLA:H112	1.85	0.44
24:A:1133:CLA:HBB1	24:A:1135:CLA:HED2	1.99	0.44
2:B:382:PHE:HE1	29:B:5003:DGD:HBE1	1.83	0.44
12:H:58:GLY:HA2	13:L:331:TYR:HB3	1.99	0.44
12:H:87:LEU:HG	13:L:388:LEU:HD11	1.99	0.44
18:6:180:LEU:HD21	24:6:601:CLA:H12	1.99	0.44
18:6:216:HIS:CG	24:6:603:CLA:HAA2	2.53	0.44
20:8:199:ARG:HA	20:8:202:MET:HE3	2.00	0.44
24:B:1207:CLA:HED2	27:L:4002:BCR:H393	2.00	0.44
6:F:416:GLY:HA3	6:F:457:TRP:CE2	2.53	0.44
11:I:21:VAL:HG11	24:2:621:CLA:HAB	2.00	0.44
24:1:612:CLA:H61	24:1:612:CLA:H41	1.64	0.44
24:4:615:CLA:H2	24:4:615:CLA:HAA2	1.99	0.44
27:6:504:BCR:H351	27:6:504:BCR:H15C	1.59	0.44
22:9:298:VAL:HG11	40:9:501:LUT:H12	1.97	0.44
1:A:121:ILE:HG23	1:A:122:VAL:HG22	2.00	0.44
1:A:674:GLY:HA2	27:A:4005:BCR:H17C	1.99	0.44
24:A:1106:CLA:C3D	24:A:1126:CLA:HBA1	2.48	0.44
24:A:1122:CLA:H93	24:A:1122:CLA:H111	1.87	0.44
24:A:1128:CLA:H61	24:A:1128:CLA:H41	1.72	0.44
2:B:677:GLU:HG2	3:C:81:TYR:CE1	2.52	0.44
24:B:1240:CLA:H41	24:B:1240:CLA:H62	1.67	0.44
24:H:1703:CLA:HAB	35:H:5001:SQD:H131	2.00	0.44
14:a:210:MET:HE1	16:4:116:TRP:HZ3	1.81	0.44
16:4:140:ASP:HB2	24:4:611:CLA:HAC2	1.99	0.44
27:5:503:BCR:HC21	28:6:801:LHG:H102	1.99	0.44
18:6:131:TRP:HE1	41:6:611:CHL:CBB	2.31	0.44
40:6:502:LUT:H15	40:6:502:LUT:H201	1.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2:166:ARG:HB3	24:2:604:CLA:HBC3	1.98	0.44
40:2:502:LUT:H381	40:2:502:LUT:H27	1.54	0.44
1:A:322:LEU:HD13	24:A:1123:CLA:HAC2	1.98	0.44
24:A:1103:CLA:H3A	24:A:1103:CLA:HBA1	1.59	0.44
24:A:1133:CLA:H61	24:A:1133:CLA:H92	1.86	0.44
24:A:1135:CLA:H61	24:A:1135:CLA:H41	1.57	0.44
24:B:1022:CLA:H101	24:B:1023:CLA:H143	2.00	0.44
27:B:4004:BCR:H391	27:B:4005:BCR:H272	1.99	0.44
4:D:222:ILE:HG23	4:D:224:TRP:HZ3	1.83	0.44
4:D:277:VAL:HG22	4:D:283:VAL:HG22	1.99	0.44
24:1:604:CLA:H61	24:1:604:CLA:H41	1.57	0.44
14:a:101:ASP:HA	14:a:104:LEU:HD23	1.99	0.44
40:a:502:LUT:H11	40:a:502:LUT:H191	1.85	0.44
24:3:605:CLA:H193	33:3:802:PTY:H191	1.99	0.44
21:2:169:MET:HE1	24:2:604:CLA:CAB	2.40	0.44
1:A:95:GLY:O	1:A:99:SER:OG	2.31	0.44
1:A:368:ALA:HB2	1:A:394:HIS:HB2	1.99	0.44
24:A:1129:CLA:HAB	24:A:1137:CLA:HBB2	1.99	0.44
24:B:1219:CLA:HBB1	24:B:1219:CLA:HMB1	1.99	0.44
7:G:1291:PRO:HG3	24:G:1602:CLA:HBC2	2.00	0.44
8:J:45:LEU:HD13	27:J:4001:BCR:H24C	2.00	0.44
20:8:109:LYS:HE2	24:8:610:CLA:HED2	1.99	0.44
29:8:802:DGD:HD1	29:8:802:DGD:HG2	1.71	0.44
21:2:116:ILE:HA	21:2:119:VAL:HG12	2.00	0.44
24:B:1203:CLA:H191	29:B:5003:DGD:HAG1	2.00	0.44
31:B:5006:LMT:H51	24:1:612:CLA:H43	2.00	0.44
9:K:52:GLY:HA2	9:K:57:ALA:HB3	2.00	0.44
41:1:609:CHL:HED2	20:8:137:LYS:HA	1.99	0.44
16:4:227:ASN:ND2	24:4:603:CLA:OBD	2.39	0.44
24:4:611:CLA:HHC	24:4:611:CLA:HBB1	1.99	0.44
28:4:801:LHG:H172	24:6:618:CLA:HAB	1.98	0.44
17:5:175:SER:O	17:5:177:GLY:N	2.48	0.44
24:6:604:CLA:H192	24:6:604:CLA:H161	1.76	0.44
1:A:169:MET:HG3	27:A:4001:BCR:H322	2.00	0.43
1:A:679:TRP:CE3	23:A:1011:CL0:H6	2.53	0.43
24:A:1110:CLA:HED2	24:A:1111:CLA:HAC1	1.99	0.43
2:B:208:VAL:HG22	2:B:216:VAL:HG11	1.99	0.43
31:B:5006:LMT:H42	24:1:605:CLA:H42	1.98	0.43
3:C:29:VAL:HG12	4:D:301:ARG:HB2	1.99	0.43
8:J:47:GLU:OE1	8:J:50:ARG:NE	2.50	0.43
15:3:477:ASN:HB2	41:3:608:CHL:HED2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:6:209:PRO:O	40:6:501:LUT:O3	2.34	0.43
40:8:501:LUT:H32	41:8:601:CHL:CBB	2.48	0.43
24:2:609:CLA:HBA2	24:2:609:CLA:H3A	1.67	0.43
24:A:1012:CLA:HAB	2:B:583:TRP:HH2	1.83	0.43
24:B:1201:CLA:HBC1	29:B:5003:DGD:HAW2	2.01	0.43
24:B:1220:CLA:H143	24:B:1220:CLA:H111	1.77	0.43
39:M:4001:ECH:H11	39:M:4001:ECH:H34	1.72	0.43
13:L:353:VAL:HA	13:L:376:ASN:ND2	2.30	0.43
24:1:608:CLA:H11	41:1:609:CHL:H42	2.01	0.43
40:a:502:LUT:H15	40:a:502:LUT:H201	1.84	0.43
40:3:501:LUT:H15	40:3:501:LUT:H201	1.85	0.43
16:4:41:HIS:O	16:4:45:ARG:NH2	2.51	0.43
17:5:81:MET:CE	24:5:601:CLA:HAB	2.48	0.43
40:6:502:LUT:H393	47:6:806:SPH:H183	1.99	0.43
22:9:414:ASN:HD22	24:9:608:CLA:HED3	1.82	0.43
13:L:401:GLN:N	13:L:414:ARG:HH12	2.16	0.43
14:1:178:ARG:NH2	24:1:604:CLA:O2D	2.52	0.43
40:3:502:LUT:H15	40:3:502:LUT:H201	1.84	0.43
24:2:603:CLA:H101	24:2:603:CLA:CAB	2.48	0.43
22:9:246:THR:HG21	28:9:801:LHG:HC31	2.00	0.43
1:A:428:ASP:OD2	1:A:432:ARG:NH1	2.48	0.43
24:A:1123:CLA:HMB1	24:A:1123:CLA:HBB1	1.99	0.43
2:B:54:GLN:HE21	24:B:1202:CLA:HMB3	1.83	0.43
8:J:33:LEU:HA	8:J:33:LEU:HD23	1.84	0.43
24:H:1701:CLA:HMB1	24:L:1501:CLA:HAA2	2.01	0.43
24:1:603:CLA:H41	24:1:603:CLA:H62	1.72	0.43
17:5:242:VAL:HG23	17:5:245:LEU:HB3	1.99	0.43
21:2:95:LEU:HD23	21:2:95:LEU:HA	1.90	0.43
1:A:539:HIS:HE1	1:A:605:ILE:HG22	1.83	0.43
28:A:5003:LHG:H142	28:A:5003:LHG:H172	1.73	0.43
2:B:300:HIS:HB3	2:B:305:ILE:HD11	1.99	0.43
2:B:356:LEU:HD13	24:B:1214:CLA:HAA2	2.01	0.43
24:B:1204:CLA:HBA1	11:I:14:VAL:HG21	2.00	0.43
24:B:1207:CLA:HHC	24:B:1207:CLA:HBB1	2.00	0.43
24:B:1219:CLA:HAA2	31:B:5006:LMT:H1'	1.99	0.43
24:K:1404:CLA:O1D	15:3:266:ASN:ND2	2.52	0.43
41:4:609:CHL:H92	41:4:609:CHL:H62	1.85	0.43
20:8:143:LYS:HG2	46:8:803:DGA:HG31	2.00	0.43
41:8:601:CHL:H61	41:8:601:CHL:H41	1.76	0.43
22:9:386:VAL:HG12	24:9:603:CLA:HAC1	2.01	0.43
24:A:1127:CLA:H102	24:A:1127:CLA:H62	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:727:ILE:O	2:B:731:SER:OG	2.33	0.43
7:G:1265:LYS:HG2	7:G:1270:THR:HG22	2.01	0.43
7:G:1316:THR:HG23	36:G:5002:ERG:H181	2.01	0.43
7:G:1323:ARG:NH1	24:G:1603:CLA:OBD	2.51	0.43
39:M:4001:ECH:H20	39:M:4001:ECH:H36	1.75	0.43
13:L:324:TYR:OH	24:L:1502:CLA:O1A	2.32	0.43
42:1:803:OLA:H111	42:1:803:OLA:H81	1.79	0.43
15:3:369:TRP:CD1	24:7:608:CLA:HED2	2.53	0.43
40:4:501:LUT:H32	24:4:601:CLA:HHC	2.00	0.43
17:5:57:MET:HG2	40:5:502:LUT:H222	1.99	0.43
40:5:505:LUT:H15	40:5:505:LUT:H201	1.69	0.43
40:2:502:LUT:H35	40:2:502:LUT:H401	1.88	0.43
28:2:802:LHG:H382	28:2:802:LHG:H352	1.75	0.43
52:9:504:A8S:H6B	24:9:606:CLA:HAB	1.99	0.43
1:A:481:PRO:HG2	1:A:528:LEU:HB3	2.00	0.43
24:A:1128:CLA:H18	24:A:1139:CLA:HBA2	2.00	0.43
28:A:5003:LHG:HC61	15:3:354:ALA:HB2	2.00	0.43
24:B:1023:CLA:H172	24:B:1207:CLA:HAC1	2.01	0.43
28:B:5002:LHG:H241	28:B:5002:LHG:H272	1.85	0.43
24:J:1901:CLA:HMC2	37:J:4002:RRX:H26	2.01	0.43
35:H:5001:SQD:H192	35:H:5001:SQD:H161	1.83	0.43
24:1:607:CLA:H141	24:1:607:CLA:H162	1.83	0.43
1:A:453:PHE:CZ	1:A:457:ILE:HD11	2.54	0.43
2:B:352:HIS:ND1	24:B:1214:CLA:OBD	2.46	0.43
24:B:1229:CLA:H2	24:B:1229:CLA:H62	1.70	0.43
5:E:44:GLN:O	5:E:98:ALA:N	2.51	0.43
24:H:1701:CLA:H62	24:H:1701:CLA:H41	1.57	0.43
24:1:604:CLA:HAC2	28:1:801:LHG:H252	2.01	0.43
40:3:501:LUT:H27	41:3:611:CHL:H42	2.01	0.43
33:5:802:PTY:H141	33:5:802:PTY:H172	1.85	0.43
32:6:803:PCW:H121	45:6:804:PLM:H52	2.00	0.43
19:7:210:ASP:O	19:7:214:THR:OG1	2.27	0.43
20:8:169:TYR:HB3	41:8:601:CHL:HED2	2.01	0.43
33:8:891:PTY:H172	33:8:891:PTY:H142	1.86	0.43
1:A:441:LEU:HG	1:A:548:LEU:HB2	2.00	0.43
24:A:1102:CLA:H203	24:A:1107:CLA:H91	2.00	0.43
24:A:1111:CLA:H61	24:A:1111:CLA:H41	1.70	0.43
24:A:1135:CLA:H141	24:A:1135:CLA:H162	1.78	0.43
2:B:49:ALA:HB3	10:M:29:LEU:HD21	2.01	0.43
2:B:191:TRP:NE1	24:B:1215:CLA:O1D	2.43	0.43
7:G:1288:THR:HG21	7:G:1295:THR:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:31:PRO:HA	8:J:34:THR:HG22	2.01	0.43
37:J:4002:RRX:H32	37:J:4002:RRX:H28	1.75	0.43
9:K:93:VAL:HG21	24:K:1404:CLA:HMA2	2.01	0.43
12:H:68:LEU:HD11	27:H:4001:BCR:H312	2.01	0.43
24:H:1703:CLA:CAB	35:H:5001:SQD:H131	2.49	0.43
24:a:612:CLA:H3A	24:a:612:CLA:HBA2	1.52	0.43
24:4:604:CLA:HBC2	41:4:609:CHL:HBB2	1.99	0.43
41:4:609:CHL:H51	41:4:609:CHL:H12	1.69	0.43
17:5:250:SER:OG	33:5:802:PTY:O10	2.34	0.43
18:6:263:LEU:HD22	24:6:615:CLA:HMB2	2.01	0.43
40:2:502:LUT:H371	40:2:502:LUT:H28	2.00	0.43
28:2:802:LHG:H301	28:2:802:LHG:H212	2.01	0.43
1:A:363:LEU:HD23	24:A:1127:CLA:HBC1	2.00	0.43
1:A:685:PHE:HA	25:A:2001:PQN:H9	2.01	0.43
23:A:1011:CL0:H8	23:A:1011:CL0:CGD	2.49	0.43
24:A:1102:CLA:HBA1	24:A:1102:CLA:H3A	1.84	0.43
24:A:1119:CLA:H72	27:A:4004:BCR:H14C	2.00	0.43
24:A:1125:CLA:C4B	24:A:1133:CLA:HMA3	2.48	0.43
2:B:653:PHE:O	2:B:657:ILE:HG13	2.19	0.43
24:B:1224:CLA:O1D	24:B:1225:CLA:HHB	2.18	0.43
12:H:108:VAL:HG11	13:L:371:ILE:HD13	1.99	0.43
15:3:350:VAL:HG13	15:3:351:ILE:HG13	2.01	0.43
40:3:501:LUT:H32	24:3:601:CLA:CAB	2.49	0.43
24:3:616:CLA:H43	17:5:231:ILE:HG21	2.00	0.43
24:5:612:CLA:H102	41:6:619:CHL:H43	2.01	0.43
18:6:225:ILE:HA	18:6:228:LYS:HG2	2.01	0.43
40:8:502:LUT:H28	41:8:604:CHL:H61	2.01	0.43
22:9:270:PRO:HD2	40:9:502:LUT:H23	2.00	0.43
1:A:430:VAL:HA	1:A:433:HIS:CE1	2.54	0.42
2:B:87:PRO:HB3	2:B:122:TYR:CG	2.54	0.42
24:B:1218:CLA:H62	24:B:1218:CLA:H41	1.42	0.42
12:H:108:VAL:HG12	24:H:1702:CLA:HAB	2.00	0.42
24:3:603:CLA:HHB	41:3:608:CHL:HBC3	2.01	0.42
16:4:83:GLY:O	16:4:87:ILE:HG12	2.19	0.42
17:5:30:GLN:NE2	17:5:51:ASP:OD2	2.52	0.42
18:6:177:LEU:HG	18:6:181:LYS:HD2	2.00	0.42
20:8:196:ARG:HD2	24:8:607:CLA:O1D	2.19	0.42
22:9:295:MET:HE3	22:9:377:ASN:HB3	2.01	0.42
1:A:264:PHE:CZ	27:K:4001:BCR:H343	2.54	0.42
33:B:5005:PTY:H181	33:B:5005:PTY:H152	1.88	0.42
6:F:360:LYS:HA	6:F:360:LYS:HD2	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:1228:LEU:N	7:G:1317:SER:OG	2.49	0.42
12:H:86:ILE:HG13	13:L:384:LEU:HD21	2.01	0.42
24:4:607:CLA:H12	24:4:607:CLA:HBA1	1.90	0.42
17:5:43:TYR:OH	17:5:55:ASP:OD2	2.35	0.42
24:5:618:CLA:HBA2	24:5:618:CLA:H3A	1.96	0.42
18:6:181:LYS:HG3	24:6:601:CLA:HMA3	2.02	0.42
40:6:501:LUT:H31	40:6:501:LUT:H391	1.59	0.42
24:6:601:CLA:H61	24:6:601:CLA:H41	1.41	0.42
22:9:295:MET:HE1	24:9:601:CLA:HAB	2.01	0.42
31:A:5008:LMT:H3O1	15:3:356:GLN:HE21	1.63	0.42
2:B:195:LEU:HA	2:B:199:ALA:HB3	2.01	0.42
24:B:1232:CLA:H3A	24:B:1232:CLA:HBA2	1.45	0.42
24:F:1301:CLA:HBC3	34:F:5003:LAP:H92	2.01	0.42
24:1:603:CLA:H93	28:1:801:LHG:H301	2.01	0.42
14:a:89:LEU:O	14:a:93:VAL:HG12	2.19	0.42
14:a:185:LEU:HD12	24:a:605:CLA:HAB	2.00	0.42
15:3:374:LEU:HB3	27:3:503:BCR:C16	2.50	0.42
18:6:261:HIS:CG	18:6:262:SER:H	2.37	0.42
19:7:154:TYR:CE2	24:7:617:CLA:HAB	2.54	0.42
40:7:501:LUT:H362	40:7:501:LUT:H23	1.81	0.42
20:8:154:PHE:HD2	20:8:157:PHE:HB3	1.83	0.42
20:8:205:PHE:CD2	40:8:502:LUT:H12	2.55	0.42
29:8:802:DGD:HA92	29:8:802:DGD:HG11	2.02	0.42
40:9:502:LUT:H181	24:9:606:CLA:HBB1	2.01	0.42
1:A:220:VAL:HG13	1:A:240:PRO:HB3	2.01	0.42
1:A:679:TRP:O	1:A:682:SER:OG	2.34	0.42
24:A:1116:CLA:HBA2	24:A:1116:CLA:H3A	1.63	0.42
2:B:499:LEU:HA	2:B:499:LEU:HD23	1.93	0.42
2:B:661:GLY:O	2:B:665:LEU:HG	2.19	0.42
24:B:1239:CLA:HBA2	24:B:1239:CLA:H3A	1.60	0.42
12:H:81:SER:HA	13:L:428:ALA:HB2	2.01	0.42
24:1:607:CLA:H151	24:1:607:CLA:H111	1.73	0.42
15:3:250:ASP:O	15:3:252:ALA:N	2.51	0.42
40:6:501:LUT:C14	24:6:602:CLA:HAB	2.50	0.42
1:A:408:HIS:HA	1:A:411:ILE:HD12	2.00	0.42
24:A:1126:CLA:H62	24:A:1126:CLA:H102	1.84	0.42
2:B:354:TYR:HB2	2:B:595:TRP:HZ2	1.84	0.42
24:B:1220:CLA:HMD3	24:B:1221:CLA:HHC	2.00	0.42
4:D:233:GLU:O	4:D:263:GLN:NE2	2.51	0.42
12:H:82:ARG:NH2	21:2:64:ASP:OD2	2.51	0.42
24:1:615:CLA:HMC2	33:8:891:PTY:H182	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:3:350:VAL:HG21	40:3:502:LUT:H172	2.00	0.42
16:4:223:HIS:CE1	16:4:225:ILE:HB	2.55	0.42
18:6:74:TRP:HZ2	24:6:612:CLA:HAA2	1.83	0.42
24:8:602:CLA:H62	24:8:602:CLA:H41	1.50	0.42
24:2:608:CLA:HMA2	22:9:321:TRP:HH2	1.85	0.42
33:9:803:PTY:H132	33:9:803:PTY:H161	1.78	0.42
1:A:297:HIS:CE1	1:A:301:ILE:HD13	2.54	0.42
24:A:1103:CLA:H61	27:A:4002:BCR:H323	2.02	0.42
24:A:1104:CLA:H52	24:A:1128:CLA:H71	2.01	0.42
2:B:430:LEU:HB3	2:B:526:LEU:HB2	2.00	0.42
4:D:276:ARG:HB3	4:D:284:GLN:HB3	2.00	0.42
24:a:607:CLA:H41	24:a:607:CLA:H61	1.76	0.42
24:3:616:CLA:H43	17:5:231:ILE:HD13	2.01	0.42
28:3:801:LHG:H202	28:3:801:LHG:H172	1.86	0.42
24:5:605:CLA:HBC1	41:5:610:CHL:HAB	2.01	0.42
24:6:603:CLA:H111	24:6:603:CLA:H152	1.78	0.42
24:6:615:CLA:H61	24:6:615:CLA:H41	1.85	0.42
19:7:177:ARG:HH11	24:7:607:CLA:CGD	2.32	0.42
2:B:137:TYR:OH	10:M:7:GLN:O	2.31	0.42
24:B:1205:CLA:O1A	24:B:1224:CLA:HBD	2.19	0.42
24:B:1210:CLA:H143	24:B:1210:CLA:H112	1.76	0.42
24:B:1235:CLA:H143	24:B:1235:CLA:H111	1.92	0.42
14:a:211:ALA:HA	14:a:216:THR:HG21	2.01	0.42
24:3:601:CLA:HBA2	24:3:601:CLA:H3A	1.60	0.42
24:3:605:CLA:HBA1	24:3:605:CLA:H3A	1.76	0.42
16:4:41:HIS:HB2	16:4:45:ARG:HH22	1.83	0.42
24:4:612:CLA:H122	24:4:612:CLA:H162	1.87	0.42
24:6:605:CLA:HHD	24:6:615:CLA:H193	2.01	0.42
20:8:68:TRP:HZ2	24:8:612:CLA:HAA2	1.84	0.42
1:A:598:TRP:HE1	24:B:1023:CLA:C1D	2.33	0.42
24:A:1116:CLA:NA	24:A:1116:CLA:H2	2.35	0.42
2:B:646:VAL:HG21	24:B:1205:CLA:HAC1	2.01	0.42
2:B:659:ALA:HB3	24:B:1023:CLA:HBB2	2.00	0.42
24:B:1228:CLA:H141	24:B:1228:CLA:H162	1.78	0.42
24:B:1238:CLA:H201	11:I:20:ALA:HB2	2.01	0.42
14:1:215:ALA:HB2	20:8:125:MET:HG3	2.02	0.42
40:4:501:LUT:H11	40:4:501:LUT:H191	1.89	0.42
18:6:66:GLY:HA3	18:6:72:LEU:HD13	2.01	0.42
24:6:601:CLA:H62	24:6:602:CLA:HBA1	2.02	0.42
32:6:803:PCW:H122	32:6:803:PCW:H321	2.02	0.42
24:7:601:CLA:H91	24:7:601:CLA:H112	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:7:801:LHG:H241	28:7:801:LHG:H271	1.64	0.42
1:A:16:VAL:HG23	1:A:187:LYS:HB2	2.02	0.42
1:A:263:PRO:HG2	1:A:272:TYR:CZ	2.55	0.42
1:A:355:ILE:HD11	27:A:4003:BCR:H24C	2.02	0.42
1:A:574:PRO:HB3	1:A:720:ILE:HB	2.01	0.42
24:A:1135:CLA:H2	24:A:1136:CLA:O1A	2.20	0.42
2:B:358:PRO:HG3	24:B:1215:CLA:HBA1	2.02	0.42
24:B:1238:CLA:H141	27:L:4002:BCR:H24C	2.02	0.42
4:D:254:LYS:HE3	4:D:286:LEU:HD13	2.01	0.42
6:F:363:ILE:O	6:F:367:GLU:HG3	2.20	0.42
13:L:404:VAL:HG13	13:L:412:ILE:HG23	2.02	0.42
13:L:405:LYS:HG2	13:L:411:SER:HA	2.02	0.42
40:4:501:LUT:H15	40:4:501:LUT:H201	1.85	0.42
24:4:611:CLA:H92	24:4:611:CLA:H62	1.74	0.42
24:8:610:CLA:HBA1	24:8:610:CLA:H3A	1.54	0.42
1:A:297:HIS:HB2	24:A:1116:CLA:CHB	2.50	0.42
24:A:1117:CLA:HBA2	24:A:1117:CLA:H3A	1.64	0.42
24:A:1138:CLA:HBA2	24:A:1138:CLA:H3A	1.58	0.42
2:B:72:GLN:NE2	24:B:1204:CLA:O1D	2.51	0.42
24:1:605:CLA:HBC1	24:1:612:CLA:HAC1	2.01	0.42
15:3:375:MET:CB	24:3:612:CLA:HAB	2.49	0.42
40:4:501:LUT:H401	40:4:501:LUT:H35	1.75	0.42
17:5:81:MET:SD	24:5:601:CLA:HAB	2.60	0.42
24:5:601:CLA:H51	24:5:602:CLA:HMA3	2.02	0.42
24:5:603:CLA:H62	24:5:603:CLA:H41	1.74	0.42
24:7:603:CLA:H2	24:7:608:CLA:HMD2	2.01	0.42
24:7:612:CLA:H91	24:7:612:CLA:H111	1.80	0.42
24:7:617:CLA:OBD	28:8:801:LHG:O2	2.35	0.42
24:A:1121:CLA:H61	24:A:1121:CLA:H41	1.63	0.41
24:A:1122:CLA:HMA1	24:A:1141:CLA:HAB	2.02	0.41
41:1:609:CHL:CGD	20:8:137:LYS:HG2	2.50	0.41
14:a:69:ARG:NH2	20:8:155:LEU:HD23	2.35	0.41
24:6:602:CLA:H11	24:6:602:CLA:H51	1.88	0.41
41:6:619:CHL:H11	41:6:619:CHL:H51	1.80	0.41
24:2:612:CLA:HBA1	24:2:612:CLA:H3A	1.65	0.41
1:A:351:ALA:HB1	27:A:4003:BCR:H393	2.02	0.41
1:A:584:CYS:N	2:B:669:ARG:O	2.53	0.41
2:B:295:ILE:HG12	24:B:1209:CLA:HMA2	2.02	0.41
24:B:1239:CLA:H141	13:L:386:LEU:HD21	2.02	0.41
4:D:212:SER:HA	4:D:215:GLN:NE2	2.35	0.41
7:G:1319:LEU:HD23	7:G:1323:ARG:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1:501:LUT:H11	40:1:501:LUT:H191	1.88	0.41
40:5:505:LUT:H181	41:5:610:CHL:H43	2.02	0.41
24:5:612:CLA:H62	24:5:612:CLA:H92	1.85	0.41
24:7:612:CLA:HBC2	41:7:613:CHL:HMB3	2.02	0.41
21:2:159:LEU:HD23	24:2:607:CLA:HED3	2.01	0.41
22:9:282:TRP:CZ2	24:9:612:CLA:HAA1	2.55	0.41
2:B:445:GLN:OE1	2:B:453:GLN:NE2	2.54	0.41
2:B:715:SER:HB2	29:B:5003:DGD:HBH2	2.02	0.41
24:B:1207:CLA:HED3	13:L:375:ILE:HD12	2.03	0.41
28:F:5002:LHG:H272	42:8:809:OLA:H51	2.03	0.41
13:L:313:THR:HB	13:L:316:THR:HG22	2.02	0.41
13:L:440:TRP:HB2	27:L:4003:BCR:H331	2.03	0.41
27:3:503:BCR:H271	24:3:606:CLA:NB	2.35	0.41
19:7:21:TYR:CZ	19:7:39:SER:HA	2.56	0.41
40:7:501:LUT:H383	24:7:611:CLA:H12	2.02	0.41
27:8:503:BCR:H351	27:8:503:BCR:H15C	1.64	0.41
24:8:606:CLA:H41	24:8:606:CLA:H8	2.02	0.41
1:A:274:ASP:N	1:A:274:ASP:OD1	2.52	0.41
1:A:457:ILE:HG23	24:B:1022:CLA:H61	2.01	0.41
24:A:1013:CLA:CGA	24:A:1013:CLA:H3A	2.51	0.41
24:A:1108:CLA:HBB1	24:A:1111:CLA:H13	2.02	0.41
24:A:1130:CLA:H92	24:A:1130:CLA:H61	1.88	0.41
24:A:1131:CLA:H141	24:A:1131:CLA:H161	1.83	0.41
2:B:682:ALA:O	2:B:686:THR:OG1	2.23	0.41
24:B:1201:CLA:H101	24:B:1201:CLA:C3	2.50	0.41
27:B:4003:BCR:H351	27:B:4003:BCR:H15C	1.83	0.41
24:F:1302:CLA:C1C	28:F:5001:LHG:HC42	2.50	0.41
28:1:802:LHG:H121	28:1:802:LHG:HC92	1.62	0.41
15:3:393:SER:HA	15:3:401:GLU:HB2	2.02	0.41
15:3:442:ARG:HA	15:3:445:MET:HE3	2.03	0.41
18:6:218:ASP:OD1	18:6:218:ASP:N	2.52	0.41
1:A:81:LEU:HB3	1:A:173:MET:HG3	2.02	0.41
24:A:1136:CLA:H11	24:A:1136:CLA:H51	1.79	0.41
2:B:632:LEU:HD22	2:B:725:PHE:HA	2.01	0.41
24:B:1236:CLA:HED2	24:B:1236:CLA:H2A	2.03	0.41
24:B:1240:CLA:H142	24:B:1240:CLA:H112	1.88	0.41
27:J:4001:BCR:H15C	27:J:4001:BCR:H351	1.86	0.41
14:1:185:LEU:HG	24:1:603:CLA:HAC1	2.01	0.41
16:4:93:LEU:HG	16:4:98:LEU:HB2	2.02	0.41
18:6:239:PRO:HA	18:6:240:PRO:HD3	1.97	0.41
19:7:125:GLN:HB3	24:7:611:CLA:HMC1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:2:604:CLA:H41	24:2:604:CLA:H62	1.60	0.41
1:A:198:LEU:HD12	1:A:322:LEU:HD11	2.02	0.41
24:B:1223:CLA:C4B	24:B:1231:CLA:HMA2	2.51	0.41
24:B:1228:CLA:H191	6:F:409:ILE:HG23	2.02	0.41
35:H:5001:SQD:H252	24:2:612:CLA:H12	2.02	0.41
17:5:104:MET:HE3	41:5:610:CHL:HED2	2.02	0.41
24:7:603:CLA:H2	24:7:608:CLA:CMD	2.50	0.41
24:7:604:CLA:H152	24:7:604:CLA:H112	1.80	0.41
20:8:56:PRO:HD2	40:8:502:LUT:H23	2.02	0.41
1:A:13:VAL:N	1:A:315:ASN:OD1	2.54	0.41
1:A:16:VAL:HB	1:A:187:LYS:HD2	2.03	0.41
24:A:1116:CLA:H111	24:A:1134:CLA:HBA1	2.02	0.41
24:A:1123:CLA:H193	24:A:1123:CLA:H161	1.86	0.41
24:A:1134:CLA:H62	24:A:1134:CLA:H92	1.79	0.41
2:B:159:GLN:O	2:B:163:GLN:HG3	2.21	0.41
25:B:2002:PQN:H141	25:B:2002:PQN:H161	1.73	0.41
34:F:5003:LAP:H131	34:F:5003:LAP:H21	1.89	0.41
24:1:612:CLA:HBA2	24:1:612:CLA:H3A	1.47	0.41
28:7:801:LHG:HC81	28:7:801:LHG:HC5	1.67	0.41
24:9:612:CLA:H12	28:9:802:LHG:H311	2.03	0.41
2:B:70:ALA:HB2	2:B:136:LEU:HB2	2.02	0.41
2:B:374:THR:HB	24:B:1224:CLA:HMB1	2.03	0.41
4:D:221:VAL:HA	4:D:250:LYS:HA	2.02	0.41
27:K:4001:BCR:H351	27:K:4001:BCR:H15C	1.83	0.41
12:H:92:ILE:HD12	12:H:92:ILE:HA	1.97	0.41
12:H:93:GLY:O	12:H:97:ILE:HG12	2.20	0.41
40:a:503:LUT:H41	41:a:606:CHL:H62	2.02	0.41
15:3:312:ILE:HD11	24:3:612:CLA:CGD	2.51	0.41
15:3:361:TRP:CH2	15:3:362:MET:HE2	2.56	0.41
24:3:606:CLA:H91	24:3:606:CLA:H112	1.93	0.41
18:6:149:ASP:HB3	18:6:152:PHE:O	2.21	0.41
40:8:502:LUT:H30	41:8:604:CHL:H72	2.03	0.41
21:2:66:LEU:HA	21:2:69:TYR:HD2	1.85	0.41
24:9:612:CLA:H61	24:9:612:CLA:H2	1.88	0.41
1:A:29:TRP:HE1	24:A:1109:CLA:CHB	2.34	0.41
1:A:279:GLN:HG3	1:A:503:LEU:HD12	2.03	0.41
1:A:372:TYR:HA	1:A:387:GLN:OE1	2.21	0.41
1:A:509:SER:HB3	1:A:523:MET:HE2	2.03	0.41
24:A:1107:CLA:HBB1	27:J:4001:BCR:C23	2.51	0.41
24:A:1109:CLA:CHA	24:A:1109:CLA:HBA1	2.50	0.41
24:A:1120:CLA:HMB2	24:A:1121:CLA:H2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:2001:PQN:H222	25:A:2001:PQN:H261	1.83	0.41
27:A:4002:BCR:H383	24:3:612:CLA:H18	2.02	0.41
2:B:520:VAL:HG21	2:B:594:TYR:HB2	2.03	0.41
24:B:1203:CLA:HAB	24:B:1225:CLA:HBB1	2.03	0.41
24:B:1216:CLA:H111	24:B:1216:CLA:H152	1.78	0.41
24:B:1229:CLA:HHC	24:B:1229:CLA:HBB1	2.03	0.41
25:B:2002:PQN:H302	25:B:2002:PQN:H262	1.79	0.41
27:B:4001:BCR:H351	27:B:4001:BCR:H15C	1.68	0.41
6:F:353:SER:HB2	6:F:355:PRO:HD2	2.03	0.41
28:F:5001:LHG:H121	40:8:502:LUT:H363	2.01	0.41
28:F:5002:LHG:H271	28:F:5002:LHG:H241	1.70	0.41
12:H:71:GLU:HA	12:H:74:GLU:HG3	2.02	0.41
13:L:301:PRO:HB3	13:L:306:PRO:HA	2.02	0.41
13:L:355:PRO:O	13:L:359:LEU:HB2	2.21	0.41
14:1:34:GLY:HA3	14:1:53:TYR:CD1	2.55	0.41
14:1:88:VAL:HG22	14:1:99:TRP:HB3	2.03	0.41
14:1:205:HIS:CG	24:1:603:CLA:HAA2	2.55	0.41
40:a:502:LUT:H35	40:a:502:LUT:H401	1.84	0.41
15:3:330:LEU:HD22	15:3:335:LEU:HD12	2.01	0.41
16:4:157:LYS:HE2	16:4:157:LYS:HB2	1.96	0.41
24:4:604:CLA:H2A	24:4:604:CLA:HED2	2.03	0.41
24:4:612:CLA:H61	24:4:612:CLA:H41	1.56	0.41
18:6:219:ASN:O	18:6:223:THR:OG1	2.32	0.41
27:7:503:BCR:H15C	27:7:503:BCR:H351	1.80	0.41
20:8:93:LEU:HD23	20:8:99:LEU:HD12	2.03	0.41
20:8:154:PHE:HB3	20:8:155:LEU:H	1.58	0.41
1:A:249:LEU:HA	1:A:252:GLN:HG3	2.03	0.41
2:B:561:ASP:OD1	3:C:66:ARG:NH1	2.54	0.41
24:B:1022:CLA:H192	24:B:1207:CLA:HMC1	2.03	0.41
24:B:1209:CLA:HBB2	24:B:1217:CLA:H102	2.01	0.41
24:1:601:CLA:H62	24:1:601:CLA:H41	1.94	0.41
24:1:608:CLA:H121	24:a:612:CLA:H8	2.02	0.41
15:3:446:ILE:HD11	24:3:604:CLA:HAC1	2.03	0.41
40:6:501:LUT:H191	40:6:501:LUT:H11	1.94	0.41
28:6:802:LHG:H292	28:6:802:LHG:H321	1.74	0.41
1:A:429:ARG:HE	24:A:1129:CLA:CGD	2.33	0.40
1:A:435:ASP:OD1	1:A:556:TYR:OH	2.29	0.40
1:A:603:ILE:O	1:A:607:ILE:HG12	2.22	0.40
24:A:1133:CLA:H71	27:A:4004:BCR:H372	2.03	0.40
24:A:1137:CLA:H111	24:A:1137:CLA:H91	1.84	0.40
2:B:232:ALA:HA	24:B:1213:CLA:HAA2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:575:ASP:OD1	2:B:707:ARG:NH1	2.54	0.40
24:B:1205:CLA:HBB1	24:B:1205:CLA:H71	2.03	0.40
6:F:426:LEU:HD23	6:F:426:LEU:HA	1.95	0.40
12:H:88:GLY:HA3	35:H:5001:SQD:H262	2.04	0.40
40:1:502:LUT:H15	40:1:502:LUT:H201	1.87	0.40
24:3:606:CLA:HMA2	24:3:613:CLA:C3C	2.51	0.40
16:4:179:TRP:HB3	24:4:601:CLA:HMA2	2.02	0.40
17:5:34:TRP:HE1	17:5:38:VAL:HG21	1.85	0.40
18:6:60:PHE:CZ	24:6:609:CLA:HBB1	2.56	0.40
24:8:609:CLA:H93	24:8:609:CLA:H62	1.76	0.40
21:2:42:TYR:OH	21:2:54:ASP:OD2	2.38	0.40
21:2:87:ILE:HG13	40:2:502:LUT:H382	2.02	0.40
40:9:502:LUT:H371	24:9:604:CLA:H112	2.02	0.40
1:A:658:ILE:HD12	2:B:622:ARG:HG3	2.03	0.40
1:A:683:LEU:HG	1:A:687:PHE:CZ	2.56	0.40
24:A:1115:CLA:H3A	24:A:1115:CLA:HBA2	1.78	0.40
2:B:331:LEU:HD21	24:B:1202:CLA:H192	2.02	0.40
24:B:1220:CLA:HAB	24:B:1227:CLA:CMD	2.51	0.40
24:B:1229:CLA:H192	24:B:1235:CLA:H121	2.03	0.40
32:B:5004:PCW:H342	27:F:4001:BCR:H14C	2.02	0.40
13:L:357:ILE:HA	13:L:372:VAL:HG21	2.03	0.40
40:4:502:LUT:H30	24:4:604:CLA:H72	2.02	0.40
17:5:200:PHE:HE1	40:5:501:LUT:H41	1.85	0.40
18:6:104:PHE:CE2	18:6:106:TYR:HB3	2.56	0.40
20:8:195:ILE:HD12	20:8:195:ILE:HA	1.95	0.40
24:2:603:CLA:H41	24:2:603:CLA:H62	1.81	0.40
24:9:612:CLA:H111	24:9:612:CLA:H152	1.84	0.40
1:A:588:ALA:O	1:A:592:VAL:HG23	2.21	0.40
24:A:1121:CLA:H111	27:K:4001:BCR:H381	2.03	0.40
2:B:141:ILE:HD13	2:B:141:ILE:HA	1.97	0.40
2:B:196:VAL:HG21	24:B:1212:CLA:HBC3	2.04	0.40
2:B:258:PHE:CE2	2:B:493:LEU:HB3	2.55	0.40
2:B:269:LEU:HD21	2:B:356:LEU:HB3	2.03	0.40
2:B:341:SER:HA	24:B:1223:CLA:H51	2.04	0.40
2:B:462:GLN:HG2	2:B:473:TYR:CZ	2.56	0.40
2:B:491:GLN:HA	2:B:495:LEU:HB2	2.03	0.40
24:B:1209:CLA:H62	24:B:1209:CLA:H92	1.77	0.40
24:B:1209:CLA:H93	24:9:604:CLA:H101	2.03	0.40
24:B:1212:CLA:H2A	24:B:1212:CLA:HED2	2.03	0.40
39:M:4001:ECH:H8	24:2:615:CLA:CBB	2.51	0.40
13:L:353:VAL:HG11	13:L:441:GLY:HA3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1:501:LUT:H35	40:1:501:LUT:H401	1.78	0.40
24:a:607:CLA:HAB	27:4:503:BCR:HC21	2.03	0.40
40:3:501:LUT:H162	41:3:608:CHL:HBC1	2.04	0.40
24:3:607:CLA:H91	24:3:607:CLA:H112	1.81	0.40
16:4:81:MET:SD	24:4:601:CLA:HAB	2.62	0.40
24:4:611:CLA:H52	24:4:611:CLA:H11	1.84	0.40
18:6:190:LEU:HD12	18:6:190:LEU:HA	1.93	0.40
18:6:203:GLN:HA	18:6:243:ILE:HD12	2.02	0.40
24:6:601:CLA:H91	24:6:601:CLA:H112	1.82	0.40
20:8:215:THR:HB	20:8:217:LYS:NZ	2.37	0.40
40:8:502:LUT:H15	40:8:502:LUT:H201	1.93	0.40
40:2:501:LUT:H221	24:2:601:CLA:H12	2.02	0.40
24:2:603:CLA:H71	24:2:603:CLA:H112	1.91	0.40
1:A:326:LEU:O	1:A:338:HIS:HB2	2.21	0.40
24:A:1131:CLA:H162	24:A:1131:CLA:H193	1.83	0.40
24:A:1138:CLA:NC	24:A:1138:CLA:H51	2.36	0.40
24:B:1216:CLA:HBB1	24:B:1221:CLA:H72	2.02	0.40
29:B:5003:DGD:HAF1	29:B:5003:DGD:HAE1	1.76	0.40
37:J:4002:RRX:H40	37:J:4002:RRX:H36	1.89	0.40
24:1:604:CLA:H18	24:8:618:CLA:H112	2.04	0.40
14:a:88:VAL:HA	14:a:91:VAL:HG12	2.03	0.40
24:3:603:CLA:H172	28:3:801:LHG:H302	2.04	0.40
24:3:605:CLA:OBD	24:3:612:CLA:HBA2	2.21	0.40
24:7:605:CLA:OBD	24:7:612:CLA:HBA2	2.22	0.40
1:A:413:MET:HE1	1:A:427:LEU:HD11	2.03	0.40
1:A:458:HIS:O	1:A:462:MET:HG2	2.21	0.40
24:A:1013:CLA:H141	24:A:1013:CLA:H161	1.82	0.40
24:A:1104:CLA:H43	28:A:5002:LHG:H262	2.04	0.40
24:A:1112:CLA:H8	24:A:1114:CLA:H112	2.02	0.40
25:A:2001:PQN:H111	25:A:2001:PQN:H2M1	1.92	0.40
2:B:590:TRP:CD1	24:B:1021:CLA:H121	2.56	0.40
24:B:1239:CLA:HBC1	25:B:2002:PQN:H2M2	2.02	0.40
14:1:148:LYS:HA	14:1:148:LYS:HD3	1.86	0.40
20:8:52:PHE:HZ	20:8:196:ARG:HE	1.70	0.40
20:8:84:VAL:HG11	40:8:501:LUT:H12	2.04	0.40
40:2:502:LUT:H201	40:2:502:LUT:H15	1.83	0.40
24:2:604:CLA:CGA	24:2:604:CLA:H3A	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	739/741 (100%)	715 (97%)	24 (3%)	0	100	100
2	B	729/731 (100%)	697 (96%)	32 (4%)	0	100	100
3	C	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
4	D	141/143 (99%)	133 (94%)	8 (6%)	0	100	100
5	E	62/64 (97%)	58 (94%)	4 (6%)	0	100	100
6	F	163/165 (99%)	158 (97%)	5 (3%)	0	100	100
7	G	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
8	J	39/41 (95%)	39 (100%)	0	0	100	100
9	K	84/86 (98%)	80 (95%)	4 (5%)	0	100	100
10	M	29/31 (94%)	29 (100%)	0	0	100	100
11	I	33/35 (94%)	30 (91%)	3 (9%)	0	100	100
12	H	92/94 (98%)	75 (82%)	15 (16%)	2 (2%)	5	25
13	L	155/157 (99%)	141 (91%)	13 (8%)	1 (1%)	21	52
14	1	190/192 (99%)	174 (92%)	15 (8%)	1 (0%)	24	55
14	a	190/192 (99%)	169 (89%)	20 (10%)	1 (0%)	24	55
15	3	239/241 (99%)	221 (92%)	17 (7%)	1 (0%)	30	59
16	4	205/207 (99%)	188 (92%)	17 (8%)	0	100	100
17	5	225/227 (99%)	204 (91%)	21 (9%)	0	100	100
18	6	229/231 (99%)	208 (91%)	20 (9%)	1 (0%)	30	59
19	7	219/221 (99%)	206 (94%)	13 (6%)	0	100	100
20	8	217/219 (99%)	203 (94%)	14 (6%)	0	100	100
21	2	213/215 (99%)	199 (93%)	13 (6%)	1 (0%)	24	55
22	9	180/182 (99%)	166 (92%)	14 (8%)	0	100	100
All	All	4548/4594 (99%)	4261 (94%)	279 (6%)	8 (0%)	44	71

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	H	118	PRO
14	1	36	TRP
14	a	107	VAL
18	6	46	PRO
12	H	110	LEU
13	L	415	ASP
15	3	280	LEU
21	2	109	PHE

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	600/600 (100%)	600 (100%)	0	100	100
2	B	588/588 (100%)	588 (100%)	0	100	100
3	C	69/69 (100%)	69 (100%)	0	100	100
4	D	121/121 (100%)	121 (100%)	0	100	100
5	E	55/55 (100%)	55 (100%)	0	100	100
6	F	126/126 (100%)	126 (100%)	0	100	100
7	G	71/71 (100%)	71 (100%)	0	100	100
8	J	35/35 (100%)	35 (100%)	0	100	100
9	K	66/66 (100%)	66 (100%)	0	100	100
10	M	23/23 (100%)	23 (100%)	0	100	100
11	I	30/30 (100%)	30 (100%)	0	100	100
12	H	71/71 (100%)	71 (100%)	0	100	100
13	L	122/122 (100%)	122 (100%)	0	100	100
14	1	134/134 (100%)	134 (100%)	0	100	100
14	a	134/134 (100%)	134 (100%)	0	100	100
15	3	186/186 (100%)	186 (100%)	0	100	100
16	4	165/165 (100%)	165 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	5	183/183 (100%)	182 (100%)	1 (0%)	81	82
18	6	187/187 (100%)	187 (100%)	0	100	100
19	7	176/176 (100%)	176 (100%)	0	100	100
20	8	168/168 (100%)	168 (100%)	0	100	100
21	2	173/173 (100%)	173 (100%)	0	100	100
22	9	140/140 (100%)	140 (100%)	0	100	100
All	All	3623/3623 (100%)	3622 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	5	159	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	ASN
1	A	225	ASN
1	A	442	ASN
1	A	539	HIS
1	A	722	GLN
2	B	54	GLN
2	B	277	HIS
2	B	278	HIS
2	B	433	HIS
2	B	453	GLN
2	B	468	HIS
2	B	503	ASN
2	B	604	GLN
2	B	609	GLN
2	B	690	ASN
4	D	280	ASN
8	J	49	ASN
12	H	116	GLN
12	H	120	GLN
13	L	376	ASN
13	L	396	GLN
14	1	176	ASN
14	a	111	GLN

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Mol	Chain	Res	Type
14	a	205	HIS
15	3	271	GLN
15	3	356	GLN
15	3	416	GLN
15	3	454	GLN
15	3	465	ASN
15	3	476	ASN
16	4	201	HIS
17	5	30	GLN
17	5	76	ASN
17	5	117	ASN
17	5	189	ASN
17	5	214	ASN
17	5	233	HIS
18	6	68	ASN
18	6	250	GLN
19	7	121	ASN
19	7	141	GLN
19	7	167	GLN
19	7	213	HIS
20	8	58	ASN
20	8	76	ASN
20	8	197	ASN
21	2	76	ASN
21	2	164	ASN
21	2	182	GLN
22	9	391	GLN
22	9	424	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

379 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
28	LHG	7	802	-	35,35,48	0.44	0	38,41,54	1.12	2 (5%)
38	LPX	a	804	-	29,29,29	1.04	2 (6%)	31,33,33	0.98	1 (3%)
28	LHG	4	801	-	48,48,48	0.40	0	51,54,54	1.02	3 (5%)
27	BCR	5	504	-	41,41,41	1.61	4 (9%)	56,56,56	4.65	20 (35%)
29	DGD	B	5003	-	67,67,67	1.30	7 (10%)	81,81,81	0.94	2 (2%)
27	BCR	A	4001	-	41,41,41	1.60	4 (9%)	56,56,56	4.40	16 (28%)
28	LHG	7	801	-	48,48,48	0.39	0	51,54,54	1.10	3 (5%)
24	CLA	8	620	20	69,73,73	1.35	7 (10%)	82,113,113	1.86	19 (23%)
24	CLA	B	1220	-	64,68,73	1.41	7 (10%)	76,107,113	1.96	19 (25%)
24	CLA	A	1130	-	60,64,73	1.48	6 (10%)	71,102,113	2.02	18 (25%)
41	CHL	4	609	16	60,74,74	1.75	10 (16%)	58,114,114	1.63	10 (17%)
40	LUT	1	503	-	42,43,43	2.47	1 (2%)	51,60,60	2.19	14 (27%)
38	LPX	J	5001	-	16,16,29	1.33	2 (12%)	18,20,33	1.11	1 (5%)
41	CHL	5	610	-	60,74,74	1.25	8 (13%)	58,114,114	1.57	11 (18%)
24	CLA	A	1124	-	59,63,73	1.47	7 (11%)	70,101,113	2.00	21 (30%)
24	CLA	B	1237	-	69,73,73	1.37	6 (8%)	82,113,113	1.82	15 (18%)
24	CLA	9	605	-	64,68,73	1.43	8 (12%)	76,107,113	1.96	20 (26%)
41	CHL	a	606	-	50,64,74	1.49	9 (18%)	46,102,114	1.90	11 (23%)
40	LUT	6	502	-	42,43,43	2.47	1 (2%)	51,60,60	2.07	14 (27%)
24	CLA	3	610	15	64,68,73	1.40	6 (9%)	76,107,113	1.92	19 (25%)
24	CLA	B	1208	-	64,68,73	1.42	7 (10%)	76,107,113	2.00	21 (27%)
24	CLA	6	617	-	49,53,73	1.60	7 (14%)	58,89,113	2.05	17 (29%)
24	CLA	L	1501	13	54,58,73	1.52	7 (12%)	64,95,113	2.10	17 (26%)
24	CLA	B	1240	-	69,73,73	1.36	7 (10%)	82,113,113	1.93	22 (26%)
24	CLA	A	1120	-	53,57,73	1.53	7 (13%)	61,93,113	2.24	18 (29%)
24	CLA	K	1404	-	56,60,73	1.50	7 (12%)	65,97,113	2.09	20 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	1	607	-	69,73,73	1.36	6 (8%)	82,113,113	1.90	20 (24%)
27	BCR	6	503	-	41,41,41	1.61	4 (9%)	56,56,56	4.49	13 (23%)
24	CLA	1	605	-	69,73,73	1.38	7 (10%)	82,113,113	1.94	18 (21%)
24	CLA	7	602	-	47,52,73	1.64	7 (14%)	55,87,113	2.08	17 (30%)
24	CLA	3	618	-	50,54,73	1.59	8 (16%)	59,90,113	2.11	18 (30%)
24	CLA	9	606	-	59,63,73	1.46	7 (11%)	70,101,113	1.96	19 (27%)
24	CLA	A	1108	-	69,73,73	1.34	6 (8%)	82,113,113	1.95	19 (23%)
37	RRX	J	4002	-	42,42,42	5.02	24 (57%)	56,58,58	2.35	18 (32%)
51	P5S	8	806	-	35,36,53	1.20	3 (8%)	37,43,60	1.21	2 (5%)
24	CLA	5	605	-	50,54,73	1.60	7 (14%)	59,90,113	2.06	15 (25%)
41	CHL	3	611	-	49,63,74	1.59	9 (18%)	44,100,114	2.03	13 (29%)
24	CLA	9	607	-	51,55,73	1.59	8 (15%)	60,91,113	2.12	16 (26%)
24	CLA	H	1701	-	59,63,73	1.46	7 (11%)	70,101,113	2.16	17 (24%)
27	BCR	B	4001	-	41,41,41	1.62	4 (9%)	56,56,56	4.40	15 (26%)
24	CLA	A	1116	-	64,68,73	1.42	7 (10%)	76,107,113	1.93	19 (25%)
24	CLA	A	1111	-	69,73,73	1.36	7 (10%)	82,113,113	1.88	17 (20%)
24	CLA	A	1127	-	69,73,73	1.38	8 (11%)	82,113,113	1.80	16 (19%)
24	CLA	A	1104	-	69,73,73	1.35	7 (10%)	82,113,113	1.88	18 (21%)
27	BCR	3	504	-	41,41,41	1.62	4 (9%)	56,56,56	4.40	16 (28%)
24	CLA	5	602	-	56,60,73	1.51	6 (10%)	65,97,113	2.02	18 (27%)
24	CLA	3	602	-	50,54,73	1.59	8 (16%)	59,90,113	2.03	18 (30%)
24	CLA	5	606	-	54,58,73	1.54	7 (12%)	64,95,113	2.06	17 (26%)
24	CLA	4	603	-	60,64,73	1.44	7 (11%)	71,102,113	2.03	19 (26%)
34	LAP	F	5003	-	28,28,28	1.25	2 (7%)	33,35,35	0.99	1 (3%)
24	CLA	1	604	-	69,73,73	1.37	7 (10%)	82,113,113	1.82	18 (21%)
24	CLA	2	603	-	64,68,73	1.41	7 (10%)	76,107,113	1.98	21 (27%)
24	CLA	A	1106	-	69,73,73	1.36	6 (8%)	82,113,113	1.93	21 (25%)
31	LMT	1	804	-	36,36,36	1.14	5 (13%)	47,47,47	1.02	2 (4%)
23	CL0	A	1011	-	58,73,73	3.20	17 (29%)	60,113,113	2.88	18 (30%)
24	CLA	a	608	-	59,63,73	1.47	8 (13%)	70,101,113	2.00	19 (27%)
24	CLA	2	608	-	49,53,73	1.59	6 (12%)	58,89,113	2.06	16 (27%)
41	CHL	5	611	-	45,59,74	1.44	8 (17%)	40,96,114	2.03	12 (30%)
28	LHG	3	801	-	48,48,48	0.39	0	51,54,54	1.04	3 (5%)
24	CLA	A	1122	-	69,73,73	1.36	7 (10%)	82,113,113	1.90	20 (24%)
24	CLA	7	604	-	69,73,73	1.36	6 (8%)	82,113,113	1.89	21 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	LUT	7	501	-	42,43,43	2.49	1 (2%)	51,60,60	1.86	12 (23%)
43	QTB	a	504	-	19,19,19	2.50	4 (21%)	23,26,26	2.89	10 (43%)
26	SF4	C	3002	3	0,12,12	-	-	-		
24	CLA	A	1119	-	69,73,73	1.37	7 (10%)	82,113,113	1.72	18 (21%)
24	CLA	3	605	-	69,73,73	1.37	6 (8%)	82,113,113	1.86	19 (23%)
24	CLA	A	1103	-	69,73,73	1.33	6 (8%)	82,113,113	1.92	18 (21%)
24	CLA	B	1212	-	69,73,73	1.36	6 (8%)	82,113,113	1.90	19 (23%)
24	CLA	1	608	-	64,68,73	1.40	7 (10%)	76,107,113	1.95	18 (23%)
27	BCR	B	4002	-	41,41,41	1.61	4 (9%)	56,56,56	4.60	16 (28%)
24	CLA	a	607	-	62,66,73	1.43	8 (12%)	73,104,113	2.01	19 (26%)
24	CLA	A	1112	-	59,63,73	1.47	6 (10%)	70,101,113	2.03	20 (28%)
27	BCR	B	4007	-	41,41,41	1.60	4 (9%)	56,56,56	4.47	14 (25%)
24	CLA	9	608	-	49,53,73	1.60	7 (14%)	58,89,113	2.02	15 (25%)
35	SQD	G	5001	-	44,46,54	0.82	0	54,57,65	0.90	2 (3%)
28	LHG	F	5002	-	35,35,48	0.45	0	38,41,54	1.19	4 (10%)
24	CLA	8	611	-	54,58,73	1.51	6 (11%)	64,95,113	2.10	19 (29%)
24	CLA	7	612	-	64,68,73	1.41	7 (10%)	76,107,113	1.93	17 (22%)
24	CLA	6	607	-	59,63,73	1.47	7 (11%)	70,101,113	2.00	17 (24%)
24	CLA	9	612	-	69,73,73	1.36	7 (10%)	82,113,113	1.92	18 (21%)
41	CHL	4	618	16	50,64,74	1.64	9 (18%)	46,102,114	1.83	12 (26%)
28	LHG	9	802	-	48,48,48	0.39	0	51,54,54	1.11	4 (7%)
24	CLA	A	1129	-	54,58,73	1.56	8 (14%)	64,95,113	2.04	17 (26%)
24	CLA	6	609	18	69,73,73	1.36	6 (8%)	82,113,113	1.94	19 (23%)
24	CLA	a	602	-	54,58,73	1.54	7 (12%)	64,95,113	2.06	19 (29%)
24	CLA	2	612	-	54,58,73	1.52	6 (11%)	64,95,113	2.16	17 (26%)
24	CLA	A	1140	-	59,63,73	1.48	7 (11%)	70,101,113	1.93	17 (24%)
40	LUT	6	501	-	42,43,43	2.48	1 (2%)	51,60,60	3.21	21 (41%)
43	QTB	3	506	-	19,19,19	2.50	4 (21%)	23,26,26	2.91	10 (43%)
24	CLA	A	1109	24	69,73,73	1.34	7 (10%)	82,113,113	1.97	17 (20%)
40	LUT	4	502	-	42,43,43	2.42	1 (2%)	51,60,60	1.67	11 (21%)
24	CLA	B	1206	-	59,63,73	1.47	6 (10%)	70,101,113	2.02	17 (24%)
24	CLA	2	601	-	64,68,73	1.41	7 (10%)	76,107,113	4.16	23 (30%)
26	SF4	C	3003	3	0,12,12	-	-	-		
28	LHG	A	5001	24	28,28,48	0.49	0	31,34,54	1.25	3 (9%)
27	BCR	4	503	-	41,41,41	1.63	4 (9%)	56,56,56	4.47	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
44	GG0	a	805	-	7,8,8	1.37	2 (28%)	6,9,9	0.73	0
24	CLA	B	1223	-	69,73,73	1.37	8 (11%)	82,113,113	1.94	21 (25%)
24	CLA	A	1105	-	61,65,73	1.45	7 (11%)	72,103,113	1.99	18 (25%)
40	LUT	a	503	-	42,43,43	2.49	1 (2%)	51,60,60	2.33	11 (21%)
52	A8S	9	504	-	17,19,19	0.76	0	17,29,29	1.62	3 (17%)
24	CLA	1	610	-	49,53,73	1.61	6 (12%)	58,89,113	1.99	12 (20%)
24	CLA	8	615	-	50,54,73	1.60	7 (14%)	59,90,113	2.06	16 (27%)
27	BCR	J	4001	-	41,41,41	1.60	4 (9%)	56,56,56	4.44	15 (26%)
28	LHG	F	5001	-	42,42,48	0.42	0	45,48,54	1.12	3 (6%)
24	CLA	2	605	-	64,68,73	1.43	7 (10%)	76,107,113	1.93	20 (26%)
41	CHL	9	610	-	45,59,74	1.57	9 (20%)	40,96,114	2.00	12 (30%)
28	LHG	A	5002	-	48,48,48	0.39	0	51,54,54	1.00	2 (3%)
24	CLA	1	601	-	64,68,73	1.43	8 (12%)	76,107,113	1.97	21 (27%)
24	CLA	9	603	-	69,73,73	1.37	7 (10%)	82,113,113	1.98	19 (23%)
28	LHG	7	803	-	42,42,48	0.42	0	45,48,54	1.07	4 (8%)
24	CLA	A	1135	-	69,73,73	1.37	8 (11%)	82,113,113	1.90	19 (23%)
24	CLA	7	615	19	59,63,73	1.48	7 (11%)	70,101,113	1.94	16 (22%)
24	CLA	5	614	-	50,54,73	1.59	7 (14%)	59,90,113	2.06	16 (27%)
29	DGD	A	5005	-	52,52,67	0.95	3 (5%)	66,66,81	1.03	4 (6%)
24	CLA	a	611	-	54,58,73	1.54	7 (12%)	64,95,113	2.03	19 (29%)
24	CLA	2	615	-	61,65,73	1.43	7 (11%)	72,103,113	2.03	19 (26%)
24	CLA	2	610	-	50,54,73	1.59	8 (16%)	59,90,113	2.06	15 (25%)
45	PLM	4	803	-	15,16,17	0.40	0	14,15,17	0.90	0
41	CHL	6	613	-	45,59,74	1.29	7 (15%)	40,96,114	2.03	13 (32%)
24	CLA	5	603	-	60,64,73	1.45	6 (10%)	71,102,113	2.03	17 (23%)
45	PLM	6	804	-	17,17,17	0.59	0	17,17,17	1.10	1 (5%)
41	CHL	3	608	-	37,51,74	1.58	7 (18%)	30,86,114	2.40	11 (36%)
40	LUT	2	502	-	42,43,43	2.40	1 (2%)	51,60,60	2.17	14 (27%)
27	BCR	A	4004	-	41,41,41	1.63	4 (9%)	56,56,56	4.46	15 (26%)
24	CLA	a	612	-	61,65,73	1.44	7 (11%)	72,103,113	1.95	17 (23%)
24	CLA	A	1115	-	64,68,73	1.41	7 (10%)	76,107,113	1.97	20 (26%)
24	CLA	1	602	-	49,53,73	1.61	7 (14%)	58,89,113	2.04	16 (27%)
24	CLA	a	615	-	50,54,73	1.60	7 (14%)	59,90,113	2.01	14 (23%)
27	BCR	L	4001	-	41,41,41	1.60	4 (9%)	56,56,56	4.56	14 (25%)
24	CLA	9	602	-	50,54,73	1.59	7 (14%)	59,90,113	2.02	15 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
50	4RF	7	807	-	31,31,56	1.16	6 (19%)	34,34,59	1.28	3 (8%)
24	CLA	A	1101	-	69,73,73	1.34	6 (8%)	82,113,113	2.01	21 (25%)
27	BCR	G	4001	-	41,41,41	1.61	4 (9%)	56,56,56	4.44	13 (23%)
27	BCR	5	503	-	41,41,41	1.60	4 (9%)	56,56,56	4.54	13 (23%)
24	CLA	3	603	-	69,73,73	1.37	7 (10%)	82,113,113	1.88	17 (20%)
50	4RF	8	807	-	41,41,56	1.01	6 (14%)	44,44,59	1.09	3 (6%)
34	LAP	B	5007	-	28,28,28	1.26	2 (7%)	33,35,35	0.99	1 (3%)
28	LHG	A	5003	-	41,41,48	0.42	0	44,47,54	1.14	2 (4%)
27	BCR	I	4001	-	41,41,41	1.60	4 (9%)	56,56,56	4.42	19 (33%)
24	CLA	B	1224	-	69,73,73	1.37	7 (10%)	82,113,113	1.90	18 (21%)
24	CLA	2	602	-	56,60,73	1.50	7 (12%)	65,97,113	2.06	20 (30%)
28	LHG	6	802	-	36,36,48	0.45	0	39,42,54	1.16	3 (7%)
24	CLA	6	615	-	69,73,73	1.36	7 (10%)	82,113,113	1.90	18 (21%)
27	BCR	B	4006	-	41,41,41	1.61	4 (9%)	56,56,56	4.59	11 (19%)
46	DGA	8	803	-	29,29,43	1.31	2 (6%)	31,31,45	1.37	3 (9%)
24	CLA	A	1102	24	69,73,73	1.34	7 (10%)	82,113,113	1.94	21 (25%)
24	CLA	4	607	-	59,63,73	1.48	8 (13%)	70,101,113	2.04	18 (25%)
24	CLA	3	613	-	65,69,73	1.40	6 (9%)	77,108,113	1.90	17 (22%)
28	LHG	2	801	-	48,48,48	0.36	0	51,54,54	1.12	3 (5%)
26	SF4	A	3001	2,1	0,12,12	-	-	-	-	-
24	CLA	1	611	-	59,63,73	1.47	6 (10%)	70,101,113	2.01	17 (24%)
24	CLA	A	1132	-	69,73,73	1.34	6 (8%)	82,113,113	1.89	17 (20%)
24	CLA	a	601	-	64,68,73	1.40	7 (10%)	76,107,113	1.94	20 (26%)
27	BCR	B	4005	-	41,41,41	1.64	5 (12%)	56,56,56	4.65	13 (23%)
41	CHL	8	604	-	56,70,74	1.62	9 (16%)	53,109,114	1.84	13 (24%)
40	LUT	9	502	-	42,43,43	2.46	1 (2%)	51,60,60	1.93	14 (27%)
24	CLA	6	612	-	54,58,73	1.54	7 (12%)	64,95,113	2.05	17 (26%)
27	BCR	K	4002	-	41,41,41	1.60	4 (9%)	56,56,56	4.47	14 (25%)
41	CHL	8	613	-	45,59,74	1.58	9 (20%)	40,96,114	2.05	11 (27%)
24	CLA	B	1207	-	64,68,73	1.40	6 (9%)	76,107,113	1.89	18 (23%)
28	LHG	1	801	-	34,34,48	0.45	0	37,40,54	1.21	4 (10%)
24	CLA	B	1234	-	60,64,73	1.47	7 (11%)	71,102,113	1.99	19 (26%)
24	CLA	9	604	-	64,68,73	1.45	8 (12%)	76,107,113	1.96	19 (25%)
40	LUT	3	501	-	42,43,43	2.47	1 (2%)	51,60,60	1.92	18 (35%)
24	CLA	B	1216	-	65,69,73	1.41	6 (9%)	77,108,113	1.87	18 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	LUT	8	501	-	42,43,43	2.42	1 (2%)	51,60,60	1.83	15 (29%)
29	DGD	8	802	-	67,67,67	1.30	7 (10%)	81,81,81	1.07	2 (2%)
24	CLA	B	1022	-	69,73,73	1.37	6 (8%)	82,113,113	1.84	21 (25%)
31	LMT	B	5006	-	36,36,36	1.15	5 (13%)	47,47,47	0.98	1 (2%)
32	PCW	B	5004	-	29,29,53	1.40	5 (17%)	35,37,61	1.11	2 (5%)
24	CLA	4	611	-	60,64,73	1.44	6 (10%)	71,102,113	1.98	20 (28%)
28	LHG	9	801	-	32,32,48	0.46	0	35,38,54	1.17	3 (8%)
24	CLA	B	1217	-	60,64,73	1.46	8 (13%)	71,102,113	2.06	17 (23%)
24	CLA	2	609	21	59,63,73	1.47	7 (11%)	70,101,113	1.99	17 (24%)
27	BCR	A	4003	-	41,41,41	1.58	4 (9%)	56,56,56	4.67	17 (30%)
24	CLA	B	1210	-	69,73,73	1.38	6 (8%)	82,113,113	1.87	17 (20%)
27	BCR	3	503	-	41,41,41	1.63	5 (12%)	56,56,56	4.57	16 (28%)
24	CLA	A	1012	-	69,73,73	1.37	8 (11%)	82,113,113	1.85	19 (23%)
27	BCR	K	4001	-	41,41,41	1.60	4 (9%)	56,56,56	4.53	11 (19%)
24	CLA	7	601	-	64,68,73	1.41	7 (10%)	76,107,113	1.95	19 (25%)
24	CLA	A	1117	-	69,73,73	1.36	6 (8%)	82,113,113	1.87	16 (19%)
24	CLA	8	612	20	50,54,73	1.60	7 (14%)	59,90,113	1.98	12 (20%)
24	CLA	A	1121	-	61,65,73	1.45	7 (11%)	72,103,113	2.17	20 (27%)
24	CLA	K	1403	9	50,54,73	1.58	6 (12%)	59,90,113	2.06	15 (25%)
27	BCR	L	4002	-	41,41,41	1.61	4 (9%)	56,56,56	4.47	16 (28%)
24	CLA	3	601	-	69,73,73	1.38	6 (8%)	82,113,113	1.93	17 (20%)
24	CLA	B	1213	-	64,68,73	1.41	7 (10%)	76,107,113	1.97	19 (25%)
35	SQD	7	805	-	37,39,54	0.90	0	47,50,65	0.93	2 (4%)
24	CLA	B	1215	-	64,68,73	1.40	6 (9%)	76,107,113	1.87	16 (21%)
24	CLA	8	605	-	49,53,73	1.60	7 (14%)	58,89,113	2.05	17 (29%)
40	LUT	a	501	-	42,43,43	2.47	1 (2%)	51,60,60	1.92	14 (27%)
24	CLA	5	608	-	49,53,73	1.60	8 (16%)	58,89,113	2.18	16 (27%)
24	CLA	2	604	-	60,64,73	1.46	8 (13%)	71,102,113	2.12	20 (28%)
24	CLA	K	1402	-	64,68,73	1.40	7 (10%)	76,107,113	1.99	20 (26%)
24	CLA	8	608	-	56,60,73	1.48	6 (10%)	65,97,113	2.23	20 (30%)
24	CLA	A	1136	-	69,73,73	1.35	7 (10%)	82,113,113	1.86	19 (23%)
24	CLA	7	605	-	47,52,73	1.66	8 (17%)	55,88,113	1.94	12 (21%)
24	CLA	G	1603	-	49,53,73	1.61	7 (14%)	58,89,113	2.05	16 (27%)
24	CLA	A	1110	-	64,68,73	1.41	6 (9%)	76,107,113	1.90	16 (21%)
27	BCR	L	4003	-	41,41,41	1.61	4 (9%)	56,56,56	4.57	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	L	1502	-	64,68,73	1.41	6 (9%)	76,107,113	1.98	20 (26%)
24	CLA	6	603	-	69,73,73	1.34	7 (10%)	82,113,113	1.93	19 (23%)
24	CLA	7	608	-	46,50,73	1.66	6 (13%)	53,85,113	2.13	13 (24%)
24	CLA	4	617	-	49,53,73	1.60	7 (14%)	58,89,113	2.08	14 (24%)
33	PTY	B	5005	-	40,40,49	0.97	4 (10%)	43,45,54	1.19	2 (4%)
28	LHG	B	5002	-	48,48,48	0.40	0	51,54,54	1.03	3 (5%)
24	CLA	A	1113	-	56,60,73	1.50	6 (10%)	65,97,113	2.05	20 (30%)
24	CLA	A	1133	-	69,73,73	1.36	7 (10%)	82,113,113	1.80	16 (19%)
24	CLA	B	1023	-	69,73,73	1.36	6 (8%)	82,113,113	1.84	20 (24%)
24	CLA	B	1230	-	62,66,73	1.43	6 (9%)	73,104,113	1.98	18 (24%)
33	PTY	8	891	-	34,34,49	1.05	4 (11%)	37,39,54	1.16	2 (5%)
27	BCR	A	4005	-	41,41,41	1.59	4 (9%)	56,56,56	4.45	15 (26%)
24	CLA	A	1114	-	69,73,73	1.35	6 (8%)	82,113,113	1.92	18 (21%)
24	CLA	G	1602	-	50,54,73	1.60	7 (14%)	59,90,113	2.10	18 (30%)
27	BCR	7	503	-	41,41,41	1.60	4 (9%)	56,56,56	4.52	13 (23%)
24	CLA	a	605	-	69,73,73	1.36	7 (10%)	82,113,113	1.88	19 (23%)
24	CLA	5	616	-	50,54,73	1.60	8 (16%)	59,90,113	2.02	15 (25%)
24	CLA	7	607	-	63,67,73	1.42	7 (11%)	74,105,113	1.99	16 (21%)
24	CLA	7	611	-	64,68,73	1.39	6 (9%)	76,107,113	1.94	16 (21%)
40	LUT	1	502	-	42,43,43	2.41	1 (2%)	51,60,60	2.00	18 (35%)
40	LUT	a	502	-	42,43,43	2.39	1 (2%)	51,60,60	1.91	14 (27%)
41	CHL	1	613	-	42,56,74	1.38	7 (16%)	36,92,114	2.18	12 (33%)
24	CLA	F	1302	-	59,63,73	1.48	8 (13%)	70,101,113	1.97	17 (24%)
27	BCR	6	504	-	41,41,41	1.60	4 (9%)	56,56,56	4.53	14 (25%)
24	CLA	6	604	-	69,73,73	1.35	6 (8%)	82,113,113	1.92	19 (23%)
27	BCR	B	4004	-	41,41,41	1.59	4 (9%)	56,56,56	4.50	13 (23%)
41	CHL	6	610	-	50,64,74	1.47	8 (16%)	46,102,114	1.80	12 (26%)
24	CLA	6	605	-	50,54,73	1.58	6 (12%)	59,90,113	2.17	19 (32%)
24	CLA	8	610	-	59,63,73	1.48	6 (10%)	70,101,113	2.00	18 (25%)
33	PTY	7	804	-	32,32,49	1.06	4 (12%)	35,37,54	1.21	2 (5%)
41	CHL	4	613	-	46,60,74	1.72	8 (17%)	40,97,114	1.98	11 (27%)
24	CLA	1	603	-	69,73,73	1.35	7 (10%)	82,113,113	1.91	18 (21%)
28	LHG	6	801	-	48,48,48	0.40	0	51,54,54	1.07	3 (5%)
24	CLA	8	606	-	61,65,73	1.44	6 (9%)	72,103,113	1.96	16 (22%)
27	BCR	F	4001	-	41,41,41	1.54	4 (9%)	56,56,56	4.25	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	BCR	H	4001	-	41,41,41	1.60	4 (9%)	56,56,56	4.76	16 (28%)
24	CLA	B	1218	-	59,63,73	1.46	6 (10%)	70,101,113	2.11	21 (30%)
24	CLA	A	1107	1	59,63,73	1.47	6 (10%)	70,101,113	2.01	19 (27%)
24	CLA	8	618	-	64,68,73	1.41	6 (9%)	76,107,113	1.94	18 (23%)
24	CLA	6	602	-	56,60,73	1.51	7 (12%)	65,97,113	2.01	17 (26%)
28	LHG	1	802	-	41,41,48	0.42	0	44,47,54	1.09	4 (9%)
24	CLA	6	606	-	56,60,73	1.51	6 (10%)	65,97,113	2.06	18 (27%)
24	CLA	5	607	-	59,63,73	1.48	8 (13%)	70,101,113	2.01	19 (27%)
24	CLA	K	1401	-	50,54,73	1.59	7 (14%)	59,90,113	2.10	15 (25%)
24	CLA	1	615	14	50,54,73	1.59	8 (16%)	59,90,113	2.08	16 (27%)
24	CLA	3	607	-	69,73,73	1.36	8 (11%)	82,113,113	1.87	15 (18%)
28	LHG	5	801	-	48,48,48	0.39	0	51,54,54	1.08	4 (7%)
24	CLA	8	607	-	50,54,73	1.59	7 (14%)	59,90,113	2.05	15 (25%)
24	CLA	1	612	-	69,73,73	1.35	7 (10%)	82,113,113	1.86	17 (20%)
34	LAP	K	5001	-	28,28,28	1.24	2 (7%)	33,35,35	1.00	1 (3%)
24	CLA	B	1236	-	57,61,73	1.49	8 (14%)	67,98,113	1.98	17 (25%)
24	CLA	3	616	-	60,64,73	1.45	6 (10%)	71,102,113	2.01	20 (28%)
24	CLA	2	606	-	50,54,73	1.58	7 (14%)	59,90,113	2.05	15 (25%)
24	CLA	A	1134	1	64,68,73	1.40	7 (10%)	76,107,113	1.91	19 (25%)
24	CLA	8	602	-	56,60,73	1.52	7 (12%)	65,97,113	2.05	19 (29%)
24	CLA	B	1227	-	54,58,73	1.54	7 (12%)	64,95,113	2.04	16 (25%)
24	CLA	B	1226	-	69,73,73	1.41	7 (10%)	82,113,113	1.88	18 (21%)
24	CLA	B	1204	-	69,73,73	1.35	7 (10%)	82,113,113	1.96	20 (24%)
24	CLA	B	1211	-	59,63,73	1.47	8 (13%)	70,101,113	1.97	18 (25%)
24	CLA	6	601	-	64,68,73	1.41	7 (10%)	76,107,113	1.96	19 (25%)
24	CLA	4	601	-	64,68,73	1.41	7 (10%)	76,107,113	1.95	18 (23%)
24	CLA	7	617	19	58,62,73	1.49	7 (12%)	69,100,113	2.02	18 (26%)
24	CLA	2	613	-	45,49,73	1.67	7 (15%)	54,84,113	2.13	15 (27%)
24	CLA	B	1238	-	69,73,73	1.35	8 (11%)	82,113,113	1.90	19 (23%)
24	CLA	5	609	17	55,59,73	1.53	8 (14%)	64,96,113	2.08	19 (29%)
24	CLA	G	1601	-	54,58,73	1.54	8 (14%)	64,95,113	2.05	19 (29%)
41	CHL	a	609	-	47,61,74	1.35	7 (14%)	41,98,114	1.99	11 (26%)
24	CLA	8	609	20	64,68,73	1.40	6 (9%)	76,107,113	1.95	18 (23%)
24	CLA	2	621	-	54,58,73	1.55	8 (14%)	64,95,113	2.14	17 (26%)
46	DGA	5	803	-	22,22,43	1.46	3 (13%)	24,24,45	1.38	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	LHG	a	801	-	34,34,48	0.46	0	37,40,54	1.24	4 (10%)
24	CLA	A	1137	-	64,68,73	1.40	7 (10%)	76,107,113	1.99	22 (28%)
24	CLA	A	1128	-	69,73,73	1.39	6 (8%)	82,113,113	1.88	16 (19%)
24	CLA	B	1202	-	69,73,73	1.35	6 (8%)	82,113,113	1.86	18 (21%)
24	CLA	B	1219	-	63,67,73	1.44	7 (11%)	74,105,113	1.94	15 (20%)
41	CHL	6	611	-	45,59,74	1.53	8 (17%)	40,96,114	2.06	13 (32%)
24	CLA	B	1021	-	69,73,73	1.35	7 (10%)	82,113,113	1.86	17 (20%)
24	CLA	7	609	19	64,68,73	1.40	6 (9%)	76,107,113	2.05	20 (26%)
24	CLA	a	604	-	69,73,73	1.35	7 (10%)	82,113,113	1.87	20 (24%)
41	CHL	7	613	-	60,74,74	1.43	9 (15%)	58,114,114	1.63	10 (17%)
41	CHL	9	613	-	36,50,74	1.51	8 (22%)	29,85,114	2.30	10 (34%)
24	CLA	5	617	-	54,58,73	1.53	6 (11%)	64,95,113	2.05	19 (29%)
24	CLA	9	609	-	50,54,73	1.59	7 (14%)	59,90,113	2.01	13 (22%)
24	CLA	4	610	-	69,73,73	1.40	8 (11%)	82,113,113	1.86	18 (21%)
24	CLA	H	1703	-	59,63,73	1.47	6 (10%)	70,101,113	2.02	17 (24%)
24	CLA	4	608	-	55,59,73	1.52	7 (12%)	64,96,113	2.11	17 (26%)
24	CLA	4	615	16	64,68,73	1.42	7 (10%)	76,107,113	1.96	17 (22%)
24	CLA	5	612	-	69,73,73	1.35	6 (8%)	82,113,113	1.88	17 (20%)
47	SPH	6	806	-	19,20,20	0.65	0	18,21,21	1.13	1 (5%)
27	BCR	A	4002	-	41,41,41	1.61	4 (9%)	56,56,56	4.44	14 (25%)
24	CLA	A	1118	-	59,63,73	1.46	7 (11%)	70,101,113	1.99	18 (25%)
41	CHL	1	609	14	60,74,74	1.10	7 (11%)	58,114,114	1.90	13 (22%)
24	CLA	1	606	-	61,65,73	1.44	7 (11%)	72,103,113	1.94	15 (20%)
24	CLA	9	601	-	64,68,73	1.42	8 (12%)	76,107,113	1.96	19 (25%)
27	BCR	B	4003	-	41,41,41	1.60	4 (9%)	56,56,56	4.61	17 (30%)
40	LUT	5	502	-	42,43,43	2.47	2 (4%)	51,60,60	2.02	18 (35%)
40	LUT	3	502	-	42,43,43	2.43	1 (2%)	51,60,60	1.85	15 (29%)
24	CLA	J	1901	8	46,50,73	1.65	8 (17%)	53,85,113	2.12	16 (30%)
24	CLA	A	1138	-	69,73,73	1.35	6 (8%)	82,113,113	1.83	15 (18%)
40	LUT	8	502	-	42,43,43	2.41	1 (2%)	51,60,60	1.77	13 (25%)
41	CHL	5	613	-	50,64,74	1.34	7 (14%)	46,102,114	1.97	12 (26%)
24	CLA	8	603	-	69,73,73	1.35	7 (10%)	82,113,113	1.91	18 (21%)
32	PCW	6	803	-	35,35,53	1.32	4 (11%)	41,43,61	1.14	2 (4%)
24	CLA	A	1131	-	69,73,73	1.36	7 (10%)	82,113,113	1.89	16 (19%)
24	CLA	4	616	-	54,58,73	1.54	8 (14%)	64,95,113	2.10	20 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	A	1126	-	69,73,73	1.36	7 (10%)	82,113,113	1.90	17 (20%)
40	LUT	2	501	-	42,43,43	2.45	1 (2%)	51,60,60	2.00	13 (25%)
25	PQN	B	2002	-	34,34,34	0.38	0	43,45,45	1.17	4 (9%)
40	LUT	4	501	-	42,43,43	2.45	1 (2%)	51,60,60	2.12	14 (27%)
24	CLA	B	1225	-	69,73,73	1.37	7 (10%)	82,113,113	1.79	14 (17%)
25	PQN	A	2001	-	34,34,34	0.40	0	43,45,45	1.13	3 (6%)
31	LMT	2	804	-	36,36,36	1.14	6 (16%)	47,47,47	0.99	2 (4%)
24	CLA	B	1209	-	69,73,73	1.34	6 (8%)	82,113,113	1.89	18 (21%)
24	CLA	B	1228	-	69,73,73	1.36	6 (8%)	82,113,113	1.82	19 (23%)
24	CLA	B	1229	-	69,73,73	1.34	7 (10%)	82,113,113	1.92	22 (26%)
24	CLA	5	601	-	64,68,73	1.43	7 (10%)	76,107,113	2.00	24 (31%)
50	4RF	8	808	-	53,53,56	0.90	6 (11%)	56,56,59	0.95	3 (5%)
24	CLA	5	604	-	69,73,73	1.38	7 (10%)	82,113,113	1.90	18 (21%)
24	CLA	3	604	-	64,68,73	1.39	7 (10%)	76,107,113	1.95	21 (27%)
40	LUT	5	505	-	42,43,43	2.50	2 (4%)	51,60,60	2.32	16 (31%)
24	CLA	A	1141	28	49,53,73	1.60	8 (16%)	58,89,113	2.07	14 (24%)
24	CLA	A	1123	-	69,73,73	1.38	7 (10%)	82,113,113	1.93	16 (19%)
24	CLA	4	602	-	56,60,73	1.52	7 (12%)	65,97,113	2.05	19 (29%)
24	CLA	6	618	-	50,54,73	1.59	7 (14%)	59,90,113	2.01	14 (23%)
28	LHG	4	802	-	31,31,48	0.48	0	34,37,54	1.15	3 (8%)
24	CLA	B	1214	-	66,70,73	1.39	7 (10%)	78,109,113	1.90	18 (23%)
31	LMT	A	5008	-	36,36,36	1.09	4 (11%)	47,47,47	1.03	3 (6%)
35	SQD	H	5001	-	43,45,54	0.84	1 (2%)	53,56,65	0.90	2 (3%)
24	CLA	a	603	-	69,73,73	1.35	7 (10%)	82,113,113	1.94	19 (23%)
49	C7Z	7	504	-	43,43,43	5.45	26 (60%)	56,60,60	2.78	18 (32%)
24	CLA	4	605	-	50,54,73	1.61	8 (16%)	59,90,113	2.02	14 (23%)
41	CHL	8	601	-	55,69,74	1.67	9 (16%)	52,108,114	1.82	12 (23%)
39	ECH	M	4001	-	42,42,42	0.89	3 (7%)	55,58,58	2.23	13 (23%)
28	LHG	2	802	-	48,48,48	0.39	0	51,54,54	1.07	3 (5%)
33	PTY	5	802	-	37,37,49	1.00	4 (10%)	40,42,54	1.11	2 (5%)
24	CLA	B	1231	-	69,73,73	1.35	7 (10%)	82,113,113	1.86	16 (19%)
24	CLA	B	1222	-	62,66,73	1.44	7 (11%)	73,104,113	1.99	21 (28%)
40	LUT	9	501	-	42,43,43	2.43	1 (2%)	51,60,60	1.92	13 (25%)
24	CLA	7	610	-	59,63,73	1.49	9 (15%)	70,101,113	2.02	17 (24%)
41	CHL	6	619	18	60,74,74	1.62	8 (13%)	58,114,114	1.61	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	A	1139	-	59,63,73	1.47	7 (11%)	70,101,113	1.98	18 (25%)
24	CLA	4	604	-	64,68,73	1.41	7 (10%)	76,107,113	1.93	21 (27%)
24	CLA	4	606	-	54,58,73	1.53	7 (12%)	64,95,113	2.06	19 (29%)
40	LUT	1	501	-	42,43,43	2.44	1 (2%)	51,60,60	1.97	16 (31%)
24	CLA	3	612	-	69,73,73	1.36	6 (8%)	82,113,113	1.84	15 (18%)
48	XAT	7	502	-	41,47,47	0.68	1 (2%)	54,74,74	1.84	11 (20%)
24	CLA	H	1702	-	50,54,73	1.59	8 (16%)	59,90,113	2.10	14 (23%)
24	CLA	7	606	-	59,63,73	1.46	7 (11%)	70,101,113	2.00	18 (25%)
41	CHL	a	610	-	42,56,74	1.42	7 (16%)	36,92,114	2.01	11 (30%)
40	LUT	5	501	-	42,43,43	2.45	1 (2%)	51,60,60	1.86	15 (29%)
24	CLA	B	1203	-	69,73,73	1.36	7 (10%)	82,113,113	1.82	18 (21%)
24	CLA	7	603	-	69,73,73	1.35	7 (10%)	82,113,113	1.90	18 (21%)
24	CLA	2	607	-	50,54,73	1.59	8 (16%)	59,90,113	2.02	13 (22%)
42	OLA	1	803	-	19,19,19	0.58	0	19,19,19	1.02	1 (5%)
27	BCR	3	505	-	41,41,41	1.60	4 (9%)	56,56,56	4.50	14 (25%)
24	CLA	L	1503	-	49,53,73	1.61	8 (16%)	58,89,113	2.05	14 (24%)
24	CLA	B	1235	-	69,73,73	1.35	7 (10%)	82,113,113	1.96	19 (23%)
24	CLA	B	1205	-	69,73,73	1.34	7 (10%)	82,113,113	1.98	18 (21%)
24	CLA	B	1201	-	69,73,73	1.35	7 (10%)	82,113,113	1.91	22 (26%)
30	3PH	A	5007	-	32,32,47	1.04	4 (12%)	35,37,52	1.24	2 (5%)
24	CLA	6	608	-	49,53,73	1.60	8 (16%)	58,89,113	2.07	15 (25%)
24	CLA	A	1125	-	69,73,73	1.38	6 (8%)	82,113,113	1.93	22 (26%)
24	CLA	B	1239	-	69,73,73	1.34	6 (8%)	82,113,113	1.92	21 (25%)
27	BCR	8	503	-	41,41,41	1.60	4 (9%)	56,56,56	4.57	14 (25%)
33	PTY	9	803	-	47,47,49	0.90	4 (8%)	50,52,54	1.11	2 (4%)
33	PTY	3	802	-	37,37,49	1.01	4 (10%)	40,42,54	1.09	2 (5%)
24	CLA	B	1221	-	69,73,73	1.38	9 (13%)	82,113,113	1.89	16 (19%)
42	OLA	8	809	-	19,19,19	0.58	0	19,19,19	1.02	0
24	CLA	3	606	-	69,73,73	1.36	6 (8%)	82,113,113	1.87	15 (18%)
24	CLA	A	1013	-	69,73,73	1.36	7 (10%)	82,113,113	1.78	18 (21%)
28	LHG	B	5001	-	45,45,48	0.40	0	48,51,54	1.08	3 (6%)
24	CLA	5	618	17	56,60,73	1.51	8 (14%)	65,97,113	2.04	19 (29%)
24	CLA	F	1301	-	54,58,73	1.53	7 (12%)	64,95,113	2.09	19 (29%)
28	LHG	8	801	-	36,36,48	0.44	0	39,42,54	1.17	3 (7%)
41	CHL	a	613	-	40,54,74	1.51	7 (17%)	34,90,114	2.16	11 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	B	1232	-	49,53,73	1.60	7 (14%)	58,89,113	2.05	16 (27%)
36	ERG	G	5002	-	32,32,32	8.13	20 (62%)	45,50,50	3.79	18 (40%)
24	CLA	4	612	-	66,70,73	1.38	7 (10%)	78,109,113	1.99	19 (24%)

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
28	LHG	7	802	-	-	19/40/40/53	-
38	LPX	a	804	-	-	7/31/31/31	-
28	LHG	4	801	-	-	27/53/53/53	-
27	BCR	5	504	-	-	11/29/63/63	0/2/2/2
29	DGD	B	5003	-	-	16/55/95/95	0/2/2/2
27	BCR	A	4001	-	-	13/29/63/63	0/2/2/2
28	LHG	7	801	-	-	24/53/53/53	-
24	CLA	8	620	20	1/1/15/20	15/39/115/115	-
24	CLA	B	1220	-	1/1/14/20	19/33/109/115	-
24	CLA	A	1130	-	1/1/13/20	12/29/105/115	-
41	CHL	4	609	16	4/4/20/26	7/39/137/137	-
40	LUT	1	503	-	1/1/12/27	4/29/67/67	0/2/2/2
38	LPX	J	5001	-	-	10/18/18/31	-
41	CHL	5	610	-	4/4/20/26	9/39/137/137	-
24	CLA	A	1124	-	1/1/13/20	7/27/103/115	-
24	CLA	B	1237	-	1/1/15/20	18/39/115/115	-
24	CLA	9	605	-	1/1/14/20	16/33/109/115	-
41	CHL	a	606	-	4/4/18/26	4/27/125/137	-
40	LUT	6	502	-	1/1/12/27	7/29/67/67	0/2/2/2
24	CLA	3	610	15	1/1/14/20	13/33/109/115	-
24	CLA	B	1208	-	1/1/14/20	15/33/109/115	-
24	CLA	6	617	-	1/1/11/20	7/15/91/115	-
24	CLA	L	1501	13	1/1/12/20	10/21/97/115	-
24	CLA	B	1240	-	1/1/15/20	12/39/115/115	-
24	CLA	A	1120	-	1/1/11/20	10/20/96/115	-
24	CLA	K	1404	-	1/1/12/20	10/24/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	1	607	-	1/1/15/20	7/39/115/115	-
27	BCR	6	503	-	-	12/29/63/63	0/2/2/2
24	CLA	1	605	-	1/1/15/20	18/39/115/115	-
24	CLA	7	602	-	1/1/10/20	6/14/90/115	-
24	CLA	3	618	-	1/1/11/20	8/17/93/115	-
24	CLA	9	606	-	1/1/13/20	7/27/103/115	-
24	CLA	A	1108	-	1/1/15/20	17/39/115/115	-
37	RRX	J	4002	-	1/1/11/25	9/29/65/65	0/2/2/2
51	P5S	8	806	-	-	15/42/42/59	-
24	CLA	5	605	-	1/1/11/20	6/17/93/115	-
41	CHL	3	611	-	3/3/17/26	7/26/124/137	-
24	CLA	9	607	-	1/1/11/20	11/18/94/115	-
24	CLA	H	1701	-	1/1/13/20	12/27/103/115	-
27	BCR	B	4001	-	-	10/29/63/63	0/2/2/2
24	CLA	A	1116	-	1/1/14/20	16/33/109/115	-
24	CLA	A	1111	-	1/1/15/20	19/39/115/115	-
24	CLA	A	1127	-	1/1/15/20	14/39/115/115	-
24	CLA	A	1104	-	1/1/15/20	17/39/115/115	-
27	BCR	3	504	-	-	12/29/63/63	0/2/2/2
24	CLA	5	602	-	1/1/12/20	9/24/100/115	-
24	CLA	3	602	-	1/1/11/20	5/17/93/115	-
24	CLA	5	606	-	1/1/12/20	5/21/97/115	-
24	CLA	4	603	-	1/1/13/20	12/29/105/115	-
34	LAP	F	5003	-	-	15/30/30/30	-
24	CLA	1	604	-	1/1/15/20	22/39/115/115	-
24	CLA	2	603	-	1/1/14/20	14/33/109/115	-
24	CLA	A	1106	-	1/1/15/20	13/39/115/115	-
31	LMT	1	804	-	-	8/21/61/61	0/2/2/2
23	CL0	A	1011	-	3/3/20/25	9/37/135/135	-
24	CLA	a	608	-	1/1/13/20	13/27/103/115	-
24	CLA	2	608	-	1/1/11/20	5/15/91/115	-
41	CHL	5	611	-	3/3/17/26	3/21/119/137	-
28	LHG	3	801	-	-	31/53/53/53	-
24	CLA	A	1122	-	1/1/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	7	604	-	1/1/15/20	14/39/115/115	-
40	LUT	7	501	-	1/1/12/27	6/29/67/67	0/2/2/2
43	QTB	a	504	-	1/1/5/10	4/11/28/28	0/1/1/1
26	SF4	C	3002	3	-	-	0/6/5/5
24	CLA	A	1119	-	1/1/15/20	17/39/115/115	-
24	CLA	3	605	-	1/1/15/20	17/39/115/115	-
24	CLA	A	1103	-	1/1/15/20	22/39/115/115	-
24	CLA	B	1212	-	1/1/15/20	21/39/115/115	-
24	CLA	1	608	-	1/1/14/20	13/33/109/115	-
27	BCR	B	4002	-	-	13/29/63/63	0/2/2/2
24	CLA	a	607	-	1/1/13/20	15/31/107/115	-
24	CLA	A	1112	-	1/1/13/20	15/27/103/115	-
27	BCR	B	4007	-	-	12/29/63/63	0/2/2/2
24	CLA	9	608	-	1/1/11/20	6/15/91/115	-
35	SQD	G	5001	-	-	16/41/61/69	0/1/1/1
28	LHG	F	5002	-	-	25/40/40/53	-
24	CLA	8	611	-	1/1/12/20	8/21/97/115	-
24	CLA	7	612	-	1/1/14/20	11/33/109/115	-
24	CLA	6	607	-	1/1/13/20	12/27/103/115	-
24	CLA	9	612	-	1/1/15/20	17/39/115/115	-
41	CHL	4	618	16	4/4/18/26	5/27/125/137	-
28	LHG	9	802	-	-	30/53/53/53	-
24	CLA	A	1129	-	1/1/12/20	10/21/97/115	-
24	CLA	6	609	18	1/1/15/20	17/39/115/115	-
24	CLA	a	602	-	1/1/12/20	9/21/97/115	-
24	CLA	2	612	-	1/1/12/20	8/21/97/115	-
24	CLA	A	1140	-	1/1/13/20	7/27/103/115	-
40	LUT	6	501	-	1/1/12/27	8/29/67/67	0/2/2/2
43	QTB	3	506	-	2/2/5/10	1/11/28/28	0/1/1/1
24	CLA	A	1109	24	1/1/15/20	17/39/115/115	-
40	LUT	4	502	-	-	3/29/67/67	0/2/2/2
24	CLA	B	1206	-	1/1/13/20	13/27/103/115	-
24	CLA	2	601	-	1/1/14/20	14/33/109/115	-
28	LHG	A	5001	24	-	14/33/33/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	SF4	C	3003	3	-	-	0/6/5/5
27	BCR	4	503	-	-	13/29/63/63	0/2/2/2
44	GG0	a	805	-	-	2/7/7/7	-
24	CLA	B	1223	-	1/1/15/20	19/39/115/115	-
24	CLA	A	1105	-	1/1/13/20	11/30/106/115	-
40	LUT	a	503	-	-	5/29/67/67	0/2/2/2
52	A8S	9	504	-	-	2/10/34/34	0/1/1/1
24	CLA	1	610	-	1/1/11/20	7/15/91/115	-
24	CLA	8	615	-	1/1/11/20	7/17/93/115	-
27	BCR	J	4001	-	-	10/29/63/63	0/2/2/2
28	LHG	F	5001	-	-	22/47/47/53	-
24	CLA	2	605	-	1/1/14/20	15/33/109/115	-
41	CHL	9	610	-	3/3/17/26	4/21/119/137	-
28	LHG	A	5002	-	-	32/53/53/53	-
24	CLA	1	601	-	1/1/14/20	8/33/109/115	-
24	CLA	9	603	-	1/1/15/20	15/39/115/115	-
28	LHG	7	803	-	-	22/47/47/53	-
24	CLA	A	1135	-	1/1/15/20	20/39/115/115	-
24	CLA	7	615	19	1/1/13/20	11/27/103/115	-
24	CLA	5	614	-	1/1/11/20	6/17/93/115	-
29	DGD	A	5005	-	-	13/40/80/95	0/2/2/2
24	CLA	a	611	-	1/1/12/20	10/21/97/115	-
24	CLA	2	615	-	1/1/13/20	15/30/106/115	-
24	CLA	2	610	-	1/1/11/20	9/17/93/115	-
45	PLM	4	803	-	-	2/14/14/15	-
41	CHL	6	613	-	3/3/17/26	2/21/119/137	-
24	CLA	5	603	-	1/1/13/20	18/29/105/115	-
45	PLM	6	804	-	-	4/15/15/15	-
41	CHL	3	608	-	3/3/15/26	4/12/110/137	-
40	LUT	2	502	-	-	3/29/67/67	0/2/2/2
27	BCR	A	4004	-	-	11/29/63/63	0/2/2/2
24	CLA	a	612	-	1/1/13/20	10/30/106/115	-
24	CLA	A	1115	-	1/1/14/20	18/33/109/115	-
24	CLA	1	602	-	1/1/11/20	9/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	a	615	-	1/1/11/20	6/17/93/115	-
27	BCR	L	4001	-	-	12/29/63/63	0/2/2/2
24	CLA	9	602	-	1/1/11/20	6/17/93/115	-
50	4RF	7	807	-	-	10/34/34/59	-
24	CLA	A	1101	-	1/1/15/20	15/39/115/115	-
27	BCR	G	4001	-	-	14/29/63/63	0/2/2/2
27	BCR	5	503	-	-	13/29/63/63	0/2/2/2
24	CLA	3	603	-	1/1/15/20	11/39/115/115	-
50	4RF	8	807	-	-	24/44/44/59	-
34	LAP	B	5007	-	-	14/30/30/30	-
28	LHG	A	5003	-	-	22/46/46/53	-
27	BCR	I	4001	-	-	12/29/63/63	0/2/2/2
24	CLA	B	1224	-	1/1/15/20	21/39/115/115	-
24	CLA	2	602	-	1/1/12/20	9/24/100/115	-
28	LHG	6	802	-	-	22/41/41/53	-
24	CLA	6	615	-	1/1/15/20	18/39/115/115	-
27	BCR	B	4006	-	-	11/29/63/63	0/2/2/2
46	DGA	8	803	-	-	17/31/31/45	-
24	CLA	A	1102	24	1/1/15/20	17/39/115/115	-
24	CLA	4	607	-	1/1/13/20	12/27/103/115	-
24	CLA	3	613	-	1/1/14/20	11/35/111/115	-
28	LHG	2	801	-	-	33/53/53/53	-
26	SF4	A	3001	2,1	-	-	0/6/5/5
24	CLA	1	611	-	1/1/13/20	10/27/103/115	-
24	CLA	A	1132	-	1/1/15/20	15/39/115/115	-
24	CLA	a	601	-	1/1/14/20	11/33/109/115	-
27	BCR	B	4005	-	-	10/29/63/63	0/2/2/2
41	CHL	8	604	-	4/4/19/26	13/35/133/137	-
40	LUT	9	502	-	1/1/12/27	7/29/67/67	0/2/2/2
24	CLA	6	612	-	1/1/12/20	9/21/97/115	-
27	BCR	K	4002	-	-	12/29/63/63	0/2/2/2
41	CHL	8	613	-	3/3/17/26	2/21/119/137	-
24	CLA	B	1207	-	1/1/14/20	13/33/109/115	-
28	LHG	1	801	-	-	24/39/39/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	1234	-	1/1/13/20	9/29/105/115	-
24	CLA	9	604	-	1/1/14/20	9/33/109/115	-
40	LUT	3	501	-	-	3/29/67/67	0/2/2/2
24	CLA	B	1216	-	1/1/14/20	18/35/111/115	-
40	LUT	8	501	-	-	3/29/67/67	0/2/2/2
29	DGD	8	802	-	-	19/55/95/95	0/2/2/2
24	CLA	B	1022	-	1/1/15/20	12/39/115/115	-
31	LMT	B	5006	-	-	15/21/61/61	0/2/2/2
32	PCW	B	5004	-	-	19/33/33/57	-
24	CLA	4	611	-	1/1/13/20	9/29/105/115	-
28	LHG	9	801	-	-	20/37/37/53	-
24	CLA	B	1217	-	1/1/13/20	14/29/105/115	-
24	CLA	2	609	21	1/1/13/20	7/27/103/115	-
27	BCR	A	4003	-	-	11/29/63/63	0/2/2/2
24	CLA	B	1210	-	1/1/15/20	19/39/115/115	-
27	BCR	3	503	-	-	12/29/63/63	0/2/2/2
24	CLA	A	1012	-	1/1/15/20	13/39/115/115	-
27	BCR	K	4001	-	-	10/29/63/63	0/2/2/2
24	CLA	7	601	-	1/1/14/20	14/33/109/115	-
24	CLA	A	1117	-	1/1/15/20	21/39/115/115	-
24	CLA	8	612	20	1/1/11/20	11/17/93/115	-
24	CLA	A	1121	-	1/1/13/20	15/30/106/115	-
24	CLA	K	1403	9	1/1/11/20	9/17/93/115	-
27	BCR	L	4002	-	-	7/29/63/63	0/2/2/2
24	CLA	3	601	-	1/1/15/20	15/39/115/115	-
24	CLA	B	1213	-	1/1/14/20	11/33/109/115	-
35	SQD	7	805	-	-	15/34/54/69	0/1/1/1
24	CLA	B	1215	-	1/1/14/20	18/33/109/115	-
24	CLA	8	605	-	1/1/11/20	6/15/91/115	-
40	LUT	a	501	-	-	8/29/67/67	0/2/2/2
24	CLA	5	608	-	1/1/11/20	8/15/91/115	-
24	CLA	2	604	-	1/1/13/20	16/29/105/115	-
24	CLA	K	1402	-	1/1/14/20	15/33/109/115	-
24	CLA	8	608	-	1/1/12/20	11/24/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	1136	-	1/1/15/20	18/39/115/115	-
24	CLA	7	605	-	1/1/11/20	2/13/89/115	-
24	CLA	G	1603	-	1/1/11/20	5/15/91/115	-
24	CLA	A	1110	-	1/1/14/20	13/33/109/115	-
27	BCR	L	4003	-	-	12/29/63/63	0/2/2/2
24	CLA	L	1502	-	1/1/14/20	15/33/109/115	-
24	CLA	6	603	-	1/1/15/20	14/39/115/115	-
24	CLA	7	608	-	1/1/10/20	5/12/88/115	-
24	CLA	4	617	-	1/1/11/20	8/15/91/115	-
33	PTY	B	5005	-	-	25/44/44/53	-
28	LHG	B	5002	-	-	26/53/53/53	-
24	CLA	A	1113	-	1/1/12/20	6/24/100/115	-
24	CLA	A	1133	-	1/1/15/20	18/39/115/115	-
24	CLA	B	1023	-	1/1/15/20	11/39/115/115	-
24	CLA	B	1230	-	1/1/13/20	15/31/107/115	-
33	PTY	8	891	-	-	14/38/38/53	-
27	BCR	A	4005	-	-	13/29/63/63	0/2/2/2
24	CLA	A	1114	-	1/1/15/20	15/39/115/115	-
24	CLA	G	1602	-	1/1/11/20	10/17/93/115	-
27	BCR	7	503	-	-	10/29/63/63	0/2/2/2
24	CLA	a	605	-	1/1/15/20	18/39/115/115	-
24	CLA	5	616	-	1/1/11/20	9/17/93/115	-
24	CLA	7	607	-	1/1/13/20	16/31/107/115	-
24	CLA	7	611	-	1/1/14/20	11/33/109/115	-
40	LUT	1	502	-	-	1/29/67/67	0/2/2/2
40	LUT	a	502	-	-	1/29/67/67	0/2/2/2
41	CHL	1	613	-	3/3/16/26	4/18/116/137	-
24	CLA	F	1302	-	1/1/13/20	10/27/103/115	-
27	BCR	6	504	-	-	9/29/63/63	0/2/2/2
24	CLA	6	604	-	1/1/15/20	15/39/115/115	-
27	BCR	B	4004	-	-	12/29/63/63	0/2/2/2
41	CHL	6	610	-	4/4/18/26	4/27/125/137	-
24	CLA	6	605	-	1/1/11/20	5/17/93/115	-
24	CLA	8	610	-	1/1/13/20	16/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	PTY	7	804	-	-	15/36/36/53	-
41	CHL	4	613	-	3/3/17/26	1/23/121/137	-
24	CLA	1	603	-	1/1/15/20	18/39/115/115	-
28	LHG	6	801	-	-	28/53/53/53	-
24	CLA	8	606	-	1/1/13/20	16/30/106/115	-
27	BCR	F	4001	-	-	14/29/63/63	0/2/2/2
27	BCR	H	4001	-	-	10/29/63/63	0/2/2/2
24	CLA	B	1218	-	1/1/13/20	11/27/103/115	-
24	CLA	A	1107	1	1/1/13/20	10/27/103/115	-
24	CLA	8	618	-	1/1/14/20	15/33/109/115	-
24	CLA	6	602	-	1/1/12/20	6/24/100/115	-
24	CLA	6	606	-	1/1/12/20	11/24/100/115	-
28	LHG	1	802	-	-	28/46/46/53	-
24	CLA	5	607	-	1/1/13/20	10/27/103/115	-
24	CLA	K	1401	-	1/1/11/20	6/17/93/115	-
24	CLA	1	615	14	1/1/11/20	8/17/93/115	-
24	CLA	3	607	-	1/1/15/20	16/39/115/115	-
28	LHG	5	801	-	-	25/53/53/53	-
24	CLA	8	607	-	1/1/11/20	4/17/93/115	-
24	CLA	1	612	-	1/1/15/20	22/39/115/115	-
34	LAP	K	5001	-	-	10/30/30/30	-
24	CLA	B	1236	-	1/1/12/20	9/25/101/115	-
24	CLA	3	616	-	1/1/13/20	13/29/105/115	-
24	CLA	2	606	-	1/1/11/20	10/17/93/115	-
24	CLA	A	1134	1	1/1/14/20	17/33/109/115	-
24	CLA	8	602	-	1/1/12/20	11/24/100/115	-
24	CLA	B	1227	-	1/1/12/20	8/21/97/115	-
24	CLA	B	1226	-	1/1/15/20	14/39/115/115	-
24	CLA	B	1204	-	1/1/15/20	18/39/115/115	-
24	CLA	B	1211	-	1/1/13/20	14/27/103/115	-
24	CLA	6	601	-	1/1/14/20	17/33/109/115	-
24	CLA	4	601	-	1/1/14/20	8/33/109/115	-
24	CLA	7	617	19	1/1/13/20	14/25/101/115	-
24	CLA	2	613	-	1/1/10/20	4/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	1238	-	1/1/15/20	13/39/115/115	-
24	CLA	5	609	17	1/1/12/20	11/23/99/115	-
24	CLA	G	1601	-	1/1/12/20	10/21/97/115	-
41	CHL	a	609	-	3/3/17/26	4/24/122/137	-
24	CLA	8	609	20	1/1/14/20	19/33/109/115	-
24	CLA	2	621	-	1/1/12/20	10/21/97/115	-
46	DGA	5	803	-	-	12/24/24/45	-
28	LHG	a	801	-	-	21/39/39/53	-
24	CLA	A	1137	-	1/1/14/20	13/33/109/115	-
24	CLA	A	1128	-	1/1/15/20	14/39/115/115	-
24	CLA	B	1202	-	1/1/15/20	17/39/115/115	-
41	CHL	6	611	-	3/3/17/26	1/21/119/137	-
24	CLA	B	1219	-	1/1/13/20	9/32/108/115	-
24	CLA	B	1021	-	1/1/15/20	17/39/115/115	-
24	CLA	7	609	19	1/1/14/20	14/33/109/115	-
24	CLA	a	604	-	1/1/15/20	19/39/115/115	-
41	CHL	7	613	-	4/4/20/26	5/39/137/137	-
41	CHL	9	613	-	3/3/15/26	0/10/108/137	-
24	CLA	5	617	-	1/1/12/20	9/21/97/115	-
24	CLA	9	609	-	1/1/11/20	8/17/93/115	-
24	CLA	4	610	-	1/1/15/20	25/39/115/115	-
24	CLA	H	1703	-	1/1/13/20	10/27/103/115	-
24	CLA	4	608	-	1/1/12/20	4/23/99/115	-
24	CLA	4	615	16	1/1/14/20	16/33/109/115	-
24	CLA	5	612	-	1/1/15/20	14/39/115/115	-
47	SPH	6	806	-	-	7/21/21/21	-
27	BCR	A	4002	-	-	8/29/63/63	0/2/2/2
24	CLA	A	1118	-	1/1/13/20	14/27/103/115	-
41	CHL	1	609	14	4/4/20/26	8/39/137/137	-
24	CLA	1	606	-	1/1/13/20	15/30/106/115	-
24	CLA	9	601	-	1/1/14/20	14/33/109/115	-
27	BCR	B	4003	-	-	10/29/63/63	0/2/2/2
40	LUT	5	502	-	-	5/29/67/67	0/2/2/2
40	LUT	3	502	-	-	1/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	J	1901	8	1/1/10/20	5/12/88/115	-
24	CLA	A	1138	-	1/1/15/20	10/39/115/115	-
41	CHL	5	613	-	4/4/18/26	1/27/125/137	-
40	LUT	8	502	-	-	1/29/67/67	0/2/2/2
24	CLA	8	603	-	1/1/15/20	17/39/115/115	-
32	PCW	6	803	-	-	15/39/39/57	-
24	CLA	A	1131	-	1/1/15/20	16/39/115/115	-
24	CLA	4	616	-	1/1/12/20	8/21/97/115	-
24	CLA	A	1126	-	1/1/15/20	22/39/115/115	-
40	LUT	2	501	-	-	1/29/67/67	0/2/2/2
25	PQN	B	2002	-	-	3/23/43/43	0/2/2/2
40	LUT	4	501	-	-	2/29/67/67	0/2/2/2
24	CLA	B	1225	-	1/1/15/20	7/39/115/115	-
25	PQN	A	2001	-	-	8/23/43/43	0/2/2/2
31	LMT	2	804	-	-	7/21/61/61	0/2/2/2
24	CLA	B	1209	-	1/1/15/20	16/39/115/115	-
24	CLA	B	1228	-	1/1/15/20	15/39/115/115	-
24	CLA	B	1229	-	1/1/15/20	13/39/115/115	-
24	CLA	5	601	-	1/1/14/20	13/33/109/115	-
50	4RF	8	808	-	-	24/56/56/59	-
24	CLA	5	604	-	1/1/15/20	14/39/115/115	-
24	CLA	3	604	-	1/1/14/20	11/33/109/115	-
40	LUT	5	505	-	-	7/29/67/67	0/2/2/2
24	CLA	A	1141	28	1/1/11/20	10/15/91/115	-
24	CLA	A	1123	-	1/1/15/20	19/39/115/115	-
24	CLA	4	602	-	1/1/12/20	7/24/100/115	-
24	CLA	6	618	-	1/1/11/20	8/17/93/115	-
28	LHG	4	802	-	-	20/36/36/53	-
24	CLA	B	1214	-	1/1/14/20	19/36/112/115	-
31	LMT	A	5008	-	-	8/21/61/61	0/2/2/2
35	SQD	H	5001	-	-	8/40/60/69	0/1/1/1
24	CLA	a	603	-	1/1/15/20	15/39/115/115	-
49	C7Z	7	504	-	1/1/12/26	9/29/67/67	0/2/2/2
24	CLA	4	605	-	1/1/11/20	6/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	CHL	8	601	-	4/4/19/26	6/33/131/137	-
39	ECH	M	4001	-	-	5/29/66/66	0/2/2/2
28	LHG	2	802	-	-	33/53/53/53	-
33	PTY	5	802	-	-	19/41/41/53	-
24	CLA	B	1231	-	1/1/15/20	15/39/115/115	-
24	CLA	B	1222	-	1/1/13/20	4/31/107/115	-
40	LUT	9	501	-	-	2/29/67/67	0/2/2/2
24	CLA	7	610	-	1/1/13/20	12/27/103/115	-
41	CHL	6	619	18	4/4/20/26	9/39/137/137	-
24	CLA	A	1139	-	1/1/13/20	13/27/103/115	-
24	CLA	4	604	-	1/1/14/20	12/33/109/115	-
24	CLA	4	606	-	1/1/12/20	6/21/97/115	-
40	LUT	1	501	-	-	5/29/67/67	0/2/2/2
24	CLA	3	612	-	1/1/15/20	10/39/115/115	-
48	XAT	7	502	-	2/2/12/26	1/31/93/93	0/4/4/4
24	CLA	H	1702	-	1/1/11/20	9/17/93/115	-
24	CLA	7	606	-	1/1/13/20	15/27/103/115	-
41	CHL	a	610	-	4/4/16/26	3/18/116/137	-
40	LUT	5	501	-	-	3/29/67/67	0/2/2/2
24	CLA	B	1203	-	1/1/15/20	14/39/115/115	-
24	CLA	7	603	-	1/1/15/20	20/39/115/115	-
24	CLA	2	607	-	1/1/11/20	6/17/93/115	-
42	OLA	1	803	-	-	5/17/17/17	-
27	BCR	3	505	-	-	11/29/63/63	0/2/2/2
24	CLA	L	1503	-	1/1/11/20	6/15/91/115	-
24	CLA	B	1235	-	1/1/15/20	12/39/115/115	-
24	CLA	B	1205	-	1/1/15/20	10/39/115/115	-
24	CLA	B	1201	-	1/1/15/20	14/39/115/115	-
30	3PH	A	5007	-	-	17/34/34/49	-
24	CLA	6	608	-	1/1/11/20	5/15/91/115	-
24	CLA	A	1125	-	1/1/15/20	20/39/115/115	-
24	CLA	B	1239	-	1/1/15/20	15/39/115/115	-
27	BCR	8	503	-	-	11/29/63/63	0/2/2/2
33	PTY	9	803	-	-	25/51/51/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	PTY	3	802	-	-	13/41/41/53	-
24	CLA	B	1221	-	1/1/15/20	13/39/115/115	-
42	OLA	8	809	-	-	10/17/17/17	-
24	CLA	3	606	-	1/1/15/20	17/39/115/115	-
24	CLA	A	1013	-	1/1/15/20	11/39/115/115	-
28	LHG	B	5001	-	-	27/50/50/53	-
24	CLA	5	618	17	1/1/12/20	4/24/100/115	-
24	CLA	F	1301	-	1/1/12/20	7/21/97/115	-
41	CHL	a	613	-	4/4/16/26	2/15/113/137	-
28	LHG	8	801	-	-	28/41/41/53	-
24	CLA	B	1232	-	1/1/11/20	9/15/91/115	-
36	ERG	G	5002	-	4/4/11/15	7/13/71/71	0/4/4/4
24	CLA	4	612	-	1/1/14/20	21/36/112/115	-

All (2130) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	G	5002	ERG	C1-C10	-24.32	1.09	1.54
36	G	5002	ERG	C10-C9	-22.35	1.27	1.55
49	7	504	C7Z	C25-C26	16.05	1.61	1.34
37	J	4002	RRX	C26-C25	15.89	1.61	1.34
49	7	504	C7Z	C5-C6	15.64	1.60	1.34
40	7	501	LUT	C24-C25	15.45	1.51	1.33
36	G	5002	ERG	C10-C5	-15.45	1.23	1.52
40	5	505	LUT	C24-C25	15.40	1.51	1.33
37	J	4002	RRX	C5-C6	15.39	1.60	1.34
40	a	503	LUT	C24-C25	15.37	1.51	1.33
40	6	501	LUT	C24-C25	15.33	1.51	1.33
40	1	503	LUT	C24-C25	15.29	1.51	1.33
40	3	501	LUT	C24-C25	15.28	1.51	1.33
40	a	501	LUT	C24-C25	15.27	1.51	1.33
40	6	502	LUT	C24-C25	15.21	1.51	1.33
40	9	502	LUT	C24-C25	15.20	1.51	1.33
40	2	501	LUT	C24-C25	15.17	1.51	1.33
40	5	502	LUT	C24-C25	15.17	1.51	1.33
40	5	501	LUT	C24-C25	15.16	1.51	1.33
40	1	501	LUT	C24-C25	15.12	1.51	1.33
40	4	501	LUT	C24-C25	15.08	1.51	1.33
40	9	501	LUT	C24-C25	15.05	1.51	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	3	502	LUT	C24-C25	15.05	1.51	1.33
40	4	502	LUT	C24-C25	14.98	1.50	1.33
40	1	502	LUT	C24-C25	14.94	1.50	1.33
40	8	501	LUT	C24-C25	14.91	1.50	1.33
40	8	502	LUT	C24-C25	14.88	1.50	1.33
40	2	502	LUT	C24-C25	14.84	1.50	1.33
40	a	502	LUT	C24-C25	14.79	1.50	1.33
36	G	5002	ERG	C4-C3	-13.51	1.28	1.52
49	7	504	C7Z	C24-C23	11.85	1.73	1.52
36	G	5002	ERG	C2-C3	-11.50	1.25	1.51
49	7	504	C7Z	C22-C23	-10.70	1.37	1.52
49	7	504	C7Z	C2-C3	-10.32	1.37	1.52
37	J	4002	RRX	C29-C28	-10.12	1.38	1.52
23	A	1011	CL0	C1A-CHA	9.95	1.51	1.40
36	G	5002	ERG	O1-C3	9.32	1.70	1.43
36	G	5002	ERG	C12-C13	9.25	1.70	1.54
23	A	1011	CL0	C1B-C2B	9.11	1.49	1.39
41	4	609	CHL	C3A-C2A	-8.81	1.47	1.54
41	6	619	CHL	C3A-C2A	-8.67	1.47	1.54
36	G	5002	ERG	C6-C5	8.60	1.54	1.34
49	7	504	C7Z	C4-C3	8.35	1.66	1.52
23	A	1011	CL0	C1D-C2D	8.16	1.48	1.39
43	a	504	QTB	C11-C12	-8.16	1.36	1.54
43	3	506	QTB	C11-C12	-8.10	1.36	1.54
41	4	613	CHL	C3A-C2A	-7.96	1.47	1.54
37	J	4002	RRX	C27-C28	7.82	1.65	1.52
41	8	601	CHL	C3B-C4B	7.16	1.48	1.41
41	8	604	CHL	C3B-C4B	7.04	1.48	1.41
23	A	1011	CL0	C3B-C4B	6.85	1.48	1.41
37	J	4002	RRX	C2-C3	-6.77	1.36	1.52
24	A	1130	CLA	MG-NA	6.53	2.21	2.06
24	G	1601	CLA	MG-NA	6.50	2.21	2.06
24	9	605	CLA	MG-NA	6.49	2.21	2.06
24	4	605	CLA	MG-NA	6.49	2.21	2.06
24	5	607	CLA	MG-NA	6.48	2.21	2.06
24	G	1602	CLA	MG-NA	6.48	2.21	2.06
24	2	605	CLA	MG-NA	6.48	2.21	2.06
24	2	607	CLA	MG-NA	6.47	2.21	2.06
24	a	602	CLA	MG-NA	6.47	2.21	2.06
24	7	605	CLA	MG-NA	6.47	2.21	2.06
24	4	602	CLA	MG-NA	6.47	2.21	2.06
24	9	603	CLA	MG-NA	6.46	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	4	615	CLA	MG-NA	6.46	2.21	2.06
24	3	605	CLA	MG-NA	6.46	2.21	2.06
24	5	616	CLA	MG-NA	6.46	2.21	2.06
24	a	611	CLA	MG-NA	6.46	2.21	2.06
24	4	616	CLA	MG-NA	6.45	2.21	2.06
24	5	602	CLA	MG-NA	6.45	2.21	2.06
24	7	615	CLA	MG-NA	6.45	2.21	2.06
24	A	1125	CLA	MG-NA	6.45	2.21	2.06
24	6	617	CLA	MG-NA	6.45	2.21	2.06
24	9	607	CLA	MG-NA	6.45	2.21	2.06
24	7	617	CLA	MG-NA	6.44	2.21	2.06
24	8	602	CLA	MG-NA	6.44	2.21	2.06
24	2	621	CLA	MG-NA	6.44	2.21	2.06
24	B	1240	CLA	MG-NA	6.44	2.21	2.06
24	4	610	CLA	MG-NA	6.44	2.21	2.06
24	2	610	CLA	MG-NA	6.43	2.21	2.06
24	A	1127	CLA	MG-NA	6.43	2.21	2.06
24	8	610	CLA	MG-NA	6.43	2.21	2.06
24	7	602	CLA	MG-NA	6.43	2.21	2.06
24	B	1223	CLA	MG-NA	6.43	2.21	2.06
24	8	615	CLA	MG-NA	6.43	2.21	2.06
24	5	605	CLA	MG-NA	6.42	2.21	2.06
24	3	618	CLA	MG-NA	6.42	2.21	2.06
24	1	605	CLA	MG-NA	6.42	2.21	2.06
24	2	613	CLA	MG-NA	6.42	2.21	2.06
24	9	602	CLA	MG-NA	6.42	2.21	2.06
24	B	1220	CLA	MG-NA	6.42	2.21	2.06
24	A	1129	CLA	MG-NA	6.42	2.21	2.06
24	6	602	CLA	MG-NA	6.42	2.21	2.06
24	a	608	CLA	MG-NA	6.41	2.21	2.06
24	5	608	CLA	MG-NA	6.41	2.21	2.06
24	A	1115	CLA	MG-NA	6.41	2.21	2.06
24	5	614	CLA	MG-NA	6.41	2.21	2.06
24	6	607	CLA	MG-NA	6.41	2.21	2.06
24	A	1123	CLA	MG-NA	6.41	2.21	2.06
24	A	1140	CLA	MG-NA	6.41	2.21	2.06
24	4	607	CLA	MG-NA	6.41	2.21	2.06
24	F	1302	CLA	MG-NA	6.41	2.21	2.06
24	7	610	CLA	MG-NA	6.40	2.21	2.06
37	J	4002	RRX	C1-C6	-6.40	1.45	1.53
24	1	602	CLA	MG-NA	6.40	2.21	2.06
24	4	617	CLA	MG-NA	6.40	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	607	CLA	MG-NA	6.40	2.21	2.06
24	1	607	CLA	MG-NA	6.40	2.21	2.06
24	5	618	CLA	MG-NA	6.40	2.21	2.06
24	B	1219	CLA	MG-NA	6.40	2.21	2.06
24	6	609	CLA	MG-NA	6.40	2.21	2.06
24	B	1234	CLA	MG-NA	6.40	2.21	2.06
24	9	609	CLA	MG-NA	6.39	2.21	2.06
24	G	1603	CLA	MG-NA	6.39	2.21	2.06
24	B	1228	CLA	MG-NA	6.39	2.21	2.06
24	B	1215	CLA	MG-NA	6.39	2.21	2.06
24	B	1227	CLA	MG-NA	6.39	2.21	2.06
24	B	1213	CLA	MG-NA	6.38	2.21	2.06
24	B	1229	CLA	MG-NA	6.38	2.21	2.06
24	B	1232	CLA	MG-NA	6.38	2.21	2.06
24	H	1702	CLA	MG-NA	6.38	2.21	2.06
24	J	1901	CLA	MG-NA	6.38	2.21	2.06
24	A	1135	CLA	MG-NA	6.38	2.21	2.06
24	8	620	CLA	MG-NA	6.38	2.21	2.06
24	3	602	CLA	MG-NA	6.38	2.21	2.06
24	6	615	CLA	MG-NA	6.37	2.21	2.06
24	A	1139	CLA	MG-NA	6.37	2.21	2.06
24	8	618	CLA	MG-NA	6.37	2.21	2.06
24	8	605	CLA	MG-NA	6.37	2.21	2.06
24	6	606	CLA	MG-NA	6.37	2.21	2.06
24	6	618	CLA	MG-NA	6.37	2.21	2.06
24	a	604	CLA	MG-NA	6.37	2.21	2.06
24	A	1141	CLA	MG-NA	6.37	2.21	2.06
24	B	1217	CLA	MG-NA	6.37	2.21	2.06
24	F	1301	CLA	MG-NA	6.37	2.21	2.06
24	K	1403	CLA	MG-NA	6.37	2.21	2.06
24	7	607	CLA	MG-NA	6.37	2.21	2.06
24	K	1402	CLA	MG-NA	6.37	2.21	2.06
24	A	1122	CLA	MG-NA	6.37	2.21	2.06
24	2	602	CLA	MG-NA	6.36	2.21	2.06
24	H	1703	CLA	MG-NA	6.36	2.21	2.06
24	5	617	CLA	MG-NA	6.36	2.21	2.06
24	3	607	CLA	MG-NA	6.36	2.21	2.06
24	5	609	CLA	MG-NA	6.36	2.21	2.06
24	9	612	CLA	MG-NA	6.36	2.21	2.06
24	A	1107	CLA	MG-NA	6.36	2.21	2.06
24	a	605	CLA	MG-NA	6.35	2.21	2.06
24	8	607	CLA	MG-NA	6.35	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1101	CLA	MG-NA	6.35	2.21	2.06
24	a	615	CLA	MG-NA	6.35	2.21	2.06
24	A	1110	CLA	MG-NA	6.35	2.21	2.06
24	9	608	CLA	MG-NA	6.35	2.21	2.06
24	1	601	CLA	MG-NA	6.35	2.21	2.06
24	B	1212	CLA	MG-NA	6.35	2.21	2.06
24	7	608	CLA	MG-NA	6.35	2.21	2.06
24	K	1404	CLA	MG-NA	6.35	2.21	2.06
24	B	1218	CLA	MG-NA	6.35	2.21	2.06
41	6	610	CHL	C3A-C2A	-6.35	1.49	1.54
24	A	1114	CLA	MG-NA	6.35	2.21	2.06
24	1	611	CLA	MG-NA	6.35	2.21	2.06
24	L	1503	CLA	MG-NA	6.35	2.21	2.06
24	5	606	CLA	MG-NA	6.35	2.21	2.06
24	2	601	CLA	MG-NA	6.34	2.21	2.06
24	K	1401	CLA	MG-NA	6.34	2.21	2.06
24	2	606	CLA	MG-NA	6.34	2.21	2.06
24	1	615	CLA	MG-NA	6.34	2.21	2.06
24	1	612	CLA	MG-NA	6.34	2.21	2.06
24	2	604	CLA	MG-NA	6.34	2.21	2.06
24	1	610	CLA	MG-NA	6.34	2.21	2.06
24	7	603	CLA	MG-NA	6.34	2.21	2.06
24	B	1214	CLA	MG-NA	6.34	2.21	2.06
24	9	604	CLA	MG-NA	6.34	2.21	2.06
24	3	603	CLA	MG-NA	6.34	2.21	2.06
24	B	1224	CLA	MG-NA	6.33	2.21	2.06
24	A	1137	CLA	MG-NA	6.33	2.21	2.06
24	A	1136	CLA	MG-NA	6.33	2.21	2.06
24	B	1237	CLA	MG-NA	6.33	2.21	2.06
24	a	612	CLA	MG-NA	6.33	2.21	2.06
24	B	1022	CLA	MG-NA	6.33	2.21	2.06
41	4	618	CHL	C3A-C2A	-6.32	1.49	1.54
24	6	608	CLA	MG-NA	6.32	2.21	2.06
24	B	1221	CLA	MG-NA	6.32	2.21	2.06
24	8	603	CLA	MG-NA	6.32	2.21	2.06
24	6	604	CLA	MG-NA	6.32	2.21	2.06
24	6	601	CLA	MG-NA	6.32	2.21	2.06
24	1	608	CLA	MG-NA	6.31	2.21	2.06
24	9	606	CLA	MG-NA	6.31	2.21	2.06
24	A	1134	CLA	MG-NA	6.31	2.21	2.06
24	a	603	CLA	MG-NA	6.31	2.21	2.06
24	L	1502	CLA	MG-NA	6.31	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	1225	CLA	MG-NA	6.31	2.21	2.06
24	B	1208	CLA	MG-NA	6.31	2.21	2.06
24	3	612	CLA	MG-NA	6.30	2.21	2.06
24	1	604	CLA	MG-NA	6.30	2.21	2.06
24	B	1201	CLA	MG-NA	6.30	2.21	2.06
24	B	1226	CLA	MG-NA	6.30	2.21	2.06
24	6	605	CLA	MG-NA	6.30	2.21	2.06
24	A	1112	CLA	MG-NA	6.30	2.21	2.06
24	7	606	CLA	MG-NA	6.30	2.21	2.06
24	2	603	CLA	MG-NA	6.29	2.21	2.06
24	5	603	CLA	MG-NA	6.29	2.21	2.06
24	2	609	CLA	MG-NA	6.29	2.21	2.06
24	A	1105	CLA	MG-NA	6.29	2.21	2.06
24	H	1701	CLA	MG-NA	6.29	2.21	2.06
24	A	1121	CLA	MG-NA	6.29	2.21	2.06
24	A	1012	CLA	MG-NA	6.28	2.21	2.06
24	8	609	CLA	MG-NA	6.28	2.21	2.06
24	B	1202	CLA	MG-NA	6.28	2.21	2.06
24	2	615	CLA	MG-NA	6.28	2.21	2.06
24	3	616	CLA	MG-NA	6.28	2.21	2.06
24	B	1210	CLA	MG-NA	6.28	2.21	2.06
24	A	1113	CLA	MG-NA	6.28	2.21	2.06
24	4	611	CLA	MG-NA	6.28	2.21	2.06
24	A	1118	CLA	MG-NA	6.28	2.21	2.06
24	A	1126	CLA	MG-NA	6.28	2.21	2.06
24	A	1116	CLA	MG-NA	6.28	2.21	2.06
24	B	1239	CLA	MG-NA	6.27	2.21	2.06
24	A	1104	CLA	MG-NA	6.27	2.21	2.06
24	A	1131	CLA	MG-NA	6.27	2.21	2.06
24	6	612	CLA	MG-NA	6.27	2.21	2.06
24	4	604	CLA	MG-NA	6.27	2.21	2.06
24	7	604	CLA	MG-NA	6.27	2.21	2.06
24	L	1501	CLA	MG-NA	6.26	2.21	2.06
24	A	1117	CLA	MG-NA	6.26	2.21	2.06
24	B	1209	CLA	MG-NA	6.26	2.21	2.06
24	1	603	CLA	MG-NA	6.26	2.21	2.06
24	A	1133	CLA	MG-NA	6.26	2.21	2.06
24	B	1230	CLA	MG-NA	6.26	2.21	2.06
24	2	612	CLA	MG-NA	6.26	2.21	2.06
24	B	1203	CLA	MG-NA	6.25	2.21	2.06
24	B	1207	CLA	MG-NA	6.25	2.21	2.06
24	A	1120	CLA	MG-NA	6.25	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	2	608	CLA	MG-NA	6.25	2.21	2.06
24	4	612	CLA	MG-NA	6.25	2.21	2.06
24	A	1124	CLA	MG-NA	6.25	2.21	2.06
24	7	611	CLA	MG-NA	6.25	2.21	2.06
24	5	612	CLA	MG-NA	6.24	2.21	2.06
36	G	5002	ERG	C16-C17	-6.24	1.41	1.54
24	A	1128	CLA	MG-NA	6.24	2.21	2.06
24	5	601	CLA	MG-NA	6.24	2.21	2.06
24	A	1106	CLA	MG-NA	6.23	2.21	2.06
24	4	603	CLA	MG-NA	6.23	2.21	2.06
24	4	606	CLA	MG-NA	6.23	2.21	2.06
24	8	612	CLA	MG-NA	6.23	2.21	2.06
24	9	601	CLA	MG-NA	6.23	2.21	2.06
24	3	613	CLA	MG-NA	6.23	2.21	2.06
24	B	1236	CLA	MG-NA	6.23	2.21	2.06
24	8	606	CLA	MG-NA	6.22	2.21	2.06
24	A	1109	CLA	MG-NA	6.22	2.21	2.06
24	6	603	CLA	MG-NA	6.22	2.21	2.06
24	3	601	CLA	MG-NA	6.22	2.21	2.06
24	7	609	CLA	MG-NA	6.22	2.21	2.06
24	B	1238	CLA	MG-NA	6.21	2.21	2.06
24	B	1222	CLA	MG-NA	6.21	2.21	2.06
24	B	1216	CLA	MG-NA	6.21	2.21	2.06
24	a	601	CLA	MG-NA	6.21	2.21	2.06
24	A	1108	CLA	MG-NA	6.20	2.21	2.06
24	B	1235	CLA	MG-NA	6.20	2.21	2.06
24	5	604	CLA	MG-NA	6.20	2.21	2.06
24	A	1119	CLA	MG-NA	6.19	2.21	2.06
24	A	1138	CLA	MG-NA	6.19	2.21	2.06
24	B	1023	CLA	MG-NA	6.19	2.21	2.06
24	8	611	CLA	MG-NA	6.19	2.21	2.06
24	1	606	CLA	MG-NA	6.19	2.21	2.06
24	8	608	CLA	MG-NA	6.17	2.20	2.06
24	A	1103	CLA	MG-NA	6.17	2.20	2.06
24	3	610	CLA	MG-NA	6.17	2.20	2.06
24	B	1211	CLA	MG-NA	6.17	2.20	2.06
24	7	601	CLA	MG-NA	6.16	2.20	2.06
24	7	612	CLA	MG-NA	6.16	2.20	2.06
24	B	1206	CLA	MG-NA	6.16	2.20	2.06
24	A	1111	CLA	MG-NA	6.16	2.20	2.06
24	B	1204	CLA	MG-NA	6.15	2.20	2.06
24	4	601	CLA	MG-NA	6.15	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	1231	CLA	MG-NA	6.15	2.20	2.06
24	3	606	CLA	MG-NA	6.14	2.20	2.06
24	A	1102	CLA	MG-NA	6.13	2.20	2.06
41	8	601	CHL	C3A-C2A	-6.11	1.49	1.54
24	B	1205	CLA	MG-NA	6.10	2.20	2.06
24	A	1132	CLA	MG-NA	6.09	2.20	2.06
24	4	608	CLA	MG-NA	6.09	2.20	2.06
24	3	604	CLA	MG-NA	6.04	2.20	2.06
24	B	1021	CLA	MG-NA	6.02	2.20	2.06
27	B	4005	BCR	C24-C23	5.98	1.50	1.33
27	G	4001	BCR	C24-C23	5.97	1.50	1.33
24	A	1013	CLA	MG-NA	5.96	2.20	2.06
27	L	4003	BCR	C24-C23	5.90	1.50	1.33
27	5	503	BCR	C24-C23	5.90	1.50	1.33
27	4	503	BCR	C24-C23	5.90	1.50	1.33
27	6	503	BCR	C24-C23	5.89	1.50	1.33
27	K	4002	BCR	C24-C23	5.89	1.50	1.33
27	3	503	BCR	C24-C23	5.88	1.50	1.33
27	B	4006	BCR	C24-C23	5.88	1.50	1.33
27	L	4001	BCR	C24-C23	5.84	1.50	1.33
27	3	505	BCR	C24-C23	5.84	1.50	1.33
27	H	4001	BCR	C24-C23	5.84	1.50	1.33
49	7	504	C7Z	C1-C6	-5.83	1.46	1.53
27	6	504	BCR	C24-C23	5.83	1.50	1.33
27	8	503	BCR	C24-C23	5.82	1.50	1.33
27	B	4002	BCR	C24-C23	5.80	1.50	1.33
27	A	4001	BCR	C24-C23	5.80	1.50	1.33
27	F	4001	BCR	C24-C23	5.79	1.50	1.33
27	5	504	BCR	C24-C23	5.79	1.50	1.33
37	J	4002	RRX	C30-C25	-5.78	1.46	1.53
27	3	504	BCR	C24-C23	5.78	1.50	1.33
27	A	4003	BCR	C24-C23	5.77	1.50	1.33
27	7	503	BCR	C24-C23	5.76	1.50	1.33
41	7	613	CHL	C3B-C4B	5.75	1.47	1.41
27	K	4001	BCR	C24-C23	5.75	1.50	1.33
27	B	4003	BCR	C24-C23	5.74	1.50	1.33
27	J	4001	BCR	C24-C23	5.74	1.50	1.33
27	I	4001	BCR	C24-C23	5.73	1.50	1.33
27	B	4001	BCR	C24-C23	5.72	1.50	1.33
27	B	4007	BCR	C24-C23	5.71	1.50	1.33
27	A	4002	BCR	C24-C23	5.70	1.50	1.33
27	B	4004	BCR	C24-C23	5.70	1.50	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	7	504	C7Z	C12-C13	5.67	1.58	1.46
41	a	613	CHL	C3B-C4B	5.67	1.46	1.41
27	L	4002	BCR	C24-C23	5.64	1.49	1.33
27	A	4004	BCR	C24-C23	5.63	1.49	1.33
36	G	5002	ERG	C1-C2	5.62	1.64	1.53
27	A	4005	BCR	C24-C23	5.57	1.49	1.33
23	A	1011	CL0	O2A-C1	5.55	1.61	1.46
41	8	604	CHL	C3A-C2A	-5.55	1.49	1.54
41	4	609	CHL	C3B-C4B	5.43	1.46	1.41
27	A	4004	BCR	C11-C12	-5.43	1.20	1.34
27	A	4002	BCR	C11-C12	-5.38	1.20	1.34
41	a	610	CHL	C3B-C4B	5.38	1.46	1.41
23	A	1011	CL0	CHB-C1B	5.36	1.48	1.39
27	L	4002	BCR	C11-C12	-5.32	1.20	1.34
41	8	613	CHL	C3B-C4B	5.32	1.46	1.41
36	G	5002	ERG	C12-C11	-5.31	1.42	1.53
27	B	4006	BCR	C11-C12	-5.27	1.20	1.34
41	9	610	CHL	C3B-C4B	5.26	1.46	1.41
27	B	4001	BCR	C11-C12	-5.25	1.21	1.34
27	J	4001	BCR	C11-C12	-5.23	1.21	1.34
37	J	4002	RRX	C19-C18	5.22	1.57	1.46
27	K	4001	BCR	C11-C12	-5.21	1.21	1.34
27	5	504	BCR	C11-C12	-5.20	1.21	1.34
36	G	5002	ERG	C7-C6	-5.20	1.27	1.41
27	A	4001	BCR	C11-C12	-5.18	1.21	1.34
27	A	4005	BCR	C11-C12	-5.17	1.21	1.34
37	J	4002	RRX	C2-C1	5.15	1.65	1.54
27	3	504	BCR	C11-C12	-5.14	1.21	1.34
27	I	4001	BCR	C11-C12	-5.13	1.21	1.34
41	3	608	CHL	C3A-C2A	-5.13	1.50	1.54
27	3	503	BCR	C11-C12	-5.13	1.21	1.34
23	A	1011	CL0	CHC-C4B	5.13	1.47	1.39
27	L	4001	BCR	C11-C12	-5.12	1.21	1.34
41	6	611	CHL	C3B-C4B	5.12	1.46	1.41
27	4	503	BCR	C11-C12	-5.12	1.21	1.34
27	G	4001	BCR	C11-C12	-5.11	1.21	1.34
36	G	5002	ERG	C13-C14	-5.11	1.47	1.56
27	B	4002	BCR	C11-C12	-5.10	1.21	1.34
27	B	4004	BCR	C11-C12	-5.10	1.21	1.34
27	7	503	BCR	C11-C12	-5.10	1.21	1.34
41	4	618	CHL	C3B-C4B	5.10	1.46	1.41
23	A	1011	CL0	O2D-CGD	5.09	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	H	4001	BCR	C11-C12	-5.08	1.21	1.34
27	3	505	BCR	C11-C12	-5.07	1.21	1.34
27	6	503	BCR	C11-C12	-5.07	1.21	1.34
27	5	503	BCR	C11-C12	-5.07	1.21	1.34
27	B	4007	BCR	C11-C12	-5.07	1.21	1.34
41	6	619	CHL	C3B-C4B	5.06	1.46	1.41
27	8	503	BCR	C11-C12	-5.06	1.21	1.34
27	B	4003	BCR	C11-C12	-5.05	1.21	1.34
41	3	611	CHL	C3A-C2A	-5.05	1.50	1.54
27	6	504	BCR	C11-C12	-5.04	1.21	1.34
27	B	4005	BCR	C11-C12	-5.03	1.21	1.34
27	L	4003	BCR	C11-C12	-5.02	1.21	1.34
41	a	606	CHL	C3B-C4B	5.00	1.46	1.41
27	K	4002	BCR	C11-C12	-4.99	1.21	1.34
27	A	4003	BCR	C11-C12	-4.99	1.21	1.34
23	A	1011	CL0	OBD-CAD	4.95	1.28	1.22
43	3	506	QTB	C11-C10	-4.91	1.43	1.50
23	A	1011	CL0	C3B-C2B	4.87	1.47	1.40
37	J	4002	RRX	C8-C9	4.83	1.56	1.46
27	F	4001	BCR	C11-C12	-4.77	1.22	1.34
41	7	613	CHL	C3A-C2A	-4.71	1.50	1.54
49	7	504	C7Z	C28-C29	4.71	1.56	1.46
23	A	1011	CL0	C3D-C4D	-4.65	1.34	1.41
23	A	1011	CL0	C3D-C2D	4.64	1.47	1.39
41	5	611	CHL	C3A-C2A	-4.63	1.50	1.54
23	A	1011	CL0	CHD-C1D	4.62	1.47	1.39
49	7	504	C7Z	C24-C25	-4.61	1.43	1.51
41	5	610	CHL	C3B-C4B	4.57	1.45	1.41
36	G	5002	ERG	C13-C17	4.57	1.63	1.55
49	7	504	C7Z	C32-C33	4.54	1.55	1.46
41	5	613	CHL	C3B-C4B	4.54	1.45	1.41
43	a	504	QTB	C17-C11	-4.51	1.51	1.55
41	6	611	CHL	C3A-C2A	-4.48	1.50	1.54
24	B	1207	CLA	CBB-CAB	4.47	1.51	1.30
24	5	604	CLA	CBB-CAB	4.46	1.51	1.30
24	2	601	CLA	CBB-CAB	4.46	1.51	1.30
24	4	611	CLA	CBB-CAB	4.45	1.51	1.30
24	9	612	CLA	CBB-CAB	4.45	1.51	1.30
24	4	608	CLA	CBB-CAB	4.44	1.51	1.30
49	7	504	C7Z	C8-C9	4.44	1.55	1.46
24	1	606	CLA	CBB-CAB	4.44	1.51	1.30
24	2	605	CLA	CBB-CAB	4.43	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	1011	CL0	CHD-C4C	4.43	1.47	1.39
24	A	1128	CLA	CBB-CAB	4.43	1.51	1.30
24	A	1013	CLA	CBB-CAB	4.43	1.51	1.30
24	6	605	CLA	CBB-CAB	4.43	1.51	1.30
24	B	1219	CLA	CBB-CAB	4.42	1.51	1.30
24	B	1226	CLA	CBB-CAB	4.42	1.51	1.30
24	K	1401	CLA	CBB-CAB	4.42	1.51	1.30
24	H	1701	CLA	CBB-CAB	4.42	1.51	1.30
24	3	613	CLA	CBB-CAB	4.42	1.51	1.30
24	5	618	CLA	CBB-CAB	4.42	1.51	1.30
24	5	606	CLA	CBB-CAB	4.42	1.51	1.30
24	9	603	CLA	CBB-CAB	4.42	1.51	1.30
24	B	1023	CLA	CBB-CAB	4.42	1.51	1.30
24	A	1123	CLA	CBB-CAB	4.42	1.51	1.30
24	7	615	CLA	CBB-CAB	4.42	1.51	1.30
24	B	1239	CLA	CBB-CAB	4.42	1.51	1.30
24	7	608	CLA	CBB-CAB	4.42	1.51	1.30
24	1	607	CLA	CBB-CAB	4.42	1.51	1.30
24	a	608	CLA	CBB-CAB	4.42	1.51	1.30
24	9	602	CLA	CBB-CAB	4.42	1.51	1.30
24	B	1228	CLA	CBB-CAB	4.42	1.51	1.30
24	A	1124	CLA	CBB-CAB	4.42	1.51	1.30
24	6	601	CLA	CBB-CAB	4.42	1.51	1.30
24	H	1703	CLA	CBB-CAB	4.42	1.51	1.30
24	1	603	CLA	CBB-CAB	4.42	1.51	1.30
24	L	1503	CLA	CBB-CAB	4.41	1.51	1.30
24	4	615	CLA	CBB-CAB	4.41	1.51	1.30
24	4	616	CLA	CBB-CAB	4.41	1.51	1.30
24	1	604	CLA	CBB-CAB	4.41	1.51	1.30
24	1	605	CLA	CBB-CAB	4.41	1.51	1.30
24	5	605	CLA	CBB-CAB	4.41	1.51	1.30
24	2	613	CLA	CBB-CAB	4.41	1.51	1.30
24	a	611	CLA	CBB-CAB	4.41	1.51	1.30
24	3	610	CLA	CBB-CAB	4.41	1.51	1.30
24	A	1120	CLA	CBB-CAB	4.41	1.51	1.30
41	3	611	CHL	C3B-C4B	4.41	1.45	1.41
24	L	1501	CLA	CBB-CAB	4.41	1.51	1.30
24	2	621	CLA	CBB-CAB	4.41	1.51	1.30
24	F	1302	CLA	CBB-CAB	4.41	1.51	1.30
24	8	615	CLA	CBB-CAB	4.41	1.51	1.30
24	5	612	CLA	CBB-CAB	4.41	1.51	1.30
24	B	1227	CLA	CBB-CAB	4.41	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	1	601	CLA	CBB-CAB	4.41	1.51	1.30
24	9	608	CLA	CBB-CAB	4.41	1.51	1.30
24	1	611	CLA	CBB-CAB	4.41	1.51	1.30
24	A	1103	CLA	CBB-CAB	4.41	1.51	1.30
24	9	609	CLA	CBB-CAB	4.41	1.51	1.30
24	A	1110	CLA	CBB-CAB	4.41	1.51	1.30
24	3	602	CLA	CBB-CAB	4.41	1.51	1.30
24	A	1106	CLA	CBB-CAB	4.41	1.51	1.30
24	G	1602	CLA	CBB-CAB	4.41	1.51	1.30
24	1	615	CLA	CBB-CAB	4.41	1.51	1.30
24	3	605	CLA	CBB-CAB	4.41	1.51	1.30
24	9	604	CLA	CBB-CAB	4.41	1.51	1.30
43	a	504	QTB	C11-C10	-4.41	1.44	1.50
24	6	617	CLA	CBB-CAB	4.41	1.51	1.30
24	2	612	CLA	CBB-CAB	4.41	1.51	1.30
24	9	606	CLA	CBB-CAB	4.41	1.51	1.30
24	4	617	CLA	CBB-CAB	4.41	1.51	1.30
24	a	615	CLA	CBB-CAB	4.41	1.51	1.30
24	6	608	CLA	CBB-CAB	4.40	1.51	1.30
24	7	605	CLA	CBB-CAB	4.40	1.51	1.30
24	1	602	CLA	CBB-CAB	4.40	1.51	1.30
24	A	1105	CLA	CBB-CAB	4.40	1.51	1.30
24	3	606	CLA	CBB-CAB	4.40	1.51	1.30
24	6	618	CLA	CBB-CAB	4.40	1.51	1.30
24	B	1222	CLA	CBB-CAB	4.40	1.51	1.30
24	a	607	CLA	CBB-CAB	4.40	1.51	1.30
24	B	1217	CLA	CBB-CAB	4.40	1.51	1.30
24	3	607	CLA	CBB-CAB	4.40	1.51	1.30
24	G	1601	CLA	CBB-CAB	4.40	1.51	1.30
24	K	1404	CLA	CBB-CAB	4.40	1.51	1.30
24	a	612	CLA	CBB-CAB	4.40	1.51	1.30
24	B	1240	CLA	CBB-CAB	4.40	1.51	1.30
24	4	606	CLA	CBB-CAB	4.40	1.51	1.30
24	4	601	CLA	CBB-CAB	4.40	1.51	1.30
24	2	607	CLA	CBB-CAB	4.40	1.51	1.30
24	B	1211	CLA	CBB-CAB	4.40	1.51	1.30
24	2	603	CLA	CBB-CAB	4.40	1.51	1.30
24	9	605	CLA	CBB-CAB	4.40	1.51	1.30
24	1	608	CLA	CBB-CAB	4.40	1.51	1.30
24	5	602	CLA	CBB-CAB	4.40	1.51	1.30
24	6	602	CLA	CBB-CAB	4.40	1.51	1.30
24	4	602	CLA	CBB-CAB	4.40	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	603	CLA	CBB-CAB	4.40	1.51	1.30
24	A	1136	CLA	CBB-CAB	4.40	1.51	1.30
24	6	604	CLA	CBB-CAB	4.40	1.51	1.30
24	8	618	CLA	CBB-CAB	4.40	1.51	1.30
24	A	1119	CLA	CBB-CAB	4.40	1.51	1.30
24	4	612	CLA	CBB-CAB	4.40	1.51	1.30
24	1	610	CLA	CBB-CAB	4.40	1.51	1.30
24	L	1502	CLA	CBB-CAB	4.40	1.51	1.30
24	7	610	CLA	CBB-CAB	4.40	1.51	1.30
24	2	610	CLA	CBB-CAB	4.40	1.51	1.30
24	A	1102	CLA	CBB-CAB	4.40	1.51	1.30
24	8	607	CLA	CBB-CAB	4.40	1.51	1.30
24	8	609	CLA	CBB-CAB	4.40	1.51	1.30
24	8	620	CLA	CBB-CAB	4.40	1.51	1.30
24	B	1206	CLA	CBB-CAB	4.40	1.51	1.30
24	4	610	CLA	CBB-CAB	4.40	1.51	1.30
24	B	1223	CLA	CBB-CAB	4.40	1.51	1.30
24	B	1236	CLA	CBB-CAB	4.40	1.51	1.30
24	A	1132	CLA	CBB-CAB	4.40	1.51	1.30
24	6	607	CLA	CBB-CAB	4.40	1.51	1.30
24	a	603	CLA	CBB-CAB	4.40	1.51	1.30
24	5	614	CLA	CBB-CAB	4.39	1.51	1.30
24	B	1235	CLA	CBB-CAB	4.39	1.51	1.30
24	2	608	CLA	CBB-CAB	4.39	1.51	1.30
24	9	607	CLA	CBB-CAB	4.39	1.51	1.30
24	5	616	CLA	CBB-CAB	4.39	1.51	1.30
24	7	617	CLA	CBB-CAB	4.39	1.51	1.30
24	8	602	CLA	CBB-CAB	4.39	1.51	1.30
24	2	615	CLA	CBB-CAB	4.39	1.51	1.30
24	A	1115	CLA	CBB-CAB	4.39	1.51	1.30
24	8	608	CLA	CBB-CAB	4.39	1.51	1.30
24	a	602	CLA	CBB-CAB	4.39	1.51	1.30
24	J	1901	CLA	CBB-CAB	4.39	1.51	1.30
24	A	1125	CLA	CBB-CAB	4.39	1.51	1.30
24	6	615	CLA	CBB-CAB	4.39	1.51	1.30
24	B	1213	CLA	CBB-CAB	4.39	1.51	1.30
24	B	1203	CLA	CBB-CAB	4.39	1.51	1.30
24	3	618	CLA	CBB-CAB	4.39	1.51	1.30
24	4	607	CLA	CBB-CAB	4.39	1.51	1.30
24	8	612	CLA	CBB-CAB	4.39	1.51	1.30
24	K	1402	CLA	CBB-CAB	4.39	1.51	1.30
24	B	1224	CLA	CBB-CAB	4.39	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	2	606	CLA	CBB-CAB	4.39	1.51	1.30
24	A	1012	CLA	CBB-CAB	4.39	1.51	1.30
24	5	608	CLA	CBB-CAB	4.39	1.51	1.30
37	J	4002	RRX	C12-C13	4.39	1.55	1.46
24	A	1118	CLA	CBB-CAB	4.39	1.51	1.30
24	4	604	CLA	CBB-CAB	4.39	1.51	1.30
24	7	611	CLA	CBB-CAB	4.39	1.51	1.30
24	A	1117	CLA	CBB-CAB	4.39	1.51	1.30
24	A	1134	CLA	CBB-CAB	4.39	1.51	1.30
24	5	609	CLA	CBB-CAB	4.39	1.51	1.30
24	3	616	CLA	CBB-CAB	4.39	1.51	1.30
24	B	1208	CLA	CBB-CAB	4.39	1.51	1.30
24	7	602	CLA	CBB-CAB	4.39	1.51	1.30
24	8	611	CLA	CBB-CAB	4.39	1.51	1.30
24	7	606	CLA	CBB-CAB	4.38	1.51	1.30
24	5	607	CLA	CBB-CAB	4.38	1.51	1.30
24	A	1130	CLA	CBB-CAB	4.38	1.51	1.30
24	8	605	CLA	CBB-CAB	4.38	1.51	1.30
24	A	1141	CLA	CBB-CAB	4.38	1.51	1.30
24	5	601	CLA	CBB-CAB	4.38	1.51	1.30
24	6	606	CLA	CBB-CAB	4.38	1.51	1.30
24	A	1121	CLA	CBB-CAB	4.38	1.51	1.30
24	3	604	CLA	CBB-CAB	4.38	1.51	1.30
24	a	605	CLA	CBB-CAB	4.38	1.51	1.30
24	6	612	CLA	CBB-CAB	4.38	1.51	1.30
24	1	612	CLA	CBB-CAB	4.38	1.51	1.30
24	2	604	CLA	CBB-CAB	4.38	1.51	1.30
24	3	601	CLA	CBB-CAB	4.38	1.51	1.30
24	B	1232	CLA	CBB-CAB	4.38	1.51	1.30
24	A	1113	CLA	CBB-CAB	4.38	1.51	1.30
24	A	1109	CLA	CBB-CAB	4.38	1.51	1.30
24	2	602	CLA	CBB-CAB	4.38	1.51	1.30
24	B	1209	CLA	CBB-CAB	4.38	1.51	1.30
24	A	1137	CLA	CBB-CAB	4.38	1.51	1.30
24	B	1210	CLA	CBB-CAB	4.38	1.51	1.30
24	B	1231	CLA	CBB-CAB	4.38	1.51	1.30
24	8	610	CLA	CBB-CAB	4.38	1.51	1.30
24	4	605	CLA	CBB-CAB	4.38	1.51	1.30
24	7	601	CLA	CBB-CAB	4.38	1.51	1.30
24	B	1212	CLA	CBB-CAB	4.38	1.51	1.30
24	A	1111	CLA	CBB-CAB	4.37	1.51	1.30
24	8	606	CLA	CBB-CAB	4.37	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	1201	CLA	CBB-CAB	4.37	1.51	1.30
24	B	1230	CLA	CBB-CAB	4.37	1.51	1.30
24	A	1140	CLA	CBB-CAB	4.37	1.51	1.30
24	3	603	CLA	CBB-CAB	4.37	1.51	1.30
24	7	603	CLA	CBB-CAB	4.37	1.51	1.30
24	7	607	CLA	CBB-CAB	4.37	1.51	1.30
24	2	609	CLA	CBB-CAB	4.37	1.51	1.30
24	8	603	CLA	CBB-CAB	4.37	1.51	1.30
24	A	1138	CLA	CBB-CAB	4.37	1.51	1.30
24	a	604	CLA	CBB-CAB	4.37	1.51	1.30
24	B	1225	CLA	CBB-CAB	4.37	1.51	1.30
24	A	1126	CLA	CBB-CAB	4.37	1.51	1.30
24	G	1603	CLA	CBB-CAB	4.37	1.51	1.30
24	A	1139	CLA	CBB-CAB	4.37	1.51	1.30
23	A	1011	CL0	CHC-C1C	4.37	1.47	1.39
24	B	1204	CLA	CBB-CAB	4.36	1.51	1.30
24	A	1116	CLA	CBB-CAB	4.36	1.51	1.30
49	7	504	C7Z	C31-C30	4.36	1.56	1.43
24	A	1122	CLA	CBB-CAB	4.36	1.51	1.30
24	A	1101	CLA	CBB-CAB	4.36	1.51	1.30
24	B	1022	CLA	CBB-CAB	4.36	1.51	1.30
24	B	1215	CLA	CBB-CAB	4.36	1.51	1.30
24	F	1301	CLA	CBB-CAB	4.36	1.51	1.30
24	B	1221	CLA	CBB-CAB	4.36	1.51	1.30
24	7	609	CLA	CBB-CAB	4.36	1.51	1.30
24	B	1220	CLA	CBB-CAB	4.36	1.51	1.30
24	K	1403	CLA	CBB-CAB	4.35	1.51	1.30
24	A	1114	CLA	CBB-CAB	4.35	1.51	1.30
24	A	1127	CLA	CBB-CAB	4.35	1.51	1.30
27	A	4004	BCR	C16-C17	-4.35	1.29	1.43
24	A	1108	CLA	CBB-CAB	4.35	1.51	1.30
24	A	1133	CLA	CBB-CAB	4.35	1.51	1.30
24	H	1702	CLA	CBB-CAB	4.35	1.51	1.30
24	6	609	CLA	CBB-CAB	4.35	1.51	1.30
24	B	1238	CLA	CBB-CAB	4.35	1.51	1.30
24	B	1205	CLA	CBB-CAB	4.35	1.51	1.30
24	7	612	CLA	CBB-CAB	4.34	1.51	1.30
24	7	604	CLA	CBB-CAB	4.34	1.51	1.30
24	9	601	CLA	CBB-CAB	4.34	1.51	1.30
37	J	4002	RRX	C27-C26	-4.34	1.44	1.51
24	B	1229	CLA	CBB-CAB	4.34	1.51	1.30
24	3	612	CLA	CBB-CAB	4.34	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	1218	CLA	CBB-CAB	4.34	1.51	1.30
24	A	1104	CLA	CBB-CAB	4.34	1.51	1.30
24	A	1107	CLA	CBB-CAB	4.34	1.51	1.30
24	B	1214	CLA	CBB-CAB	4.34	1.51	1.30
29	A	5005	DGD	O1G-C1A	4.34	1.46	1.33
24	A	1112	CLA	CBB-CAB	4.34	1.51	1.30
24	4	603	CLA	CBB-CAB	4.33	1.51	1.30
24	B	1216	CLA	CBB-CAB	4.33	1.51	1.30
24	5	617	CLA	CBB-CAB	4.32	1.51	1.30
24	A	1131	CLA	CBB-CAB	4.32	1.51	1.30
24	A	1129	CLA	CBB-CAB	4.32	1.51	1.30
24	a	601	CLA	CBB-CAB	4.32	1.51	1.30
49	7	504	C7Z	C4-C5	-4.31	1.44	1.51
27	K	4002	BCR	C10-C9	4.31	1.45	1.35
24	6	603	CLA	CBB-CAB	4.31	1.51	1.30
24	B	1202	CLA	CBB-CAB	4.31	1.51	1.30
27	4	503	BCR	C10-C9	4.30	1.45	1.35
24	B	1237	CLA	CBB-CAB	4.30	1.51	1.30
29	8	802	DGD	O1G-C1A	4.29	1.45	1.33
27	J	4001	BCR	C16-C17	-4.28	1.29	1.43
24	B	1021	CLA	CBB-CAB	4.27	1.50	1.30
27	7	503	BCR	C16-C17	-4.27	1.30	1.43
49	7	504	C7Z	C11-C10	4.27	1.56	1.43
27	L	4003	BCR	C10-C9	4.26	1.45	1.35
24	B	1221	CLA	MG-ND	-4.26	1.97	2.05
24	B	1226	CLA	MG-ND	-4.26	1.97	2.05
37	J	4002	RRX	C3-C4	4.25	1.65	1.52
24	A	1135	CLA	CBB-CAB	4.25	1.50	1.30
27	L	4002	BCR	C16-C17	-4.24	1.30	1.43
27	I	4001	BCR	C16-C17	-4.24	1.30	1.43
29	B	5003	DGD	O1G-C1A	4.24	1.45	1.33
27	A	4001	BCR	C16-C17	-4.23	1.30	1.43
27	A	4003	BCR	C10-C9	4.23	1.45	1.35
27	B	4005	BCR	C16-C17	-4.23	1.30	1.43
24	B	1234	CLA	CBB-CAB	4.22	1.50	1.30
27	A	4005	BCR	C16-C17	-4.22	1.30	1.43
27	F	4001	BCR	C16-C17	-4.21	1.30	1.43
27	A	4002	BCR	C16-C17	-4.21	1.30	1.43
27	B	4003	BCR	C10-C9	4.20	1.45	1.35
27	B	4004	BCR	C16-C17	-4.20	1.30	1.43
24	A	1128	CLA	MG-ND	-4.19	1.97	2.05
27	B	4001	BCR	C16-C17	-4.19	1.30	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	1	613	CHL	C3B-C4B	4.19	1.45	1.41
27	H	4001	BCR	C10-C9	4.19	1.45	1.35
27	B	4006	BCR	C16-C17	-4.18	1.30	1.43
27	K	4001	BCR	C16-C17	-4.18	1.30	1.43
27	3	504	BCR	C16-C17	-4.18	1.30	1.43
27	8	503	BCR	C10-C9	4.17	1.45	1.35
27	B	4002	BCR	C10-C9	4.17	1.45	1.35
27	3	505	BCR	C10-C9	4.17	1.45	1.35
41	5	613	CHL	C3A-C2A	-4.16	1.51	1.54
37	J	4002	RRX	C20-C21	4.16	1.56	1.43
41	a	609	CHL	C3B-C4B	4.16	1.45	1.41
27	B	4003	BCR	C16-C17	-4.15	1.30	1.43
27	5	503	BCR	C10-C9	4.15	1.45	1.35
41	9	610	CHL	C3A-C2A	-4.15	1.51	1.54
41	4	609	CHL	C2C-C3C	4.15	1.40	1.36
27	B	4007	BCR	C10-C9	4.15	1.45	1.35
27	L	4003	BCR	C16-C17	-4.14	1.30	1.43
27	B	4007	BCR	C16-C17	-4.14	1.30	1.43
27	6	504	BCR	C10-C9	4.13	1.45	1.35
27	4	503	BCR	C16-C17	-4.13	1.30	1.43
27	5	503	BCR	C16-C17	-4.13	1.30	1.43
27	6	503	BCR	C16-C17	-4.12	1.30	1.43
27	8	503	BCR	C16-C17	-4.12	1.30	1.43
27	B	4002	BCR	C16-C17	-4.12	1.30	1.43
27	3	503	BCR	C16-C17	-4.12	1.30	1.43
27	6	504	BCR	C16-C17	-4.12	1.30	1.43
27	H	4001	BCR	C16-C17	-4.11	1.30	1.43
27	3	505	BCR	C16-C17	-4.11	1.30	1.43
27	A	4003	BCR	C16-C17	-4.11	1.30	1.43
27	B	4004	BCR	C10-C9	4.10	1.45	1.35
27	G	4001	BCR	C16-C17	-4.10	1.30	1.43
27	3	504	BCR	C10-C9	4.10	1.45	1.35
27	3	503	BCR	C10-C9	4.08	1.45	1.35
27	7	503	BCR	C10-C9	4.08	1.45	1.35
41	3	611	CHL	C3B-C2B	-4.08	1.34	1.40
37	J	4002	RRX	C23-C22	4.07	1.54	1.46
27	K	4002	BCR	C16-C17	-4.07	1.30	1.43
24	A	1116	CLA	MG-ND	-4.06	1.97	2.05
24	A	1129	CLA	MG-ND	-4.06	1.97	2.05
27	5	504	BCR	C16-C17	-4.06	1.30	1.43
27	B	4005	BCR	C10-C9	4.05	1.45	1.35
27	L	4001	BCR	C16-C17	-4.05	1.30	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	6	503	BCR	C10-C9	4.05	1.45	1.35
27	K	4001	BCR	C10-C9	4.04	1.45	1.35
27	L	4001	BCR	C10-C9	4.04	1.45	1.35
27	A	4005	BCR	C10-C9	4.04	1.45	1.35
24	B	1237	CLA	MG-ND	-4.04	1.97	2.05
27	5	504	BCR	C10-C9	4.03	1.45	1.35
24	A	1012	CLA	MG-ND	-4.02	1.97	2.05
27	G	4001	BCR	C10-C9	4.02	1.45	1.35
24	A	1127	CLA	MG-ND	-4.01	1.97	2.05
24	B	1225	CLA	MG-ND	-4.01	1.97	2.05
41	6	613	CHL	C3A-C2A	-4.01	1.51	1.54
24	B	1223	CLA	MG-ND	-4.01	1.97	2.05
41	a	606	CHL	C2C-C3C	4.00	1.40	1.36
27	I	4001	BCR	C10-C9	4.00	1.45	1.35
24	A	1013	CLA	MG-ND	-3.98	1.97	2.05
24	B	1021	CLA	MG-ND	-3.98	1.97	2.05
24	2	609	CLA	MG-ND	-3.98	1.97	2.05
24	A	1123	CLA	MG-ND	-3.98	1.97	2.05
24	A	1125	CLA	MG-ND	-3.98	1.97	2.05
24	9	605	CLA	MG-ND	-3.97	1.97	2.05
24	B	1216	CLA	MG-ND	-3.97	1.97	2.05
24	B	1023	CLA	MG-ND	-3.96	1.97	2.05
24	A	1133	CLA	MG-ND	-3.96	1.97	2.05
24	B	1022	CLA	MG-ND	-3.96	1.97	2.05
24	a	615	CLA	MG-ND	-3.96	1.97	2.05
27	B	4001	BCR	C10-C9	3.96	1.44	1.35
24	B	1210	CLA	MG-ND	-3.95	1.98	2.05
24	7	610	CLA	MG-ND	-3.95	1.98	2.05
41	a	609	CHL	C3A-C2A	-3.95	1.51	1.54
37	J	4002	RRX	C15-C14	3.94	1.55	1.43
24	B	1219	CLA	MG-ND	-3.94	1.98	2.05
24	B	1202	CLA	MG-ND	-3.94	1.98	2.05
49	7	504	C7Z	C22-C21	3.93	1.66	1.54
24	3	612	CLA	MG-ND	-3.93	1.98	2.05
24	A	1135	CLA	MG-ND	-3.92	1.98	2.05
24	7	605	CLA	MG-ND	-3.92	1.98	2.05
24	4	612	CLA	MG-ND	-3.91	1.98	2.05
24	B	1217	CLA	MG-ND	-3.91	1.98	2.05
27	A	4001	BCR	C10-C9	3.91	1.44	1.35
24	A	1126	CLA	MG-ND	-3.91	1.98	2.05
27	L	4002	BCR	C10-C9	3.91	1.44	1.35
24	B	1206	CLA	MG-ND	-3.90	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	1234	CLA	MG-ND	-3.90	1.98	2.05
24	3	603	CLA	MG-ND	-3.89	1.98	2.05
36	G	5002	ERG	C16-C15	3.89	1.64	1.54
24	A	1117	CLA	MG-ND	-3.89	1.98	2.05
24	9	604	CLA	MG-ND	-3.89	1.98	2.05
49	7	504	C7Z	C2-C1	3.88	1.66	1.54
24	A	1131	CLA	MG-ND	-3.88	1.98	2.05
24	A	1139	CLA	MG-ND	-3.88	1.98	2.05
24	B	1205	CLA	MG-ND	-3.88	1.98	2.05
24	2	621	CLA	MG-ND	-3.88	1.98	2.05
24	5	616	CLA	MG-ND	-3.88	1.98	2.05
24	3	607	CLA	MG-ND	-3.87	1.98	2.05
24	4	610	CLA	MG-ND	-3.87	1.98	2.05
24	6	612	CLA	MG-ND	-3.87	1.98	2.05
24	6	615	CLA	MG-ND	-3.87	1.98	2.05
24	2	604	CLA	MG-ND	-3.87	1.98	2.05
27	F	4001	BCR	C10-C9	3.87	1.44	1.35
24	B	1224	CLA	MG-ND	-3.87	1.98	2.05
24	7	612	CLA	MG-ND	-3.86	1.98	2.05
49	7	504	C7Z	C15-C14	3.86	1.55	1.43
27	J	4001	BCR	C10-C9	3.86	1.44	1.35
24	1	615	CLA	MG-ND	-3.86	1.98	2.05
24	7	608	CLA	MG-ND	-3.85	1.98	2.05
24	L	1502	CLA	MG-ND	-3.85	1.98	2.05
24	A	1119	CLA	MG-ND	-3.85	1.98	2.05
24	6	609	CLA	MG-ND	-3.85	1.98	2.05
24	7	607	CLA	MG-ND	-3.85	1.98	2.05
24	B	1236	CLA	MG-ND	-3.85	1.98	2.05
24	7	615	CLA	MG-ND	-3.85	1.98	2.05
24	8	607	CLA	MG-ND	-3.85	1.98	2.05
24	5	607	CLA	MG-ND	-3.85	1.98	2.05
24	8	612	CLA	MG-ND	-3.84	1.98	2.05
24	A	1107	CLA	MG-ND	-3.84	1.98	2.05
24	5	612	CLA	MG-ND	-3.84	1.98	2.05
24	B	1214	CLA	MG-ND	-3.84	1.98	2.05
41	3	608	CHL	C3B-C4B	3.84	1.45	1.41
24	A	1124	CLA	MG-ND	-3.84	1.98	2.05
24	B	1230	CLA	MG-ND	-3.84	1.98	2.05
24	8	615	CLA	MG-ND	-3.84	1.98	2.05
27	B	4006	BCR	C10-C9	3.84	1.44	1.35
24	B	1215	CLA	MG-ND	-3.83	1.98	2.05
24	1	612	CLA	MG-ND	-3.83	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	605	CLA	MG-ND	-3.83	1.98	2.05
24	8	610	CLA	MG-ND	-3.83	1.98	2.05
24	A	1112	CLA	MG-ND	-3.83	1.98	2.05
24	B	1227	CLA	MG-ND	-3.83	1.98	2.05
24	1	610	CLA	MG-ND	-3.83	1.98	2.05
24	8	602	CLA	MG-ND	-3.83	1.98	2.05
24	4	607	CLA	MG-ND	-3.83	1.98	2.05
24	4	615	CLA	MG-ND	-3.82	1.98	2.05
24	5	609	CLA	MG-ND	-3.82	1.98	2.05
24	7	601	CLA	MG-ND	-3.82	1.98	2.05
24	A	1111	CLA	MG-ND	-3.82	1.98	2.05
24	3	606	CLA	MG-ND	-3.82	1.98	2.05
24	2	613	CLA	MG-ND	-3.82	1.98	2.05
24	7	617	CLA	MG-ND	-3.82	1.98	2.05
27	A	4004	BCR	C10-C9	3.82	1.44	1.35
24	A	1113	CLA	MG-ND	-3.82	1.98	2.05
24	B	1220	CLA	MG-ND	-3.81	1.98	2.05
23	A	1011	CL0	C3A-C2A	-3.81	1.51	1.54
24	B	1211	CLA	MG-ND	-3.81	1.98	2.05
24	A	1118	CLA	MG-ND	-3.81	1.98	2.05
24	a	602	CLA	MG-ND	-3.81	1.98	2.05
24	3	601	CLA	MG-ND	-3.81	1.98	2.05
24	9	609	CLA	MG-ND	-3.81	1.98	2.05
24	a	611	CLA	MG-ND	-3.80	1.98	2.05
24	7	609	CLA	MG-ND	-3.80	1.98	2.05
24	1	601	CLA	MG-ND	-3.80	1.98	2.05
24	5	608	CLA	MG-ND	-3.80	1.98	2.05
24	G	1601	CLA	MG-ND	-3.80	1.98	2.05
24	F	1302	CLA	MG-ND	-3.80	1.98	2.05
24	8	611	CLA	MG-ND	-3.79	1.98	2.05
24	L	1503	CLA	MG-ND	-3.79	1.98	2.05
24	2	605	CLA	MG-ND	-3.79	1.98	2.05
24	4	602	CLA	MG-ND	-3.79	1.98	2.05
24	K	1401	CLA	MG-ND	-3.79	1.98	2.05
24	2	612	CLA	MG-ND	-3.79	1.98	2.05
24	1	602	CLA	MG-ND	-3.79	1.98	2.05
24	B	1238	CLA	MG-ND	-3.79	1.98	2.05
24	A	1122	CLA	MG-ND	-3.79	1.98	2.05
24	8	620	CLA	MG-ND	-3.79	1.98	2.05
24	A	1141	CLA	MG-ND	-3.79	1.98	2.05
24	9	608	CLA	MG-ND	-3.79	1.98	2.05
24	3	613	CLA	MG-ND	-3.79	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	H	1702	CLA	MG-ND	-3.78	1.98	2.05
24	B	1228	CLA	MG-ND	-3.78	1.98	2.05
24	6	602	CLA	MG-ND	-3.78	1.98	2.05
24	5	618	CLA	MG-ND	-3.78	1.98	2.05
24	9	607	CLA	MG-ND	-3.78	1.98	2.05
24	6	607	CLA	MG-ND	-3.78	1.98	2.05
24	B	1208	CLA	MG-ND	-3.78	1.98	2.05
24	1	607	CLA	MG-ND	-3.78	1.98	2.05
24	4	605	CLA	MG-ND	-3.78	1.98	2.05
24	J	1901	CLA	MG-ND	-3.78	1.98	2.05
24	2	615	CLA	MG-ND	-3.78	1.98	2.05
24	B	1212	CLA	MG-ND	-3.78	1.98	2.05
24	H	1701	CLA	MG-ND	-3.78	1.98	2.05
24	5	601	CLA	MG-ND	-3.78	1.98	2.05
27	A	4002	BCR	C10-C9	3.78	1.44	1.35
24	A	1106	CLA	MG-ND	-3.77	1.98	2.05
24	8	618	CLA	MG-ND	-3.77	1.98	2.05
24	6	618	CLA	MG-ND	-3.77	1.98	2.05
24	5	602	CLA	MG-ND	-3.77	1.98	2.05
24	B	1239	CLA	MG-ND	-3.77	1.98	2.05
24	G	1603	CLA	MG-ND	-3.77	1.98	2.05
24	A	1140	CLA	MG-ND	-3.77	1.98	2.05
24	B	1235	CLA	MG-ND	-3.77	1.98	2.05
24	3	605	CLA	MG-ND	-3.77	1.98	2.05
24	9	612	CLA	MG-ND	-3.77	1.98	2.05
24	B	1232	CLA	MG-ND	-3.77	1.98	2.05
24	1	604	CLA	MG-ND	-3.77	1.98	2.05
24	A	1110	CLA	MG-ND	-3.77	1.98	2.05
24	B	1240	CLA	MG-ND	-3.77	1.98	2.05
24	8	605	CLA	MG-ND	-3.77	1.98	2.05
24	K	1403	CLA	MG-ND	-3.76	1.98	2.05
24	A	1130	CLA	MG-ND	-3.76	1.98	2.05
24	1	611	CLA	MG-ND	-3.76	1.98	2.05
24	6	601	CLA	MG-ND	-3.76	1.98	2.05
24	2	610	CLA	MG-ND	-3.76	1.98	2.05
24	2	606	CLA	MG-ND	-3.76	1.98	2.05
24	8	609	CLA	MG-ND	-3.76	1.98	2.05
24	A	1114	CLA	MG-ND	-3.76	1.98	2.05
24	B	1203	CLA	MG-ND	-3.76	1.98	2.05
24	B	1231	CLA	MG-ND	-3.76	1.98	2.05
24	3	616	CLA	MG-ND	-3.76	1.98	2.05
24	A	1137	CLA	MG-ND	-3.75	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	1222	CLA	MG-ND	-3.75	1.98	2.05
24	a	605	CLA	MG-ND	-3.75	1.98	2.05
24	2	602	CLA	MG-ND	-3.75	1.98	2.05
24	9	602	CLA	MG-ND	-3.75	1.98	2.05
24	4	601	CLA	MG-ND	-3.75	1.98	2.05
24	5	604	CLA	MG-ND	-3.75	1.98	2.05
24	a	608	CLA	MG-ND	-3.75	1.98	2.05
24	A	1121	CLA	MG-ND	-3.75	1.98	2.05
24	7	604	CLA	MG-ND	-3.75	1.98	2.05
41	4	618	CHL	C2C-C3C	3.74	1.40	1.36
24	5	614	CLA	MG-ND	-3.74	1.98	2.05
24	6	606	CLA	MG-ND	-3.74	1.98	2.05
24	A	1102	CLA	MG-ND	-3.74	1.98	2.05
24	B	1218	CLA	MG-ND	-3.74	1.98	2.05
24	6	605	CLA	MG-ND	-3.74	1.98	2.05
24	a	604	CLA	MG-ND	-3.74	1.98	2.05
24	5	606	CLA	MG-ND	-3.74	1.98	2.05
24	5	617	CLA	MG-ND	-3.74	1.98	2.05
24	A	1103	CLA	MG-ND	-3.74	1.98	2.05
24	F	1301	CLA	MG-ND	-3.74	1.98	2.05
24	4	606	CLA	MG-ND	-3.74	1.98	2.05
24	1	605	CLA	MG-ND	-3.73	1.98	2.05
24	2	608	CLA	MG-ND	-3.73	1.98	2.05
24	9	606	CLA	MG-ND	-3.73	1.98	2.05
24	8	606	CLA	MG-ND	-3.73	1.98	2.05
24	6	608	CLA	MG-ND	-3.73	1.98	2.05
29	B	5003	DGD	CAB-C9B	-3.73	1.33	1.51
29	B	5003	DGD	CDB-CCB	-3.73	1.33	1.51
24	7	611	CLA	MG-ND	-3.73	1.98	2.05
29	B	5003	DGD	CGB-CFB	-3.73	1.33	1.51
24	7	602	CLA	MG-ND	-3.73	1.98	2.05
24	9	603	CLA	MG-ND	-3.73	1.98	2.05
24	G	1602	CLA	MG-ND	-3.72	1.98	2.05
24	1	608	CLA	MG-ND	-3.72	1.98	2.05
24	a	607	CLA	MG-ND	-3.72	1.98	2.05
41	4	613	CHL	C3B-C4B	3.72	1.45	1.41
24	6	604	CLA	MG-ND	-3.72	1.98	2.05
24	a	612	CLA	MG-ND	-3.72	1.98	2.05
24	A	1115	CLA	MG-ND	-3.72	1.98	2.05
24	K	1404	CLA	MG-ND	-3.72	1.98	2.05
24	7	603	CLA	MG-ND	-3.72	1.98	2.05
24	B	1213	CLA	MG-ND	-3.72	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1105	CLA	MG-ND	-3.71	1.98	2.05
24	A	1104	CLA	MG-ND	-3.71	1.98	2.05
29	B	5003	DGD	CGA-CFA	-3.71	1.33	1.51
24	2	603	CLA	MG-ND	-3.71	1.98	2.05
24	A	1120	CLA	MG-ND	-3.71	1.98	2.05
24	B	1204	CLA	MG-ND	-3.71	1.98	2.05
24	4	617	CLA	MG-ND	-3.71	1.98	2.05
29	8	802	DGD	CAB-C9B	-3.71	1.33	1.51
24	2	607	CLA	MG-ND	-3.71	1.98	2.05
24	4	604	CLA	MG-ND	-3.71	1.98	2.05
24	3	610	CLA	MG-ND	-3.71	1.98	2.05
24	A	1132	CLA	MG-ND	-3.70	1.98	2.05
29	8	802	DGD	CDA-CCA	-3.70	1.33	1.51
24	4	616	CLA	MG-ND	-3.70	1.98	2.05
24	a	601	CLA	MG-ND	-3.70	1.98	2.05
24	8	603	CLA	MG-ND	-3.70	1.98	2.05
24	A	1136	CLA	MG-ND	-3.70	1.98	2.05
24	H	1703	CLA	MG-ND	-3.70	1.98	2.05
43	3	506	QTB	C17-C11	-3.70	1.52	1.55
24	K	1402	CLA	MG-ND	-3.69	1.98	2.05
24	3	602	CLA	MG-ND	-3.69	1.98	2.05
24	A	1138	CLA	MG-ND	-3.69	1.98	2.05
24	2	601	CLA	MG-ND	-3.69	1.98	2.05
24	4	608	CLA	MG-ND	-3.69	1.98	2.05
24	A	1108	CLA	MG-ND	-3.69	1.98	2.05
24	B	1201	CLA	MG-ND	-3.69	1.98	2.05
24	B	1207	CLA	MG-ND	-3.68	1.98	2.05
24	7	606	CLA	MG-ND	-3.68	1.98	2.05
29	8	802	DGD	CDB-CCB	-3.68	1.33	1.51
29	8	802	DGD	CGB-CFB	-3.68	1.33	1.51
24	A	1134	CLA	MG-ND	-3.68	1.98	2.05
24	3	618	CLA	MG-ND	-3.68	1.98	2.05
24	A	1101	CLA	MG-ND	-3.68	1.98	2.05
24	B	1209	CLA	MG-ND	-3.68	1.98	2.05
24	4	611	CLA	MG-ND	-3.68	1.98	2.05
29	B	5003	DGD	CAA-C9A	-3.68	1.33	1.51
29	8	802	DGD	CGA-CFA	-3.67	1.33	1.51
24	6	603	CLA	MG-ND	-3.67	1.98	2.05
24	6	617	CLA	MG-ND	-3.67	1.98	2.05
24	3	604	CLA	MG-ND	-3.67	1.98	2.05
24	a	603	CLA	MG-ND	-3.67	1.98	2.05
41	5	610	CHL	C3A-C2A	-3.67	1.51	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	9	601	CLA	MG-ND	-3.67	1.98	2.05
24	5	603	CLA	MG-ND	-3.67	1.98	2.05
24	L	1501	CLA	MG-ND	-3.67	1.98	2.05
29	8	802	DGD	CAA-C9A	-3.67	1.33	1.51
49	7	504	C7Z	C27-C26	3.66	1.57	1.45
24	8	608	CLA	MG-ND	-3.65	1.98	2.05
24	1	606	CLA	MG-ND	-3.65	1.98	2.05
41	4	613	CHL	CBB-CAB	3.65	1.52	1.29
29	B	5003	DGD	CDA-CCA	-3.65	1.33	1.51
46	8	803	DGA	OG2-CB1	3.64	1.44	1.34
41	1	609	CHL	C3B-C4B	3.64	1.44	1.41
24	A	1109	CLA	MG-ND	-3.63	1.98	2.05
24	4	603	CLA	MG-ND	-3.62	1.98	2.05
24	1	603	CLA	MG-ND	-3.62	1.98	2.05
24	B	1210	CLA	C1C-NC	-3.62	1.32	1.37
41	6	619	CHL	CBB-CAB	3.61	1.52	1.29
49	7	504	C7Z	C35-C34	3.61	1.54	1.43
41	a	613	CHL	CBB-CAB	3.61	1.51	1.29
41	3	608	CHL	CBB-CAB	3.60	1.51	1.29
41	5	611	CHL	CBB-CAB	3.59	1.51	1.29
41	5	613	CHL	CBB-CAB	3.58	1.51	1.29
41	9	613	CHL	CBB-CAB	3.58	1.51	1.29
34	B	5007	LAP	P9-O6	3.57	1.73	1.59
41	1	609	CHL	CBB-CAB	3.56	1.51	1.29
41	9	610	CHL	CBB-CAB	3.56	1.51	1.29
41	a	610	CHL	CBB-CAB	3.56	1.51	1.29
24	A	1128	CLA	C1C-NC	-3.56	1.32	1.37
34	F	5003	LAP	P9-O6	3.55	1.73	1.59
41	1	613	CHL	CBB-CAB	3.55	1.51	1.29
34	K	5001	LAP	P9-O6	3.55	1.73	1.59
49	7	504	C7Z	C7-C6	3.54	1.57	1.45
41	a	609	CHL	CBB-CAB	3.54	1.51	1.29
37	J	4002	RRX	C11-C10	3.53	1.54	1.43
49	7	504	C7Z	C38-C25	3.52	1.56	1.50
41	9	613	CHL	C2A-C3A	-3.51	1.51	1.54
37	J	4002	RRX	C29-C30	3.51	1.65	1.54
41	5	610	CHL	CBB-CAB	3.50	1.51	1.29
41	4	609	CHL	CBB-CAB	3.50	1.51	1.29
41	4	618	CHL	CBB-CAB	3.49	1.51	1.29
41	9	610	CHL	C2C-C3C	3.48	1.39	1.36
37	J	4002	RRX	C16-C17	3.47	1.54	1.43
41	8	613	CHL	CBB-CAB	3.47	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	5	803	DGA	OG2-CB1	3.47	1.44	1.34
24	4	610	CLA	C1C-NC	-3.46	1.32	1.37
41	8	604	CHL	C3B-C2B	-3.46	1.35	1.40
24	B	1229	CLA	MG-ND	-3.46	1.98	2.05
41	8	613	CHL	C2C-C3C	3.46	1.39	1.36
24	B	1206	CLA	C1C-NC	-3.43	1.32	1.37
41	9	613	CHL	C2C-C3C	3.43	1.39	1.36
24	3	601	CLA	C1C-NC	-3.42	1.32	1.37
32	B	5004	PCW	O3-C11	3.41	1.43	1.33
24	A	1111	CLA	C1C-NC	-3.40	1.32	1.37
37	J	4002	RRX	C24-C25	3.40	1.56	1.45
41	6	613	CHL	CBB-CAB	3.39	1.50	1.29
24	7	601	CLA	C1C-NC	-3.39	1.32	1.37
41	8	613	CHL	C3A-C2A	-3.37	1.51	1.54
41	6	611	CHL	CBB-CAB	3.37	1.50	1.29
24	B	1225	CLA	C1C-NC	-3.36	1.32	1.37
46	5	803	DGA	OG1-CA1	3.36	1.43	1.33
24	A	1125	CLA	C1C-NC	-3.36	1.32	1.37
24	A	1132	CLA	C1C-NC	-3.36	1.32	1.37
32	6	803	PCW	O3-C11	3.35	1.43	1.33
24	B	1230	CLA	C1C-NC	-3.35	1.32	1.37
24	1	610	CLA	C1C-NC	-3.34	1.32	1.37
24	A	1112	CLA	C1C-NC	-3.33	1.32	1.37
24	A	1106	CLA	C1C-NC	-3.32	1.32	1.37
24	3	606	CLA	C1C-NC	-3.31	1.32	1.37
46	8	803	DGA	OG1-CA1	3.31	1.43	1.33
24	4	611	CLA	C1C-NC	-3.30	1.32	1.37
24	9	604	CLA	C1C-NC	-3.30	1.32	1.37
24	5	605	CLA	C1C-NC	-3.30	1.32	1.37
24	5	601	CLA	C1C-NC	-3.30	1.32	1.37
24	A	1138	CLA	C1C-NC	-3.30	1.32	1.37
41	7	613	CHL	CBB-CAB	3.30	1.50	1.29
24	5	604	CLA	C1C-NC	-3.29	1.32	1.37
41	a	606	CHL	CBB-CAB	3.29	1.50	1.29
41	6	610	CHL	C2C-C3C	3.29	1.39	1.36
41	3	611	CHL	C2C-C3C	3.29	1.39	1.36
24	B	1207	CLA	C1C-NC	-3.29	1.32	1.37
24	A	1108	CLA	C1C-NC	-3.28	1.32	1.37
41	1	613	CHL	C3A-C2A	-3.28	1.51	1.54
41	5	611	CHL	C3B-C4B	3.28	1.44	1.41
24	A	1109	CLA	C1C-NC	-3.28	1.32	1.37
24	4	601	CLA	C1C-NC	-3.27	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	1212	CLA	C1C-NC	-3.27	1.32	1.37
24	9	612	CLA	C1C-NC	-3.27	1.32	1.37
24	7	610	CLA	C1C-NC	-3.27	1.32	1.37
24	B	1209	CLA	C1C-NC	-3.27	1.32	1.37
24	7	609	CLA	C1C-NC	-3.26	1.32	1.37
24	A	1101	CLA	C1C-NC	-3.26	1.32	1.37
24	B	1234	CLA	C1C-NC	-3.26	1.32	1.37
24	A	1114	CLA	C1C-NC	-3.25	1.32	1.37
24	B	1204	CLA	C1C-NC	-3.25	1.32	1.37
41	6	610	CHL	CBB-CAB	3.25	1.49	1.29
24	A	1127	CLA	C1C-NC	-3.24	1.32	1.37
24	A	1135	CLA	C1C-NC	-3.24	1.32	1.37
24	B	1239	CLA	C1C-NC	-3.24	1.32	1.37
24	A	1103	CLA	C1C-NC	-3.24	1.32	1.37
24	4	605	CLA	C1C-NC	-3.24	1.32	1.37
24	B	1236	CLA	C1C-NC	-3.23	1.32	1.37
24	A	1124	CLA	C1C-NC	-3.23	1.32	1.37
24	A	1116	CLA	C1C-NC	-3.23	1.32	1.37
41	3	611	CHL	CBB-CAB	3.23	1.49	1.29
24	8	605	CLA	C1C-NC	-3.23	1.32	1.37
24	A	1117	CLA	C1C-NC	-3.23	1.32	1.37
24	B	1023	CLA	C1C-NC	-3.22	1.32	1.37
24	8	612	CLA	C1C-NC	-3.22	1.32	1.37
24	B	1226	CLA	C1C-NC	-3.22	1.32	1.37
24	3	613	CLA	C1C-NC	-3.22	1.32	1.37
24	B	1237	CLA	C1C-NC	-3.22	1.32	1.37
24	8	609	CLA	C1C-NC	-3.22	1.32	1.37
24	B	1203	CLA	C1C-NC	-3.22	1.32	1.37
24	B	1223	CLA	C1C-NC	-3.21	1.32	1.37
24	A	1133	CLA	C1C-NC	-3.21	1.32	1.37
24	B	1229	CLA	C1C-NC	-3.21	1.32	1.37
24	G	1603	CLA	C1C-NC	-3.21	1.32	1.37
24	3	610	CLA	C1C-NC	-3.21	1.32	1.37
24	A	1130	CLA	C1C-NC	-3.20	1.32	1.37
24	3	616	CLA	C1C-NC	-3.20	1.32	1.37
24	A	1121	CLA	C1C-NC	-3.20	1.32	1.37
24	6	612	CLA	C1C-NC	-3.20	1.32	1.37
24	B	1205	CLA	C1C-NC	-3.20	1.32	1.37
24	3	605	CLA	C1C-NC	-3.20	1.32	1.37
24	B	1214	CLA	C1C-NC	-3.20	1.32	1.37
24	A	1105	CLA	C1C-NC	-3.20	1.32	1.37
24	1	607	CLA	C1C-NC	-3.20	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1120	CLA	C1C-NC	-3.19	1.32	1.37
24	B	1216	CLA	C1C-NC	-3.19	1.32	1.37
24	7	604	CLA	C1C-NC	-3.19	1.32	1.37
24	3	604	CLA	C1C-NC	-3.19	1.32	1.37
24	B	1211	CLA	C1C-NC	-3.19	1.32	1.37
24	1	605	CLA	C1C-NC	-3.18	1.32	1.37
24	2	603	CLA	C1C-NC	-3.18	1.32	1.37
24	B	1021	CLA	C1C-NC	-3.18	1.32	1.37
24	5	618	CLA	C1C-NC	-3.18	1.32	1.37
24	A	1113	CLA	C1C-NC	-3.18	1.32	1.37
41	8	601	CHL	CBB-CAB	3.18	1.49	1.29
41	8	604	CHL	CBB-CAB	3.17	1.49	1.29
24	6	609	CLA	C1C-NC	-3.17	1.32	1.37
24	A	1107	CLA	C1C-NC	-3.17	1.32	1.37
24	5	617	CLA	C1C-NC	-3.17	1.32	1.37
24	3	612	CLA	C1C-NC	-3.17	1.32	1.37
24	5	603	CLA	C1C-NC	-3.17	1.32	1.37
41	8	601	CHL	CHB-C4A	-3.16	1.34	1.38
24	K	1401	CLA	C1C-NC	-3.16	1.32	1.37
24	K	1403	CLA	C1C-NC	-3.16	1.32	1.37
24	A	1119	CLA	C1C-NC	-3.15	1.32	1.37
24	A	1140	CLA	C1C-NC	-3.15	1.32	1.37
24	4	603	CLA	C1C-NC	-3.15	1.32	1.37
24	7	608	CLA	C1C-NC	-3.15	1.32	1.37
24	A	1122	CLA	C1C-NC	-3.15	1.32	1.37
41	8	604	CHL	C1A-CHA	-3.15	1.36	1.40
24	8	610	CLA	C1C-NC	-3.15	1.32	1.37
41	a	606	CHL	C3B-C2B	-3.15	1.36	1.40
24	L	1503	CLA	C1C-NC	-3.15	1.32	1.37
24	5	612	CLA	C1C-NC	-3.15	1.32	1.37
24	B	1215	CLA	C1C-NC	-3.14	1.32	1.37
24	7	612	CLA	C1C-NC	-3.14	1.32	1.37
24	B	1222	CLA	C1C-NC	-3.14	1.32	1.37
24	4	615	CLA	C1C-NC	-3.14	1.32	1.37
24	B	1228	CLA	C1C-NC	-3.14	1.32	1.37
37	J	4002	RRX	C4-C5	-3.14	1.45	1.51
24	A	1131	CLA	C1C-NC	-3.14	1.32	1.37
24	B	1238	CLA	C1C-NC	-3.13	1.33	1.37
24	a	605	CLA	C1C-NC	-3.13	1.33	1.37
24	6	605	CLA	C1C-NC	-3.13	1.33	1.37
24	A	1136	CLA	C1C-NC	-3.13	1.33	1.37
24	7	615	CLA	C1C-NC	-3.13	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	8	606	CLA	C1C-NC	-3.13	1.33	1.37
24	7	607	CLA	C1C-NC	-3.13	1.33	1.37
24	B	1202	CLA	C1C-NC	-3.12	1.33	1.37
24	a	601	CLA	C1C-NC	-3.12	1.33	1.37
24	a	603	CLA	C1C-NC	-3.12	1.33	1.37
24	B	1218	CLA	C1C-NC	-3.12	1.33	1.37
24	1	604	CLA	C1C-NC	-3.12	1.33	1.37
24	1	611	CLA	C1C-NC	-3.12	1.33	1.37
24	1	601	CLA	C1C-NC	-3.12	1.33	1.37
41	4	613	CHL	C1A-CHA	-3.11	1.36	1.40
24	8	602	CLA	C1C-NC	-3.11	1.33	1.37
24	A	1137	CLA	C1C-NC	-3.11	1.33	1.37
24	2	615	CLA	C1C-NC	-3.11	1.33	1.37
24	B	1231	CLA	C1C-NC	-3.11	1.33	1.37
24	6	601	CLA	C1C-NC	-3.11	1.33	1.37
24	B	1208	CLA	C1C-NC	-3.11	1.33	1.37
24	H	1703	CLA	C1C-NC	-3.11	1.33	1.37
24	9	607	CLA	C1C-NC	-3.11	1.33	1.37
41	a	606	CHL	C3A-C2A	-3.11	1.52	1.54
24	8	615	CLA	C1C-NC	-3.11	1.33	1.37
41	8	601	CHL	C3B-C2B	-3.11	1.36	1.40
24	6	617	CLA	C1C-NC	-3.11	1.33	1.37
24	5	614	CLA	C1C-NC	-3.11	1.33	1.37
24	3	601	CLA	C4B-NB	-3.11	1.33	1.37
24	a	604	CLA	C1C-NC	-3.10	1.33	1.37
24	8	618	CLA	C1C-NC	-3.10	1.33	1.37
24	8	608	CLA	C1C-NC	-3.10	1.33	1.37
24	6	618	CLA	C1C-NC	-3.10	1.33	1.37
24	A	1126	CLA	C1C-NC	-3.10	1.33	1.37
24	7	611	CLA	C1C-NC	-3.10	1.33	1.37
24	1	602	CLA	C1C-NC	-3.10	1.33	1.37
24	4	607	CLA	C1C-NC	-3.10	1.33	1.37
24	9	604	CLA	C4B-NB	-3.10	1.33	1.37
41	8	613	CHL	C3B-C2B	-3.10	1.36	1.40
37	J	4002	RRX	C7-C6	3.10	1.55	1.45
24	B	1022	CLA	C1C-NC	-3.10	1.33	1.37
24	9	605	CLA	C1C-NC	-3.09	1.33	1.37
24	5	616	CLA	C1C-NC	-3.09	1.33	1.37
24	7	602	CLA	C1C-NC	-3.09	1.33	1.37
24	B	1224	CLA	C1C-NC	-3.09	1.33	1.37
24	A	1115	CLA	C1C-NC	-3.09	1.33	1.37
24	4	604	CLA	C1C-NC	-3.09	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	4	617	CLA	C1C-NC	-3.09	1.33	1.37
24	A	1139	CLA	C1C-NC	-3.08	1.33	1.37
24	B	1232	CLA	C1C-NC	-3.08	1.33	1.37
24	A	1118	CLA	C1C-NC	-3.08	1.33	1.37
24	4	602	CLA	C1C-NC	-3.08	1.33	1.37
24	L	1502	CLA	C1C-NC	-3.08	1.33	1.37
24	6	606	CLA	C1C-NC	-3.08	1.33	1.37
24	8	603	CLA	C1C-NC	-3.08	1.33	1.37
24	B	1235	CLA	C1C-NC	-3.08	1.33	1.37
24	F	1302	CLA	C1C-NC	-3.08	1.33	1.37
24	2	605	CLA	C1C-NC	-3.08	1.33	1.37
24	7	617	CLA	C1C-NC	-3.08	1.33	1.37
24	3	603	CLA	C1C-NC	-3.08	1.33	1.37
24	3	607	CLA	C1C-NC	-3.08	1.33	1.37
24	2	612	CLA	C1C-NC	-3.08	1.33	1.37
24	a	612	CLA	C1C-NC	-3.08	1.33	1.37
24	6	607	CLA	C1C-NC	-3.08	1.33	1.37
24	6	602	CLA	C1C-NC	-3.07	1.33	1.37
24	A	1110	CLA	C1C-NC	-3.07	1.33	1.37
24	a	615	CLA	C1C-NC	-3.07	1.33	1.37
24	B	1219	CLA	C1C-NC	-3.07	1.33	1.37
24	2	608	CLA	C1C-NC	-3.07	1.33	1.37
24	B	1213	CLA	C1C-NC	-3.07	1.33	1.37
24	7	605	CLA	C1C-NC	-3.07	1.33	1.37
24	B	1227	CLA	C1C-NC	-3.07	1.33	1.37
24	1	603	CLA	C1C-NC	-3.06	1.33	1.37
24	B	1220	CLA	C1C-NC	-3.06	1.33	1.37
24	8	611	CLA	C1C-NC	-3.06	1.33	1.37
24	4	606	CLA	C1C-NC	-3.06	1.33	1.37
24	6	603	CLA	C1C-NC	-3.06	1.33	1.37
24	4	612	CLA	C1C-NC	-3.06	1.33	1.37
24	A	1104	CLA	C1C-NC	-3.06	1.33	1.37
24	6	604	CLA	C1C-NC	-3.05	1.33	1.37
24	a	608	CLA	C1C-NC	-3.05	1.33	1.37
24	2	613	CLA	C1C-NC	-3.05	1.33	1.37
24	9	608	CLA	C1C-NC	-3.05	1.33	1.37
24	a	602	CLA	C1C-NC	-3.05	1.33	1.37
24	B	1240	CLA	C1C-NC	-3.05	1.33	1.37
49	7	504	C7Z	C21-C26	-3.05	1.49	1.53
24	F	1301	CLA	C1C-NC	-3.05	1.33	1.37
24	5	609	CLA	C1C-NC	-3.05	1.33	1.37
24	2	607	CLA	C1C-NC	-3.05	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	8	607	CLA	C1C-NC	-3.05	1.33	1.37
24	7	606	CLA	C1C-NC	-3.05	1.33	1.37
24	1	606	CLA	C1C-NC	-3.05	1.33	1.37
24	5	606	CLA	C1C-NC	-3.05	1.33	1.37
24	5	607	CLA	C1C-NC	-3.05	1.33	1.37
41	7	613	CHL	C3B-C2B	-3.05	1.36	1.40
24	3	602	CLA	C1C-NC	-3.05	1.33	1.37
24	K	1404	CLA	C1C-NC	-3.05	1.33	1.37
24	1	612	CLA	C1C-NC	-3.04	1.33	1.37
24	9	609	CLA	C1C-NC	-3.04	1.33	1.37
24	2	621	CLA	C1C-NC	-3.04	1.33	1.37
34	B	5007	LAP	P9-O4	3.04	1.71	1.59
24	9	603	CLA	C1C-NC	-3.04	1.33	1.37
24	7	603	CLA	C1C-NC	-3.03	1.33	1.37
24	2	602	CLA	C1C-NC	-3.03	1.33	1.37
24	L	1501	CLA	C1C-NC	-3.03	1.33	1.37
51	8	806	P5S	O37-C38	3.03	1.42	1.34
24	5	608	CLA	C1C-NC	-3.03	1.33	1.37
24	2	606	CLA	C1C-NC	-3.03	1.33	1.37
24	B	1217	CLA	C1C-NC	-3.03	1.33	1.37
24	B	1201	CLA	C1C-NC	-3.03	1.33	1.37
24	4	616	CLA	C1C-NC	-3.03	1.33	1.37
24	9	602	CLA	C1C-NC	-3.03	1.33	1.37
41	6	613	CHL	C3B-C4B	3.03	1.44	1.41
24	A	1129	CLA	C1C-NC	-3.02	1.33	1.37
24	A	1134	CLA	C1C-NC	-3.02	1.33	1.37
24	J	1901	CLA	C1C-NC	-3.02	1.33	1.37
24	3	618	CLA	C1C-NC	-3.02	1.33	1.37
24	A	1013	CLA	C1C-NC	-3.02	1.33	1.37
24	1	608	CLA	C1C-NC	-3.02	1.33	1.37
24	H	1702	CLA	C1C-NC	-3.02	1.33	1.37
24	6	608	CLA	C1C-NC	-3.01	1.33	1.37
24	a	607	CLA	C1C-NC	-3.01	1.33	1.37
24	6	615	CLA	C1C-NC	-3.01	1.33	1.37
24	A	1123	CLA	C1C-NC	-3.01	1.33	1.37
24	5	602	CLA	C1C-NC	-3.01	1.33	1.37
24	A	1012	CLA	C1C-NC	-3.00	1.33	1.37
24	2	601	CLA	C1C-NC	-3.00	1.33	1.37
24	B	1221	CLA	C1C-NC	-3.00	1.33	1.37
24	1	615	CLA	C1C-NC	-3.00	1.33	1.37
24	K	1402	CLA	C1C-NC	-2.99	1.33	1.37
24	2	604	CLA	C1C-NC	-2.99	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	1602	CLA	C1C-NC	-2.99	1.33	1.37
24	A	1141	CLA	C1C-NC	-2.99	1.33	1.37
24	9	601	CLA	C1C-NC	-2.99	1.33	1.37
24	4	608	CLA	C1C-NC	-2.98	1.33	1.37
24	a	611	CLA	C1C-NC	-2.98	1.33	1.37
24	9	606	CLA	C1C-NC	-2.98	1.33	1.37
24	2	609	CLA	C1C-NC	-2.96	1.33	1.37
24	A	1102	CLA	C1C-NC	-2.96	1.33	1.37
24	G	1601	CLA	C1C-NC	-2.96	1.33	1.37
24	8	620	CLA	C1C-NC	-2.95	1.33	1.37
24	2	610	CLA	C1C-NC	-2.95	1.33	1.37
24	B	1210	CLA	C4B-NB	-2.94	1.34	1.37
34	K	5001	LAP	P9-O4	2.93	1.70	1.59
29	A	5005	DGD	CAB-C9B	-2.93	1.33	1.51
24	A	1111	CLA	C4B-NB	-2.92	1.34	1.37
24	B	1022	CLA	C4B-NB	-2.90	1.34	1.37
24	6	612	CLA	C4B-NB	-2.90	1.34	1.37
41	7	613	CHL	CHB-C4A	-2.90	1.35	1.38
24	B	1204	CLA	C4B-NB	-2.89	1.34	1.37
24	4	601	CLA	C4B-NB	-2.89	1.34	1.37
41	4	613	CHL	C1B-C2B	2.89	1.42	1.39
24	5	601	CLA	C4B-NB	-2.89	1.34	1.37
41	3	608	CHL	C1B-C2B	2.88	1.42	1.39
34	F	5003	LAP	P9-O4	2.88	1.70	1.59
24	5	604	CLA	C4B-NB	-2.87	1.34	1.37
41	5	610	CHL	C1D-C2D	2.87	1.42	1.39
37	J	4002	RRX	C32-C1	2.86	1.59	1.53
36	G	5002	ERG	C4-C5	2.86	1.57	1.51
24	A	1126	CLA	C4B-NB	-2.86	1.34	1.37
24	B	1203	CLA	C4B-NB	-2.85	1.34	1.37
24	1	605	CLA	C4B-NB	-2.85	1.34	1.37
38	a	804	LPX	P1-O1	2.85	1.70	1.59
38	J	5001	LPX	P1-O1	2.85	1.70	1.59
41	a	613	CHL	C1A-CHA	-2.85	1.36	1.40
23	A	1011	CL0	CHB-C4A	-2.85	1.35	1.38
24	A	1112	CLA	C4B-NB	-2.85	1.34	1.37
24	7	612	CLA	C4B-NB	-2.84	1.34	1.37
24	4	604	CLA	C4B-NB	-2.84	1.34	1.37
24	A	1128	CLA	C4B-NB	-2.83	1.34	1.37
24	3	610	CLA	C4B-NB	-2.83	1.34	1.37
41	8	604	CHL	CHB-C4A	-2.83	1.35	1.38
41	6	619	CHL	C1D-C2D	2.83	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	1224	CLA	C4B-NB	-2.83	1.34	1.37
24	3	606	CLA	C4B-NB	-2.82	1.34	1.37
24	A	1135	CLA	C4B-NB	-2.82	1.34	1.37
24	A	1123	CLA	C4B-NB	-2.82	1.34	1.37
24	A	1132	CLA	C4B-NB	-2.82	1.34	1.37
24	B	1234	CLA	C4B-NB	-2.82	1.34	1.37
41	a	606	CHL	CHB-C4A	-2.82	1.35	1.38
24	H	1701	CLA	C1C-NC	-2.82	1.33	1.37
41	4	613	CHL	C1D-C2D	2.82	1.42	1.39
41	a	613	CHL	CHB-C4A	-2.81	1.35	1.38
41	a	606	CHL	C1D-C2D	2.81	1.42	1.39
24	A	1113	CLA	C4B-NB	-2.81	1.34	1.37
24	A	1117	CLA	C4B-NB	-2.81	1.34	1.37
24	B	1237	CLA	C4B-NB	-2.81	1.34	1.37
24	3	604	CLA	C4B-NB	-2.81	1.34	1.37
24	A	1125	CLA	C4B-NB	-2.80	1.34	1.37
24	1	611	CLA	C4B-NB	-2.80	1.34	1.37
24	1	604	CLA	C4B-NB	-2.80	1.34	1.37
41	5	611	CHL	C2C-C3C	2.80	1.39	1.36
41	9	613	CHL	C1B-C2B	2.80	1.42	1.39
41	8	601	CHL	C1A-CHA	-2.80	1.36	1.40
24	B	1206	CLA	C4B-NB	-2.80	1.34	1.37
24	B	1211	CLA	C4B-NB	-2.80	1.34	1.37
41	5	611	CHL	C1B-C2B	2.80	1.42	1.39
24	B	1023	CLA	C4B-NB	-2.79	1.34	1.37
41	6	610	CHL	CHB-C4A	-2.79	1.35	1.38
24	B	1222	CLA	C4B-NB	-2.79	1.34	1.37
24	A	1105	CLA	C4B-NB	-2.79	1.34	1.37
24	5	612	CLA	C4B-NB	-2.79	1.34	1.37
24	8	612	CLA	C4B-NB	-2.79	1.34	1.37
24	3	613	CLA	C4B-NB	-2.79	1.34	1.37
24	A	1130	CLA	C4B-NB	-2.79	1.34	1.37
24	A	1107	CLA	C4B-NB	-2.79	1.34	1.37
24	3	605	CLA	C4B-NB	-2.78	1.34	1.37
24	A	1116	CLA	C4B-NB	-2.78	1.34	1.37
24	B	1219	CLA	C4B-NB	-2.78	1.34	1.37
41	a	609	CHL	CHB-C4A	-2.78	1.35	1.38
24	7	601	CLA	C4B-NB	-2.78	1.34	1.37
41	4	609	CHL	C1D-C2D	2.78	1.42	1.39
41	6	613	CHL	C1B-C2B	2.78	1.42	1.39
24	3	602	CLA	C4B-NB	-2.77	1.34	1.37
41	1	613	CHL	C1B-C2B	2.77	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	1238	CLA	C4B-NB	-2.77	1.34	1.37
24	3	612	CLA	C4B-NB	-2.77	1.34	1.37
41	a	610	CHL	C1B-C2B	2.76	1.42	1.39
24	A	1129	CLA	C4B-NB	-2.76	1.34	1.37
41	1	609	CHL	C1B-C2B	2.76	1.42	1.39
41	7	613	CHL	C1D-C2D	2.76	1.42	1.39
41	5	610	CHL	CHB-C4A	-2.75	1.35	1.38
24	7	611	CLA	C4B-NB	-2.75	1.34	1.37
41	8	601	CHL	C1D-C2D	2.75	1.42	1.39
41	3	611	CHL	CHB-C4A	-2.75	1.35	1.38
24	A	1138	CLA	C4B-NB	-2.75	1.34	1.37
24	6	609	CLA	C4B-NB	-2.75	1.34	1.37
41	4	609	CHL	CHB-C4A	-2.74	1.35	1.38
41	a	609	CHL	C1D-C2D	2.74	1.42	1.39
41	9	613	CHL	C3B-C4B	2.74	1.44	1.41
24	B	1201	CLA	C4B-NB	-2.74	1.34	1.37
41	6	611	CHL	CHB-C4A	-2.74	1.35	1.38
24	A	1124	CLA	C4B-NB	-2.73	1.34	1.37
24	B	1218	CLA	C4B-NB	-2.73	1.34	1.37
24	1	612	CLA	C4B-NB	-2.73	1.34	1.37
24	A	1102	CLA	C4B-NB	-2.73	1.34	1.37
41	4	618	CHL	C1B-C2B	2.73	1.42	1.39
24	1	610	CLA	C4B-NB	-2.73	1.34	1.37
24	7	605	CLA	C4B-NB	-2.73	1.34	1.37
24	8	606	CLA	C4B-NB	-2.73	1.34	1.37
24	1	601	CLA	C4B-NB	-2.72	1.34	1.37
24	8	610	CLA	C4B-NB	-2.72	1.34	1.37
41	5	613	CHL	CHB-C4A	-2.72	1.35	1.38
24	3	603	CLA	C4B-NB	-2.72	1.34	1.37
41	6	611	CHL	C1D-C2D	2.72	1.42	1.39
41	8	613	CHL	C1B-C2B	2.72	1.42	1.39
24	A	1012	CLA	C4B-NB	-2.72	1.34	1.37
24	2	605	CLA	C4B-NB	-2.72	1.34	1.37
48	7	502	XAT	O24-C25	-2.72	1.42	1.46
41	6	619	CHL	C1B-C2B	2.72	1.42	1.39
41	a	613	CHL	C1B-C2B	2.72	1.42	1.39
24	9	605	CLA	C4B-NB	-2.71	1.34	1.37
24	1	606	CLA	C4B-NB	-2.71	1.34	1.37
41	4	618	CHL	C1D-C2D	2.71	1.42	1.39
24	B	1226	CLA	C4B-NB	-2.71	1.34	1.37
24	5	603	CLA	C4B-NB	-2.71	1.34	1.37
41	9	610	CHL	C1B-C2B	2.71	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	a	613	CHL	C1D-C2D	2.71	1.42	1.39
41	5	613	CHL	C1B-C2B	2.71	1.42	1.39
24	A	1121	CLA	C4B-NB	-2.71	1.34	1.37
24	5	606	CLA	C4B-NB	-2.71	1.34	1.37
41	5	613	CHL	C1D-C2D	2.71	1.42	1.39
30	A	5007	3PH	O21-C2	-2.70	1.40	1.46
41	8	604	CHL	C1D-C2D	2.70	1.42	1.39
41	6	610	CHL	C1D-C2D	2.70	1.42	1.39
41	6	611	CHL	C1B-C2B	2.70	1.42	1.39
24	2	612	CLA	C4B-NB	-2.70	1.34	1.37
41	1	613	CHL	C1D-C2D	2.70	1.42	1.39
24	B	1227	CLA	C4B-NB	-2.70	1.34	1.37
24	F	1302	CLA	C4B-NB	-2.70	1.34	1.37
41	3	608	CHL	C1D-C2D	2.70	1.42	1.39
24	A	1110	CLA	C4B-NB	-2.70	1.34	1.37
24	4	606	CLA	C4B-NB	-2.69	1.34	1.37
24	B	1231	CLA	C4B-NB	-2.69	1.34	1.37
24	4	608	CLA	C4B-NB	-2.69	1.34	1.37
41	8	613	CHL	C1D-C2D	2.69	1.42	1.39
51	8	806	P5S	O19-C17	2.69	1.41	1.33
41	6	611	CHL	C3B-C2B	-2.69	1.36	1.40
24	9	607	CLA	C4B-NB	-2.69	1.34	1.37
41	6	619	CHL	CHB-C4A	-2.69	1.35	1.38
24	7	610	CLA	C4B-NB	-2.69	1.34	1.37
24	7	604	CLA	C4B-NB	-2.68	1.34	1.37
41	9	613	CHL	C1D-C2D	2.68	1.42	1.39
41	a	609	CHL	C1B-C2B	2.68	1.42	1.39
24	B	1213	CLA	C4B-NB	-2.68	1.34	1.37
24	2	609	CLA	C4B-NB	-2.68	1.34	1.37
33	3	802	PTY	O7-C6	-2.68	1.40	1.46
41	6	619	CHL	C1A-CHA	-2.68	1.37	1.40
24	A	1131	CLA	C4B-NB	-2.68	1.34	1.37
24	6	607	CLA	C4B-NB	-2.68	1.34	1.37
41	a	610	CHL	CHB-C4A	-2.68	1.35	1.38
24	L	1503	CLA	C4B-NB	-2.68	1.34	1.37
24	A	1133	CLA	C4B-NB	-2.67	1.34	1.37
41	6	610	CHL	C1B-C2B	2.67	1.42	1.39
24	6	602	CLA	C4B-NB	-2.67	1.34	1.37
24	A	1013	CLA	C4B-NB	-2.67	1.34	1.37
33	8	891	PTY	O7-C6	-2.67	1.40	1.46
36	G	5002	ERG	C9-C8	2.67	1.58	1.51
24	1	603	CLA	C4B-NB	-2.67	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	6	803	PCW	O2-C2	-2.67	1.40	1.46
24	4	610	CLA	C4B-NB	-2.66	1.34	1.37
41	6	613	CHL	CHB-C4A	-2.66	1.35	1.38
24	8	603	CLA	C4B-NB	-2.66	1.34	1.37
41	6	613	CHL	C1D-C2D	2.66	1.42	1.39
24	7	606	CLA	C4B-NB	-2.66	1.34	1.37
24	6	604	CLA	C4B-NB	-2.66	1.34	1.37
24	8	611	CLA	C4B-NB	-2.66	1.34	1.37
24	2	608	CLA	C4B-NB	-2.65	1.34	1.37
41	3	611	CHL	C1D-C2D	2.65	1.42	1.39
24	B	1212	CLA	C4B-NB	-2.65	1.34	1.37
24	A	1122	CLA	C4B-NB	-2.65	1.34	1.37
24	6	606	CLA	C4B-NB	-2.65	1.34	1.37
24	4	605	CLA	C4B-NB	-2.65	1.34	1.37
24	9	603	CLA	C4B-NB	-2.65	1.34	1.37
24	A	1109	CLA	C4B-NB	-2.65	1.34	1.37
24	5	616	CLA	C4B-NB	-2.64	1.34	1.37
41	5	611	CHL	C1D-C2D	2.64	1.42	1.39
41	9	610	CHL	C1D-C2D	2.64	1.42	1.39
41	4	618	CHL	CHB-C4A	-2.64	1.35	1.38
24	B	1208	CLA	C4B-NB	-2.64	1.34	1.37
24	a	601	CLA	C4B-NB	-2.64	1.34	1.37
41	a	610	CHL	C1D-C2D	2.64	1.42	1.39
41	4	609	CHL	C1B-C2B	2.64	1.42	1.39
24	B	1240	CLA	C4B-NB	-2.64	1.34	1.37
24	a	602	CLA	C4B-NB	-2.64	1.34	1.37
24	2	603	CLA	C4B-NB	-2.64	1.34	1.37
24	A	1104	CLA	C4B-NB	-2.64	1.34	1.37
24	L	1502	CLA	C4B-NB	-2.63	1.34	1.37
24	6	601	CLA	C4B-NB	-2.63	1.34	1.37
41	8	613	CHL	CHB-C4A	-2.63	1.35	1.38
41	6	610	CHL	C3B-C4B	2.63	1.43	1.41
24	7	615	CLA	C4B-NB	-2.63	1.34	1.37
24	B	1230	CLA	C4B-NB	-2.63	1.34	1.37
24	8	618	CLA	C4B-NB	-2.63	1.34	1.37
24	3	607	CLA	C4B-NB	-2.62	1.34	1.37
33	B	5005	PTY	O7-C6	-2.62	1.40	1.46
24	2	621	CLA	C4B-NB	-2.62	1.34	1.37
24	1	615	CLA	C4B-NB	-2.62	1.34	1.37
24	B	1228	CLA	C4B-NB	-2.62	1.34	1.37
24	8	620	CLA	C4B-NB	-2.62	1.34	1.37
24	4	616	CLA	C4B-NB	-2.62	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	6	618	CLA	C4B-NB	-2.61	1.34	1.37
49	7	504	C7Z	C20-C13	2.61	1.56	1.50
41	9	610	CHL	CHB-C4A	-2.61	1.35	1.38
24	8	607	CLA	C4B-NB	-2.61	1.34	1.37
33	9	803	PTY	O7-C6	-2.61	1.40	1.46
24	A	1119	CLA	C4B-NB	-2.61	1.34	1.37
24	B	1235	CLA	C4B-NB	-2.61	1.34	1.37
24	8	615	CLA	C4B-NB	-2.61	1.34	1.37
41	1	613	CHL	CHB-C4A	-2.61	1.35	1.38
24	4	607	CLA	C4B-NB	-2.61	1.34	1.37
24	H	1702	CLA	C4B-NB	-2.60	1.34	1.37
24	6	608	CLA	C4B-NB	-2.60	1.34	1.37
24	9	608	CLA	C4B-NB	-2.60	1.34	1.37
41	5	610	CHL	C1B-C2B	2.60	1.42	1.39
24	B	1214	CLA	C4B-NB	-2.60	1.34	1.37
24	7	602	CLA	C4B-NB	-2.60	1.34	1.37
24	2	606	CLA	C4B-NB	-2.60	1.34	1.37
24	7	609	CLA	C4B-NB	-2.60	1.34	1.37
24	9	606	CLA	C4B-NB	-2.59	1.34	1.37
24	B	1205	CLA	C4B-NB	-2.59	1.34	1.37
24	5	605	CLA	C4B-NB	-2.59	1.34	1.37
24	B	1220	CLA	C4B-NB	-2.59	1.34	1.37
24	B	1216	CLA	C4B-NB	-2.59	1.34	1.37
24	6	615	CLA	C4B-NB	-2.59	1.34	1.37
24	a	604	CLA	C4B-NB	-2.59	1.34	1.37
24	a	612	CLA	C4B-NB	-2.59	1.34	1.37
24	9	602	CLA	C4B-NB	-2.59	1.34	1.37
24	7	607	CLA	C4B-NB	-2.58	1.34	1.37
41	5	611	CHL	CHB-C4A	-2.58	1.35	1.38
24	3	616	CLA	C4B-NB	-2.58	1.34	1.37
24	a	607	CLA	C4B-NB	-2.58	1.34	1.37
24	H	1701	CLA	C4B-NB	-2.58	1.34	1.37
32	B	5004	PCW	O2-C31	2.58	1.41	1.34
24	L	1501	CLA	C4B-NB	-2.58	1.34	1.37
24	2	601	CLA	C4B-NB	-2.58	1.34	1.37
24	K	1403	CLA	C4B-NB	-2.57	1.34	1.37
24	6	605	CLA	C4B-NB	-2.57	1.34	1.37
24	8	602	CLA	C4B-NB	-2.57	1.34	1.37
24	4	615	CLA	C4B-NB	-2.57	1.34	1.37
24	K	1401	CLA	C4B-NB	-2.57	1.34	1.37
24	A	1106	CLA	C4B-NB	-2.56	1.34	1.37
24	8	608	CLA	C4B-NB	-2.56	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1141	CLA	C4B-NB	-2.56	1.34	1.37
24	G	1602	CLA	C4B-NB	-2.56	1.34	1.37
24	1	608	CLA	C4B-NB	-2.56	1.34	1.37
24	a	605	CLA	C4B-NB	-2.56	1.34	1.37
24	4	602	CLA	C4B-NB	-2.56	1.34	1.37
24	5	608	CLA	C4B-NB	-2.55	1.34	1.37
24	7	608	CLA	C4B-NB	-2.55	1.34	1.37
24	8	605	CLA	C4B-NB	-2.55	1.34	1.37
24	5	609	CLA	C4B-NB	-2.55	1.34	1.37
31	A	5008	LMT	O3'-C3'	-2.54	1.36	1.43
24	2	613	CLA	C4B-NB	-2.54	1.34	1.37
24	a	608	CLA	C4B-NB	-2.54	1.34	1.37
41	1	609	CHL	C1D-C2D	2.54	1.42	1.39
50	8	808	4RF	O18-C16	2.54	1.40	1.33
41	3	611	CHL	C1B-C2B	2.54	1.42	1.39
50	7	807	4RF	O21-C20	-2.53	1.40	1.46
24	5	617	CLA	C4B-NB	-2.52	1.34	1.37
24	9	609	CLA	C4B-NB	-2.52	1.34	1.37
24	4	612	CLA	C4B-NB	-2.52	1.34	1.37
24	G	1601	CLA	C4B-NB	-2.52	1.34	1.37
24	a	611	CLA	C4B-NB	-2.52	1.34	1.37
24	B	1217	CLA	C4B-NB	-2.52	1.34	1.37
49	7	504	C7Z	C18-C5	2.51	1.54	1.50
24	6	603	CLA	C4B-NB	-2.51	1.34	1.37
24	2	610	CLA	C4B-NB	-2.51	1.34	1.37
24	F	1301	CLA	C4B-NB	-2.51	1.34	1.37
41	3	608	CHL	CHB-C4A	-2.51	1.35	1.38
41	a	606	CHL	C1B-C2B	2.50	1.42	1.39
41	8	604	CHL	C1B-C2B	2.50	1.42	1.39
24	B	1221	CLA	C4B-NB	-2.50	1.34	1.37
24	a	615	CLA	C4B-NB	-2.50	1.34	1.37
24	A	1108	CLA	C4B-NB	-2.49	1.34	1.37
24	7	617	CLA	C4B-NB	-2.49	1.34	1.37
24	H	1703	CLA	C4B-NB	-2.49	1.34	1.37
24	2	602	CLA	C4B-NB	-2.49	1.34	1.37
24	5	614	CLA	C4B-NB	-2.49	1.34	1.37
41	1	609	CHL	CHB-C4A	-2.49	1.35	1.38
24	4	617	CLA	C4B-NB	-2.48	1.34	1.37
31	1	804	LMT	O3'-C3'	-2.48	1.36	1.43
24	B	1202	CLA	C4B-NB	-2.48	1.34	1.37
50	8	807	4RF	O40-C41	2.48	1.40	1.33
24	1	607	CLA	C4B-NB	-2.48	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	5006	LMT	O3'-C3'	-2.48	1.36	1.43
41	7	613	CHL	C1B-C2B	2.48	1.42	1.39
24	3	618	CLA	C4B-NB	-2.48	1.34	1.37
24	B	1223	CLA	C4B-NB	-2.47	1.34	1.37
24	A	1115	CLA	C4B-NB	-2.47	1.34	1.37
24	7	603	CLA	C4B-NB	-2.47	1.34	1.37
24	A	1120	CLA	C4B-NB	-2.47	1.34	1.37
24	K	1402	CLA	C4B-NB	-2.47	1.34	1.37
24	A	1134	CLA	C4B-NB	-2.47	1.34	1.37
41	9	613	CHL	CHB-C4A	-2.46	1.35	1.38
37	J	4002	RRX	C35-C13	2.46	1.55	1.50
24	1	602	CLA	C4B-NB	-2.46	1.34	1.37
24	A	1118	CLA	C4B-NB	-2.46	1.34	1.37
24	2	607	CLA	C4B-NB	-2.46	1.34	1.37
24	5	607	CLA	C4B-NB	-2.46	1.34	1.37
24	9	601	CLA	C4B-NB	-2.45	1.34	1.37
24	A	1136	CLA	C4B-NB	-2.45	1.34	1.37
24	5	602	CLA	C4B-NB	-2.45	1.34	1.37
24	B	1225	CLA	C4B-NB	-2.45	1.34	1.37
50	8	807	4RF	O18-C16	2.45	1.40	1.33
50	7	807	4RF	O40-C41	2.45	1.40	1.33
24	A	1139	CLA	C4B-NB	-2.45	1.34	1.37
24	9	601	CLA	C1C-C2C	2.45	1.49	1.44
24	2	604	CLA	C4B-NB	-2.44	1.34	1.37
33	7	804	PTY	O7-C8	2.44	1.41	1.34
32	6	803	PCW	O2-C31	2.44	1.41	1.34
31	2	804	LMT	O3'-C3'	-2.43	1.36	1.43
24	B	1239	CLA	C4B-NB	-2.43	1.34	1.37
24	a	603	CLA	C4B-NB	-2.43	1.34	1.37
38	a	804	LPX	P1-O2	2.42	1.68	1.59
24	4	603	CLA	C4B-NB	-2.42	1.34	1.37
24	J	1901	CLA	C4B-NB	-2.42	1.34	1.37
24	K	1404	CLA	C4B-NB	-2.41	1.34	1.37
24	2	615	CLA	C4B-NB	-2.41	1.34	1.37
33	7	804	PTY	O4-C30	2.41	1.40	1.33
43	3	506	QTB	C14-C12	-2.41	1.47	1.53
50	8	808	4RF	O40-C41	2.41	1.40	1.33
33	9	803	PTY	O4-C30	2.40	1.40	1.33
24	B	1232	CLA	C4B-NB	-2.40	1.34	1.37
33	3	802	PTY	O4-C30	2.40	1.40	1.33
24	5	608	CLA	C1A-CHA	2.40	1.53	1.43
24	A	1101	CLA	C4B-NB	-2.39	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	a	606	CHL	CHA-CBD	2.39	1.54	1.51
30	A	5007	3PH	O31-C31	2.39	1.40	1.33
41	4	618	CHL	C3B-C2B	-2.38	1.37	1.40
41	8	601	CHL	C1B-C2B	2.38	1.42	1.39
33	5	802	PTY	O4-C30	2.38	1.40	1.33
33	B	5005	PTY	O4-C30	2.38	1.40	1.33
24	9	603	CLA	C1A-CHA	2.38	1.52	1.43
33	5	802	PTY	O7-C8	2.37	1.41	1.34
41	4	609	CHL	C1A-CHA	-2.37	1.37	1.40
36	G	5002	ERG	C7-C8	-2.37	1.28	1.34
50	7	807	4RF	O18-C16	2.36	1.40	1.33
50	8	807	4RF	O21-C20	-2.36	1.41	1.46
41	4	609	CHL	C3B-C2B	-2.36	1.37	1.40
29	A	5005	DGD	CAA-C9A	-2.36	1.33	1.50
33	8	891	PTY	O4-C30	2.36	1.40	1.33
24	B	1236	CLA	C4B-NB	-2.36	1.34	1.37
36	G	5002	ERG	C14-C8	2.35	1.57	1.51
50	8	808	4RF	O21-C22	2.35	1.40	1.34
38	J	5001	LPX	P1-O2	2.34	1.68	1.59
24	G	1603	CLA	C4B-NB	-2.33	1.34	1.37
24	8	609	CLA	C4B-NB	-2.33	1.34	1.37
41	4	613	CHL	CHB-C4A	-2.33	1.35	1.38
24	A	1141	CLA	C1A-CHA	2.33	1.52	1.43
24	A	1114	CLA	C4B-NB	-2.33	1.34	1.37
41	3	608	CHL	CHA-CBD	2.33	1.54	1.51
41	1	609	CHL	CHA-CBD	2.32	1.54	1.51
24	A	1137	CLA	C4B-NB	-2.32	1.34	1.37
24	6	615	CLA	C1A-CHA	2.32	1.52	1.43
39	M	4001	ECH	C25-C26	-2.32	1.32	1.35
51	8	806	P5S	O37-C2	-2.31	1.41	1.46
24	B	1229	CLA	C4B-NB	-2.31	1.34	1.37
50	7	807	4RF	O18-C19	-2.31	1.40	1.45
24	B	1021	CLA	C4B-NB	-2.31	1.34	1.37
24	9	603	CLA	C1C-C2C	2.31	1.49	1.44
41	a	609	CHL	CHA-CBD	2.30	1.54	1.51
24	A	1140	CLA	C4B-NB	-2.30	1.34	1.37
24	A	1103	CLA	C4B-NB	-2.30	1.34	1.37
24	4	607	CLA	C1A-CHA	2.30	1.52	1.43
24	4	612	CLA	C1A-CHA	2.30	1.52	1.43
24	B	1215	CLA	C4B-NB	-2.30	1.34	1.37
24	6	617	CLA	C4B-NB	-2.30	1.34	1.37
24	B	1207	CLA	C4B-NB	-2.29	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1125	CLA	C1A-CHA	2.29	1.52	1.43
24	G	1601	CLA	C1A-CHA	2.29	1.52	1.43
24	5	604	CLA	C1C-C2C	2.29	1.49	1.44
50	8	807	4RF	O21-C22	2.28	1.40	1.34
24	B	1221	CLA	C1A-CHA	2.28	1.52	1.43
24	2	604	CLA	C1C-C2C	2.28	1.49	1.44
41	7	613	CHL	C1A-CHA	-2.28	1.37	1.40
24	2	604	CLA	C1A-CHA	2.28	1.52	1.43
32	B	5004	PCW	O2-C2	-2.27	1.41	1.46
24	H	1701	CLA	C1C-C2C	2.27	1.49	1.44
24	8	610	CLA	C1A-CHA	2.27	1.52	1.43
41	6	611	CHL	CHA-CBD	2.27	1.54	1.51
24	5	618	CLA	C4B-NB	-2.26	1.34	1.37
24	7	607	CLA	C1A-CHA	2.26	1.52	1.43
24	1	611	CLA	C1A-CHA	2.26	1.52	1.43
41	8	613	CHL	CHA-CBD	2.26	1.54	1.51
24	2	607	CLA	C1A-CHA	2.26	1.52	1.43
41	1	609	CHL	C3A-C2A	-2.26	1.52	1.54
24	6	609	CLA	C1A-CHA	2.26	1.52	1.43
24	B	1212	CLA	C1A-CHA	2.26	1.52	1.43
24	B	1226	CLA	C3D-C4D	-2.26	1.39	1.44
24	3	605	CLA	C1A-CHA	2.26	1.52	1.43
24	8	608	CLA	C1A-CHA	2.26	1.52	1.43
24	B	1209	CLA	C4B-NB	-2.25	1.34	1.37
24	A	1012	CLA	C1C-C2C	2.25	1.49	1.44
24	B	1226	CLA	CHD-C1D	2.25	1.42	1.38
41	3	611	CHL	CHA-CBD	2.25	1.54	1.51
24	1	610	CLA	C1A-CHA	2.25	1.52	1.43
50	7	807	4RF	O21-C22	2.25	1.40	1.34
24	A	1140	CLA	C1C-C2C	2.25	1.49	1.44
24	A	1102	CLA	C1A-CHA	2.25	1.52	1.43
24	9	607	CLA	C1A-CHA	2.25	1.52	1.43
50	8	808	4RF	O21-C20	-2.25	1.41	1.46
24	9	612	CLA	C4B-NB	-2.25	1.34	1.37
41	1	613	CHL	CHA-CBD	2.25	1.54	1.51
24	7	609	CLA	C1A-CHA	2.24	1.52	1.43
24	2	603	CLA	C1A-CHA	2.24	1.52	1.43
33	5	802	PTY	O7-C6	-2.24	1.41	1.46
24	B	1202	CLA	C1A-CHA	2.24	1.52	1.43
24	5	616	CLA	C1A-CHA	2.24	1.52	1.43
41	6	610	CHL	CHA-CBD	2.24	1.54	1.51
41	4	613	CHL	CHA-CBD	2.24	1.54	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	2	804	LMT	O2B-C2B	-2.24	1.37	1.43
24	a	608	CLA	C1A-CHA	2.24	1.52	1.43
24	5	617	CLA	C1A-CHA	2.24	1.52	1.43
41	5	613	CHL	CHA-CBD	2.24	1.54	1.51
24	A	1109	CLA	C1A-CHA	2.24	1.52	1.43
24	B	1239	CLA	C1A-CHA	2.23	1.52	1.43
24	H	1701	CLA	C1A-CHA	2.23	1.52	1.43
24	B	1240	CLA	C1A-CHA	2.23	1.52	1.43
24	5	618	CLA	C1A-CHA	2.23	1.52	1.43
24	7	615	CLA	C1A-CHA	2.23	1.52	1.43
24	5	601	CLA	C1A-CHA	2.23	1.52	1.43
24	8	620	CLA	C1A-CHA	2.23	1.52	1.43
24	B	1217	CLA	C1A-CHA	2.23	1.52	1.43
32	B	5004	PCW	P-O4P	2.23	1.68	1.59
24	5	607	CLA	C1A-CHA	2.23	1.52	1.43
24	A	1124	CLA	C1A-CHA	2.23	1.52	1.43
41	7	613	CHL	CHA-CBD	2.23	1.54	1.51
24	B	1023	CLA	C1A-CHA	2.23	1.52	1.43
24	3	601	CLA	C1A-CHA	2.23	1.52	1.43
24	4	603	CLA	C1A-CHA	2.23	1.52	1.43
24	B	1220	CLA	C1A-CHA	2.23	1.52	1.43
24	2	615	CLA	C1A-CHA	2.23	1.52	1.43
41	9	613	CHL	CHA-CBD	2.23	1.54	1.51
24	a	615	CLA	C1C-C2C	2.23	1.49	1.44
24	7	617	CLA	C1A-CHA	2.23	1.52	1.43
24	6	607	CLA	C1A-CHA	2.23	1.52	1.43
24	A	1123	CLA	C1A-CHA	2.22	1.52	1.43
24	3	612	CLA	C1A-CHA	2.22	1.52	1.43
24	3	618	CLA	C1A-CHA	2.22	1.52	1.43
24	F	1302	CLA	C1A-CHA	2.22	1.52	1.43
31	1	804	LMT	O2'-C2'	-2.22	1.37	1.43
31	2	804	LMT	O2'-C2'	-2.22	1.37	1.43
24	2	605	CLA	C1A-CHA	2.22	1.52	1.43
24	7	611	CLA	C1A-CHA	2.22	1.52	1.43
24	6	617	CLA	C1A-CHA	2.22	1.52	1.43
24	H	1702	CLA	C1A-CHA	2.22	1.52	1.43
24	4	617	CLA	C1A-CHA	2.22	1.52	1.43
24	6	606	CLA	C1A-CHA	2.22	1.52	1.43
24	A	1122	CLA	C1A-CHA	2.22	1.52	1.43
41	6	613	CHL	CHA-CBD	2.22	1.54	1.51
24	1	607	CLA	C1A-CHA	2.22	1.52	1.43
24	2	613	CLA	C1A-CHA	2.22	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	3	607	CLA	C1A-CHA	2.22	1.52	1.43
24	1	612	CLA	C1A-CHA	2.22	1.52	1.43
31	B	5006	LMT	O2B-C2B	-2.22	1.37	1.43
24	a	611	CLA	C1C-C2C	2.22	1.49	1.44
41	5	610	CHL	CHA-CBD	2.22	1.54	1.51
24	9	604	CLA	C1C-C2C	2.21	1.49	1.44
24	4	605	CLA	C1A-CHA	2.21	1.52	1.43
24	L	1501	CLA	C1A-CHA	2.21	1.52	1.43
44	a	805	GG0	C06-C07	2.21	1.56	1.50
24	6	602	CLA	C1A-CHA	2.21	1.52	1.43
24	9	609	CLA	C1A-CHA	2.21	1.52	1.43
41	5	610	CHL	C3B-C2B	-2.21	1.37	1.40
41	4	609	CHL	CHA-CBD	2.21	1.54	1.51
24	B	1235	CLA	C1A-CHA	2.21	1.52	1.43
24	1	605	CLA	C1A-CHA	2.21	1.52	1.43
46	5	803	DGA	OG2-CG2	-2.21	1.41	1.46
24	a	603	CLA	C1A-CHA	2.21	1.52	1.43
24	8	607	CLA	C1A-CHA	2.21	1.52	1.43
24	3	610	CLA	C1A-CHA	2.20	1.52	1.43
24	3	603	CLA	C1C-C2C	2.20	1.49	1.44
24	A	1138	CLA	C1A-CHA	2.20	1.52	1.43
24	A	1112	CLA	C1A-CHA	2.20	1.52	1.43
24	A	1127	CLA	C4B-NB	-2.20	1.35	1.37
24	9	602	CLA	C1A-CHA	2.20	1.52	1.43
24	a	603	CLA	C1C-C2C	2.20	1.49	1.44
24	3	603	CLA	C1A-CHA	2.20	1.52	1.43
31	B	5006	LMT	O3B-C3B	-2.20	1.37	1.43
24	4	610	CLA	CHD-C1D	2.20	1.42	1.38
24	A	1101	CLA	C1A-CHA	2.20	1.52	1.43
24	4	615	CLA	C1A-CHA	2.20	1.52	1.43
24	A	1134	CLA	C1A-CHA	2.20	1.52	1.43
24	G	1603	CLA	C1C-C2C	2.20	1.49	1.44
24	B	1213	CLA	C1A-CHA	2.19	1.52	1.43
24	B	1235	CLA	C1C-C2C	2.19	1.49	1.44
24	4	602	CLA	C1A-CHA	2.19	1.52	1.43
24	A	1106	CLA	C1A-CHA	2.19	1.52	1.43
24	B	1232	CLA	C1A-CHA	2.19	1.52	1.43
24	a	615	CLA	C1A-CHA	2.19	1.52	1.43
32	6	803	PCW	P-O4P	2.19	1.68	1.59
24	A	1130	CLA	C1A-CHA	2.19	1.52	1.43
33	3	802	PTY	O7-C8	2.19	1.40	1.34
24	B	1201	CLA	C1A-CHA	2.19	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	2	621	CLA	C1A-CHA	2.19	1.52	1.43
24	4	616	CLA	C1A-CHA	2.19	1.52	1.43
41	6	619	CHL	CHA-CBD	2.19	1.54	1.51
24	a	602	CLA	C1A-CHA	2.19	1.52	1.43
24	B	1237	CLA	C1A-CHA	2.19	1.52	1.43
31	A	5008	LMT	O3B-C3B	-2.19	1.37	1.43
31	1	804	LMT	O2B-C2B	-2.19	1.37	1.43
24	B	1215	CLA	C1A-CHA	2.19	1.52	1.43
24	B	1210	CLA	C1A-CHA	2.19	1.52	1.43
24	B	1224	CLA	C1A-CHA	2.19	1.52	1.43
24	5	618	CLA	C1C-C2C	2.19	1.49	1.44
24	B	1223	CLA	C1A-CHA	2.19	1.52	1.43
24	A	1140	CLA	C1A-CHA	2.18	1.52	1.43
24	A	1119	CLA	C1C-C2C	2.18	1.49	1.44
24	9	601	CLA	CHC-C1C	2.18	1.42	1.38
24	J	1901	CLA	C1A-CHA	2.18	1.52	1.43
24	8	605	CLA	C1A-CHA	2.18	1.52	1.43
36	G	5002	ERG	C11-C9	2.18	1.57	1.53
24	3	618	CLA	C1C-C2C	2.18	1.48	1.44
24	4	610	CLA	C1A-CHA	2.18	1.52	1.43
24	B	1221	CLA	C1C-C2C	2.18	1.48	1.44
31	2	804	LMT	O3B-C3B	-2.18	1.37	1.43
24	K	1401	CLA	C1A-CHA	2.18	1.52	1.43
24	7	603	CLA	C1A-CHA	2.18	1.52	1.43
24	7	608	CLA	C1A-CHA	2.18	1.52	1.43
24	A	1139	CLA	C1A-CHA	2.18	1.52	1.43
24	5	609	CLA	C1A-CHA	2.18	1.52	1.43
24	2	610	CLA	C1A-CHA	2.18	1.52	1.43
24	5	603	CLA	C1A-CHA	2.18	1.52	1.43
24	K	1403	CLA	C1A-CHA	2.18	1.52	1.43
24	B	1021	CLA	C1C-C2C	2.18	1.48	1.44
24	2	605	CLA	C1C-C2C	2.17	1.48	1.44
24	8	603	CLA	C1A-CHA	2.17	1.52	1.43
30	A	5007	3PH	O31-C3	-2.17	1.40	1.45
24	5	601	CLA	C1C-C2C	2.17	1.48	1.44
24	2	612	CLA	C1A-CHA	2.17	1.52	1.43
24	G	1602	CLA	C1A-CHA	2.17	1.52	1.43
24	5	605	CLA	C1A-CHA	2.17	1.52	1.43
24	A	1110	CLA	C1A-CHA	2.17	1.52	1.43
24	7	606	CLA	C1A-CHA	2.17	1.52	1.43
33	B	5005	PTY	O4-C1	-2.17	1.40	1.45
24	7	601	CLA	C1A-CHA	2.17	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	8	611	CLA	C1A-CHA	2.17	1.52	1.43
24	2	602	CLA	C1A-CHA	2.17	1.52	1.43
24	6	605	CLA	C1A-CHA	2.17	1.52	1.43
24	A	1137	CLA	C1A-CHA	2.17	1.52	1.43
24	A	1107	CLA	C1A-CHA	2.17	1.52	1.43
24	5	602	CLA	C1A-CHA	2.17	1.52	1.43
49	7	504	C7Z	C40-C33	2.17	1.55	1.50
41	9	610	CHL	CHA-CBD	2.17	1.54	1.51
24	3	616	CLA	C1A-CHA	2.17	1.52	1.43
24	7	605	CLA	C1A-CHA	2.17	1.52	1.43
24	A	1139	CLA	C1C-C2C	2.17	1.48	1.44
24	a	612	CLA	C1A-CHA	2.17	1.52	1.43
24	9	608	CLA	C1A-CHA	2.17	1.52	1.43
24	2	608	CLA	C1A-CHA	2.17	1.52	1.43
41	4	618	CHL	CHA-CBD	2.17	1.54	1.51
40	5	502	LUT	C22-C21	-2.16	1.52	1.54
24	B	1201	CLA	C1C-C2C	2.16	1.48	1.44
24	A	1103	CLA	C1A-CHA	2.16	1.52	1.43
24	7	612	CLA	C1A-CHA	2.16	1.52	1.43
24	A	1126	CLA	C1A-CHA	2.16	1.52	1.43
43	a	504	QTB	C14-C12	-2.16	1.47	1.53
24	B	1223	CLA	C1C-C2C	2.16	1.48	1.44
24	6	603	CLA	C1C-C2C	2.16	1.48	1.44
24	A	1135	CLA	C1A-CHA	2.16	1.52	1.43
24	F	1301	CLA	C1A-CHA	2.16	1.52	1.43
50	8	807	4RF	O18-C19	-2.16	1.40	1.45
24	A	1108	CLA	C1A-CHA	2.16	1.52	1.43
24	K	1404	CLA	C1C-C2C	2.16	1.48	1.44
24	A	1115	CLA	C1A-CHA	2.16	1.52	1.43
24	9	606	CLA	C1A-CHA	2.16	1.52	1.43
41	a	610	CHL	C3B-C2B	-2.16	1.37	1.40
24	3	602	CLA	C1A-CHA	2.16	1.52	1.43
24	1	601	CLA	C1C-C2C	2.16	1.48	1.44
50	7	807	4RF	O40-C39	-2.16	1.40	1.45
31	B	5006	LMT	O1'-C1'	-2.16	1.36	1.40
24	B	1214	CLA	C1A-CHA	2.16	1.52	1.43
24	A	1123	CLA	MG-NC	2.16	2.11	2.06
24	7	610	CLA	C1A-CHA	2.16	1.52	1.43
24	1	615	CLA	C1A-CHA	2.16	1.52	1.43
24	2	601	CLA	C1A-CHA	2.16	1.52	1.43
24	5	614	CLA	C1A-CHA	2.15	1.52	1.43
24	A	1116	CLA	C1C-C2C	2.15	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	8	612	CLA	C1A-CHA	2.15	1.52	1.43
24	a	612	CLA	C1C-C2C	2.15	1.48	1.44
24	1	601	CLA	C1A-CHA	2.15	1.52	1.43
24	4	606	CLA	C1A-CHA	2.15	1.52	1.43
41	5	611	CHL	CHA-CBD	2.15	1.54	1.51
24	B	1022	CLA	C3D-C4D	-2.15	1.39	1.44
24	B	1228	CLA	C1A-CHA	2.15	1.52	1.43
24	A	1124	CLA	C1C-C2C	2.15	1.48	1.44
24	9	605	CLA	C1A-CHA	2.15	1.52	1.43
24	B	1209	CLA	C1A-CHA	2.15	1.52	1.43
24	K	1404	CLA	C1A-CHA	2.15	1.52	1.43
24	6	608	CLA	C1A-CHA	2.15	1.52	1.43
24	5	607	CLA	C1C-C2C	2.15	1.48	1.44
41	a	613	CHL	CHA-CBD	2.15	1.54	1.51
24	F	1302	CLA	C1C-C2C	2.15	1.48	1.44
24	K	1402	CLA	C1A-CHA	2.15	1.52	1.43
24	B	1230	CLA	C1A-CHA	2.15	1.51	1.43
24	A	1120	CLA	C1A-CHA	2.15	1.51	1.43
41	a	610	CHL	CHA-CBD	2.15	1.54	1.51
24	a	601	CLA	C1A-CHA	2.15	1.51	1.43
24	8	615	CLA	C1A-CHA	2.15	1.51	1.43
24	8	618	CLA	C1A-CHA	2.15	1.51	1.43
24	A	1118	CLA	C1A-CHA	2.15	1.51	1.43
31	A	5008	LMT	O2B-C2B	-2.15	1.37	1.43
24	B	1232	CLA	C1C-C2C	2.15	1.48	1.44
24	B	1211	CLA	C3D-C4D	-2.15	1.39	1.44
31	1	804	LMT	O3B-C3B	-2.15	1.37	1.43
24	A	1111	CLA	C1A-CHA	2.15	1.51	1.43
24	6	601	CLA	C1A-CHA	2.15	1.51	1.43
24	B	1229	CLA	C1C-C2C	2.14	1.48	1.44
24	A	1136	CLA	C1A-CHA	2.14	1.51	1.43
24	a	605	CLA	C1A-CHA	2.14	1.51	1.43
24	8	603	CLA	C1C-C2C	2.14	1.48	1.44
24	A	1121	CLA	C1A-CHA	2.14	1.51	1.43
24	1	608	CLA	C1A-CHA	2.14	1.51	1.43
24	a	607	CLA	C1A-CHA	2.14	1.51	1.43
33	5	802	PTY	O4-C1	-2.14	1.40	1.45
24	A	1132	CLA	C1A-CHA	2.14	1.51	1.43
24	a	604	CLA	C1A-CHA	2.14	1.51	1.43
50	8	808	4RF	O40-C39	-2.14	1.40	1.45
41	8	601	CHL	CHA-CBD	2.14	1.54	1.51
31	B	5006	LMT	O2'-C2'	-2.14	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	5007	3PH	O21-C21	2.14	1.40	1.34
24	A	1117	CLA	C1A-CHA	2.14	1.51	1.43
24	2	609	CLA	C1A-CHA	2.14	1.51	1.43
33	B	5005	PTY	O7-C8	2.14	1.40	1.34
24	6	603	CLA	C1A-CHA	2.14	1.51	1.43
33	8	891	PTY	O4-C1	-2.14	1.40	1.45
24	5	606	CLA	C1A-CHA	2.14	1.51	1.43
24	9	612	CLA	C1A-CHA	2.14	1.51	1.43
31	A	5008	LMT	O2'-C2'	-2.13	1.37	1.43
33	9	803	PTY	O7-C8	2.13	1.40	1.34
24	A	1127	CLA	C1A-CHA	2.13	1.51	1.43
24	B	1238	CLA	C1A-CHA	2.13	1.51	1.43
24	G	1603	CLA	C1A-CHA	2.13	1.51	1.43
33	7	804	PTY	O7-C6	-2.13	1.41	1.46
24	7	610	CLA	C1C-C2C	2.13	1.48	1.44
24	4	611	CLA	C4B-NB	-2.13	1.35	1.37
24	a	611	CLA	C1A-CHA	2.13	1.51	1.43
24	B	1208	CLA	C3D-C4D	-2.13	1.39	1.44
24	1	602	CLA	C1A-CHA	2.13	1.51	1.43
24	3	607	CLA	C1C-C2C	2.13	1.48	1.44
24	2	606	CLA	C1A-CHA	2.13	1.51	1.43
24	B	1222	CLA	C1A-CHA	2.13	1.51	1.43
31	1	804	LMT	O1'-C1'	-2.13	1.36	1.40
24	A	1114	CLA	C1A-CHA	2.13	1.51	1.43
24	4	601	CLA	C1A-CHA	2.13	1.51	1.43
24	A	1119	CLA	C3D-C4D	-2.13	1.39	1.44
24	A	1128	CLA	C1A-CHA	2.13	1.51	1.43
27	B	4005	BCR	C12-C13	-2.13	1.41	1.46
24	B	1206	CLA	C1A-CHA	2.13	1.51	1.43
24	a	602	CLA	C1C-C2C	2.13	1.48	1.44
24	8	606	CLA	C1A-CHA	2.13	1.51	1.43
24	B	1227	CLA	C1A-CHA	2.12	1.51	1.43
24	3	613	CLA	C1A-CHA	2.12	1.51	1.43
24	5	614	CLA	C1C-C2C	2.12	1.48	1.44
24	5	612	CLA	C1A-CHA	2.12	1.51	1.43
24	A	1131	CLA	C1A-CHA	2.12	1.51	1.43
24	B	1221	CLA	MG-NC	2.12	2.11	2.06
24	B	1207	CLA	C1A-CHA	2.12	1.51	1.43
24	1	608	CLA	C1C-C2C	2.12	1.48	1.44
24	G	1601	CLA	C1C-C2C	2.12	1.48	1.44
33	8	891	PTY	O7-C8	2.12	1.40	1.34
24	L	1503	CLA	C1A-CHA	2.11	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	604	CLA	C3D-C4D	-2.11	1.39	1.44
24	B	1219	CLA	C1A-CHA	2.11	1.51	1.43
24	5	609	CLA	C1C-C2C	2.11	1.48	1.44
24	A	1013	CLA	C1A-CHA	2.11	1.51	1.43
24	4	611	CLA	C1A-CHA	2.11	1.51	1.43
24	A	1129	CLA	C1A-CHA	2.11	1.51	1.43
24	2	615	CLA	C1C-C2C	2.11	1.48	1.44
24	A	1013	CLA	C1C-C2C	2.11	1.48	1.44
24	2	602	CLA	C1C-C2C	2.11	1.48	1.44
50	8	808	4RF	O18-C19	-2.11	1.40	1.45
24	A	1126	CLA	C1C-C2C	2.11	1.48	1.44
24	A	1116	CLA	C3D-C4D	-2.11	1.39	1.44
39	M	4001	ECH	C30-C25	-2.11	1.51	1.53
24	3	606	CLA	C1A-CHA	2.11	1.51	1.43
24	B	1216	CLA	C3D-C4D	-2.11	1.39	1.44
24	7	602	CLA	C1A-CHA	2.11	1.51	1.43
24	H	1703	CLA	C1A-CHA	2.11	1.51	1.43
24	4	612	CLA	C1C-C2C	2.11	1.48	1.44
24	8	615	CLA	C1C-C2C	2.11	1.48	1.44
24	K	1402	CLA	C1C-C2C	2.11	1.48	1.44
24	G	1602	CLA	C1C-C2C	2.11	1.48	1.44
33	3	802	PTY	O4-C1	-2.10	1.40	1.45
24	4	608	CLA	C3D-C4D	-2.10	1.39	1.44
44	a	805	GG0	C03-N05	2.10	1.38	1.33
24	2	607	CLA	C1C-C2C	2.10	1.48	1.44
24	B	1203	CLA	C1A-CHA	2.10	1.51	1.43
24	a	601	CLA	C1C-C2C	2.10	1.48	1.44
24	8	602	CLA	C1A-CHA	2.10	1.51	1.43
24	8	609	CLA	C1A-CHA	2.10	1.51	1.43
27	3	503	BCR	C1-C6	-2.10	1.51	1.53
24	B	1223	CLA	C3D-C4D	-2.10	1.39	1.44
33	7	804	PTY	O4-C1	-2.10	1.40	1.45
24	8	612	CLA	CHD-C1D	2.10	1.42	1.38
24	3	602	CLA	C1C-C2C	2.10	1.48	1.44
24	7	605	CLA	C1C-C2C	2.10	1.48	1.44
24	A	1105	CLA	C1C-C2C	2.10	1.48	1.44
24	6	612	CLA	C1A-CHA	2.09	1.51	1.43
24	A	1135	CLA	C1C-C2C	2.09	1.48	1.44
24	a	607	CLA	C1C-C2C	2.09	1.48	1.44
24	7	603	CLA	C1C-C2C	2.09	1.48	1.44
24	B	1205	CLA	C1A-CHA	2.09	1.51	1.43
24	9	609	CLA	C1C-C2C	2.09	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	4	617	CLA	C1C-C2C	2.09	1.48	1.44
24	A	1118	CLA	C1C-C2C	2.09	1.48	1.44
24	2	609	CLA	C1C-C2C	2.09	1.48	1.44
24	A	1113	CLA	C1A-CHA	2.09	1.51	1.43
24	A	1105	CLA	C1A-CHA	2.09	1.51	1.43
24	9	605	CLA	C3D-C4D	-2.09	1.39	1.44
24	2	603	CLA	C1C-C2C	2.09	1.48	1.44
24	5	607	CLA	MG-NC	2.09	2.11	2.06
24	6	604	CLA	C1A-CHA	2.09	1.51	1.43
40	5	505	LUT	C1-C6	-2.09	1.51	1.53
24	2	601	CLA	C1C-C2C	2.09	1.48	1.44
24	1	603	CLA	C1A-CHA	2.09	1.51	1.43
24	B	1208	CLA	C1C-C2C	2.09	1.48	1.44
24	B	1225	CLA	C1A-CHA	2.09	1.51	1.43
24	B	1240	CLA	C1C-C2C	2.08	1.48	1.44
24	4	616	CLA	C1C-C2C	2.08	1.48	1.44
31	2	804	LMT	O1'-C1'	-2.08	1.36	1.40
24	H	1702	CLA	C1C-C2C	2.08	1.48	1.44
24	6	618	CLA	C1C-C2C	2.08	1.48	1.44
24	4	607	CLA	MG-NC	2.08	2.11	2.06
24	A	1134	CLA	C1C-C2C	2.08	1.48	1.44
24	A	1137	CLA	C1C-C2C	2.08	1.48	1.44
24	a	608	CLA	C1C-C2C	2.08	1.48	1.44
24	7	606	CLA	C1C-C2C	2.08	1.48	1.44
24	9	607	CLA	C1C-C2C	2.08	1.48	1.44
24	6	618	CLA	C1A-CHA	2.08	1.51	1.43
24	B	1220	CLA	C1C-C2C	2.07	1.48	1.44
24	L	1501	CLA	C1C-C2C	2.07	1.48	1.44
24	7	605	CLA	C3D-C4D	-2.07	1.39	1.44
24	4	604	CLA	C1C-C2C	2.07	1.48	1.44
39	M	4001	ECH	C1-C6	-2.07	1.51	1.53
50	8	807	4RF	O40-C39	-2.07	1.40	1.45
24	B	1224	CLA	C1C-C2C	2.07	1.48	1.44
24	1	606	CLA	C1A-CHA	2.07	1.51	1.43
24	4	603	CLA	C1C-C2C	2.07	1.48	1.44
24	9	608	CLA	C1C-C2C	2.07	1.48	1.44
24	A	1136	CLA	C1C-C2C	2.07	1.48	1.44
24	B	1229	CLA	C1A-CHA	2.07	1.51	1.43
24	1	606	CLA	C1C-C2C	2.07	1.48	1.44
24	8	620	CLA	C1C-C2C	2.07	1.48	1.44
24	A	1127	CLA	C1C-C2C	2.07	1.48	1.44
33	9	803	PTY	O4-C1	-2.07	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	2	606	CLA	C1C-C2C	2.07	1.48	1.44
24	9	602	CLA	C1C-C2C	2.07	1.48	1.44
24	1	601	CLA	C3D-C4D	-2.07	1.39	1.44
24	9	601	CLA	C1A-CHA	2.06	1.51	1.43
41	9	610	CHL	C3B-C2B	-2.06	1.37	1.40
24	7	610	CLA	MG-NC	2.06	2.11	2.06
24	B	1217	CLA	C1C-C2C	2.06	1.48	1.44
24	B	1234	CLA	C1A-CHA	2.06	1.51	1.43
24	A	1133	CLA	C1A-CHA	2.06	1.51	1.43
24	B	1213	CLA	C1C-C2C	2.06	1.48	1.44
24	B	1234	CLA	C3D-C4D	-2.06	1.39	1.44
24	A	1104	CLA	C1A-CHA	2.06	1.51	1.43
24	4	607	CLA	C1C-C2C	2.06	1.48	1.44
24	9	607	CLA	MG-NC	2.06	2.11	2.06
24	9	606	CLA	C1C-C2C	2.06	1.48	1.44
24	2	621	CLA	C1C-C2C	2.06	1.48	1.44
24	9	604	CLA	C3D-C4D	-2.06	1.39	1.44
24	6	602	CLA	C1C-C2C	2.06	1.48	1.44
24	H	1702	CLA	MG-NC	2.06	2.11	2.06
24	B	1211	CLA	C1A-CHA	2.05	1.51	1.43
24	a	605	CLA	C3D-C4D	-2.05	1.39	1.44
41	8	604	CHL	CHA-CBD	2.05	1.54	1.51
24	B	1021	CLA	C1A-CHA	2.05	1.51	1.43
24	9	612	CLA	C1C-C2C	2.05	1.48	1.44
24	4	606	CLA	C1C-C2C	2.05	1.48	1.44
24	1	603	CLA	C1C-C2C	2.05	1.48	1.44
24	5	616	CLA	C1C-C2C	2.05	1.48	1.44
24	6	615	CLA	C1C-C2C	2.05	1.48	1.44
24	5	608	CLA	C1C-C2C	2.05	1.48	1.44
24	B	1238	CLA	C1C-C2C	2.05	1.48	1.44
24	A	1012	CLA	C3D-C4D	-2.05	1.39	1.44
24	1	604	CLA	C1C-C2C	2.05	1.48	1.44
24	1	602	CLA	C1C-C2C	2.05	1.48	1.44
24	L	1502	CLA	C1A-CHA	2.05	1.51	1.43
24	A	1115	CLA	C1C-C2C	2.05	1.48	1.44
24	5	609	CLA	MG-NC	2.05	2.11	2.06
24	6	612	CLA	C3D-C4D	-2.05	1.39	1.44
24	A	1121	CLA	C3D-C4D	-2.05	1.39	1.44
24	B	1231	CLA	C1A-CHA	2.04	1.51	1.43
24	A	1135	CLA	C3D-C4D	-2.04	1.39	1.44
24	5	605	CLA	C3D-C4D	-2.04	1.39	1.44
24	A	1120	CLA	C1C-C2C	2.04	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1012	CLA	C1A-CHA	2.04	1.51	1.43
24	G	1601	CLA	MG-NC	2.04	2.11	2.06
24	B	1222	CLA	C1C-C2C	2.04	1.48	1.44
24	J	1901	CLA	C1C-C2C	2.04	1.48	1.44
24	B	1219	CLA	C3D-C4D	-2.04	1.39	1.44
24	8	605	CLA	C3D-C4D	-2.04	1.39	1.44
24	4	608	CLA	C1C-C2C	2.04	1.48	1.44
24	B	1218	CLA	C1A-CHA	2.04	1.51	1.43
24	A	1102	CLA	C1C-C2C	2.04	1.48	1.44
24	7	601	CLA	C3D-C4D	-2.04	1.39	1.44
24	B	1225	CLA	C3D-C4D	-2.04	1.39	1.44
24	F	1302	CLA	MG-NC	2.04	2.11	2.06
24	4	604	CLA	C1A-CHA	2.04	1.51	1.43
24	6	601	CLA	C1C-C2C	2.04	1.48	1.44
24	A	1133	CLA	C3D-C4D	-2.04	1.39	1.44
24	7	604	CLA	C1C-C2C	2.04	1.48	1.44
24	4	601	CLA	C1C-C2C	2.04	1.48	1.44
24	3	607	CLA	MG-NC	2.03	2.11	2.06
24	B	1204	CLA	C1A-CHA	2.03	1.51	1.43
24	7	617	CLA	C1C-C2C	2.03	1.48	1.44
24	A	1109	CLA	C3D-C4D	-2.03	1.39	1.44
24	a	607	CLA	MG-NC	2.03	2.11	2.06
24	4	610	CLA	MG-NC	2.03	2.11	2.06
24	A	1129	CLA	C1C-C2C	2.03	1.48	1.44
24	6	617	CLA	C1C-C2C	2.03	1.48	1.44
24	7	615	CLA	C1C-C2C	2.03	1.48	1.44
24	8	607	CLA	C1C-C2C	2.03	1.48	1.44
24	B	1227	CLA	C1C-C2C	2.03	1.48	1.44
24	A	1131	CLA	C1C-C2C	2.03	1.48	1.44
24	L	1503	CLA	C1C-C2C	2.03	1.48	1.44
24	K	1401	CLA	C3D-C4D	-2.03	1.39	1.44
24	2	621	CLA	MG-NC	2.03	2.11	2.06
24	3	602	CLA	MG-NC	2.03	2.11	2.06
24	A	1104	CLA	C1C-C2C	2.03	1.48	1.44
24	B	1231	CLA	CHD-C1D	2.03	1.42	1.38
24	6	607	CLA	C1C-C2C	2.03	1.48	1.44
24	A	1141	CLA	MG-NC	2.02	2.11	2.06
24	B	1236	CLA	C1A-CHA	2.02	1.51	1.43
24	4	602	CLA	MG-NC	2.02	2.11	2.06
24	5	616	CLA	MG-NC	2.02	2.11	2.06
24	1	604	CLA	C1A-CHA	2.02	1.51	1.43
24	F	1301	CLA	C1C-C2C	2.02	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	7	610	CLA	C3D-C4D	-2.02	1.39	1.44
24	A	1122	CLA	C1C-C2C	2.02	1.48	1.44
24	a	604	CLA	C1C-C2C	2.02	1.48	1.44
24	5	606	CLA	C1C-C2C	2.02	1.48	1.44
24	B	1236	CLA	C1C-C2C	2.02	1.48	1.44
24	7	602	CLA	MG-NC	2.02	2.11	2.06
24	B	1214	CLA	C3D-C4D	-2.02	1.39	1.44
24	B	1203	CLA	C1C-C2C	2.02	1.48	1.44
31	2	804	LMT	O4'-C4B	-2.02	1.38	1.43
24	1	615	CLA	C1C-C2C	2.02	1.48	1.44
24	1	612	CLA	MG-NC	2.02	2.11	2.06
24	4	615	CLA	MG-NC	2.02	2.11	2.06
24	A	1141	CLA	C1C-C2C	2.02	1.48	1.44
24	B	1217	CLA	MG-NC	2.02	2.11	2.06
24	5	608	CLA	MG-NC	2.02	2.11	2.06
24	9	605	CLA	C1C-C2C	2.02	1.48	1.44
24	5	618	CLA	MG-NC	2.02	2.11	2.06
24	A	1127	CLA	C3D-C4D	-2.01	1.39	1.44
24	1	615	CLA	MG-NC	2.01	2.11	2.06
24	3	604	CLA	C1C-C2C	2.01	1.48	1.44
24	7	612	CLA	C1C-C2C	2.01	1.48	1.44
24	2	613	CLA	C1C-C2C	2.01	1.48	1.44
24	A	1111	CLA	C3D-C4D	-2.01	1.39	1.44
24	4	616	CLA	MG-NC	2.01	2.11	2.06
35	H	5001	SQD	O47-C45	-2.01	1.41	1.46
24	L	1503	CLA	MG-NC	2.01	2.11	2.06
24	2	604	CLA	MG-NC	2.01	2.11	2.06
24	7	607	CLA	MG-NC	2.01	2.11	2.06
24	9	604	CLA	C1A-CHA	2.01	1.51	1.43
24	B	1205	CLA	C3D-C4D	-2.01	1.39	1.44
24	6	608	CLA	C3D-C4D	-2.01	1.39	1.44
24	1	605	CLA	C3D-C4D	-2.01	1.39	1.44
24	B	1238	CLA	C3D-C4D	-2.01	1.39	1.44
24	6	608	CLA	C1C-C2C	2.01	1.48	1.44
24	a	608	CLA	MG-NC	2.01	2.11	2.06
24	2	610	CLA	C1C-C2C	2.01	1.48	1.44
24	8	602	CLA	C1C-C2C	2.01	1.48	1.44
24	2	610	CLA	MG-NC	2.01	2.11	2.06
24	B	1221	CLA	C3D-C4D	-2.01	1.39	1.44
24	B	1236	CLA	C3D-C4D	-2.00	1.39	1.44
24	3	604	CLA	C1A-CHA	2.00	1.51	1.43
24	J	1901	CLA	MG-NC	2.00	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	1211	CLA	C1C-C2C	2.00	1.48	1.44
24	3	618	CLA	MG-NC	2.00	2.11	2.06
32	B	5004	PCW	C32-C31	2.00	1.56	1.50
24	A	1129	CLA	C3D-C4D	-2.00	1.39	1.44
24	2	607	CLA	MG-NC	2.00	2.11	2.06
24	4	605	CLA	MG-NC	2.00	2.11	2.06
24	4	605	CLA	CHD-C1D	2.00	1.42	1.38
24	B	1204	CLA	C3D-C4D	-2.00	1.39	1.44

All (5386) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	2	601	CLA	C4-C3-C5	-21.81	77.37	115.23
27	F	4001	BCR	C10-C11-C12	19.59	179.95	123.20
27	5	504	BCR	C10-C11-C12	19.36	179.29	123.20
27	H	4001	BCR	C10-C11-C12	19.20	178.83	123.20
27	L	4001	BCR	C10-C11-C12	19.04	178.36	123.20
27	6	504	BCR	C10-C11-C12	18.97	178.16	123.20
27	8	503	BCR	C10-C11-C12	18.95	178.12	123.20
27	6	503	BCR	C10-C11-C12	18.92	178.03	123.20
27	A	4002	BCR	C10-C11-C12	18.90	177.97	123.20
27	B	4001	BCR	C10-C11-C12	18.89	177.92	123.20
27	K	4001	BCR	C10-C11-C12	18.89	177.92	123.20
27	3	503	BCR	C10-C11-C12	18.88	177.91	123.20
27	5	503	BCR	C10-C11-C12	18.88	177.90	123.20
27	7	503	BCR	C10-C11-C12	18.86	177.84	123.20
27	I	4001	BCR	C10-C11-C12	18.78	177.62	123.20
27	B	4002	BCR	C10-C11-C12	18.73	177.46	123.20
27	A	4004	BCR	C10-C11-C12	18.72	177.45	123.20
27	A	4003	BCR	C10-C11-C12	18.68	177.31	123.20
27	B	4004	BCR	C10-C11-C12	18.61	177.11	123.20
27	L	4003	BCR	C10-C11-C12	18.56	176.98	123.20
27	3	505	BCR	C10-C11-C12	18.54	176.91	123.20
27	B	4007	BCR	C10-C11-C12	18.48	176.75	123.20
27	B	4005	BCR	C10-C11-C12	18.43	176.60	123.20
27	B	4006	BCR	C10-C11-C12	18.43	176.60	123.20
27	3	504	BCR	C10-C11-C12	18.24	176.05	123.20
27	4	503	BCR	C10-C11-C12	18.23	176.02	123.20
27	K	4002	BCR	C10-C11-C12	18.20	175.94	123.20
27	G	4001	BCR	C10-C11-C12	18.16	175.81	123.20
27	J	4001	BCR	C10-C11-C12	18.14	175.75	123.20
27	L	4002	BCR	C10-C11-C12	18.12	175.70	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	4001	BCR	C10-C11-C12	18.09	175.63	123.20
27	A	4005	BCR	C10-C11-C12	17.27	173.25	123.20
27	B	4003	BCR	C10-C11-C12	17.25	173.18	123.20
24	2	601	CLA	C5-C3-C2	17.05	159.43	121.17
27	B	4003	BCR	C11-C10-C9	16.24	150.06	127.28
24	2	601	CLA	C4-C3-C2	-16.18	82.06	123.63
27	H	4001	BCR	C16-C15-C14	15.81	155.86	123.52
27	6	503	BCR	C16-C15-C14	15.56	155.35	123.52
27	B	4006	BCR	C16-C15-C14	15.41	155.05	123.52
27	4	503	BCR	C16-C15-C14	15.37	154.97	123.52
27	B	4002	BCR	C11-C10-C9	15.28	148.70	127.28
27	B	4005	BCR	C16-C15-C14	15.14	154.50	123.52
27	5	504	BCR	C16-C15-C14	14.53	153.24	123.52
27	L	4003	BCR	C16-C15-C14	14.48	153.15	123.52
27	G	4001	BCR	C21-C20-C19	14.43	165.02	123.20
27	A	4003	BCR	C11-C10-C9	14.37	147.43	127.28
27	3	504	BCR	C21-C20-C19	14.33	164.71	123.20
23	A	1011	CL0	C1B-CHB-C4A	14.26	130.49	121.32
27	A	4005	BCR	C11-C10-C9	14.17	147.15	127.28
27	J	4001	BCR	C11-C10-C9	14.09	147.04	127.28
27	6	504	BCR	C16-C15-C14	14.02	152.21	123.52
27	5	503	BCR	C16-C15-C14	14.00	152.17	123.52
27	A	4001	BCR	C21-C20-C19	13.96	163.66	123.20
27	B	4007	BCR	C11-C10-C9	13.88	146.74	127.28
27	7	503	BCR	C16-C15-C14	13.86	151.89	123.52
27	A	4003	BCR	C16-C15-C14	13.86	151.87	123.52
27	3	503	BCR	C16-C15-C14	13.83	151.82	123.52
27	L	4001	BCR	C21-C20-C19	13.78	163.12	123.20
27	K	4002	BCR	C21-C20-C19	13.76	163.07	123.20
27	L	4001	BCR	C16-C15-C14	13.75	151.65	123.52
27	B	4001	BCR	C21-C20-C19	13.71	162.91	123.20
27	B	4005	BCR	C11-C10-C9	13.70	146.50	127.28
27	8	503	BCR	C16-C15-C14	13.69	151.53	123.52
27	3	505	BCR	C11-C10-C9	13.62	146.38	127.28
27	K	4001	BCR	C21-C20-C19	13.61	162.64	123.20
27	B	4002	BCR	C16-C15-C14	13.61	151.37	123.52
27	B	4004	BCR	C11-C10-C9	13.60	146.35	127.28
27	B	4006	BCR	C11-C10-C9	13.52	146.25	127.28
27	A	4003	BCR	C21-C20-C19	13.52	162.38	123.20
27	H	4001	BCR	C21-C20-C19	13.48	162.27	123.20
27	L	4002	BCR	C21-C20-C19	13.48	162.26	123.20
27	L	4003	BCR	C11-C10-C9	13.47	146.17	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	8	503	BCR	C11-C10-C9	13.43	146.11	127.28
36	G	5002	ERG	C15-C14-C8	-13.38	102.26	120.42
27	B	4005	BCR	C21-C20-C19	13.36	161.90	123.20
27	J	4001	BCR	C21-C20-C19	13.28	161.68	123.20
27	B	4007	BCR	C16-C15-C14	13.27	150.67	123.52
27	K	4002	BCR	C16-C15-C14	13.27	150.66	123.52
27	K	4001	BCR	C16-C15-C14	13.27	150.66	123.52
27	5	504	BCR	C21-C20-C19	13.23	161.55	123.20
27	K	4001	BCR	C11-C10-C9	13.18	145.76	127.28
27	3	505	BCR	C21-C20-C19	13.18	161.38	123.20
27	A	4002	BCR	C16-C15-C14	13.08	150.28	123.52
27	A	4004	BCR	C21-C20-C19	13.03	160.94	123.20
27	B	4004	BCR	C16-C15-C14	13.02	150.16	123.52
27	7	503	BCR	C11-C10-C9	13.00	145.51	127.28
27	3	505	BCR	C16-C15-C14	12.98	150.09	123.52
27	A	4005	BCR	C11-C12-C13	12.89	161.72	126.36
27	5	503	BCR	C11-C10-C9	12.87	145.32	127.28
27	L	4001	BCR	C11-C10-C9	12.80	145.23	127.28
27	L	4002	BCR	C11-C10-C9	12.70	145.08	127.28
27	A	4001	BCR	C11-C10-C9	12.69	145.07	127.28
27	L	4003	BCR	C21-C20-C19	12.69	159.96	123.20
27	B	4006	BCR	C21-C20-C19	12.64	159.83	123.20
27	G	4001	BCR	C11-C10-C9	12.59	144.94	127.28
27	8	503	BCR	C21-C20-C19	12.53	159.50	123.20
27	F	4001	BCR	C16-C15-C14	12.52	149.15	123.52
27	A	4002	BCR	C21-C20-C19	12.49	159.39	123.20
27	H	4001	BCR	C11-C10-C9	12.49	144.79	127.28
27	5	503	BCR	C21-C20-C19	12.47	159.32	123.20
27	3	504	BCR	C16-C15-C14	12.44	148.98	123.52
27	F	4001	BCR	C21-C20-C19	12.41	159.17	123.20
27	6	504	BCR	C21-C20-C19	12.36	159.01	123.20
27	3	503	BCR	C11-C10-C9	12.33	144.57	127.28
27	A	4004	BCR	C11-C10-C9	12.30	144.53	127.28
27	B	4004	BCR	C21-C20-C19	12.22	158.60	123.20
27	A	4004	BCR	C16-C15-C14	12.19	148.46	123.52
27	6	504	BCR	C11-C10-C9	12.18	144.37	127.28
27	A	4002	BCR	C11-C10-C9	12.16	144.34	127.28
27	A	4005	BCR	C21-C20-C19	12.14	158.38	123.20
27	B	4003	BCR	C16-C15-C14	12.13	148.33	123.52
27	B	4002	BCR	C21-C20-C19	12.11	158.30	123.20
27	3	503	BCR	C21-C20-C19	12.11	158.29	123.20
27	B	4003	BCR	C11-C12-C13	12.10	159.54	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	L	4002	BCR	C11-C12-C13	12.08	159.48	126.36
27	K	4002	BCR	C11-C10-C9	12.08	144.21	127.28
27	6	503	BCR	C21-C20-C19	12.06	158.14	123.20
27	L	4002	BCR	C16-C15-C14	12.05	148.18	123.52
27	B	4001	BCR	C16-C15-C14	12.04	148.16	123.52
27	I	4001	BCR	C11-C10-C9	11.94	144.02	127.28
27	G	4001	BCR	C11-C12-C13	11.91	159.01	126.36
27	B	4001	BCR	C11-C10-C9	11.68	143.66	127.28
27	A	4001	BCR	C11-C12-C13	11.61	158.19	126.36
27	I	4001	BCR	C16-C15-C14	11.53	147.12	123.52
27	B	4007	BCR	C21-C20-C19	11.45	156.38	123.20
27	I	4001	BCR	C21-C20-C19	11.41	156.27	123.20
27	3	504	BCR	C11-C10-C9	11.39	143.25	127.28
27	A	4004	BCR	C11-C12-C13	11.31	157.37	126.36
27	J	4001	BCR	C16-C15-C14	11.23	146.49	123.52
27	7	503	BCR	C21-C20-C19	11.14	155.49	123.20
27	I	4001	BCR	C11-C12-C13	11.09	156.76	126.36
27	4	503	BCR	C21-C20-C19	10.99	155.06	123.20
27	5	504	BCR	C11-C12-C13	10.99	156.51	126.36
27	5	504	BCR	C11-C10-C9	10.96	142.65	127.28
27	G	4001	BCR	C16-C15-C14	10.90	145.82	123.52
27	B	4007	BCR	C11-C12-C13	10.89	156.23	126.36
27	B	4004	BCR	C11-C12-C13	10.87	156.18	126.36
27	K	4002	BCR	C11-C12-C13	10.85	156.12	126.36
27	B	4006	BCR	C11-C12-C13	10.85	156.12	126.36
27	K	4001	BCR	C11-C12-C13	10.82	156.03	126.36
27	B	4001	BCR	C11-C12-C13	10.82	156.03	126.36
27	B	4003	BCR	C21-C20-C19	10.76	154.38	123.20
27	A	4002	BCR	C11-C12-C13	10.68	155.66	126.36
27	3	504	BCR	C11-C12-C13	10.66	155.59	126.36
27	6	504	BCR	C11-C12-C13	10.62	155.49	126.36
27	L	4003	BCR	C11-C12-C13	10.58	155.36	126.36
27	A	4005	BCR	C16-C15-C14	10.46	144.92	123.52
27	7	503	BCR	C11-C12-C13	10.37	154.79	126.36
24	H	1701	CLA	C4A-NA-C1A	10.36	111.41	106.68
27	6	503	BCR	C11-C10-C9	10.30	141.72	127.28
27	J	4001	BCR	C11-C12-C13	10.26	154.50	126.36
27	3	505	BCR	C11-C12-C13	10.24	154.44	126.36
27	3	503	BCR	C11-C12-C13	10.19	154.30	126.36
27	L	4001	BCR	C11-C12-C13	10.15	154.18	126.36
27	A	4003	BCR	C11-C12-C13	10.10	154.07	126.36
27	4	503	BCR	C11-C10-C9	10.02	141.33	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	5	503	BCR	C11-C12-C13	10.02	153.83	126.36
27	6	503	BCR	C11-C12-C13	9.98	153.73	126.36
27	H	4001	BCR	C11-C12-C13	9.95	153.66	126.36
27	A	4001	BCR	C16-C15-C14	9.94	143.85	123.52
27	8	503	BCR	C11-C12-C13	9.93	153.60	126.36
27	7	503	BCR	C20-C19-C18	9.90	153.50	126.36
27	4	503	BCR	C11-C12-C13	9.84	153.34	126.36
27	B	4005	BCR	C11-C12-C13	9.80	153.22	126.36
36	G	5002	ERG	C19-C10-C9	-9.76	94.77	110.98
24	B	1205	CLA	C4A-NA-C1A	9.68	111.10	106.68
24	A	1123	CLA	C4A-NA-C1A	9.62	111.07	106.68
24	a	603	CLA	C4A-NA-C1A	9.59	111.05	106.68
27	B	4003	BCR	C20-C19-C18	9.57	152.62	126.36
24	B	1221	CLA	C4A-NA-C1A	9.55	111.04	106.68
24	A	1103	CLA	C4A-NA-C1A	9.53	111.03	106.68
24	4	612	CLA	C4A-NA-C1A	9.47	111.00	106.68
24	B	1206	CLA	C4A-NA-C1A	9.42	110.97	106.68
24	2	615	CLA	C4A-NA-C1A	9.40	110.97	106.68
24	8	608	CLA	C4A-NA-C1A	9.38	110.96	106.68
49	7	504	C7Z	C27-C28-C29	-9.38	112.36	126.23
24	6	609	CLA	C4A-NA-C1A	9.37	110.95	106.68
24	A	1109	CLA	C4A-NA-C1A	9.36	110.95	106.68
27	4	503	BCR	C20-C19-C18	9.35	151.99	126.36
27	H	4001	BCR	C20-C19-C18	9.33	151.94	126.36
24	B	1235	CLA	C4A-NA-C1A	9.33	110.93	106.68
24	A	1120	CLA	C4A-NA-C1A	9.32	110.93	106.68
24	2	612	CLA	C4A-NA-C1A	9.31	110.93	106.68
24	B	1239	CLA	C4A-NA-C1A	9.31	110.93	106.68
24	a	615	CLA	C4A-NA-C1A	9.30	110.92	106.68
24	3	606	CLA	C4A-NA-C1A	9.28	110.91	106.68
24	5	612	CLA	C4A-NA-C1A	9.26	110.90	106.68
24	4	603	CLA	C4A-NA-C1A	9.26	110.90	106.68
24	3	601	CLA	C4A-NA-C1A	9.26	110.90	106.68
24	8	611	CLA	C4A-NA-C1A	9.23	110.89	106.68
24	B	1217	CLA	C4A-NA-C1A	9.23	110.89	106.68
24	5	608	CLA	C4A-NA-C1A	9.22	110.88	106.68
24	A	1121	CLA	C4A-NA-C1A	9.20	110.88	106.68
24	A	1102	CLA	C4A-NA-C1A	9.15	110.86	106.68
24	6	607	CLA	C4A-NA-C1A	9.14	110.85	106.68
24	9	607	CLA	C4A-NA-C1A	9.10	110.83	106.68
24	1	610	CLA	C4A-NA-C1A	9.09	110.83	106.68
24	A	1141	CLA	C4A-NA-C1A	9.08	110.82	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	7	609	CLA	C4A-NA-C1A	9.07	110.82	106.68
27	I	4001	BCR	C20-C19-C18	9.07	151.24	126.36
24	K	1401	CLA	C4A-NA-C1A	9.07	110.82	106.68
24	7	608	CLA	C4A-NA-C1A	9.06	110.81	106.68
24	8	603	CLA	C4A-NA-C1A	9.06	110.81	106.68
24	7	601	CLA	C4A-NA-C1A	9.04	110.80	106.68
24	1	608	CLA	C4A-NA-C1A	9.04	110.80	106.68
24	1	612	CLA	C4A-NA-C1A	9.04	110.80	106.68
24	5	616	CLA	C4A-NA-C1A	9.03	110.80	106.68
24	7	611	CLA	C4A-NA-C1A	9.03	110.80	106.68
24	B	1021	CLA	C4A-NA-C1A	9.03	110.80	106.68
24	B	1204	CLA	C4A-NA-C1A	9.03	110.80	106.68
24	A	1108	CLA	C4A-NA-C1A	9.03	110.80	106.68
24	4	607	CLA	C4A-NA-C1A	9.03	110.80	106.68
24	A	1112	CLA	C4A-NA-C1A	9.02	110.79	106.68
24	a	608	CLA	C4A-NA-C1A	9.01	110.79	106.68
24	8	609	CLA	C4A-NA-C1A	9.01	110.79	106.68
24	L	1501	CLA	C4A-NA-C1A	9.01	110.79	106.68
24	3	618	CLA	C4A-NA-C1A	9.00	110.79	106.68
24	B	1222	CLA	C4A-NA-C1A	9.00	110.78	106.68
24	6	603	CLA	C4A-NA-C1A	9.00	110.78	106.68
24	B	1212	CLA	C4A-NA-C1A	8.99	110.78	106.68
24	5	603	CLA	C4A-NA-C1A	8.99	110.78	106.68
24	7	612	CLA	C4A-NA-C1A	8.99	110.78	106.68
24	3	616	CLA	C4A-NA-C1A	8.98	110.78	106.68
24	a	612	CLA	C4A-NA-C1A	8.97	110.77	106.68
24	6	615	CLA	C4A-NA-C1A	8.96	110.77	106.68
27	B	4002	BCR	C11-C12-C13	8.96	150.94	126.36
24	A	1118	CLA	C4A-NA-C1A	8.96	110.77	106.68
24	A	1138	CLA	C4A-NA-C1A	8.95	110.76	106.68
24	A	1132	CLA	C4A-NA-C1A	8.94	110.76	106.68
24	3	607	CLA	C4A-NA-C1A	8.94	110.76	106.68
27	A	4005	BCR	C20-C19-C18	8.94	150.87	126.36
24	7	607	CLA	C4A-NA-C1A	8.93	110.75	106.68
24	9	603	CLA	C4A-NA-C1A	8.93	110.75	106.68
24	3	613	CLA	C4A-NA-C1A	8.92	110.75	106.68
24	2	608	CLA	C4A-NA-C1A	8.91	110.75	106.68
24	6	605	CLA	C4A-NA-C1A	8.90	110.74	106.68
24	4	601	CLA	C4A-NA-C1A	8.90	110.74	106.68
24	1	615	CLA	C4A-NA-C1A	8.89	110.74	106.68
24	A	1125	CLA	C4A-NA-C1A	8.89	110.74	106.68
24	B	1230	CLA	C4A-NA-C1A	8.88	110.73	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	7	610	CLA	C4A-NA-C1A	8.88	110.73	106.68
24	A	1131	CLA	C4A-NA-C1A	8.88	110.73	106.68
24	A	1107	CLA	C4A-NA-C1A	8.88	110.73	106.68
24	5	617	CLA	C4A-NA-C1A	8.87	110.73	106.68
24	3	612	CLA	C4A-NA-C1A	8.87	110.72	106.68
24	5	614	CLA	C4A-NA-C1A	8.87	110.72	106.68
24	2	607	CLA	C4A-NA-C1A	8.85	110.72	106.68
24	2	621	CLA	C4A-NA-C1A	8.85	110.72	106.68
24	3	603	CLA	C4A-NA-C1A	8.85	110.72	106.68
24	A	1013	CLA	C4A-NA-C1A	8.84	110.71	106.68
24	6	601	CLA	C4A-NA-C1A	8.84	110.71	106.68
24	B	1220	CLA	C4A-NA-C1A	8.84	110.71	106.68
24	5	601	CLA	C4A-NA-C1A	8.83	110.71	106.68
24	a	602	CLA	C4A-NA-C1A	8.82	110.70	106.68
24	F	1301	CLA	C4A-NA-C1A	8.82	110.70	106.68
24	H	1702	CLA	C4A-NA-C1A	8.82	110.70	106.68
24	2	613	CLA	C4A-NA-C1A	8.82	110.70	106.68
24	A	1106	CLA	C4A-NA-C1A	8.82	110.70	106.68
24	3	604	CLA	C4A-NA-C1A	8.81	110.70	106.68
24	8	620	CLA	C4A-NA-C1A	8.81	110.70	106.68
24	B	1232	CLA	C4A-NA-C1A	8.80	110.70	106.68
24	8	610	CLA	C4A-NA-C1A	8.80	110.70	106.68
24	5	609	CLA	C4A-NA-C1A	8.80	110.69	106.68
24	G	1601	CLA	C4A-NA-C1A	8.80	110.69	106.68
24	5	607	CLA	C4A-NA-C1A	8.80	110.69	106.68
24	A	1101	CLA	C4A-NA-C1A	8.79	110.69	106.68
24	1	603	CLA	C4A-NA-C1A	8.79	110.69	106.68
24	2	603	CLA	C4A-NA-C1A	8.79	110.69	106.68
24	9	602	CLA	C4A-NA-C1A	8.79	110.69	106.68
24	1	611	CLA	C4A-NA-C1A	8.78	110.68	106.68
24	A	1115	CLA	C4A-NA-C1A	8.78	110.68	106.68
24	A	1134	CLA	C4A-NA-C1A	8.77	110.68	106.68
24	A	1111	CLA	C4A-NA-C1A	8.77	110.68	106.68
24	8	605	CLA	C4A-NA-C1A	8.77	110.68	106.68
24	B	1210	CLA	C4A-NA-C1A	8.77	110.68	106.68
24	1	605	CLA	C4A-NA-C1A	8.76	110.68	106.68
24	6	606	CLA	C4A-NA-C1A	8.76	110.68	106.68
24	9	609	CLA	C4A-NA-C1A	8.76	110.68	106.68
24	A	1122	CLA	C4A-NA-C1A	8.76	110.67	106.68
24	9	612	CLA	C4A-NA-C1A	8.75	110.67	106.68
24	6	617	CLA	C4A-NA-C1A	8.75	110.67	106.68
24	B	1223	CLA	C4A-NA-C1A	8.74	110.67	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	L	1503	CLA	C4A-NA-C1A	8.74	110.67	106.68
24	8	606	CLA	C4A-NA-C1A	8.74	110.67	106.68
24	a	607	CLA	C4A-NA-C1A	8.74	110.67	106.68
24	4	617	CLA	C4A-NA-C1A	8.74	110.67	106.68
24	2	610	CLA	C4A-NA-C1A	8.73	110.66	106.68
23	A	1011	CL0	O2D-CGD-CBD	8.73	120.54	110.95
27	3	503	BCR	C20-C19-C18	8.73	150.30	126.36
24	J	1901	CLA	C4A-NA-C1A	8.73	110.66	106.68
24	B	1202	CLA	C4A-NA-C1A	8.73	110.66	106.68
24	4	615	CLA	C4A-NA-C1A	8.72	110.66	106.68
24	A	1126	CLA	C4A-NA-C1A	8.71	110.66	106.68
24	3	610	CLA	C4A-NA-C1A	8.71	110.66	106.68
24	B	1237	CLA	C4A-NA-C1A	8.71	110.65	106.68
24	K	1403	CLA	C4A-NA-C1A	8.70	110.65	106.68
27	6	504	BCR	C20-C19-C18	8.70	150.22	126.36
24	a	604	CLA	C4A-NA-C1A	8.70	110.65	106.68
40	2	502	LUT	C21-C26-C27	8.69	122.82	112.83
24	A	1117	CLA	C4A-NA-C1A	8.68	110.64	106.68
24	B	1240	CLA	C4A-NA-C1A	8.68	110.64	106.68
24	6	604	CLA	C4A-NA-C1A	8.68	110.64	106.68
24	6	612	CLA	C4A-NA-C1A	8.67	110.64	106.68
24	2	606	CLA	C4A-NA-C1A	8.67	110.64	106.68
24	3	602	CLA	C4A-NA-C1A	8.66	110.63	106.68
27	B	4002	BCR	C20-C19-C18	8.66	150.10	126.36
24	A	1114	CLA	C4A-NA-C1A	8.66	110.63	106.68
24	A	1133	CLA	C4A-NA-C1A	8.66	110.63	106.68
24	B	1224	CLA	C4A-NA-C1A	8.65	110.63	106.68
24	A	1105	CLA	C4A-NA-C1A	8.65	110.63	106.68
24	7	603	CLA	C4A-NA-C1A	8.65	110.62	106.68
24	4	602	CLA	C4A-NA-C1A	8.64	110.62	106.68
24	4	611	CLA	C4A-NA-C1A	8.64	110.62	106.68
24	7	606	CLA	C4A-NA-C1A	8.64	110.62	106.68
27	F	4001	BCR	C11-C12-C13	8.63	150.03	126.36
24	G	1603	CLA	C4A-NA-C1A	8.63	110.61	106.68
24	H	1703	CLA	C4A-NA-C1A	8.62	110.61	106.68
27	8	503	BCR	C20-C19-C18	8.62	150.00	126.36
24	8	612	CLA	C4A-NA-C1A	8.62	110.61	106.68
24	A	1139	CLA	C4A-NA-C1A	8.61	110.61	106.68
24	8	615	CLA	C4A-NA-C1A	8.60	110.60	106.68
24	1	606	CLA	C4A-NA-C1A	8.59	110.60	106.68
27	B	4004	BCR	C20-C19-C18	8.59	149.90	126.36
24	1	607	CLA	C4A-NA-C1A	8.58	110.59	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	2	602	CLA	C4A-NA-C1A	8.58	110.59	106.68
24	F	1302	CLA	C4A-NA-C1A	8.58	110.59	106.68
24	8	602	CLA	C4A-NA-C1A	8.58	110.59	106.68
24	A	1113	CLA	C4A-NA-C1A	8.57	110.59	106.68
24	8	607	CLA	C4A-NA-C1A	8.57	110.59	106.68
24	A	1137	CLA	C4A-NA-C1A	8.57	110.59	106.68
24	A	1128	CLA	C4A-NA-C1A	8.57	110.59	106.68
24	A	1136	CLA	C4A-NA-C1A	8.56	110.58	106.68
24	4	616	CLA	C4A-NA-C1A	8.56	110.58	106.68
24	A	1140	CLA	C4A-NA-C1A	8.55	110.58	106.68
24	A	1124	CLA	C4A-NA-C1A	8.55	110.58	106.68
24	B	1238	CLA	C4A-NA-C1A	8.54	110.58	106.68
24	8	618	CLA	C4A-NA-C1A	8.54	110.57	106.68
24	9	605	CLA	C4A-NA-C1A	8.54	110.57	106.68
27	L	4003	BCR	C20-C19-C18	8.53	149.76	126.36
24	5	605	CLA	C4A-NA-C1A	8.52	110.57	106.68
24	9	608	CLA	C4A-NA-C1A	8.52	110.57	106.68
24	6	608	CLA	C4A-NA-C1A	8.52	110.56	106.68
24	A	1110	CLA	C4A-NA-C1A	8.51	110.56	106.68
24	B	1201	CLA	C4A-NA-C1A	8.51	110.56	106.68
24	B	1211	CLA	C4A-NA-C1A	8.51	110.56	106.68
24	6	602	CLA	C4A-NA-C1A	8.51	110.56	106.68
24	4	606	CLA	C4A-NA-C1A	8.50	110.56	106.68
27	F	4001	BCR	C11-C10-C9	8.49	139.19	127.28
24	5	618	CLA	C4A-NA-C1A	8.49	110.55	106.68
24	9	604	CLA	C4A-NA-C1A	8.48	110.55	106.68
24	4	608	CLA	C4A-NA-C1A	8.48	110.55	106.68
24	5	602	CLA	C4A-NA-C1A	8.48	110.55	106.68
27	F	4001	BCR	C20-C19-C18	8.48	149.60	126.36
24	K	1404	CLA	C4A-NA-C1A	8.47	110.55	106.68
24	B	1218	CLA	C4A-NA-C1A	8.47	110.54	106.68
24	L	1502	CLA	C4A-NA-C1A	8.47	110.54	106.68
24	2	605	CLA	C4A-NA-C1A	8.47	110.54	106.68
24	A	1104	CLA	C4A-NA-C1A	8.46	110.54	106.68
24	B	1209	CLA	C4A-NA-C1A	8.45	110.53	106.68
24	7	604	CLA	C4A-NA-C1A	8.45	110.53	106.68
24	B	1236	CLA	C4A-NA-C1A	8.45	110.53	106.68
41	1	609	CHL	C1B-CHB-C4A	8.44	126.75	121.32
24	G	1602	CLA	C4A-NA-C1A	8.44	110.53	106.68
24	2	601	CLA	C4A-NA-C1A	8.44	110.53	106.68
24	5	606	CLA	C4A-NA-C1A	8.42	110.52	106.68
24	1	602	CLA	C4A-NA-C1A	8.41	110.52	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	5	503	BCR	C20-C19-C18	8.41	149.43	126.36
24	B	1023	CLA	C4A-NA-C1A	8.41	110.52	106.68
24	7	615	CLA	C4A-NA-C1A	8.41	110.51	106.68
24	a	611	CLA	C4A-NA-C1A	8.40	110.51	106.68
24	a	601	CLA	C4A-NA-C1A	8.39	110.51	106.68
24	5	604	CLA	C4A-NA-C1A	8.39	110.51	106.68
24	K	1402	CLA	C4A-NA-C1A	8.37	110.50	106.68
41	3	608	CHL	C1B-CHB-C4A	8.37	126.71	121.32
24	B	1231	CLA	C4A-NA-C1A	8.37	110.50	106.68
24	B	1213	CLA	C4A-NA-C1A	8.36	110.49	106.68
24	6	618	CLA	C4A-NA-C1A	8.36	110.49	106.68
24	2	609	CLA	C4A-NA-C1A	8.36	110.49	106.68
24	4	605	CLA	C4A-NA-C1A	8.35	110.49	106.68
24	A	1127	CLA	C4A-NA-C1A	8.35	110.49	106.68
24	3	605	CLA	C4A-NA-C1A	8.34	110.48	106.68
24	B	1203	CLA	C4A-NA-C1A	8.33	110.48	106.68
24	9	606	CLA	C4A-NA-C1A	8.32	110.48	106.68
24	7	602	CLA	C4A-NA-C1A	8.32	110.47	106.68
24	B	1219	CLA	C4A-NA-C1A	8.31	110.47	106.68
24	4	604	CLA	C4A-NA-C1A	8.31	110.47	106.68
24	2	604	CLA	C4A-NA-C1A	8.29	110.46	106.68
24	1	601	CLA	C4A-NA-C1A	8.28	110.45	106.68
27	B	4007	BCR	C20-C19-C18	8.27	149.05	126.36
24	7	617	CLA	C4A-NA-C1A	8.27	110.45	106.68
24	B	1225	CLA	C4A-NA-C1A	8.26	110.45	106.68
24	B	1228	CLA	C4A-NA-C1A	8.26	110.45	106.68
24	B	1207	CLA	C4A-NA-C1A	8.26	110.45	106.68
24	B	1215	CLA	C4A-NA-C1A	8.24	110.44	106.68
24	B	1214	CLA	C4A-NA-C1A	8.24	110.44	106.68
24	a	605	CLA	C4A-NA-C1A	8.24	110.44	106.68
24	B	1208	CLA	C4A-NA-C1A	8.22	110.43	106.68
24	A	1012	CLA	C4A-NA-C1A	8.22	110.43	106.68
24	7	605	CLA	C4A-NA-C1A	8.21	110.42	106.68
27	A	4002	BCR	C20-C19-C18	8.20	148.86	126.36
24	B	1227	CLA	C4A-NA-C1A	8.20	110.42	106.68
40	6	501	LUT	C15-C35-C34	-8.19	106.76	123.52
24	B	1229	CLA	C4A-NA-C1A	8.17	110.41	106.68
27	B	4006	BCR	C20-C19-C18	8.16	148.74	126.36
24	A	1135	CLA	C4A-NA-C1A	8.14	110.39	106.68
24	1	604	CLA	C4A-NA-C1A	8.13	110.39	106.68
40	6	501	LUT	C21-C26-C27	8.09	122.12	112.83
24	A	1116	CLA	C4A-NA-C1A	8.07	110.36	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	4	610	CLA	C4A-NA-C1A	8.04	110.34	106.68
27	6	503	BCR	C20-C19-C18	7.96	148.19	126.36
24	A	1119	CLA	C4A-NA-C1A	7.96	110.31	106.68
24	B	1234	CLA	C4A-NA-C1A	7.91	110.29	106.68
40	6	501	LUT	C31-C30-C29	-7.84	116.28	127.28
27	A	4004	BCR	C20-C19-C18	7.81	147.78	126.36
27	A	4003	BCR	C20-C19-C18	7.80	147.75	126.36
27	B	4005	BCR	C20-C19-C18	7.76	147.63	126.36
24	B	1216	CLA	C4A-NA-C1A	7.75	110.22	106.68
27	L	4001	BCR	C20-C19-C18	7.71	147.51	126.36
24	A	1130	CLA	C4A-NA-C1A	7.70	110.19	106.68
24	A	1129	CLA	C4A-NA-C1A	7.62	110.16	106.68
27	J	4001	BCR	C20-C19-C18	7.59	147.18	126.36
27	3	505	BCR	C20-C19-C18	7.57	147.11	126.36
24	B	1226	CLA	C4A-NA-C1A	7.52	110.11	106.68
41	1	613	CHL	C1B-CHB-C4A	7.48	126.14	121.32
27	K	4001	BCR	C20-C19-C18	7.47	146.84	126.36
41	5	613	CHL	C1B-CHB-C4A	7.44	126.11	121.32
27	5	504	BCR	C20-C19-C18	7.41	146.69	126.36
36	G	5002	ERG	C14-C13-C17	7.38	107.43	99.72
40	1	503	LUT	C21-C26-C27	7.33	121.25	112.83
41	9	613	CHL	C1B-CHB-C4A	7.28	126.01	121.32
24	9	601	CLA	C4A-NA-C1A	7.28	110.00	106.68
40	6	502	LUT	C21-C26-C27	7.28	121.19	112.83
27	L	4002	BCR	C20-C19-C18	7.25	146.24	126.36
49	7	504	C7Z	C15-C14-C13	-7.24	117.13	127.28
27	K	4002	BCR	C20-C19-C18	7.22	146.15	126.36
24	B	1022	CLA	C4A-NA-C1A	7.17	109.95	106.68
41	8	613	CHL	C1B-CHB-C4A	7.10	125.89	121.32
24	2	604	CLA	O2D-CGD-CBD	7.07	123.59	111.23
41	8	604	CHL	C1B-CHB-C4A	7.07	125.87	121.32
41	7	613	CHL	C1B-CHB-C4A	6.88	125.75	121.32
24	A	1121	CLA	CMD-C2D-C1D	6.81	136.72	124.73
27	A	4001	BCR	C20-C19-C18	6.75	144.87	126.36
27	B	4001	BCR	C20-C19-C18	6.73	144.82	126.36
24	A	1101	CLA	O2D-CGD-CBD	6.73	122.99	111.23
41	8	601	CHL	C1B-CHB-C4A	6.72	125.64	121.32
27	3	504	BCR	C20-C19-C18	6.68	144.69	126.36
36	G	5002	ERG	C12-C13-C14	6.66	117.24	107.19
27	G	4001	BCR	C20-C19-C18	6.61	144.50	126.36
41	6	611	CHL	C1B-CHB-C4A	6.59	125.56	121.32
24	5	608	CLA	O2D-CGD-CBD	6.59	122.75	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	a	609	CHL	C1B-CHB-C4A	6.58	125.56	121.32
39	M	4001	ECH	C11-C10-C9	-6.54	118.11	127.28
41	4	613	CHL	C1B-CHB-C4A	6.45	125.47	121.32
40	a	503	LUT	C35-C34-C33	-6.40	118.31	127.28
40	5	505	LUT	C11-C10-C9	-6.38	118.33	127.28
24	4	612	CLA	O2D-CGD-CBD	6.36	122.34	111.23
40	6	501	LUT	C7-C8-C9	-6.36	116.83	126.23
40	7	501	LUT	C21-C26-C27	6.36	120.13	112.83
41	4	618	CHL	C1B-CHB-C4A	6.32	125.39	121.32
40	5	505	LUT	C21-C26-C27	6.31	120.08	112.83
41	6	613	CHL	C1B-CHB-C4A	6.31	125.38	121.32
24	A	1108	CLA	O2D-CGD-CBD	6.25	122.15	111.23
40	5	505	LUT	C15-C14-C13	-6.24	118.52	127.28
24	B	1218	CLA	O2D-CGD-CBD	6.24	122.14	111.23
40	9	501	LUT	C21-C26-C27	6.21	119.97	112.83
41	9	610	CHL	C1B-CHB-C4A	6.20	125.31	121.32
24	A	1121	CLA	O2D-CGD-CBD	6.18	122.04	111.23
24	4	608	CLA	CMD-C2D-C1D	6.16	135.58	124.73
41	4	609	CHL	C1B-CHB-C4A	6.13	125.27	121.32
41	a	606	CHL	C1B-CHB-C4A	6.12	125.26	121.32
24	B	1221	CLA	O2D-CGD-CBD	6.12	121.92	111.23
43	3	506	QTB	C04-C03-C02	6.10	135.84	127.28
24	A	1109	CLA	CMD-C2D-C1D	6.10	135.46	124.73
24	6	608	CLA	CMD-C2D-C1D	6.10	135.46	124.73
40	4	501	LUT	C21-C26-C27	6.09	119.83	112.83
41	6	619	CHL	C1B-CHB-C4A	6.07	125.23	121.32
24	A	1128	CLA	O2D-CGD-CBD	6.07	121.84	111.23
40	6	501	LUT	C35-C34-C33	6.04	135.75	127.28
24	K	1402	CLA	O2D-CGD-CBD	6.03	121.78	111.23
24	B	1230	CLA	O2D-CGD-CBD	6.02	121.75	111.23
24	B	1208	CLA	O2D-CGD-CBD	6.01	121.74	111.23
24	B	1226	CLA	CMD-C2D-C1D	6.01	135.31	124.73
24	8	608	CLA	O2D-CGD-CBD	6.01	121.73	111.23
24	B	1201	CLA	O2D-CGD-CBD	5.99	121.69	111.23
40	a	503	LUT	C31-C30-C29	-5.98	118.89	127.28
41	5	611	CHL	C1B-CHB-C4A	5.96	125.16	121.32
24	H	1703	CLA	CMD-C2D-C1D	5.95	135.21	124.73
24	A	1132	CLA	O2D-CGD-CBD	5.95	121.62	111.23
24	7	606	CLA	CMD-C2D-C1D	5.94	135.19	124.73
24	A	1137	CLA	O2D-CGD-CBD	5.93	121.60	111.23
40	a	503	LUT	C15-C14-C13	-5.93	118.96	127.28
24	A	1113	CLA	O2D-CGD-CBD	5.93	121.59	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	a	613	CHL	C1B-CHB-C4A	5.91	125.12	121.32
24	B	1205	CLA	O2D-CGD-CBD	5.88	121.51	111.23
37	J	4002	RRX	C11-C10-C9	-5.85	119.08	127.28
24	B	1212	CLA	O2D-CGD-CBD	5.84	121.43	111.23
24	B	1240	CLA	O2D-CGD-CBD	5.83	121.42	111.23
24	B	1211	CLA	CMD-C2D-C1D	5.83	134.99	124.73
24	5	603	CLA	CMD-C2D-C1D	5.82	134.98	124.73
40	9	502	LUT	C21-C26-C27	5.82	119.52	112.83
24	A	1106	CLA	O2D-CGD-CBD	5.82	121.41	111.23
24	1	605	CLA	CMD-C2D-C1D	5.82	134.97	124.73
37	J	4002	RRX	C16-C17-C18	-5.81	119.13	127.28
24	a	605	CLA	CMD-C2D-C1D	5.80	134.95	124.73
27	4	503	BCR	C15-C14-C13	-5.80	119.14	127.28
24	B	1219	CLA	CMD-C2D-C1D	5.80	134.94	124.73
24	6	605	CLA	CMD-C2D-C1D	5.80	134.93	124.73
24	a	607	CLA	O2D-CGD-CBD	5.80	121.36	111.23
24	G	1602	CLA	O2D-CGD-CBD	5.79	121.36	111.23
24	6	609	CLA	O2D-CGD-CBD	5.77	121.31	111.23
24	7	609	CLA	CMD-C2D-C1D	5.76	134.87	124.73
24	A	1115	CLA	O2D-CGD-CBD	5.75	121.29	111.23
24	K	1401	CLA	CMD-C2D-C1D	5.75	134.85	124.73
27	H	4001	BCR	C15-C14-C13	-5.74	119.22	127.28
24	7	617	CLA	O2D-CGD-CBD	5.74	121.27	111.23
24	2	615	CLA	O2D-CGD-CBD	5.74	121.27	111.23
24	7	601	CLA	CMD-C2D-C1D	5.73	134.82	124.73
24	A	1114	CLA	CMD-C2D-C1D	5.72	134.81	124.73
24	A	1129	CLA	O2D-CGD-CBD	5.72	121.22	111.23
24	8	608	CLA	CMD-C2D-C1D	5.72	134.79	124.73
24	1	607	CLA	O2D-CGD-CBD	5.72	121.22	111.23
24	2	603	CLA	CMD-C2D-C1D	5.71	134.79	124.73
24	A	1101	CLA	CMD-C2D-C1D	5.70	134.77	124.73
24	8	607	CLA	O2D-CGD-CBD	5.70	121.19	111.23
24	A	1105	CLA	CMD-C2D-C1D	5.70	134.76	124.73
24	3	618	CLA	O2D-CGD-CBD	5.70	121.19	111.23
24	B	1231	CLA	CMD-C2D-C1D	5.70	134.76	124.73
24	1	603	CLA	CMD-C2D-C1D	5.70	134.76	124.73
24	B	1208	CLA	CMD-C2D-C1D	5.69	134.75	124.73
24	A	1125	CLA	O2D-CGD-CBD	5.69	121.18	111.23
24	2	621	CLA	O2D-CGD-CBD	5.69	121.17	111.23
24	K	1404	CLA	O2D-CGD-CBD	5.68	121.17	111.23
40	6	501	LUT	C32-C33-C34	5.68	127.94	119.01
43	a	504	QTB	C09-C02-C03	5.68	127.94	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	4	610	CLA	CMD-C2D-C1D	5.68	134.73	124.73
24	B	1202	CLA	O2D-CGD-CBD	5.68	121.16	111.23
24	5	604	CLA	CMD-C2D-C1D	5.66	134.70	124.73
24	B	1223	CLA	CMD-C2D-C1D	5.66	134.70	124.73
24	A	1126	CLA	CMD-C2D-C1D	5.66	134.69	124.73
24	H	1702	CLA	O2D-CGD-CBD	5.65	121.11	111.23
24	B	1238	CLA	CMD-C2D-C1D	5.65	134.67	124.73
24	B	1223	CLA	O2D-CGD-CBD	5.64	121.09	111.23
36	G	5002	ERG	C1-C10-C9	5.64	119.35	108.39
24	K	1402	CLA	CMD-C2D-C1D	5.64	134.66	124.73
24	B	1214	CLA	CMD-C2D-C1D	5.63	134.64	124.73
24	4	604	CLA	O2D-CGD-CBD	5.63	121.06	111.23
24	9	605	CLA	CMD-C2D-C1D	5.62	134.62	124.73
24	B	1213	CLA	CMD-C2D-C1D	5.62	134.62	124.73
24	B	1222	CLA	CMD-C2D-C1D	5.62	134.62	124.73
24	6	617	CLA	CMD-C2D-C1D	5.61	134.61	124.73
24	2	605	CLA	CMD-C2D-C1D	5.61	134.61	124.73
24	B	1232	CLA	CMD-C2D-C1D	5.60	134.60	124.73
24	4	603	CLA	CMD-C2D-C1D	5.60	134.59	124.73
24	B	1218	CLA	CMD-C2D-C1D	5.60	134.59	124.73
24	1	615	CLA	CMD-C2D-C1D	5.60	134.59	124.73
24	7	603	CLA	CMD-C2D-C1D	5.60	134.59	124.73
24	A	1131	CLA	CMD-C2D-C1D	5.59	134.58	124.73
24	B	1229	CLA	CMD-C2D-C1D	5.59	134.58	124.73
24	3	605	CLA	CMD-C2D-C1D	5.59	134.57	124.73
24	7	604	CLA	CMD-C2D-C1D	5.59	134.57	124.73
24	1	601	CLA	CMD-C2D-C1D	5.59	134.57	124.73
24	A	1112	CLA	O2D-CGD-CBD	5.58	120.99	111.23
24	B	1217	CLA	O2D-CGD-CBD	5.58	120.99	111.23
24	4	606	CLA	O2D-CGD-CBD	5.58	120.99	111.23
24	B	1224	CLA	CMD-C2D-C1D	5.58	134.56	124.73
24	A	1102	CLA	O2D-CGD-CBD	5.58	120.98	111.23
24	4	617	CLA	CMD-C2D-C1D	5.58	134.55	124.73
24	A	1130	CLA	CMD-C2D-C1D	5.58	134.55	124.73
24	4	607	CLA	O2D-CGD-CBD	5.57	120.97	111.23
24	A	1113	CLA	CMD-C2D-C1D	5.57	134.54	124.73
24	6	606	CLA	CMD-C2D-C1D	5.57	134.54	124.73
24	4	605	CLA	CMD-C2D-C1D	5.57	134.54	124.73
24	A	1135	CLA	CMD-C2D-C1D	5.57	134.53	124.73
24	8	618	CLA	O2D-CGD-CBD	5.56	120.96	111.23
24	A	1120	CLA	O2A-C1-C2	5.56	122.23	108.99
27	6	503	BCR	C15-C14-C13	-5.56	119.48	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	L	1503	CLA	O2D-CGD-CBD	5.56	120.95	111.23
43	3	506	QTB	C13-C12-C11	5.56	123.08	112.57
24	1	606	CLA	CMD-C2D-C1D	5.56	134.51	124.73
24	K	1404	CLA	CMD-C2D-C1D	5.55	134.50	124.73
24	B	1227	CLA	CMD-C2D-C1D	5.55	134.50	124.73
24	7	605	CLA	CMD-C2D-C1D	5.55	134.50	124.73
24	8	615	CLA	CMD-C2D-C1D	5.55	134.49	124.73
24	G	1602	CLA	CMD-C2D-C1D	5.54	134.49	124.73
24	B	1203	CLA	CMD-C2D-C1D	5.54	134.48	124.73
24	5	605	CLA	CMD-C2D-C1D	5.54	134.48	124.73
40	a	503	LUT	C21-C26-C27	5.54	119.19	112.83
24	2	602	CLA	O2D-CGD-CBD	5.53	120.91	111.23
24	2	621	CLA	CMD-C2D-C1D	5.53	134.47	124.73
24	5	601	CLA	CMD-C2D-C1D	5.53	134.47	124.73
24	A	1134	CLA	CMD-C2D-C1D	5.53	134.47	124.73
24	A	1132	CLA	CMD-C2D-C1D	5.53	134.47	124.73
24	3	613	CLA	O2D-CGD-CBD	5.53	120.89	111.23
24	a	603	CLA	CMD-C2D-C1D	5.52	134.45	124.73
24	3	602	CLA	CMD-C2D-C1D	5.52	134.45	124.73
24	L	1502	CLA	CMD-C2D-C1D	5.52	134.45	124.73
43	a	504	QTB	C13-C12-C11	5.52	123.00	112.57
49	7	504	C7Z	C15-C35-C34	-5.51	112.24	123.52
24	4	616	CLA	CMD-C2D-C1D	5.51	134.44	124.73
24	A	1111	CLA	CMD-C2D-C1D	5.51	134.43	124.73
24	9	604	CLA	CMD-C2D-C1D	5.51	134.43	124.73
24	3	610	CLA	O2D-CGD-CBD	5.51	120.86	111.23
24	2	602	CLA	CMD-C2D-C1D	5.51	134.43	124.73
24	7	604	CLA	O2D-CGD-CBD	5.51	120.86	111.23
40	6	501	LUT	C40-C33-C34	-5.50	113.90	122.82
24	B	1231	CLA	O2D-CGD-CBD	5.50	120.85	111.23
24	A	1116	CLA	CMD-C2D-C1D	5.50	134.41	124.73
40	5	502	LUT	C21-C26-C27	5.49	119.14	112.83
24	1	602	CLA	CMD-C2D-C1D	5.49	134.40	124.73
24	7	602	CLA	CMD-C2D-C1D	5.49	134.40	124.73
24	8	618	CLA	CMD-C2D-C1D	5.48	134.39	124.73
24	A	1102	CLA	CMD-C2D-C1D	5.48	134.38	124.73
24	2	610	CLA	CMD-C2D-C1D	5.48	134.38	124.73
24	8	602	CLA	CMD-C2D-C1D	5.48	134.38	124.73
24	2	612	CLA	CMD-C2D-C1D	5.48	134.38	124.73
24	A	1120	CLA	O2D-CGD-CBD	5.48	120.81	111.23
24	9	601	CLA	CMD-C2D-C1D	5.48	134.38	124.73
24	1	607	CLA	CMD-C2D-C1D	5.48	134.38	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1	611	CLA	CMD-C2D-C1D	5.48	134.38	124.73
24	A	1125	CLA	CMD-C2D-C1D	5.48	134.38	124.73
24	4	611	CLA	CMD-C2D-C1D	5.48	134.38	124.73
24	8	606	CLA	CMD-C2D-C1D	5.48	134.38	124.73
24	9	606	CLA	O2D-CGD-CBD	5.48	120.81	111.23
24	7	617	CLA	CMD-C2D-C1D	5.48	134.37	124.73
24	2	601	CLA	CMD-C2D-C1D	5.48	134.37	124.73
24	3	606	CLA	CMD-C2D-C1D	5.48	134.37	124.73
24	K	1403	CLA	CMD-C2D-C1D	5.48	134.37	124.73
24	L	1501	CLA	CMD-C2D-C1D	5.48	134.37	124.73
24	A	1115	CLA	CMD-C2D-C1D	5.47	134.37	124.73
24	6	604	CLA	CMD-C2D-C1D	5.47	134.37	124.73
24	8	609	CLA	O2D-CGD-CBD	5.47	120.79	111.23
24	A	1141	CLA	CMD-C2D-C1D	5.47	134.36	124.73
24	J	1901	CLA	CMD-C2D-C1D	5.47	134.36	124.73
24	H	1702	CLA	CMD-C2D-C1D	5.47	134.36	124.73
24	4	606	CLA	CMD-C2D-C1D	5.47	134.36	124.73
24	8	603	CLA	CMD-C2D-C1D	5.46	134.35	124.73
24	A	1130	CLA	O2D-CGD-CBD	5.46	120.78	111.23
24	7	611	CLA	CMD-C2D-C1D	5.46	134.34	124.73
24	6	618	CLA	CMD-C2D-C1D	5.46	134.34	124.73
24	A	1103	CLA	CMD-C2D-C1D	5.45	134.33	124.73
24	A	1106	CLA	CMD-C2D-C1D	5.45	134.33	124.73
24	B	1239	CLA	CMD-C2D-C1D	5.45	134.33	124.73
24	8	611	CLA	CMD-C2D-C1D	5.45	134.33	124.73
24	a	601	CLA	CMD-C2D-C1D	5.45	134.33	124.73
24	A	1116	CLA	O2D-CGD-CBD	5.45	120.76	111.23
24	6	605	CLA	O2D-CGD-CBD	5.45	120.76	111.23
24	2	604	CLA	CMD-C2D-C1D	5.45	134.32	124.73
24	3	601	CLA	CMD-C2D-C1D	5.45	134.32	124.73
24	8	620	CLA	CMD-C2D-C1D	5.45	134.32	124.73
24	a	607	CLA	CMD-C2D-C1D	5.45	134.32	124.73
24	6	601	CLA	CMD-C2D-C1D	5.45	134.32	124.73
24	B	1228	CLA	CMD-C2D-C1D	5.44	134.31	124.73
24	2	606	CLA	CMD-C2D-C1D	5.44	134.31	124.73
24	9	606	CLA	CMD-C2D-C1D	5.44	134.31	124.73
24	6	602	CLA	CMD-C2D-C1D	5.44	134.31	124.73
24	B	1235	CLA	CMD-C2D-C1D	5.44	134.31	124.73
39	M	4001	ECH	C16-C17-C18	-5.44	119.65	127.28
24	5	614	CLA	CMD-C2D-C1D	5.44	134.30	124.73
24	B	1229	CLA	O2D-CGD-CBD	5.44	120.73	111.23
24	6	604	CLA	O2D-CGD-CBD	5.44	120.73	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	6	603	CLA	CMD-C2D-C1D	5.43	134.30	124.73
24	B	1234	CLA	CMD-C2D-C1D	5.43	134.30	124.73
24	B	1210	CLA	O2D-CGD-CBD	5.43	120.72	111.23
24	A	1108	CLA	CMD-C2D-C1D	5.43	134.29	124.73
24	8	605	CLA	CMD-C2D-C1D	5.43	134.28	124.73
43	a	504	QTB	C01-C02-C09	-5.43	109.80	118.09
24	2	613	CLA	CMD-C2D-C1D	5.43	134.28	124.73
24	3	604	CLA	O2D-CGD-CBD	5.43	120.71	111.23
24	B	1216	CLA	CMD-C2D-C1D	5.42	134.28	124.73
24	1	604	CLA	O2D-CGD-CBD	5.42	120.71	111.23
24	B	1022	CLA	CMD-C2D-C1D	5.42	134.28	124.73
24	2	607	CLA	CMD-C2D-C1D	5.42	134.27	124.73
24	5	618	CLA	CMD-C2D-C1D	5.42	134.27	124.73
24	A	1136	CLA	CMD-C2D-C1D	5.42	134.27	124.73
24	B	1201	CLA	CMD-C2D-C1D	5.42	134.27	124.73
24	5	608	CLA	CMD-C2D-C1D	5.42	134.27	124.73
39	M	4001	ECH	C15-C14-C13	-5.42	119.68	127.28
24	A	1104	CLA	CMD-C2D-C1D	5.42	134.27	124.73
24	7	615	CLA	CMD-C2D-C1D	5.42	134.26	124.73
24	9	609	CLA	CMD-C2D-C1D	5.41	134.26	124.73
24	K	1401	CLA	O2D-CGD-CBD	5.41	120.69	111.23
24	2	609	CLA	CMD-C2D-C1D	5.41	134.25	124.73
24	B	1227	CLA	O2D-CGD-CBD	5.41	120.68	111.23
24	L	1502	CLA	O2D-CGD-CBD	5.41	120.68	111.23
24	4	604	CLA	CMD-C2D-C1D	5.41	134.25	124.73
24	5	606	CLA	CMD-C2D-C1D	5.41	134.25	124.73
24	5	607	CLA	CMD-C2D-C1D	5.40	134.25	124.73
24	8	610	CLA	CMD-C2D-C1D	5.40	134.25	124.73
24	A	1122	CLA	O2D-CGD-CBD	5.40	120.68	111.23
24	1	608	CLA	O2D-CGD-CBD	5.40	120.67	111.23
39	M	4001	ECH	C20-C21-C22	-5.40	119.71	127.28
41	5	610	CHL	C1B-CHB-C4A	5.40	124.80	121.32
24	A	1129	CLA	CMD-C2D-C1D	5.40	134.23	124.73
24	a	608	CLA	CMD-C2D-C1D	5.40	134.23	124.73
24	a	604	CLA	O2D-CGD-CBD	5.40	120.66	111.23
24	B	1212	CLA	CMD-C2D-C1D	5.39	134.22	124.73
24	A	1103	CLA	O2D-CGD-CBD	5.39	120.65	111.23
24	6	612	CLA	CMD-C2D-C1D	5.39	134.21	124.73
24	B	1235	CLA	O2D-CGD-CBD	5.38	120.64	111.23
40	1	503	LUT	C35-C34-C33	-5.38	119.73	127.28
24	1	612	CLA	CMD-C2D-C1D	5.38	134.21	124.73
24	4	615	CLA	CMD-C2D-C1D	5.38	134.21	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1123	CLA	CMD-C2D-C1D	5.38	134.20	124.73
24	A	1110	CLA	O2D-CGD-CBD	5.38	120.64	111.23
24	A	1137	CLA	CMD-C2D-C1D	5.38	134.20	124.73
24	3	604	CLA	CMD-C2D-C1D	5.38	134.20	124.73
24	3	618	CLA	CMD-C2D-C1D	5.37	134.19	124.73
24	5	616	CLA	CMD-C2D-C1D	5.37	134.19	124.73
24	3	610	CLA	CMD-C2D-C1D	5.37	134.19	124.73
40	6	501	LUT	C31-C32-C33	-5.37	111.63	126.36
24	L	1503	CLA	CMD-C2D-C1D	5.37	134.19	124.73
24	B	1021	CLA	O2D-CGD-CBD	5.37	120.62	111.23
24	B	1209	CLA	O2D-CGD-CBD	5.37	120.61	111.23
24	4	608	CLA	O2D-CGD-CBD	5.37	120.61	111.23
24	A	1112	CLA	CMD-C2D-C1D	5.37	134.18	124.73
24	4	602	CLA	CMD-C2D-C1D	5.36	134.18	124.73
40	4	501	LUT	C26-C27-C28	-5.36	116.23	124.58
24	G	1601	CLA	CMD-C2D-C1D	5.36	134.17	124.73
49	7	504	C7Z	C31-C30-C29	-5.36	119.76	127.28
24	B	1207	CLA	CMD-C2D-C1D	5.36	134.16	124.73
24	A	1111	CLA	O2D-CGD-CBD	5.35	120.59	111.23
24	B	1215	CLA	CMD-C2D-C1D	5.35	134.15	124.73
24	A	1107	CLA	O2D-CGD-CBD	5.35	120.58	111.23
24	9	607	CLA	CMD-C2D-C1D	5.35	134.15	124.73
24	B	1204	CLA	CMD-C2D-C1D	5.35	134.15	124.73
24	4	601	CLA	CMD-C2D-C1D	5.35	134.15	124.73
24	a	604	CLA	CMD-C2D-C1D	5.35	134.14	124.73
24	a	612	CLA	CMD-C2D-C1D	5.34	134.14	124.73
24	A	1124	CLA	O2D-CGD-CBD	5.34	120.56	111.23
40	1	503	LUT	C15-C14-C13	-5.34	119.79	127.28
24	9	604	CLA	O2D-CGD-CBD	5.34	120.56	111.23
41	3	611	CHL	C1B-CHB-C4A	5.34	124.75	121.32
24	5	606	CLA	O2D-CGD-CBD	5.34	120.56	111.23
24	5	609	CLA	O2D-CGD-CBD	5.34	120.56	111.23
24	B	1209	CLA	CMD-C2D-C1D	5.33	134.12	124.73
24	7	609	CLA	O2D-CGD-CBD	5.33	120.56	111.23
24	8	609	CLA	CMD-C2D-C1D	5.33	134.12	124.73
24	7	612	CLA	CMD-C2D-C1D	5.33	134.12	124.73
24	A	1110	CLA	CMD-C2D-C1D	5.33	134.11	124.73
24	2	608	CLA	CMD-C2D-C1D	5.33	134.11	124.73
37	J	4002	RRX	C20-C21-C22	-5.32	119.81	127.28
24	A	1139	CLA	CMD-C2D-C1D	5.32	134.10	124.73
24	F	1301	CLA	CMD-C2D-C1D	5.32	134.10	124.73
24	7	607	CLA	O2D-CGD-CBD	5.32	120.53	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	2	501	LUT	C21-C26-C27	5.32	118.94	112.83
40	2	501	LUT	C35-C34-C33	-5.31	119.83	127.28
24	8	602	CLA	O2D-CGD-CBD	5.31	120.52	111.23
24	3	602	CLA	O2D-CGD-CBD	5.31	120.52	111.23
40	4	501	LUT	C35-C34-C33	-5.31	119.83	127.28
24	B	1202	CLA	CMD-C2D-C1D	5.31	134.08	124.73
24	A	1139	CLA	O2D-CGD-CBD	5.31	120.51	111.23
24	8	607	CLA	CMD-C2D-C1D	5.30	134.07	124.73
24	A	1122	CLA	CMD-C2D-C1D	5.30	134.06	124.73
24	1	601	CLA	O2D-CGD-CBD	5.30	120.50	111.23
24	5	605	CLA	O2D-CGD-CBD	5.30	120.50	111.23
24	B	1240	CLA	CMD-C2D-C1D	5.30	134.06	124.73
24	9	602	CLA	CMD-C2D-C1D	5.30	134.06	124.73
24	4	605	CLA	O2D-CGD-CBD	5.29	120.48	111.23
24	B	1239	CLA	O2D-CGD-CBD	5.29	120.48	111.23
24	3	607	CLA	O2D-CGD-CBD	5.29	120.48	111.23
24	9	605	CLA	O2D-CGD-CBD	5.29	120.47	111.23
24	5	609	CLA	CMD-C2D-C1D	5.28	134.03	124.73
24	1	608	CLA	CMD-C2D-C1D	5.28	134.03	124.73
24	G	1603	CLA	CMD-C2D-C1D	5.28	134.03	124.73
24	F	1302	CLA	CMD-C2D-C1D	5.28	134.03	124.73
24	3	616	CLA	CMD-C2D-C1D	5.28	134.02	124.73
24	K	1403	CLA	O2D-CGD-CBD	5.28	120.46	111.23
24	1	604	CLA	CMD-C2D-C1D	5.27	134.01	124.73
24	a	611	CLA	CMD-C2D-C1D	5.27	134.01	124.73
24	5	601	CLA	O2D-CGD-CBD	5.27	120.45	111.23
24	5	602	CLA	CMD-C2D-C1D	5.27	134.01	124.73
24	B	1214	CLA	O2D-CGD-CBD	5.27	120.44	111.23
24	5	617	CLA	CMD-C2D-C1D	5.27	134.00	124.73
24	A	1138	CLA	CMD-C2D-C1D	5.26	134.00	124.73
24	3	601	CLA	O2D-CGD-CBD	5.26	120.43	111.23
24	9	603	CLA	CAA-C2A-C3A	-5.26	98.78	113.00
24	5	602	CLA	O2D-CGD-CBD	5.26	120.42	111.23
24	A	1123	CLA	O2D-CGD-CBD	5.25	120.42	111.23
24	8	612	CLA	CMD-C2D-C1D	5.25	133.98	124.73
24	A	1105	CLA	O2D-CGD-CBD	5.24	120.40	111.23
24	7	607	CLA	O2A-C1-C2	5.24	121.47	108.99
43	a	504	QTB	C04-C03-C02	5.24	134.63	127.28
24	5	604	CLA	O2D-CGD-CBD	5.24	120.39	111.23
24	9	602	CLA	O2D-CGD-CBD	5.24	120.38	111.23
24	A	1012	CLA	O2D-CGD-CBD	5.23	120.38	111.23
24	7	602	CLA	O2D-CGD-CBD	5.23	120.38	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	1213	CLA	O2D-CGD-CBD	5.23	120.37	111.23
24	a	602	CLA	CMD-C2D-C1D	5.22	133.93	124.73
24	6	617	CLA	O2D-CGD-CBD	5.22	120.35	111.23
24	A	1135	CLA	O2D-CGD-CBD	5.22	120.35	111.23
24	A	1119	CLA	CMD-C2D-C1D	5.21	133.91	124.73
24	H	1703	CLA	O2D-CGD-CBD	5.21	120.34	111.23
24	4	607	CLA	CMD-C2D-C1D	5.21	133.90	124.73
24	1	605	CLA	O2D-CGD-CBD	5.21	120.33	111.23
36	G	5002	ERG	C1-C2-C3	5.21	117.38	110.48
24	B	1204	CLA	O2D-CGD-CBD	5.21	120.33	111.23
24	4	616	CLA	O2D-CGD-CBD	5.20	120.33	111.23
24	6	609	CLA	CMD-C2D-C1D	5.20	133.89	124.73
24	7	608	CLA	O2D-CGD-CBD	5.20	120.32	111.23
24	A	1131	CLA	O2D-CGD-CBD	5.20	120.31	111.23
24	9	608	CLA	CMD-C2D-C1D	5.19	133.87	124.73
24	F	1301	CLA	O2D-CGD-CBD	5.19	120.31	111.23
24	7	607	CLA	CMD-C2D-C1D	5.19	133.87	124.73
24	2	608	CLA	O2D-CGD-CBD	5.19	120.30	111.23
24	4	601	CLA	O2D-CGD-CBD	5.19	120.30	111.23
24	1	602	CLA	O2D-CGD-CBD	5.18	120.29	111.23
24	6	602	CLA	O2D-CGD-CBD	5.18	120.29	111.23
24	9	612	CLA	CMD-C2D-C1D	5.18	133.85	124.73
24	2	605	CLA	O2D-CGD-CBD	5.18	120.28	111.23
24	7	603	CLA	O2D-CGD-CBD	5.17	120.27	111.23
27	5	504	BCR	C15-C14-C13	-5.17	120.03	127.28
24	A	1104	CLA	O2D-CGD-CBD	5.17	120.26	111.23
24	a	605	CLA	O2D-CGD-CBD	5.17	120.26	111.23
24	3	613	CLA	CMD-C2D-C1D	5.16	133.82	124.73
24	9	601	CLA	O2D-CGD-CBD	5.16	120.25	111.23
24	A	1120	CLA	CMD-C2D-C1D	5.16	133.81	124.73
24	B	1205	CLA	CMD-C2D-C1D	5.16	133.81	124.73
37	J	4002	RRX	C33-C5-C6	-5.16	118.86	124.48
24	A	1133	CLA	O2D-CGD-CBD	5.15	120.24	111.23
49	7	504	C7Z	C38-C25-C26	-5.15	118.86	124.48
24	B	1207	CLA	O2D-CGD-CBD	5.15	120.23	111.23
24	A	1118	CLA	CMD-C2D-C1D	5.15	133.80	124.73
24	B	1226	CLA	O2D-CGD-CBD	5.15	120.23	111.23
24	B	1238	CLA	O2D-CGD-CBD	5.14	120.22	111.23
24	2	606	CLA	O2D-CGD-CBD	5.14	120.22	111.23
24	4	602	CLA	O2D-CGD-CBD	5.14	120.22	111.23
24	B	1236	CLA	CMD-C2D-C1D	5.14	133.78	124.73
24	2	601	CLA	O2D-CGD-CBD	5.14	120.21	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	8	502	LUT	C21-C26-C27	5.13	118.72	112.83
24	5	607	CLA	O2D-CGD-CBD	5.13	120.19	111.23
24	6	615	CLA	CMD-C2D-C1D	5.13	133.76	124.73
24	5	614	CLA	O2D-CGD-CBD	5.12	120.19	111.23
24	A	1107	CLA	CMD-C2D-C1D	5.12	133.75	124.73
24	1	606	CLA	O2D-CGD-CBD	5.12	120.18	111.23
24	B	1217	CLA	CMD-C2D-C1D	5.12	133.74	124.73
24	2	609	CLA	O2D-CGD-CBD	5.11	120.16	111.23
24	B	1206	CLA	CMD-C2D-C1D	5.10	133.71	124.73
24	A	1117	CLA	CMD-C2D-C1D	5.09	133.69	124.73
24	H	1701	CLA	O2D-CGD-CBD	5.09	120.13	111.23
24	A	1114	CLA	O2D-CGD-CBD	5.09	120.12	111.23
24	J	1901	CLA	O2D-CGD-CBD	5.09	120.12	111.23
40	6	502	LUT	C35-C34-C33	-5.09	120.14	127.28
24	6	608	CLA	O2D-CGD-CBD	5.09	120.12	111.23
24	7	610	CLA	CMD-C2D-C1D	5.09	133.69	124.73
24	7	608	CLA	CMD-C2D-C1D	5.08	133.67	124.73
48	7	502	XAT	C31-C30-C29	-5.08	120.16	127.28
24	6	607	CLA	CMD-C2D-C1D	5.07	133.66	124.73
24	B	1215	CLA	O2D-CGD-CBD	5.07	120.09	111.23
24	1	603	CLA	O2D-CGD-CBD	5.07	120.08	111.23
24	6	615	CLA	O2D-CGD-CBD	5.06	120.08	111.23
24	B	1211	CLA	O2D-CGD-CBD	5.06	120.08	111.23
24	2	612	CLA	O2D-CGD-CBD	5.06	120.07	111.23
24	B	1023	CLA	CMD-C2D-C1D	5.05	133.62	124.73
28	7	801	LHG	O7-C7-C8	5.05	122.41	111.48
41	3	611	CHL	C1-O2A-CGA	5.05	128.87	116.65
24	9	609	CLA	O2D-CGD-CBD	5.05	120.05	111.23
24	F	1302	CLA	O2D-CGD-CBD	5.04	120.04	111.23
24	3	607	CLA	CMD-C2D-C1D	5.04	133.60	124.73
41	a	610	CHL	C1B-CHB-C4A	5.04	124.56	121.32
48	7	502	XAT	C38-C25-C24	5.04	119.90	114.24
36	G	5002	ERG	C19-C10-C1	-5.04	101.77	109.43
24	a	608	CLA	O2D-CGD-CBD	5.03	120.03	111.23
24	B	1210	CLA	CMD-C2D-C1D	5.03	133.59	124.73
43	3	506	QTB	C09-C02-C03	5.03	126.92	119.01
24	4	615	CLA	O2D-CGD-CBD	5.03	120.02	111.23
24	4	603	CLA	O2D-CGD-CBD	5.02	120.01	111.23
24	8	606	CLA	O2D-CGD-CBD	5.02	120.01	111.23
24	A	1126	CLA	O2D-CGD-CBD	5.02	120.00	111.23
24	8	620	CLA	O2D-CGD-CBD	5.01	119.99	111.23
24	2	610	CLA	O2D-CGD-CBD	5.01	119.99	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	1206	CLA	O2D-CGD-CBD	5.01	119.99	111.23
40	6	502	LUT	C31-C30-C29	-5.01	120.25	127.28
24	8	615	CLA	O2D-CGD-CBD	5.00	119.98	111.23
24	9	612	CLA	O2D-CGD-CBD	5.00	119.97	111.23
24	9	608	CLA	O2D-CGD-CBD	4.99	119.96	111.23
24	B	1224	CLA	O2D-CGD-CBD	4.99	119.96	111.23
24	7	611	CLA	O2D-CGD-CBD	4.99	119.95	111.23
41	a	610	CHL	C1C-CHC-C4B	4.99	133.92	116.07
24	a	601	CLA	O2D-CGD-CBD	4.98	119.93	111.23
24	1	615	CLA	O2D-CGD-CBD	4.97	119.92	111.23
40	7	501	LUT	C35-C34-C33	-4.97	120.31	127.28
24	4	611	CLA	O2D-CGD-CBD	4.97	119.92	111.23
24	1	611	CLA	O2D-CGD-CBD	4.97	119.92	111.23
24	3	612	CLA	CMD-C2D-C1D	4.97	133.47	124.73
24	2	613	CLA	O2D-CGD-CBD	4.97	119.91	111.23
41	5	610	CHL	C1C-CHC-C4B	4.96	133.83	116.07
41	6	610	CHL	C1C-CHC-C4B	4.96	133.82	116.07
24	a	603	CLA	O2D-CGD-CBD	4.96	119.90	111.23
24	3	616	CLA	O2D-CGD-CBD	4.96	119.90	111.23
24	8	610	CLA	O2D-CGD-CBD	4.96	119.89	111.23
40	9	502	LUT	C31-C30-C29	-4.96	120.33	127.28
24	1	610	CLA	CMD-C2D-C1D	4.95	133.45	124.73
24	6	601	CLA	O2D-CGD-CBD	4.95	119.89	111.23
24	6	606	CLA	O2D-CGD-CBD	4.95	119.89	111.23
24	G	1603	CLA	O2D-CGD-CBD	4.94	119.87	111.23
24	3	603	CLA	O2D-CGD-CBD	4.94	119.87	111.23
24	A	1127	CLA	O2D-CGD-CBD	4.94	119.86	111.23
24	3	612	CLA	O2D-CGD-CBD	4.94	119.86	111.23
24	6	603	CLA	O2D-CGD-CBD	4.93	119.86	111.23
24	3	606	CLA	O2D-CGD-CBD	4.93	119.85	111.23
24	4	617	CLA	O2D-CGD-CBD	4.93	119.85	111.23
24	6	607	CLA	O2D-CGD-CBD	4.93	119.85	111.23
40	3	502	LUT	C21-C26-C27	4.93	118.49	112.83
24	A	1118	CLA	O2D-CGD-CBD	4.93	119.84	111.23
24	B	1220	CLA	O2D-CGD-CBD	4.92	119.83	111.23
24	9	607	CLA	O2D-CGD-CBD	4.92	119.83	111.23
24	L	1501	CLA	O2D-CGD-CBD	4.92	119.83	111.23
24	A	1134	CLA	O2D-CGD-CBD	4.92	119.82	111.23
24	5	603	CLA	O2D-CGD-CBD	4.91	119.82	111.23
24	4	610	CLA	O2D-CGD-CBD	4.91	119.81	111.23
24	A	1109	CLA	O2D-CGD-CBD	4.91	119.81	111.23
24	B	1203	CLA	O2D-CGD-CBD	4.91	119.81	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	602	CLA	O2D-CGD-CBD	4.91	119.81	111.23
24	a	611	CLA	O2D-CGD-CBD	4.90	119.80	111.23
24	B	1230	CLA	CMD-C2D-C1D	4.90	133.36	124.73
24	B	1220	CLA	CMD-C2D-C1D	4.90	133.36	124.73
28	2	801	LHG	O7-C7-C8	4.90	122.08	111.48
24	B	1216	CLA	O2D-CGD-CBD	4.90	119.79	111.23
24	B	1236	CLA	O2D-CGD-CBD	4.89	119.78	111.23
24	7	615	CLA	O2D-CGD-CBD	4.89	119.77	111.23
24	5	617	CLA	O2D-CGD-CBD	4.89	119.77	111.23
24	6	612	CLA	O2D-CGD-CBD	4.88	119.76	111.23
24	A	1133	CLA	CMD-C2D-C1D	4.88	133.32	124.73
49	7	504	C7Z	C21-C26-C25	-4.88	115.97	122.64
24	5	618	CLA	O2D-CGD-CBD	4.87	119.75	111.23
49	7	504	C7Z	C30-C31-C32	-4.87	109.08	123.20
24	7	610	CLA	O2D-CGD-CBD	4.87	119.74	111.23
24	B	1022	CLA	O2D-CGD-CBD	4.86	119.73	111.23
24	5	612	CLA	CMD-C2D-C1D	4.85	133.27	124.73
40	1	501	LUT	C21-C26-C27	4.85	118.40	112.83
24	2	615	CLA	CMD-C2D-C1D	4.85	133.26	124.73
24	8	603	CLA	O2D-CGD-CBD	4.84	119.69	111.23
24	B	1219	CLA	O2D-CGD-CBD	4.84	119.69	111.23
40	1	502	LUT	C35-C34-C33	-4.84	120.50	127.28
24	H	1701	CLA	CMD-C2D-C1D	4.84	133.24	124.73
24	a	612	CLA	O2D-CGD-CBD	4.83	119.68	111.23
24	B	1225	CLA	O2D-CGD-CBD	4.83	119.67	111.23
40	1	501	LUT	C35-C34-C33	-4.83	120.50	127.28
24	A	1140	CLA	CMD-C2D-C1D	4.82	133.21	124.73
41	9	610	CHL	C1C-CHC-C4B	4.82	133.31	116.07
24	2	607	CLA	O2D-CGD-CBD	4.81	119.65	111.23
24	8	605	CLA	O2D-CGD-CBD	4.81	119.64	111.23
24	B	1228	CLA	O2D-CGD-CBD	4.80	119.62	111.23
24	G	1601	CLA	O2D-CGD-CBD	4.79	119.60	111.23
24	A	1141	CLA	O2D-CGD-CBD	4.79	119.60	111.23
24	a	615	CLA	O2D-CGD-CBD	4.79	119.60	111.23
23	A	1011	CL0	CBC-CAC-C3C	-4.78	106.02	112.87
24	B	1213	CLA	C1-C2-C3	-4.78	118.37	126.20
24	8	612	CLA	O2D-CGD-CBD	4.78	119.58	111.23
43	3	506	QTB	C01-C02-C09	-4.78	110.79	118.09
24	8	611	CLA	O2D-CGD-CBD	4.78	119.58	111.23
40	3	501	LUT	C21-C26-C27	4.77	118.31	112.83
28	A	5003	LHG	O7-C7-C8	4.77	121.80	111.48
24	9	603	CLA	O2D-CGD-CBD	4.77	119.57	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	5	612	CLA	O2D-CGD-CBD	4.76	119.55	111.23
41	4	613	CHL	C1C-CHC-C4B	4.76	133.10	116.07
24	1	610	CLA	O2D-CGD-CBD	4.75	119.54	111.23
24	B	1234	CLA	O2D-CGD-CBD	4.75	119.53	111.23
41	8	613	CHL	C1C-CHC-C4B	4.74	133.04	116.07
24	A	1136	CLA	O2D-CGD-CBD	4.74	119.52	111.23
24	A	1119	CLA	O2D-CGD-CBD	4.74	119.52	111.23
24	A	1117	CLA	O2D-CGD-CBD	4.74	119.51	111.23
41	5	611	CHL	C1C-CHC-C4B	4.74	133.02	116.07
41	6	611	CHL	C1C-CHC-C4B	4.73	133.00	116.07
24	3	605	CLA	O2D-CGD-CBD	4.72	119.49	111.23
24	7	601	CLA	O2D-CGD-CBD	4.72	119.49	111.23
41	4	618	CHL	C1C-CHC-C4B	4.72	132.97	116.07
40	a	502	LUT	C7-C8-C9	-4.72	119.25	126.23
24	B	1237	CLA	CMD-C2D-C1D	4.72	133.04	124.73
24	7	606	CLA	O2D-CGD-CBD	4.71	119.47	111.23
41	6	619	CHL	C1C-CHC-C4B	4.71	132.93	116.07
24	B	1237	CLA	O2D-CGD-CBD	4.71	119.46	111.23
37	J	4002	RRX	C15-C14-C13	-4.70	120.69	127.28
41	a	609	CHL	C1C-CHC-C4B	4.69	132.87	116.07
41	4	609	CHL	C1C-CHC-C4B	4.69	132.86	116.07
41	a	606	CHL	C1C-CHC-C4B	4.68	132.83	116.07
24	B	1232	CLA	O2D-CGD-CBD	4.68	119.41	111.23
41	a	613	CHL	C1C-CHC-C4B	4.68	132.81	116.07
24	7	612	CLA	O2D-CGD-CBD	4.66	119.38	111.23
24	9	603	CLA	CMD-C2D-C1D	4.65	132.92	124.73
40	8	501	LUT	C21-C26-C27	4.64	118.16	112.83
24	B	1225	CLA	CMD-C2D-C1D	4.64	132.90	124.73
41	3	611	CHL	C1C-CHC-C4B	4.64	132.67	116.07
24	A	1124	CLA	CMD-C2D-C1D	4.64	132.89	124.73
41	6	613	CHL	C1C-CHC-C4B	4.63	132.65	116.07
36	G	5002	ERG	C1-C10-C5	4.60	116.68	108.74
24	4	612	CLA	CMD-C2D-C1D	4.60	132.83	124.73
29	8	802	DGD	O2G-C1B-C2B	4.60	121.43	111.48
37	J	4002	RRX	C38-C26-C25	-4.59	119.48	124.48
24	A	1012	CLA	CMD-C2D-C1D	4.58	132.79	124.73
41	5	613	CHL	C1C-CHC-C4B	4.57	132.41	116.07
24	B	1021	CLA	CMD-C2D-C1D	4.56	132.77	124.73
41	7	613	CHL	C1C-CHC-C4B	4.55	132.37	116.07
41	1	613	CHL	C1C-CHC-C4B	4.55	132.35	116.07
24	A	1140	CLA	O2D-CGD-CBD	4.53	119.15	111.23
24	6	618	CLA	O2D-CGD-CBD	4.52	119.13	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	615	CLA	CMD-C2D-C1D	4.50	132.66	124.73
24	A	1013	CLA	O2D-CGD-CBD	4.50	119.09	111.23
41	9	613	CHL	C1C-CHC-C4B	4.49	132.15	116.07
41	1	609	CHL	C1C-CHC-C4B	4.49	132.15	116.07
28	2	802	LHG	O7-C7-C8	4.48	121.18	111.48
40	5	502	LUT	C26-C27-C28	-4.48	117.61	124.58
49	7	504	C7Z	C11-C10-C9	-4.47	121.00	127.28
40	5	502	LUT	C35-C34-C33	-4.47	121.01	127.28
39	M	4001	ECH	C24-C23-C22	-4.46	119.63	126.23
40	a	502	LUT	C21-C26-C27	4.45	117.95	112.83
24	6	601	CLA	C1-C2-C3	-4.45	118.91	126.20
41	8	604	CHL	C1C-CHC-C4B	4.44	131.95	116.07
36	G	5002	ERG	C13-C17-C20	-4.43	114.07	119.38
40	a	501	LUT	C21-C26-C27	4.43	117.92	112.83
40	5	501	LUT	C21-C26-C27	4.43	117.92	112.83
24	3	603	CLA	CMD-C2D-C1D	4.42	132.51	124.73
24	A	1128	CLA	CMD-C2D-C1D	4.41	132.50	124.73
40	a	501	LUT	C15-C14-C13	-4.41	121.10	127.28
27	B	4005	BCR	C15-C14-C13	-4.40	121.10	127.28
23	A	1011	CL0	O2A-CGA-O1A	-4.40	112.62	123.63
41	8	601	CHL	C1C-CHC-C4B	4.40	131.82	116.07
41	3	608	CHL	C1C-CHC-C4B	4.40	131.80	116.07
40	2	501	LUT	C7-C8-C9	-4.39	119.74	126.23
24	1	612	CLA	O2D-CGD-CBD	4.38	118.88	111.23
40	1	502	LUT	C26-C27-C28	-4.38	117.77	124.58
28	5	801	LHG	O7-C7-C8	4.37	120.93	111.48
36	G	5002	ERG	C18-C13-C12	-4.37	104.17	110.61
40	6	501	LUT	C35-C15-C14	4.36	132.44	123.52
40	4	502	LUT	C35-C34-C33	-4.36	121.17	127.28
39	M	4001	ECH	C33-C5-C6	-4.35	119.74	124.48
24	2	601	CLA	C1-C2-C3	-4.35	119.07	126.20
40	6	501	LUT	C18-C5-C6	-4.35	119.74	124.48
40	2	502	LUT	C27-C28-C29	-4.34	117.00	126.32
27	B	4002	BCR	C15-C14-C13	-4.33	121.21	127.28
41	3	608	CHL	C3D-C4D-CHA	4.33	115.11	108.54
24	H	1701	CLA	C1C-C2C-C3C	-4.32	102.44	106.98
27	A	4003	BCR	C28-C27-C26	-4.31	106.36	114.06
37	J	4002	RRX	C24-C23-C22	-4.31	119.86	126.23
24	B	1021	CLA	C1-C2-C3	-4.31	119.14	126.20
36	G	5002	ERG	C18-C13-C14	-4.31	103.20	110.35
24	9	601	CLA	O2A-C1-C2	4.30	124.66	108.11
28	9	802	LHG	O7-C7-C8	4.30	120.77	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	6	803	PCW	O2-C31-C32	4.29	120.77	111.48
27	B	4003	BCR	C23-C22-C21	4.29	125.75	119.01
34	K	5001	LAP	O7-P9-O5	4.27	132.33	112.44
28	a	801	LHG	O7-C7-C8	4.27	120.73	111.48
40	9	502	LUT	C35-C34-C33	-4.27	121.28	127.28
41	a	606	CHL	C1-O2A-CGA	4.27	126.99	116.65
41	6	610	CHL	C3D-C4D-CHA	4.27	115.03	108.54
34	B	5007	LAP	O7-P9-O5	4.27	132.29	112.44
34	F	5003	LAP	O7-P9-O5	4.26	132.28	112.44
41	a	606	CHL	C3D-C4D-CHA	4.26	115.01	108.54
24	B	1222	CLA	O2D-CGD-CBD	4.26	118.67	111.23
28	6	802	LHG	O7-C7-C8	4.25	120.68	111.48
41	a	609	CHL	C3D-C4D-CHA	4.25	114.99	108.54
41	3	611	CHL	C3D-C4D-CHA	4.25	114.99	108.54
24	A	1130	CLA	C1-C2-C3	-4.24	119.24	126.20
40	5	501	LUT	C7-C8-C9	-4.24	119.96	126.23
24	A	1101	CLA	C1-C2-C3	-4.24	119.25	126.20
41	4	609	CHL	C3D-C4D-CHA	4.24	114.99	108.54
49	7	504	C7Z	C7-C8-C9	-4.24	119.96	126.23
41	3	611	CHL	C1-C2-C3	-4.24	119.25	126.20
43	3	506	QTB	C19-C17-C11	-4.24	104.61	110.58
24	A	1130	CLA	O2A-C1-C2	4.23	124.40	108.11
24	5	616	CLA	O2D-CGD-CBD	4.23	118.62	111.23
24	B	1023	CLA	O2D-CGD-CBD	4.22	118.62	111.23
41	8	601	CHL	C3D-C4D-CHA	4.22	114.95	108.54
41	6	611	CHL	C3D-C4D-CHA	4.22	114.95	108.54
24	2	604	CLA	O2A-C1-C2	4.22	124.33	108.11
24	7	609	CLA	O2A-CGA-CBA	4.21	124.68	111.83
41	5	613	CHL	C3D-C4D-CHA	4.21	114.94	108.54
23	A	1011	CL0	O2A-C1-C2	4.20	124.28	108.11
28	B	5002	LHG	O7-C7-C8	4.20	120.57	111.48
50	7	807	4RF	O21-C22-C24	4.20	120.56	111.48
41	6	613	CHL	C3D-C4D-CHA	4.20	114.92	108.54
51	8	806	P5S	O37-C38-C39	4.19	120.55	111.48
41	9	613	CHL	C3D-C4D-CHA	4.19	114.91	108.54
24	B	1221	CLA	CMD-C2D-C1D	4.19	132.10	124.73
32	B	5004	PCW	O2-C31-C32	4.18	120.53	111.48
36	G	5002	ERG	C2-C1-C10	4.18	121.69	112.78
49	7	504	C7Z	C18-C5-C6	-4.18	119.92	124.48
40	1	502	LUT	C21-C26-C27	4.17	117.62	112.83
24	2	603	CLA	O2D-CGD-CBD	4.16	118.51	111.23
40	8	502	LUT	C35-C34-C33	-4.16	121.44	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	B	5001	LHG	O7-C7-C8	4.16	120.49	111.48
33	7	804	PTY	O7-C8-C11	4.16	120.48	111.48
28	1	801	LHG	O7-C7-C8	4.16	120.48	111.48
27	K	4002	BCR	C8-C9-C10	4.16	125.55	119.01
23	A	1011	CL0	CHA-C1A-C2A	-4.16	123.54	133.31
24	8	608	CLA	C1-C2-C3	-4.15	119.39	126.20
24	A	1127	CLA	CMD-C2D-C1D	4.15	132.04	124.73
28	7	803	LHG	O7-C7-C8	4.15	120.45	111.48
28	9	801	LHG	O7-C7-C8	4.15	120.45	111.48
24	A	1116	CLA	C1-C2-C3	-4.14	119.41	126.20
41	5	611	CHL	C3D-C4D-CHA	4.14	114.84	108.54
40	5	505	LUT	C18-C5-C6	-4.14	119.96	124.48
28	F	5001	LHG	O7-C7-C8	4.14	120.44	111.48
24	1	601	CLA	C1-C2-C3	-4.14	119.42	126.20
40	a	501	LUT	C18-C5-C6	-4.13	119.98	124.48
40	6	501	LUT	C27-C28-C29	-4.13	117.44	126.32
40	3	501	LUT	C35-C34-C33	-4.13	121.49	127.28
24	2	609	CLA	C1-C2-C3	-4.12	119.45	126.20
41	1	613	CHL	C3D-C4D-CHA	4.10	114.77	108.54
24	9	612	CLA	O2A-C1-C2	4.09	123.86	108.11
24	B	1023	CLA	O2A-C1-C2	4.09	123.85	108.11
41	a	610	CHL	C3D-C4D-CHA	4.09	114.76	108.54
48	7	502	XAT	C18-C5-C4	4.09	118.83	114.24
43	a	504	QTB	C10-C09-C02	-4.09	117.53	126.32
28	A	5001	LHG	O7-C7-C8	4.09	120.32	111.48
27	L	4002	BCR	C33-C5-C6	-4.09	120.03	124.48
27	A	4003	BCR	C15-C14-C13	-4.09	121.55	127.28
28	3	801	LHG	O7-C7-C8	4.08	120.32	111.48
41	4	618	CHL	C3D-C4D-CHA	4.08	114.75	108.54
40	6	501	LUT	C15-C14-C13	4.08	133.01	127.28
41	9	610	CHL	C3D-C4D-CHA	4.08	114.74	108.54
40	a	503	LUT	C7-C8-C9	-4.08	120.20	126.23
33	B	5005	PTY	O7-C8-C11	4.08	120.30	111.48
41	a	613	CHL	C3D-C4D-CHA	4.07	114.73	108.54
24	B	1220	CLA	O2A-C1-C2	4.07	123.78	108.11
23	A	1011	CL0	O2A-CGA-CBA	4.07	124.25	111.83
27	8	503	BCR	C15-C14-C13	-4.07	121.57	127.28
24	6	609	CLA	O2A-C1-C2	4.07	123.78	108.11
24	6	601	CLA	O2A-C1-C2	4.06	123.73	108.11
24	B	1213	CLA	O2A-C1-C2	4.06	123.72	108.11
24	B	1209	CLA	O2A-C1-C2	4.05	123.71	108.11
24	B	1224	CLA	C1-C2-C3	-4.05	119.57	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	8	604	CHL	C1-C2-C3	-4.05	119.57	126.20
40	a	501	LUT	C35-C34-C33	-4.04	121.61	127.28
41	6	619	CHL	C3D-C4D-CHA	4.04	114.69	108.54
46	5	803	DGA	OG2-CB1-CB2	4.04	120.23	111.48
28	F	5002	LHG	O7-C7-C8	4.04	120.21	111.48
27	B	4007	BCR	C33-C5-C6	-4.04	120.08	124.48
24	a	601	CLA	C1-C2-C3	-4.03	119.59	126.20
24	A	1125	CLA	O2A-C1-C2	4.03	123.61	108.11
40	a	501	LUT	C11-C10-C9	-4.03	121.63	127.28
30	A	5007	3PH	O21-C21-C22	4.03	120.19	111.48
33	5	802	PTY	O7-C8-C11	4.02	120.19	111.48
24	A	1138	CLA	O2D-CGD-CBD	4.02	118.26	111.23
24	4	615	CLA	O2A-C1-C2	4.02	123.59	108.11
24	A	1114	CLA	O2A-C1-C2	4.02	123.58	108.11
27	I	4001	BCR	C23-C24-C25	-4.02	116.27	127.00
40	1	503	LUT	C11-C10-C9	-4.01	121.65	127.28
41	5	610	CHL	C3D-C4D-CHA	4.01	114.64	108.54
39	M	4001	ECH	C28-C27-C26	-4.01	115.04	118.64
28	4	801	LHG	O7-C7-C8	4.01	120.15	111.48
40	a	502	LUT	C11-C10-C9	-4.00	121.66	127.28
40	1	502	LUT	C7-C8-C9	-4.00	120.32	126.23
33	8	891	PTY	O7-C8-C11	3.99	120.12	111.48
41	8	604	CHL	C3D-C4D-CHA	3.99	114.61	108.54
28	7	802	LHG	O7-C7-C8	3.99	120.12	111.48
41	8	613	CHL	C3D-C4D-CHA	3.99	114.61	108.54
24	2	601	CLA	O2A-C1-C2	3.99	123.45	108.11
43	a	504	QTB	C17-C11-C10	3.98	119.58	113.07
28	6	801	LHG	O7-C7-C8	3.98	120.09	111.48
33	9	803	PTY	O7-C8-C11	3.98	120.09	111.48
41	1	609	CHL	C3D-C4D-CHA	3.98	114.59	108.54
24	A	1126	CLA	C1-C2-C3	-3.97	119.69	126.20
24	A	1101	CLA	O2A-C1-C2	3.97	123.39	108.11
40	a	502	LUT	C35-C34-C33	-3.97	121.71	127.28
24	B	1217	CLA	C1-C2-C3	-3.97	119.69	126.20
43	3	506	QTB	C17-C11-C10	3.97	119.55	113.07
28	8	801	LHG	O7-C7-C8	3.96	120.05	111.48
40	4	501	LUT	C15-C14-C13	-3.96	121.73	127.28
24	H	1703	CLA	C1-C2-C3	-3.96	119.72	126.20
28	1	802	LHG	O7-C7-C8	3.95	120.03	111.48
24	B	1238	CLA	O2A-C1-C2	3.94	123.29	108.11
24	A	1128	CLA	C1-C2-C3	-3.94	119.74	126.20
24	4	608	CLA	C1-C2-C3	-3.94	119.74	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	4	607	CLA	O2A-C1-C2	3.93	123.24	108.11
24	3	605	CLA	O2A-C1-C2	3.93	123.24	108.11
36	G	5002	ERG	C19-C10-C5	-3.92	102.40	108.38
50	8	808	4RF	O21-C22-C24	3.91	119.94	111.48
40	2	501	LUT	C11-C10-C9	-3.91	121.79	127.28
27	I	4001	BCR	C27-C26-C25	-3.91	117.42	122.70
24	B	1217	CLA	O2A-C1-C2	3.91	123.14	108.11
24	2	612	CLA	C1-C2-C3	-3.90	120.45	126.76
24	B	1203	CLA	O2A-C1-C2	3.90	123.12	108.11
40	2	501	LUT	C18-C5-C6	-3.90	120.23	124.48
52	9	504	A8S	C8-C9-C10	-3.90	119.82	123.84
40	3	502	LUT	C15-C14-C13	-3.90	121.81	127.28
28	A	5002	LHG	O7-C7-C8	3.90	119.92	111.48
50	8	807	4RF	O21-C22-C24	3.90	119.91	111.48
24	A	1127	CLA	C1-C2-C3	-3.90	119.81	126.20
24	1	601	CLA	O2A-C1-C2	3.89	123.09	108.11
48	7	502	XAT	C15-C14-C13	-3.89	121.83	127.28
46	8	803	DGA	CDB-CCB-CBB	-3.88	81.18	115.25
27	G	4001	BCR	C19-C18-C17	3.88	125.11	119.01
24	B	1205	CLA	O2A-C1-C2	3.87	122.99	108.11
27	B	4001	BCR	C33-C5-C6	-3.86	120.27	124.48
40	4	502	LUT	C21-C26-C27	3.86	117.26	112.83
24	3	605	CLA	C1-C2-C3	-3.85	119.89	126.20
23	A	1011	CL0	C1C-CHC-C4B	3.85	129.84	116.07
24	A	1136	CLA	C1-C2-C3	-3.85	119.89	126.20
24	L	1502	CLA	C1-C2-C3	-3.84	119.90	126.20
24	6	603	CLA	C1-C2-C3	-3.84	119.90	126.20
24	B	1234	CLA	C1-C2-C3	-3.83	119.91	126.20
43	3	506	QTB	C10-C09-C02	-3.83	118.08	126.32
40	6	501	LUT	C12-C13-C14	-3.83	112.98	119.01
28	4	802	LHG	O7-C7-C8	3.83	119.77	111.48
24	B	1216	CLA	O2A-C1-C2	3.83	122.85	108.11
40	6	502	LUT	C7-C8-C9	-3.82	120.58	126.23
24	a	605	CLA	O2A-C1-C2	3.82	122.82	108.11
24	A	1135	CLA	O2A-C1-C2	3.82	122.81	108.11
24	B	1218	CLA	O2A-C1-C2	3.82	122.79	108.11
41	7	613	CHL	C3D-C4D-CHA	3.81	114.34	108.54
24	7	601	CLA	O2A-C1-C2	3.81	122.78	108.11
24	A	1114	CLA	C1-C2-C3	-3.81	119.95	126.20
40	9	501	LUT	C7-C8-C9	-3.81	120.60	126.23
40	1	503	LUT	C7-C8-C9	-3.80	120.61	126.23
36	G	5002	ERG	C9-C10-C5	3.80	115.72	109.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	9	601	CLA	C3B-C4B-NB	-3.80	107.14	110.53
24	B	1227	CLA	C1-C2-C3	-3.79	120.62	126.76
27	5	503	BCR	C33-C5-C6	-3.79	120.35	124.48
24	9	612	CLA	C1-C2-C3	-3.79	119.99	126.20
27	F	4001	BCR	C12-C13-C14	3.79	124.97	119.01
24	2	609	CLA	O2A-C1-C2	3.79	122.69	108.11
40	2	502	LUT	C11-C10-C9	-3.79	121.97	127.28
24	K	1402	CLA	O2A-C1-C2	3.78	122.67	108.11
24	A	1108	CLA	C1-C2-C3	-3.78	120.00	126.20
37	J	4002	RRX	C7-C8-C9	-3.78	120.64	126.23
24	L	1502	CLA	O2A-C1-C2	3.78	122.64	108.11
24	4	610	CLA	C2C-C1C-NC	3.78	113.95	109.98
24	6	615	CLA	O2A-C1-C2	3.77	122.64	108.11
24	A	1106	CLA	O2A-C1-C2	3.77	122.63	108.11
24	A	1138	CLA	O2A-C1-C2	3.77	122.63	108.11
24	1	606	CLA	C1-C2-C3	-3.77	120.02	126.20
41	6	610	CHL	C1-O2A-CGA	3.77	125.78	116.65
24	L	1501	CLA	C1-C2-C3	-3.77	120.66	126.76
24	8	608	CLA	O2A-C1-C2	3.77	122.61	108.11
24	4	611	CLA	O2A-C1-C2	3.76	122.59	108.11
40	9	502	LUT	C15-C14-C13	-3.76	122.00	127.28
24	K	1402	CLA	C1-C2-C3	-3.76	120.03	126.20
24	2	612	CLA	O2A-C1-C2	3.76	122.59	108.11
24	B	1208	CLA	O2A-C1-C2	3.76	122.58	108.11
24	A	1105	CLA	O2A-C1-C2	3.76	122.58	108.11
52	9	504	A8S	C1-C2-C3	-3.76	122.81	128.40
41	4	613	CHL	C3D-C4D-CHA	3.76	114.25	108.54
46	8	803	DGA	OG2-CB1-CB2	3.76	119.61	111.48
27	3	503	BCR	C33-C5-C4	3.75	121.60	113.60
41	4	613	CHL	CHA-C1A-C2A	-3.75	124.50	133.31
24	B	1225	CLA	O2A-C1-C2	3.75	122.54	108.11
27	6	504	BCR	C15-C14-C13	-3.75	122.02	127.28
24	5	603	CLA	O2A-C1-C2	3.75	122.53	108.11
24	8	603	CLA	O2A-C1-C2	3.75	122.52	108.11
24	A	1013	CLA	CMD-C2D-C1D	3.74	131.32	124.73
40	5	501	LUT	C35-C15-C14	-3.74	115.86	123.52
40	a	502	LUT	C26-C27-C28	-3.74	118.76	124.58
24	8	611	CLA	C1-C2-C3	-3.74	120.71	126.76
24	B	1222	CLA	O2A-C1-C2	3.73	122.47	108.11
24	4	606	CLA	C1-C2-C3	-3.73	120.73	126.76
24	2	621	CLA	C1-C2-C3	-3.73	120.73	126.76
24	3	606	CLA	C1-C2-C3	-3.73	120.09	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	9	607	CLA	O2A-C1-C2	3.73	121.77	108.40
24	H	1703	CLA	O2A-C1-C2	3.73	122.45	108.11
24	5	602	CLA	O2A-C1-C2	3.73	122.45	108.11
24	B	1206	CLA	C2C-C1C-NC	3.73	113.90	109.98
24	7	609	CLA	O2A-C1-C2	3.73	122.45	108.11
24	5	601	CLA	O2A-C1-C2	3.72	122.44	108.11
24	B	1230	CLA	O2A-C1-C2	3.72	122.43	108.11
24	3	606	CLA	O2A-C1-C2	3.72	122.43	108.11
24	A	1122	CLA	O2A-C1-C2	3.72	122.42	108.11
24	a	612	CLA	O2A-C1-C2	3.72	122.42	108.11
24	B	1205	CLA	C1-C2-C3	-3.72	120.11	126.20
24	5	606	CLA	C1-C2-C3	-3.72	120.75	126.76
27	B	4005	BCR	C33-C5-C6	-3.71	120.43	124.48
49	7	504	C7Z	C32-C33-C34	-3.71	113.17	119.01
24	B	1207	CLA	O2A-C1-C2	3.71	122.39	108.11
27	5	503	BCR	C15-C14-C13	-3.71	122.08	127.28
40	1	503	LUT	C31-C30-C29	-3.71	122.08	127.28
40	2	502	LUT	C7-C8-C9	-3.71	120.75	126.23
24	A	1108	CLA	O2A-C1-C2	3.71	122.38	108.11
40	a	503	LUT	C31-C32-C33	-3.71	116.20	126.36
24	B	1235	CLA	O2A-C1-C2	3.71	122.37	108.11
41	1	609	CHL	C1-O2A-CGA	3.70	125.62	116.65
24	A	1139	CLA	O2A-C1-C2	3.70	122.36	108.11
24	G	1601	CLA	O2A-C1-C2	3.70	122.35	108.11
29	B	5003	DGD	O2G-C1B-C2B	3.70	119.49	111.48
24	9	601	CLA	CAA-C2A-C3A	-3.70	103.01	113.00
24	5	618	CLA	O2A-C1-C2	3.70	122.33	108.11
27	G	4001	BCR	C33-C5-C6	-3.69	120.45	124.48
24	7	606	CLA	O2A-C1-C2	3.69	122.32	108.11
24	B	1206	CLA	O2A-C1-C2	3.69	122.32	108.11
40	5	501	LUT	C18-C5-C6	-3.69	120.45	124.48
24	A	1115	CLA	O2A-C1-C2	3.69	122.32	108.11
24	A	1136	CLA	O2A-C1-C2	3.69	122.31	108.11
24	A	1128	CLA	O2A-C1-C2	3.69	122.30	108.11
24	A	1107	CLA	O2A-C1-C2	3.68	122.28	108.11
43	a	504	QTB	C19-C17-C11	-3.68	105.39	110.58
24	5	606	CLA	O2A-C1-C2	3.68	122.27	108.11
24	A	1127	CLA	O2A-C1-C2	3.68	122.27	108.11
24	B	1225	CLA	C1-C2-C3	-3.68	120.17	126.20
24	B	1240	CLA	O2A-C1-C2	3.67	122.25	108.11
24	2	603	CLA	O2A-C1-C2	3.67	122.23	108.11
24	A	1111	CLA	O2A-C1-C2	3.67	122.22	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	1	501	LUT	C15-C14-C13	-3.67	122.14	127.28
40	4	501	LUT	C7-C8-C9	-3.66	120.81	126.23
27	3	503	BCR	C2-C1-C6	-3.66	105.13	110.44
27	3	503	BCR	C4-C5-C6	-3.66	117.76	122.70
40	a	503	LUT	C18-C5-C6	-3.66	120.50	124.48
40	3	502	LUT	C35-C34-C33	-3.66	122.15	127.28
24	B	1231	CLA	O2A-C1-C2	3.65	122.17	108.11
24	K	1404	CLA	O2A-C1-C2	3.65	122.15	108.11
24	5	612	CLA	O2A-C1-C2	3.65	122.15	108.11
24	A	1115	CLA	C1-C2-C3	-3.65	120.22	126.20
24	F	1301	CLA	C1-C2-C3	-3.65	120.86	126.76
24	B	1203	CLA	C1-C2-C3	-3.65	120.22	126.20
24	B	1224	CLA	O2A-C1-C2	3.64	122.13	108.11
24	2	602	CLA	O2A-C1-C2	3.64	122.12	108.11
40	3	501	LUT	C15-C14-C13	-3.64	122.17	127.28
24	4	601	CLA	C1-C2-C3	-3.64	120.24	126.20
24	3	612	CLA	O2A-C1-C2	3.64	122.10	108.11
24	A	1117	CLA	O2A-C1-C2	3.64	122.10	108.11
40	8	502	LUT	C26-C27-C28	-3.64	118.92	124.58
24	a	603	CLA	C1-C2-C3	-3.63	120.24	126.20
24	B	1219	CLA	C1-C2-C3	-3.63	120.25	126.20
24	2	605	CLA	O2A-C1-C2	3.62	122.06	108.11
40	a	503	LUT	C11-C10-C9	-3.62	122.19	127.28
24	9	604	CLA	CMA-C3A-C4A	3.62	121.51	111.77
29	A	5005	DGD	O2G-C1B-C2B	3.62	119.32	111.48
24	B	1229	CLA	O2A-C1-C2	3.62	122.04	108.11
40	1	502	LUT	C15-C14-C13	-3.62	122.20	127.28
24	A	1121	CLA	O2A-C1-C2	3.62	122.03	108.11
24	3	603	CLA	O2A-C1-C2	3.62	122.03	108.11
24	5	618	CLA	C1-C2-C3	-3.62	120.27	126.20
33	3	802	PTY	O7-C8-C11	3.61	119.30	111.48
24	a	607	CLA	O2A-C1-C2	3.61	122.01	108.11
40	a	503	LUT	C27-C28-C29	-3.61	118.56	126.32
24	6	615	CLA	C1-C2-C3	-3.61	120.28	126.20
24	B	1211	CLA	O2A-C1-C2	3.61	121.99	108.11
27	6	503	BCR	C33-C5-C6	-3.61	120.55	124.48
41	1	609	CHL	C1-C2-C3	-3.61	120.29	126.20
24	A	1137	CLA	O2A-C1-C2	3.60	121.98	108.11
24	B	1234	CLA	O2A-C1-C2	3.60	121.98	108.11
24	1	606	CLA	O2A-C1-C2	3.60	121.97	108.11
24	1	604	CLA	O2A-C1-C2	3.60	121.96	108.11
24	6	603	CLA	O2A-C1-C2	3.60	121.95	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1109	CLA	O2A-C1-C2	3.60	121.95	108.11
24	8	609	CLA	O2A-C1-C2	3.59	121.93	108.11
24	B	1202	CLA	C2C-C1C-NC	3.59	113.75	109.98
24	B	1210	CLA	O2A-C1-C2	3.59	121.93	108.11
24	B	1226	CLA	O2A-C1-C2	3.59	121.92	108.11
24	6	612	CLA	O2A-C1-C2	3.59	121.92	108.11
24	9	603	CLA	O2A-C1-C2	3.59	121.92	108.11
40	5	502	LUT	C15-C14-C13	-3.59	122.25	127.28
24	7	610	CLA	O2A-C1-C2	3.59	121.91	108.11
24	A	1104	CLA	O2A-C1-C2	3.58	121.90	108.11
24	5	612	CLA	C1-C2-C3	-3.58	120.33	126.20
24	A	1140	CLA	O2A-C1-C2	3.58	121.89	108.11
24	A	1012	CLA	C3B-C4B-NB	-3.58	107.33	110.53
24	7	615	CLA	O2A-C1-C2	3.57	121.86	108.11
41	8	604	CHL	CHA-C1A-C2A	-3.57	124.92	133.31
24	B	1216	CLA	C1-C2-C3	-3.57	120.35	126.20
24	A	1120	CLA	CMA-C3A-C4A	3.57	121.36	111.77
24	8	610	CLA	O2A-C1-C2	3.57	121.84	108.11
40	2	501	LUT	C35-C15-C14	-3.57	116.22	123.52
24	2	604	CLA	C1-C2-C3	-3.57	120.36	126.20
27	6	504	BCR	C33-C5-C6	-3.57	120.59	124.48
24	A	1102	CLA	C1-C2-C3	-3.56	120.36	126.20
24	7	603	CLA	O2A-C1-C2	3.56	121.82	108.11
24	3	603	CLA	C1-C2-C3	-3.56	120.36	126.20
40	a	502	LUT	C15-C14-C13	-3.56	122.28	127.28
40	2	502	LUT	C15-C14-C13	-3.56	122.29	127.28
24	A	1118	CLA	O2A-C1-C2	3.56	121.80	108.11
27	A	4005	BCR	C23-C24-C25	-3.56	117.49	127.00
24	a	602	CLA	O2A-C1-C2	3.56	121.79	108.11
40	7	501	LUT	C7-C8-C9	-3.56	120.97	126.23
24	1	612	CLA	O2A-C1-C2	3.56	121.79	108.11
40	8	501	LUT	C26-C27-C28	-3.55	119.05	124.58
24	B	1227	CLA	O2A-C1-C2	3.55	121.78	108.11
24	4	604	CLA	O2A-C1-C2	3.55	121.77	108.11
40	4	501	LUT	C18-C5-C6	-3.55	120.61	124.48
24	B	1218	CLA	C1-C2-C3	-3.55	120.38	126.20
24	F	1301	CLA	O2A-C1-C2	3.55	121.77	108.11
24	8	602	CLA	O2A-C1-C2	3.55	121.77	108.11
24	2	621	CLA	O2A-C1-C2	3.55	121.76	108.11
24	A	1112	CLA	O2A-C1-C2	3.54	121.73	108.11
27	B	4003	BCR	C33-C5-C6	-3.54	120.62	124.48
24	4	616	CLA	O2A-C1-C2	3.54	121.72	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	4004	BCR	C23-C24-C25	-3.54	117.55	127.00
24	A	1116	CLA	O2A-C1-C2	3.53	121.71	108.11
40	4	502	LUT	C7-C8-C9	-3.53	121.01	126.23
24	B	1022	CLA	O2A-C1-C2	3.53	121.70	108.11
27	A	4003	BCR	C27-C26-C25	-3.53	117.94	122.70
24	A	1103	CLA	C1-C2-C3	-3.53	120.42	126.20
24	B	1240	CLA	C1-C2-C3	-3.53	120.42	126.20
27	3	503	BCR	C33-C5-C6	-3.53	120.64	124.48
24	A	1133	CLA	O2A-C1-C2	3.52	121.67	108.11
24	A	1106	CLA	C1-C2-C3	-3.52	120.43	126.20
24	B	1223	CLA	O2A-C1-C2	3.52	121.65	108.11
24	B	1204	CLA	C1-C2-C3	-3.52	120.43	126.20
24	6	606	CLA	O2A-C1-C2	3.52	121.65	108.11
24	B	1021	CLA	O2A-C1-C2	3.52	121.64	108.11
24	9	605	CLA	O2A-C1-C2	3.51	121.62	108.11
27	F	4001	BCR	C35-C13-C14	-3.51	117.13	122.82
24	B	1219	CLA	O2A-C1-C2	3.51	121.61	108.11
24	A	1012	CLA	O2A-C1-C2	3.51	121.61	108.11
24	4	616	CLA	C1-C2-C3	-3.51	121.08	126.76
24	1	607	CLA	O2A-C1-C2	3.51	121.61	108.11
41	6	610	CHL	C1A-CHA-C4D	3.51	124.83	118.98
24	F	1302	CLA	O2A-C1-C2	3.51	121.60	108.11
24	B	1237	CLA	O2A-C1-C2	3.51	121.60	108.11
24	3	601	CLA	O2A-C1-C2	3.50	121.59	108.11
24	4	606	CLA	O2A-C1-C2	3.50	121.59	108.11
24	B	1221	CLA	O2A-C1-C2	3.50	121.59	108.11
24	6	602	CLA	O2A-C1-C2	3.50	121.58	108.11
24	a	604	CLA	O2A-C1-C2	3.50	121.56	108.11
24	a	601	CLA	O2A-C1-C2	3.50	121.56	108.11
24	K	1404	CLA	C1-C2-C3	-3.49	120.48	126.20
24	a	607	CLA	C1-C2-C3	-3.48	120.49	126.20
24	7	601	CLA	C1-C2-C3	-3.48	120.49	126.20
24	A	1129	CLA	O2A-C1-C2	3.48	121.51	108.11
24	A	1131	CLA	C1-C2-C3	-3.48	120.50	126.20
24	4	601	CLA	O2A-C1-C2	3.48	121.50	108.11
24	A	1123	CLA	O2A-C1-C2	3.48	121.50	108.11
24	A	1134	CLA	O2A-C1-C2	3.48	121.50	108.11
24	B	1236	CLA	O2A-C1-C2	3.48	121.49	108.11
24	A	1103	CLA	O2A-C1-C2	3.48	121.49	108.11
24	2	613	CLA	CAA-C2A-C3A	-3.48	108.26	116.23
24	8	606	CLA	O2A-C1-C2	3.48	121.49	108.11
24	A	1013	CLA	O2A-C1-C2	3.48	121.49	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1129	CLA	C1-C2-C3	-3.48	121.14	126.76
24	1	603	CLA	O2A-C1-C2	3.48	121.48	108.11
24	7	612	CLA	O2A-C1-C2	3.48	121.48	108.11
24	B	1206	CLA	C1-C2-C3	-3.47	120.50	126.20
24	A	1112	CLA	C1-C2-C3	-3.47	120.50	126.20
24	L	1501	CLA	O2A-C1-C2	3.47	121.47	108.11
24	a	602	CLA	C1-C2-C3	-3.47	121.14	126.76
24	B	1228	CLA	O2A-C1-C2	3.47	121.46	108.11
24	2	603	CLA	C1-C2-C3	-3.47	120.52	126.20
24	7	604	CLA	O2A-C1-C2	3.47	121.45	108.11
41	3	611	CHL	CHA-C1A-C2A	-3.47	125.17	133.31
24	7	604	CLA	C1-C2-C3	-3.47	120.52	126.20
24	A	1132	CLA	O2A-C1-C2	3.46	121.44	108.11
40	5	501	LUT	C35-C34-C33	-3.46	122.42	127.28
24	3	616	CLA	O2A-C1-C2	3.46	121.44	108.11
41	6	610	CHL	C1B-CHB-C4A	3.46	123.55	121.32
24	2	604	CLA	C3B-C4B-NB	-3.46	107.44	110.53
24	6	612	CLA	C1-C2-C3	-3.46	121.17	126.76
24	8	603	CLA	C1-C2-C3	-3.46	120.53	126.20
24	A	1138	CLA	C1-C2-C3	-3.46	120.53	126.20
24	B	1209	CLA	C1-O2A-CGA	3.46	125.02	116.65
24	4	608	CLA	O2A-C1-C2	3.45	121.40	108.11
24	5	607	CLA	O2A-C1-C2	3.45	121.40	108.11
24	5	601	CLA	C1-C2-C3	-3.45	120.54	126.20
24	A	1109	CLA	C1-C2-C3	-3.45	120.54	126.20
24	A	1124	CLA	O2A-C1-C2	3.45	121.39	108.11
24	B	1212	CLA	O2A-C1-C2	3.45	121.39	108.11
24	A	1125	CLA	C1-C2-C3	-3.45	120.54	126.20
41	a	613	CHL	CMA-C3A-C2A	3.45	127.45	114.13
24	7	606	CLA	C1-C2-C3	-3.45	120.55	126.20
24	B	1239	CLA	C1C-C2C-C3C	-3.45	103.36	106.98
24	7	617	CLA	O2A-C1-C2	3.44	121.35	108.11
24	B	1022	CLA	C3B-C4B-NB	-3.44	107.46	110.53
24	8	610	CLA	C1-C2-C3	-3.44	120.56	126.20
40	8	501	LUT	C35-C34-C33	-3.44	122.46	127.28
24	1	608	CLA	O2A-C1-C2	3.44	121.33	108.11
24	4	602	CLA	O2A-C1-C2	3.44	121.33	108.11
41	a	610	CHL	C1A-CHA-C4D	3.44	124.72	118.98
27	K	4002	BCR	C33-C5-C6	-3.44	120.73	124.48
24	8	609	CLA	C1-C2-C3	-3.44	120.57	126.20
24	6	618	CLA	CMA-C3A-C4A	3.43	121.00	111.77
41	5	611	CHL	C1A-CHA-C4D	3.43	124.71	118.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	608	CLA	O2A-C1-C2	3.43	121.32	108.11
40	5	505	LUT	C35-C34-C33	-3.43	122.47	127.28
24	A	1102	CLA	O2A-C1-C2	3.43	121.31	108.11
24	8	620	CLA	O2A-C1-C2	3.43	121.30	108.11
24	7	611	CLA	O2A-C1-C2	3.43	121.30	108.11
24	6	604	CLA	CMA-C3A-C4A	3.43	120.98	111.77
41	a	610	CHL	CHA-C1A-C2A	-3.42	125.27	133.31
24	A	1117	CLA	C1-C2-C3	-3.42	120.59	126.20
24	5	602	CLA	C1-C2-C3	-3.42	120.59	126.20
40	1	502	LUT	C35-C15-C14	-3.42	116.52	123.52
24	a	611	CLA	CMA-C3A-C4A	3.42	120.96	111.77
24	B	1210	CLA	C1-C2-C3	-3.42	120.60	126.20
24	a	611	CLA	C1-C2-C3	-3.42	121.23	126.76
24	6	607	CLA	O2A-C1-C2	3.41	121.25	108.11
24	B	1239	CLA	O2A-C1-C2	3.41	121.25	108.11
40	1	501	LUT	C26-C27-C28	-3.41	119.27	124.58
40	5	502	LUT	C10-C11-C12	-3.41	113.31	123.20
27	5	504	BCR	C19-C18-C17	3.41	124.38	119.01
27	3	504	BCR	C27-C26-C25	-3.40	118.10	122.70
24	A	1105	CLA	C1-C2-C3	-3.40	120.62	126.20
24	F	1302	CLA	C1-C2-C3	-3.40	120.63	126.20
24	8	608	CLA	O2A-CGA-CBA	3.39	122.18	111.83
48	7	502	XAT	C7-C8-C9	-3.39	120.27	125.53
24	A	1122	CLA	C1-C2-C3	-3.39	120.64	126.20
24	5	609	CLA	O2A-C1-C2	3.39	121.15	108.11
27	B	4001	BCR	C19-C18-C17	3.39	124.34	119.01
40	9	501	LUT	C18-C5-C6	-3.39	120.79	124.48
24	9	606	CLA	O2A-C1-C2	3.39	121.14	108.11
40	3	501	LUT	C22-C23-C24	-3.38	106.16	111.18
24	2	615	CLA	O2A-C1-C2	3.38	121.12	108.11
24	a	603	CLA	O2A-C1-C2	3.38	121.10	108.11
24	B	1206	CLA	C1C-C2C-C3C	-3.38	103.43	106.98
24	8	611	CLA	O2A-C1-C2	3.38	121.10	108.11
24	a	604	CLA	C1-C2-C3	-3.38	120.67	126.20
24	4	605	CLA	C2C-C1C-NC	3.37	113.53	109.98
24	3	613	CLA	O2A-C1-C2	3.37	121.09	108.11
41	1	609	CHL	C4D-CHA-CBD	-3.37	105.57	108.97
24	9	603	CLA	CBA-CAA-C2A	3.37	123.82	113.79
24	B	1239	CLA	C2C-C1C-NC	3.37	113.52	109.98
24	B	1222	CLA	CMA-C3A-C4A	3.37	120.82	111.77
24	A	1107	CLA	C1-C2-C3	-3.36	120.69	126.20
39	M	4001	ECH	C11-C12-C13	-3.36	117.15	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1104	CLA	C1-C2-C3	-3.36	120.69	126.20
24	6	604	CLA	C1-C2-C3	-3.36	120.69	126.20
24	1	611	CLA	O2A-C1-C2	3.36	121.03	108.11
24	H	1701	CLA	O2A-C1-C2	3.35	121.02	108.11
24	A	1139	CLA	C1-C2-C3	-3.35	120.70	126.20
24	3	601	CLA	C1-C2-C3	-3.35	120.70	126.20
27	B	4003	BCR	C8-C9-C10	3.35	124.28	119.01
27	A	4004	BCR	C33-C5-C6	-3.35	120.83	124.48
24	4	610	CLA	O2A-C1-C2	3.35	121.00	108.11
24	B	1220	CLA	CMA-C3A-C4A	3.35	120.77	111.77
27	5	504	BCR	C36-C18-C17	-3.35	117.39	122.82
24	B	1208	CLA	CAA-C2A-C3A	-3.34	103.96	113.00
24	5	604	CLA	O2A-C1-C2	3.34	120.97	108.11
24	8	618	CLA	O2A-C1-C2	3.34	120.97	108.11
24	3	607	CLA	O2A-C1-C2	3.34	120.97	108.11
41	9	610	CHL	CHA-C1A-C2A	-3.34	125.47	133.31
24	B	1237	CLA	C1-C2-C3	-3.34	120.73	126.20
24	H	1701	CLA	C2C-C1C-NC	3.34	113.48	109.98
27	8	503	BCR	C33-C5-C6	-3.33	120.84	124.48
24	7	612	CLA	C1-C2-C3	-3.33	120.73	126.20
24	A	1137	CLA	C1-C2-C3	-3.33	120.74	126.20
24	1	603	CLA	CMA-C3A-C4A	3.33	120.73	111.77
24	6	603	CLA	CMA-C3A-C4A	3.33	120.73	111.77
24	6	604	CLA	O2A-C1-C2	3.33	120.93	108.11
27	A	4001	BCR	C19-C18-C17	3.33	124.24	119.01
36	G	5002	ERG	C13-C14-C8	3.32	119.45	113.59
41	a	606	CHL	CHA-C1A-C2A	-3.32	125.50	133.31
40	a	502	LUT	C18-C5-C6	-3.32	120.86	124.48
41	4	613	CHL	C3C-C4C-NC	-3.32	106.53	114.65
41	6	619	CHL	CHA-C1A-C2A	-3.32	125.52	133.31
24	4	603	CLA	C1-O2A-CGA	3.32	124.68	116.65
24	B	1235	CLA	O2A-CGA-CBA	3.31	121.94	111.83
41	8	601	CHL	C3C-C4C-NC	-3.31	106.55	114.65
24	B	1212	CLA	C1-C2-C3	-3.31	120.77	126.20
24	A	1124	CLA	C1-C2-C3	-3.31	120.77	126.20
24	a	605	CLA	C1-C2-C3	-3.31	120.78	126.20
24	9	601	CLA	C1-O2A-CGA	3.31	124.66	116.65
24	3	601	CLA	C2C-C1C-NC	3.31	113.46	109.98
40	8	502	LUT	C7-C8-C9	-3.31	121.34	126.23
24	A	1121	CLA	C1-C2-C3	-3.30	120.78	126.20
24	8	620	CLA	C1-C2-C3	-3.30	120.79	126.20
24	5	617	CLA	O2A-C1-C2	3.30	120.81	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	6	610	CHL	C4D-CHA-CBD	-3.30	105.64	108.97
24	7	617	CLA	C1-C2-C3	-3.30	120.79	126.20
24	A	1135	CLA	C1-C2-C3	-3.30	120.79	126.20
24	B	1201	CLA	O2A-C1-C2	3.30	120.80	108.11
49	7	504	C7Z	C1-C6-C5	-3.30	118.13	122.64
27	3	503	BCR	C15-C14-C13	-3.30	122.65	127.28
39	M	4001	ECH	C7-C8-C9	-3.29	121.36	126.23
24	5	617	CLA	C1-C2-C3	-3.29	121.43	126.76
41	9	610	CHL	C1A-CHA-C4D	3.29	124.47	118.98
24	4	612	CLA	O2A-C1-C2	3.29	120.76	108.11
24	1	605	CLA	O2A-CGA-CBA	3.29	121.86	111.83
41	7	613	CHL	CHA-C1A-C2A	-3.28	125.60	133.31
24	2	612	CLA	C1C-C2C-C3C	-3.28	103.53	106.98
24	9	603	CLA	CMA-C3A-C4A	3.28	120.59	111.77
24	B	1230	CLA	C1-C2-C3	-3.28	120.82	126.20
41	3	608	CHL	C3C-C4C-NC	-3.28	106.63	114.65
40	9	501	LUT	C26-C27-C28	-3.28	119.47	124.58
24	A	1101	CLA	O2D-CGD-O1D	-3.28	117.47	123.85
40	4	501	LUT	C35-C15-C14	-3.28	116.81	123.52
24	3	603	CLA	CMA-C3A-C4A	3.28	120.58	111.77
41	6	611	CHL	C3C-C4C-NC	-3.28	106.64	114.65
24	A	1131	CLA	O2A-C1-C2	3.27	120.71	108.11
24	G	1601	CLA	C1-C2-C3	-3.27	121.47	126.76
24	A	1121	CLA	CMA-C3A-C4A	3.27	120.56	111.77
27	B	4003	BCR	C37-C22-C21	-3.27	117.52	122.82
24	9	605	CLA	C1-C2-C3	-3.27	120.84	126.20
41	8	613	CHL	CHA-C1A-C2A	-3.27	125.63	133.31
41	6	610	CHL	CHA-C1A-C2A	-3.27	125.63	133.31
24	9	603	CLA	C1-C2-C3	-3.27	120.84	126.20
41	3	611	CHL	C1A-CHA-C4D	3.27	124.43	118.98
41	a	613	CHL	CHA-C1A-C2A	-3.27	125.64	133.31
41	6	611	CHL	C1A-CHA-C4D	3.27	124.43	118.98
24	B	1229	CLA	C3B-C4B-NB	-3.27	107.61	110.53
24	B	1226	CLA	CMD-C2D-C3D	-3.26	120.20	127.69
40	6	501	LUT	C20-C13-C12	3.26	123.07	118.09
24	B	1021	CLA	C3B-C4B-NB	-3.26	107.62	110.53
24	B	1234	CLA	C3B-C4B-NB	-3.26	107.62	110.53
27	B	4002	BCR	C23-C24-C25	-3.26	118.30	127.00
24	A	1123	CLA	CMA-C3A-C4A	3.26	120.52	111.77
41	5	610	CHL	C3C-C4C-NC	-3.25	106.70	114.65
40	1	503	LUT	C18-C5-C6	-3.25	120.94	124.48
24	2	612	CLA	C2C-C1C-NC	3.25	113.40	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	5	603	CLA	C1-C2-C3	-3.25	120.87	126.20
41	6	619	CHL	C3C-C4C-NC	-3.25	106.70	114.65
24	A	1118	CLA	C1-C2-C3	-3.25	120.87	126.20
24	6	607	CLA	C1-C2-C3	-3.25	120.88	126.20
24	H	1701	CLA	C1-C2-C3	-3.24	120.88	126.20
24	1	607	CLA	C1-C2-C3	-3.24	120.88	126.20
24	B	1226	CLA	C2C-C1C-NC	3.24	113.39	109.98
24	A	1121	CLA	CMD-C2D-C3D	-3.24	120.26	127.69
24	7	603	CLA	C1-O2A-CGA	3.24	124.49	116.65
41	a	609	CHL	CHA-C1A-C2A	-3.24	125.71	133.31
27	A	4005	BCR	C35-C13-C12	3.23	123.03	118.09
40	9	501	LUT	C31-C30-C29	-3.23	122.74	127.28
24	3	607	CLA	C1-C2-C3	-3.23	120.90	126.20
24	5	604	CLA	CMA-C3A-C4A	3.23	120.45	111.77
27	A	4005	BCR	C12-C13-C14	-3.23	113.93	119.01
24	8	618	CLA	C1-C2-C3	-3.23	120.91	126.20
40	8	501	LUT	C7-C8-C9	-3.23	121.46	126.23
41	a	613	CHL	C3C-C4C-NC	-3.23	106.77	114.65
41	3	608	CHL	CHA-C1A-C2A	-3.22	125.74	133.31
24	B	1214	CLA	O2A-C1-C2	3.22	120.50	108.11
40	a	501	LUT	C35-C15-C14	-3.22	116.93	123.52
24	3	610	CLA	O2A-C1-C2	3.22	120.48	108.11
24	9	604	CLA	O2A-C1-C2	3.21	120.47	108.11
40	2	502	LUT	C18-C5-C6	-3.21	120.98	124.48
27	B	4002	BCR	C27-C26-C25	-3.21	118.37	122.70
24	B	1204	CLA	O2A-C1-C2	3.21	120.46	108.11
37	J	4002	RRX	C1-C6-C5	-3.21	118.25	122.64
24	A	1109	CLA	CMA-C3A-C4A	3.21	120.39	111.77
24	8	606	CLA	C1-C2-C3	-3.21	120.94	126.20
40	1	501	LUT	C11-C10-C9	-3.21	122.78	127.28
24	A	1123	CLA	C2C-C1C-NC	3.20	113.35	109.98
24	B	1239	CLA	C1-C2-C3	-3.20	120.95	126.20
40	3	502	LUT	C7-C8-C9	-3.20	121.50	126.23
24	5	608	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
39	M	4001	ECH	C23-C24-C25	-3.20	118.45	127.00
40	5	505	LUT	C11-C12-C13	-3.20	117.59	126.36
41	5	613	CHL	CHA-C1A-C2A	-3.20	125.80	133.31
41	6	613	CHL	CHA-C1A-C2A	-3.19	125.81	133.31
27	B	4007	BCR	C23-C24-C25	-3.19	118.47	127.00
40	3	502	LUT	C26-C27-C28	-3.19	119.61	124.58
24	a	608	CLA	C1-C2-C3	-3.19	120.97	126.20
27	L	4001	BCR	C23-C22-C21	3.19	124.03	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	6	606	CLA	C1-C2-C3	-3.19	120.97	126.20
24	A	1117	CLA	C2C-C1C-NC	3.19	113.33	109.98
24	4	603	CLA	O2A-C1-C2	3.19	120.37	108.11
24	A	1127	CLA	CMA-C3A-C4A	3.19	120.34	111.77
41	a	609	CHL	C3C-C4C-NC	-3.18	106.87	114.65
24	B	1215	CLA	O2A-C1-C2	3.18	120.36	108.11
41	6	611	CHL	CHA-C1A-C2A	-3.18	125.83	133.31
40	1	502	LUT	C11-C10-C9	-3.18	122.82	127.28
41	5	610	CHL	C4D-CHA-CBD	-3.18	105.76	108.97
27	G	4001	BCR	C36-C18-C17	-3.18	117.67	122.82
24	A	1128	CLA	C2C-C1C-NC	3.18	113.32	109.98
28	9	802	LHG	O8-C23-C24	3.18	121.52	111.83
40	8	502	LUT	C10-C11-C12	-3.18	113.99	123.20
40	1	502	LUT	C10-C11-C12	-3.17	114.00	123.20
41	8	604	CHL	C3C-C4C-NC	-3.17	106.90	114.65
24	a	611	CLA	O2A-C1-C2	3.17	120.31	108.11
24	A	1012	CLA	C1-C2-C3	-3.17	121.00	126.20
24	6	602	CLA	C1-C2-C3	-3.17	121.00	126.20
24	B	1202	CLA	C1C-C2C-C3C	-3.17	103.65	106.98
24	4	611	CLA	CMA-C3A-C4A	3.17	120.29	111.77
27	A	4002	BCR	C23-C24-C25	-3.17	118.54	127.00
24	A	1111	CLA	C1-C2-C3	-3.16	121.01	126.20
40	a	501	LUT	C7-C8-C9	-3.16	121.56	126.23
24	3	604	CLA	O2A-C1-C2	3.16	120.26	108.11
40	1	501	LUT	C18-C5-C6	-3.16	121.04	124.48
24	A	1130	CLA	C2C-C1C-NC	3.16	113.30	109.98
24	8	603	CLA	CMA-C3A-C4A	3.16	120.26	111.77
27	7	503	BCR	C33-C5-C6	-3.16	121.04	124.48
41	5	611	CHL	C4D-CHA-CBD	-3.16	105.78	108.97
24	4	617	CLA	CMA-C3A-C4A	3.16	120.26	111.77
24	4	602	CLA	C1-C2-C3	-3.15	121.03	126.20
24	A	1135	CLA	C3B-C4B-NB	-3.15	107.72	110.53
40	3	502	LUT	C10-C11-C12	-3.15	114.07	123.20
23	A	1011	CL0	CAA-C2A-C3A	-3.15	104.48	113.00
24	2	615	CLA	C1-C2-C3	-3.15	121.04	126.20
27	8	503	BCR	C33-C5-C4	3.15	120.31	113.60
24	B	1211	CLA	C1-C2-C3	-3.14	121.05	126.20
27	7	503	BCR	C23-C24-C25	-3.14	118.61	127.00
24	a	612	CLA	C1-C2-C3	-3.14	121.05	126.20
24	8	602	CLA	C1-C2-C3	-3.14	121.06	126.20
24	2	602	CLA	C1-C2-C3	-3.14	121.06	126.20
48	7	502	XAT	O4-C5-C18	-3.14	111.54	115.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	4003	BCR	C33-C5-C6	-3.14	121.06	124.48
24	7	617	CLA	C1C-C2C-C3C	-3.13	104.17	107.09
24	3	601	CLA	C1C-C2C-C3C	-3.13	103.69	106.98
24	L	1502	CLA	CMA-C3A-C4A	3.13	120.19	111.77
24	6	605	CLA	C1C-C2C-C3C	-3.13	103.69	106.98
40	5	505	LUT	C18-C5-C4	3.13	120.18	114.42
24	A	1121	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
27	A	4001	BCR	C36-C18-C17	-3.13	117.75	122.82
24	9	604	CLA	C1-C2-C3	-3.13	121.08	126.20
40	2	501	LUT	C31-C30-C29	-3.12	122.90	127.28
41	9	613	CHL	C1A-CHA-C4D	3.12	124.19	118.98
24	B	1238	CLA	CMA-C3A-C4A	3.12	120.17	111.77
24	5	609	CLA	CMA-C3A-C4A	3.12	120.16	111.77
24	K	1402	CLA	CMA-C3A-C4A	3.12	120.15	111.77
24	7	609	CLA	C1-C2-C3	-3.12	121.09	126.20
41	1	613	CHL	C1A-CHA-C4D	3.12	124.18	118.98
24	4	607	CLA	C1-C2-C3	-3.12	121.09	126.20
41	1	613	CHL	C4D-CHA-CBD	-3.11	105.83	108.97
24	8	618	CLA	CMA-C3A-C4A	3.11	120.14	111.77
41	1	613	CHL	CHA-C1A-C2A	-3.11	126.00	133.31
24	A	1117	CLA	CMA-C3A-C4A	3.11	120.14	111.77
24	4	615	CLA	C1-O2A-CGA	3.11	124.18	116.65
41	5	611	CHL	CHA-C1A-C2A	-3.11	126.00	133.31
24	4	612	CLA	C1-C2-C3	-3.11	121.10	126.20
27	B	4003	BCR	C34-C9-C10	-3.11	117.78	122.82
40	5	505	LUT	C1-C6-C5	-3.11	118.39	122.64
24	B	1226	CLA	C1-C2-C3	-3.11	121.10	126.20
40	6	501	LUT	C10-C11-C12	-3.11	114.19	123.20
24	9	607	CLA	CMA-C3A-C4A	3.11	120.12	111.77
24	A	1134	CLA	C1-C2-C3	-3.11	121.11	126.20
24	9	606	CLA	C1-C2-C3	-3.11	121.11	126.20
24	B	1023	CLA	C3B-C4B-NB	-3.11	107.76	110.53
41	7	613	CHL	C3C-C4C-NC	-3.10	107.07	114.65
40	9	502	LUT	C18-C5-C6	-3.10	121.10	124.48
24	1	608	CLA	CMA-C3A-C4A	3.10	120.10	111.77
24	7	615	CLA	C1-C2-C3	-3.10	121.12	126.20
24	1	605	CLA	O2A-C1-C2	3.10	120.03	108.11
50	7	807	4RF	O18-C16-C15	3.10	121.28	111.83
40	2	502	LUT	C30-C31-C32	-3.10	114.23	123.20
24	1	603	CLA	C1-C2-C3	-3.09	121.13	126.20
24	7	611	CLA	C1-C2-C3	-3.09	121.13	126.20
41	5	611	CHL	C1-O2A-CGA	3.09	124.14	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	4	609	CHL	C3C-C4C-NC	-3.09	107.10	114.65
24	B	1201	CLA	C1-C2-C3	-3.09	121.14	126.20
41	6	613	CHL	C3C-C4C-NC	-3.09	107.10	114.65
24	B	1228	CLA	C1-C2-C3	-3.09	121.14	126.20
24	7	608	CLA	C2C-C1C-NC	3.08	113.22	109.98
24	3	603	CLA	O2A-CGA-CBA	3.08	121.24	111.83
40	5	505	LUT	C7-C8-C9	-3.08	121.67	126.23
24	H	1702	CLA	CMA-C3A-C4A	3.08	120.06	111.77
41	5	613	CHL	C3C-C4C-NC	-3.08	107.12	114.65
40	9	501	LUT	C10-C11-C12	-3.08	114.27	123.20
40	8	501	LUT	C35-C15-C14	-3.08	117.21	123.52
24	B	1204	CLA	O2A-CGA-CBA	3.08	121.23	111.83
24	A	1108	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
24	4	603	CLA	CMA-C3A-C4A	3.08	120.05	111.77
37	J	4002	RRX	C20-C19-C18	-3.08	117.92	126.36
40	1	501	LUT	C35-C15-C14	-3.08	117.22	123.52
27	3	503	BCR	C8-C7-C6	-3.07	118.78	127.00
24	H	1701	CLA	CMA-C3A-C4A	3.07	120.04	111.77
41	1	613	CHL	C3C-C4C-NC	-3.07	107.14	114.65
27	3	504	BCR	C19-C18-C17	3.07	123.84	119.01
24	2	604	CLA	O1D-CGD-CBD	-3.07	118.46	124.52
27	3	505	BCR	C33-C5-C6	-3.07	121.14	124.48
24	9	603	CLA	O2A-CGA-CBA	3.07	121.19	111.83
24	B	1232	CLA	CMA-C3A-C4A	3.07	120.02	111.77
31	1	804	LMT	C1'-O5'-C5'	-3.07	107.73	113.72
41	a	610	CHL	C3C-C4C-NC	-3.07	107.16	114.65
24	A	1110	CLA	O2A-C1-C2	3.06	119.90	108.11
24	B	1225	CLA	C2C-C1C-NC	3.06	113.20	109.98
24	2	605	CLA	C1-C2-C3	-3.06	121.18	126.20
24	B	1218	CLA	CMA-C3A-C4A	3.06	120.00	111.77
24	G	1603	CLA	CMA-C3A-C4A	3.06	120.00	111.77
24	4	615	CLA	C2C-C1C-NC	3.06	113.20	109.98
24	1	605	CLA	CAA-C2A-C3A	-3.06	104.73	113.00
24	B	1202	CLA	O2A-CGA-CBA	3.06	121.17	111.83
24	4	604	CLA	C1-C2-C3	-3.06	121.18	126.20
24	K	1403	CLA	CMA-C3A-C4A	3.06	120.00	111.77
24	5	604	CLA	C1-C2-C3	-3.06	121.19	126.20
24	3	616	CLA	C1-C2-C3	-3.06	121.19	126.20
24	5	607	CLA	C1-C2-C3	-3.06	121.19	126.20
40	6	502	LUT	C18-C5-C6	-3.06	121.15	124.48
49	7	504	C7Z	C18-C5-C4	3.06	120.04	114.42
24	4	611	CLA	C1C-C2C-C3C	-3.05	103.77	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1	612	CLA	C1-C2-C3	-3.05	121.20	126.20
24	5	607	CLA	CMA-C3A-C4A	3.05	119.97	111.77
27	4	503	BCR	C4-C5-C6	-3.04	118.59	122.70
24	A	1113	CLA	O2A-C1-C2	3.04	119.81	108.11
27	8	503	BCR	C38-C26-C25	-3.04	121.17	124.48
24	A	1126	CLA	O2A-C1-C2	3.04	119.80	108.11
24	A	1127	CLA	C3B-C4B-NB	-3.04	107.82	110.53
24	A	1140	CLA	C3B-C4B-NB	-3.04	107.82	110.53
24	L	1501	CLA	CMA-C3A-C4A	3.04	119.94	111.77
24	A	1125	CLA	C2C-C1C-NC	3.04	113.17	109.98
24	A	1133	CLA	C1-C2-C3	-3.04	121.22	126.20
24	2	604	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
24	B	1215	CLA	C1C-C2C-C3C	-3.03	103.79	106.98
40	3	501	LUT	C7-C8-C9	-3.03	121.75	126.23
24	B	1236	CLA	C1-C2-C3	-3.03	121.23	126.20
24	6	609	CLA	CMA-C3A-C4A	3.03	119.92	111.77
40	8	502	LUT	C35-C15-C14	-3.03	117.32	123.52
24	6	609	CLA	C2C-C1C-NC	3.03	113.16	109.98
24	1	608	CLA	C1-C2-C3	-3.03	121.24	126.20
24	2	610	CLA	CMA-C3A-C4A	3.03	119.91	111.77
24	A	1122	CLA	CMA-C3A-C4A	3.03	119.91	111.77
24	2	612	CLA	CBC-CAC-C3C	-3.03	104.22	112.42
24	A	1102	CLA	O2A-CGA-CBA	3.03	121.06	111.83
40	9	501	LUT	C35-C15-C14	-3.03	117.33	123.52
50	8	807	4RF	O40-C41-C43	3.02	121.06	111.83
40	a	501	LUT	C26-C27-C28	-3.02	119.87	124.58
24	2	603	CLA	CMA-C3A-C4A	3.02	119.90	111.77
24	B	1207	CLA	C1-C2-C3	-3.02	121.25	126.20
24	B	1237	CLA	C2C-C1C-NC	3.02	113.16	109.98
24	9	601	CLA	CMA-C3A-C4A	3.02	119.89	111.77
24	7	603	CLA	CMA-C3A-C4A	3.02	119.89	111.77
24	A	1114	CLA	C2C-C1C-NC	3.02	113.15	109.98
24	A	1135	CLA	C2C-C1C-NC	3.02	113.15	109.98
24	B	1022	CLA	C2C-C1C-NC	3.02	113.15	109.98
24	3	607	CLA	CMA-C3A-C4A	3.02	119.88	111.77
24	4	615	CLA	C1-C2-C3	-3.02	121.25	126.20
24	1	612	CLA	C2C-C1C-NC	3.02	113.15	109.98
27	B	4001	BCR	C36-C18-C17	-3.02	117.93	122.82
24	5	614	CLA	CMA-C3A-C4A	3.02	119.88	111.77
27	A	4002	BCR	C33-C5-C6	-3.02	121.19	124.48
41	3	611	CHL	C4D-CHA-CBD	-3.01	105.93	108.97
40	7	501	LUT	C18-C5-C6	-3.01	121.19	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	2001	PQN	C14-C13-C15	3.01	120.46	115.23
24	A	1107	CLA	CMA-C3A-C4A	3.01	119.87	111.77
24	B	1226	CLA	C1C-C2C-C3C	-3.01	103.81	106.98
24	B	1218	CLA	C1C-C2C-C3C	-3.01	103.81	106.98
24	1	607	CLA	C2C-C1C-NC	3.01	113.14	109.98
24	7	610	CLA	C2C-C1C-NC	3.01	113.14	109.98
24	B	1222	CLA	C1-C2-C3	-3.01	121.27	126.20
24	a	603	CLA	C1C-C2C-C3C	-3.01	103.81	106.98
24	B	1235	CLA	CMA-C3A-C4A	3.01	119.86	111.77
41	4	618	CHL	C1A-CHA-C4D	3.01	124.00	118.98
27	5	504	BCR	C33-C5-C4	3.01	120.01	113.60
27	K	4001	BCR	C15-C14-C13	-3.01	123.06	127.28
24	B	1223	CLA	OBD-CAD-C3D	-3.01	121.39	128.42
24	5	616	CLA	CMA-C3A-C4A	3.01	119.85	111.77
27	A	4001	BCR	C35-C13-C12	3.00	122.68	118.09
41	6	613	CHL	C4D-CHA-CBD	-3.00	105.94	108.97
41	8	601	CHL	C1-C2-C3	-3.00	121.28	126.20
24	7	602	CLA	CMA-C3A-C4A	3.00	119.85	111.77
27	F	4001	BCR	C33-C5-C6	-3.00	121.21	124.48
49	7	504	C7Z	C38-C25-C24	3.00	119.94	114.42
24	B	1205	CLA	O2A-CGA-CBA	3.00	120.99	111.83
24	A	1126	CLA	C3B-C4B-NB	-3.00	107.85	110.53
24	A	1112	CLA	C2C-C1C-NC	3.00	113.13	109.98
27	5	504	BCR	C33-C5-C6	-3.00	121.21	124.48
41	6	611	CHL	C4D-CHA-CBD	-3.00	105.94	108.97
24	B	1234	CLA	O2A-CGA-CBA	3.00	120.98	111.83
27	5	504	BCR	C28-C27-C26	-3.00	108.71	114.06
41	6	611	CHL	C1-C2-C3	-3.00	121.91	126.76
24	8	611	CLA	C1C-C2C-C3C	-3.00	103.83	106.98
24	1	611	CLA	C1-C2-C3	-3.00	121.29	126.20
24	3	616	CLA	CMA-C3A-C4A	3.00	119.82	111.77
24	3	616	CLA	C2C-C1C-NC	2.99	113.13	109.98
27	L	4003	BCR	C33-C5-C6	-2.99	121.22	124.48
41	1	609	CHL	CHA-C1A-C2A	-2.99	126.28	133.31
27	B	4006	BCR	C33-C5-C6	-2.99	121.22	124.48
40	5	501	LUT	C11-C10-C9	-2.99	123.08	127.28
40	8	501	LUT	C18-C5-C6	-2.99	121.22	124.48
24	5	609	CLA	C1-C2-C3	-2.99	121.30	126.20
41	8	613	CHL	C4D-CHA-CBD	-2.99	105.95	108.97
24	4	608	CLA	CMD-C2D-C3D	-2.99	120.83	127.69
24	B	1223	CLA	C3B-C4B-NB	-2.99	107.86	110.53
24	6	606	CLA	CMA-C3A-C4A	2.99	119.80	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	1223	CLA	C1-C2-C3	-2.99	121.30	126.20
24	9	607	CLA	C2C-C1C-NC	2.99	113.12	109.98
28	F	5002	LHG	O8-C23-C24	2.98	120.93	111.83
24	2	603	CLA	C1D-ND-C4D	-2.98	104.22	106.31
24	7	607	CLA	C2C-C1C-NC	2.98	113.11	109.98
24	B	1232	CLA	C3B-C4B-NB	-2.98	107.87	110.53
24	5	605	CLA	C2C-C1C-NC	2.98	113.11	109.98
24	4	607	CLA	C2C-C1C-NC	2.98	113.11	109.98
25	B	2002	PQN	C14-C13-C15	2.97	120.39	115.23
24	B	1209	CLA	C1-C2-C3	-2.97	121.33	126.20
24	3	612	CLA	C1-C2-C3	-2.97	121.33	126.20
41	9	610	CHL	C4D-CHA-CBD	-2.97	105.97	108.97
24	7	610	CLA	CMA-C3A-C4A	2.97	119.75	111.77
27	L	4001	BCR	C33-C5-C6	-2.97	121.25	124.48
24	6	607	CLA	CMA-C3A-C4A	2.96	119.74	111.77
24	2	613	CLA	CMA-C3A-C4A	2.96	119.74	111.77
40	5	505	LUT	C31-C30-C29	-2.96	123.12	127.28
24	J	1901	CLA	CMA-C3A-C4A	2.96	119.74	111.77
40	1	501	LUT	C7-C8-C9	-2.96	121.85	126.23
24	A	1140	CLA	C1-C2-C3	-2.96	121.34	126.20
24	L	1503	CLA	CMA-C3A-C4A	2.96	119.73	111.77
48	7	502	XAT	C26-C27-C28	-2.96	119.74	125.99
41	5	610	CHL	C1A-CHA-C4D	2.96	123.92	118.98
24	B	1216	CLA	C3B-C4B-NB	-2.96	107.89	110.53
24	1	605	CLA	C1C-C2C-C3C	-2.96	103.87	106.98
41	8	604	CHL	C1A-CHA-C4D	2.96	123.92	118.98
24	2	613	CLA	C2C-C1C-NC	2.96	113.09	109.98
24	G	1603	CLA	C3B-C4B-NB	-2.95	107.89	110.53
41	8	604	CHL	C1-O2A-CGA	2.95	123.80	116.65
24	6	612	CLA	C2C-C1C-NC	2.95	113.08	109.98
24	9	604	CLA	C4B-CHC-C1C	2.95	133.19	126.25
24	B	1215	CLA	CMA-C3A-C4A	2.95	119.71	111.77
24	F	1302	CLA	CMA-C3A-C4A	2.95	119.70	111.77
24	4	610	CLA	CMA-C3A-C4A	2.95	119.70	111.77
41	9	613	CHL	C3C-C4C-NC	-2.95	107.44	114.65
24	a	608	CLA	C2C-C1C-NC	2.95	113.08	109.98
24	4	615	CLA	O2A-CGA-CBA	2.95	120.82	111.83
24	A	1130	CLA	CMA-C3A-C4A	2.95	119.69	111.77
24	1	610	CLA	CMA-C3A-C4A	2.95	119.69	111.77
24	7	615	CLA	C2C-C1C-NC	2.95	113.08	109.98
24	6	603	CLA	C3B-C4B-NB	-2.95	107.90	110.53
24	A	1131	CLA	C2C-C1C-NC	2.95	113.08	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	4004	BCR	C33-C5-C6	-2.95	121.27	124.48
27	4	503	BCR	C30-C25-C24	2.94	123.64	115.65
24	1	605	CLA	CMA-C3A-C4A	2.94	119.69	111.77
27	A	4001	BCR	C12-C13-C14	-2.94	114.38	119.01
24	4	602	CLA	C2C-C1C-NC	2.94	113.07	109.98
40	5	505	LUT	C22-C23-C24	-2.94	106.81	111.18
24	B	1229	CLA	C1-C2-C3	-2.94	121.38	126.20
24	A	1114	CLA	CMA-C3A-C4A	2.94	119.68	111.77
41	9	613	CHL	C4D-CHA-CBD	-2.94	106.00	108.97
24	a	603	CLA	CMA-C3A-C4A	2.94	119.68	111.77
24	1	603	CLA	O2A-CGA-CBA	2.94	120.80	111.83
41	4	618	CHL	CHA-C1A-C2A	-2.94	126.40	133.31
24	1	605	CLA	C2C-C1C-NC	2.94	113.07	109.98
41	1	609	CHL	C3C-C4C-NC	-2.94	107.47	114.65
24	B	1223	CLA	CMA-C3A-C4A	2.94	119.67	111.77
24	B	1221	CLA	C1-C2-C3	-2.94	121.38	126.20
24	B	1217	CLA	CMA-C3A-C4A	2.94	119.67	111.77
40	4	502	LUT	C26-C27-C28	-2.94	120.01	124.58
24	5	603	CLA	CMA-C3A-C4A	2.94	119.67	111.77
41	8	601	CHL	CHA-C1A-C2A	-2.94	126.41	133.31
29	8	802	DGD	O1G-C1A-C2A	2.94	120.79	111.83
24	1	607	CLA	CMA-C3A-C4A	2.94	119.67	111.77
24	9	605	CLA	C2C-C1C-NC	2.94	113.07	109.98
24	4	611	CLA	C2C-C1C-NC	2.94	113.06	109.98
27	J	4001	BCR	C36-C18-C17	-2.93	118.06	122.82
24	B	1204	CLA	C1D-ND-C4D	-2.93	104.25	106.31
24	A	1107	CLA	C2C-C1C-NC	2.93	113.06	109.98
24	5	604	CLA	C4B-CHC-C1C	2.93	133.15	126.25
24	A	1124	CLA	CMA-C3A-C4A	2.93	119.65	111.77
24	7	608	CLA	CMA-C3A-C4A	2.93	119.65	111.77
24	a	604	CLA	CMA-C3A-C4A	2.93	119.65	111.77
24	2	621	CLA	C2C-C1C-NC	2.93	113.06	109.98
24	K	1401	CLA	CMA-C3A-C4A	2.93	119.65	111.77
40	6	501	LUT	C11-C10-C9	-2.93	123.17	127.28
24	1	611	CLA	CMA-C3A-C4A	2.93	119.64	111.77
24	7	617	CLA	CMA-C3A-C4A	2.93	119.64	111.77
24	4	612	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
24	B	1215	CLA	C2C-C1C-NC	2.93	113.06	109.98
24	H	1702	CLA	C2C-C1C-NC	2.93	113.06	109.98
24	7	604	CLA	CMA-C3A-C4A	2.93	119.64	111.77
50	7	807	4RF	O40-C41-C43	2.93	120.76	111.83
24	3	612	CLA	C2C-C1C-NC	2.92	113.05	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	K	1402	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
24	6	605	CLA	CBC-CAC-C3C	-2.92	104.50	112.42
24	A	1130	CLA	C1C-C2C-C3C	-2.92	103.91	106.98
24	3	604	CLA	O2A-CGA-CBA	2.92	120.75	111.83
40	5	502	LUT	C35-C15-C14	-2.92	117.54	123.52
24	B	1208	CLA	C1-O2A-CGA	2.92	123.72	116.65
24	8	608	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
41	5	611	CHL	C3C-C4C-NC	-2.92	107.51	114.65
24	B	1235	CLA	C3B-C4B-NB	-2.92	107.92	110.53
24	4	617	CLA	C2C-C1C-NC	2.92	113.05	109.98
40	7	501	LUT	C35-C15-C14	-2.92	117.55	123.52
24	a	607	CLA	CMA-C3A-C4A	2.92	119.61	111.77
41	5	613	CHL	C1A-CHA-C4D	2.92	123.85	118.98
24	K	1403	CLA	C2C-C1C-NC	2.92	113.05	109.98
24	2	607	CLA	C2C-C1C-NC	2.92	113.04	109.98
41	8	613	CHL	C1A-CHA-C4D	2.92	123.85	118.98
40	4	501	LUT	C31-C30-C29	-2.91	123.19	127.28
24	4	604	CLA	CMA-C3A-C4A	2.91	119.61	111.77
24	8	607	CLA	C2C-C1C-NC	2.91	113.04	109.98
40	9	501	LUT	C35-C34-C33	-2.91	123.19	127.28
24	A	1141	CLA	CMA-C3A-C4A	2.91	119.61	111.77
24	5	601	CLA	C4B-CHC-C1C	2.91	133.10	126.25
41	4	609	CHL	C1-C2-C3	-2.91	121.42	126.20
24	B	1236	CLA	C2C-C1C-NC	2.91	113.04	109.98
24	8	606	CLA	C2C-C1C-NC	2.91	113.04	109.98
36	G	5002	ERG	C2-C3-C4	2.91	114.39	110.29
41	4	609	CHL	CHA-C1A-C2A	-2.91	126.47	133.31
24	B	1240	CLA	CMA-C3A-C4A	2.91	119.60	111.77
24	B	1226	CLA	CAC-C3C-C4C	2.91	128.58	124.79
27	A	4004	BCR	C27-C26-C25	-2.91	118.77	122.70
24	8	612	CLA	C2C-C1C-NC	2.91	113.04	109.98
24	A	1130	CLA	C3B-C4B-NB	-2.91	107.93	110.53
27	B	4005	BCR	C33-C5-C4	2.91	119.80	113.60
24	1	611	CLA	C2C-C1C-NC	2.91	113.04	109.98
24	1	615	CLA	CMA-C3A-C4A	2.91	119.58	111.77
24	9	612	CLA	CAA-C2A-C3A	-2.90	105.15	113.00
27	5	504	BCR	C4-C5-C6	-2.90	118.78	122.70
24	9	612	CLA	C2C-C1C-NC	2.90	113.03	109.98
24	5	602	CLA	C2C-C1C-NC	2.90	113.03	109.98
24	9	603	CLA	C1C-C2C-C3C	-2.90	103.93	106.98
24	2	621	CLA	CMA-C3A-C4A	2.90	119.57	111.77
24	A	1130	CLA	CHD-C1D-ND	-2.90	120.72	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	1217	CLA	C2C-C1C-NC	2.90	113.03	109.98
40	5	501	LUT	C26-C27-C28	-2.90	120.07	124.58
24	A	1103	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
24	a	608	CLA	CMA-C3A-C4A	2.90	119.56	111.77
24	B	1208	CLA	C1-C2-C3	-2.90	121.45	126.20
24	5	604	CLA	O2A-CGA-CBA	2.89	120.66	111.83
27	H	4001	BCR	C33-C5-C6	-2.89	121.33	124.48
24	7	611	CLA	CMA-C3A-C4A	2.89	119.54	111.77
24	9	609	CLA	C2C-C1C-NC	2.89	113.02	109.98
40	9	501	LUT	C11-C10-C9	-2.89	123.23	127.28
24	6	606	CLA	C2C-C1C-NC	2.89	113.02	109.98
40	2	502	LUT	C40-C33-C32	2.89	122.50	118.09
24	5	618	CLA	C3B-C4B-NB	-2.89	107.95	110.53
24	B	1214	CLA	C1-C2-C3	-2.89	121.47	126.20
27	6	504	BCR	C33-C5-C4	2.88	119.75	113.60
27	F	4001	BCR	C27-C26-C25	-2.88	118.81	122.70
24	A	1123	CLA	C1-C2-C3	-2.88	121.47	126.20
24	B	1235	CLA	C1-C2-C3	-2.88	121.47	126.20
24	7	608	CLA	C1C-C2C-C3C	-2.88	103.95	106.98
41	9	610	CHL	C1-C2-C3	-2.88	122.10	126.76
24	8	618	CLA	C2C-C1C-NC	2.88	113.01	109.98
24	9	612	CLA	CMA-C3A-C4A	2.88	119.51	111.77
24	A	1106	CLA	C4B-CHC-C1C	2.88	133.02	126.25
28	5	801	LHG	C5-O7-C7	-2.88	110.91	117.80
24	B	1229	CLA	CMA-C3A-C4A	2.88	119.51	111.77
40	4	501	LUT	C11-C10-C9	-2.88	123.24	127.28
38	J	5001	LPX	O3-P1-O4	2.88	125.83	112.44
24	A	1141	CLA	C2C-C1C-NC	2.88	113.00	109.98
24	6	604	CLA	O2A-CGA-CBA	2.88	120.61	111.83
39	M	4001	ECH	C8-C7-C6	-2.88	119.31	127.00
24	1	604	CLA	CMA-C3A-C4A	2.88	119.50	111.77
24	9	612	CLA	C4B-CHC-C1C	2.88	133.01	126.25
24	B	1231	CLA	C1-C2-C3	-2.87	121.49	126.20
41	6	610	CHL	C3C-C4C-NC	-2.87	107.62	114.65
49	7	504	C7Z	C40-C33-C32	2.87	122.48	118.09
40	3	501	LUT	C11-C10-C9	-2.87	123.25	127.28
24	3	601	CLA	C4B-CHC-C1C	2.87	133.00	126.25
24	A	1120	CLA	C2C-C1C-NC	2.87	113.00	109.98
24	4	616	CLA	CMA-C3A-C4A	2.87	119.49	111.77
24	8	606	CLA	C1C-C2C-C3C	-2.87	103.96	106.98
24	A	1108	CLA	CMA-C3A-C4A	2.87	119.49	111.77
24	A	1140	CLA	C4B-CHC-C1C	2.87	133.00	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	8	613	CHL	C1-C2-C3	-2.87	122.12	126.76
28	2	801	LHG	O8-C23-C24	2.86	120.57	111.83
24	1	601	CLA	O2A-CGA-CBA	2.86	120.57	111.83
24	L	1503	CLA	C2C-C1C-NC	2.86	112.99	109.98
24	B	1202	CLA	O2A-C1-C2	2.86	119.13	108.11
24	2	607	CLA	CMA-C3A-C4A	2.86	119.47	111.77
24	A	1121	CLA	C2C-C1C-NC	2.86	112.99	109.98
24	B	1204	CLA	C2C-C1C-NC	2.86	112.99	109.98
24	7	611	CLA	C1C-C2C-C3C	-2.86	103.97	106.98
41	a	606	CHL	C3C-C4C-NC	-2.86	107.65	114.65
24	6	615	CLA	C2C-C1C-NC	2.86	112.99	109.98
24	A	1136	CLA	CMA-C3A-C4A	2.86	119.46	111.77
38	a	804	LPX	O3-P1-O4	2.86	125.75	112.44
24	B	1229	CLA	C4B-CHC-C1C	2.86	132.97	126.25
24	6	612	CLA	C1C-C2C-C3C	-2.86	103.97	106.98
23	A	1011	CL0	C1-O2A-CGA	2.86	123.57	116.65
24	5	608	CLA	C2C-C1C-NC	2.86	112.98	109.98
40	3	501	LUT	C31-C30-C29	-2.86	123.27	127.28
24	a	605	CLA	C2C-C1C-NC	2.86	112.98	109.98
24	5	609	CLA	C2C-C1C-NC	2.86	112.98	109.98
41	6	613	CHL	C1A-CHA-C4D	2.86	123.75	118.98
41	a	609	CHL	C1A-CHA-C4D	2.86	123.75	118.98
24	3	618	CLA	CMA-C3A-C4A	2.86	119.45	111.77
41	6	613	CHL	C1-C2-C3	-2.86	122.14	126.76
24	2	610	CLA	C2C-C1C-NC	2.86	112.98	109.98
24	5	612	CLA	C1C-C2C-C3C	-2.86	103.98	106.98
27	8	503	BCR	C4-C5-C6	-2.85	118.85	122.70
24	G	1601	CLA	C2C-C1C-NC	2.85	112.98	109.98
24	A	1110	CLA	CMA-C3A-C4A	2.85	119.44	111.77
40	8	501	LUT	C10-C11-C12	-2.85	114.94	123.20
27	L	4001	BCR	C27-C26-C25	-2.85	118.85	122.70
24	A	1115	CLA	CMA-C3A-C4A	2.85	119.43	111.77
24	1	611	CLA	C1C-C2C-C3C	-2.85	103.98	106.98
24	9	609	CLA	C1C-C2C-C3C	-2.85	103.98	106.98
33	B	5005	PTY	O4-C30-C31	2.85	120.52	111.83
24	7	611	CLA	C2C-C1C-NC	2.85	112.97	109.98
24	A	1120	CLA	C1C-C2C-C3C	-2.85	103.98	106.98
24	3	604	CLA	C1-C2-C3	-2.85	121.53	126.20
27	7	503	BCR	C15-C14-C13	-2.85	123.29	127.28
24	A	1135	CLA	C1C-C2C-C3C	-2.85	103.99	106.98
41	5	611	CHL	C1-C2-C3	-2.85	122.16	126.76
24	6	608	CLA	CMD-C2D-C3D	-2.84	121.17	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	I	4001	BCR	C1-C6-C5	-2.84	118.75	122.64
24	A	1119	CLA	C3B-C4B-NB	-2.84	107.99	110.53
24	A	1139	CLA	C3B-C4B-NB	-2.84	107.99	110.53
24	5	612	CLA	C2C-C1C-NC	2.84	112.97	109.98
41	a	613	CHL	CMA-C3A-C4A	2.84	120.74	114.61
24	A	1109	CLA	CMD-C2D-C3D	-2.84	121.17	127.69
24	B	1207	CLA	C4B-CHC-C1C	2.84	132.93	126.25
40	4	502	LUT	C15-C14-C13	-2.84	123.29	127.28
24	6	615	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
24	1	612	CLA	C1C-C2C-C3C	-2.84	103.99	106.98
40	6	502	LUT	C15-C14-C13	-2.84	123.30	127.28
24	A	1110	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
41	3	611	CHL	C3C-C4C-NC	-2.84	107.71	114.65
50	8	808	4RF	O18-C16-C15	2.84	120.49	111.83
24	F	1301	CLA	C2C-C1C-NC	2.84	112.96	109.98
24	6	609	CLA	C1-O2A-CGA	2.84	123.52	116.65
24	a	602	CLA	C2C-C1C-NC	2.84	112.96	109.98
27	L	4001	BCR	C37-C22-C21	-2.84	118.22	122.82
24	7	602	CLA	C2C-C1C-NC	2.84	112.96	109.98
40	4	502	LUT	C10-C11-C12	-2.84	114.98	123.20
27	B	4003	BCR	C33-C5-C4	2.84	119.64	113.60
29	A	5005	DGD	O6D-C5D-C6D	2.84	112.32	106.69
24	G	1602	CLA	CMA-C3A-C4A	2.84	119.39	111.77
24	B	1205	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
41	5	613	CHL	C4D-CHA-CBD	-2.83	106.11	108.97
28	1	802	LHG	O8-C23-C24	2.83	120.48	111.83
28	a	801	LHG	O8-C23-C24	2.83	120.48	111.83
27	B	4005	BCR	C37-C22-C23	2.83	122.42	118.09
24	4	610	CLA	C1-C2-C3	-2.83	121.55	126.20
24	H	1703	CLA	C2C-C1C-NC	2.83	112.96	109.98
24	A	1114	CLA	C1C-C2C-C3C	-2.83	104.00	106.98
46	5	803	DGA	OG1-CA1-CA2	2.83	120.47	111.83
24	A	1106	CLA	C2C-C1C-NC	2.83	112.96	109.98
24	3	607	CLA	C2C-C1C-NC	2.83	112.96	109.98
24	9	612	CLA	C1C-C2C-C3C	-2.83	104.00	106.98
40	5	502	LUT	C7-C8-C9	-2.83	122.05	126.23
40	4	502	LUT	C18-C5-C6	-2.83	121.40	124.48
24	5	612	CLA	CMA-C3A-C4A	2.83	119.38	111.77
24	A	1123	CLA	C1C-C2C-C3C	-2.83	104.01	106.98
24	1	615	CLA	C2C-C1C-NC	2.83	112.95	109.98
24	8	610	CLA	C2C-C1C-NC	2.83	112.95	109.98
40	1	503	LUT	C31-C32-C33	-2.83	118.61	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	601	CLA	C3B-C4B-NB	-2.83	108.01	110.53
41	5	610	CHL	CHA-C1A-C2A	-2.83	126.67	133.31
41	5	613	CHL	C1-C2-C3	-2.82	121.57	126.20
43	3	506	QTB	C03-C04-C05	-2.82	115.02	123.20
27	A	4001	BCR	C33-C5-C6	-2.82	121.41	124.48
24	B	1219	CLA	C2C-C1C-NC	2.82	112.94	109.98
24	4	607	CLA	CMA-C3A-C4A	2.82	119.35	111.77
24	9	608	CLA	C2C-C1C-NC	2.82	112.94	109.98
24	A	1128	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
27	I	4001	BCR	C35-C13-C12	2.82	122.39	118.09
27	J	4001	BCR	C33-C5-C6	-2.82	121.41	124.48
40	7	501	LUT	C15-C14-C13	-2.82	123.33	127.28
24	L	1502	CLA	C2C-C1C-NC	2.82	112.94	109.98
27	4	503	BCR	C33-C5-C4	2.82	119.60	113.60
24	6	607	CLA	C2C-C1C-NC	2.82	112.94	109.98
24	8	615	CLA	CMA-C3A-C4A	2.82	119.34	111.77
24	7	601	CLA	O2A-CGA-CBA	2.81	120.42	111.83
24	7	607	CLA	CMA-C3A-C4A	2.81	119.33	111.77
24	A	1121	CLA	CHD-C1D-ND	-2.81	120.84	124.80
24	7	612	CLA	C2C-C1C-NC	2.81	112.94	109.98
24	6	603	CLA	O2A-CGA-CBA	2.81	120.40	111.83
24	8	607	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
24	9	607	CLA	C1C-C2C-C3C	-2.81	104.03	106.98
24	B	1208	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
24	A	1117	CLA	C1C-C2C-C3C	-2.81	104.03	106.98
24	8	603	CLA	O2A-CGA-CBA	2.81	120.39	111.83
41	5	610	CHL	C1-C2-C3	-2.81	121.60	126.20
24	A	1118	CLA	C2C-C1C-NC	2.81	112.93	109.98
24	A	1105	CLA	CMA-C3A-C4A	2.81	119.31	111.77
24	4	611	CLA	C4B-CHC-C1C	2.80	132.84	126.25
24	9	604	CLA	C2C-C1C-NC	2.80	112.93	109.98
24	4	615	CLA	C1C-C2C-C3C	-2.80	104.03	106.98
50	8	808	4RF	O40-C41-C43	2.80	120.38	111.83
40	8	501	LUT	C15-C14-C13	-2.80	123.35	127.28
41	4	618	CHL	C3C-C4C-NC	-2.80	107.80	114.65
24	B	1208	CLA	CMA-C3A-C4A	2.80	119.30	111.77
24	8	615	CLA	C2C-C1C-NC	2.80	112.92	109.98
40	a	503	LUT	C22-C23-C24	-2.80	107.02	111.18
27	L	4001	BCR	C28-C27-C26	-2.80	109.06	114.06
24	A	1131	CLA	C1C-C2C-C3C	-2.80	104.03	106.98
24	B	1237	CLA	CMA-C3A-C4A	2.80	119.30	111.77
24	A	1013	CLA	C3B-C4B-NB	-2.80	108.03	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	5	616	CLA	C2C-C1C-NC	2.80	112.92	109.98
24	B	1236	CLA	C1C-C2C-C3C	-2.80	104.04	106.98
24	6	601	CLA	CMA-C3A-C4A	2.80	119.29	111.77
24	3	604	CLA	C1D-ND-C4D	-2.80	104.35	106.31
24	B	1220	CLA	C1-C2-C3	-2.80	121.61	126.20
24	B	1209	CLA	C4B-CHC-C1C	2.80	132.82	126.25
24	7	617	CLA	C2C-C1C-NC	2.80	112.92	109.98
24	5	617	CLA	C2C-C1C-NC	2.79	112.92	109.98
24	6	604	CLA	C1C-C2C-C3C	-2.79	104.04	106.98
24	1	607	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
24	A	1114	CLA	C4B-CHC-C1C	2.79	132.81	126.25
24	8	609	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
24	8	602	CLA	C3B-C4B-NB	-2.79	108.04	110.53
24	3	612	CLA	C1C-C2C-C3C	-2.79	104.04	106.98
24	B	1022	CLA	C1C-C2C-C3C	-2.79	104.04	106.98
24	A	1129	CLA	C2C-C1C-NC	2.79	112.91	109.98
24	J	1901	CLA	C2C-C1C-NC	2.79	112.91	109.98
24	5	614	CLA	C2C-C1C-NC	2.79	112.91	109.98
27	J	4001	BCR	C35-C13-C12	2.79	122.35	118.09
24	B	1238	CLA	C3B-C4B-NB	-2.79	108.04	110.53
24	B	1212	CLA	CMA-C3A-C4A	2.79	119.27	111.77
24	a	605	CLA	C1C-C2C-C3C	-2.79	104.05	106.98
27	K	4002	BCR	C34-C9-C10	-2.79	118.30	122.82
24	G	1603	CLA	C2D-C1D-ND	2.79	112.89	110.13
27	L	4002	BCR	C35-C13-C12	2.79	122.35	118.09
24	B	1220	CLA	C2C-C1C-NC	2.79	112.91	109.98
29	A	5005	DGD	C1D-O6D-C5D	2.79	119.16	113.72
24	A	1118	CLA	CMA-C3A-C4A	2.78	119.26	111.77
24	3	607	CLA	C1C-C2C-C3C	-2.78	104.05	106.98
24	4	608	CLA	CHD-C1D-ND	-2.78	120.88	124.80
24	a	607	CLA	C2C-C1C-NC	2.78	112.91	109.98
24	6	602	CLA	C2C-C1C-NC	2.78	112.91	109.98
51	8	806	P5S	O19-C17-C20	2.78	120.32	111.83
24	A	1122	CLA	C3B-C4B-NB	-2.78	108.05	110.53
24	6	604	CLA	C2C-C1C-NC	2.78	112.90	109.98
24	3	616	CLA	C1C-C2C-C3C	-2.78	104.05	106.98
41	8	613	CHL	C3C-C4C-NC	-2.78	107.85	114.65
24	L	1503	CLA	C1C-C2C-C3C	-2.78	104.06	106.98
24	B	1223	CLA	CHA-C4D-ND	2.78	138.28	132.55
24	B	1226	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
24	B	1023	CLA	CAA-C2A-C3A	-2.78	105.49	113.00
24	3	602	CLA	C2C-C1C-NC	2.78	112.90	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	6	609	CLA	C1-C2-C3	-2.78	121.64	126.20
41	a	610	CHL	C4D-CHA-CBD	-2.78	106.17	108.97
24	A	1134	CLA	CMA-C3A-C4A	2.78	119.24	111.77
24	1	602	CLA	CMA-C3A-C4A	2.78	119.24	111.77
24	5	618	CLA	C4B-CHC-C1C	2.78	132.78	126.25
24	3	606	CLA	C2C-C1C-NC	2.78	112.90	109.98
24	2	605	CLA	C2C-C1C-NC	2.78	112.90	109.98
24	B	1226	CLA	CHA-C4D-ND	2.78	138.28	132.55
24	A	1141	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
27	J	4001	BCR	C27-C26-C25	-2.78	118.95	122.70
24	B	1238	CLA	C1C-C2C-C3C	-2.78	104.06	106.98
24	A	1137	CLA	C3B-C4B-NB	-2.77	108.05	110.53
24	B	1218	CLA	C2C-C1C-NC	2.77	112.90	109.98
24	A	1103	CLA	CMA-C3A-C4A	2.77	119.23	111.77
24	7	617	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
25	B	2002	PQN	C11-C12-C13	-2.77	122.06	126.83
24	a	612	CLA	CMA-C3A-C4A	2.77	119.22	111.77
24	A	1140	CLA	CMA-C3A-C4A	2.77	119.22	111.77
24	6	609	CLA	C1C-C2C-C3C	-2.77	104.07	106.98
24	7	609	CLA	C1C-C2C-C3C	-2.77	104.07	106.98
28	7	802	LHG	O8-C23-C24	2.77	120.28	111.83
24	1	607	CLA	C1C-C2C-C3C	-2.77	104.07	106.98
24	a	615	CLA	CMA-C3A-C4A	2.77	119.21	111.77
24	B	1209	CLA	C3B-C4B-NB	-2.77	108.06	110.53
28	6	801	LHG	C5-O7-C7	-2.77	111.17	117.80
24	8	607	CLA	C1C-C2C-C3C	-2.77	104.07	106.98
24	A	1136	CLA	C3B-C4B-NB	-2.77	108.06	110.53
24	A	1108	CLA	C3B-C4B-NB	-2.76	108.06	110.53
24	a	603	CLA	C2C-C1C-NC	2.76	112.89	109.98
28	7	801	LHG	O7-C7-O9	-2.76	117.24	123.70
24	9	612	CLA	C3B-C4B-NB	-2.76	108.06	110.53
24	2	615	CLA	C3B-C4B-NB	-2.76	108.06	110.53
24	B	1224	CLA	C2C-C1C-NC	2.76	112.88	109.98
24	A	1110	CLA	O2A-CGA-CBA	2.76	120.25	111.83
28	6	801	LHG	O8-C23-C24	2.76	120.25	111.83
24	5	607	CLA	C2C-C1C-NC	2.76	112.88	109.98
24	B	1218	CLA	O2A-CGA-CBA	2.76	120.25	111.83
40	2	501	LUT	C26-C27-C28	-2.76	120.28	124.58
28	A	5001	LHG	O8-C23-C24	2.76	120.25	111.83
24	B	1229	CLA	C1C-C2C-C3C	-2.76	104.08	106.98
24	4	610	CLA	C1C-C2C-C3C	-2.76	104.08	106.98
24	8	611	CLA	CMA-C3A-C4A	2.76	119.19	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	1218	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
41	3	611	CHL	CMA-C3A-C4A	2.76	120.56	114.61
24	B	1216	CLA	C2C-C1C-NC	2.76	112.88	109.98
24	2	602	CLA	C2C-C1C-NC	2.76	112.88	109.98
24	A	1119	CLA	O2A-C1-C2	2.76	118.72	108.11
24	4	611	CLA	C1-C2-C3	-2.76	121.68	126.20
24	9	605	CLA	CMA-C3A-C4A	2.76	119.18	111.77
24	9	602	CLA	C2C-C1C-NC	2.76	112.88	109.98
41	8	601	CHL	C1A-CHA-C4D	2.76	123.58	118.98
24	K	1404	CLA	C3B-C4B-NB	-2.76	108.07	110.53
24	3	610	CLA	C2C-C1C-NC	2.76	112.88	109.98
24	A	1104	CLA	C3B-C4B-NB	-2.76	108.07	110.53
30	A	5007	3PH	O31-C31-C32	2.75	120.23	111.83
24	L	1502	CLA	C1C-C2C-C3C	-2.75	104.08	106.98
24	8	602	CLA	C2C-C1C-NC	2.75	112.88	109.98
35	G	5001	SQD	O7-S-C6	-2.75	102.64	106.76
24	A	1129	CLA	C3B-C4B-NB	-2.75	108.07	110.53
24	K	1401	CLA	C2C-C1C-NC	2.75	112.87	109.98
27	3	503	BCR	C38-C26-C25	-2.75	121.48	124.48
31	B	5006	LMT	C1'-O5'-C5'	-2.75	108.35	113.72
24	a	608	CLA	C1C-C2C-C3C	-2.75	104.09	106.98
24	3	605	CLA	C2C-C1C-NC	2.75	112.87	109.98
41	a	613	CHL	C1A-CHA-C4D	2.75	123.57	118.98
33	5	802	PTY	O4-C30-C31	2.75	120.21	111.83
24	A	1134	CLA	C3B-C4B-NB	-2.75	108.08	110.53
24	B	1214	CLA	O2A-CGA-CBA	2.75	120.21	111.83
24	A	1124	CLA	C1C-C2C-C3C	-2.75	104.09	106.98
24	B	1221	CLA	C2C-C1C-NC	2.75	112.87	109.98
24	1	602	CLA	C2C-C1C-NC	2.75	112.87	109.98
24	A	1012	CLA	OBD-CAD-C3D	-2.75	122.00	128.42
24	7	610	CLA	O2A-CGA-CBA	2.75	120.20	111.83
24	K	1403	CLA	C1C-C2C-C3C	-2.74	104.09	106.98
41	5	613	CHL	C1-O2A-CGA	2.74	123.30	116.65
24	B	1220	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
24	B	1201	CLA	O2A-CGA-CBA	2.74	120.20	111.83
24	3	604	CLA	CMA-C3A-C4A	2.74	119.15	111.77
24	3	618	CLA	C2C-C1C-NC	2.74	112.86	109.98
24	H	1703	CLA	CMD-C2D-C3D	-2.74	121.40	127.69
24	7	604	CLA	O2A-CGA-CBA	2.74	120.20	111.83
24	A	1101	CLA	CMA-C3A-C4A	2.74	119.14	111.77
24	H	1703	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
24	A	1122	CLA	O2D-CGD-O1D	-2.74	118.51	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1132	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
24	8	608	CLA	C1C-C2C-C3C	-2.74	104.10	106.98
24	B	1205	CLA	C2C-C1C-NC	2.74	112.86	109.98
24	6	608	CLA	C2C-C1C-NC	2.74	112.86	109.98
41	4	613	CHL	C1A-CHA-C4D	2.74	123.55	118.98
24	a	602	CLA	CMA-C3A-C4A	2.74	119.13	111.77
24	B	1203	CLA	C1C-C2C-C3C	-2.74	104.10	106.98
24	2	605	CLA	C1C-C2C-C3C	-2.74	104.10	106.98
24	a	607	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
28	6	802	LHG	O8-C23-C24	2.74	120.18	111.83
40	5	501	LUT	C15-C14-C13	-2.74	123.44	127.28
41	9	610	CHL	C3C-C4C-NC	-2.74	107.96	114.65
24	B	1221	CLA	C1C-C2C-C3C	-2.74	104.10	106.98
24	B	1207	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
24	A	1141	CLA	C1C-C2C-C3C	-2.74	104.10	106.98
24	5	618	CLA	C2C-C1C-NC	2.74	112.86	109.98
24	F	1302	CLA	C2C-C1C-NC	2.73	112.85	109.98
27	3	504	BCR	C33-C5-C6	-2.73	121.50	124.48
24	G	1602	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
24	3	618	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
24	B	1230	CLA	C2C-C1C-NC	2.73	112.85	109.98
24	B	1240	CLA	C2C-C1C-NC	2.73	112.85	109.98
24	7	609	CLA	C2C-C1C-NC	2.73	112.85	109.98
24	3	618	CLA	C3B-C4B-NB	-2.73	108.09	110.53
23	A	1011	CL0	O2D-CGD-O1D	-2.73	118.53	123.85
24	B	1231	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
24	B	1203	CLA	C2C-C1C-NC	2.73	112.85	109.98
24	B	1204	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
24	A	1105	CLA	C2C-C1C-NC	2.73	112.85	109.98
24	A	1013	CLA	CAA-C2A-C3A	-2.73	105.62	113.00
24	4	616	CLA	C2C-C1C-NC	2.73	112.85	109.98
24	A	1112	CLA	CMA-C3A-C4A	2.73	119.11	111.77
24	8	618	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
37	J	4002	RRX	C30-C25-C26	-2.73	118.91	122.64
24	2	615	CLA	C2D-C1D-ND	2.73	112.83	110.13
27	A	4002	BCR	C27-C26-C25	-2.73	119.02	122.70
24	8	609	CLA	C2C-C1C-NC	2.73	112.85	109.98
24	8	620	CLA	C2C-C1C-NC	2.73	112.85	109.98
24	A	1137	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
24	B	1217	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
24	6	618	CLA	C2C-C1C-NC	2.73	112.85	109.98
28	B	5001	LHG	O8-C23-C24	2.73	120.15	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	3	604	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
27	H	4001	BCR	C33-C5-C4	2.72	119.41	113.60
24	B	1022	CLA	C1-C2-C3	-2.72	121.73	126.20
24	7	612	CLA	C1C-C2C-C3C	-2.72	104.11	106.98
24	G	1602	CLA	C3B-C4B-NB	-2.72	108.10	110.53
24	4	617	CLA	C1C-C2C-C3C	-2.72	104.12	106.98
27	G	4001	BCR	C35-C13-C12	2.72	122.25	118.09
24	B	1211	CLA	CMD-C2D-C3D	-2.72	121.45	127.69
24	7	610	CLA	C1-C2-C3	-2.72	121.74	126.20
23	A	1011	CL0	CMC-C2C-C1C	2.72	129.63	124.73
24	7	615	CLA	C1C-C2C-C3C	-2.72	104.12	106.98
24	4	601	CLA	C2C-C1C-NC	2.72	112.84	109.98
24	B	1225	CLA	CMA-C3A-C4A	2.72	119.09	111.77
50	8	807	4RF	O18-C16-C15	2.72	120.13	111.83
24	2	613	CLA	C1C-C2C-C3C	-2.72	104.12	106.98
24	a	615	CLA	C3B-C4B-NB	-2.72	108.10	110.53
24	5	607	CLA	C3B-C4B-NB	-2.72	108.10	110.53
24	1	615	CLA	C1C-C2C-C3C	-2.72	104.12	106.98
24	B	1209	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
24	A	1132	CLA	C2C-C1C-NC	2.72	112.84	109.98
41	a	610	CHL	CMA-C3A-C2A	2.72	124.62	114.13
24	B	1219	CLA	CMA-C3A-C4A	2.72	119.08	111.77
24	7	607	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
24	1	608	CLA	C1C-C2C-C3C	-2.72	104.12	106.98
29	B	5003	DGD	O1G-C1A-C2A	2.72	120.12	111.83
24	1	606	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
27	B	4005	BCR	C34-C9-C10	-2.72	118.42	122.82
24	7	603	CLA	C1-C2-C3	-2.71	121.75	126.20
24	B	1236	CLA	C4B-CHC-C1C	2.71	132.63	126.25
24	7	610	CLA	C4B-CHC-C1C	2.71	132.63	126.25
24	A	1101	CLA	C3B-C4B-NB	-2.71	108.11	110.53
24	B	1223	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
28	3	801	LHG	O8-C23-C24	2.71	120.11	111.83
33	7	804	PTY	O4-C30-C31	2.71	120.11	111.83
24	5	606	CLA	C2C-C1C-NC	2.71	112.83	109.98
24	B	1205	CLA	C1C-C2C-C3C	-2.71	104.13	106.98
24	H	1702	CLA	C1C-C2C-C3C	-2.71	104.13	106.98
23	A	1011	CL0	C4-C3-C5	2.71	119.93	115.23
24	A	1139	CLA	CMA-C3A-C4A	2.71	119.06	111.77
24	A	1125	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
40	7	501	LUT	C10-C11-C12	-2.71	115.35	123.20
24	A	1109	CLA	C2C-C1C-NC	2.71	112.83	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	4	605	CLA	C1C-C2C-C3C	-2.71	104.13	106.98
24	7	610	CLA	OBD-CAD-C3D	-2.71	122.09	128.42
24	7	605	CLA	C2C-C1C-NC	2.71	112.83	109.98
24	8	611	CLA	C2C-C1C-NC	2.71	112.83	109.98
24	G	1601	CLA	C1C-C2C-C3C	-2.71	104.13	106.98
24	B	1214	CLA	C3B-C4B-NB	-2.71	108.11	110.53
24	7	610	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
24	2	602	CLA	C3B-C4B-NB	-2.70	108.12	110.53
24	2	605	CLA	O2A-CGA-CBA	2.70	120.08	111.83
24	2	615	CLA	O2D-CGD-O1D	-2.70	118.58	123.85
28	8	801	LHG	O8-C23-C24	2.70	120.08	111.83
24	A	1116	CLA	O2A-CGA-CBA	2.70	120.08	111.83
24	2	621	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
24	6	602	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
24	4	601	CLA	C4B-CHC-C1C	2.70	132.60	126.25
24	B	1216	CLA	CAA-C2A-C3A	-2.70	105.69	113.00
24	A	1102	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
24	2	615	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
24	A	1138	CLA	C2C-C1C-NC	2.70	112.82	109.98
24	2	606	CLA	C2C-C1C-NC	2.70	112.82	109.98
27	I	4001	BCR	C38-C26-C27	2.70	119.36	113.60
24	4	604	CLA	O2A-CGA-CBA	2.70	120.07	111.83
24	4	601	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
24	a	602	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
24	a	607	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
24	K	1404	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
24	2	602	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
24	G	1602	CLA	C2C-C1C-NC	2.70	112.82	109.98
31	2	804	LMT	C1'-O5'-C5'	-2.70	108.45	113.72
24	4	607	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
24	B	1227	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
40	2	502	LUT	C26-C27-C28	2.70	128.78	124.58
24	8	615	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
24	K	1403	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
24	A	1135	CLA	OBD-CAD-C3D	-2.70	122.11	128.42
24	3	603	CLA	C3B-C4B-NB	-2.70	108.12	110.53
24	2	608	CLA	C2C-C1C-NC	2.70	112.81	109.98
24	8	615	CLA	C3B-C4B-NB	-2.70	108.12	110.53
24	B	1219	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
24	B	1212	CLA	C2C-C1C-NC	2.69	112.81	109.98
24	B	1220	CLA	C1-O2A-CGA	2.69	123.17	116.65
24	B	1201	CLA	O2D-CGD-O1D	-2.69	118.61	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	1208	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
24	6	605	CLA	C2C-C1C-NC	2.69	112.81	109.98
40	3	502	LUT	C11-C10-C9	-2.69	123.50	127.28
43	3	506	QTB	C11-C10-C09	2.69	131.01	125.25
24	K	1402	CLA	C3B-C4B-NB	-2.69	108.13	110.53
24	A	1115	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
24	B	1210	CLA	O2A-CGA-CBA	2.69	120.04	111.83
24	A	1137	CLA	C2C-C1C-NC	2.69	112.81	109.98
27	3	504	BCR	C36-C18-C17	-2.69	118.46	122.82
24	a	603	CLA	C3B-C4B-NB	-2.69	108.13	110.53
28	A	5002	LHG	O8-C23-C24	2.69	120.04	111.83
24	B	1222	CLA	CAA-C2A-C3A	-2.69	105.73	113.00
24	B	1230	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
24	2	621	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
24	1	608	CLA	C2C-C1C-NC	2.69	112.81	109.98
24	7	603	CLA	C2C-C1C-NC	2.69	112.81	109.98
40	6	502	LUT	C35-C15-C14	-2.69	118.02	123.52
24	5	606	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
24	1	602	CLA	C3B-C4B-NB	-2.69	108.13	110.53
24	7	602	CLA	C3B-C4B-NB	-2.69	108.13	110.53
24	5	601	CLA	CAA-C2A-C3A	-2.69	105.73	113.00
49	7	504	C7Z	C24-C25-C26	-2.69	115.23	120.76
33	9	803	PTY	O4-C30-C31	2.69	120.03	111.83
24	B	1225	CLA	C3B-C4B-NB	-2.69	108.13	110.53
24	A	1129	CLA	C1C-C2C-C3C	-2.69	104.16	106.98
24	9	605	CLA	CHA-C4D-ND	2.69	138.09	132.55
24	4	607	CLA	O2D-CGD-O1D	-2.68	118.62	123.85
24	1	601	CLA	CMA-C3A-C4A	2.68	118.99	111.77
24	5	603	CLA	C2C-C1C-NC	2.68	112.80	109.98
40	3	501	LUT	C10-C11-C12	-2.68	115.42	123.20
28	A	5003	LHG	O8-C23-C24	2.68	120.02	111.83
24	1	607	CLA	C4B-CHC-C1C	2.68	132.56	126.25
24	B	1237	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
24	3	610	CLA	C1-C2-C3	-2.68	121.81	126.20
24	a	611	CLA	C3B-C4B-NB	-2.68	108.14	110.53
24	6	618	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
24	H	1701	CLA	C1D-ND-C4D	-2.68	104.43	106.31
24	B	1221	CLA	CHA-C4D-ND	2.68	138.08	132.55
43	a	504	QTB	C13-C12-C14	2.68	116.06	111.06
24	B	1224	CLA	C3B-C4B-NB	-2.68	108.14	110.53
24	5	617	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
24	7	603	CLA	O2A-CGA-CBA	2.68	120.00	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	6	502	LUT	C31-C32-C33	-2.68	119.02	126.36
24	B	1217	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
27	B	4007	BCR	C38-C26-C25	-2.68	121.56	124.48
24	B	1221	CLA	O1D-CGD-CBD	-2.68	119.24	124.52
24	A	1134	CLA	C2C-C1C-NC	2.68	112.79	109.98
24	A	1140	CLA	C2C-C1C-NC	2.68	112.79	109.98
24	A	1123	CLA	O2D-CGD-O1D	-2.67	118.64	123.85
24	A	1124	CLA	C4B-CHC-C1C	2.67	132.54	126.25
27	B	4007	BCR	C19-C18-C17	2.67	123.22	119.01
24	9	604	CLA	O2A-CGA-CBA	2.67	119.99	111.83
24	B	1209	CLA	CMA-C3A-C4A	2.67	118.96	111.77
27	I	4001	BCR	C33-C5-C6	-2.67	121.57	124.48
24	A	1135	CLA	C4B-CHC-C1C	2.67	132.53	126.25
24	A	1104	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
24	2	610	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
24	7	606	CLA	CMD-C2D-C3D	-2.67	121.56	127.69
24	4	601	CLA	O2A-CGA-CBA	2.67	119.98	111.83
24	A	1137	CLA	C4B-CHC-C1C	2.67	132.53	126.25
24	6	607	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
24	A	1101	CLA	C2C-C1C-NC	2.67	112.79	109.98
24	3	612	CLA	CMA-C3A-C4A	2.67	118.95	111.77
24	B	1240	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
24	a	612	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
24	A	1118	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
24	B	1207	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
24	A	1128	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
24	K	1404	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
24	G	1603	CLA	C4B-CHC-C1C	2.67	132.52	126.25
27	L	4002	BCR	C23-C24-C25	-2.67	119.87	127.00
27	J	4001	BCR	C23-C24-C25	-2.67	119.87	127.00
24	9	604	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
41	a	609	CHL	C1-C2-C3	-2.67	121.83	126.20
24	2	603	CLA	CHD-C1D-ND	-2.67	121.05	124.80
41	4	618	CHL	C4D-CHA-CBD	-2.67	106.28	108.97
24	7	601	CLA	CMA-C3A-C4A	2.67	118.94	111.77
40	5	501	LUT	C10-C11-C12	-2.67	115.47	123.20
40	4	502	LUT	C35-C15-C14	-2.67	118.06	123.52
24	A	1115	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
24	5	616	CLA	C3B-C4B-NB	-2.67	108.15	110.53
32	B	5004	PCW	O3-C11-C12	2.67	119.96	111.83
24	6	606	CLA	C1C-C2C-C3C	-2.67	104.18	106.98
24	A	1127	CLA	C2C-C1C-NC	2.67	112.78	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	5	617	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
24	A	1105	CLA	C1C-C2C-C3C	-2.67	104.18	106.98
24	B	1225	CLA	C1C-C2C-C3C	-2.67	104.18	106.98
24	H	1702	CLA	O2D-CGD-O1D	-2.66	118.66	123.85
24	A	1138	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
24	6	605	CLA	CMA-C3A-C4A	2.66	118.93	111.77
24	4	615	CLA	CMA-C3A-C4A	2.66	118.93	111.77
40	2	502	LUT	C35-C34-C33	-2.66	123.54	127.28
24	7	605	CLA	CHA-C4D-ND	2.66	138.04	132.55
24	6	617	CLA	C3B-C4B-NB	-2.66	108.15	110.53
24	8	610	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
24	B	1220	CLA	C3B-C4B-NB	-2.66	108.16	110.53
24	A	1134	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
24	7	607	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
24	A	1107	CLA	O2A-CGA-CBA	2.66	119.94	111.83
24	B	1212	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
24	9	608	CLA	C1C-C2C-C3C	-2.66	104.19	106.98
24	2	607	CLA	C1C-C2C-C3C	-2.66	104.19	106.98
24	H	1703	CLA	C1C-C2C-C3C	-2.66	104.19	106.98
24	6	608	CLA	C1C-C2C-C3C	-2.66	104.19	106.98
24	K	1402	CLA	C2C-C1C-NC	2.66	112.77	109.98
24	8	618	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
28	1	802	LHG	C5-O7-C7	-2.65	111.44	117.80
24	A	1118	CLA	C3B-C4B-NB	-2.65	108.16	110.53
24	8	620	CLA	C1C-C2C-C3C	-2.65	104.19	106.98
24	9	605	CLA	C1C-C2C-C3C	-2.65	104.19	106.98
24	B	1210	CLA	C4B-CHC-C1C	2.65	132.49	126.25
24	A	1106	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
24	6	609	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
24	1	603	CLA	C1C-C2C-C3C	-2.65	104.19	106.98
24	3	601	CLA	C1-O2A-CGA	2.65	123.07	116.65
24	B	1236	CLA	C3B-C4B-NB	-2.65	108.16	110.53
40	3	501	LUT	C38-C25-C24	-2.65	117.09	123.36
24	8	609	CLA	C1C-C2C-C3C	-2.65	104.19	106.98
40	6	501	LUT	C1-C6-C7	2.65	122.84	115.65
24	A	1106	CLA	C1C-C2C-C3C	-2.65	104.19	106.98
24	9	603	CLA	C2C-C1C-NC	2.65	112.77	109.98
28	F	5001	LHG	O8-C23-C24	2.65	119.91	111.83
28	4	802	LHG	O8-C23-C24	2.65	119.91	111.83
24	A	1116	CLA	C3B-C4B-NB	-2.65	108.17	110.53
24	6	612	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
24	A	1109	CLA	C1C-C2C-C3C	-2.65	104.19	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	L	1503	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
24	A	1104	CLA	C2C-C1C-NC	2.65	112.76	109.98
24	B	1229	CLA	CAA-CBA-CGA	-2.65	105.69	113.21
24	A	1102	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
24	A	1013	CLA	C2D-C1D-ND	2.65	112.75	110.13
41	6	619	CHL	C1A-CHA-C4D	2.65	123.40	118.98
24	A	1107	CLA	C1C-C2C-C3C	-2.65	104.20	106.98
24	8	612	CLA	C1C-C2C-C3C	-2.65	104.20	106.98
24	A	1111	CLA	O2A-CGA-CBA	2.65	119.90	111.83
24	5	607	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
24	A	1111	CLA	C2C-C1C-NC	2.64	112.76	109.98
24	A	1124	CLA	C3B-C4B-NB	-2.64	108.17	110.53
24	2	608	CLA	O2D-CGD-O1D	-2.64	118.70	123.85
40	3	501	LUT	C18-C5-C6	-2.64	121.60	124.48
24	1	604	CLA	O2D-CGD-O1D	-2.64	118.70	123.85
24	7	610	CLA	C3B-C4B-NB	-2.64	108.17	110.53
41	8	604	CHL	CMA-C3A-C4A	2.64	120.31	114.61
24	8	609	CLA	C4B-CHC-C1C	2.64	132.46	126.25
24	B	1218	CLA	CHD-C1D-ND	-2.64	121.08	124.80
24	3	616	CLA	O2A-CGA-CBA	2.64	119.89	111.83
24	A	1140	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
24	B	1216	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
24	B	1220	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
24	6	615	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
41	8	601	CHL	C1C-C2C-CMC	2.64	131.56	126.80
33	8	891	PTY	O4-C30-C31	2.64	119.88	111.83
24	A	1127	CLA	C4B-CHC-C1C	2.64	132.45	126.25
24	F	1301	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
24	9	608	CLA	CMA-C3A-C4A	2.64	118.86	111.77
24	1	602	CLA	C1C-C2C-C3C	-2.64	104.21	106.98
24	A	1110	CLA	C1-O2A-CGA	2.64	123.03	116.65
24	6	612	CLA	CMA-C3A-C4A	2.64	118.86	111.77
24	A	1109	CLA	CHD-C1D-ND	-2.64	121.09	124.80
24	B	1209	CLA	O2A-CGA-CBA	2.64	119.87	111.83
24	2	603	CLA	C3B-C4B-NB	-2.64	108.18	110.53
24	5	614	CLA	C1C-C2C-C3C	-2.64	104.21	106.98
35	H	5001	SQD	O7-S-C6	-2.64	102.82	106.76
24	a	605	CLA	CHA-C4D-ND	2.64	137.99	132.55
24	9	601	CLA	CHD-C1D-ND	-2.64	121.09	124.80
24	A	1115	CLA	C3B-C4B-NB	-2.63	108.18	110.53
24	4	603	CLA	C3B-C4B-NB	-2.63	108.18	110.53
24	A	1137	CLA	C1C-C2C-C3C	-2.63	104.21	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	L	4003	BCR	C27-C26-C25	-2.63	119.14	122.70
37	J	4002	RRX	C2-C1-C6	2.63	114.27	110.44
24	F	1301	CLA	C3B-C4B-NB	-2.63	108.18	110.53
24	A	1012	CLA	O2A-CGA-CBA	2.63	119.86	111.83
24	B	1240	CLA	O2A-CGA-CBA	2.63	119.86	111.83
24	A	1131	CLA	CMA-C3A-C4A	2.63	118.85	111.77
24	5	618	CLA	C1D-ND-C4D	-2.63	104.47	106.31
24	A	1128	CLA	CMA-C3A-C4A	2.63	118.84	111.77
24	2	608	CLA	C1C-C2C-C3C	-2.63	104.21	106.98
24	2	609	CLA	C1C-C2C-C3C	-2.63	104.21	106.98
40	9	501	LUT	C15-C14-C13	-2.63	123.59	127.28
24	4	602	CLA	CMA-C3A-C4A	2.63	118.84	111.77
24	1	608	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
24	5	608	CLA	C1C-C2C-C3C	-2.63	104.22	106.98
24	B	1023	CLA	O2A-CGA-CBA	2.63	119.85	111.83
24	3	616	CLA	C1-O2A-CGA	2.63	123.01	116.65
24	9	606	CLA	C1C-C2C-C3C	-2.63	104.22	106.98
24	1	603	CLA	C2C-C1C-NC	2.63	112.74	109.98
24	A	1138	CLA	O2A-CGA-CBA	2.63	119.85	111.83
24	8	609	CLA	C3B-C4B-NB	-2.63	108.19	110.53
40	8	501	LUT	C30-C31-C32	-2.63	115.59	123.20
24	3	602	CLA	C1C-C2C-C3C	-2.63	104.22	106.98
24	J	1901	CLA	C1C-C2C-C3C	-2.63	104.22	106.98
40	5	505	LUT	C8-C7-C6	-2.62	119.99	127.00
24	B	1208	CLA	CMD-C2D-C3D	-2.62	121.67	127.69
24	3	601	CLA	CMA-C3A-C4A	2.62	118.83	111.77
24	7	603	CLA	C1C-C2C-C3C	-2.62	104.22	106.98
24	2	603	CLA	C2C-C1C-NC	2.62	112.74	109.98
24	B	1229	CLA	O2A-CGA-CBA	2.62	119.83	111.83
40	9	502	LUT	C7-C8-C9	-2.62	122.35	126.23
24	4	607	CLA	O2A-CGA-CBA	2.62	119.83	111.83
24	3	605	CLA	CHA-C4D-ND	2.62	137.96	132.55
24	6	605	CLA	CHD-C1D-ND	-2.62	121.11	124.80
24	B	1204	CLA	C2D-C1D-ND	2.62	112.72	110.13
24	9	602	CLA	CMA-C3A-C4A	2.62	118.82	111.77
37	J	4002	RRX	C4-C5-C6	-2.62	119.16	122.70
24	3	613	CLA	C2C-C1C-NC	2.62	112.73	109.98
24	8	605	CLA	C2C-C1C-NC	2.62	112.73	109.98
46	8	803	DGA	OG1-CA1-CA2	2.62	119.83	111.83
28	a	801	LHG	C5-O7-C7	-2.62	111.53	117.80
24	B	1208	CLA	C2C-C1C-NC	2.62	112.73	109.98
24	2	621	CLA	C3B-C4B-NB	-2.62	108.19	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	5	502	LUT	C18-C5-C6	-2.62	121.62	124.48
24	4	606	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
41	8	601	CHL	C4D-CHA-CBD	-2.62	106.33	108.97
24	B	1227	CLA	C2C-C1C-NC	2.62	112.73	109.98
28	4	801	LHG	O8-C23-C24	2.62	119.82	111.83
24	3	605	CLA	C1C-C2C-C3C	-2.62	104.23	106.98
24	3	610	CLA	C1C-C2C-C3C	-2.62	104.23	106.98
24	4	603	CLA	C1C-C2C-C3C	-2.62	104.23	106.98
24	9	602	CLA	C1C-C2C-C3C	-2.62	104.23	106.98
24	A	1101	CLA	C4B-CHC-C1C	2.62	132.40	126.25
24	B	1236	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
24	H	1701	CLA	CMC-C2C-C1C	2.62	129.12	125.03
24	8	610	CLA	CMA-C3A-C4A	2.62	118.81	111.77
27	5	504	BCR	C34-C9-C10	-2.62	118.58	122.82
40	8	502	LUT	C18-C5-C6	-2.62	121.63	124.48
24	B	1214	CLA	C2C-C1C-NC	2.62	112.73	109.98
24	G	1603	CLA	C2C-C1C-NC	2.62	112.73	109.98
40	5	505	LUT	C15-C35-C34	-2.62	118.17	123.52
24	B	1224	CLA	O1D-CGD-CBD	-2.62	119.36	124.52
27	4	503	BCR	C1-C6-C5	-2.62	119.06	122.64
24	B	1227	CLA	C1C-C2C-C3C	-2.62	104.23	106.98
24	5	618	CLA	C1C-C2C-C3C	-2.62	104.23	106.98
24	1	605	CLA	CHA-C4D-ND	2.61	137.94	132.55
24	A	1105	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
24	3	604	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
24	2	615	CLA	C1D-ND-C4D	-2.61	104.48	106.31
24	K	1401	CLA	C1C-C2C-C3C	-2.61	104.23	106.98
24	8	609	CLA	O2A-CGA-CBA	2.61	119.80	111.83
41	4	613	CHL	CMA-C3A-C4A	2.61	120.24	114.61
48	7	502	XAT	C6-C7-C8	-2.61	120.47	125.99
24	9	601	CLA	C4B-CHC-C1C	2.61	132.39	126.25
24	A	1125	CLA	CHA-C4D-ND	2.61	137.94	132.55
24	B	1204	CLA	CHD-C1D-ND	-2.61	121.13	124.80
24	A	1124	CLA	C2C-C1C-NC	2.61	112.72	109.98
24	A	1133	CLA	C1C-C2C-C3C	-2.61	104.23	106.98
24	5	606	CLA	C1C-C2C-C3C	-2.61	104.23	106.98
24	A	1113	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
28	7	801	LHG	O8-C23-C24	2.61	119.79	111.83
40	3	501	LUT	C26-C27-C28	-2.61	120.52	124.58
24	B	1207	CLA	C3B-C4B-NB	-2.61	108.20	110.53
24	5	614	CLA	C3B-C4B-NB	-2.61	108.20	110.53
24	K	1404	CLA	C2C-C1C-NC	2.61	112.72	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	1223	CLA	C3D-C2D-C1D	-2.61	102.27	105.83
24	5	605	CLA	CHA-C4D-ND	2.61	137.93	132.55
24	G	1603	CLA	C1D-ND-C4D	-2.61	104.48	106.31
35	7	805	SQD	O7-S-C6	-2.61	102.86	106.76
28	7	803	LHG	O8-C23-C24	2.61	119.78	111.83
24	a	605	CLA	CMD-C2D-C3D	-2.61	121.71	127.69
24	B	1219	CLA	CMD-C2D-C3D	-2.60	121.72	127.69
24	B	1210	CLA	C2C-C1C-NC	2.60	112.72	109.98
24	B	1226	CLA	CMA-C3A-C4A	2.60	118.77	111.77
27	3	505	BCR	C36-C18-C17	-2.60	118.60	122.82
24	B	1231	CLA	O2A-CGA-CBA	2.60	119.78	111.83
24	A	1115	CLA	C2C-C1C-NC	2.60	112.72	109.98
24	8	608	CLA	C2C-C1C-NC	2.60	112.72	109.98
24	B	1022	CLA	CHD-C1D-ND	-2.60	121.14	124.80
40	1	502	LUT	C31-C32-C33	-2.60	119.22	126.36
24	8	605	CLA	C3B-C4B-NB	-2.60	108.21	110.53
24	3	603	CLA	C2C-C1C-NC	2.60	112.72	109.98
24	B	1218	CLA	O1D-CGD-CBD	-2.60	119.38	124.52
40	4	501	LUT	C10-C11-C12	-2.60	115.66	123.20
24	9	601	CLA	C1-C2-C3	-2.60	121.93	126.20
24	7	609	CLA	C3B-C4B-NB	-2.60	108.21	110.53
24	8	605	CLA	CHA-C4D-ND	2.60	137.91	132.55
24	5	605	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
24	A	1110	CLA	C2C-C1C-NC	2.60	112.71	109.98
24	G	1602	CLA	CHA-C4D-ND	2.60	137.91	132.55
24	3	606	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
24	7	605	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
24	9	606	CLA	C2C-C1C-NC	2.60	112.71	109.98
24	5	618	CLA	C2D-C1D-ND	2.60	112.70	110.13
24	5	601	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
24	4	601	CLA	O1D-CGD-CBD	-2.60	119.39	124.52
24	A	1103	CLA	C4B-CHC-C1C	2.60	132.36	126.25
24	4	608	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
24	B	1201	CLA	CAA-C2A-C3A	-2.60	105.98	113.00
24	4	612	CLA	C3B-C4B-NB	-2.60	108.21	110.53
24	7	606	CLA	C2C-C1C-NC	2.60	112.71	109.98
24	7	606	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
24	A	1013	CLA	O2D-CGD-O1D	-2.60	118.80	123.85
24	8	603	CLA	C1C-C2C-C3C	-2.59	104.25	106.98
24	A	1104	CLA	O2A-CGA-CBA	2.59	119.75	111.83
24	A	1109	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
24	A	1139	CLA	O2D-CGD-O1D	-2.59	118.80	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	4	602	CLA	C3B-C4B-NB	-2.59	108.22	110.53
24	A	1136	CLA	C2C-C1C-NC	2.59	112.70	109.98
24	2	606	CLA	C1C-C2C-C3C	-2.59	104.26	106.98
40	1	501	LUT	C31-C30-C29	-2.59	123.65	127.28
24	K	1401	CLA	CMD-C2D-C3D	-2.59	121.75	127.69
24	4	610	CLA	C4B-CHC-C1C	2.59	132.34	126.25
24	L	1501	CLA	C1C-C2C-C3C	-2.59	104.26	106.98
24	8	605	CLA	C1C-C2C-C3C	-2.59	104.26	106.98
24	L	1501	CLA	C2C-C1C-NC	2.59	112.70	109.98
24	4	605	CLA	CHA-C4D-ND	2.59	137.89	132.55
24	2	609	CLA	C2C-C1C-NC	2.59	112.70	109.98
24	1	607	CLA	C3B-C4B-NB	-2.59	108.22	110.53
24	6	603	CLA	C1D-ND-C4D	-2.59	104.50	106.31
24	L	1502	CLA	CHD-C1D-ND	-2.59	121.16	124.80
24	B	1201	CLA	C1C-C2C-C3C	-2.59	104.26	106.98
24	F	1302	CLA	C1C-C2C-C3C	-2.59	104.26	106.98
24	2	602	CLA	C1C-C2C-C3C	-2.59	104.26	106.98
24	A	1103	CLA	C2C-C1C-NC	2.59	112.70	109.98
24	K	1401	CLA	C3B-C4B-NB	-2.59	108.22	110.53
24	2	606	CLA	CMA-C3A-C4A	2.58	118.72	111.77
41	a	609	CHL	C1-O2A-CGA	2.58	122.91	116.65
24	A	1129	CLA	CMA-C3A-C4A	2.58	118.72	111.77
24	B	1238	CLA	C2C-C1C-NC	2.58	112.70	109.98
24	5	601	CLA	C2C-C1C-NC	2.58	112.70	109.98
24	5	601	CLA	O2A-CGA-CBA	2.58	119.71	111.83
24	3	607	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
24	1	605	CLA	CMD-C2D-C3D	-2.58	121.76	127.69
41	6	619	CHL	C1-C2-C3	-2.58	121.96	126.20
24	B	1224	CLA	C1C-C2C-C3C	-2.58	104.26	106.98
24	5	607	CLA	CHA-C4D-ND	2.58	137.88	132.55
24	A	1136	CLA	C1C-C2C-C3C	-2.58	104.26	106.98
24	A	1120	CLA	C3B-C4B-NB	-2.58	108.22	110.53
24	7	617	CLA	C3B-C4B-NB	-2.58	108.22	110.53
40	a	502	LUT	C35-C15-C14	-2.58	118.24	123.52
27	B	4001	BCR	C15-C14-C13	-2.58	123.66	127.28
24	A	1129	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
24	A	1127	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
24	5	609	CLA	C1C-C2C-C3C	-2.58	104.27	106.98
24	5	602	CLA	C1C-C2C-C3C	-2.58	104.27	106.98
28	A	5001	LHG	C5-O7-C7	-2.58	111.62	117.80
24	8	607	CLA	CMA-C3A-C4A	2.58	118.70	111.77
24	B	1231	CLA	CHD-C1D-ND	-2.58	121.17	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1	601	CLA	O1D-CGD-CBD	-2.58	119.43	124.52
27	I	4001	BCR	C33-C5-C4	2.58	119.09	113.60
24	B	1221	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
24	A	1113	CLA	C2C-C1C-NC	2.58	112.69	109.98
24	6	617	CLA	C2C-C1C-NC	2.58	112.69	109.98
41	7	613	CHL	C1A-CHA-C4D	2.58	123.28	118.98
24	2	603	CLA	C1C-C2C-C3C	-2.58	104.27	106.98
24	A	1136	CLA	C4B-CHC-C1C	2.58	132.30	126.25
24	a	601	CLA	CAA-C2A-C3A	-2.58	106.04	113.00
24	8	602	CLA	C1C-C2C-C3C	-2.57	104.27	106.98
24	7	601	CLA	C4B-CHC-C1C	2.57	132.30	126.25
41	9	610	CHL	CMA-C3A-C4A	2.57	120.16	114.61
40	1	502	LUT	C18-C5-C6	-2.57	121.67	124.48
29	A	5005	DGD	O1G-C1A-C2A	2.57	119.68	111.83
24	a	602	CLA	C3B-C4B-NB	-2.57	108.23	110.53
24	5	605	CLA	C4B-CHC-C1C	2.57	132.30	126.25
24	3	610	CLA	CAA-C2A-C3A	-2.57	106.05	113.00
24	7	603	CLA	C3B-C4B-NB	-2.57	108.23	110.53
24	A	1106	CLA	CMA-C3A-C4A	2.57	118.69	111.77
40	3	502	LUT	C18-C5-C6	-2.57	121.68	124.48
24	B	1202	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
24	7	609	CLA	C4B-CHC-C1C	2.57	132.29	126.25
24	3	603	CLA	C1C-C2C-C3C	-2.57	104.28	106.98
24	B	1231	CLA	C2C-C1C-NC	2.57	112.68	109.98
25	A	2001	PQN	C11-C12-C13	-2.57	122.40	126.83
40	3	501	LUT	C35-C15-C14	-2.57	118.26	123.52
28	2	802	LHG	C5-O7-C7	-2.57	111.64	117.80
37	J	4002	RRX	C11-C12-C13	-2.57	119.31	126.36
24	B	1231	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
24	A	1141	CLA	CHA-C4D-ND	2.57	137.85	132.55
24	4	603	CLA	C2C-C1C-NC	2.57	112.68	109.98
24	1	604	CLA	C2C-C1C-NC	2.57	112.68	109.98
24	B	1240	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
24	K	1401	CLA	CHA-C4D-ND	2.57	137.85	132.55
33	3	802	PTY	O4-C30-C31	2.57	119.67	111.83
24	1	606	CLA	C1C-C2C-C3C	-2.57	104.28	106.98
41	9	613	CHL	CMA-C3A-C4A	2.57	120.14	114.61
24	A	1116	CLA	CMA-C3A-C4A	2.57	118.67	111.77
24	1	610	CLA	C2C-C1C-NC	2.57	112.68	109.98
24	A	1126	CLA	CMA-C3A-C4A	2.57	118.67	111.77
24	7	605	CLA	CMA-C3A-C4A	2.57	118.67	111.77
24	2	601	CLA	CMA-C3A-C4A	2.57	118.67	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	9	502	LUT	C31-C32-C33	-2.57	119.33	126.36
24	5	617	CLA	C3B-C4B-NB	-2.57	108.24	110.53
24	7	609	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
24	B	1209	CLA	C2C-C1C-NC	2.57	112.68	109.98
40	5	502	LUT	C22-C23-C24	-2.57	107.37	111.18
24	A	1121	CLA	CHA-C4D-ND	2.57	137.84	132.55
27	B	4002	BCR	C34-C9-C10	-2.57	118.66	122.82
24	A	1116	CLA	CHA-C4D-ND	2.56	137.84	132.55
24	A	1105	CLA	C4B-CHC-C1C	2.56	132.28	126.25
24	A	1114	CLA	C3B-C4B-NB	-2.56	108.24	110.53
24	4	611	CLA	C3B-C4B-NB	-2.56	108.24	110.53
24	B	1214	CLA	OBD-CAD-C3D	-2.56	122.42	128.42
24	A	1113	CLA	C1C-C2C-C3C	-2.56	104.28	106.98
24	9	606	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
24	5	608	CLA	CHA-C4D-ND	2.56	137.84	132.55
24	G	1602	CLA	C1C-C2C-C3C	-2.56	104.28	106.98
27	G	4001	BCR	C12-C13-C14	-2.56	114.98	119.01
24	6	617	CLA	C4B-CHC-C1C	2.56	132.27	126.25
41	4	613	CHL	C1-O2A-CGA	2.56	122.85	116.65
24	4	606	CLA	C1C-C2C-C3C	-2.56	104.29	106.98
24	A	1129	CLA	CHA-C4D-ND	2.56	137.83	132.55
24	A	1130	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
24	a	603	CLA	CHD-C1D-ND	-2.56	121.20	124.80
27	A	4004	BCR	C34-C9-C10	-2.56	118.67	122.82
24	8	602	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
24	a	601	CLA	CMA-C3A-C4A	2.56	118.65	111.77
28	F	5002	LHG	C5-O7-C7	-2.56	111.67	117.80
24	7	610	CLA	CHA-C4D-ND	2.56	137.83	132.55
27	5	503	BCR	C33-C5-C4	2.56	119.05	113.60
24	A	1121	CLA	C1C-C2C-C3C	-2.56	104.29	106.98
24	5	616	CLA	C1C-C2C-C3C	-2.56	104.29	106.98
27	3	503	BCR	C1-C6-C5	-2.56	119.14	122.64
24	A	1125	CLA	OBD-CAD-C3D	-2.56	122.44	128.42
24	5	603	CLA	C1C-C2C-C3C	-2.56	104.29	106.98
24	A	1133	CLA	C2C-C1C-NC	2.56	112.67	109.98
24	2	606	CLA	C3B-C4B-NB	-2.56	108.25	110.53
40	5	501	LUT	C39-C29-C28	2.56	121.99	118.09
24	B	1225	CLA	C4B-CHC-C1C	2.56	132.26	126.25
24	B	1235	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
24	5	604	CLA	C1D-ND-C4D	-2.55	104.52	106.31
41	8	613	CHL	C1-O2A-CGA	2.55	122.83	116.65
24	B	1203	CLA	CHA-C4D-ND	2.55	137.82	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	7	617	CLA	CHA-C4D-ND	2.55	137.82	132.55
24	4	616	CLA	C1C-C2C-C3C	-2.55	104.29	106.98
24	3	604	CLA	C1-O2A-CGA	2.55	122.83	116.65
24	J	1901	CLA	C3B-C4B-NB	-2.55	108.25	110.53
24	G	1603	CLA	C1C-C2C-C3C	-2.55	104.30	106.98
24	2	604	CLA	CHA-C4D-ND	2.55	137.82	132.55
24	a	612	CLA	O2A-CGA-CBA	2.55	119.62	111.83
24	a	612	CLA	C2C-C1C-NC	2.55	112.66	109.98
24	3	612	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
24	9	603	CLA	CHA-C4D-ND	2.55	137.81	132.55
28	2	802	LHG	O8-C23-C24	2.55	119.61	111.83
24	1	602	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
40	8	501	LUT	C22-C23-C24	-2.55	107.40	111.18
24	B	1228	CLA	O2A-CGA-CBA	2.55	119.61	111.83
27	5	504	BCR	C8-C7-C6	-2.55	120.19	127.00
24	5	617	CLA	CMA-C3A-C4A	2.55	118.62	111.77
24	B	1022	CLA	CHA-C4D-ND	2.55	137.81	132.55
24	8	605	CLA	CMA-C3A-C4A	2.55	118.62	111.77
24	4	607	CLA	CHA-C4D-ND	2.55	137.81	132.55
24	A	1135	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
27	H	4001	BCR	C4-C5-C6	-2.55	119.26	122.70
24	B	1228	CLA	CMA-C3A-C4A	2.55	118.62	111.77
24	B	1212	CLA	C1C-C2C-C3C	-2.55	104.30	106.98
24	B	1229	CLA	C1D-ND-C4D	-2.55	104.53	106.31
24	2	601	CLA	CAA-C2A-C3A	-2.55	106.12	113.00
24	A	1137	CLA	CMA-C3A-C4A	2.55	118.62	111.77
24	4	604	CLA	C4B-CHC-C1C	2.55	132.24	126.25
24	6	618	CLA	C3B-C4B-NB	-2.55	108.26	110.53
24	B	1220	CLA	O2A-CGA-CBA	2.55	119.60	111.83
28	5	801	LHG	O8-C23-C24	2.55	119.60	111.83
24	A	1135	CLA	CHA-C4D-ND	2.55	137.80	132.55
24	A	1116	CLA	C4B-CHC-C1C	2.55	132.23	126.25
41	1	613	CHL	CMA-C3A-C4A	2.55	120.09	114.61
28	F	5001	LHG	C5-O7-C7	-2.54	111.71	117.80
24	9	604	CLA	CHA-C4D-ND	2.54	137.80	132.55
24	A	1110	CLA	C1C-C2C-C3C	-2.54	104.30	106.98
24	4	612	CLA	O1D-CGD-CBD	-2.54	119.50	124.52
24	A	1112	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
24	A	1114	CLA	CMD-C2D-C3D	-2.54	121.86	127.69
41	9	610	CHL	C1-O2A-CGA	2.54	122.81	116.65
27	5	503	BCR	C38-C26-C25	-2.54	121.71	124.48
24	H	1703	CLA	CHA-C4D-ND	2.54	137.80	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	6	605	CLA	C1D-ND-C4D	-2.54	104.53	106.31
40	1	503	LUT	C27-C28-C29	-2.54	120.86	126.32
28	9	801	LHG	O8-C23-C24	2.54	119.59	111.83
41	a	606	CHL	C1A-CHA-C4D	2.54	123.22	118.98
24	B	1231	CLA	CMD-C2D-C3D	-2.54	121.86	127.69
24	A	1012	CLA	CHA-C4D-ND	2.54	137.79	132.55
24	9	605	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
24	4	603	CLA	C1D-ND-C4D	-2.54	104.53	106.31
24	4	610	CLA	CMD-C2D-C3D	-2.54	121.86	127.69
24	B	1215	CLA	C3B-C4B-NB	-2.54	108.26	110.53
24	1	601	CLA	C3B-C4B-NB	-2.54	108.26	110.53
24	5	602	CLA	C3B-C4B-NB	-2.54	108.26	110.53
24	6	617	CLA	CMA-C3A-C4A	2.54	118.60	111.77
24	B	1230	CLA	O2A-CGA-CBA	2.54	119.58	111.83
28	3	801	LHG	C5-O7-C7	-2.54	111.72	117.80
24	5	603	CLA	CMD-C2D-C3D	-2.54	121.87	127.69
27	B	4003	BCR	C23-C24-C25	-2.54	120.22	127.00
24	1	612	CLA	CMA-C3A-C4A	2.54	118.59	111.77
24	4	604	CLA	C1C-C2C-C3C	-2.54	104.31	106.98
24	A	1138	CLA	CMA-C3A-C4A	2.54	118.59	111.77
32	6	803	PCW	O3-C11-C12	2.54	119.57	111.83
24	5	605	CLA	CMA-C3A-C4A	2.54	118.59	111.77
24	6	608	CLA	CHA-C4D-ND	2.53	137.78	132.55
24	1	604	CLA	C1C-C2C-C3C	-2.53	104.31	106.98
24	5	604	CLA	C1C-C2C-C3C	-2.53	104.31	106.98
24	1	601	CLA	C4B-CHC-C1C	2.53	132.21	126.25
24	B	1232	CLA	C2C-C1C-NC	2.53	112.64	109.98
24	B	1211	CLA	CHA-C4D-ND	2.53	137.78	132.55
24	B	1219	CLA	CHD-C1D-ND	-2.53	121.24	124.80
24	3	605	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
24	4	604	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
24	6	612	CLA	CHA-C4D-ND	2.53	137.77	132.55
27	F	4001	BCR	C28-C27-C26	-2.53	109.54	114.06
24	L	1501	CLA	C3B-C4B-NB	-2.53	108.27	110.53
24	B	1223	CLA	C2C-C1C-NC	2.53	112.64	109.98
27	B	4003	BCR	C29-C28-C27	2.53	116.84	111.28
24	G	1601	CLA	CHA-C4D-ND	2.53	137.77	132.55
24	7	608	CLA	C3B-C4B-NB	-2.53	108.27	110.53
27	B	4003	BCR	C35-C13-C12	2.53	121.95	118.09
24	B	1217	CLA	C3B-C4B-NB	-2.53	108.27	110.53
24	2	605	CLA	CHA-C4D-ND	2.53	137.77	132.55
24	K	1402	CLA	C1C-C2C-C3C	-2.53	104.32	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	1	502	LUT	C39-C29-C28	2.53	121.95	118.09
41	3	608	CHL	C4C-CHD-C1D	2.53	125.12	116.07
24	8	607	CLA	CHA-C4D-ND	2.53	137.76	132.55
24	A	1101	CLA	O1D-CGD-CBD	-2.53	119.53	124.52
24	B	1207	CLA	C2C-C1C-NC	2.53	112.64	109.98
24	B	1208	CLA	CHD-C1D-ND	-2.53	121.25	124.80
24	8	610	CLA	O2A-CGA-CBA	2.53	119.53	111.83
24	1	606	CLA	C4B-CHC-C1C	2.52	132.18	126.25
27	A	4001	BCR	C30-C25-C24	2.52	122.50	115.65
24	A	1131	CLA	CHA-C4D-ND	2.52	137.76	132.55
24	A	1120	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
24	B	1234	CLA	CHA-C4D-ND	2.52	137.76	132.55
24	B	1232	CLA	C4B-CHC-C1C	2.52	132.18	126.25
27	3	504	BCR	C38-C26-C27	2.52	118.97	113.60
24	B	1214	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
24	8	602	CLA	CHA-C4D-ND	2.52	137.75	132.55
24	B	1215	CLA	CHD-C1D-ND	-2.52	121.25	124.80
24	5	603	CLA	O2A-CGA-CBA	2.52	119.52	111.83
28	B	5002	LHG	O8-C23-C24	2.52	119.52	111.83
24	6	612	CLA	C4B-CHC-C1C	2.52	132.18	126.25
24	4	616	CLA	C3B-C4B-NB	-2.52	108.28	110.53
24	5	604	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
24	4	603	CLA	C4B-CHC-C1C	2.52	132.18	126.25
24	B	1205	CLA	CMA-C3A-C4A	2.52	118.55	111.77
24	3	603	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
24	A	1137	CLA	CHA-C4D-ND	2.52	137.75	132.55
24	7	608	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
40	5	502	LUT	C30-C31-C32	-2.52	115.90	123.20
24	5	606	CLA	CHA-C4D-ND	2.52	137.75	132.55
41	7	613	CHL	C1-O2A-CGA	2.52	122.75	116.65
24	7	612	CLA	CHA-C4D-ND	2.52	137.75	132.55
41	1	609	CHL	CGD-CBD-CAD	-2.52	102.69	110.85
24	B	1202	CLA	C4B-CHC-C1C	2.52	132.17	126.25
24	A	1122	CLA	C2C-C1C-NC	2.52	112.63	109.98
24	5	607	CLA	C1C-C2C-C3C	-2.52	104.33	106.98
24	7	609	CLA	CHA-C4D-ND	2.52	137.74	132.55
41	8	601	CHL	CMA-C3A-C4A	2.52	120.03	114.61
24	B	1224	CLA	O2A-CGA-CBA	2.52	119.51	111.83
40	6	501	LUT	C7-C6-C5	-2.52	115.76	121.56
40	3	502	LUT	C35-C15-C14	-2.52	118.37	123.52
24	4	608	CLA	C2C-C1C-NC	2.52	112.62	109.98
40	2	502	LUT	C22-C23-C24	-2.52	107.45	111.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1	602	CLA	CHA-C4D-ND	2.52	137.74	132.55
24	5	604	CLA	C2C-C1C-NC	2.52	112.62	109.98
27	3	505	BCR	C33-C5-C4	2.52	118.96	113.60
24	B	1238	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
24	6	618	CLA	C4B-CHC-C1C	2.51	132.16	126.25
41	4	609	CHL	C1A-CHA-C4D	2.51	123.18	118.98
24	4	602	CLA	O2D-CGD-O1D	-2.51	118.95	123.85
24	4	612	CLA	CMC-C2C-C1C	2.51	128.96	125.03
24	A	1116	CLA	O2D-CGD-O1D	-2.51	118.95	123.85
24	B	1239	CLA	O2D-CGD-O1D	-2.51	118.95	123.85
24	4	610	CLA	CHA-C4D-ND	2.51	137.74	132.55
24	B	1229	CLA	C2C-C1C-NC	2.51	112.62	109.98
24	8	608	CLA	C3B-C4B-NB	-2.51	108.29	110.53
24	a	601	CLA	C4B-CHC-C1C	2.51	132.16	126.25
27	K	4002	BCR	C36-C18-C17	-2.51	118.75	122.82
24	6	603	CLA	C1C-C2C-C3C	-2.51	104.34	106.98
27	I	4001	BCR	C12-C13-C14	-2.51	115.06	119.01
24	B	1214	CLA	CHA-C4D-ND	2.51	137.73	132.55
24	2	621	CLA	CHA-C4D-ND	2.51	137.73	132.55
24	A	1102	CLA	C2C-C1C-NC	2.51	112.62	109.98
24	F	1302	CLA	O2A-CGA-CBA	2.51	119.49	111.83
24	7	615	CLA	O2A-CGA-CBA	2.51	119.49	111.83
41	7	613	CHL	C4D-CHA-CBD	-2.51	106.44	108.97
24	B	1204	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
24	B	1228	CLA	C3B-C4B-NB	-2.51	108.29	110.53
24	a	605	CLA	C3B-C4B-NB	-2.51	108.29	110.53
24	7	606	CLA	CHA-C4D-ND	2.51	137.73	132.55
24	A	1111	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
24	9	601	CLA	C1D-ND-C4D	-2.51	104.55	106.31
24	5	602	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
24	B	1202	CLA	CHA-C4D-ND	2.51	137.73	132.55
24	8	609	CLA	CMA-C3A-C4A	2.51	118.52	111.77
24	6	605	CLA	C2D-C1D-ND	2.51	112.61	110.13
24	A	1139	CLA	C2C-C1C-NC	2.51	112.62	109.98
24	5	607	CLA	O2A-CGA-CBA	2.51	119.48	111.83
49	7	504	C7Z	C8-C7-C6	-2.51	120.30	127.00
24	9	601	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
24	7	612	CLA	C3B-C4B-NB	-2.51	108.29	110.53
24	B	1227	CLA	CHA-C4D-ND	2.51	137.72	132.55
24	8	608	CLA	CHD-C1D-ND	-2.51	121.28	124.80
24	8	602	CLA	C4B-CHC-C1C	2.51	132.14	126.25
24	4	617	CLA	C3B-C4B-NB	-2.51	108.29	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1139	CLA	CHA-C4D-ND	2.51	137.72	132.55
24	B	1213	CLA	C1C-C2C-C3C	-2.51	104.34	106.98
24	A	1130	CLA	C4B-CHC-C1C	2.51	132.14	126.25
24	3	607	CLA	O2A-CGA-CBA	2.51	119.47	111.83
24	1	611	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
28	1	801	LHG	O8-C23-C24	2.50	119.47	111.83
41	a	606	CHL	C4D-CHA-CBD	-2.50	106.44	108.97
24	A	1118	CLA	O2D-CGD-O1D	-2.50	118.97	123.85
24	a	603	CLA	C2D-C1D-ND	2.50	112.60	110.13
24	1	601	CLA	CAA-C2A-C3A	-2.50	106.23	113.00
24	K	1404	CLA	CHA-C4D-ND	2.50	137.71	132.55
24	4	616	CLA	O2A-CGA-CBA	2.50	119.47	111.83
24	1	607	CLA	CHA-C4D-ND	2.50	137.71	132.55
24	8	603	CLA	C2C-C1C-NC	2.50	112.61	109.98
24	6	617	CLA	CHA-C4D-ND	2.50	137.71	132.55
24	1	603	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
23	A	1011	CL0	O1D-CGD-CBD	-2.50	120.93	124.72
27	4	503	BCR	C8-C7-C6	-2.50	120.32	127.00
41	4	618	CHL	C1-C2-C3	-2.50	122.10	126.20
24	B	1217	CLA	O2A-CGA-CBA	2.50	119.46	111.83
24	A	1123	CLA	CHA-C4D-ND	2.50	137.71	132.55
24	H	1701	CLA	C2D-C1D-ND	2.50	112.60	110.13
24	5	606	CLA	CMA-C3A-C4A	2.50	118.49	111.77
24	A	1104	CLA	CHA-C4D-ND	2.50	137.71	132.55
27	3	503	BCR	C36-C18-C17	-2.50	118.77	122.82
24	A	1124	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
24	2	604	CLA	CMA-C3A-C4A	2.50	118.49	111.77
24	H	1702	CLA	CHA-C4D-ND	2.50	137.70	132.55
24	A	1117	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
24	F	1301	CLA	O2A-CGA-CBA	2.50	119.45	111.83
24	6	604	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
24	3	607	CLA	CHA-C4D-ND	2.50	137.70	132.55
24	3	612	CLA	CHA-C4D-ND	2.50	137.70	132.55
24	A	1140	CLA	O2A-CGA-CBA	2.50	119.45	111.83
24	B	1215	CLA	C4B-CHC-C1C	2.50	132.12	126.25
24	8	615	CLA	CHA-C4D-ND	2.50	137.70	132.55
24	7	612	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
24	A	1111	CLA	C4B-CHC-C1C	2.49	132.11	126.25
24	1	608	CLA	C3B-C4B-NB	-2.49	108.30	110.53
24	2	601	CLA	C3B-C4B-NB	-2.49	108.30	110.53
24	6	602	CLA	CHA-C4D-ND	2.49	137.70	132.55
24	3	602	CLA	CHA-C4D-ND	2.49	137.69	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	7	607	CLA	CHA-C4D-ND	2.49	137.69	132.55
24	B	1219	CLA	CHA-C4D-ND	2.49	137.69	132.55
24	H	1703	CLA	C4B-CHC-C1C	2.49	132.11	126.25
24	B	1236	CLA	CHD-C1D-ND	-2.49	121.29	124.80
24	A	1119	CLA	CHA-C4D-ND	2.49	137.69	132.55
24	4	604	CLA	C2C-C1C-NC	2.49	112.60	109.98
24	B	1231	CLA	CHA-C4D-ND	2.49	137.69	132.55
24	2	612	CLA	CHA-C4D-ND	2.49	137.69	132.55
24	9	609	CLA	CHA-C4D-ND	2.49	137.69	132.55
25	B	2002	PQN	C11-C3-C2	-2.49	120.62	124.89
27	3	505	BCR	C19-C18-C17	2.49	122.93	119.01
24	B	1021	CLA	C4B-CHC-C1C	2.49	132.11	126.25
24	B	1216	CLA	CHA-C4D-ND	2.49	137.69	132.55
24	3	602	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
24	B	1021	CLA	CHA-C4D-ND	2.49	137.69	132.55
24	4	602	CLA	C1C-C2C-C3C	-2.49	104.36	106.98
24	8	620	CLA	CMA-C3A-C4A	2.49	118.47	111.77
24	B	1207	CLA	CHA-C4D-ND	2.49	137.69	132.55
24	8	612	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
24	A	1102	CLA	CHA-C4D-ND	2.49	137.69	132.55
24	A	1113	CLA	CHD-C1D-ND	-2.49	121.30	124.80
24	B	1239	CLA	O2A-CGA-CBA	2.49	119.42	111.83
27	A	4001	BCR	C38-C26-C25	-2.49	121.77	124.48
24	B	1201	CLA	C2C-C1C-NC	2.49	112.60	109.98
24	5	604	CLA	CMD-C2D-C3D	-2.49	121.98	127.69
24	2	606	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
27	I	4001	BCR	C4-C5-C6	-2.49	119.34	122.70
24	4	607	CLA	C3B-C4B-NB	-2.49	108.31	110.53
24	A	1113	CLA	O2A-CGA-CBA	2.49	119.42	111.83
24	B	1223	CLA	C2D-C1D-ND	2.49	112.59	110.13
24	F	1302	CLA	O2D-CGD-O1D	-2.49	119.01	123.85
24	4	605	CLA	O2D-CGD-O1D	-2.49	119.01	123.85
24	6	601	CLA	O2A-CGA-CBA	2.49	119.42	111.83
24	1	604	CLA	C4B-CHC-C1C	2.49	132.09	126.25
40	6	502	LUT	C11-C10-C9	-2.49	123.79	127.28
24	3	618	CLA	CHA-C4D-ND	2.49	137.68	132.55
24	B	1218	CLA	C3B-C4B-NB	-2.48	108.31	110.53
24	B	1215	CLA	O2D-CGD-O1D	-2.48	119.01	123.85
24	A	1134	CLA	C4B-CHC-C1C	2.48	132.09	126.25
24	4	602	CLA	C4B-CHC-C1C	2.48	132.09	126.25
24	B	1222	CLA	CHD-C1D-ND	-2.48	121.31	124.80
24	2	613	CLA	CHA-C4D-ND	2.48	137.67	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1132	CLA	CHA-C4D-ND	2.48	137.67	132.55
24	5	602	CLA	CHA-C4D-ND	2.48	137.67	132.55
24	5	608	CLA	O1D-CGD-CBD	-2.48	119.62	124.52
24	a	602	CLA	CHA-C4D-ND	2.48	137.67	132.55
24	4	617	CLA	C4B-CHC-C1C	2.48	132.08	126.25
24	2	601	CLA	C4B-CHC-C1C	2.48	132.08	126.25
24	2	612	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
24	B	1228	CLA	C2C-C1C-NC	2.48	112.59	109.98
24	4	602	CLA	CHA-C4D-ND	2.48	137.67	132.55
24	4	612	CLA	CHA-C4D-ND	2.48	137.67	132.55
41	4	609	CHL	C1-O2A-CGA	2.48	122.66	116.65
24	2	609	CLA	CHA-C4D-ND	2.48	137.67	132.55
24	a	608	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
24	7	606	CLA	CHD-C1D-ND	-2.48	121.31	124.80
24	2	609	CLA	CHD-C1D-ND	-2.48	121.31	124.80
24	B	1223	CLA	C4B-CHC-C1C	2.48	132.08	126.25
24	H	1703	CLA	CMA-C3A-C4A	2.48	118.44	111.77
24	9	603	CLA	C4B-CHC-C1C	2.48	132.08	126.25
24	2	603	CLA	C2D-C1D-ND	2.48	112.58	110.13
24	A	1125	CLA	C4B-CHC-C1C	2.48	132.08	126.25
24	4	615	CLA	C3B-C4B-NB	-2.48	108.32	110.53
24	5	609	CLA	CHA-C4D-ND	2.48	137.66	132.55
41	a	609	CHL	C4D-CHA-CBD	-2.48	106.47	108.97
24	a	611	CLA	C4B-CHC-C1C	2.48	132.07	126.25
24	B	1232	CLA	CHA-C4D-ND	2.48	137.66	132.55
24	B	1226	CLA	O2A-CGA-CBA	2.48	119.39	111.83
24	J	1901	CLA	C4B-CHC-C1C	2.48	132.07	126.25
24	1	602	CLA	C4B-CHC-C1C	2.48	132.07	126.25
48	7	502	XAT	O24-C25-C38	-2.48	112.28	115.05
41	4	609	CHL	C4C-CHD-C1D	2.48	124.93	116.07
24	8	608	CLA	CHA-C4D-ND	2.48	137.66	132.55
24	B	1230	CLA	O1D-CGD-CBD	-2.48	119.63	124.52
24	3	613	CLA	C1C-C2C-C3C	-2.48	104.38	106.98
24	H	1702	CLA	C3B-C4B-NB	-2.48	108.32	110.53
24	A	1111	CLA	CHA-C4D-ND	2.48	137.66	132.55
24	a	607	CLA	CHA-C4D-ND	2.48	137.66	132.55
24	7	615	CLA	CHA-C4D-ND	2.48	137.66	132.55
24	J	1901	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
24	4	615	CLA	CHA-C4D-ND	2.48	137.66	132.55
27	A	4005	BCR	C37-C22-C23	2.48	121.87	118.09
41	5	611	CHL	CMA-C3A-C4A	2.48	119.94	114.61
24	A	1122	CLA	O2A-CGA-CBA	2.48	119.38	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	2	601	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
24	B	1238	CLA	C1-C2-C3	-2.47	122.14	126.20
24	5	607	CLA	C4B-CHC-C1C	2.47	132.07	126.25
24	B	1206	CLA	O2A-CGA-CBA	2.47	119.38	111.83
47	6	806	SPH	C3-C4-C5	-2.47	119.56	124.69
24	A	1113	CLA	O1D-CGD-CBD	-2.47	119.64	124.52
24	B	1238	CLA	CMD-C2D-C3D	-2.47	122.01	127.69
24	A	1126	CLA	CHD-C1D-ND	-2.47	121.32	124.80
24	1	603	CLA	CHD-C1D-ND	-2.47	121.32	124.80
24	a	615	CLA	C2D-C1D-ND	2.47	112.58	110.13
24	2	607	CLA	CHA-C4D-ND	2.47	137.65	132.55
40	6	501	LUT	C22-C23-C24	-2.47	107.51	111.18
24	1	606	CLA	CHA-C4D-ND	2.47	137.65	132.55
24	9	603	CLA	O2D-CGD-O1D	-2.47	119.03	123.85
24	a	604	CLA	C2C-C1C-NC	2.47	112.58	109.98
24	4	607	CLA	C1-O2A-CGA	2.47	122.64	116.65
24	2	607	CLA	C3B-C4B-NB	-2.47	108.32	110.53
24	7	612	CLA	O2A-CGA-CBA	2.47	119.38	111.83
24	5	609	CLA	O2D-CGD-O1D	-2.47	119.03	123.85
24	6	602	CLA	O2D-CGD-O1D	-2.47	119.03	123.85
24	9	602	CLA	O2D-CGD-O1D	-2.47	119.03	123.85
24	2	615	CLA	C2C-C1C-NC	2.47	112.58	109.98
24	a	615	CLA	CHA-C4D-ND	2.47	137.65	132.55
40	8	501	LUT	C39-C29-C28	2.47	121.86	118.09
24	B	1210	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
24	2	609	CLA	C3B-C4B-NB	-2.47	108.32	110.53
24	6	603	CLA	C4B-CHC-C1C	2.47	132.06	126.25
24	B	1209	CLA	C1C-C2C-C3C	-2.47	104.38	106.98
24	5	616	CLA	CHA-C4D-ND	2.47	137.65	132.55
24	5	612	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
24	9	612	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
24	F	1301	CLA	CHA-C4D-ND	2.47	137.65	132.55
24	8	618	CLA	C3B-C4B-NB	-2.47	108.33	110.53
24	A	1108	CLA	CHA-C4D-ND	2.47	137.65	132.55
24	1	601	CLA	CHA-C4D-ND	2.47	137.65	132.55
24	2	602	CLA	CHA-C4D-ND	2.47	137.65	132.55
24	a	612	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
24	B	1201	CLA	C4B-CHC-C1C	2.47	132.05	126.25
24	B	1204	CLA	CAA-C2A-C3A	-2.47	106.33	113.00
24	A	1124	CLA	CAA-C2A-C1A	-2.47	103.88	111.97
24	K	1403	CLA	CHA-C4D-ND	2.47	137.64	132.55
24	1	612	CLA	CHA-C4D-ND	2.47	137.64	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	612	CLA	C3B-C4B-NB	-2.47	108.33	110.53
24	6	608	CLA	CHD-C1D-ND	-2.47	121.33	124.80
24	A	1119	CLA	C4B-CHC-C1C	2.47	132.05	126.25
41	1	609	CHL	CMA-C3A-C4A	2.47	119.93	114.61
24	a	608	CLA	C3B-C4B-NB	-2.47	108.33	110.53
24	4	608	CLA	O2A-CGA-CBA	2.47	119.36	111.83
24	A	1101	CLA	CHA-C4D-ND	2.47	137.64	132.55
24	6	615	CLA	CHA-C4D-ND	2.47	137.64	132.55
24	B	1205	CLA	C3B-C4B-NB	-2.47	108.33	110.53
27	B	4006	BCR	C28-C27-C26	-2.47	109.66	114.06
24	6	608	CLA	CMA-C3A-C4A	2.47	118.40	111.77
24	1	603	CLA	CMD-C2D-C3D	-2.47	122.03	127.69
41	a	610	CHL	CMA-C3A-C4A	2.47	119.92	114.61
24	4	617	CLA	CHA-C4D-ND	2.47	137.64	132.55
24	8	612	CLA	CHA-C4D-ND	2.47	137.63	132.55
24	F	1301	CLA	CMA-C3A-C4A	2.46	118.40	111.77
24	K	1402	CLA	CHA-C4D-ND	2.46	137.63	132.55
24	5	603	CLA	CHA-C4D-ND	2.46	137.63	132.55
24	6	604	CLA	CHA-C4D-ND	2.46	137.63	132.55
24	8	606	CLA	CHA-C4D-ND	2.46	137.63	132.55
24	4	606	CLA	CHA-C4D-ND	2.46	137.63	132.55
24	4	608	CLA	CHA-C4D-ND	2.46	137.63	132.55
24	2	601	CLA	C2C-C1C-NC	2.46	112.57	109.98
24	1	604	CLA	C1-C2-C3	-2.46	122.16	126.20
24	4	603	CLA	CHD-C1D-ND	-2.46	121.33	124.80
24	2	610	CLA	CHA-C4D-ND	2.46	137.63	132.55
24	4	615	CLA	C4B-CHC-C1C	2.46	132.04	126.25
24	7	608	CLA	C4B-CHC-C1C	2.46	132.04	126.25
24	7	617	CLA	C4B-CHC-C1C	2.46	132.04	126.25
24	2	607	CLA	C4B-CHC-C1C	2.46	132.04	126.25
24	B	1213	CLA	CHD-C1D-ND	-2.46	121.34	124.80
24	9	602	CLA	CHA-C4D-ND	2.46	137.63	132.55
24	A	1132	CLA	CAA-C2A-C3A	-2.46	106.34	113.00
24	4	606	CLA	C2C-C1C-NC	2.46	112.57	109.98
24	A	1114	CLA	CHA-C4D-ND	2.46	137.63	132.55
24	2	602	CLA	C4B-CHC-C1C	2.46	132.04	126.25
24	A	1133	CLA	CHA-C4D-ND	2.46	137.63	132.55
24	8	618	CLA	CHA-C4D-ND	2.46	137.63	132.55
40	7	501	LUT	C31-C32-C33	-2.46	119.61	126.36
24	A	1109	CLA	CAA-C2A-C3A	-2.46	106.35	113.00
24	B	1201	CLA	CMA-C3A-C4A	2.46	118.39	111.77
28	8	801	LHG	C5-O7-C7	-2.46	111.91	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	1204	CLA	C4B-CHC-C1C	2.46	132.03	126.25
24	7	603	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
24	A	1118	CLA	C4B-CHC-C1C	2.46	132.03	126.25
24	4	611	CLA	C1D-ND-C4D	-2.46	104.59	106.31
24	A	1133	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
24	A	1115	CLA	CHA-C4D-ND	2.46	137.62	132.55
24	1	615	CLA	CHA-C4D-ND	2.46	137.62	132.55
24	B	1217	CLA	CHA-C4D-ND	2.46	137.62	132.55
24	6	602	CLA	C3B-C4B-NB	-2.46	108.34	110.53
40	5	505	LUT	C1-C6-C7	2.46	122.32	115.65
24	2	603	CLA	C1-O2A-CGA	2.46	122.60	116.65
24	A	1114	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
24	2	607	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
27	4	503	BCR	C33-C5-C6	-2.46	121.80	124.48
24	B	1229	CLA	C1-O2A-CGA	2.46	122.60	116.65
24	B	1210	CLA	CHA-C4D-ND	2.46	137.62	132.55
24	9	606	CLA	CHA-C4D-ND	2.46	137.62	132.55
24	7	602	CLA	O2D-CGD-O1D	-2.46	119.07	123.85
24	K	1404	CLA	C4B-CHC-C1C	2.46	132.02	126.25
24	A	1134	CLA	CHA-C4D-ND	2.46	137.62	132.55
24	3	604	CLA	C4B-CHC-C1C	2.46	132.02	126.25
24	7	606	CLA	C4B-CHC-C1C	2.45	132.02	126.25
24	3	618	CLA	O2D-CGD-O1D	-2.45	119.07	123.85
24	A	1109	CLA	O2A-CGA-CBA	2.45	119.32	111.83
24	8	610	CLA	CHA-C4D-ND	2.45	137.61	132.55
24	a	605	CLA	C4B-CHC-C1C	2.45	132.02	126.25
24	5	603	CLA	CHD-C1D-ND	-2.45	121.35	124.80
24	A	1126	CLA	CHA-C4D-ND	2.45	137.61	132.55
24	B	1208	CLA	CHA-C4D-ND	2.45	137.61	132.55
24	B	1240	CLA	C4B-CHC-C1C	2.45	132.02	126.25
24	B	1207	CLA	O2A-CGA-CBA	2.45	119.31	111.83
24	G	1603	CLA	CHA-C4D-ND	2.45	137.61	132.55
24	7	602	CLA	CHA-C4D-ND	2.45	137.61	132.55
24	2	609	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
24	A	1114	CLA	O2A-CGA-CBA	2.45	119.31	111.83
31	A	5008	LMT	O5'-C5'-C4'	2.45	114.79	109.72
24	A	1139	CLA	C1C-C2C-C3C	-2.45	104.40	106.98
24	B	1021	CLA	C1C-C2C-C3C	-2.45	104.40	106.98
24	7	601	CLA	C3B-C4B-NB	-2.45	108.34	110.53
24	B	1217	CLA	C4B-CHC-C1C	2.45	132.01	126.25
24	7	604	CLA	C4B-CHC-C1C	2.45	132.01	126.25
24	B	1201	CLA	CHA-C4D-ND	2.45	137.60	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	1215	CLA	CHA-C4D-ND	2.45	137.60	132.55
24	A	1126	CLA	O1D-CGD-CBD	-2.45	119.69	124.52
24	B	1235	CLA	C1C-C2C-C3C	-2.45	104.40	106.98
41	8	601	CHL	C4C-CHD-C1D	2.45	124.83	116.07
24	4	604	CLA	CHA-C4D-ND	2.45	137.60	132.55
24	A	1126	CLA	C2C-C1C-NC	2.45	112.55	109.98
24	B	1228	CLA	CHA-C4D-ND	2.45	137.60	132.55
24	H	1701	CLA	CHA-C4D-ND	2.45	137.60	132.55
27	3	504	BCR	C37-C22-C21	-2.45	118.85	122.82
24	A	1121	CLA	O2A-CGA-CBA	2.45	119.30	111.83
24	B	1214	CLA	CMA-C3A-C4A	2.45	118.35	111.77
24	5	602	CLA	C4B-CHC-C1C	2.45	132.00	126.25
24	A	1103	CLA	C3B-C4B-NB	-2.45	108.34	110.53
40	8	501	LUT	C20-C13-C12	2.45	121.83	118.09
24	B	1023	CLA	CHA-C1A-NA	-2.45	120.85	126.39
27	5	504	BCR	C1-C6-C5	-2.45	119.29	122.64
24	A	1109	CLA	CHA-C4D-ND	2.45	137.60	132.55
24	7	601	CLA	CHA-C4D-ND	2.45	137.60	132.55
24	5	617	CLA	O2A-CGA-CBA	2.45	119.30	111.83
24	L	1502	CLA	C3B-C4B-NB	-2.45	108.35	110.53
24	3	616	CLA	C4B-CHC-C1C	2.45	132.00	126.25
24	A	1101	CLA	C1C-C2C-C3C	-2.45	104.41	106.98
24	7	602	CLA	C1C-C2C-C3C	-2.45	104.41	106.98
24	2	601	CLA	C1C-C2C-C3C	-2.45	104.41	106.98
24	3	610	CLA	CHD-C1D-ND	-2.45	121.36	124.80
24	8	609	CLA	C1D-ND-C4D	-2.45	104.60	106.31
48	7	502	XAT	C38-C25-C26	-2.45	118.28	122.30
24	A	1125	CLA	C2D-C1D-ND	2.45	112.55	110.13
40	8	501	LUT	C11-C10-C9	-2.45	123.85	127.28
24	A	1120	CLA	C4B-CHC-C1C	2.44	132.00	126.25
24	B	1234	CLA	C4B-CHC-C1C	2.44	132.00	126.25
24	B	1225	CLA	CHA-C4D-ND	2.44	137.59	132.55
24	4	608	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
24	a	612	CLA	CHA-C4D-ND	2.44	137.59	132.55
40	a	501	LUT	C22-C23-C24	-2.44	107.55	111.18
28	9	802	LHG	C5-O7-C7	-2.44	111.95	117.80
24	A	1013	CLA	CMB-C2B-C3B	2.44	132.30	126.55
24	3	606	CLA	CHA-C4D-ND	2.44	137.59	132.55
24	B	1238	CLA	C1-O2A-CGA	2.44	122.56	116.65
24	B	1201	CLA	O1D-CGD-CBD	-2.44	119.70	124.52
27	K	4002	BCR	C19-C18-C17	2.44	122.85	119.01
24	H	1701	CLA	C4B-CHC-C1C	2.44	131.99	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1128	CLA	CHA-C4D-ND	2.44	137.59	132.55
24	B	1213	CLA	C2C-C1C-NC	2.44	112.55	109.98
24	1	615	CLA	CHD-C1D-ND	-2.44	121.37	124.80
27	3	505	BCR	C38-C26-C25	-2.44	121.82	124.48
27	J	4001	BCR	C19-C18-C17	2.44	122.85	119.01
24	3	616	CLA	C3B-C4B-NB	-2.44	108.35	110.53
27	A	4003	BCR	C8-C9-C10	2.44	122.85	119.01
24	9	606	CLA	CAA-C2A-C3A	-2.44	106.40	113.00
24	a	601	CLA	CHD-C1D-ND	-2.44	121.37	124.80
24	A	1135	CLA	O2A-CGA-CBA	2.44	119.28	111.83
24	4	603	CLA	C1-C2-C3	-2.44	122.20	126.20
24	A	1120	CLA	C2D-C1D-ND	2.44	112.54	110.13
24	K	1401	CLA	C4B-CHC-C1C	2.44	131.99	126.25
24	4	608	CLA	C4B-CHC-C1C	2.44	131.99	126.25
24	A	1106	CLA	CHA-C4D-ND	2.44	137.58	132.55
24	5	601	CLA	C3B-C4B-NB	-2.44	108.35	110.53
24	a	605	CLA	CMA-C3A-C4A	2.44	118.33	111.77
24	B	1212	CLA	CHA-C4D-ND	2.44	137.58	132.55
24	7	608	CLA	CHA-C4D-ND	2.44	137.58	132.55
24	A	1107	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
24	a	608	CLA	C4B-CHC-C1C	2.44	131.98	126.25
24	A	1102	CLA	CHD-C1D-ND	-2.44	121.37	124.80
40	9	502	LUT	C18-C5-C4	2.44	118.90	114.42
24	B	1211	CLA	C1C-C2C-C3C	-2.44	104.42	106.98
24	B	1203	CLA	O2D-CGD-O1D	-2.44	119.11	123.85
24	A	1108	CLA	C4B-CHC-C1C	2.44	131.98	126.25
24	B	1211	CLA	C4B-CHC-C1C	2.44	131.98	126.25
24	a	607	CLA	C3B-C4B-NB	-2.44	108.36	110.53
24	B	1211	CLA	C2C-C1C-NC	2.44	112.54	109.98
24	A	1136	CLA	O2D-CGD-O1D	-2.44	119.11	123.85
24	9	612	CLA	CHA-C4D-ND	2.44	137.57	132.55
24	A	1133	CLA	C3B-C4B-NB	-2.44	108.36	110.53
24	3	613	CLA	O2A-CGA-CBA	2.44	119.26	111.83
24	B	1204	CLA	CMA-C3A-C4A	2.44	118.32	111.77
24	8	606	CLA	O2D-CGD-O1D	-2.44	119.11	123.85
24	9	607	CLA	O2D-CGD-O1D	-2.44	119.11	123.85
24	A	1104	CLA	C4B-CHC-C1C	2.43	131.97	126.25
24	2	612	CLA	CHD-C1D-ND	-2.43	121.38	124.80
24	1	603	CLA	C1-O2A-CGA	2.43	122.54	116.65
24	a	608	CLA	CHA-C4D-ND	2.43	137.57	132.55
24	2	608	CLA	CHA-C4D-ND	2.43	137.57	132.55
24	2	603	CLA	C4B-CHC-C1C	2.43	131.97	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	L	1502	CLA	O2D-CGD-O1D	-2.43	119.11	123.85
24	8	612	CLA	CHD-C1D-ND	-2.43	121.38	124.80
24	6	617	CLA	C1C-C2C-C3C	-2.43	104.42	106.98
24	1	611	CLA	C4B-CHC-C1C	2.43	131.97	126.25
24	A	1127	CLA	CHA-C4D-ND	2.43	137.57	132.55
24	F	1302	CLA	CHA-C4D-ND	2.43	137.57	132.55
24	A	1131	CLA	O2D-CGD-O1D	-2.43	119.11	123.85
24	7	604	CLA	O2D-CGD-O1D	-2.43	119.11	123.85
24	a	601	CLA	C1C-C2C-C3C	-2.43	104.42	106.98
24	B	1206	CLA	O2D-CGD-O1D	-2.43	119.11	123.85
24	9	604	CLA	O2D-CGD-O1D	-2.43	119.11	123.85
27	A	4003	BCR	C34-C9-C10	-2.43	118.88	122.82
24	6	618	CLA	CHA-C4D-ND	2.43	137.57	132.55
24	1	610	CLA	CHA-C4D-ND	2.43	137.57	132.55
24	9	607	CLA	CHA-C4D-ND	2.43	137.56	132.55
24	3	610	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
41	4	609	CHL	C4D-CHA-CBD	-2.43	106.52	108.97
24	B	1208	CLA	C4B-CHC-C1C	2.43	131.96	126.25
24	5	614	CLA	C4B-CHC-C1C	2.43	131.96	126.25
24	B	1240	CLA	O1D-CGD-CBD	-2.43	119.72	124.52
24	1	610	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
24	a	603	CLA	C1D-ND-C4D	-2.43	104.61	106.31
40	4	501	LUT	C39-C29-C28	2.43	121.80	118.09
24	K	1402	CLA	C4B-CHC-C1C	2.43	131.96	126.25
24	2	601	CLA	CHA-C4D-ND	2.43	137.56	132.55
24	3	618	CLA	O1D-CGD-CBD	-2.43	119.73	124.52
24	A	1104	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
24	6	605	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
24	B	1214	CLA	C4B-CHC-C1C	2.43	131.96	126.25
27	8	503	BCR	C1-C6-C5	-2.43	119.32	122.64
24	3	605	CLA	C4B-CHC-C1C	2.43	131.96	126.25
24	6	604	CLA	C4B-CHC-C1C	2.43	131.96	126.25
24	B	1240	CLA	CHA-C4D-ND	2.43	137.56	132.55
24	1	604	CLA	CHA-C4D-ND	2.43	137.56	132.55
24	B	1205	CLA	CHA-C4D-ND	2.43	137.56	132.55
24	6	605	CLA	CHA-C4D-ND	2.43	137.56	132.55
24	3	604	CLA	CHD-C1D-ND	-2.43	121.39	124.80
24	A	1013	CLA	O2A-CGA-CBA	2.43	119.24	111.83
24	B	1209	CLA	C1D-ND-C4D	-2.43	104.61	106.31
24	A	1103	CLA	C1-O2A-CGA	2.43	122.52	116.65
24	A	1104	CLA	C1-O2A-CGA	2.43	122.52	116.65
24	B	1228	CLA	CHD-C1D-ND	-2.43	121.39	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	5	601	CLA	CHA-C4D-ND	2.43	137.55	132.55
24	A	1105	CLA	CHD-C1D-ND	-2.43	121.39	124.80
24	B	1239	CLA	CHA-C4D-ND	2.43	137.55	132.55
24	J	1901	CLA	CHA-C4D-ND	2.43	137.55	132.55
24	G	1601	CLA	O2A-CGA-CBA	2.43	119.23	111.83
24	2	604	CLA	O2A-CGA-CBA	2.43	119.23	111.83
24	A	1110	CLA	C3B-C4B-NB	-2.43	108.36	110.53
24	1	606	CLA	C2C-C1C-NC	2.42	112.53	109.98
24	a	604	CLA	CHA-C4D-ND	2.42	137.55	132.55
24	B	1228	CLA	C1C-C2C-C3C	-2.42	104.43	106.98
24	B	1229	CLA	CHD-C1D-ND	-2.42	121.39	124.80
24	3	603	CLA	C4B-CHC-C1C	2.42	131.95	126.25
24	2	605	CLA	C4B-CHC-C1C	2.42	131.95	126.25
24	A	1107	CLA	CHA-C4D-ND	2.42	137.55	132.55
27	I	4001	BCR	C1-C6-C7	2.42	122.22	115.65
24	B	1223	CLA	C1C-C2C-C3C	-2.42	104.43	106.98
24	3	606	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
24	H	1703	CLA	C3B-C4B-NB	-2.42	108.37	110.53
24	A	1012	CLA	C2D-C1D-ND	2.42	112.52	110.13
24	a	611	CLA	CHA-C4D-ND	2.42	137.55	132.55
24	B	1203	CLA	C4B-CHC-C1C	2.42	131.94	126.25
27	L	4003	BCR	C15-C14-C13	-2.42	123.88	127.28
24	8	609	CLA	C2D-C1D-ND	2.42	112.52	110.13
24	6	601	CLA	C3B-C4B-NB	-2.42	108.37	110.53
24	B	1222	CLA	C4B-CHC-C1C	2.42	131.94	126.25
24	A	1112	CLA	C1C-C2C-C3C	-2.42	104.43	106.98
24	L	1503	CLA	CHA-C4D-ND	2.42	137.54	132.55
24	7	607	CLA	CAA-C2A-C3A	-2.42	106.46	113.00
24	4	606	CLA	C4B-CHC-C1C	2.42	131.94	126.25
24	8	615	CLA	C4B-CHC-C1C	2.42	131.94	126.25
41	a	613	CHL	C4C-CHD-C1D	2.42	124.73	116.07
24	2	602	CLA	CMA-C3A-C4A	2.42	118.28	111.77
24	B	1224	CLA	CHD-C1D-ND	-2.42	121.40	124.80
24	A	1122	CLA	C1C-C2C-C3C	-2.42	104.44	106.98
24	4	615	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
27	4	503	BCR	C27-C26-C25	-2.42	119.44	122.70
24	B	1223	CLA	O2A-CGA-CBA	2.42	119.21	111.83
24	8	610	CLA	C3B-C4B-NB	-2.42	108.37	110.53
24	4	616	CLA	CHA-C4D-ND	2.42	137.54	132.55
24	a	604	CLA	C4B-CHC-C1C	2.42	131.93	126.25
24	1	606	CLA	CHD-C1D-ND	-2.42	121.40	124.80
27	K	4001	BCR	C33-C5-C6	-2.42	121.85	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	1229	CLA	CHA-C4D-ND	2.42	137.53	132.55
24	B	1204	CLA	C1-O2A-CGA	2.42	122.50	116.65
24	8	606	CLA	O2A-CGA-CBA	2.42	119.20	111.83
24	B	1021	CLA	O2A-CGA-CBA	2.42	119.20	111.83
24	A	1120	CLA	C1D-ND-C4D	-2.42	104.62	106.31
24	7	604	CLA	CHA-C4D-ND	2.42	137.53	132.55
24	a	607	CLA	O2A-CGA-CBA	2.42	119.20	111.83
24	B	1231	CLA	C4B-CHC-C1C	2.42	131.93	126.25
24	6	609	CLA	CHA-C4D-ND	2.41	137.53	132.55
24	B	1216	CLA	CHD-C1D-ND	-2.41	121.41	124.80
24	3	606	CLA	C4B-CHC-C1C	2.41	131.92	126.25
40	1	501	LUT	C38-C25-C24	-2.41	117.65	123.36
24	9	606	CLA	C4B-CHC-C1C	2.41	131.92	126.25
24	7	601	CLA	CMD-C2D-C3D	-2.41	122.15	127.69
24	B	1234	CLA	C2C-C1C-NC	2.41	112.52	109.98
24	7	611	CLA	CHA-C4D-ND	2.41	137.53	132.55
24	6	603	CLA	CHD-C1D-ND	-2.41	121.41	124.80
24	B	1023	CLA	CHA-C4D-ND	2.41	137.53	132.55
24	A	1105	CLA	CMD-C2D-C3D	-2.41	122.16	127.69
24	6	615	CLA	O2A-CGA-CBA	2.41	119.19	111.83
24	A	1115	CLA	C4B-CHC-C1C	2.41	131.92	126.25
24	4	605	CLA	CMD-C2D-C3D	-2.41	122.16	127.69
24	5	601	CLA	CMA-C3A-C4A	2.41	118.25	111.77
24	G	1602	CLA	C4B-CHC-C1C	2.41	131.92	126.25
24	B	1236	CLA	O2A-CGA-CBA	2.41	119.19	111.83
24	6	607	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
24	B	1230	CLA	C1C-C2C-C3C	-2.41	104.44	106.98
24	B	1230	CLA	CHA-C4D-ND	2.41	137.52	132.55
24	A	1102	CLA	C3B-C4B-NB	-2.41	108.38	110.53
24	5	605	CLA	C3B-C4B-NB	-2.41	108.38	110.53
41	6	613	CHL	C1-O2A-CGA	2.41	122.49	116.65
28	1	801	LHG	C5-O7-C7	-2.41	112.03	117.80
24	L	1501	CLA	C4B-CHC-C1C	2.41	131.91	126.25
24	2	610	CLA	C3B-C4B-NB	-2.41	108.38	110.53
24	F	1302	CLA	C4B-CHC-C1C	2.41	131.91	126.25
24	B	1213	CLA	CHA-C4D-ND	2.41	137.52	132.55
24	1	608	CLA	CHA-C4D-ND	2.41	137.52	132.55
24	2	605	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
24	6	603	CLA	C2C-C1C-NC	2.41	112.51	109.98
24	7	602	CLA	C4B-CHC-C1C	2.41	131.91	126.25
24	B	1206	CLA	CHA-C4D-ND	2.41	137.52	132.55
24	5	616	CLA	C4B-CHC-C1C	2.41	131.91	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	7	612	CLA	CMA-C3A-C4A	2.41	118.24	111.77
24	6	607	CLA	CHA-C4D-ND	2.41	137.52	132.55
24	7	603	CLA	CHA-C4D-ND	2.41	137.52	132.55
24	7	604	CLA	C3B-C4B-NB	-2.41	108.38	110.53
24	2	615	CLA	CMA-C3A-C4A	2.41	118.24	111.77
40	4	502	LUT	C38-C25-C24	-2.41	117.67	123.36
24	B	1218	CLA	C4B-CHC-C1C	2.41	131.91	126.25
24	9	602	CLA	C4B-CHC-C1C	2.41	131.91	126.25
24	6	617	CLA	O2D-CGD-O1D	-2.41	119.17	123.85
24	7	603	CLA	C4B-CHC-C1C	2.41	131.90	126.25
24	A	1118	CLA	CHA-C4D-ND	2.41	137.51	132.55
24	8	620	CLA	CHA-C4D-ND	2.41	137.51	132.55
24	6	606	CLA	CHD-C1D-ND	-2.40	121.42	124.80
24	L	1501	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
24	4	616	CLA	C4B-CHC-C1C	2.40	131.90	126.25
27	B	4004	BCR	C23-C24-C25	-2.40	120.57	127.00
27	L	4001	BCR	C30-C25-C24	2.40	122.17	115.65
24	B	1213	CLA	CMD-C2D-C3D	-2.40	122.17	127.69
24	4	605	CLA	C4B-CHC-C1C	2.40	131.90	126.25
24	6	601	CLA	C4B-CHC-C1C	2.40	131.90	126.25
24	8	603	CLA	C3B-C4B-NB	-2.40	108.38	110.53
24	9	603	CLA	C3B-C4B-NB	-2.40	108.38	110.53
24	9	608	CLA	C3B-C4B-NB	-2.40	108.38	110.53
24	1	606	CLA	CMD-C2D-C3D	-2.40	122.18	127.69
24	A	1139	CLA	C4B-CHC-C1C	2.40	131.90	126.25
24	3	618	CLA	C4B-CHC-C1C	2.40	131.90	126.25
24	A	1122	CLA	CHA-C4D-ND	2.40	137.51	132.55
24	a	603	CLA	CHA-C4D-ND	2.40	137.51	132.55
24	5	614	CLA	CHA-C4D-ND	2.40	137.51	132.55
24	6	608	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
24	A	1108	CLA	CAA-C2A-C3A	-2.40	106.51	113.00
24	7	605	CLA	C4B-CHC-C1C	2.40	131.90	126.25
24	L	1501	CLA	CHA-C4D-ND	2.40	137.51	132.55
40	1	502	LUT	C38-C25-C24	-2.40	117.67	123.36
40	2	502	LUT	C38-C25-C24	-2.40	117.67	123.36
24	1	611	CLA	CHA-C4D-ND	2.40	137.50	132.55
24	A	1130	CLA	C3D-C2D-C1D	-2.40	102.55	105.83
24	3	612	CLA	O2A-CGA-CBA	2.40	119.16	111.83
24	B	1232	CLA	C1C-C2C-C3C	-2.40	104.45	106.98
24	9	606	CLA	CHD-C1D-ND	-2.40	121.42	124.80
24	a	607	CLA	C4B-CHC-C1C	2.40	131.89	126.25
24	F	1301	CLA	C4B-CHC-C1C	2.40	131.89	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1132	CLA	C1C-C2C-C3C	-2.40	104.45	106.98
24	B	1205	CLA	C4B-CHC-C1C	2.40	131.89	126.25
24	5	606	CLA	C4B-CHC-C1C	2.40	131.89	126.25
27	5	503	BCR	C36-C18-C17	-2.40	118.93	122.82
24	2	610	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
24	A	1113	CLA	CHA-C4D-ND	2.40	137.50	132.55
24	B	1238	CLA	CHA-C4D-ND	2.40	137.50	132.55
24	8	609	CLA	CHA-C4D-ND	2.40	137.50	132.55
24	8	608	CLA	CMA-C3A-C4A	2.40	118.22	111.77
24	8	606	CLA	CHD-C1D-ND	-2.40	121.42	124.80
24	B	1228	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
24	a	604	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
24	A	1135	CLA	CHA-C1A-NA	-2.40	120.96	126.39
41	3	608	CHL	C4D-CHA-CBD	-2.40	106.55	108.97
24	9	609	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
24	5	609	CLA	O2A-CGA-CBA	2.40	119.15	111.83
24	B	1213	CLA	C4B-CHC-C1C	2.40	131.89	126.25
24	B	1222	CLA	C3B-C4B-NB	-2.40	108.39	110.53
24	9	607	CLA	O2A-CGA-CBA	2.40	119.15	111.83
24	A	1127	CLA	C1C-C2C-C3C	-2.40	104.46	106.98
24	2	608	CLA	CHD-C1D-ND	-2.40	121.43	124.80
24	L	1501	CLA	O2A-CGA-CBA	2.40	119.15	111.83
24	5	618	CLA	CHA-C4D-ND	2.40	137.50	132.55
40	1	503	LUT	C18-C5-C4	2.40	118.83	114.42
24	a	603	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
27	A	4005	BCR	C33-C5-C6	-2.40	121.87	124.48
24	8	605	CLA	C1D-ND-C4D	-2.40	104.63	106.31
24	7	607	CLA	C3B-C4B-NB	-2.40	108.39	110.53
40	8	502	LUT	C15-C14-C13	-2.40	123.92	127.28
43	a	504	QTB	C03-C04-C05	-2.40	116.26	123.20
24	3	613	CLA	C4B-CHC-C1C	2.40	131.88	126.25
24	A	1125	CLA	CHA-C1A-NA	-2.40	120.97	126.39
24	A	1138	CLA	C4B-CHC-C1C	2.40	131.88	126.25
24	5	604	CLA	CHA-C4D-ND	2.40	137.49	132.55
24	2	606	CLA	CHA-C4D-ND	2.40	137.49	132.55
24	A	1110	CLA	CHA-C4D-ND	2.40	137.49	132.55
24	4	611	CLA	CHA-C4D-ND	2.39	137.49	132.55
24	6	606	CLA	CHA-C4D-ND	2.39	137.49	132.55
24	F	1301	CLA	O2D-CGD-O1D	-2.39	119.19	123.85
24	6	601	CLA	C1D-ND-C4D	-2.39	104.63	106.31
24	B	1227	CLA	CMD-C2D-C3D	-2.39	122.20	127.69
24	8	605	CLA	C4B-CHC-C1C	2.39	131.88	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1140	CLA	CHA-C4D-ND	2.39	137.49	132.55
40	1	502	LUT	C22-C23-C24	-2.39	107.63	111.18
24	A	1128	CLA	O1D-CGD-CBD	-2.39	119.80	124.52
24	4	608	CLA	C1D-ND-C4D	-2.39	104.63	106.31
24	3	613	CLA	C1-C2-C3	-2.39	122.28	126.20
27	8	503	BCR	C30-C25-C24	2.39	122.14	115.65
37	J	4002	RRX	C23-C24-C25	-2.39	120.61	127.00
24	2	604	CLA	C1-O2A-CGA	2.39	122.44	116.65
24	5	605	CLA	O2D-CGD-O1D	-2.39	119.19	123.85
27	A	4004	BCR	C35-C13-C12	2.39	121.74	118.09
24	B	1222	CLA	C1C-C2C-C3C	-2.39	104.47	106.98
24	K	1403	CLA	C3B-C4B-NB	-2.39	108.40	110.53
24	a	611	CLA	C1C-C2C-C3C	-2.39	104.47	106.98
24	A	1013	CLA	C1D-ND-C4D	-2.39	104.64	106.31
24	6	601	CLA	CHD-C1D-ND	-2.39	121.44	124.80
24	5	612	CLA	O2A-CGA-CBA	2.39	119.12	111.83
24	2	605	CLA	CMA-C3A-C4A	2.39	118.19	111.77
24	L	1503	CLA	C4B-CHC-C1C	2.39	131.87	126.25
24	B	1022	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
24	K	1401	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
24	A	1103	CLA	C1D-ND-C4D	-2.39	104.64	106.31
24	A	1105	CLA	CHA-C4D-ND	2.39	137.48	132.55
24	A	1138	CLA	CHA-C4D-ND	2.39	137.48	132.55
24	B	1214	CLA	C1C-C2C-C3C	-2.39	104.47	106.98
24	A	1106	CLA	C3B-C4B-NB	-2.39	108.40	110.53
24	a	601	CLA	O2A-CGA-CBA	2.39	119.12	111.83
24	1	615	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
24	a	605	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
24	B	1240	CLA	CAA-CBA-CGA	-2.39	106.43	113.21
24	B	1224	CLA	CHA-C4D-ND	2.39	137.47	132.55
41	a	606	CHL	C4C-CHD-C1D	2.39	124.61	116.07
24	1	605	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
27	A	4005	BCR	C27-C26-C25	-2.39	119.48	122.70
40	9	502	LUT	C3-C4-C5	-2.39	106.23	112.18
24	A	1136	CLA	CHD-C1D-ND	-2.39	121.44	124.80
24	K	1402	CLA	CHD-C1D-ND	-2.39	121.44	124.80
24	8	611	CLA	CHA-C4D-ND	2.39	137.47	132.55
24	1	603	CLA	C4B-CHC-C1C	2.39	131.86	126.25
24	A	1110	CLA	C4B-CHC-C1C	2.39	131.86	126.25
24	6	608	CLA	C3B-C4B-NB	-2.39	108.40	110.53
24	B	1221	CLA	O2A-CGA-CBA	2.39	119.11	111.83
27	H	4001	BCR	C27-C26-C25	-2.39	119.48	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	6	603	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
24	2	606	CLA	CHD-C1D-ND	-2.39	121.44	124.80
24	a	603	CLA	C4B-CHC-C1C	2.39	131.86	126.25
24	3	602	CLA	C4B-CHC-C1C	2.39	131.86	126.25
24	A	1134	CLA	CHD-C1D-ND	-2.39	121.45	124.80
27	J	4001	BCR	C34-C9-C10	-2.39	118.95	122.82
24	2	615	CLA	C4B-CHC-C1C	2.38	131.85	126.25
24	A	1103	CLA	CHA-C4D-ND	2.38	137.47	132.55
24	a	602	CLA	C4B-CHC-C1C	2.38	131.85	126.25
24	A	1012	CLA	CHA-C1A-NA	-2.38	120.99	126.39
24	5	602	CLA	CMA-C3A-C4A	2.38	118.18	111.77
24	3	613	CLA	CHA-C4D-ND	2.38	137.47	132.55
24	3	610	CLA	CHA-C4D-ND	2.38	137.47	132.55
24	4	610	CLA	CAA-C2A-C3A	-2.38	106.56	113.00
24	3	607	CLA	C3B-C4B-NB	-2.38	108.40	110.53
41	6	611	CHL	CMA-C3A-C4A	2.38	119.74	114.61
24	A	1132	CLA	C4B-CHC-C1C	2.38	131.85	126.25
24	8	608	CLA	C4B-CHC-C1C	2.38	131.85	126.25
24	2	606	CLA	C4B-CHC-C1C	2.38	131.85	126.25
24	8	603	CLA	CHA-C4D-ND	2.38	137.46	132.55
24	6	608	CLA	C4B-CHC-C1C	2.38	131.85	126.25
24	B	1211	CLA	O2A-CGA-CBA	2.38	119.10	111.83
24	B	1218	CLA	C1-O2A-CGA	2.38	122.42	116.65
24	7	609	CLA	CMD-C2D-C3D	-2.38	122.23	127.69
24	a	601	CLA	CHA-C4D-ND	2.38	137.46	132.55
24	4	601	CLA	CHA-C4D-ND	2.38	137.46	132.55
24	B	1220	CLA	CHA-C4D-ND	2.38	137.46	132.55
24	6	606	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
24	B	1023	CLA	CHD-C1D-ND	-2.38	121.45	124.80
24	4	612	CLA	O2A-CGA-CBA	2.38	119.09	111.83
24	A	1012	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
24	A	1112	CLA	CHA-C4D-ND	2.38	137.46	132.55
24	B	1211	CLA	CAA-C2A-C3A	-2.38	106.57	113.00
24	B	1023	CLA	CAC-C3C-C4C	2.38	127.89	124.79
40	4	502	LUT	C22-C23-C24	-2.38	107.65	111.18
24	B	1022	CLA	CHA-C1A-NA	-2.38	121.00	126.39
27	K	4001	BCR	C34-C9-C10	-2.38	118.96	122.82
27	B	4006	BCR	C35-C13-C12	2.38	121.72	118.09
24	5	609	CLA	C3B-C4B-NB	-2.38	108.41	110.53
24	1	601	CLA	CHD-C1D-ND	-2.38	121.46	124.80
24	A	1136	CLA	CHA-C4D-ND	2.38	137.46	132.55
40	1	501	LUT	C22-C23-C24	-2.38	107.65	111.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	615	CLA	C4B-CHC-C1C	2.38	131.84	126.25
24	4	603	CLA	CHA-C4D-ND	2.38	137.45	132.55
24	B	1202	CLA	CHA-C1A-NA	-2.38	121.01	126.39
24	B	1209	CLA	CHA-C4D-ND	2.38	137.45	132.55
24	6	601	CLA	CHA-C4D-ND	2.38	137.45	132.55
24	B	1213	CLA	O1D-CGD-CBD	-2.38	119.83	124.52
24	2	609	CLA	O2A-CGA-CBA	2.38	119.08	111.83
24	7	604	CLA	C2C-C1C-NC	2.38	112.48	109.98
24	G	1603	CLA	C3D-C2D-C1D	-2.38	102.59	105.83
24	5	614	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
24	5	618	CLA	CMA-C3A-C4A	2.38	118.16	111.77
24	A	1117	CLA	CHD-C1D-ND	-2.38	121.46	124.80
24	A	1130	CLA	CHA-C4D-ND	2.38	137.45	132.55
24	a	601	CLA	C2C-C1C-NC	2.38	112.48	109.98
24	8	611	CLA	CHD-C1D-ND	-2.38	121.46	124.80
24	8	618	CLA	C4B-CHC-C1C	2.37	131.83	126.25
24	5	612	CLA	CHA-C4D-ND	2.37	137.45	132.55
24	B	1220	CLA	C4B-CHC-C1C	2.37	131.83	126.25
27	A	4003	BCR	C31-C1-C6	-2.37	106.52	110.24
24	3	612	CLA	CHA-C1A-NA	-2.37	121.02	126.39
24	A	1117	CLA	CHA-C4D-ND	2.37	137.45	132.55
24	9	608	CLA	C4B-CHC-C1C	2.37	131.83	126.25
24	B	1211	CLA	CHD-C1D-ND	-2.37	121.46	124.80
24	B	1238	CLA	C4B-CHC-C1C	2.37	131.83	126.25
24	3	616	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
24	A	1110	CLA	CHD-C1D-ND	-2.37	121.46	124.80
24	2	621	CLA	C4B-CHC-C1C	2.37	131.83	126.25
24	A	1112	CLA	O2A-CGA-CBA	2.37	119.07	111.83
24	8	610	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
25	B	2002	PQN	C2M-C2-C3	-2.37	120.55	124.45
24	6	607	CLA	C3B-C4B-NB	-2.37	108.41	110.53
24	8	607	CLA	C3B-C4B-NB	-2.37	108.41	110.53
24	B	1211	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
28	6	802	LHG	C5-O7-C7	-2.37	112.12	117.80
24	6	603	CLA	CHA-C4D-ND	2.37	137.44	132.55
24	3	604	CLA	CAA-C2A-C3A	-2.37	106.59	113.00
24	3	606	CLA	CMD-C2D-C3D	-2.37	122.25	127.69
24	4	611	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
24	B	1213	CLA	C3B-C4B-NB	-2.37	108.41	110.53
24	B	1221	CLA	C3B-C4B-NB	-2.37	108.41	110.53
24	A	1120	CLA	CHA-C4D-ND	2.37	137.44	132.55
24	7	609	CLA	CMA-C3A-C4A	2.37	118.14	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1	608	CLA	O2A-CGA-CBA	2.37	119.06	111.83
24	9	604	CLA	CMD-C2D-C3D	-2.37	122.25	127.69
24	A	1134	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
24	B	1239	CLA	C4B-CHC-C1C	2.37	131.82	126.25
24	A	1121	CLA	C1D-ND-C4D	-2.37	104.65	106.31
24	L	1501	CLA	CHD-C1D-ND	-2.37	121.47	124.80
27	B	4002	BCR	C38-C26-C27	2.37	118.64	113.60
24	7	603	CLA	CHD-C1D-ND	-2.37	121.47	124.80
40	4	501	LUT	C20-C13-C12	2.37	121.70	118.09
24	5	617	CLA	CHA-C4D-ND	2.37	137.43	132.55
24	9	608	CLA	CHA-C4D-ND	2.37	137.43	132.55
37	J	4002	RRX	C33-C5-C4	2.37	118.64	113.60
24	B	1212	CLA	C4B-CHC-C1C	2.37	131.81	126.25
24	a	607	CLA	CHD-C1D-ND	-2.37	121.47	124.80
40	9	501	LUT	C20-C13-C12	2.37	121.70	118.09
27	7	503	BCR	C38-C26-C25	-2.37	121.90	124.48
24	A	1126	CLA	C1C-C2C-C3C	-2.37	104.49	106.98
24	8	603	CLA	C4B-CHC-C1C	2.37	131.81	126.25
24	B	1235	CLA	CHA-C4D-ND	2.36	137.43	132.55
24	a	604	CLA	C3B-C4B-NB	-2.36	108.42	110.53
24	B	1236	CLA	CHA-C4D-ND	2.36	137.43	132.55
24	7	604	CLA	CHD-C1D-ND	-2.36	121.48	124.80
24	3	613	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
24	A	1137	CLA	O1D-CGD-CBD	-2.36	119.86	124.52
24	6	606	CLA	CMD-C2D-C3D	-2.36	122.27	127.69
24	B	1224	CLA	C4B-CHC-C1C	2.36	131.80	126.25
24	9	606	CLA	CMA-C3A-C4A	2.36	118.12	111.77
41	1	609	CHL	C1A-CHA-C4D	2.36	122.92	118.98
24	7	605	CLA	OBD-CAD-C3D	-2.36	122.89	128.42
24	3	613	CLA	O1D-CGD-CBD	-2.36	119.86	124.52
24	B	1234	CLA	CMA-C3A-C4A	2.36	118.12	111.77
24	4	617	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
24	A	1118	CLA	C1D-ND-C4D	-2.36	104.66	106.31
24	7	605	CLA	CMD-C2D-C3D	-2.36	122.28	127.69
27	K	4002	BCR	C38-C26-C25	-2.36	121.91	124.48
24	1	602	CLA	CAA-C2A-C3A	-2.36	106.62	113.00
27	3	505	BCR	C15-C14-C13	-2.36	123.97	127.28
24	A	1107	CLA	C4B-CHC-C1C	2.36	131.80	126.25
24	A	1132	CLA	O1D-CGD-CBD	-2.36	119.86	124.52
24	L	1502	CLA	CHA-C4D-ND	2.36	137.42	132.55
24	1	606	CLA	O2A-CGA-CBA	2.36	119.03	111.83
24	A	1125	CLA	C3D-C2D-C1D	-2.36	102.61	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	7	601	CLA	CHD-C1D-ND	-2.36	121.48	124.80
24	7	609	CLA	CHD-C1D-ND	-2.36	121.48	124.80
24	a	615	CLA	C1D-ND-C4D	-2.36	104.66	106.31
24	a	612	CLA	C4B-CHC-C1C	2.36	131.79	126.25
24	B	1214	CLA	CMD-C2D-C3D	-2.36	122.28	127.69
24	A	1115	CLA	CHD-C1D-ND	-2.36	121.48	124.80
27	B	4002	BCR	C33-C5-C6	-2.36	121.91	124.48
24	H	1701	CLA	C3B-C4B-NB	-2.36	108.42	110.53
24	8	612	CLA	C4B-CHC-C1C	2.36	131.79	126.25
24	6	604	CLA	CHD-C1D-ND	-2.36	121.48	124.80
24	6	612	CLA	CHD-C1D-ND	-2.36	121.48	124.80
24	A	1131	CLA	CMD-C2D-C3D	-2.36	122.28	127.69
24	2	603	CLA	CMD-C2D-C3D	-2.36	122.28	127.69
24	B	1237	CLA	CHA-C4D-ND	2.36	137.41	132.55
24	9	601	CLA	CHA-C4D-ND	2.36	137.41	132.55
24	B	1208	CLA	O1D-CGD-CBD	-2.36	119.87	124.52
43	a	504	QTB	C11-C10-C09	2.36	130.29	125.25
24	A	1131	CLA	C3B-C4B-NB	-2.36	108.43	110.53
24	6	601	CLA	C2C-C1C-NC	2.36	112.46	109.98
24	8	606	CLA	C4B-CHC-C1C	2.36	131.79	126.25
41	1	609	CHL	C4C-CHD-C1D	2.36	124.50	116.07
24	K	1404	CLA	O2A-CGA-CBA	2.36	119.02	111.83
24	1	603	CLA	CHA-C4D-ND	2.36	137.41	132.55
24	5	603	CLA	O2D-CGD-O1D	-2.36	119.26	123.85
24	7	604	CLA	C1C-C2C-C3C	-2.36	104.50	106.98
24	8	618	CLA	CMD-C2D-C3D	-2.36	122.29	127.69
24	B	1021	CLA	C1D-ND-C4D	-2.36	104.66	106.31
24	7	601	CLA	C1D-ND-C4D	-2.36	104.66	106.31
28	B	5002	LHG	C5-O7-C7	-2.36	112.16	117.80
24	8	610	CLA	CHA-C1A-NA	-2.36	121.06	126.39
41	6	619	CHL	C4C-CHD-C1D	2.36	124.50	116.07
24	3	604	CLA	C2D-C1D-ND	2.36	112.46	110.13
24	6	615	CLA	C2D-C1D-ND	2.36	112.46	110.13
24	5	603	CLA	C4B-CHC-C1C	2.36	131.78	126.25
24	A	1116	CLA	CMD-C2D-C3D	-2.35	122.29	127.69
24	A	1108	CLA	CHD-C1D-ND	-2.35	121.49	124.80
24	6	606	CLA	C4B-CHC-C1C	2.35	131.78	126.25
24	1	604	CLA	C1-O2A-CGA	2.35	122.35	116.65
27	7	503	BCR	C3-C4-C5	-2.35	109.86	114.06
24	A	1102	CLA	C4B-CHC-C1C	2.35	131.78	126.25
24	7	606	CLA	C3B-C4B-NB	-2.35	108.43	110.53
24	3	616	CLA	CHA-C4D-ND	2.35	137.40	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1120	CLA	CAA-C2A-C3A	-2.35	106.65	113.00
24	B	1229	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
24	8	612	CLA	CMD-C2D-C3D	-2.35	122.30	127.69
24	3	601	CLA	CHA-C4D-ND	2.35	137.40	132.55
40	5	502	LUT	C19-C9-C8	2.35	121.68	118.09
39	M	4001	ECH	C20-C19-C18	-2.35	119.92	126.36
24	6	602	CLA	C4B-CHC-C1C	2.35	131.77	126.25
24	7	603	CLA	CMD-C2D-C3D	-2.35	122.30	127.69
24	A	1122	CLA	C4B-CHC-C1C	2.35	131.77	126.25
24	4	610	CLA	CMC-C2C-C3C	2.35	132.50	126.15
24	B	1237	CLA	C3B-C4B-NB	-2.35	108.43	110.53
24	G	1601	CLA	O2D-CGD-O1D	-2.35	119.28	123.85
41	8	604	CHL	C4D-CHA-CBD	-2.35	106.60	108.97
24	4	611	CLA	CHD-C1D-ND	-2.35	121.50	124.80
24	5	601	CLA	CHD-C1D-ND	-2.35	121.50	124.80
24	B	1022	CLA	CMA-C3A-C4A	2.35	118.08	111.77
24	6	609	CLA	O2A-CGA-CBA	2.35	118.99	111.83
27	6	503	BCR	C38-C26-C25	-2.35	121.92	124.48
24	A	1101	CLA	CMD-C2D-C3D	-2.35	122.31	127.69
24	B	1230	CLA	C3B-C4B-NB	-2.35	108.44	110.53
24	G	1601	CLA	C4B-CHC-C1C	2.35	131.76	126.25
23	A	1011	CL0	CMB-C2B-C3B	2.35	129.37	124.68
24	A	1129	CLA	CHD-C1D-ND	-2.35	121.50	124.80
24	B	1222	CLA	CMD-C2D-C3D	-2.35	122.31	127.69
24	G	1603	CLA	O2D-CGD-O1D	-2.35	119.28	123.85
24	a	615	CLA	O2D-CGD-O1D	-2.35	119.28	123.85
40	2	502	LUT	C15-C35-C34	-2.35	118.72	123.52
24	B	1212	CLA	O1D-CGD-CBD	-2.35	119.89	124.52
24	1	608	CLA	C4B-CHC-C1C	2.35	131.76	126.25
23	A	1011	CL0	C1-C2-C3	-2.34	122.36	126.20
24	3	603	CLA	CHA-C4D-ND	2.34	137.39	132.55
24	B	1218	CLA	CMD-C2D-C3D	-2.34	122.31	127.69
24	9	608	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
24	A	1125	CLA	C1C-C2C-C3C	-2.34	104.52	106.98
24	2	608	CLA	C3B-C4B-NB	-2.34	108.44	110.53
24	4	616	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
24	A	1119	CLA	C1-C2-C3	-2.34	122.36	126.20
24	A	1113	CLA	C4B-CHC-C1C	2.34	131.76	126.25
24	5	612	CLA	C4B-CHC-C1C	2.34	131.76	126.25
24	B	1238	CLA	C1D-ND-C4D	-2.34	104.67	106.31
24	8	603	CLA	C1D-ND-C4D	-2.34	104.67	106.31
24	7	605	CLA	C3B-C4B-NB	-2.34	108.44	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	1224	CLA	CMA-C3A-C4A	2.34	118.07	111.77
24	H	1703	CLA	CHD-C1D-ND	-2.34	121.51	124.80
24	4	601	CLA	CHD-C1D-ND	-2.34	121.51	124.80
24	4	603	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
24	5	617	CLA	C4B-CHC-C1C	2.34	131.75	126.25
24	3	604	CLA	C2C-C1C-NC	2.34	112.44	109.98
24	L	1503	CLA	CHD-C1D-ND	-2.34	121.51	124.80
24	8	603	CLA	CHD-C1D-ND	-2.34	121.51	124.80
40	3	502	LUT	C38-C25-C24	-2.34	117.82	123.36
24	7	610	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
24	6	615	CLA	C3B-C4B-NB	-2.34	108.44	110.53
27	B	4002	BCR	C30-C25-C26	-2.34	119.44	122.64
24	9	604	CLA	C1-O2A-CGA	2.34	122.31	116.65
24	5	609	CLA	C4B-CHC-C1C	2.34	131.75	126.25
24	B	1216	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
41	8	613	CHL	CMA-C3A-C4A	2.34	119.65	114.61
24	H	1701	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
24	a	602	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
24	1	603	CLA	C3B-C4B-NB	-2.34	108.44	110.53
27	A	4004	BCR	C38-C26-C27	2.34	118.58	113.60
24	7	607	CLA	C4B-CHC-C1C	2.34	131.75	126.25
24	8	608	CLA	CMD-C2D-C3D	-2.34	122.33	127.69
24	7	607	CLA	O2A-CGA-CBA	2.34	118.96	111.83
24	B	1021	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
24	B	1023	CLA	C1-C2-C3	-2.34	122.37	126.20
40	a	503	LUT	C20-C13-C14	-2.34	119.03	122.82
24	K	1402	CLA	CMD-C2D-C3D	-2.34	122.33	127.69
27	3	504	BCR	C23-C24-C25	-2.34	120.75	127.00
24	5	616	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
24	A	1118	CLA	O2A-CGA-CBA	2.34	118.96	111.83
24	B	1235	CLA	C4B-CHC-C1C	2.34	131.74	126.25
24	8	618	CLA	O2A-CGA-CBA	2.34	118.96	111.83
24	4	617	CLA	CMD-C2D-C3D	-2.34	122.33	127.69
24	8	606	CLA	CMD-C2D-C3D	-2.34	122.33	127.69
24	A	1106	CLA	O1D-CGD-CBD	-2.34	119.91	124.52
24	9	609	CLA	CMA-C3A-C4A	2.34	118.05	111.77
41	3	608	CHL	CMA-C3A-C4A	2.34	119.64	114.61
24	a	604	CLA	C1C-C2C-C3C	-2.34	104.52	106.98
24	8	620	CLA	O2A-CGA-CBA	2.33	118.95	111.83
43	3	506	QTB	C13-C12-C14	2.33	115.42	111.06
24	5	617	CLA	C2D-C1D-ND	2.33	112.44	110.13
24	A	1120	CLA	CHD-C1D-ND	-2.33	121.52	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	1222	CLA	CHA-C4D-ND	2.33	137.36	132.55
24	7	612	CLA	CHD-C1D-ND	-2.33	121.52	124.80
27	A	4002	BCR	C36-C18-C17	-2.33	119.04	122.82
24	B	1228	CLA	C4B-CHC-C1C	2.33	131.73	126.25
40	5	502	LUT	C8-C7-C6	-2.33	120.77	127.00
24	A	1012	CLA	CHD-C1D-ND	-2.33	121.52	124.80
24	1	608	CLA	CHD-C1D-ND	-2.33	121.52	124.80
37	J	4002	RRX	C8-C7-C6	-2.33	120.77	127.00
24	7	609	CLA	CAA-C2A-C3A	-2.33	106.70	113.00
40	5	501	LUT	C30-C31-C32	-2.33	116.44	123.20
24	4	610	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
24	6	618	CLA	CHD-C1D-ND	-2.33	121.52	124.80
24	9	607	CLA	C4B-CHC-C1C	2.33	131.73	126.25
24	A	1102	CLA	CHA-C1A-NA	-2.33	121.11	126.39
24	8	607	CLA	C4B-CHC-C1C	2.33	131.73	126.25
24	A	1101	CLA	O2A-CGA-CBA	2.33	118.94	111.83
24	6	605	CLA	C3B-C4B-NB	-2.33	108.45	110.53
24	B	1227	CLA	C4B-CHC-C1C	2.33	131.73	126.25
24	B	1218	CLA	CHA-C4D-ND	2.33	137.36	132.55
24	7	615	CLA	C4B-CHC-C1C	2.33	131.73	126.25
24	a	611	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
24	2	613	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
24	B	1221	CLA	CHA-C1A-NA	-2.33	121.11	126.39
37	J	4002	RRX	C38-C26-C27	2.33	118.71	114.42
24	A	1109	CLA	C1D-ND-C4D	-2.33	104.68	106.31
24	1	605	CLA	C4B-CHC-C1C	2.33	131.73	126.25
24	4	606	CLA	CMD-C2D-C3D	-2.33	122.35	127.69
40	3	501	LUT	C39-C29-C28	2.33	121.65	118.09
24	a	615	CLA	C2C-C1C-NC	2.33	112.43	109.98
27	L	4002	BCR	C36-C18-C17	-2.33	119.04	122.82
24	4	616	CLA	CHA-C1A-NA	-2.33	121.12	126.39
24	1	610	CLA	C4B-CHC-C1C	2.33	131.72	126.25
24	A	1132	CLA	CMD-C2D-C3D	-2.33	122.35	127.69
24	B	1235	CLA	CHD-C1D-ND	-2.33	121.53	124.80
24	A	1111	CLA	C1C-C2C-C3C	-2.33	104.53	106.98
24	1	611	CLA	CAA-C2A-C3A	-2.33	106.71	113.00
24	8	615	CLA	O2D-CGD-O1D	-2.33	119.32	123.85
24	2	609	CLA	C4B-CHC-C1C	2.33	131.72	126.25
24	2	601	CLA	CHD-C1D-ND	-2.33	121.53	124.80
40	7	501	LUT	C31-C30-C29	-2.33	124.01	127.28
24	2	608	CLA	C4B-CHC-C1C	2.33	131.72	126.25
24	B	1236	CLA	C1D-ND-C4D	-2.33	104.68	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	3	610	CLA	C4B-CHC-C1C	2.33	131.72	126.25
24	5	605	CLA	CMD-C2D-C3D	-2.33	122.35	127.69
24	7	611	CLA	CHD-C1D-ND	-2.33	121.53	124.80
24	2	604	CLA	CHD-C1D-ND	-2.33	121.53	124.80
24	8	620	CLA	C4B-CHC-C1C	2.33	131.72	126.25
24	6	617	CLA	CMD-C2D-C3D	-2.33	122.36	127.69
24	5	606	CLA	CHD-C1D-ND	-2.33	121.53	124.80
24	4	612	CLA	C2D-C1D-ND	2.32	112.43	110.13
24	B	1237	CLA	O2D-CGD-O1D	-2.32	119.32	123.85
24	8	620	CLA	O2D-CGD-O1D	-2.32	119.32	123.85
24	B	1219	CLA	CHA-C1A-NA	-2.32	121.13	126.39
24	B	1220	CLA	CAA-CBA-CGA	-2.32	106.61	113.21
24	2	610	CLA	C4B-CHC-C1C	2.32	131.71	126.25
27	A	4003	BCR	C38-C26-C27	2.32	118.55	113.60
24	2	605	CLA	CMD-C2D-C3D	-2.32	122.36	127.69
24	A	1119	CLA	CHD-C1D-ND	-2.32	121.53	124.80
27	B	4004	BCR	C33-C5-C4	2.32	118.55	113.60
24	1	605	CLA	C1-C2-C3	-2.32	122.39	126.20
24	1	611	CLA	O2A-CGA-CBA	2.32	118.92	111.83
24	A	1012	CLA	C4B-CHC-C1C	2.32	131.71	126.25
24	B	1231	CLA	C3B-C4B-NB	-2.32	108.46	110.53
24	9	605	CLA	O2A-CGA-CBA	2.32	118.92	111.83
24	G	1601	CLA	CHA-C1A-NA	-2.32	121.13	126.39
24	A	1112	CLA	CHD-C1D-ND	-2.32	121.53	124.80
28	9	801	LHG	C5-O7-C7	-2.32	112.24	117.80
24	A	1108	CLA	C2C-C1C-NC	2.32	112.42	109.98
24	B	1202	CLA	C3B-C4B-NB	-2.32	108.46	110.53
27	3	504	BCR	C30-C25-C26	-2.32	119.46	122.64
24	9	601	CLA	CMC-C2C-C1C	2.32	128.66	125.03
24	a	611	CLA	O2A-CGA-CBA	2.32	118.91	111.83
24	1	611	CLA	CMD-C2D-C3D	-2.32	122.37	127.69
24	A	1104	CLA	CHD-C1D-ND	-2.32	121.54	124.80
24	1	605	CLA	CBC-CAC-C3C	-2.32	106.13	112.42
24	7	612	CLA	C4B-CHC-C1C	2.32	131.70	126.25
24	8	611	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
24	2	621	CLA	CMD-C2D-C3D	-2.32	122.37	127.69
24	2	604	CLA	C4B-CHC-C1C	2.32	131.70	126.25
24	B	1239	CLA	CHD-C1D-ND	-2.32	121.54	124.80
27	H	4001	BCR	C37-C22-C21	-2.32	119.06	122.82
27	L	4002	BCR	C34-C9-C10	-2.32	119.06	122.82
24	K	1404	CLA	CHD-C1D-ND	-2.32	121.54	124.80
24	B	1023	CLA	C2A-C1A-CHA	2.32	127.89	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	6	607	CLA	C4B-CHC-C1C	2.32	131.70	126.25
24	B	1022	CLA	OBD-CAD-C3D	-2.32	123.00	128.42
24	a	612	CLA	CHD-C1D-ND	-2.32	121.54	124.80
24	a	611	CLA	C2C-C1C-NC	2.32	112.42	109.98
40	1	501	LUT	C10-C11-C12	-2.32	116.49	123.20
24	9	603	CLA	CMC-C2C-C1C	2.32	128.65	125.03
24	6	601	CLA	O1D-CGD-CBD	-2.32	119.95	124.52
24	B	1210	CLA	CAA-C2A-C3A	-2.32	106.74	113.00
24	A	1129	CLA	O1D-CGD-CBD	-2.32	119.95	124.52
24	9	605	CLA	C3B-C4B-NB	-2.32	108.46	110.53
24	6	605	CLA	CMD-C2D-C3D	-2.32	122.38	127.69
24	B	1223	CLA	CHA-C1A-NA	-2.32	121.15	126.39
28	4	801	LHG	C5-O7-C7	-2.32	112.25	117.80
24	L	1502	CLA	CMD-C2D-C3D	-2.32	122.38	127.69
24	1	611	CLA	CHD-C1D-ND	-2.31	121.55	124.80
24	8	618	CLA	CHD-C1D-ND	-2.31	121.55	124.80
24	3	601	CLA	O1D-CGD-CBD	-2.31	119.95	124.52
41	6	613	CHL	CMA-C3A-C4A	2.31	119.60	114.61
24	A	1111	CLA	CAA-C2A-C3A	-2.31	106.75	113.00
24	B	1213	CLA	O2A-CGA-CBA	2.31	118.89	111.83
24	5	603	CLA	C1D-ND-C4D	-2.31	104.69	106.31
24	7	604	CLA	C1D-ND-C4D	-2.31	104.69	106.31
28	B	5001	LHG	C5-O7-C7	-2.31	112.26	117.80
27	J	4001	BCR	C33-C5-C4	2.31	118.53	113.60
40	4	501	LUT	C31-C32-C33	-2.31	120.02	126.36
27	F	4001	BCR	C32-C1-C6	-2.31	106.62	110.24
24	A	1131	CLA	CHD-C1D-ND	-2.31	121.55	124.80
24	B	1240	CLA	C3B-C4B-NB	-2.31	108.47	110.53
24	5	608	CLA	C3B-C4B-NB	-2.31	108.47	110.53
24	B	1224	CLA	CHA-C1A-NA	-2.31	121.16	126.39
24	B	1023	CLA	C2D-C1D-ND	2.31	112.41	110.13
24	A	1119	CLA	C1C-C2C-C3C	-2.31	104.55	106.98
24	4	612	CLA	C1C-C2C-C3C	-2.31	104.55	106.98
27	L	4002	BCR	C12-C13-C14	-2.31	115.38	119.01
24	3	607	CLA	C4B-CHC-C1C	2.31	131.68	126.25
24	4	607	CLA	C4B-CHC-C1C	2.31	131.68	126.25
24	5	608	CLA	CMA-C3A-C4A	2.31	117.98	111.77
24	2	608	CLA	CMA-C3A-C4A	2.31	117.98	111.77
24	5	618	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
24	B	1227	CLA	C3B-C4B-NB	-2.31	108.47	110.53
40	6	502	LUT	C27-C28-C29	-2.31	121.36	126.32
24	4	603	CLA	CMD-C2D-C3D	-2.31	122.39	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	1215	CLA	O2A-CGA-CBA	2.31	118.87	111.83
27	A	4005	BCR	C19-C18-C17	-2.31	115.38	119.01
24	4	610	CLA	CHD-C1D-ND	-2.31	121.56	124.80
24	B	1239	CLA	C3B-C4B-NB	-2.31	108.47	110.53
24	H	1702	CLA	C4B-CHC-C1C	2.31	131.67	126.25
24	4	605	CLA	CHA-C1A-NA	-2.31	121.17	126.39
24	B	1022	CLA	C1-O2A-CGA	2.31	122.23	116.65
24	B	1235	CLA	C2C-C1C-NC	2.31	112.41	109.98
24	B	1238	CLA	CHD-C1D-ND	-2.31	121.56	124.80
24	3	616	CLA	CHD-C1D-ND	-2.31	121.56	124.80
40	9	502	LUT	C38-C25-C24	-2.31	117.90	123.36
24	A	1103	CLA	C2D-C1D-ND	2.31	112.41	110.13
24	9	603	CLA	CHA-C1A-NA	-2.31	121.17	126.39
24	7	605	CLA	O2D-CGD-O1D	-2.31	118.85	124.08
24	3	601	CLA	CHD-C1D-ND	-2.30	121.56	124.80
24	6	605	CLA	C3D-C2D-C1D	-2.30	102.69	105.83
23	A	1011	CL0	C4C-CHD-C1D	2.30	124.31	116.07
24	9	605	CLA	C4B-CHC-C1C	2.30	131.67	126.25
24	7	615	CLA	C3B-C4B-NB	-2.30	108.47	110.53
40	5	505	LUT	C27-C28-C29	-2.30	121.37	126.32
24	7	617	CLA	O2A-CGA-CBA	2.30	118.86	111.83
24	A	1116	CLA	C1D-ND-C4D	-2.30	104.70	106.31
24	G	1601	CLA	C3B-C4B-NB	-2.30	108.47	110.53
40	1	503	LUT	C35-C15-C14	-2.30	118.81	123.52
41	7	613	CHL	C4C-CHD-C1D	2.30	124.31	116.07
24	B	1238	CLA	O2A-CGA-CBA	2.30	118.86	111.83
24	9	601	CLA	O2A-CGA-CBA	2.30	118.86	111.83
24	7	611	CLA	O2A-CGA-CBA	2.30	118.86	111.83
24	A	1122	CLA	CHD-C1D-ND	-2.30	121.56	124.80
24	3	604	CLA	CHA-C4D-ND	2.30	137.30	132.55
41	5	613	CHL	CMA-C3A-C4A	2.30	119.57	114.61
24	8	620	CLA	C2D-C1D-ND	2.30	112.40	110.13
24	A	1126	CLA	CMD-C2D-C3D	-2.30	122.41	127.69
24	A	1138	CLA	CHD-C1D-ND	-2.30	121.57	124.80
24	2	602	CLA	CHD-C1D-ND	-2.30	121.57	124.80
27	3	504	BCR	C15-C14-C13	-2.30	124.05	127.28
24	A	1141	CLA	C4B-CHC-C1C	2.30	131.65	126.25
24	4	606	CLA	CAA-C2A-C3A	-2.30	106.79	113.00
24	8	603	CLA	O2D-CGD-O1D	-2.30	119.37	123.85
24	1	601	CLA	C1C-C2C-C3C	-2.30	104.56	106.98
24	A	1106	CLA	C1-O2A-CGA	2.30	122.22	116.65
24	B	1229	CLA	CMD-C2D-C3D	-2.30	122.42	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1	615	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
24	4	606	CLA	CHD-C1D-ND	-2.30	121.57	124.80
24	1	601	CLA	C2C-C1C-NC	2.30	112.40	109.98
24	B	1210	CLA	CHA-C1A-NA	-2.30	121.19	126.39
24	2	609	CLA	CHA-C1A-NA	-2.30	121.19	126.39
24	7	611	CLA	C4B-CHC-C1C	2.30	131.65	126.25
24	K	1404	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
40	a	501	LUT	C31-C32-C33	-2.30	120.06	126.36
24	1	615	CLA	C4B-CHC-C1C	2.30	131.65	126.25
24	A	1106	CLA	C1D-ND-C4D	-2.30	104.70	106.31
40	a	502	LUT	C10-C11-C12	-2.30	116.54	123.20
24	2	615	CLA	CHA-C4D-ND	2.30	137.29	132.55
24	5	608	CLA	C4B-CHC-C1C	2.30	131.65	126.25
24	4	616	CLA	CHD-C1D-ND	-2.30	121.57	124.80
24	8	605	CLA	O2D-CGD-O1D	-2.30	119.38	123.85
41	a	609	CHL	C4C-CHD-C1D	2.30	124.29	116.07
40	a	502	LUT	C38-C25-C24	-2.30	117.92	123.36
24	9	606	CLA	C3B-C4B-NB	-2.30	108.48	110.53
24	A	1123	CLA	C4B-CHC-C1C	2.30	131.65	126.25
24	B	1216	CLA	C4B-CHC-C1C	2.30	131.65	126.25
24	A	1129	CLA	CHA-C1A-NA	-2.30	121.19	126.39
40	a	502	LUT	C31-C32-C33	-2.30	120.07	126.36
24	a	601	CLA	C1D-ND-C4D	-2.30	104.70	106.31
24	3	605	CLA	CMA-C3A-C4A	2.30	117.94	111.77
24	2	612	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
24	3	606	CLA	CHD-C1D-ND	-2.30	121.57	124.80
24	4	610	CLA	CHA-C1A-NA	-2.30	121.19	126.39
24	B	1227	CLA	CHD-C1D-ND	-2.29	121.57	124.80
24	B	1229	CLA	O1D-CGD-CBD	-2.29	119.99	124.52
24	B	1222	CLA	C2C-C1C-NC	2.29	112.39	109.98
24	8	611	CLA	O2A-CGA-CBA	2.29	118.83	111.83
24	4	612	CLA	CMA-C3A-C4A	2.29	117.94	111.77
24	B	1207	CLA	CAA-C2A-C3A	-2.29	106.80	113.00
24	9	609	CLA	C4B-CHC-C1C	2.29	131.64	126.25
24	7	601	CLA	OBD-CAD-C3D	-2.29	123.06	128.42
24	K	1403	CLA	CHD-C1D-ND	-2.29	121.58	124.80
24	6	603	CLA	C2D-C1D-ND	2.29	112.39	110.13
24	B	1201	CLA	C1-O2A-CGA	2.29	122.20	116.65
24	B	1023	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
40	9	502	LUT	C10-C11-C12	-2.29	116.56	123.20
24	A	1108	CLA	O1D-CGD-CBD	-2.29	120.00	124.52
24	A	1137	CLA	C1-O2A-CGA	2.29	122.19	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	1202	CLA	O1D-CGD-CBD	-2.29	120.00	124.52
41	a	606	CHL	C1-C2-C3	-2.29	122.45	126.20
41	8	604	CHL	C4C-CHD-C1D	2.29	124.26	116.07
24	A	1132	CLA	C1-C2-C3	-2.29	122.45	126.20
24	A	1013	CLA	CHA-C4D-ND	2.29	137.27	132.55
27	A	4005	BCR	C34-C9-C10	-2.29	119.11	122.82
24	6	609	CLA	O1D-CGD-CBD	-2.29	120.00	124.52
24	8	615	CLA	CHD-C1D-ND	-2.29	121.58	124.80
24	5	603	CLA	C3B-C4B-NB	-2.29	108.49	110.53
24	9	602	CLA	C3B-C4B-NB	-2.29	108.49	110.53
41	5	613	CHL	C4C-CHD-C1D	2.29	124.25	116.07
24	7	611	CLA	O2D-CGD-O1D	-2.29	119.40	123.85
24	7	615	CLA	O2D-CGD-O1D	-2.29	119.40	123.85
24	9	605	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
24	3	610	CLA	O1D-CGD-CBD	-2.29	120.01	124.52
24	4	603	CLA	C2D-C1D-ND	2.29	112.39	110.13
24	3	605	CLA	CMD-C2D-C3D	-2.29	122.45	127.69
24	9	608	CLA	CHA-C1A-NA	-2.29	121.22	126.39
24	6	615	CLA	C4B-CHC-C1C	2.29	131.62	126.25
24	A	1121	CLA	CAA-C2A-C3A	-2.29	106.82	113.00
24	A	1131	CLA	C4B-CHC-C1C	2.29	131.62	126.25
24	J	1901	CLA	CHD-C1D-ND	-2.28	121.59	124.80
27	L	4002	BCR	C19-C18-C17	2.28	122.60	119.01
40	7	501	LUT	C20-C13-C12	2.28	121.58	118.09
24	B	1229	CLA	C2D-C1D-ND	2.28	112.39	110.13
24	B	1214	CLA	CHD-C1D-ND	-2.28	121.59	124.80
40	6	501	LUT	C30-C31-C32	2.28	129.82	123.20
35	G	5001	SQD	O3-C3-C2	-2.28	104.99	110.38
24	2	613	CLA	C4B-CHC-C1C	2.28	131.62	126.25
24	A	1124	CLA	C2D-C1D-ND	2.28	112.39	110.13
24	B	1232	CLA	CMD-C2D-C3D	-2.28	122.45	127.69
24	L	1501	CLA	CMD-C2D-C3D	-2.28	122.45	127.69
24	6	604	CLA	CMD-C2D-C3D	-2.28	122.45	127.69
24	B	1230	CLA	C4B-CHC-C1C	2.28	131.62	126.25
24	A	1012	CLA	C1C-C2C-C3C	-2.28	104.58	106.98
24	5	614	CLA	CHD-C1D-ND	-2.28	121.59	124.80
24	L	1502	CLA	C4B-CHC-C1C	2.28	131.62	126.25
24	A	1133	CLA	O2A-CGA-CBA	2.28	118.80	111.83
24	4	604	CLA	O1D-CGD-CBD	-2.28	120.02	124.52
24	3	605	CLA	CHA-C1A-NA	-2.28	121.22	126.39
40	3	502	LUT	C22-C23-C24	-2.28	107.80	111.18
24	7	602	CLA	C1D-ND-C4D	-2.28	104.71	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	G	1603	CLA	CHD-C1D-ND	-2.28	121.59	124.80
24	B	1240	CLA	CHA-C1A-NA	-2.28	121.22	126.39
24	6	609	CLA	C4B-CHC-C1C	2.28	131.61	126.25
24	1	615	CLA	C3B-C4B-NB	-2.28	108.49	110.53
24	8	620	CLA	CHD-C1D-ND	-2.28	121.59	124.80
24	1	605	CLA	CHA-C1A-NA	-2.28	121.23	126.39
41	4	613	CHL	C1-C2-C3	-2.28	122.46	126.20
24	2	601	CLA	CMD-C2D-C3D	-2.28	122.46	127.69
24	A	1139	CLA	CHD-C1D-ND	-2.28	121.59	124.80
40	8	501	LUT	C38-C25-C24	-2.28	117.97	123.36
24	4	606	CLA	C3B-C4B-NB	-2.28	108.50	110.53
24	3	603	CLA	CAA-C2A-C3A	-2.28	106.84	113.00
24	7	615	CLA	CHA-C1A-NA	-2.28	121.23	126.39
24	A	1121	CLA	C4B-CHC-C1C	2.28	131.61	126.25
24	A	1013	CLA	C1-O2A-CGA	2.28	122.17	116.65
27	A	4001	BCR	C31-C1-C6	-2.28	106.67	110.24
24	B	1234	CLA	O2D-CGD-O1D	-2.28	119.41	123.85
24	B	1216	CLA	CMD-C2D-C3D	-2.28	122.47	127.69
35	7	805	SQD	O3-C3-C2	-2.28	105.01	110.38
41	4	618	CHL	C4C-CHD-C1D	2.28	124.21	116.07
24	A	1126	CLA	C4B-CHC-C1C	2.27	131.60	126.25
24	7	615	CLA	CMA-C3A-C4A	2.27	117.89	111.77
24	7	604	CLA	O1D-CGD-CBD	-2.27	120.03	124.52
24	B	1203	CLA	CHD-C1D-ND	-2.27	121.60	124.80
24	B	1209	CLA	CHD-C1D-ND	-2.27	121.60	124.80
24	5	601	CLA	O1D-CGD-CBD	-2.27	120.03	124.52
24	6	601	CLA	C2D-C1D-ND	2.27	112.38	110.13
24	a	608	CLA	CHA-C1A-NA	-2.27	121.24	126.39
24	7	604	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
40	5	502	LUT	C20-C13-C12	2.27	121.56	118.09
24	6	602	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
24	A	1103	CLA	C1C-C2C-C3C	-2.27	104.59	106.98
24	2	605	CLA	CHA-C1A-NA	-2.27	121.25	126.39
24	9	606	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
40	5	502	LUT	C11-C10-C9	-2.27	124.09	127.28
24	A	1129	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
24	B	1214	CLA	CHA-C1A-NA	-2.27	121.25	126.39
24	2	606	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
24	A	1137	CLA	O2A-CGA-CBA	2.27	118.76	111.83
28	4	802	LHG	C5-O7-C7	-2.27	112.36	117.80
27	6	504	BCR	C28-C27-C26	-2.27	110.01	114.06
24	6	603	CLA	C1-O2A-CGA	2.27	122.15	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	607	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
24	3	612	CLA	CHD-C1D-ND	-2.27	121.61	124.80
24	3	605	CLA	C3B-C4B-NB	-2.27	108.50	110.53
24	A	1114	CLA	CHD-C1D-ND	-2.27	121.61	124.80
24	5	612	CLA	CHD-C1D-ND	-2.27	121.61	124.80
24	B	1207	CLA	C1D-ND-C4D	-2.27	104.72	106.31
24	L	1501	CLA	C1D-ND-C4D	-2.27	104.72	106.31
24	1	612	CLA	CHD-C1D-ND	-2.27	121.61	124.80
24	9	612	CLA	CHA-C1A-NA	-2.27	121.25	126.39
24	8	610	CLA	C4B-CHC-C1C	2.27	131.58	126.25
41	9	613	CHL	C4C-CHD-C1D	2.27	124.18	116.07
24	2	604	CLA	CHA-C1A-NA	-2.27	121.26	126.39
24	A	1113	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
24	B	1219	CLA	C4B-CHC-C1C	2.27	131.58	126.25
24	A	1132	CLA	CHD-C1D-ND	-2.27	121.61	124.80
24	2	610	CLA	CHD-C1D-ND	-2.27	121.61	124.80
24	A	1111	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
24	6	618	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
24	1	603	CLA	CAA-C2A-C3A	-2.27	106.87	113.00
24	5	618	CLA	C3D-C2D-C1D	-2.27	102.74	105.83
24	1	604	CLA	CHD-C1D-ND	-2.27	121.61	124.80
24	A	1134	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
24	1	602	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
27	A	4002	BCR	C15-C14-C13	-2.27	124.10	127.28
27	B	4007	BCR	C34-C9-C10	-2.27	119.14	122.82
24	K	1403	CLA	C4B-CHC-C1C	2.27	131.57	126.25
24	7	602	CLA	CHD-C1D-ND	-2.27	121.61	124.80
24	B	1219	CLA	O2D-CGD-O1D	-2.27	119.44	123.85
24	A	1113	CLA	CMA-C3A-C4A	2.26	117.86	111.77
27	5	503	BCR	C30-C25-C24	2.26	121.79	115.65
24	5	607	CLA	CHA-C1A-NA	-2.26	121.26	126.39
41	8	613	CHL	C4C-CHD-C1D	2.26	124.17	116.07
24	3	610	CLA	CMD-C2D-C3D	-2.26	122.50	127.69
24	B	1201	CLA	CHD-C1D-ND	-2.26	121.62	124.80
24	A	1115	CLA	O1D-CGD-CBD	-2.26	120.05	124.52
24	3	610	CLA	CMA-C3A-C4A	2.26	117.86	111.77
24	B	1209	CLA	CMD-C2D-C3D	-2.26	122.50	127.69
24	G	1602	CLA	CMD-C2D-C3D	-2.26	122.50	127.69
24	A	1111	CLA	CHD-C1D-ND	-2.26	121.62	124.80
41	6	610	CHL	C3D-C4D-ND	-2.26	109.31	112.94
24	A	1133	CLA	C4B-CHC-C1C	2.26	131.57	126.25
24	1	612	CLA	C4B-CHC-C1C	2.26	131.57	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	4	605	CLA	C3B-C4B-NB	-2.26	108.51	110.53
24	7	605	CLA	CHA-C1A-NA	-2.26	121.27	126.39
24	4	616	CLA	CMD-C2D-C3D	-2.26	122.50	127.69
24	2	621	CLA	O2A-CGA-CBA	2.26	118.73	111.83
24	6	601	CLA	C1C-C2C-C3C	-2.26	104.60	106.98
24	K	1402	CLA	O1D-CGD-CBD	-2.26	120.06	124.52
24	B	1224	CLA	CMD-C2D-C3D	-2.26	122.50	127.69
24	5	617	CLA	CHD-C1D-ND	-2.26	121.62	124.80
24	8	612	CLA	C3B-C4B-NB	-2.26	108.51	110.53
24	1	605	CLA	CHD-C1D-ND	-2.26	121.62	124.80
24	2	612	CLA	CHA-C1A-NA	-2.26	121.27	126.39
24	2	610	CLA	CMD-C2D-C3D	-2.26	122.51	127.69
24	a	615	CLA	C1C-C2C-C3C	-2.26	104.60	106.98
24	A	1141	CLA	CHD-C1D-ND	-2.26	121.62	124.80
24	4	615	CLA	CHA-C1A-NA	-2.26	121.28	126.39
24	9	601	CLA	CMD-C2D-C3D	-2.26	122.51	127.69
24	8	611	CLA	C4B-CHC-C1C	2.26	131.56	126.25
24	A	1123	CLA	CHA-C1A-NA	-2.26	121.28	126.39
24	8	615	CLA	CHA-C1A-NA	-2.26	121.28	126.39
24	3	618	CLA	CHD-C1D-ND	-2.26	121.63	124.80
24	3	602	CLA	CMD-C2D-C3D	-2.26	122.51	127.69
24	7	611	CLA	CMD-C2D-C3D	-2.26	122.51	127.69
24	B	1230	CLA	CMA-C3A-C4A	2.26	117.84	111.77
24	A	1101	CLA	C1D-ND-C4D	-2.26	104.73	106.31
24	5	606	CLA	C3B-C4B-NB	-2.26	108.52	110.53
48	7	502	XAT	O4-C6-C7	-2.26	110.41	116.88
24	G	1601	CLA	CMA-C3A-C4A	2.26	117.84	111.77
40	1	501	LUT	C8-C7-C6	-2.26	120.97	127.00
24	1	611	CLA	CHA-C1A-NA	-2.26	121.28	126.39
40	1	501	LUT	C39-C29-C28	2.26	121.53	118.09
31	2	804	LMT	C3'-C4'-C5'	-2.25	105.93	110.93
24	5	606	CLA	CMD-C2D-C3D	-2.25	122.52	127.69
24	8	605	CLA	C2D-C1D-ND	2.25	112.36	110.13
24	2	602	CLA	CMD-C2D-C3D	-2.25	122.52	127.69
24	A	1130	CLA	CHA-C1A-NA	-2.25	121.29	126.39
24	A	1119	CLA	C2C-C1C-NC	2.25	112.35	109.98
24	6	602	CLA	CHA-C1A-NA	-2.25	121.29	126.39
24	1	603	CLA	C1D-ND-C4D	-2.25	104.73	106.31
24	8	603	CLA	CMD-C2D-C3D	-2.25	122.52	127.69
27	6	504	BCR	C4-C5-C6	-2.25	119.66	122.70
24	A	1108	CLA	O2A-CGA-CBA	2.25	118.70	111.83
24	B	1204	CLA	CHA-C4D-ND	2.25	137.20	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	1202	CLA	C1-C2-C3	-2.25	122.51	126.20
24	4	604	CLA	CHD-C1D-ND	-2.25	121.63	124.80
24	H	1702	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
40	6	502	LUT	C10-C11-C12	-2.25	116.68	123.20
24	A	1119	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
24	B	1226	CLA	CHD-C4C-C3C	2.25	128.06	124.77
24	1	612	CLA	C1-O2A-CGA	2.25	122.10	116.65
24	A	1103	CLA	CHD-C1D-ND	-2.25	121.64	124.80
24	3	613	CLA	CHD-C1D-ND	-2.25	121.64	124.80
24	7	610	CLA	CHA-C1A-NA	-2.25	121.30	126.39
24	K	1403	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
24	A	1101	CLA	CHD-C1D-ND	-2.25	121.64	124.80
24	F	1301	CLA	CHD-C1D-ND	-2.25	121.64	124.80
24	A	1115	CLA	C1D-ND-C4D	-2.25	104.73	106.31
24	H	1702	CLA	CHD-C1D-ND	-2.25	121.64	124.80
24	A	1112	CLA	CHA-C1A-NA	-2.25	121.30	126.39
41	1	613	CHL	C4C-CHD-C1D	2.25	124.11	116.07
24	2	602	CLA	O2A-CGA-CBA	2.25	118.69	111.83
24	B	1021	CLA	O1D-CGD-CBD	-2.25	120.08	124.52
24	F	1302	CLA	CHD-C1D-ND	-2.25	121.64	124.80
24	B	1201	CLA	C3B-C4B-NB	-2.25	108.52	110.53
27	8	503	BCR	C24-C25-C26	-2.25	116.38	121.56
41	6	613	CHL	C4C-CHD-C1D	2.25	124.11	116.07
24	B	1212	CLA	C3B-C4B-NB	-2.25	108.53	110.53
24	F	1302	CLA	C3B-C4B-NB	-2.25	108.53	110.53
24	A	1141	CLA	CMD-C2D-C3D	-2.25	122.54	127.69
24	B	1218	CLA	C1D-ND-C4D	-2.24	104.74	106.31
24	a	611	CLA	C1D-ND-C4D	-2.24	104.74	106.31
24	a	601	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
24	8	602	CLA	CHA-C1A-NA	-2.24	121.31	126.39
40	5	501	LUT	C20-C13-C12	2.24	121.51	118.09
24	3	602	CLA	CMA-C3A-C4A	2.24	117.80	111.77
24	A	1118	CLA	C2D-C1D-ND	2.24	112.34	110.13
24	B	1021	CLA	C2D-C1D-ND	2.24	112.34	110.13
24	A	1131	CLA	O2A-CGA-CBA	2.24	118.67	111.83
24	A	1105	CLA	C1D-ND-C4D	-2.24	104.74	106.31
40	5	502	LUT	C18-C5-C4	2.24	118.54	114.42
24	9	609	CLA	CHA-C1A-NA	-2.24	121.32	126.39
24	4	615	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
24	2	601	CLA	C1D-ND-C4D	-2.24	104.74	106.31
24	4	611	CLA	C2D-C1D-ND	2.24	112.34	110.13
24	7	615	CLA	CMD-C2D-C3D	-2.24	122.56	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	1234	CLA	CHA-C1A-NA	-2.24	121.32	126.39
24	8	608	CLA	O1D-CGD-CBD	-2.24	120.10	124.52
24	6	606	CLA	O2A-CGA-CBA	2.24	118.66	111.83
24	9	607	CLA	C3B-C4B-NB	-2.24	108.53	110.53
24	A	1126	CLA	CHA-C1A-NA	-2.24	121.32	126.39
24	3	616	CLA	C2D-C1D-ND	2.24	112.34	110.13
24	a	605	CLA	CHD-C1D-ND	-2.24	121.65	124.80
24	K	1401	CLA	O1D-CGD-CBD	-2.24	120.10	124.52
40	1	501	LUT	C18-C5-C4	2.24	118.54	114.42
24	2	607	CLA	CMD-C2D-C3D	-2.24	122.56	127.69
24	3	616	CLA	C1D-ND-C4D	-2.24	104.74	106.31
24	6	603	CLA	CMD-C2D-C3D	-2.24	122.56	127.69
24	8	602	CLA	CMD-C2D-C3D	-2.24	122.56	127.69
24	4	606	CLA	CMA-C3A-C4A	2.24	117.78	111.77
40	8	502	LUT	C30-C31-C32	-2.24	116.72	123.20
24	8	620	CLA	CHA-C1A-NA	-2.24	121.33	126.39
24	A	1112	CLA	O1D-CGD-CBD	-2.24	120.11	124.52
24	A	1117	CLA	C4B-CHC-C1C	2.24	131.50	126.25
24	2	612	CLA	C4B-CHC-C1C	2.24	131.50	126.25
24	A	1133	CLA	CHD-C1D-ND	-2.24	121.66	124.80
24	9	607	CLA	CHD-C1D-ND	-2.24	121.66	124.80
24	6	607	CLA	O2A-CGA-CBA	2.24	118.65	111.83
24	B	1232	CLA	CHD-C1D-ND	-2.24	121.66	124.80
24	B	1222	CLA	O2A-CGA-CBA	2.24	118.65	111.83
24	B	1207	CLA	CHA-C1A-NA	-2.23	121.33	126.39
24	A	1111	CLA	CHA-C1A-NA	-2.23	121.33	126.39
24	2	615	CLA	CHD-C1D-ND	-2.23	121.66	124.80
24	B	1023	CLA	C4B-CHC-C1C	2.23	131.50	126.25
24	1	607	CLA	CHA-C1A-NA	-2.23	121.33	126.39
24	9	609	CLA	CMD-C2D-C3D	-2.23	122.57	127.69
24	2	612	CLA	C3B-C4B-NB	-2.23	108.54	110.53
24	7	617	CLA	CMD-C2D-C3D	-2.23	122.57	127.69
27	L	4003	BCR	C38-C26-C27	2.23	118.36	113.60
24	G	1602	CLA	O1D-CGD-CBD	-2.23	120.11	124.52
27	L	4003	BCR	C36-C18-C17	-2.23	119.20	122.82
27	6	503	BCR	C34-C9-C10	-2.23	119.20	122.82
24	a	602	CLA	CHA-C1A-NA	-2.23	121.34	126.39
24	5	618	CLA	CHA-C1A-NA	-2.23	121.34	126.39
24	5	601	CLA	CMD-C2D-C3D	-2.23	122.57	127.69
24	8	602	CLA	C1D-ND-C4D	-2.23	104.75	106.31
24	2	602	CLA	C1D-ND-C4D	-2.23	104.75	106.31
24	B	1239	CLA	C2D-C1D-ND	2.23	112.33	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	8	607	CLA	CHD-C1D-ND	-2.23	121.66	124.80
27	A	4002	BCR	C33-C5-C4	2.23	118.35	113.60
24	a	607	CLA	O1D-CGD-CBD	-2.23	120.12	124.52
24	3	602	CLA	CHA-C1A-NA	-2.23	121.34	126.39
24	5	606	CLA	CAA-C2A-C3A	-2.23	106.97	113.00
41	6	619	CHL	C1-O2A-CGA	2.23	122.05	116.65
40	5	502	LUT	C27-C28-C29	-2.23	121.53	126.32
41	a	613	CHL	C4D-CHA-CBD	-2.23	106.72	108.97
24	A	1116	CLA	CHA-C1A-NA	-2.23	121.34	126.39
24	1	610	CLA	CHA-C1A-NA	-2.23	121.34	126.39
24	2	621	CLA	CHA-C1A-NA	-2.23	121.34	126.39
24	B	1212	CLA	O2A-CGA-CBA	2.23	118.63	111.83
27	B	4001	BCR	C27-C26-C25	-2.23	119.69	122.70
24	6	605	CLA	O1D-CGD-CBD	-2.23	120.12	124.52
24	A	1108	CLA	CMD-C2D-C3D	-2.23	122.58	127.69
24	B	1211	CLA	CMA-C3A-C4A	2.23	117.76	111.77
24	B	1203	CLA	CMD-C2D-C3D	-2.23	122.58	127.69
24	A	1124	CLA	CHA-C4D-ND	2.23	137.15	132.55
24	A	1121	CLA	C3B-C4B-NB	-2.23	108.54	110.53
24	B	1226	CLA	CHD-C1D-ND	-2.23	121.67	124.80
24	a	604	CLA	CHD-C1D-ND	-2.23	121.67	124.80
24	7	602	CLA	CMD-C2D-C3D	-2.23	122.58	127.69
35	H	5001	SQD	O3-C3-C2	-2.23	105.13	110.38
24	1	612	CLA	CHA-C1A-NA	-2.23	121.35	126.39
24	A	1129	CLA	O2A-CGA-CBA	2.23	118.62	111.83
24	A	1102	CLA	C2A-C1A-CHA	2.23	127.73	123.87
24	B	1205	CLA	C1D-ND-C4D	-2.23	104.75	106.31
24	B	1220	CLA	C1D-ND-C4D	-2.23	104.75	106.31
24	8	620	CLA	C1D-ND-C4D	-2.23	104.75	106.31
24	a	611	CLA	CHA-C1A-NA	-2.23	121.35	126.39
24	3	601	CLA	CMD-C2D-C3D	-2.23	122.58	127.69
24	2	615	CLA	C3D-C2D-C1D	-2.23	102.79	105.83
24	7	617	CLA	CHA-C1A-NA	-2.23	121.35	126.39
31	A	5008	LMT	O5'-C5'-C6'	2.23	111.95	106.44
24	5	601	CLA	O2D-CGD-O1D	-2.23	119.52	123.85
24	5	606	CLA	O2A-CGA-CBA	2.22	118.62	111.83
24	A	1104	CLA	CMD-C2D-C3D	-2.22	122.59	127.69
24	8	609	CLA	CHD-C1D-ND	-2.22	121.67	124.80
24	B	1207	CLA	CMD-C2D-C3D	-2.22	122.59	127.69
24	5	616	CLA	CMD-C2D-C3D	-2.22	122.59	127.69
24	A	1101	CLA	C2D-C1D-ND	2.22	112.33	110.13
24	A	1116	CLA	C2C-C1C-NC	2.22	112.32	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1128	CLA	O2A-CGA-CBA	2.22	118.61	111.83
40	3	502	LUT	C31-C30-C29	-2.22	124.16	127.28
24	1	601	CLA	C6-C5-C3	-2.22	108.05	113.47
24	A	1137	CLA	CHD-C1D-ND	-2.22	121.67	124.80
24	7	606	CLA	CHA-C1A-NA	-2.22	121.36	126.39
24	4	612	CLA	CBC-CAC-C3C	-2.22	106.40	112.42
24	7	612	CLA	CMD-C2D-C3D	-2.22	122.59	127.69
24	A	1135	CLA	CMA-C3A-C4A	2.22	117.75	111.77
24	B	1206	CLA	CMC-C2C-C3C	2.22	132.16	126.15
27	4	503	BCR	C30-C25-C26	-2.22	119.60	122.64
24	A	1124	CLA	O2A-CGA-CBA	2.22	118.61	111.83
24	B	1211	CLA	C1D-ND-C4D	-2.22	104.75	106.31
24	B	1201	CLA	C6-C5-C3	-2.22	108.06	113.47
24	7	601	CLA	C2C-C1C-NC	2.22	112.31	109.98
24	3	610	CLA	O2A-CGA-CBA	2.22	118.60	111.83
24	6	617	CLA	CHA-C1A-NA	-2.22	121.36	126.39
40	1	502	LUT	C31-C30-C29	-2.22	124.17	127.28
24	B	1201	CLA	CMD-C2D-C3D	-2.22	122.60	127.69
24	1	607	CLA	CMD-C2D-C3D	-2.22	122.60	127.69
24	B	1022	CLA	CMD-C2D-C3D	-2.22	122.60	127.69
24	B	1228	CLA	CMD-C2D-C3D	-2.22	122.60	127.69
24	6	615	CLA	CHA-C1A-NA	-2.22	121.37	126.39
24	B	1212	CLA	CHD-C1D-ND	-2.22	121.68	124.80
40	a	502	LUT	C39-C29-C28	2.22	121.48	118.09
24	2	615	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
27	H	4001	BCR	C38-C26-C27	2.22	118.32	113.60
24	A	1109	CLA	C4B-CHC-C1C	2.22	131.46	126.25
24	A	1125	CLA	CMA-C3A-C4A	2.22	117.73	111.77
24	B	1203	CLA	C1D-ND-C4D	-2.22	104.76	106.31
24	L	1502	CLA	O2A-CGA-CBA	2.22	118.59	111.83
24	8	615	CLA	CMD-C2D-C3D	-2.22	122.61	127.69
24	3	602	CLA	CHD-C1D-ND	-2.22	121.69	124.80
24	7	603	CLA	C1D-ND-C4D	-2.21	104.76	106.31
24	B	1204	CLA	C3B-C4B-NB	-2.21	108.55	110.53
24	2	604	CLA	C1C-C2C-C3C	-2.21	104.65	106.98
24	2	604	CLA	C2D-C1D-ND	2.21	112.32	110.13
24	F	1302	CLA	CHA-C1A-NA	-2.21	121.38	126.39
24	9	609	CLA	C3B-C4B-NB	-2.21	108.55	110.53
24	5	616	CLA	CHA-C1A-NA	-2.21	121.38	126.39
24	A	1125	CLA	O2A-CGA-CBA	2.21	118.58	111.83
24	3	612	CLA	C4B-CHC-C1C	2.21	131.45	126.25
24	B	1205	CLA	O1D-CGD-CBD	-2.21	120.15	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	7	615	CLA	CHD-C1D-ND	-2.21	121.69	124.80
40	6	502	LUT	C3-C4-C5	-2.21	106.67	112.18
28	1	801	LHG	C6-C5-C4	-2.21	106.63	111.78
24	J	1901	CLA	CMD-C2D-C3D	-2.21	122.62	127.69
24	5	614	CLA	CMD-C2D-C3D	-2.21	122.62	127.69
24	1	601	CLA	C3D-C2D-C1D	-2.21	102.81	105.83
24	1	601	CLA	CMD-C2D-C3D	-2.21	122.62	127.69
41	5	611	CHL	C3D-C4D-ND	-2.21	109.39	112.94
24	7	602	CLA	CHA-C1A-NA	-2.21	121.39	126.39
24	1	606	CLA	C1D-ND-C4D	-2.21	104.76	106.31
24	5	617	CLA	C1D-ND-C4D	-2.21	104.76	106.31
24	A	1115	CLA	CMD-C2D-C3D	-2.21	122.62	127.69
24	A	1118	CLA	CHD-C1D-ND	-2.21	121.69	124.80
24	7	612	CLA	CAA-C2A-C3A	-2.21	107.03	113.00
24	6	606	CLA	CHA-C1A-NA	-2.21	121.39	126.39
27	H	4001	BCR	C1-C6-C5	-2.21	119.62	122.64
24	4	617	CLA	CHD-C1D-ND	-2.21	121.69	124.80
24	a	604	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
24	A	1140	CLA	O2D-CGD-O1D	-2.21	119.55	123.85
24	4	602	CLA	CHA-C1A-NA	-2.21	121.39	126.39
24	2	621	CLA	CHD-C1D-ND	-2.21	121.69	124.80
27	A	4004	BCR	C12-C13-C14	-2.21	115.53	119.01
27	B	4004	BCR	C36-C18-C17	-2.21	119.24	122.82
40	a	501	LUT	C39-C29-C28	2.21	121.46	118.09
24	2	613	CLA	CMD-C2D-C3D	-2.21	122.63	127.69
24	5	614	CLA	C1D-ND-C4D	-2.21	104.76	106.31
24	5	602	CLA	CHA-C1A-NA	-2.21	121.39	126.39
27	J	4001	BCR	C38-C26-C27	2.21	118.30	113.60
24	4	612	CLA	C4B-CHC-C1C	2.21	131.44	126.25
24	6	612	CLA	O2A-CGA-CBA	2.21	118.56	111.83
24	B	1022	CLA	C4B-CHC-C1C	2.21	131.44	126.25
24	B	1213	CLA	C1D-ND-C4D	-2.21	104.76	106.31
24	2	607	CLA	CHA-C1A-NA	-2.21	121.39	126.39
24	B	1225	CLA	O2A-CGA-CBA	2.21	118.56	111.83
40	9	502	LUT	C27-C28-C29	-2.21	121.58	126.32
24	3	618	CLA	CHA-C1A-NA	-2.21	121.40	126.39
24	A	1012	CLA	C2C-C1C-NC	2.21	112.30	109.98
24	A	1136	CLA	C1D-ND-C4D	-2.20	104.77	106.31
24	L	1502	CLA	C1D-ND-C4D	-2.20	104.77	106.31
24	A	1106	CLA	CMD-C2D-C3D	-2.20	122.63	127.69
40	3	501	LUT	C8-C7-C6	-2.20	121.11	127.00
24	3	607	CLA	CHA-C1A-NA	-2.20	121.40	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	9	607	CLA	CHA-C1A-NA	-2.20	121.40	126.39
24	A	1135	CLA	C3D-C2D-C1D	-2.20	102.82	105.83
24	4	602	CLA	O2A-CGA-CBA	2.20	118.55	111.83
24	6	617	CLA	CHD-C1D-ND	-2.20	121.70	124.80
40	a	501	LUT	C27-C28-C29	-2.20	121.59	126.32
24	3	613	CLA	C2D-C1D-ND	2.20	112.31	110.13
24	B	1202	CLA	CHD-C1D-ND	-2.20	121.70	124.80
24	A	1138	CLA	C3B-C4B-NB	-2.20	108.56	110.53
27	B	4002	BCR	C8-C9-C10	2.20	122.47	119.01
24	8	607	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
24	A	1112	CLA	C4B-CHC-C1C	2.20	131.43	126.25
41	5	610	CHL	CMA-C3A-C2A	2.20	122.63	114.13
24	A	1135	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
24	6	605	CLA	C4B-CHC-C1C	2.20	131.42	126.25
24	B	1232	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
24	A	1102	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
24	4	607	CLA	CHA-C1A-NA	-2.20	121.41	126.39
24	B	1203	CLA	C2D-C1D-ND	2.20	112.30	110.13
24	6	607	CLA	CHA-C1A-NA	-2.20	121.41	126.39
24	2	608	CLA	CHA-C1A-NA	-2.20	121.41	126.39
24	B	1204	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
24	B	1235	CLA	CMD-C2D-C3D	-2.20	122.65	127.69
24	2	609	CLA	CMD-C2D-C3D	-2.20	122.65	127.69
24	5	605	CLA	CHA-C1A-NA	-2.20	121.42	126.39
27	B	4003	BCR	C4-C5-C6	-2.20	119.73	122.70
24	A	1132	CLA	O2A-CGA-CBA	2.20	118.53	111.83
24	3	606	CLA	O2A-CGA-CBA	2.20	118.53	111.83
24	5	609	CLA	CHA-C1A-NA	-2.20	121.42	126.39
24	9	602	CLA	CHA-C1A-NA	-2.20	121.42	126.39
24	B	1239	CLA	CMA-C3A-C4A	2.20	117.68	111.77
24	9	612	CLA	O2A-CGA-CBA	2.20	118.53	111.83
24	4	611	CLA	CMD-C2D-C3D	-2.20	122.65	127.69
40	3	502	LUT	C39-C29-C28	2.20	121.44	118.09
24	A	1121	CLA	O1D-CGD-CBD	-2.20	120.19	124.52
24	2	603	CLA	CHA-C4D-ND	2.20	137.08	132.55
24	B	1215	CLA	C1-C2-C3	-2.20	122.60	126.20
24	5	604	CLA	CHD-C1D-ND	-2.20	121.71	124.80
24	9	608	CLA	CHD-C1D-ND	-2.20	121.71	124.80
24	B	1205	CLA	CAA-C2A-C3A	-2.20	107.07	113.00
27	B	4001	BCR	C35-C13-C12	2.19	121.44	118.09
24	A	1101	CLA	CHA-C1A-NA	-2.19	121.42	126.39
24	B	1237	CLA	C4B-CHC-C1C	2.19	131.41	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	5	609	CLA	CHD-C1D-ND	-2.19	121.71	124.80
24	9	612	CLA	CHD-C1D-ND	-2.19	121.72	124.80
24	B	1023	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
24	6	602	CLA	O2A-CGA-CBA	2.19	118.52	111.83
27	A	4002	BCR	C38-C26-C27	2.19	118.27	113.60
24	A	1122	CLA	C1D-ND-C4D	-2.19	104.77	106.31
40	a	502	LUT	C31-C30-C29	-2.19	124.20	127.28
24	B	1226	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
24	a	612	CLA	CMD-C2D-C3D	-2.19	122.66	127.69
24	2	606	CLA	C1D-ND-C4D	-2.19	104.77	106.31
24	1	602	CLA	CHD-C1D-ND	-2.19	121.72	124.80
24	a	608	CLA	CHD-C1D-ND	-2.19	121.72	124.80
24	9	602	CLA	CHD-C1D-ND	-2.19	121.72	124.80
24	B	1231	CLA	CHA-C1A-NA	-2.19	121.43	126.39
24	B	1205	CLA	CMD-C2D-C3D	-2.19	122.66	127.69
28	7	803	LHG	C5-O7-C7	-2.19	112.55	117.80
24	7	604	CLA	CAA-C2A-C3A	-2.19	107.08	113.00
24	2	613	CLA	CHA-C1A-NA	-2.19	121.43	126.39
24	B	1230	CLA	C2D-C1D-ND	2.19	112.29	110.13
24	J	1901	CLA	CHA-C1A-NA	-2.19	121.43	126.39
24	A	1135	CLA	CHD-C1D-ND	-2.19	121.72	124.80
27	3	503	BCR	C30-C25-C24	2.19	121.59	115.65
24	B	1207	CLA	CHD-C1D-ND	-2.19	121.72	124.80
24	B	1216	CLA	CMA-C3A-C4A	2.19	117.66	111.77
24	A	1134	CLA	CHA-C1A-NA	-2.19	121.44	126.39
24	8	605	CLA	CBC-CAC-C3C	-2.19	106.49	112.42
41	6	611	CHL	C1-O2A-CGA	2.19	121.95	116.65
24	2	613	CLA	CHD-C1D-ND	-2.19	121.72	124.80
24	L	1502	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
27	A	4002	BCR	C34-C9-C10	-2.19	119.27	122.82
24	B	1021	CLA	CMC-C2C-C1C	2.19	128.45	125.03
24	A	1107	CLA	C1D-ND-C4D	-2.19	104.78	106.31
24	8	612	CLA	CHA-C1A-NA	-2.19	121.44	126.39
24	2	610	CLA	CHA-C1A-NA	-2.19	121.44	126.39
27	4	503	BCR	C23-C24-C25	-2.19	121.15	127.00
24	1	604	CLA	O2A-CGA-CBA	2.19	118.50	111.83
24	A	1013	CLA	C4B-CHC-C1C	2.19	131.39	126.25
24	A	1110	CLA	CMD-C2D-C3D	-2.19	122.67	127.69
24	2	601	CLA	C1-O2A-CGA	2.19	121.94	116.65
41	4	613	CHL	C4C-CHD-C1D	2.19	123.89	116.07
24	K	1402	CLA	CHA-C1A-NA	-2.19	121.44	126.39
24	A	1141	CLA	C3B-C4B-NB	-2.19	108.58	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	1232	CLA	C2D-C1D-ND	2.19	112.29	110.13
40	7	501	LUT	C38-C25-C24	-2.19	118.19	123.36
24	A	1113	CLA	CHA-C1A-NA	-2.19	121.44	126.39
40	5	501	LUT	C22-C23-C24	-2.19	107.94	111.18
24	4	611	CLA	CAA-C2A-C3A	-2.19	107.09	113.00
24	6	603	CLA	CAA-C2A-C3A	-2.19	107.09	113.00
24	A	1139	CLA	O2A-CGA-CBA	2.19	118.50	111.83
24	6	615	CLA	CMA-C3A-C4A	2.19	117.65	111.77
24	B	1229	CLA	CHA-C1A-NA	-2.19	121.44	126.39
24	8	611	CLA	CMD-C2D-C3D	-2.18	122.68	127.69
24	4	608	CLA	C3B-C4B-NB	-2.18	108.58	110.53
24	A	1136	CLA	CMD-C2D-C3D	-2.18	122.68	127.69
24	2	612	CLA	O2A-CGA-CBA	2.18	118.49	111.83
24	B	1237	CLA	CHA-C1A-NA	-2.18	121.45	126.39
24	5	612	CLA	C3B-C4B-NB	-2.18	108.58	110.53
40	8	502	LUT	C20-C13-C12	2.18	121.42	118.09
24	A	1139	CLA	C1-O2A-CGA	2.18	121.94	116.65
24	1	612	CLA	CMD-C2D-C3D	-2.18	122.68	127.69
24	1	601	CLA	C1D-ND-C4D	-2.18	104.78	106.31
27	I	4001	BCR	C30-C25-C26	-2.18	119.65	122.64
24	6	615	CLA	CHD-C1D-ND	-2.18	121.73	124.80
24	B	1215	CLA	CHA-C1A-NA	-2.18	121.45	126.39
24	A	1134	CLA	O2A-CGA-CBA	2.18	118.48	111.83
24	B	1225	CLA	O2D-CGD-O1D	-2.18	119.60	123.85
24	6	601	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
24	2	615	CLA	CHA-C1A-NA	-2.18	121.45	126.39
24	B	1232	CLA	C1D-ND-C4D	-2.18	104.78	106.31
24	4	602	CLA	C2D-C1D-ND	2.18	112.28	110.13
24	2	602	CLA	C2D-C1D-ND	2.18	112.28	110.13
24	8	610	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
24	B	1230	CLA	C1D-ND-C4D	-2.18	104.78	106.31
24	B	1240	CLA	CHD-C1D-ND	-2.18	121.74	124.80
24	a	603	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
24	8	611	CLA	C3B-C4B-NB	-2.18	108.58	110.53
27	L	4003	BCR	C35-C13-C12	2.18	121.42	118.09
24	a	608	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
24	9	607	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
24	5	602	CLA	O2A-CGA-CBA	2.18	118.48	111.83
24	3	601	CLA	O2D-CGD-O1D	-2.18	119.61	123.85
24	H	1702	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
24	B	1236	CLA	CHA-C1A-NA	-2.18	121.46	126.39
24	5	601	CLA	CHA-C1A-NA	-2.18	121.46	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	1	503	LUT	C8-C7-C6	-2.18	121.18	127.00
24	a	603	CLA	C3D-C2D-C1D	-2.18	102.86	105.83
24	9	606	CLA	C1D-ND-C4D	-2.18	104.78	106.31
31	A	5008	LMT	O1'-C1'-C2'	2.18	111.58	108.27
24	B	1234	CLA	CAA-C2A-C3A	-2.18	107.11	113.00
24	7	606	CLA	CAA-C2A-C3A	-2.18	107.12	113.00
24	2	604	CLA	C2C-C1C-NC	2.18	112.27	109.98
41	8	604	CHL	C1C-C2C-CMC	2.18	130.72	126.80
24	L	1503	CLA	CMD-C2D-C3D	-2.18	122.70	127.69
24	5	605	CLA	C1D-ND-C4D	-2.18	104.78	106.31
24	4	608	CLA	OBD-CAD-C3D	-2.18	123.33	128.42
24	B	1206	CLA	CHD-C1D-ND	-2.18	121.74	124.80
24	8	610	CLA	CHD-C1D-ND	-2.18	121.74	124.80
24	B	1218	CLA	CHA-C1A-NA	-2.18	121.47	126.39
24	3	602	CLA	C1D-ND-C4D	-2.17	104.79	106.31
24	A	1125	CLA	C1-O2A-CGA	2.17	121.92	116.65
24	A	1122	CLA	C2D-C1D-ND	2.17	112.28	110.13
24	a	604	CLA	CHA-C1A-NA	-2.17	121.47	126.39
27	G	4001	BCR	C37-C22-C21	-2.17	119.29	122.82
24	B	1021	CLA	CHA-C1A-NA	-2.17	121.47	126.39
24	A	1140	CLA	C1D-ND-C4D	-2.17	104.79	106.31
24	K	1404	CLA	C1D-ND-C4D	-2.17	104.79	106.31
40	4	502	LUT	C20-C13-C12	2.17	121.41	118.09
24	4	604	CLA	CMD-C2D-C3D	-2.17	122.71	127.69
27	B	4005	BCR	C4-C5-C6	-2.17	119.77	122.70
24	4	617	CLA	CHA-C1A-NA	-2.17	121.47	126.39
24	A	1140	CLA	C2D-C1D-ND	2.17	112.28	110.13
24	7	604	CLA	C2D-C1D-ND	2.17	112.28	110.13
24	a	602	CLA	O2A-CGA-CBA	2.17	118.46	111.83
24	1	602	CLA	CHA-C1A-NA	-2.17	121.47	126.39
24	3	613	CLA	CHA-C1A-NA	-2.17	121.47	126.39
24	9	605	CLA	CHA-C1A-NA	-2.17	121.47	126.39
24	B	1236	CLA	C2D-C1D-ND	2.17	112.28	110.13
24	A	1106	CLA	O2A-CGA-CBA	2.17	118.45	111.83
24	B	1022	CLA	O2A-CGA-CBA	2.17	118.45	111.83
24	L	1502	CLA	CHA-C1A-NA	-2.17	121.47	126.39
24	K	1401	CLA	C1D-ND-C4D	-2.17	104.79	106.31
24	4	604	CLA	C1D-ND-C4D	-2.17	104.79	106.31
24	a	608	CLA	O2A-CGA-CBA	2.17	118.45	111.83
24	7	606	CLA	O2A-CGA-CBA	2.17	118.45	111.83
24	A	1131	CLA	CHA-C1A-NA	-2.17	121.48	126.39
24	1	601	CLA	C2D-C1D-ND	2.17	112.27	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1137	CLA	CHA-C1A-NA	-2.17	121.48	126.39
24	1	615	CLA	CHA-C1A-NA	-2.17	121.48	126.39
24	B	1210	CLA	O1D-CGD-CBD	-2.17	120.24	124.52
24	1	607	CLA	CHD-C1D-ND	-2.17	121.75	124.80
24	2	621	CLA	O1D-CGD-CBD	-2.17	120.24	124.52
24	A	1115	CLA	C2D-C1D-ND	2.17	112.27	110.13
24	6	607	CLA	C2D-C1D-ND	2.17	112.27	110.13
24	9	602	CLA	C1D-ND-C4D	-2.17	104.79	106.31
27	7	503	BCR	C33-C5-C4	2.17	118.22	113.60
40	2	501	LUT	C38-C25-C24	-2.17	118.23	123.36
28	5	801	LHG	O7-C7-O9	-2.17	118.63	123.70
24	4	604	CLA	CAA-C2A-C3A	-2.17	107.14	113.00
24	6	608	CLA	CAA-C2A-C3A	-2.17	107.14	113.00
24	B	1210	CLA	C6-C5-C3	-2.17	108.19	113.47
24	8	620	CLA	C3B-C4B-NB	-2.17	108.59	110.53
24	a	604	CLA	O2A-CGA-CBA	2.17	118.45	111.83
24	2	603	CLA	O2D-CGD-O1D	-2.17	119.63	123.85
24	4	601	CLA	CMD-C2D-C3D	-2.17	122.72	127.69
24	K	1404	CLA	O1D-CGD-CBD	-2.17	120.24	124.52
24	2	607	CLA	CHD-C1D-ND	-2.17	121.75	124.80
24	a	602	CLA	C2D-C1D-ND	2.17	112.27	110.13
24	3	618	CLA	C2D-C1D-ND	2.17	112.27	110.13
24	G	1602	CLA	OBD-CAD-C3D	-2.17	123.35	128.42
41	5	610	CHL	C4C-CHD-C1D	2.17	123.83	116.07
27	5	503	BCR	C1-C6-C7	2.17	121.53	115.65
24	2	604	CLA	C3D-C2D-C1D	-2.17	102.87	105.83
28	9	802	LHG	O7-C7-O9	-2.17	118.64	123.70
24	B	1212	CLA	CHA-C1A-NA	-2.17	121.48	126.39
24	A	1125	CLA	O1D-CGD-CBD	-2.17	120.25	124.52
24	B	1238	CLA	CAA-C2A-C3A	-2.17	107.14	113.00
24	B	1022	CLA	CAA-C2A-C3A	-2.17	107.15	113.00
27	K	4001	BCR	C31-C1-C6	-2.17	106.85	110.24
24	5	618	CLA	CHD-C1D-ND	-2.17	121.75	124.80
24	8	606	CLA	C3B-C4B-NB	-2.17	108.60	110.53
24	B	1217	CLA	C2D-C1D-ND	2.17	112.27	110.13
24	B	1208	CLA	O2A-CGA-CBA	2.16	118.44	111.83
24	K	1402	CLA	O2A-CGA-CBA	2.16	118.44	111.83
24	A	1104	CLA	C1D-ND-C4D	-2.16	104.79	106.31
24	4	602	CLA	C1D-ND-C4D	-2.16	104.79	106.31
24	B	1213	CLA	CMA-C3A-C4A	2.16	117.59	111.77
36	G	5002	ERG	C16-C17-C13	2.16	106.39	103.84
24	A	1136	CLA	O2A-CGA-CBA	2.16	118.43	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1114	CLA	C1-O2A-CGA	2.16	121.89	116.65
49	7	504	C7Z	C11-C12-C13	-2.16	120.43	126.36
24	a	607	CLA	CAA-C2A-C3A	-2.16	107.15	113.00
24	4	616	CLA	C1D-ND-C4D	-2.16	104.79	106.31
24	A	1139	CLA	CHA-C1A-NA	-2.16	121.49	126.39
24	A	1106	CLA	CHD-C1D-ND	-2.16	121.76	124.80
24	A	1137	CLA	C2D-C1D-ND	2.16	112.27	110.13
24	B	1220	CLA	C2D-C1D-ND	2.16	112.27	110.13
24	5	601	CLA	C2D-C1D-ND	2.16	112.27	110.13
24	A	1127	CLA	O2A-CGA-CBA	2.16	118.43	111.83
24	A	1120	CLA	O1D-CGD-CBD	-2.16	120.25	124.52
24	7	606	CLA	O2D-CGD-O1D	-2.16	119.64	123.85
24	3	603	CLA	C1-O2A-CGA	2.16	121.89	116.65
24	8	608	CLA	C3D-C2D-C1D	-2.16	102.88	105.83
24	G	1601	CLA	C2D-C1D-ND	2.16	112.27	110.13
27	I	4001	BCR	C34-C9-C10	-2.16	119.31	122.82
24	6	606	CLA	C1D-ND-C4D	-2.16	104.80	106.31
24	1	612	CLA	C3B-C4B-NB	-2.16	108.60	110.53
24	8	602	CLA	CHD-C1D-ND	-2.16	121.76	124.80
27	F	4001	BCR	C38-C26-C27	2.16	118.20	113.60
24	B	1217	CLA	CHA-C1A-NA	-2.16	121.50	126.39
24	A	1113	CLA	C1-C2-C3	-2.16	122.66	126.20
24	2	602	CLA	CHA-C1A-NA	-2.16	121.50	126.39
24	B	1239	CLA	CMD-C2D-C3D	-2.16	122.73	127.69
24	6	609	CLA	CHA-C1A-NA	-2.16	121.50	126.39
24	2	601	CLA	CHA-C1A-NA	-2.16	121.50	126.39
24	A	1103	CLA	CMD-C2D-C3D	-2.16	122.74	127.69
24	5	607	CLA	C3D-C2D-C1D	-2.16	102.88	105.83
24	B	1239	CLA	C1D-ND-C4D	-2.16	104.80	106.31
24	1	604	CLA	C1D-ND-C4D	-2.16	104.80	106.31
24	6	604	CLA	C1D-ND-C4D	-2.16	104.80	106.31
24	8	615	CLA	C2D-C1D-ND	2.16	112.26	110.13
27	A	4004	BCR	C36-C18-C17	-2.16	119.32	122.82
27	B	4003	BCR	C36-C18-C17	-2.16	119.32	122.82
24	B	1239	CLA	CHA-C1A-NA	-2.16	121.50	126.39
24	6	601	CLA	CHA-C1A-NA	-2.16	121.50	126.39
24	7	608	CLA	CHA-C1A-NA	-2.16	121.50	126.39
24	1	601	CLA	CHA-C1A-NA	-2.16	121.50	126.39
24	a	605	CLA	CHA-C1A-NA	-2.16	121.50	126.39
24	B	1222	CLA	C1D-ND-C4D	-2.16	104.80	106.31
24	a	604	CLA	C1D-ND-C4D	-2.16	104.80	106.31
24	F	1301	CLA	CHA-C1A-NA	-2.16	121.50	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	1212	CLA	CMD-C2D-C3D	-2.16	122.74	127.69
24	4	606	CLA	O1D-CGD-CBD	-2.16	120.26	124.52
24	B	1227	CLA	CHA-C1A-NA	-2.16	121.51	126.39
24	B	1215	CLA	CMD-C2D-C3D	-2.16	122.74	127.69
41	6	619	CHL	C4D-CHA-CBD	-2.16	106.79	108.97
24	5	604	CLA	C3B-C4B-NB	-2.16	108.61	110.53
24	1	602	CLA	C1D-ND-C4D	-2.16	104.80	106.31
24	7	611	CLA	CAA-C2A-C3A	-2.16	107.17	113.00
24	B	1235	CLA	C2D-C1D-ND	2.16	112.26	110.13
24	4	605	CLA	CMA-C3A-C4A	2.16	117.57	111.77
24	8	620	CLA	CMD-C2D-C3D	-2.16	122.75	127.69
24	A	1130	CLA	C2D-C1D-ND	2.16	112.26	110.13
24	A	1126	CLA	C3D-C2D-C1D	-2.16	102.89	105.83
27	K	4002	BCR	C33-C5-C4	2.15	118.19	113.60
24	B	1216	CLA	CHA-C1A-NA	-2.15	121.51	126.39
24	6	615	CLA	C3D-C2D-C1D	-2.15	102.89	105.83
24	B	1234	CLA	CHD-C1D-ND	-2.15	121.77	124.80
24	5	608	CLA	CHA-C1A-NA	-2.15	121.51	126.39
24	A	1129	CLA	C4B-CHC-C1C	2.15	131.31	126.25
24	B	1203	CLA	CHA-C1A-NA	-2.15	121.51	126.39
24	4	606	CLA	C1D-ND-C4D	-2.15	104.80	106.31
24	6	612	CLA	CHA-C1A-NA	-2.15	121.52	126.39
24	8	603	CLA	C2D-C1D-ND	2.15	112.26	110.13
24	A	1132	CLA	C3B-C4B-NB	-2.15	108.61	110.53
24	7	607	CLA	CHD-C1D-ND	-2.15	121.77	124.80
24	7	617	CLA	CHD-C1D-ND	-2.15	121.77	124.80
24	9	609	CLA	CHD-C1D-ND	-2.15	121.77	124.80
24	A	1107	CLA	CHA-C1A-NA	-2.15	121.52	126.39
24	A	1114	CLA	CHA-C1A-NA	-2.15	121.52	126.39
24	8	606	CLA	CHA-C1A-NA	-2.15	121.52	126.39
24	7	617	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
24	1	608	CLA	CAA-CBA-CGA	-2.15	107.10	113.21
24	4	608	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
24	3	603	CLA	C1D-ND-C4D	-2.15	104.80	106.31
24	F	1301	CLA	CMD-C2D-C3D	-2.15	122.76	127.69
24	A	1128	CLA	CHA-C1A-NA	-2.15	121.52	126.39
24	7	612	CLA	CHA-C1A-NA	-2.15	121.52	126.39
24	A	1123	CLA	CHD-C1D-ND	-2.15	121.78	124.80
40	1	502	LUT	C20-C13-C12	2.15	121.37	118.09
24	6	604	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
24	1	610	CLA	C3B-C4B-NB	-2.15	108.61	110.53
24	J	1901	CLA	C1D-ND-C4D	-2.15	104.80	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	8	605	CLA	CMD-C2D-C3D	-2.15	122.76	127.69
24	A	1116	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
24	8	615	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
27	L	4003	BCR	C23-C24-C25	-2.15	121.26	127.00
41	3	611	CHL	CMD-C2D-C3D	2.15	128.97	124.68
24	7	607	CLA	CHA-C1A-NA	-2.15	121.53	126.39
24	G	1601	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
40	5	502	LUT	C31-C30-C29	-2.15	124.27	127.28
24	B	1225	CLA	CHA-C1A-NA	-2.15	121.53	126.39
24	8	608	CLA	C2D-C1D-ND	2.15	112.25	110.13
24	A	1123	CLA	CMD-C2D-C3D	-2.15	122.77	127.69
40	8	502	LUT	C39-C29-C28	2.15	121.37	118.09
24	6	618	CLA	CHA-C1A-NA	-2.15	121.53	126.39
41	4	613	CHL	C4D-CHA-CBD	-2.15	106.80	108.97
41	4	618	CHL	CMA-C3A-C4A	2.15	119.23	114.61
24	8	602	CLA	C2D-C1D-ND	2.15	112.25	110.13
24	3	613	CLA	C1D-ND-C4D	-2.14	104.81	106.31
24	A	1112	CLA	CMD-C2D-C3D	-2.14	122.77	127.69
24	B	1234	CLA	C3D-C2D-C1D	-2.14	102.90	105.83
24	8	605	CLA	CHA-C1A-NA	-2.14	121.53	126.39
27	B	4004	BCR	C34-C9-C10	-2.14	119.34	122.82
24	B	1205	CLA	CHD-C1D-ND	-2.14	121.78	124.80
24	5	608	CLA	CMD-C2D-C3D	-2.14	122.77	127.69
24	2	606	CLA	CHA-C1A-NA	-2.14	121.54	126.39
24	a	605	CLA	C1-O2A-CGA	2.14	121.84	116.65
41	9	613	CHL	CAA-C2A-C3A	-2.14	111.31	116.23
24	A	1137	CLA	CMD-C2D-C3D	-2.14	122.77	127.69
24	8	611	CLA	C1D-ND-C4D	-2.14	104.81	106.31
24	6	604	CLA	C6-C5-C3	-2.14	108.25	113.47
24	A	1139	CLA	CMD-C2D-C3D	-2.14	122.77	127.69
24	A	1135	CLA	C2D-C1D-ND	2.14	112.25	110.13
24	8	611	CLA	C2D-C1D-ND	2.14	112.25	110.13
24	A	1123	CLA	O2A-CGA-CBA	2.14	118.37	111.83
24	7	609	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
24	B	1201	CLA	C1D-ND-C4D	-2.14	104.81	106.31
24	3	606	CLA	C1D-ND-C4D	-2.14	104.81	106.31
24	A	1116	CLA	C1C-C2C-C3C	-2.14	104.73	106.98
24	5	608	CLA	C2D-C1D-ND	2.14	112.25	110.13
24	7	602	CLA	C2D-C1D-ND	2.14	112.25	110.13
24	1	615	CLA	C1D-ND-C4D	-2.14	104.81	106.31
24	A	1108	CLA	C1C-C2C-C3C	-2.14	104.73	106.98
24	A	1106	CLA	C2D-C1D-ND	2.14	112.24	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	1011	CL0	C4C-C3C-C2C	-2.14	104.92	113.37
24	3	604	CLA	CMD-C2D-C3D	-2.14	122.78	127.69
24	5	617	CLA	CHA-C1A-NA	-2.14	121.55	126.39
24	A	1013	CLA	CMC-C2C-C1C	2.14	128.38	125.03
24	5	603	CLA	C1-O2A-CGA	2.14	121.83	116.65
24	A	1102	CLA	C2D-C1D-ND	2.14	112.24	110.13
24	4	601	CLA	C1D-ND-C4D	-2.14	104.81	106.31
24	3	610	CLA	CHA-C1A-NA	-2.14	121.55	126.39
24	5	614	CLA	CHA-C1A-NA	-2.14	121.55	126.39
24	A	1136	CLA	C2D-C1D-ND	2.14	112.24	110.13
24	6	605	CLA	CHA-C1A-NA	-2.14	121.55	126.39
24	B	1232	CLA	CHA-C1A-NA	-2.14	121.55	126.39
24	5	612	CLA	CHA-C1A-NA	-2.14	121.55	126.39
24	2	610	CLA	C1D-ND-C4D	-2.14	104.81	106.31
24	4	601	CLA	C3B-C4B-NB	-2.14	108.62	110.53
24	B	1228	CLA	CHA-C1A-NA	-2.14	121.55	126.39
24	4	602	CLA	CHD-C1D-ND	-2.14	121.80	124.80
24	5	617	CLA	C3D-C2D-C1D	-2.14	102.92	105.83
41	4	618	CHL	CAA-C2A-C3A	-2.14	107.23	113.00
24	B	1221	CLA	C4B-CHC-C1C	2.14	131.27	126.25
24	H	1703	CLA	C1D-ND-C4D	-2.13	104.81	106.31
24	A	1116	CLA	CHD-C1D-ND	-2.13	121.80	124.80
24	4	602	CLA	CMD-C2D-C3D	-2.13	122.79	127.69
24	B	1231	CLA	O1D-CGD-CBD	-2.13	120.31	124.52
24	8	602	CLA	CMA-C3A-C4A	2.13	117.51	111.77
24	5	605	CLA	O1D-CGD-CBD	-2.13	120.31	124.52
24	8	611	CLA	CHA-C1A-NA	-2.13	121.56	126.39
24	G	1602	CLA	CAA-C2A-C3A	-2.13	107.23	113.00
25	A	2001	PQN	C2M-C2-C3	-2.13	120.94	124.45
24	2	612	CLA	CMA-C3A-C4A	2.13	117.51	111.77
24	B	1023	CLA	C3B-C2B-C1B	-2.13	104.66	107.17
24	2	609	CLA	OBD-CAD-C3D	-2.13	123.43	128.42
41	6	611	CHL	C4C-CHD-C1D	2.13	123.70	116.07
24	A	1107	CLA	O1D-CGD-CBD	-2.13	120.31	124.52
24	B	1234	CLA	CMD-C2D-C3D	-2.13	122.80	127.69
24	9	612	CLA	CMD-C2D-C3D	-2.13	122.80	127.69
24	4	601	CLA	CHA-C1A-NA	-2.13	121.56	126.39
24	5	604	CLA	CMC-C2C-C1C	2.13	128.37	125.03
24	L	1502	CLA	C1-O2A-CGA	2.13	121.81	116.65
40	5	501	LUT	C18-C5-C4	2.13	118.34	114.42
24	B	1208	CLA	C1D-ND-C4D	-2.13	104.82	106.31
24	B	1235	CLA	C1D-ND-C4D	-2.13	104.82	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	2	604	CLA	CMD-C2D-C3D	-2.13	122.80	127.69
24	G	1602	CLA	CHA-C1A-NA	-2.13	121.57	126.39
24	A	1101	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
24	L	1501	CLA	C2D-C1D-ND	2.13	112.23	110.13
24	9	602	CLA	C2D-C1D-ND	2.13	112.23	110.13
24	K	1404	CLA	CMA-C3A-C4A	2.13	117.50	111.77
24	B	1237	CLA	O2A-CGA-CBA	2.13	118.33	111.83
24	2	608	CLA	CMD-C2D-C3D	-2.13	122.81	127.69
24	3	616	CLA	C3D-C2D-C1D	-2.13	102.93	105.83
24	6	612	CLA	C3B-C4B-NB	-2.13	108.63	110.53
41	5	611	CHL	CMD-C2D-C3D	2.13	128.94	124.68
27	L	4001	BCR	C8-C7-C6	-2.13	121.31	127.00
24	A	1102	CLA	O1D-CGD-CBD	-2.13	120.32	124.52
24	8	615	CLA	C1D-ND-C4D	-2.13	104.82	106.31
27	K	4001	BCR	C36-C18-C17	-2.13	119.37	122.82
24	1	608	CLA	CMD-C2D-C3D	-2.13	122.81	127.69
27	4	503	BCR	C37-C22-C23	2.13	121.34	118.09
24	1	612	CLA	O2D-CGD-O1D	-2.13	119.71	123.85
24	5	602	CLA	C2D-C1D-ND	2.13	112.23	110.13
24	G	1603	CLA	CHA-C1A-NA	-2.13	121.58	126.39
27	6	504	BCR	C8-C7-C6	-2.13	121.32	127.00
24	A	1103	CLA	C3D-C2D-C1D	-2.13	102.93	105.83
40	8	502	LUT	C31-C30-C29	-2.13	124.30	127.28
24	2	603	CLA	C3D-C2D-C1D	-2.13	102.93	105.83
24	B	1239	CLA	C3D-C2D-C1D	-2.13	102.93	105.83
24	8	609	CLA	C3D-C2D-C1D	-2.13	102.93	105.83
24	9	605	CLA	C3D-C2D-C1D	-2.13	102.93	105.83
24	G	1602	CLA	CHD-C1D-ND	-2.13	121.81	124.80
24	9	605	CLA	C2D-C1D-ND	2.12	112.23	110.13
24	a	601	CLA	O2D-CGD-O1D	-2.12	119.71	123.85
24	9	604	CLA	O1D-CGD-CBD	-2.12	120.33	124.52
24	5	609	CLA	CMD-C2D-C3D	-2.12	122.82	127.69
41	5	613	CHL	CMD-C2D-C3D	2.12	128.93	124.68
40	3	501	LUT	C18-C5-C4	2.12	118.33	114.42
24	8	620	CLA	C3D-C2D-C1D	-2.12	102.93	105.83
27	B	4007	BCR	C35-C13-C12	2.12	121.33	118.09
24	A	1128	CLA	CAA-C2A-C3A	-2.12	107.26	113.00
24	A	1124	CLA	CHD-C1D-ND	-2.12	121.81	124.80
24	3	601	CLA	CHA-C1A-NA	-2.12	121.58	126.39
24	2	603	CLA	CHA-C1A-NA	-2.12	121.58	126.39
24	4	606	CLA	O2A-CGA-CBA	2.12	118.31	111.83
24	7	611	CLA	CHA-C1A-NA	-2.12	121.59	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	615	CLA	CMC-C2C-C1C	2.12	128.35	125.03
24	9	606	CLA	O1D-CGD-CBD	-2.12	120.33	124.52
24	F	1302	CLA	CMD-C2D-C3D	-2.12	122.83	127.69
41	8	604	CHL	CMD-C2D-C3D	2.12	128.92	124.68
24	6	612	CLA	CMD-C2D-C3D	-2.12	122.83	127.69
24	A	1012	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
24	J	1901	CLA	C2D-C1D-ND	2.12	112.22	110.13
41	a	610	CHL	CMD-C2D-C3D	2.12	128.92	124.68
24	B	1203	CLA	C1-O2A-CGA	2.12	121.78	116.65
24	a	611	CLA	C2D-C1D-ND	2.12	112.22	110.13
24	B	1224	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
24	B	1223	CLA	O1D-CGD-CBD	-2.12	120.34	124.52
24	B	1203	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
24	K	1401	CLA	CHA-C1A-NA	-2.12	121.60	126.39
24	8	618	CLA	CHA-C1A-NA	-2.12	121.60	126.39
24	9	602	CLA	CMD-C2D-C3D	-2.12	122.83	127.69
27	3	504	BCR	C23-C22-C21	2.12	122.34	119.01
24	3	603	CLA	C2D-C1D-ND	2.12	112.22	110.13
24	B	1206	CLA	CMA-C3A-C4A	2.12	117.46	111.77
27	B	4007	BCR	C33-C5-C4	2.12	118.11	113.60
24	B	1220	CLA	CHD-C1D-ND	-2.12	121.82	124.80
24	8	605	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
24	5	602	CLA	CHD-C1D-ND	-2.12	121.83	124.80
24	6	602	CLA	CHD-C1D-ND	-2.12	121.83	124.80
24	A	1127	CLA	CHA-C1A-NA	-2.12	121.60	126.39
24	a	607	CLA	CHA-C1A-NA	-2.12	121.60	126.39
24	7	601	CLA	C1C-C2C-C3C	-2.12	104.75	106.98
24	A	1013	CLA	CHA-C1A-NA	-2.12	121.60	126.39
36	G	5002	ERG	C16-C15-C14	-2.12	101.80	105.25
24	a	601	CLA	O1D-CGD-CBD	-2.12	120.35	124.52
24	B	1222	CLA	CAA-CBA-CGA	-2.11	107.20	113.21
24	a	611	CLA	CMD-C2D-C3D	-2.11	122.84	127.69
24	A	1138	CLA	CMD-C2D-C3D	-2.11	122.84	127.69
24	a	604	CLA	CMD-C2D-C3D	-2.11	122.84	127.69
24	4	612	CLA	CHA-C1A-NA	-2.11	121.60	126.39
24	9	608	CLA	C2D-C1D-ND	2.11	112.22	110.13
24	A	1119	CLA	C1D-ND-C4D	-2.11	104.83	106.31
24	A	1140	CLA	CHA-C1A-NA	-2.11	121.61	126.39
24	K	1403	CLA	CHA-C1A-NA	-2.11	121.61	126.39
24	3	612	CLA	CMB-C2B-C3B	2.11	131.52	126.55
27	F	4001	BCR	C36-C18-C17	-2.11	119.39	122.82
24	2	613	CLA	C3B-C4B-NB	-2.11	108.64	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1118	CLA	CHA-C1A-NA	-2.11	121.61	126.39
24	B	1222	CLA	CHA-C1A-NA	-2.11	121.61	126.39
24	A	1012	CLA	C1D-ND-C4D	-2.11	104.83	106.31
24	K	1402	CLA	C1D-ND-C4D	-2.11	104.83	106.31
24	a	607	CLA	C1D-ND-C4D	-2.11	104.83	106.31
24	B	1232	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
24	3	618	CLA	CMD-C2D-C3D	-2.11	122.85	127.69
24	6	609	CLA	C2D-C1D-ND	2.11	112.22	110.13
27	B	4007	BCR	C36-C18-C17	-2.11	119.39	122.82
24	7	604	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
24	5	602	CLA	C1D-ND-C4D	-2.11	104.83	106.31
24	9	601	CLA	C2D-C1D-ND	2.11	112.22	110.13
24	B	1240	CLA	CMD-C2D-C3D	-2.11	122.85	127.69
24	2	605	CLA	C3B-C4B-NB	-2.11	108.65	110.53
24	a	605	CLA	O2A-CGA-CBA	2.11	118.27	111.83
24	5	604	CLA	CAA-C2A-C3A	-2.11	107.30	113.00
40	a	501	LUT	C11-C12-C13	-2.11	120.58	126.36
24	3	605	CLA	O2A-CGA-CBA	2.11	118.27	111.83
27	L	4003	BCR	C30-C25-C26	-2.11	119.75	122.64
24	A	1124	CLA	CAA-C2A-C3A	-2.11	107.30	113.00
24	A	1130	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
24	1	604	CLA	CMD-C2D-C3D	-2.11	122.85	127.69
24	B	1227	CLA	O2A-CGA-CBA	2.11	118.26	111.83
24	L	1503	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
24	8	618	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
24	3	605	CLA	C1D-ND-C4D	-2.11	104.83	106.31
24	5	602	CLA	CMD-C2D-C3D	-2.11	122.86	127.69
24	A	1117	CLA	CAA-C2A-C1A	-2.11	105.07	111.97
41	9	610	CHL	CMD-C2D-C3D	2.11	128.89	124.68
24	5	601	CLA	CMC-C2C-C1C	2.11	128.33	125.03
24	A	1137	CLA	C1D-ND-C4D	-2.11	104.83	106.31
24	A	1105	CLA	O2A-CGA-CBA	2.11	118.26	111.83
24	4	616	CLA	C2D-C1D-ND	2.11	112.21	110.13
24	1	607	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
40	1	502	LUT	C3-C4-C5	-2.11	106.94	112.18
24	5	601	CLA	C3D-C2D-C1D	-2.11	102.96	105.83
24	B	1228	CLA	C1D-ND-C4D	-2.11	104.83	106.31
24	6	618	CLA	C1D-ND-C4D	-2.11	104.83	106.31
27	A	4001	BCR	C38-C26-C27	2.10	118.08	113.60
41	3	608	CHL	C1A-CHA-C4D	2.10	122.49	118.98
41	1	613	CHL	C1-O2A-CGA	2.10	122.65	116.67
24	A	1141	CLA	CHA-C1A-NA	-2.10	121.63	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	3	618	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
24	5	608	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
24	6	612	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
27	A	4005	BCR	C38-C26-C27	2.10	118.08	113.60
24	A	1013	CLA	CHD-C1D-ND	-2.10	121.84	124.80
24	6	617	CLA	C2D-C1D-ND	2.10	112.21	110.13
24	B	1208	CLA	CHA-C1A-NA	-2.10	121.63	126.39
40	7	501	LUT	C27-C28-C29	-2.10	121.80	126.32
27	A	4003	BCR	C2-C1-C6	2.10	113.49	110.44
24	4	606	CLA	CHA-C1A-NA	-2.10	121.63	126.39
24	5	606	CLA	CHA-C1A-NA	-2.10	121.63	126.39
24	B	1217	CLA	O1D-CGD-CBD	-2.10	120.37	124.52
24	5	607	CLA	CMD-C2D-C3D	-2.10	122.87	127.69
24	1	612	CLA	O2A-CGA-CBA	2.10	118.24	111.83
24	B	1023	CLA	C2C-C1C-NC	2.10	112.19	109.98
27	B	4002	BCR	C33-C5-C4	2.10	118.08	113.60
24	a	604	CLA	C2D-C1D-ND	2.10	112.20	110.13
40	9	502	LUT	C35-C15-C14	-2.10	119.22	123.52
24	B	1206	CLA	CHA-C1A-NA	-2.10	121.64	126.39
24	9	605	CLA	OBD-CAD-C3D	-2.10	123.51	128.42
24	H	1701	CLA	O2A-CGA-CBA	2.10	118.24	111.83
24	B	1224	CLA	C2D-C1D-ND	2.10	112.20	110.13
24	4	615	CLA	CHD-C1D-ND	-2.10	121.85	124.80
24	9	604	CLA	CHA-C1A-NA	-2.10	121.64	126.39
24	2	603	CLA	O2A-CGA-CBA	2.10	118.24	111.83
24	B	1206	CLA	C4B-CHC-C1C	2.10	131.18	126.25
24	B	1201	CLA	CHA-C1A-NA	-2.10	121.64	126.39
27	H	4001	BCR	C38-C26-C25	-2.10	122.19	124.48
24	B	1213	CLA	O2D-CGD-O1D	-2.10	119.76	123.85
24	1	615	CLA	C2D-C1D-ND	2.10	112.20	110.13
24	2	605	CLA	CHD-C1D-ND	-2.10	121.85	124.80
27	5	504	BCR	C27-C26-C25	-2.10	119.87	122.70
24	7	606	CLA	C1D-ND-C4D	-2.10	104.84	106.31
24	9	605	CLA	C1D-ND-C4D	-2.10	104.84	106.31
24	A	1113	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
24	5	614	CLA	C2D-C1D-ND	2.10	112.20	110.13
24	8	607	CLA	CAA-C2A-C3A	-2.10	107.33	113.00
27	I	4001	BCR	C36-C18-C17	-2.10	119.42	122.82
24	6	618	CLA	O2D-CGD-O1D	-2.10	119.77	123.85
24	6	617	CLA	C1D-ND-C4D	-2.10	104.84	106.31
24	4	611	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
24	4	616	CLA	O1D-CGD-CBD	-2.10	120.38	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	9	502	LUT	C22-C23-C24	-2.10	108.07	111.18
24	4	607	CLA	CMD-C2D-C3D	-2.10	122.88	127.69
41	a	610	CHL	C1-O2A-CGA	2.10	122.62	116.67
24	8	605	CLA	CHD-C1D-ND	-2.10	121.85	124.80
24	A	1101	CLA	C1-O2A-CGA	2.10	121.72	116.65
24	B	1221	CLA	CMC-C2C-C1C	2.10	128.31	125.03
24	6	615	CLA	C1D-ND-C4D	-2.10	104.84	106.31
24	B	1208	CLA	C3B-C4B-NB	-2.09	108.66	110.53
24	3	602	CLA	C3B-C4B-NB	-2.09	108.66	110.53
41	8	601	CHL	CMD-C2D-C3D	2.09	128.87	124.68
40	1	502	LUT	C19-C9-C8	2.09	121.29	118.09
24	3	605	CLA	CHD-C1D-ND	-2.09	121.86	124.80
24	6	607	CLA	CHD-C1D-ND	-2.09	121.86	124.80
24	7	610	CLA	C1-O2A-CGA	2.09	121.72	116.65
24	5	601	CLA	C1D-ND-C4D	-2.09	104.84	106.31
24	B	1234	CLA	C1C-C2C-C3C	-2.09	104.78	106.98
24	B	1221	CLA	C2D-C1D-ND	2.09	112.20	110.13
24	B	1222	CLA	C2D-C1D-ND	2.09	112.20	110.13
24	1	604	CLA	C3B-C4B-NB	-2.09	108.66	110.53
24	5	601	CLA	C6-C5-C3	-2.09	108.37	113.47
24	a	612	CLA	CHA-C1A-NA	-2.09	121.65	126.39
39	M	4001	ECH	C4-C5-C6	-2.09	119.88	122.70
24	A	1102	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
24	3	605	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
24	A	1012	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
27	B	4006	BCR	C34-C9-C10	-2.09	119.43	122.82
24	7	601	CLA	O2D-CGD-O1D	-2.09	119.78	123.85
27	A	4003	BCR	C29-C30-C25	2.09	113.48	110.44
40	2	502	LUT	C10-C11-C12	-2.09	117.14	123.20
24	B	1213	CLA	CHA-C1A-NA	-2.09	121.66	126.39
24	H	1702	CLA	CHA-C1A-NA	-2.09	121.66	126.39
27	4	503	BCR	C24-C25-C26	-2.09	116.74	121.56
52	9	504	A8S	O7-C7-C12	-2.09	104.82	109.72
24	A	1140	CLA	CAA-C2A-C3A	-2.09	107.35	113.00
41	6	611	CHL	CMD-C2D-C3D	2.09	128.86	124.68
24	A	1130	CLA	CMD-C2D-C3D	-2.09	122.90	127.69
24	A	1108	CLA	C1D-ND-C4D	-2.09	104.85	106.31
24	5	612	CLA	C1D-ND-C4D	-2.09	104.85	106.31
24	A	1013	CLA	C1C-C2C-C3C	-2.09	104.78	106.98
27	A	4001	BCR	C30-C25-C26	-2.09	119.78	122.64
24	A	1126	CLA	C2D-C1D-ND	2.09	112.19	110.13
24	2	608	CLA	C2D-C1D-ND	2.09	112.19	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	1202	CLA	CMD-C2D-C3D	-2.09	122.90	127.69
24	7	608	CLA	CHD-C1D-ND	-2.09	121.86	124.80
40	a	501	LUT	C8-C7-C6	-2.09	121.42	127.00
41	6	613	CHL	CMD-C2D-C3D	2.09	128.85	124.68
24	4	612	CLA	C2C-C1C-NC	2.09	112.17	109.98
24	B	1203	CLA	O2A-CGA-CBA	2.09	118.19	111.83
24	4	607	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
24	A	1107	CLA	CMD-C2D-C3D	-2.09	122.91	127.69
24	9	606	CLA	CHA-C1A-NA	-2.08	121.67	126.39
24	A	1128	CLA	CHD-C1D-ND	-2.08	121.87	124.80
24	K	1401	CLA	CHD-C1D-ND	-2.08	121.87	124.80
24	3	602	CLA	C2D-C1D-ND	2.08	112.19	110.13
24	5	612	CLA	C2D-C1D-ND	2.08	112.19	110.13
24	2	610	CLA	C2D-C1D-ND	2.08	112.19	110.13
41	3	611	CHL	C4C-CHD-C1D	2.08	123.53	116.07
24	5	609	CLA	O1D-CGD-CBD	-2.08	120.41	124.52
24	8	611	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
24	4	605	CLA	CHD-C1D-ND	-2.08	121.87	124.80
24	9	608	CLA	C1D-ND-C4D	-2.08	104.85	106.31
24	B	1228	CLA	C2D-C1D-ND	2.08	112.19	110.13
24	A	1117	CLA	CMD-C2D-C3D	-2.08	122.91	127.69
24	A	1122	CLA	CMD-C2D-C3D	-2.08	122.91	127.69
40	4	501	LUT	C8-C7-C6	-2.08	121.44	127.00
24	5	616	CLA	C2D-C1D-ND	2.08	112.19	110.13
24	B	1022	CLA	C6-C5-C3	-2.08	108.40	113.47
24	8	607	CLA	O1D-CGD-CBD	-2.08	120.41	124.52
24	A	1120	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
27	6	504	BCR	C1-C6-C5	-2.08	119.79	122.64
24	F	1301	CLA	C1D-ND-C4D	-2.08	104.85	106.31
24	6	602	CLA	CMA-C3A-C4A	2.08	117.36	111.77
24	4	603	CLA	O2A-CGA-CBA	2.08	118.18	111.83
24	1	615	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
31	1	804	LMT	O5B-C5B-C4B	2.08	113.45	109.70
24	6	604	CLA	C3B-C4B-NB	-2.08	108.67	110.53
24	1	610	CLA	C1C-C2C-C3C	-2.08	104.79	106.98
24	7	606	CLA	CMA-C3A-C4A	2.08	117.36	111.77
40	8	502	LUT	C38-C25-C24	-2.08	118.44	123.36
24	6	601	CLA	C3D-C2D-C1D	-2.08	103.00	105.83
24	G	1601	CLA	CMD-C2D-C3D	-2.08	122.92	127.69
40	5	501	LUT	C38-C25-C24	-2.08	118.44	123.36
24	5	607	CLA	C2D-C1D-ND	2.08	112.18	110.13
27	3	505	BCR	C4-C5-C6	-2.08	119.90	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	611	CLA	CMC-C2C-C1C	2.08	128.28	125.03
24	B	1211	CLA	C3B-C4B-NB	-2.08	108.68	110.53
24	a	608	CLA	C2D-C1D-ND	2.08	112.18	110.13
24	B	1216	CLA	C1-O2A-CGA	2.08	121.68	116.65
24	A	1117	CLA	C1-O2A-CGA	2.08	121.67	116.65
41	1	613	CHL	C1C-C2C-CMC	2.08	130.54	126.80
24	5	607	CLA	OBD-CAD-C3D	-2.08	123.57	128.42
24	A	1115	CLA	O2A-CGA-CBA	2.07	118.16	111.83
24	4	610	CLA	O2A-CGA-CBA	2.07	118.16	111.83
24	G	1602	CLA	C2D-C1D-ND	2.07	112.18	110.13
40	1	503	LUT	C22-C23-C24	-2.07	108.10	111.18
24	5	618	CLA	O2A-CGA-CBA	2.07	118.16	111.83
24	B	1208	CLA	CBA-CAA-C2A	2.07	119.96	113.79
24	B	1229	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
24	K	1404	CLA	CHA-C1A-NA	-2.07	121.70	126.39
41	1	613	CHL	CMD-C2D-C3D	2.07	128.82	124.68
40	2	501	LUT	C22-C23-C24	-2.07	108.11	111.18
24	7	607	CLA	CMD-C2D-C3D	-2.07	122.94	127.69
24	7	609	CLA	CHA-C1A-NA	-2.07	121.70	126.39
24	G	1601	CLA	CHD-C1D-ND	-2.07	121.89	124.80
24	a	605	CLA	C1D-ND-C4D	-2.07	104.86	106.31
24	a	608	CLA	C1D-ND-C4D	-2.07	104.86	106.31
24	L	1503	CLA	CAA-C2A-C3A	-2.07	107.40	113.00
27	6	503	BCR	C29-C28-C27	2.07	115.83	111.28
24	A	1127	CLA	C2D-C1D-ND	2.07	112.17	110.13
24	7	601	CLA	C2D-C1D-ND	2.07	112.17	110.13
24	A	1122	CLA	C1-O2A-CGA	2.07	121.66	116.65
24	A	1110	CLA	CHA-C1A-NA	-2.07	121.70	126.39
27	6	504	BCR	C27-C26-C25	-2.07	119.91	122.70
24	B	1238	CLA	C6-C5-C3	-2.07	108.43	113.47
24	B	1216	CLA	O2A-CGA-CBA	2.07	118.15	111.83
27	K	4002	BCR	C37-C22-C21	-2.07	119.46	122.82
24	A	1137	CLA	CAA-CBA-CGA	-2.07	107.34	113.21
24	A	1134	CLA	C1D-ND-C4D	-2.07	104.86	106.31
24	4	603	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
24	G	1601	CLA	C1-O2A-CGA	2.07	121.66	116.65
24	2	615	CLA	O2A-CGA-CBA	2.07	118.14	111.83
24	8	609	CLA	CMD-C2D-C3D	-2.07	122.95	127.69
24	H	1703	CLA	O2A-CGA-CBA	2.07	118.14	111.83
24	A	1119	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
27	6	503	BCR	C8-C9-C10	2.07	122.26	119.01
24	6	606	CLA	C3B-C4B-NB	-2.07	108.69	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	1226	CLA	C4B-CHC-C1C	2.07	131.11	126.25
24	5	609	CLA	C1D-ND-C4D	-2.07	104.86	106.31
24	8	618	CLA	C1D-ND-C4D	-2.07	104.86	106.31
24	A	1115	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
41	4	618	CHL	CMD-C2D-C3D	2.07	128.81	124.68
24	9	601	CLA	C1C-C2C-C3C	-2.07	104.81	106.98
24	G	1602	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
24	B	1206	CLA	CMD-C2D-C3D	-2.07	122.95	127.69
24	5	608	CLA	CHD-C1D-ND	-2.07	121.90	124.80
24	A	1114	CLA	C1D-ND-C4D	-2.07	104.86	106.31
24	A	1121	CLA	C3D-C2D-C1D	-2.06	103.01	105.83
24	B	1220	CLA	CHA-C1A-NA	-2.06	121.72	126.39
27	B	4001	BCR	C29-C28-C27	2.06	115.82	111.28
24	A	1134	CLA	C2D-C1D-ND	2.06	112.17	110.13
24	3	605	CLA	C2D-C1D-ND	2.06	112.17	110.13
24	a	611	CLA	CHD-C1D-ND	-2.06	121.90	124.80
24	A	1120	CLA	O2A-CGA-CBA	2.06	118.13	111.83
24	1	608	CLA	C1D-ND-C4D	-2.06	104.86	106.31
24	8	608	CLA	C1D-ND-C4D	-2.06	104.86	106.31
24	A	1111	CLA	O1D-CGD-CBD	-2.06	120.45	124.52
24	K	1402	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
24	4	604	CLA	C2D-C1D-ND	2.06	112.17	110.13
24	a	604	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
27	L	4001	BCR	C38-C26-C27	2.06	117.99	113.60
24	B	1206	CLA	CAA-C2A-C3A	-2.06	107.42	113.00
27	L	4002	BCR	C27-C26-C25	-2.06	119.92	122.70
24	A	1124	CLA	C1D-ND-C4D	-2.06	104.86	106.31
24	2	608	CLA	C1D-ND-C4D	-2.06	104.86	106.31
24	B	1202	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
24	A	1124	CLA	O1D-CGD-CBD	-2.06	120.45	124.52
24	3	618	CLA	CAA-C2A-C3A	-2.06	107.43	113.00
24	1	605	CLA	O1D-CGD-CBD	-2.06	120.45	124.52
24	3	604	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
24	6	609	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
24	A	1112	CLA	C2D-C1D-ND	2.06	112.17	110.13
24	A	1116	CLA	C2D-C1D-ND	2.06	112.17	110.13
24	9	604	CLA	CHD-C1D-ND	-2.06	121.90	124.80
24	2	605	CLA	C1D-ND-C4D	-2.06	104.87	106.31
24	A	1133	CLA	CAA-C2A-C3A	-2.06	107.43	113.00
24	J	1901	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
24	a	601	CLA	C2D-C1D-ND	2.06	112.16	110.13
24	A	1122	CLA	C3D-C2D-C1D	-2.06	103.02	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	7	602	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
24	a	602	CLA	CHD-C1D-ND	-2.06	121.91	124.80
24	6	608	CLA	CHA-C1A-NA	-2.06	121.73	126.39
40	8	501	LUT	C37-C21-C22	-2.06	105.57	109.41
27	6	503	BCR	C35-C13-C14	-2.06	119.48	122.82
24	4	611	CLA	O2A-CGA-CBA	2.06	118.11	111.83
24	A	1119	CLA	C2D-C1D-ND	2.06	112.16	110.13
24	K	1404	CLA	C2D-C1D-ND	2.06	112.16	110.13
24	1	604	CLA	C2D-C1D-ND	2.06	112.16	110.13
24	A	1127	CLA	C1D-ND-C4D	-2.06	104.87	106.31
24	A	1133	CLA	C1D-ND-C4D	-2.06	104.87	106.31
24	1	607	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
42	1	803	OLA	C3-C2-C1	-2.06	109.14	114.51
24	B	1021	CLA	C2C-C1C-NC	2.06	112.14	109.98
41	6	611	CHL	C1C-C2C-CMC	2.06	130.51	126.80
24	A	1137	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
41	1	609	CHL	CMD-C2D-C3D	2.06	128.79	124.68
24	9	612	CLA	C1D-ND-C4D	-2.06	104.87	106.31
24	4	604	CLA	CHA-C1A-NA	-2.06	121.73	126.39
24	A	1113	CLA	C2D-C1D-ND	2.06	112.16	110.13
24	F	1301	CLA	C2D-C1D-ND	2.06	112.16	110.13
24	7	609	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
40	9	501	LUT	C27-C28-C29	-2.06	121.90	126.32
24	1	606	CLA	CMA-C3A-C4A	2.06	117.30	111.77
24	A	1112	CLA	C3B-C4B-NB	-2.06	108.69	110.53
24	7	601	CLA	C3D-C2D-C1D	-2.06	103.03	105.83
41	a	609	CHL	CMD-C2D-C3D	2.05	128.79	124.68
41	9	613	CHL	CMD-C2D-C3D	2.05	128.79	124.68
24	6	609	CLA	CHD-C1D-ND	-2.05	121.91	124.80
24	4	611	CLA	CHA-C1A-NA	-2.05	121.74	126.39
24	A	1118	CLA	CMD-C2D-C3D	-2.05	122.98	127.69
24	4	601	CLA	C2D-C1D-ND	2.05	112.16	110.13
24	5	609	CLA	C2D-C1D-ND	2.05	112.16	110.13
24	A	1123	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
40	6	502	LUT	C16-C1-C6	-2.05	107.02	110.24
41	6	610	CHL	CMA-C3A-C4A	2.05	119.04	114.61
24	7	604	CLA	C6-C5-C3	-2.05	108.47	113.47
24	A	1104	CLA	C2D-C1D-ND	2.05	112.16	110.13
24	a	615	CLA	CHA-C1A-NA	-2.05	121.74	126.39
27	7	503	BCR	C37-C22-C23	2.05	121.22	118.09
24	2	605	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
27	5	504	BCR	C35-C13-C14	-2.05	119.49	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	8	606	CLA	C1-O2A-CGA	2.05	121.62	116.65
24	5	605	CLA	CHD-C1D-ND	-2.05	121.92	124.80
24	4	602	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
27	3	505	BCR	C34-C9-C10	-2.05	119.49	122.82
40	1	501	LUT	C30-C31-C32	-2.05	117.26	123.20
41	6	613	CHL	C3D-C4D-ND	-2.05	109.65	112.94
24	A	1106	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
28	F	5002	LHG	O7-C7-O9	-2.05	118.91	123.70
24	6	617	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
24	L	1502	CLA	C2D-C1D-ND	2.05	112.16	110.13
41	5	610	CHL	C3D-C4D-ND	-2.05	109.65	112.94
24	3	618	CLA	C1D-ND-C4D	-2.05	104.87	106.31
24	B	1239	CLA	CBC-CAC-C3C	-2.05	106.86	112.42
24	4	610	CLA	C3B-C4B-NB	-2.05	108.70	110.53
24	B	1212	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
24	3	607	CLA	CHD-C1D-ND	-2.05	121.92	124.80
40	2	501	LUT	C20-C13-C12	2.05	121.22	118.09
24	B	1223	CLA	CAA-C2A-C3A	-2.05	107.46	113.00
24	5	618	CLA	CMD-C2D-C3D	-2.05	122.99	127.69
24	1	607	CLA	C1D-ND-C4D	-2.05	104.88	106.31
24	5	616	CLA	CHD-C1D-ND	-2.05	121.92	124.80
28	1	802	LHG	O7-C7-O9	-2.05	118.92	123.70
28	2	801	LHG	O7-C7-O9	-2.05	118.92	123.70
24	2	605	CLA	C2D-C1D-ND	2.05	112.15	110.13
24	5	607	CLA	CHD-C1D-ND	-2.05	121.92	124.80
24	3	602	CLA	O1D-CGD-CBD	-2.05	120.48	124.52
24	6	608	CLA	C1D-ND-C4D	-2.05	104.88	106.31
24	A	1125	CLA	C3B-C4B-NB	-2.05	108.70	110.53
24	B	1235	CLA	O1D-CGD-CBD	-2.05	120.48	124.52
41	3	608	CHL	C1C-C2C-CMC	2.05	130.49	126.80
24	3	602	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
24	3	613	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
40	3	501	LUT	C3-C4-C5	-2.05	107.08	112.18
24	6	617	CLA	O1D-CGD-CBD	-2.05	120.48	124.52
24	A	1134	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
41	3	611	CHL	C3D-C4D-ND	-2.05	109.66	112.94
24	1	602	CLA	C2D-C1D-ND	2.05	112.15	110.13
40	2	501	LUT	C30-C31-C32	-2.04	117.28	123.20
27	L	4002	BCR	C38-C26-C25	-2.04	122.25	124.48
40	3	502	LUT	C30-C31-C32	-2.04	117.28	123.20
24	a	602	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
40	a	502	LUT	C22-C23-C24	-2.04	108.15	111.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1132	CLA	CHA-C1A-NA	-2.04	121.76	126.39
24	A	1107	CLA	C3B-C4B-NB	-2.04	108.71	110.53
41	6	610	CHL	CMD-C2D-C3D	2.04	128.77	124.68
24	B	1240	CLA	C2D-C1D-ND	2.04	112.15	110.13
24	7	610	CLA	CMD-C2D-C3D	-2.04	123.00	127.69
40	2	501	LUT	C27-C28-C29	-2.04	121.93	126.32
24	A	1124	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
24	B	1201	CLA	C2D-C1D-ND	2.04	112.15	110.13
24	A	1113	CLA	CAA-C2A-C3A	-2.04	107.48	113.00
24	a	603	CLA	C1-O2A-CGA	2.04	121.59	116.65
40	5	502	LUT	C3-C4-C5	-2.04	107.09	112.18
24	B	1235	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
24	4	604	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
28	a	801	LHG	O7-C7-O9	-2.04	118.94	123.70
40	9	501	LUT	C30-C31-C32	-2.04	117.29	123.20
24	B	1210	CLA	C2D-C1D-ND	2.04	112.14	110.13
24	A	1125	CLA	CMD-C2D-C3D	-2.04	123.01	127.69
27	A	4003	BCR	C23-C24-C25	-2.04	121.55	127.00
24	9	604	CLA	CAA-C2A-C3A	-2.04	107.49	113.00
27	B	4001	BCR	C33-C5-C4	2.04	117.94	113.60
24	6	606	CLA	CAA-C2A-C3A	-2.04	107.49	113.00
24	9	608	CLA	CMD-C2D-C3D	-2.04	123.02	127.69
24	9	606	CLA	C2D-C1D-ND	2.04	112.14	110.13
24	B	1210	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
24	A	1107	CLA	CAA-CBA-CGA	-2.04	107.42	113.21
24	2	602	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
24	A	1112	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
24	9	603	CLA	C2A-C1A-CHA	2.04	127.40	123.87
24	A	1136	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
24	3	602	CLA	O2A-CGA-CBA	2.04	119.83	112.14
24	7	608	CLA	CMD-C2D-C3D	-2.04	123.02	127.69
24	B	1202	CLA	C2A-C1A-CHA	2.04	127.40	123.87
24	F	1301	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
24	4	607	CLA	CHD-C1D-ND	-2.04	121.94	124.80
24	B	1204	CLA	CMD-C2D-C3D	-2.04	123.02	127.69
40	1	502	LUT	C16-C1-C6	-2.04	107.05	110.24
24	2	602	CLA	C3D-C2D-C1D	-2.03	103.05	105.83
27	B	4001	BCR	C23-C24-C25	-2.03	121.56	127.00
27	B	4006	BCR	C23-C24-C25	-2.03	121.56	127.00
24	8	603	CLA	C6-C5-C3	-2.03	108.51	113.47
24	3	606	CLA	C3B-C4B-NB	-2.03	108.71	110.53
24	A	1107	CLA	CHD-C1D-ND	-2.03	121.94	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	4004	BCR	C34-C9-C8	2.03	121.19	118.09
24	3	610	CLA	C1D-ND-C4D	-2.03	104.89	106.31
41	a	613	CHL	CMD-C2D-C3D	2.03	128.75	124.68
40	3	502	LUT	C19-C9-C8	2.03	121.19	118.09
24	B	1210	CLA	C3B-C4B-NB	-2.03	108.72	110.53
24	A	1128	CLA	C4B-CHC-C1C	2.03	131.03	126.25
24	1	607	CLA	C2D-C1D-ND	2.03	112.14	110.13
24	4	605	CLA	O1D-CGD-CBD	-2.03	120.51	124.52
41	9	610	CHL	C4C-CHD-C1D	2.03	123.34	116.07
24	3	604	CLA	C3B-C4B-NB	-2.03	108.72	110.53
24	a	602	CLA	CMD-C2D-C3D	-2.03	123.03	127.69
24	7	617	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
24	3	616	CLA	CHA-C1A-NA	-2.03	121.79	126.39
24	B	1223	CLA	CMD-C2D-C3D	-2.03	123.03	127.69
24	A	1136	CLA	CHA-C1A-NA	-2.03	121.79	126.39
27	L	4002	BCR	C33-C5-C4	2.03	117.93	113.60
24	8	602	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
24	K	1403	CLA	CAA-C2A-C3A	-2.03	107.51	113.00
24	B	1218	CLA	C2D-C1D-ND	2.03	112.14	110.13
24	8	602	CLA	O2A-CGA-CBA	2.03	118.03	111.83
24	B	1022	CLA	CBB-CAB-C3B	-2.03	117.38	127.53
24	F	1302	CLA	C2D-C1D-ND	2.03	112.14	110.13
24	A	1117	CLA	C3B-C4B-NB	-2.03	108.72	110.53
24	5	616	CLA	C1D-ND-C4D	-2.03	104.89	106.31
24	8	608	CLA	CHA-C1A-NA	-2.03	121.80	126.39
24	a	603	CLA	O2A-CGA-CBA	2.03	118.02	111.83
24	4	616	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
24	6	607	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
24	A	1139	CLA	C2D-C1D-ND	2.03	112.13	110.13
24	A	1125	CLA	C2A-C1A-CHA	2.03	127.39	123.87
41	6	619	CHL	CMD-C2D-C3D	2.03	128.74	124.68
24	A	1109	CLA	C3B-C4B-NB	-2.03	108.72	110.53
24	6	605	CLA	CAA-C2A-C3A	-2.03	107.52	113.00
24	A	1133	CLA	CHA-C1A-NA	-2.03	121.80	126.39
24	A	1102	CLA	C3B-C2B-C1B	-2.03	104.78	107.17
41	3	608	CHL	CMD-C2D-C3D	2.03	128.73	124.68
24	G	1603	CLA	CAA-C2A-C3A	-2.03	107.52	113.00
28	7	803	LHG	O7-C7-O9	-2.03	118.97	123.70
24	8	610	CLA	C3D-C2D-C1D	-2.03	103.07	105.83
24	B	1222	CLA	O2D-CGD-O1D	-2.03	119.91	123.85
24	B	1226	CLA	CAA-C2A-C3A	-2.02	107.53	113.00
24	B	1213	CLA	C2D-C1D-ND	2.02	112.13	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	4005	BCR	C23-C24-C25	-2.02	121.59	127.00
41	a	606	CHL	CMD-C2D-C3D	2.02	128.73	124.68
24	B	1211	CLA	CHA-C1A-NA	-2.02	121.81	126.39
24	3	604	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
24	a	601	CLA	CHA-C1A-NA	-2.02	121.81	126.39
24	3	616	CLA	CMD-C2D-C3D	-2.02	123.05	127.69
24	B	1237	CLA	CHD-C1D-ND	-2.02	121.95	124.80
40	6	502	LUT	C38-C25-C24	-2.02	118.57	123.36
24	A	1121	CLA	C2D-C1D-ND	2.02	112.13	110.13
24	B	1209	CLA	C2D-C1D-ND	2.02	112.13	110.13
24	B	1023	CLA	C1-O2A-CGA	2.02	121.55	116.65
40	3	501	LUT	C20-C13-C12	2.02	121.18	118.09
24	B	1240	CLA	C1D-ND-C4D	-2.02	104.89	106.31
24	6	602	CLA	C1D-ND-C4D	-2.02	104.89	106.31
24	A	1112	CLA	CAA-C2A-C3A	-2.02	107.53	113.00
24	A	1105	CLA	C2D-C1D-ND	2.02	112.13	110.13
24	B	1222	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
24	B	1234	CLA	OBD-CAD-C3D	-2.02	123.69	128.42
24	1	607	CLA	O2A-CGA-CBA	2.02	118.00	111.83
24	a	605	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
24	2	601	CLA	O2A-CGA-CBA	2.02	117.99	111.83
24	B	1214	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
24	K	1404	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
24	a	608	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
24	A	1108	CLA	C2D-C1D-ND	2.02	112.12	110.13
24	A	1113	CLA	C3B-C4B-NB	-2.02	108.73	110.53
27	H	4001	BCR	C23-C22-C21	2.02	122.18	119.01
24	A	1111	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
24	4	604	CLA	C1-O2A-CGA	2.02	121.53	116.65
24	A	1102	CLA	CMA-C3A-C2A	2.02	121.78	113.98
24	9	607	CLA	CAA-C2A-C3A	-2.02	107.55	113.00
24	2	603	CLA	C2A-C1A-CHA	2.02	127.37	123.87
27	5	504	BCR	C30-C25-C24	2.02	121.12	115.65
24	1	610	CLA	C2D-C1D-ND	2.02	112.12	110.13
24	7	609	CLA	C2D-C1D-ND	2.02	112.12	110.13
24	2	601	CLA	C2D-C1D-ND	2.02	112.12	110.13
24	a	602	CLA	C1D-ND-C4D	-2.02	104.90	106.31
24	5	614	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
24	B	1217	CLA	CHD-C1D-ND	-2.02	121.97	124.80
24	A	1105	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
24	4	601	CLA	CMA-C3A-C4A	2.02	117.19	111.77
27	B	4002	BCR	C36-C18-C17	-2.02	119.55	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	4	617	CLA	C1D-ND-C4D	-2.02	104.90	106.31
24	A	1119	CLA	CHA-C1A-NA	-2.01	121.83	126.39
24	1	611	CLA	C1D-ND-C4D	-2.01	104.90	106.31
24	a	612	CLA	C1D-ND-C4D	-2.01	104.90	106.31
24	A	1105	CLA	CAA-C2A-C3A	-2.01	107.56	113.00
24	7	603	CLA	C2D-C1D-ND	2.01	112.12	110.13
27	5	504	BCR	C23-C24-C25	-2.01	121.62	127.00
40	1	503	LUT	C11-C12-C13	-2.01	120.84	126.36
24	2	608	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
24	B	1230	CLA	CHA-C1A-NA	-2.01	121.83	126.39
40	3	501	LUT	C31-C32-C33	-2.01	120.84	126.36
24	A	1115	CLA	CHA-C1A-NA	-2.01	121.83	126.39
40	6	501	LUT	C28-C29-C30	2.01	122.17	119.01
24	9	605	CLA	CHD-C1D-ND	-2.01	121.97	124.80
24	B	1230	CLA	CAA-CBA-CGA	-2.01	107.50	113.21
24	9	604	CLA	C1D-ND-C4D	-2.01	104.90	106.31
27	G	4001	BCR	C23-C24-C25	-2.01	121.63	127.00
24	B	1240	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
24	B	1212	CLA	C2D-C1D-ND	2.01	112.12	110.13
24	B	1236	CLA	CMD-C2D-C3D	-2.01	123.08	127.69
24	B	1228	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
24	A	1119	CLA	CMD-C2D-C3D	-2.01	123.08	127.69
24	B	1223	CLA	C1D-ND-C4D	-2.01	104.90	106.31
24	L	1503	CLA	CHA-C1A-NA	-2.01	121.84	126.39
24	5	617	CLA	CMD-C2D-C3D	-2.01	123.08	127.69
24	A	1138	CLA	CHA-C1A-NA	-2.01	121.84	126.39
24	H	1701	CLA	CHA-C1A-NA	-2.01	121.84	126.39
24	7	602	CLA	O1D-CGD-CBD	-2.01	120.56	124.52
24	3	601	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
27	B	4004	BCR	C35-C13-C12	2.01	121.16	118.09
24	6	604	CLA	C2D-C1D-ND	2.01	112.11	110.13
24	B	1240	CLA	C2A-C1A-CHA	2.01	127.35	123.87
24	2	613	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
41	6	610	CHL	C4D-ND-C1D	2.01	106.74	105.22
24	4	612	CLA	C1D-ND-C4D	-2.01	104.90	106.31
24	2	605	CLA	O1D-CGD-CBD	-2.01	120.56	124.52
24	6	609	CLA	CMD-C2D-C3D	-2.01	123.09	127.69
24	B	1227	CLA	C1D-ND-C4D	-2.01	104.91	106.31
24	B	1239	CLA	O1D-CGD-CBD	-2.01	120.56	124.52
24	3	610	CLA	C3B-C4B-NB	-2.01	108.74	110.53
24	A	1119	CLA	O2A-CGA-CBA	2.00	117.95	111.83
24	B	1218	CLA	C3D-C2D-C1D	-2.00	103.09	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	1207	CLA	C2D-C1D-ND	2.00	112.11	110.13
24	8	610	CLA	C2A-C1A-CHA	2.00	127.34	123.87
24	9	603	CLA	C1D-ND-C4D	-2.00	104.91	106.31
24	K	1402	CLA	C2D-C1D-ND	2.00	112.11	110.13
24	A	1104	CLA	CHA-C1A-NA	-2.00	121.86	126.39
24	8	607	CLA	CHA-C1A-NA	-2.00	121.86	126.39
24	B	1219	CLA	O2A-CGA-CBA	2.00	117.94	111.83
24	A	1125	CLA	C1D-ND-C4D	-2.00	104.91	106.31
27	B	4004	BCR	C31-C1-C6	-2.00	107.10	110.24
24	A	1141	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
24	A	1124	CLA	CHA-C1A-NA	-2.00	121.86	126.39
24	2	606	CLA	C2D-C1D-ND	2.00	112.11	110.13
41	7	613	CHL	C3D-C4D-ND	-2.00	109.73	112.94
24	A	1122	CLA	CHA-C1A-NA	-2.00	121.86	126.39
24	H	1703	CLA	CHA-C1A-NA	-2.00	121.86	126.39
24	5	601	CLA	C2A-C1A-CHA	2.00	127.34	123.87
24	K	1403	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
24	2	609	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
24	1	608	CLA	CHA-C1A-NA	-2.00	121.86	126.39
45	6	804	PLM	O1-C1-C2	2.00	120.32	114.00
24	A	1106	CLA	CAA-C2A-C1A	-2.00	105.42	111.97
40	5	505	LUT	C38-C25-C24	-2.00	118.63	123.36

All (331) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	1011	CL0	ND
23	A	1011	CL0	NA
23	A	1011	CL0	NC
24	A	1012	CLA	ND
24	A	1013	CLA	ND
24	A	1101	CLA	ND
24	A	1102	CLA	ND
24	A	1103	CLA	ND
24	A	1104	CLA	ND
24	A	1105	CLA	ND
24	A	1106	CLA	ND
24	A	1107	CLA	ND
24	A	1108	CLA	ND
24	A	1109	CLA	ND
24	A	1110	CLA	ND
24	A	1111	CLA	ND

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Mol	Chain	Res	Type	Atom
24	A	1112	CLA	ND
24	A	1113	CLA	ND
24	A	1114	CLA	ND
24	A	1115	CLA	ND
24	A	1116	CLA	ND
24	A	1117	CLA	ND
24	A	1118	CLA	ND
24	A	1119	CLA	ND
24	A	1120	CLA	ND
24	A	1121	CLA	ND
24	A	1122	CLA	ND
24	A	1123	CLA	ND
24	A	1124	CLA	ND
24	A	1125	CLA	ND
24	A	1126	CLA	ND
24	A	1127	CLA	ND
24	A	1128	CLA	ND
24	A	1129	CLA	ND
24	A	1130	CLA	ND
24	A	1131	CLA	ND
24	A	1132	CLA	ND
24	A	1133	CLA	ND
24	A	1134	CLA	ND
24	A	1135	CLA	ND
24	A	1136	CLA	ND
24	A	1137	CLA	ND
24	A	1138	CLA	ND
24	A	1139	CLA	ND
24	A	1140	CLA	ND
24	A	1141	CLA	ND
24	B	1021	CLA	ND
24	B	1022	CLA	ND
24	B	1023	CLA	ND
24	B	1201	CLA	ND
24	B	1202	CLA	ND
24	B	1203	CLA	ND
24	B	1204	CLA	ND
24	B	1205	CLA	ND
24	B	1206	CLA	ND
24	B	1207	CLA	ND
24	B	1208	CLA	ND
24	B	1209	CLA	ND

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Mol	Chain	Res	Type	Atom
24	B	1210	CLA	ND
24	B	1211	CLA	ND
24	B	1212	CLA	ND
24	B	1213	CLA	ND
24	B	1214	CLA	ND
24	B	1215	CLA	ND
24	B	1216	CLA	ND
24	B	1217	CLA	ND
24	B	1218	CLA	ND
24	B	1219	CLA	ND
24	B	1220	CLA	ND
24	B	1221	CLA	ND
24	B	1222	CLA	ND
24	B	1223	CLA	ND
24	B	1224	CLA	ND
24	B	1225	CLA	ND
24	B	1226	CLA	ND
24	B	1227	CLA	ND
24	B	1228	CLA	ND
24	B	1229	CLA	ND
24	B	1230	CLA	ND
24	B	1231	CLA	ND
24	B	1232	CLA	ND
24	B	1234	CLA	ND
24	B	1235	CLA	ND
24	B	1236	CLA	ND
24	B	1237	CLA	ND
24	B	1238	CLA	ND
24	B	1239	CLA	ND
24	B	1240	CLA	ND
24	F	1301	CLA	ND
24	F	1302	CLA	ND
24	G	1601	CLA	ND
24	G	1602	CLA	ND
24	G	1603	CLA	ND
24	J	1901	CLA	ND
24	K	1401	CLA	ND
24	K	1402	CLA	ND
24	K	1403	CLA	ND
24	K	1404	CLA	ND
24	H	1701	CLA	ND
24	H	1702	CLA	ND

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Mol	Chain	Res	Type	Atom
24	H	1703	CLA	ND
24	L	1501	CLA	ND
24	L	1502	CLA	ND
24	L	1503	CLA	ND
24	1	601	CLA	ND
24	1	602	CLA	ND
24	1	603	CLA	ND
24	1	604	CLA	ND
24	1	605	CLA	ND
24	1	606	CLA	ND
24	1	607	CLA	ND
24	1	608	CLA	ND
24	1	610	CLA	ND
24	1	611	CLA	ND
24	1	612	CLA	ND
24	1	615	CLA	ND
24	a	601	CLA	ND
24	a	602	CLA	ND
24	a	603	CLA	ND
24	a	604	CLA	ND
24	a	605	CLA	ND
24	a	607	CLA	ND
24	a	608	CLA	ND
24	a	611	CLA	ND
24	a	612	CLA	ND
24	a	615	CLA	ND
24	3	601	CLA	ND
24	3	602	CLA	ND
24	3	603	CLA	ND
24	3	604	CLA	ND
24	3	605	CLA	ND
24	3	606	CLA	ND
24	3	607	CLA	ND
24	3	610	CLA	ND
24	3	612	CLA	ND
24	3	613	CLA	ND
24	3	616	CLA	ND
24	3	618	CLA	ND
24	4	601	CLA	ND
24	4	602	CLA	ND
24	4	603	CLA	ND
24	4	604	CLA	ND

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Mol	Chain	Res	Type	Atom
24	4	605	CLA	ND
24	4	606	CLA	ND
24	4	607	CLA	ND
24	4	608	CLA	ND
24	4	610	CLA	ND
24	4	611	CLA	ND
24	4	612	CLA	ND
24	4	615	CLA	ND
24	4	616	CLA	ND
24	4	617	CLA	ND
24	5	601	CLA	ND
24	5	602	CLA	ND
24	5	603	CLA	ND
24	5	604	CLA	ND
24	5	605	CLA	ND
24	5	606	CLA	ND
24	5	607	CLA	ND
24	5	608	CLA	ND
24	5	609	CLA	ND
24	5	612	CLA	ND
24	5	614	CLA	ND
24	5	616	CLA	ND
24	5	617	CLA	ND
24	5	618	CLA	ND
24	6	601	CLA	ND
24	6	602	CLA	ND
24	6	603	CLA	ND
24	6	604	CLA	ND
24	6	605	CLA	ND
24	6	606	CLA	ND
24	6	607	CLA	ND
24	6	608	CLA	ND
24	6	609	CLA	ND
24	6	612	CLA	ND
24	6	615	CLA	ND
24	6	617	CLA	ND
24	6	618	CLA	ND
24	7	601	CLA	ND
24	7	602	CLA	ND
24	7	603	CLA	ND
24	7	604	CLA	ND
24	7	605	CLA	ND

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Mol	Chain	Res	Type	Atom
24	7	606	CLA	ND
24	7	607	CLA	ND
24	7	608	CLA	ND
24	7	609	CLA	ND
24	7	610	CLA	ND
24	7	611	CLA	ND
24	7	612	CLA	ND
24	7	615	CLA	ND
24	7	617	CLA	ND
24	8	602	CLA	ND
24	8	603	CLA	ND
24	8	605	CLA	ND
24	8	606	CLA	ND
24	8	607	CLA	ND
24	8	608	CLA	ND
24	8	609	CLA	ND
24	8	610	CLA	ND
24	8	611	CLA	ND
24	8	612	CLA	ND
24	8	615	CLA	ND
24	8	618	CLA	ND
24	8	620	CLA	ND
24	2	601	CLA	ND
24	2	602	CLA	ND
24	2	603	CLA	ND
24	2	604	CLA	ND
24	2	605	CLA	ND
24	2	606	CLA	ND
24	2	607	CLA	ND
24	2	608	CLA	ND
24	2	609	CLA	ND
24	2	610	CLA	ND
24	2	612	CLA	ND
24	2	613	CLA	ND
24	2	615	CLA	ND
24	2	621	CLA	ND
24	9	601	CLA	ND
24	9	602	CLA	ND
24	9	603	CLA	ND
24	9	604	CLA	ND
24	9	605	CLA	ND
24	9	606	CLA	ND

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Mol	Chain	Res	Type	Atom
24	9	607	CLA	ND
24	9	608	CLA	ND
24	9	609	CLA	ND
24	9	612	CLA	ND
36	G	5002	ERG	C20
36	G	5002	ERG	C9
36	G	5002	ERG	C24
36	G	5002	ERG	C14
37	J	4002	RRX	C28
40	1	503	LUT	C26
40	6	501	LUT	C26
40	6	502	LUT	C26
40	7	501	LUT	C26
40	9	502	LUT	C26
41	1	609	CHL	ND
41	1	609	CHL	NA
41	1	609	CHL	C8
41	1	609	CHL	NC
41	1	613	CHL	ND
41	1	613	CHL	NA
41	1	613	CHL	NC
41	a	606	CHL	ND
41	a	606	CHL	NA
41	a	606	CHL	C8
41	a	606	CHL	NC
41	a	609	CHL	ND
41	a	609	CHL	NA
41	a	609	CHL	NC
41	a	610	CHL	C3A
41	a	610	CHL	NA
41	a	610	CHL	ND
41	a	610	CHL	NC
41	a	613	CHL	C3A
41	a	613	CHL	NA
41	a	613	CHL	ND
41	a	613	CHL	NC
41	3	608	CHL	ND
41	3	608	CHL	NA
41	3	608	CHL	NC
41	3	611	CHL	ND
41	3	611	CHL	NA
41	3	611	CHL	NC

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Mol	Chain	Res	Type	Atom
41	4	609	CHL	ND
41	4	609	CHL	NA
41	4	609	CHL	C8
41	4	609	CHL	NC
41	4	613	CHL	ND
41	4	613	CHL	NA
41	4	613	CHL	NC
41	4	618	CHL	ND
41	4	618	CHL	NA
41	4	618	CHL	C8
41	4	618	CHL	NC
41	5	610	CHL	ND
41	5	610	CHL	NA
41	5	610	CHL	C8
41	5	610	CHL	NC
41	5	611	CHL	ND
41	5	611	CHL	NA
41	5	611	CHL	NC
41	5	613	CHL	ND
41	5	613	CHL	NA
41	5	613	CHL	C8
41	5	613	CHL	NC
41	6	610	CHL	ND
41	6	610	CHL	NA
41	6	610	CHL	C8
41	6	610	CHL	NC
41	6	611	CHL	ND
41	6	611	CHL	NA
41	6	611	CHL	NC
41	6	613	CHL	ND
41	6	613	CHL	NA
41	6	613	CHL	NC
41	6	619	CHL	ND
41	6	619	CHL	NA
41	6	619	CHL	C8
41	6	619	CHL	NC
41	7	613	CHL	ND
41	7	613	CHL	NA
41	7	613	CHL	C8
41	7	613	CHL	NC
41	8	601	CHL	ND
41	8	601	CHL	NA

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Mol	Chain	Res	Type	Atom
41	8	601	CHL	C8
41	8	601	CHL	NC
41	8	604	CHL	ND
41	8	604	CHL	NA
41	8	604	CHL	C8
41	8	604	CHL	NC
41	8	613	CHL	ND
41	8	613	CHL	NA
41	8	613	CHL	NC
41	9	610	CHL	ND
41	9	610	CHL	NA
41	9	610	CHL	NC
41	9	613	CHL	ND
41	9	613	CHL	NA
41	9	613	CHL	NC
43	a	504	QTB	C12
43	3	506	QTB	C12
43	3	506	QTB	C11
48	7	502	XAT	C26
48	7	502	XAT	C6
49	7	504	C7Z	C3

All (4492) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	1011	CL0	C2-C1-O2A-CGA
24	A	1101	CLA	CBA-CGA-O2A-C1
24	A	1101	CLA	O1A-CGA-O2A-C1
24	A	1101	CLA	CHA-CBD-CGD-O1D
24	A	1101	CLA	CHA-CBD-CGD-O2D
24	A	1103	CLA	C3A-C2A-CAA-CBA
24	A	1103	CLA	CAD-CBD-CGD-O1D
24	A	1103	CLA	CAD-CBD-CGD-O2D
24	A	1104	CLA	C4B-C3B-CAB-CBB
24	A	1104	CLA	CBD-CGD-O2D-CED
24	A	1105	CLA	CBD-CGD-O2D-CED
24	A	1106	CLA	C3A-C2A-CAA-CBA
24	A	1106	CLA	CHA-CBD-CGD-O1D
24	A	1106	CLA	CHA-CBD-CGD-O2D
24	A	1107	CLA	CBD-CGD-O2D-CED
24	A	1108	CLA	CBD-CGD-O2D-CED
24	A	1109	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	A	1109	CLA	CBD-CGD-O2D-CED
24	A	1110	CLA	CBA-CGA-O2A-C1
24	A	1110	CLA	O1A-CGA-O2A-C1
24	A	1111	CLA	C1A-C2A-CAA-CBA
24	A	1112	CLA	CBD-CGD-O2D-CED
24	A	1115	CLA	CHA-CBD-CGD-O1D
24	A	1115	CLA	CHA-CBD-CGD-O2D
24	A	1115	CLA	C2-C3-C5-C6
24	A	1115	CLA	C4-C3-C5-C6
24	A	1116	CLA	C3A-C2A-CAA-CBA
24	A	1117	CLA	C1A-C2A-CAA-CBA
24	A	1117	CLA	C3A-C2A-CAA-CBA
24	A	1118	CLA	C3A-C2A-CAA-CBA
24	A	1120	CLA	C2-C1-O2A-CGA
24	A	1120	CLA	CHA-CBD-CGD-O1D
24	A	1120	CLA	CHA-CBD-CGD-O2D
24	A	1121	CLA	CHA-CBD-CGD-O1D
24	A	1121	CLA	CHA-CBD-CGD-O2D
24	A	1121	CLA	CBD-CGD-O2D-CED
24	A	1122	CLA	C4B-C3B-CAB-CBB
24	A	1123	CLA	C1A-C2A-CAA-CBA
24	A	1123	CLA	C2-C1-O2A-CGA
24	A	1123	CLA	CAD-CBD-CGD-O2D
24	A	1124	CLA	C1A-C2A-CAA-CBA
24	A	1125	CLA	C1A-C2A-CAA-CBA
24	A	1125	CLA	C3A-C2A-CAA-CBA
24	A	1126	CLA	C1A-C2A-CAA-CBA
24	A	1126	CLA	C3A-C2A-CAA-CBA
24	A	1126	CLA	CBD-CGD-O2D-CED
24	A	1128	CLA	CHA-CBD-CGD-O1D
24	A	1128	CLA	CHA-CBD-CGD-O2D
24	A	1132	CLA	CHA-CBD-CGD-O1D
24	A	1132	CLA	CHA-CBD-CGD-O2D
24	A	1133	CLA	CHA-CBD-CGD-O2D
24	A	1134	CLA	CHA-CBD-CGD-O1D
24	A	1134	CLA	CHA-CBD-CGD-O2D
24	A	1135	CLA	C2-C3-C5-C6
24	A	1135	CLA	C4-C3-C5-C6
24	A	1136	CLA	CBD-CGD-O2D-CED
24	A	1137	CLA	C2-C1-O2A-CGA
24	A	1137	CLA	CHA-CBD-CGD-O1D
24	A	1137	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	A	1138	CLA	C1A-C2A-CAA-CBA
24	A	1138	CLA	C3A-C2A-CAA-CBA
24	A	1139	CLA	C1A-C2A-CAA-CBA
24	A	1139	CLA	C3A-C2A-CAA-CBA
24	A	1139	CLA	CBD-CGD-O2D-CED
24	A	1141	CLA	CAD-CBD-CGD-O1D
24	A	1141	CLA	CAD-CBD-CGD-O2D
24	B	1021	CLA	CBD-CGD-O2D-CED
24	B	1022	CLA	C2B-C3B-CAB-CBB
24	B	1022	CLA	C4B-C3B-CAB-CBB
24	B	1022	CLA	CBD-CGD-O2D-CED
24	B	1023	CLA	C2-C1-O2A-CGA
24	B	1023	CLA	CBD-CGD-O2D-CED
24	B	1201	CLA	C1A-C2A-CAA-CBA
24	B	1201	CLA	CHA-CBD-CGD-O1D
24	B	1201	CLA	CHA-CBD-CGD-O2D
24	B	1202	CLA	C1A-C2A-CAA-CBA
24	B	1202	CLA	C3A-C2A-CAA-CBA
24	B	1203	CLA	CBD-CGD-O2D-CED
24	B	1205	CLA	CHA-CBD-CGD-O1D
24	B	1205	CLA	CHA-CBD-CGD-O2D
24	B	1207	CLA	C2-C1-O2A-CGA
24	B	1207	CLA	CBD-CGD-O2D-CED
24	B	1208	CLA	C1A-C2A-CAA-CBA
24	B	1208	CLA	C3A-C2A-CAA-CBA
24	B	1210	CLA	C1A-C2A-CAA-CBA
24	B	1210	CLA	C3A-C2A-CAA-CBA
24	B	1211	CLA	CHA-CBD-CGD-O1D
24	B	1211	CLA	CHA-CBD-CGD-O2D
24	B	1214	CLA	CBD-CGD-O2D-CED
24	B	1215	CLA	C1A-C2A-CAA-CBA
24	B	1215	CLA	C3A-C2A-CAA-CBA
24	B	1215	CLA	CBD-CGD-O2D-CED
24	B	1215	CLA	C6-C7-C8-C9
24	B	1216	CLA	C2B-C3B-CAB-CBB
24	B	1216	CLA	C4B-C3B-CAB-CBB
24	B	1216	CLA	CBD-CGD-O2D-CED
24	B	1218	CLA	CBA-CGA-O2A-C1
24	B	1218	CLA	O1A-CGA-O2A-C1
24	B	1221	CLA	CHA-CBD-CGD-O1D
24	B	1221	CLA	CHA-CBD-CGD-O2D
24	B	1223	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	B	1223	CLA	C3A-C2A-CAA-CBA
24	B	1224	CLA	C1A-C2A-CAA-CBA
24	B	1225	CLA	C1A-C2A-CAA-CBA
24	B	1225	CLA	C3A-C2A-CAA-CBA
24	B	1226	CLA	C2-C1-O2A-CGA
24	B	1226	CLA	CBD-CGD-O2D-CED
24	B	1228	CLA	CBD-CGD-O2D-CED
24	B	1229	CLA	C2-C1-O2A-CGA
24	B	1230	CLA	C1A-C2A-CAA-CBA
24	B	1230	CLA	C3A-C2A-CAA-CBA
24	B	1230	CLA	CHA-CBD-CGD-O1D
24	B	1230	CLA	CHA-CBD-CGD-O2D
24	B	1231	CLA	C2-C1-O2A-CGA
24	B	1232	CLA	C1A-C2A-CAA-CBA
24	B	1232	CLA	C3A-C2A-CAA-CBA
24	B	1234	CLA	C2B-C3B-CAB-CBB
24	B	1234	CLA	C4B-C3B-CAB-CBB
24	B	1234	CLA	CBD-CGD-O2D-CED
24	B	1235	CLA	CAD-CBD-CGD-O2D
24	B	1236	CLA	CHA-CBD-CGD-O1D
24	B	1236	CLA	CHA-CBD-CGD-O2D
24	B	1236	CLA	CBD-CGD-O2D-CED
24	B	1237	CLA	C2-C1-O2A-CGA
24	B	1238	CLA	C2-C1-O2A-CGA
24	B	1239	CLA	CBD-CGD-O2D-CED
24	F	1301	CLA	O1A-CGA-O2A-C1
24	F	1301	CLA	CBD-CGD-O2D-CED
24	F	1302	CLA	CBD-CGD-O2D-CED
24	G	1601	CLA	C1A-C2A-CAA-CBA
24	G	1601	CLA	C3A-C2A-CAA-CBA
24	G	1602	CLA	C1A-C2A-CAA-CBA
24	G	1602	CLA	C3A-C2A-CAA-CBA
24	G	1602	CLA	C4B-C3B-CAB-CBB
24	G	1602	CLA	CHA-CBD-CGD-O1D
24	G	1602	CLA	CHA-CBD-CGD-O2D
24	J	1901	CLA	C1A-C2A-CAA-CBA
24	J	1901	CLA	CBD-CGD-O2D-CED
24	K	1401	CLA	CBA-CGA-O2A-C1
24	K	1402	CLA	C4B-C3B-CAB-CBB
24	K	1403	CLA	CBA-CGA-O2A-C1
24	K	1403	CLA	CAD-CBD-CGD-O1D
24	K	1403	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	K	1403	CLA	CBD-CGD-O2D-CED
24	K	1404	CLA	CHA-CBD-CGD-O1D
24	K	1404	CLA	CHA-CBD-CGD-O2D
24	H	1701	CLA	C2-C1-O2A-CGA
24	H	1701	CLA	C2-C3-C5-C6
24	H	1701	CLA	C4-C3-C5-C6
24	H	1702	CLA	CBA-CGA-O2A-C1
24	H	1702	CLA	CHA-CBD-CGD-O1D
24	H	1702	CLA	CHA-CBD-CGD-O2D
24	L	1501	CLA	C1A-C2A-CAA-CBA
24	L	1501	CLA	C3A-C2A-CAA-CBA
24	L	1501	CLA	CBD-CGD-O2D-CED
24	L	1503	CLA	CHA-CBD-CGD-O1D
24	L	1503	CLA	CHA-CBD-CGD-O2D
24	1	601	CLA	CBD-CGD-O2D-CED
24	1	604	CLA	C3A-C2A-CAA-CBA
24	1	605	CLA	C1A-C2A-CAA-CBA
24	1	605	CLA	CBD-CGD-O2D-CED
24	1	606	CLA	CBD-CGD-O2D-CED
24	1	610	CLA	C1A-C2A-CAA-CBA
24	1	610	CLA	C3A-C2A-CAA-CBA
24	1	612	CLA	C1A-C2A-CAA-CBA
24	1	612	CLA	C3A-C2A-CAA-CBA
24	1	612	CLA	CBD-CGD-O2D-CED
24	1	615	CLA	C1A-C2A-CAA-CBA
24	1	615	CLA	C3A-C2A-CAA-CBA
24	1	615	CLA	CBA-CGA-O2A-C1
24	1	615	CLA	O1A-CGA-O2A-C1
24	a	601	CLA	C4B-C3B-CAB-CBB
24	a	604	CLA	C1A-C2A-CAA-CBA
24	a	604	CLA	C3A-C2A-CAA-CBA
24	a	607	CLA	CHA-CBD-CGD-O1D
24	a	607	CLA	CHA-CBD-CGD-O2D
24	a	608	CLA	C1A-C2A-CAA-CBA
24	a	608	CLA	C3A-C2A-CAA-CBA
24	a	608	CLA	CBD-CGD-O2D-CED
24	a	611	CLA	C3A-C2A-CAA-CBA
24	a	611	CLA	C2-C1-O2A-CGA
24	a	612	CLA	C1A-C2A-CAA-CBA
24	a	612	CLA	C3A-C2A-CAA-CBA
24	a	615	CLA	CBA-CGA-O2A-C1
24	3	601	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	3	602	CLA	CHA-CBD-CGD-O1D
24	3	602	CLA	CHA-CBD-CGD-O2D
24	3	603	CLA	CBD-CGD-O2D-CED
24	3	606	CLA	C1A-C2A-CAA-CBA
24	3	606	CLA	CBD-CGD-O2D-CED
24	3	613	CLA	CBD-CGD-O2D-CED
24	3	616	CLA	C4-C3-C5-C6
24	4	601	CLA	CBD-CGD-O2D-CED
24	4	602	CLA	C3-C5-C6-C7
24	4	603	CLA	CBD-CGD-O2D-CED
24	4	605	CLA	CBD-CGD-O2D-CED
24	4	606	CLA	CBD-CGD-O2D-CED
24	4	607	CLA	C3A-C2A-CAA-CBA
24	4	607	CLA	CBA-CGA-O2A-C1
24	4	607	CLA	O1A-CGA-O2A-C1
24	4	610	CLA	CBD-CGD-O2D-CED
24	4	611	CLA	C2-C1-O2A-CGA
24	4	611	CLA	CBD-CGD-O2D-CED
24	4	612	CLA	C2-C1-O2A-CGA
24	4	612	CLA	CHA-CBD-CGD-O1D
24	4	612	CLA	CHA-CBD-CGD-O2D
24	4	612	CLA	CBD-CGD-O2D-CED
24	4	615	CLA	CBA-CGA-O2A-C1
24	4	615	CLA	O1A-CGA-O2A-C1
24	4	616	CLA	CBD-CGD-O2D-CED
24	5	601	CLA	CBD-CGD-O2D-CED
24	5	602	CLA	CBD-CGD-O2D-CED
24	5	609	CLA	CBD-CGD-O2D-CED
24	5	609	CLA	C2-C3-C5-C6
24	5	612	CLA	CBD-CGD-O2D-CED
24	5	614	CLA	CBA-CGA-O2A-C1
24	5	614	CLA	CBD-CGD-O2D-CED
24	5	616	CLA	C1A-C2A-CAA-CBA
24	5	616	CLA	C3A-C2A-CAA-CBA
24	5	616	CLA	CBA-CGA-O2A-C1
24	5	616	CLA	CBD-CGD-O2D-CED
24	5	617	CLA	C1A-C2A-CAA-CBA
24	5	617	CLA	C3A-C2A-CAA-CBA
24	5	617	CLA	C2-C1-O2A-CGA
24	6	601	CLA	CBD-CGD-O2D-CED
24	6	602	CLA	CBD-CGD-O2D-CED
24	6	605	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	6	607	CLA	CBD-CGD-O2D-CED
24	6	608	CLA	CBD-CGD-O2D-CED
24	6	609	CLA	C2-C1-O2A-CGA
24	6	615	CLA	CAD-CBD-CGD-O1D
24	6	615	CLA	CAD-CBD-CGD-O2D
24	6	617	CLA	C1A-C2A-CAA-CBA
24	6	617	CLA	C3A-C2A-CAA-CBA
24	6	618	CLA	CBA-CGA-O2A-C1
24	6	618	CLA	CBD-CGD-O2D-CED
24	7	602	CLA	CBD-CGD-O2D-CED
24	7	603	CLA	CBD-CGD-O2D-CED
24	7	606	CLA	C1A-C2A-CAA-CBA
24	7	606	CLA	CBD-CGD-O2D-CED
24	7	607	CLA	C2B-C3B-CAB-CBB
24	7	607	CLA	C4B-C3B-CAB-CBB
24	7	609	CLA	CAD-CBD-CGD-O1D
24	7	609	CLA	CAD-CBD-CGD-O2D
24	7	610	CLA	CBD-CGD-O2D-CED
24	7	611	CLA	CBD-CGD-O2D-CED
24	7	612	CLA	CBD-CGD-O2D-CED
24	7	615	CLA	CBD-CGD-O2D-CED
24	7	617	CLA	CAD-CBD-CGD-O2D
24	8	602	CLA	C2-C1-O2A-CGA
24	8	602	CLA	C3-C5-C6-C7
24	8	603	CLA	CBD-CGD-O2D-CED
24	8	606	CLA	CBD-CGD-O2D-CED
24	8	606	CLA	C2-C3-C5-C6
24	8	606	CLA	C4-C3-C5-C6
24	8	607	CLA	CBA-CGA-O2A-C1
24	8	608	CLA	CHA-CBD-CGD-O1D
24	8	608	CLA	CHA-CBD-CGD-O2D
24	8	609	CLA	CAD-CBD-CGD-O1D
24	8	609	CLA	CAD-CBD-CGD-O2D
24	8	610	CLA	C3A-C2A-CAA-CBA
24	8	610	CLA	CBD-CGD-O2D-CED
24	8	612	CLA	C3A-C2A-CAA-CBA
24	8	615	CLA	C1A-C2A-CAA-CBA
24	8	615	CLA	C3A-C2A-CAA-CBA
24	8	618	CLA	C2-C1-O2A-CGA
24	8	620	CLA	C1A-C2A-CAA-CBA
24	8	620	CLA	C3A-C2A-CAA-CBA
24	2	601	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	2	601	CLA	CBD-CGD-O2D-CED
24	2	601	CLA	C2-C3-C5-C6
24	2	602	CLA	CHA-CBD-CGD-O1D
24	2	602	CLA	CHA-CBD-CGD-O2D
24	2	603	CLA	CBD-CGD-O2D-CED
24	2	604	CLA	C1A-C2A-CAA-CBA
24	2	604	CLA	CHA-CBD-CGD-O1D
24	2	604	CLA	CHA-CBD-CGD-O2D
24	2	605	CLA	C2-C1-O2A-CGA
24	2	605	CLA	CBD-CGD-O2D-CED
24	2	606	CLA	CBA-CGA-O2A-C1
24	2	607	CLA	CBA-CGA-O2A-C1
24	2	607	CLA	CBD-CGD-O2D-CED
24	2	610	CLA	CBA-CGA-O2A-C1
24	2	612	CLA	CBD-CGD-O2D-CED
24	2	615	CLA	C1A-C2A-CAA-CBA
24	2	615	CLA	C3A-C2A-CAA-CBA
24	2	621	CLA	C3A-C2A-CAA-CBA
24	2	621	CLA	CBD-CGD-O2D-CED
24	9	601	CLA	C1A-C2A-CAA-CBA
24	9	601	CLA	C2B-C3B-CAB-CBB
24	9	601	CLA	C4B-C3B-CAB-CBB
24	9	602	CLA	CBD-CGD-O2D-CED
24	9	603	CLA	CBD-CGD-O2D-CED
24	9	604	CLA	CBD-CGD-O2D-CED
24	9	606	CLA	CBD-CGD-O2D-CED
24	9	607	CLA	C1A-C2A-CAA-CBA
24	9	609	CLA	CBD-CGD-O2D-CED
24	9	612	CLA	C1A-C2A-CAA-CBA
24	9	612	CLA	C3A-C2A-CAA-CBA
24	9	612	CLA	CBD-CGD-O2D-CED
25	B	2002	PQN	C14-C13-C15-C16
27	A	4001	BCR	C11-C10-C9-C8
27	A	4001	BCR	C11-C10-C9-C34
27	A	4001	BCR	C10-C11-C12-C13
27	A	4001	BCR	C21-C22-C23-C24
27	A	4001	BCR	C37-C22-C23-C24
27	A	4001	BCR	C23-C24-C25-C26
27	A	4001	BCR	C23-C24-C25-C30
27	A	4002	BCR	C7-C8-C9-C10
27	A	4002	BCR	C7-C8-C9-C34
27	A	4002	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
27	A	4002	BCR	C11-C10-C9-C34
27	A	4002	BCR	C10-C11-C12-C13
27	A	4002	BCR	C13-C14-C15-C16
27	A	4003	BCR	C11-C10-C9-C8
27	A	4003	BCR	C11-C10-C9-C34
27	A	4003	BCR	C9-C10-C11-C12
27	A	4003	BCR	C10-C11-C12-C13
27	A	4003	BCR	C17-C18-C19-C20
27	A	4004	BCR	C7-C8-C9-C10
27	A	4004	BCR	C7-C8-C9-C34
27	A	4004	BCR	C11-C10-C9-C8
27	A	4004	BCR	C11-C10-C9-C34
27	A	4005	BCR	C7-C8-C9-C10
27	A	4005	BCR	C11-C10-C9-C8
27	A	4005	BCR	C11-C10-C9-C34
27	A	4005	BCR	C21-C22-C23-C24
27	A	4005	BCR	C37-C22-C23-C24
27	B	4001	BCR	C11-C10-C9-C8
27	B	4001	BCR	C11-C10-C9-C34
27	B	4001	BCR	C9-C10-C11-C12
27	B	4001	BCR	C10-C11-C12-C13
27	B	4001	BCR	C17-C18-C19-C20
27	B	4001	BCR	C36-C18-C19-C20
27	B	4001	BCR	C21-C22-C23-C24
27	B	4001	BCR	C37-C22-C23-C24
27	B	4002	BCR	C7-C8-C9-C10
27	B	4002	BCR	C7-C8-C9-C34
27	B	4002	BCR	C11-C10-C9-C8
27	B	4002	BCR	C11-C10-C9-C34
27	B	4002	BCR	C9-C10-C11-C12
27	B	4002	BCR	C10-C11-C12-C13
27	B	4002	BCR	C17-C18-C19-C20
27	B	4002	BCR	C36-C18-C19-C20
27	B	4002	BCR	C21-C22-C23-C24
27	B	4003	BCR	C21-C22-C23-C24
27	B	4003	BCR	C37-C22-C23-C24
27	B	4004	BCR	C7-C8-C9-C10
27	B	4004	BCR	C7-C8-C9-C34
27	B	4004	BCR	C11-C10-C9-C8
27	B	4004	BCR	C11-C10-C9-C34
27	B	4004	BCR	C10-C11-C12-C13
27	B	4004	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
27	B	4005	BCR	C11-C10-C9-C8
27	B	4005	BCR	C11-C10-C9-C34
27	B	4005	BCR	C9-C10-C11-C12
27	B	4005	BCR	C10-C11-C12-C13
27	B	4005	BCR	C21-C22-C23-C24
27	B	4005	BCR	C37-C22-C23-C24
27	B	4006	BCR	C11-C10-C9-C8
27	B	4006	BCR	C11-C10-C9-C34
27	B	4006	BCR	C10-C11-C12-C13
27	B	4006	BCR	C13-C14-C15-C16
27	B	4006	BCR	C17-C18-C19-C20
27	B	4006	BCR	C36-C18-C19-C20
27	B	4006	BCR	C21-C22-C23-C24
27	B	4007	BCR	C11-C10-C9-C8
27	B	4007	BCR	C11-C10-C9-C34
27	B	4007	BCR	C10-C11-C12-C13
27	B	4007	BCR	C13-C14-C15-C16
27	F	4001	BCR	C10-C11-C12-C13
27	F	4001	BCR	C21-C22-C23-C24
27	G	4001	BCR	C11-C10-C9-C8
27	G	4001	BCR	C11-C10-C9-C34
27	G	4001	BCR	C10-C11-C12-C13
27	G	4001	BCR	C17-C18-C19-C20
27	G	4001	BCR	C36-C18-C19-C20
27	J	4001	BCR	C7-C8-C9-C10
27	J	4001	BCR	C7-C8-C9-C34
27	J	4001	BCR	C11-C10-C9-C8
27	J	4001	BCR	C11-C10-C9-C34
27	J	4001	BCR	C10-C11-C12-C13
27	J	4001	BCR	C11-C12-C13-C14
27	J	4001	BCR	C11-C12-C13-C35
27	J	4001	BCR	C17-C18-C19-C20
27	J	4001	BCR	C36-C18-C19-C20
27	K	4001	BCR	C7-C8-C9-C10
27	K	4001	BCR	C7-C8-C9-C34
27	K	4001	BCR	C11-C10-C9-C8
27	K	4001	BCR	C11-C10-C9-C34
27	K	4001	BCR	C10-C11-C12-C13
27	K	4001	BCR	C21-C22-C23-C24
27	K	4001	BCR	C37-C22-C23-C24
27	K	4002	BCR	C11-C10-C9-C8
27	K	4002	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
27	K	4002	BCR	C10-C11-C12-C13
27	K	4002	BCR	C11-C12-C13-C14
27	K	4002	BCR	C17-C18-C19-C20
27	K	4002	BCR	C36-C18-C19-C20
27	K	4002	BCR	C23-C24-C25-C26
27	K	4002	BCR	C23-C24-C25-C30
27	I	4001	BCR	C7-C8-C9-C10
27	I	4001	BCR	C7-C8-C9-C34
27	I	4001	BCR	C11-C10-C9-C8
27	I	4001	BCR	C11-C10-C9-C34
27	I	4001	BCR	C11-C12-C13-C14
27	I	4001	BCR	C11-C12-C13-C35
27	H	4001	BCR	C11-C10-C9-C8
27	H	4001	BCR	C11-C10-C9-C34
27	H	4001	BCR	C10-C11-C12-C13
27	H	4001	BCR	C15-C16-C17-C18
27	H	4001	BCR	C21-C22-C23-C24
27	L	4001	BCR	C11-C10-C9-C8
27	L	4001	BCR	C11-C10-C9-C34
27	L	4001	BCR	C10-C11-C12-C13
27	L	4001	BCR	C23-C24-C25-C26
27	L	4002	BCR	C11-C10-C9-C8
27	L	4002	BCR	C11-C10-C9-C34
27	L	4003	BCR	C11-C10-C9-C8
27	L	4003	BCR	C11-C10-C9-C34
27	L	4003	BCR	C10-C11-C12-C13
27	3	503	BCR	C7-C8-C9-C10
27	3	503	BCR	C7-C8-C9-C34
27	3	503	BCR	C11-C10-C9-C8
27	3	503	BCR	C11-C10-C9-C34
27	3	503	BCR	C9-C10-C11-C12
27	3	503	BCR	C10-C11-C12-C13
27	3	503	BCR	C23-C24-C25-C26
27	3	503	BCR	C23-C24-C25-C30
27	3	504	BCR	C11-C10-C9-C8
27	3	504	BCR	C11-C10-C9-C34
27	3	504	BCR	C9-C10-C11-C12
27	3	504	BCR	C10-C11-C12-C13
27	3	504	BCR	C11-C12-C13-C14
27	3	504	BCR	C11-C12-C13-C35
27	3	504	BCR	C17-C18-C19-C20
27	3	504	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
27	3	504	BCR	C37-C22-C23-C24
27	3	505	BCR	C11-C10-C9-C8
27	3	505	BCR	C11-C10-C9-C34
27	3	505	BCR	C9-C10-C11-C12
27	3	505	BCR	C10-C11-C12-C13
27	3	505	BCR	C17-C18-C19-C20
27	3	505	BCR	C21-C22-C23-C24
27	3	505	BCR	C37-C22-C23-C24
27	3	505	BCR	C23-C24-C25-C26
27	3	505	BCR	C23-C24-C25-C30
27	4	503	BCR	C11-C10-C9-C8
27	4	503	BCR	C11-C10-C9-C34
27	4	503	BCR	C10-C11-C12-C13
27	4	503	BCR	C17-C18-C19-C20
27	4	503	BCR	C19-C20-C21-C22
27	5	503	BCR	C5-C6-C7-C8
27	5	503	BCR	C11-C10-C9-C8
27	5	503	BCR	C11-C10-C9-C34
27	5	503	BCR	C10-C11-C12-C13
27	5	503	BCR	C21-C22-C23-C24
27	5	503	BCR	C37-C22-C23-C24
27	5	503	BCR	C23-C24-C25-C26
27	5	503	BCR	C23-C24-C25-C30
27	6	503	BCR	C11-C10-C9-C8
27	6	503	BCR	C11-C10-C9-C34
27	6	503	BCR	C21-C22-C23-C24
27	6	503	BCR	C37-C22-C23-C24
27	6	503	BCR	C23-C24-C25-C26
27	6	503	BCR	C23-C24-C25-C30
27	6	504	BCR	C11-C10-C9-C8
27	6	504	BCR	C11-C10-C9-C34
27	6	504	BCR	C17-C18-C19-C20
27	7	503	BCR	C11-C10-C9-C8
27	7	503	BCR	C11-C10-C9-C34
27	7	503	BCR	C10-C11-C12-C13
27	8	503	BCR	C7-C8-C9-C10
27	8	503	BCR	C7-C8-C9-C34
27	8	503	BCR	C11-C10-C9-C8
27	8	503	BCR	C11-C10-C9-C34
27	8	503	BCR	C9-C10-C11-C12
27	8	503	BCR	C10-C11-C12-C13
27	8	503	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
27	8	503	BCR	C37-C22-C23-C24
27	8	503	BCR	C23-C24-C25-C26
27	8	503	BCR	C23-C24-C25-C30
28	A	5001	LHG	O1-C1-C2-C3
28	A	5001	LHG	C3-O3-P-O5
28	A	5001	LHG	C4-O6-P-O3
28	A	5001	LHG	C4-O6-P-O4
28	A	5001	LHG	C4-O6-P-O5
28	A	5002	LHG	O1-C1-C2-C3
28	A	5002	LHG	C1-C2-C3-O3
28	A	5002	LHG	C3-O3-P-O4
28	A	5002	LHG	C3-O3-P-O6
28	A	5002	LHG	C4-O6-P-O3
28	A	5002	LHG	C4-O6-P-O4
28	A	5003	LHG	C4-O6-P-O3
28	A	5003	LHG	C4-O6-P-O4
28	A	5003	LHG	O9-C7-O7-C5
28	A	5003	LHG	C8-C7-O7-C5
28	B	5001	LHG	C8-C7-O7-C5
28	B	5002	LHG	O1-C1-C2-C3
28	F	5001	LHG	C3-O3-P-O5
28	F	5001	LHG	C8-C7-O7-C5
28	F	5002	LHG	C4-O6-P-O5
28	1	801	LHG	C3-O3-P-O5
28	1	801	LHG	C4-O6-P-O3
28	1	801	LHG	C4-O6-P-O4
28	1	801	LHG	C4-O6-P-O5
28	1	801	LHG	O7-C5-C6-O8
28	1	802	LHG	O1-C1-C2-C3
28	1	802	LHG	C1-C2-C3-O3
28	1	802	LHG	C4-O6-P-O3
28	1	802	LHG	C4-O6-P-O5
28	1	802	LHG	O7-C5-C6-O8
28	1	802	LHG	C8-C7-O7-C5
28	a	801	LHG	O1-C1-C2-C3
28	a	801	LHG	C1-C2-C3-O3
28	a	801	LHG	C3-O3-P-O5
28	a	801	LHG	C4-O6-P-O3
28	a	801	LHG	C8-C7-O7-C5
28	3	801	LHG	O1-C1-C2-C3
28	3	801	LHG	C3-O3-P-O6
28	3	801	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
28	3	801	LHG	O9-C7-O7-C5
28	3	801	LHG	C8-C7-O7-C5
28	4	801	LHG	O1-C1-C2-C3
28	4	801	LHG	C1-C2-C3-O3
28	4	801	LHG	C3-O3-P-O4
28	4	801	LHG	C3-O3-P-O6
28	4	801	LHG	C4-O6-P-O3
28	4	801	LHG	C4-O6-P-O4
28	4	802	LHG	O1-C1-C2-C3
28	4	802	LHG	C8-C7-O7-C5
28	5	801	LHG	C1-C2-C3-O3
28	5	801	LHG	C3-O3-P-O5
28	5	801	LHG	C3-O3-P-O6
28	6	801	LHG	O1-C1-C2-C3
28	6	801	LHG	O2-C2-C3-O3
28	6	801	LHG	C3-O3-P-O5
28	6	801	LHG	C4-O6-P-O3
28	6	802	LHG	C1-C2-C3-O3
28	6	802	LHG	C3-O3-P-O4
28	6	802	LHG	C3-O3-P-O6
28	6	802	LHG	C8-C7-O7-C5
28	7	801	LHG	O1-C1-C2-C3
28	7	801	LHG	C4-O6-P-O3
28	7	801	LHG	C4-O6-P-O4
28	7	801	LHG	C4-O6-P-O5
28	7	801	LHG	O9-C7-O7-C5
28	7	801	LHG	C8-C7-O7-C5
28	7	802	LHG	C3-O3-P-O5
28	7	802	LHG	C3-O3-P-O6
28	7	803	LHG	C4-O6-P-O3
28	7	803	LHG	C4-O6-P-O4
28	7	803	LHG	C8-C7-O7-C5
28	8	801	LHG	C3-O3-P-O5
28	8	801	LHG	C3-O3-P-O6
28	8	801	LHG	C4-O6-P-O3
28	8	801	LHG	C4-O6-P-O4
28	8	801	LHG	C4-O6-P-O5
28	2	801	LHG	O1-C1-C2-O2
28	2	801	LHG	C1-C2-C3-O3
28	2	801	LHG	C3-O3-P-O5
28	2	801	LHG	C8-C7-O7-C5
28	2	802	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
28	2	802	LHG	C4-O6-P-O3
28	2	802	LHG	C4-O6-P-O4
28	9	801	LHG	O1-C1-C2-C3
28	9	801	LHG	C1-C2-C3-O3
28	9	802	LHG	O1-C1-C2-C3
28	9	802	LHG	C1-C2-C3-O3
28	9	802	LHG	O2-C2-C3-O3
28	9	802	LHG	C4-O6-P-O3
28	9	802	LHG	C4-O6-P-O4
28	9	802	LHG	O9-C7-O7-C5
29	A	5005	DGD	C2A-C1A-O1G-C1G
29	A	5005	DGD	O1A-C1A-O1G-C1G
29	A	5005	DGD	O6D-C1D-O3G-C3G
29	8	802	DGD	C2B-C1B-O2G-C2G
30	A	5007	3PH	C1-O11-P-O13
30	A	5007	3PH	C1-O11-P-O14
30	A	5007	3PH	C1-O11-P-O12
30	A	5007	3PH	C22-C21-O21-C2
31	B	5006	LMT	O5'-C1'-O1'-C1
31	1	804	LMT	C2'-C1'-O1'-C1
31	1	804	LMT	C2-C1-O1'-C1'
32	B	5004	PCW	O31-C31-O2-C2
32	B	5004	PCW	C1-O3P-P-O4P
32	B	5004	PCW	C4-O4P-P-O1P
32	6	803	PCW	O4P-C4-C5-N
33	B	5005	PTY	C5-O14-P1-O11
33	B	5005	PTY	C5-O14-P1-O12
33	3	802	PTY	N1-C2-C3-O11
33	3	802	PTY	C5-O14-P1-O13
33	5	802	PTY	C11-C8-O7-C6
33	7	804	PTY	C11-C8-O7-C6
33	8	891	PTY	N1-C2-C3-O11
33	8	891	PTY	C5-O14-P1-O11
33	8	891	PTY	C5-O14-P1-O12
33	8	891	PTY	C5-O14-P1-O13
33	9	803	PTY	O10-C8-O7-C6
34	B	5007	LAP	O1-C13-C14-C15
34	B	5007	LAP	O1-C13-C14-O3
34	B	5007	LAP	C14-C15-O4-P9
34	B	5007	LAP	C15-O4-P9-O6
34	K	5001	LAP	C14-C15-O4-P9
34	K	5001	LAP	O6-C16-C17-N8

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Mol	Chain	Res	Type	Atoms
34	K	5001	LAP	C15-O4-P9-O6
34	K	5001	LAP	C15-O4-P9-O7
35	G	5001	SQD	C8-C7-O47-C45
35	G	5001	SQD	C5-C6-S-O7
35	G	5001	SQD	C5-C6-S-O8
35	G	5001	SQD	C5-C6-S-O9
35	7	805	SQD	O5-C5-C6-S
36	G	5002	ERG	C13-C17-C20-C21
36	G	5002	ERG	C16-C17-C20-C21
36	G	5002	ERG	C16-C17-C20-C22
37	J	4002	RRX	C21-C22-C23-C24
37	J	4002	RRX	C19-C20-C21-C22
37	J	4002	RRX	C7-C8-C9-C34
38	J	5001	LPX	C3-O1-P1-O3
38	J	5001	LPX	C3-O1-P1-O2
38	J	5001	LPX	C3-O1-P1-O4
38	J	5001	LPX	C1-O2-P1-O3
38	a	804	LPX	C1-O2-P1-O1
38	a	804	LPX	C1-O2-P1-O3
39	M	4001	ECH	C11-C12-C13-C35
40	1	503	LUT	C21-C26-C27-C28
40	1	503	LUT	C27-C28-C29-C30
40	1	503	LUT	C27-C28-C29-C39
40	a	501	LUT	C5-C6-C7-C8
40	a	501	LUT	C7-C8-C9-C10
40	a	501	LUT	C7-C8-C9-C19
40	a	503	LUT	C21-C26-C27-C28
40	a	503	LUT	C31-C32-C33-C34
40	4	501	LUT	C25-C26-C27-C28
40	5	502	LUT	C25-C26-C27-C28
40	5	505	LUT	C21-C26-C27-C28
40	6	501	LUT	C1-C6-C7-C8
40	6	501	LUT	C5-C6-C7-C8
40	6	501	LUT	C7-C8-C9-C10
40	6	501	LUT	C7-C8-C9-C19
40	6	501	LUT	C13-C14-C15-C35
40	6	501	LUT	C25-C26-C27-C28
40	6	502	LUT	C21-C26-C27-C28
40	7	501	LUT	C21-C26-C27-C28
40	7	501	LUT	C27-C28-C29-C30
40	7	501	LUT	C27-C28-C29-C39
40	7	501	LUT	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
40	2	502	LUT	C21-C26-C27-C28
40	2	502	LUT	C25-C26-C27-C28
40	2	502	LUT	C29-C30-C31-C32
40	9	502	LUT	C21-C26-C27-C28
41	1	609	CHL	C1A-C2A-CAA-CBA
41	1	609	CHL	C3A-C2A-CAA-CBA
41	1	613	CHL	C1A-C2A-CAA-CBA
41	a	606	CHL	C3A-C2A-CAA-CBA
41	a	606	CHL	CAD-CBD-CGD-O1D
41	a	606	CHL	CAD-CBD-CGD-O2D
41	3	608	CHL	C1A-C2A-CAA-CBA
41	3	608	CHL	CAD-CBD-CGD-O1D
41	3	608	CHL	CAD-CBD-CGD-O2D
41	3	611	CHL	CHA-CBD-CGD-O1D
41	8	601	CHL	C1A-C2A-CAA-CBA
41	8	601	CHL	C4-C3-C5-C6
41	8	604	CHL	C3A-C2A-CAA-CBA
41	9	610	CHL	CHA-CBD-CGD-O1D
43	a	504	QTB	C01-C02-C09-C10
43	a	504	QTB	C03-C02-C09-C10
43	a	504	QTB	C09-C10-C11-C12
44	a	805	GG0	N05-C06-C07-O08
44	a	805	GG0	N05-C06-C07-O09
46	5	803	DGA	CB2-CB1-OG2-CG2
46	8	803	DGA	OG2-CG2-CG3-OXT
47	6	806	SPH	O1-C1-C2-N2
47	6	806	SPH	C2-C3-C4-C5
47	6	806	SPH	O3-C3-C4-C5
49	7	504	C7Z	C31-C32-C33-C34
49	7	504	C7Z	C31-C32-C33-C40
50	7	807	4RF	O18-C19-C20-O21
50	7	807	4RF	C43-C41-O40-C39
50	8	807	4RF	C24-C22-O21-C20
50	8	807	4RF	O42-C41-O40-C39
50	8	807	4RF	C43-C41-O40-C39
50	8	808	4RF	C24-C22-O21-C20
50	8	808	4RF	O23-C22-O21-C20
50	8	808	4RF	C43-C41-O40-C39
51	8	806	P5S	C3-O16-P12-OG
51	8	806	P5S	C3-O16-P12-O13
51	8	806	P5S	C20-C17-O19-C1
24	A	1122	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	A	1126	CLA	O1D-CGD-O2D-CED
24	A	1136	CLA	O1D-CGD-O2D-CED
24	B	1021	CLA	O1D-CGD-O2D-CED
24	B	1023	CLA	O1D-CGD-O2D-CED
24	B	1219	CLA	O1D-CGD-O2D-CED
24	1	608	CLA	O1D-CGD-O2D-CED
24	1	612	CLA	O1D-CGD-O2D-CED
24	a	611	CLA	O1D-CGD-O2D-CED
24	4	610	CLA	O1D-CGD-O2D-CED
24	6	606	CLA	O1D-CGD-O2D-CED
24	8	605	CLA	O1D-CGD-O2D-CED
24	A	1108	CLA	O1D-CGD-O2D-CED
24	A	1119	CLA	O1D-CGD-O2D-CED
24	A	1140	CLA	O1D-CGD-O2D-CED
24	B	1206	CLA	O1D-CGD-O2D-CED
24	K	1402	CLA	O1D-CGD-O2D-CED
24	H	1701	CLA	O1D-CGD-O2D-CED
24	1	615	CLA	O1D-CGD-O2D-CED
24	a	615	CLA	O1D-CGD-O2D-CED
24	3	605	CLA	O1D-CGD-O2D-CED
24	4	603	CLA	O1D-CGD-O2D-CED
24	4	615	CLA	O1D-CGD-O2D-CED
24	5	616	CLA	O1D-CGD-O2D-CED
24	5	618	CLA	O1D-CGD-O2D-CED
24	7	606	CLA	O1D-CGD-O2D-CED
24	8	611	CLA	O1D-CGD-O2D-CED
24	2	609	CLA	O1D-CGD-O2D-CED
24	2	613	CLA	O1D-CGD-O2D-CED
24	A	1012	CLA	CBD-CGD-O2D-CED
24	A	1102	CLA	CBD-CGD-O2D-CED
24	A	1111	CLA	CBD-CGD-O2D-CED
24	A	1114	CLA	CBD-CGD-O2D-CED
24	A	1116	CLA	CBD-CGD-O2D-CED
24	A	1118	CLA	CBD-CGD-O2D-CED
24	A	1119	CLA	CBD-CGD-O2D-CED
24	A	1120	CLA	CBD-CGD-O2D-CED
24	A	1122	CLA	CBD-CGD-O2D-CED
24	A	1123	CLA	CBD-CGD-O2D-CED
24	A	1125	CLA	CBD-CGD-O2D-CED
24	A	1129	CLA	CBD-CGD-O2D-CED
24	A	1130	CLA	CBD-CGD-O2D-CED
24	A	1131	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	A	1132	CLA	CBD-CGD-O2D-CED
24	A	1134	CLA	CBD-CGD-O2D-CED
24	A	1135	CLA	CBD-CGD-O2D-CED
24	A	1137	CLA	CBD-CGD-O2D-CED
24	A	1140	CLA	CBD-CGD-O2D-CED
24	B	1206	CLA	CBD-CGD-O2D-CED
24	B	1210	CLA	CBD-CGD-O2D-CED
24	B	1217	CLA	CBD-CGD-O2D-CED
24	B	1219	CLA	CBD-CGD-O2D-CED
24	B	1224	CLA	CBD-CGD-O2D-CED
24	B	1229	CLA	CBD-CGD-O2D-CED
24	B	1231	CLA	CBD-CGD-O2D-CED
24	B	1232	CLA	CBD-CGD-O2D-CED
24	B	1237	CLA	CBD-CGD-O2D-CED
24	G	1601	CLA	CBD-CGD-O2D-CED
24	G	1603	CLA	CBD-CGD-O2D-CED
24	K	1401	CLA	CBD-CGD-O2D-CED
24	K	1402	CLA	CBD-CGD-O2D-CED
24	H	1701	CLA	CBD-CGD-O2D-CED
24	H	1703	CLA	CBD-CGD-O2D-CED
24	1	602	CLA	CBD-CGD-O2D-CED
24	1	603	CLA	CBD-CGD-O2D-CED
24	1	604	CLA	CBD-CGD-O2D-CED
24	1	608	CLA	CBD-CGD-O2D-CED
24	1	610	CLA	CBD-CGD-O2D-CED
24	1	611	CLA	CBD-CGD-O2D-CED
24	1	615	CLA	CBD-CGD-O2D-CED
24	a	601	CLA	CBD-CGD-O2D-CED
24	a	602	CLA	CBD-CGD-O2D-CED
24	a	603	CLA	CBD-CGD-O2D-CED
24	a	604	CLA	CBD-CGD-O2D-CED
24	a	605	CLA	CBD-CGD-O2D-CED
24	a	611	CLA	CBD-CGD-O2D-CED
24	a	612	CLA	CBD-CGD-O2D-CED
24	a	615	CLA	CBD-CGD-O2D-CED
24	3	602	CLA	CBD-CGD-O2D-CED
24	3	604	CLA	CBD-CGD-O2D-CED
24	3	605	CLA	CBD-CGD-O2D-CED
24	3	607	CLA	CBD-CGD-O2D-CED
24	3	616	CLA	CBD-CGD-O2D-CED
24	3	618	CLA	CBD-CGD-O2D-CED
24	4	602	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	4	604	CLA	CBD-CGD-O2D-CED
24	4	607	CLA	CBD-CGD-O2D-CED
24	4	615	CLA	CBD-CGD-O2D-CED
24	4	617	CLA	CBD-CGD-O2D-CED
24	5	603	CLA	CBD-CGD-O2D-CED
24	5	605	CLA	CBD-CGD-O2D-CED
24	5	606	CLA	CBD-CGD-O2D-CED
24	5	607	CLA	CBD-CGD-O2D-CED
24	5	608	CLA	CBD-CGD-O2D-CED
24	5	617	CLA	CBD-CGD-O2D-CED
24	5	618	CLA	CBD-CGD-O2D-CED
24	6	603	CLA	CBD-CGD-O2D-CED
24	6	604	CLA	CBD-CGD-O2D-CED
24	6	606	CLA	CBD-CGD-O2D-CED
24	6	612	CLA	CBD-CGD-O2D-CED
24	6	615	CLA	CBD-CGD-O2D-CED
24	6	617	CLA	CBD-CGD-O2D-CED
24	7	604	CLA	CBD-CGD-O2D-CED
24	8	602	CLA	CBD-CGD-O2D-CED
24	8	605	CLA	CBD-CGD-O2D-CED
24	8	608	CLA	CBD-CGD-O2D-CED
24	8	611	CLA	CBD-CGD-O2D-CED
24	8	620	CLA	CBD-CGD-O2D-CED
24	2	602	CLA	CBD-CGD-O2D-CED
24	2	606	CLA	CBD-CGD-O2D-CED
24	2	608	CLA	CBD-CGD-O2D-CED
24	2	609	CLA	CBD-CGD-O2D-CED
24	2	610	CLA	CBD-CGD-O2D-CED
24	2	613	CLA	CBD-CGD-O2D-CED
24	9	605	CLA	CBD-CGD-O2D-CED
24	9	607	CLA	CBD-CGD-O2D-CED
24	A	1114	CLA	O1A-CGA-O2A-C1
24	A	1122	CLA	O1A-CGA-O2A-C1
24	B	1228	CLA	O1A-CGA-O2A-C1
24	K	1404	CLA	O1A-CGA-O2A-C1
24	L	1501	CLA	O1A-CGA-O2A-C1
24	a	604	CLA	O1A-CGA-O2A-C1
24	2	603	CLA	O1A-CGA-O2A-C1
32	B	5004	PCW	O11-C11-O3-C3
50	7	807	4RF	O42-C41-O40-C39
50	8	808	4RF	O42-C41-O40-C39
51	8	806	P5S	O18-C17-O19-C1

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Mol	Chain	Res	Type	Atoms
24	K	1401	CLA	O1A-CGA-O2A-C1
24	K	1403	CLA	O1A-CGA-O2A-C1
24	H	1702	CLA	O1A-CGA-O2A-C1
24	a	615	CLA	O1A-CGA-O2A-C1
24	5	614	CLA	O1A-CGA-O2A-C1
24	5	616	CLA	O1A-CGA-O2A-C1
24	6	618	CLA	O1A-CGA-O2A-C1
24	8	607	CLA	O1A-CGA-O2A-C1
24	2	606	CLA	O1A-CGA-O2A-C1
24	2	607	CLA	O1A-CGA-O2A-C1
24	2	610	CLA	O1A-CGA-O2A-C1
24	4	605	CLA	CBA-CGA-O2A-C1
24	A	1012	CLA	O1D-CGD-O2D-CED
24	A	1116	CLA	O1D-CGD-O2D-CED
24	A	1118	CLA	O1D-CGD-O2D-CED
24	B	1224	CLA	O1D-CGD-O2D-CED
24	B	1232	CLA	O1D-CGD-O2D-CED
24	G	1601	CLA	O1D-CGD-O2D-CED
24	G	1603	CLA	O1D-CGD-O2D-CED
24	a	602	CLA	O1D-CGD-O2D-CED
24	a	603	CLA	O1D-CGD-O2D-CED
24	a	612	CLA	O1D-CGD-O2D-CED
24	4	602	CLA	O1D-CGD-O2D-CED
24	5	603	CLA	O1D-CGD-O2D-CED
24	6	603	CLA	O1D-CGD-O2D-CED
24	6	617	CLA	O1D-CGD-O2D-CED
24	8	620	CLA	O1D-CGD-O2D-CED
24	9	607	CLA	O1D-CGD-O2D-CED
24	A	1114	CLA	CBA-CGA-O2A-C1
24	A	1122	CLA	CBA-CGA-O2A-C1
24	B	1228	CLA	CBA-CGA-O2A-C1
24	K	1404	CLA	CBA-CGA-O2A-C1
24	2	603	CLA	CBA-CGA-O2A-C1
32	B	5004	PCW	C12-C11-O3-C3
24	B	1238	CLA	CBD-CGD-O2D-CED
24	a	607	CLA	CBD-CGD-O2D-CED
24	A	1102	CLA	O1A-CGA-O2A-C1
24	A	1104	CLA	O1A-CGA-O2A-C1
24	A	1119	CLA	O1A-CGA-O2A-C1
24	B	1201	CLA	O1A-CGA-O2A-C1
24	B	1204	CLA	O1A-CGA-O2A-C1
24	B	1213	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	B	1219	CLA	O1A-CGA-O2A-C1
24	B	1226	CLA	O1A-CGA-O2A-C1
24	1	607	CLA	O1A-CGA-O2A-C1
24	3	603	CLA	O1A-CGA-O2A-C1
24	3	610	CLA	O1A-CGA-O2A-C1
24	3	612	CLA	O1A-CGA-O2A-C1
24	4	612	CLA	O1A-CGA-O2A-C1
24	4	616	CLA	O1A-CGA-O2A-C1
24	6	607	CLA	O1A-CGA-O2A-C1
24	6	615	CLA	O1A-CGA-O2A-C1
24	7	610	CLA	O1A-CGA-O2A-C1
24	7	615	CLA	O1A-CGA-O2A-C1
24	8	606	CLA	O1A-CGA-O2A-C1
24	8	620	CLA	O1A-CGA-O2A-C1
28	F	5002	LHG	O10-C23-O8-C6
32	6	803	PCW	O11-C11-O3-C3
33	B	5005	PTY	O30-C30-O4-C1
33	5	802	PTY	O30-C30-O4-C1
34	F	5003	LAP	O2-C1-O1-C13
35	G	5001	SQD	O10-C23-O48-C46
35	7	805	SQD	O10-C23-O48-C46
46	5	803	DGA	OA1-CA1-OG1-CG1
50	8	807	4RF	O17-C16-O18-C19
24	A	1104	CLA	O1D-CGD-O2D-CED
24	A	1109	CLA	O1D-CGD-O2D-CED
24	A	1114	CLA	O1D-CGD-O2D-CED
24	A	1131	CLA	O1D-CGD-O2D-CED
24	B	1203	CLA	O1D-CGD-O2D-CED
24	B	1234	CLA	O1D-CGD-O2D-CED
24	B	1236	CLA	O1D-CGD-O2D-CED
24	J	1901	CLA	O1D-CGD-O2D-CED
24	L	1501	CLA	O1D-CGD-O2D-CED
24	1	602	CLA	O1D-CGD-O2D-CED
24	1	605	CLA	O1D-CGD-O2D-CED
24	3	606	CLA	O1D-CGD-O2D-CED
24	3	616	CLA	O1D-CGD-O2D-CED
24	4	601	CLA	O1D-CGD-O2D-CED
24	4	607	CLA	O1D-CGD-O2D-CED
24	4	611	CLA	O1D-CGD-O2D-CED
24	4	617	CLA	O1D-CGD-O2D-CED
24	5	608	CLA	O1D-CGD-O2D-CED
24	6	602	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	6	607	CLA	O1D-CGD-O2D-CED
24	7	603	CLA	O1D-CGD-O2D-CED
24	7	610	CLA	O1D-CGD-O2D-CED
24	2	601	CLA	O1D-CGD-O2D-CED
24	2	610	CLA	O1D-CGD-O2D-CED
24	2	621	CLA	O1D-CGD-O2D-CED
24	9	604	CLA	O1D-CGD-O2D-CED
24	9	609	CLA	O1D-CGD-O2D-CED
24	A	1112	CLA	O1D-CGD-O2D-CED
24	A	1139	CLA	O1D-CGD-O2D-CED
24	B	1022	CLA	O1D-CGD-O2D-CED
24	B	1207	CLA	O1D-CGD-O2D-CED
24	B	1228	CLA	O1D-CGD-O2D-CED
24	B	1239	CLA	O1D-CGD-O2D-CED
24	F	1301	CLA	O1D-CGD-O2D-CED
24	1	601	CLA	O1D-CGD-O2D-CED
24	1	606	CLA	O1D-CGD-O2D-CED
24	4	616	CLA	O1D-CGD-O2D-CED
24	5	602	CLA	O1D-CGD-O2D-CED
24	5	609	CLA	O1D-CGD-O2D-CED
24	5	612	CLA	O1D-CGD-O2D-CED
24	6	601	CLA	O1D-CGD-O2D-CED
24	6	618	CLA	O1D-CGD-O2D-CED
24	7	602	CLA	O1D-CGD-O2D-CED
24	7	612	CLA	O1D-CGD-O2D-CED
24	7	615	CLA	O1D-CGD-O2D-CED
24	8	603	CLA	O1D-CGD-O2D-CED
24	8	606	CLA	O1D-CGD-O2D-CED
24	2	603	CLA	O1D-CGD-O2D-CED
24	2	605	CLA	O1D-CGD-O2D-CED
24	2	607	CLA	O1D-CGD-O2D-CED
24	2	612	CLA	O1D-CGD-O2D-CED
24	9	603	CLA	O1D-CGD-O2D-CED
24	9	606	CLA	O1D-CGD-O2D-CED
24	B	1205	CLA	CBD-CGD-O2D-CED
24	L	1503	CLA	CBD-CGD-O2D-CED
24	7	608	CLA	CBD-CGD-O2D-CED
24	1	603	CLA	O1A-CGA-O2A-C1
24	9	604	CLA	O1A-CGA-O2A-C1
50	8	808	4RF	O17-C16-O18-C19
28	B	5001	LHG	O9-C7-O7-C5
28	F	5001	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
28	1	802	LHG	O9-C7-O7-C5
28	4	802	LHG	O9-C7-O7-C5
28	6	802	LHG	O9-C7-O7-C5
28	2	801	LHG	O9-C7-O7-C5
29	8	802	DGD	O1B-C1B-O2G-C2G
30	A	5007	3PH	O22-C21-O21-C2
33	5	802	PTY	O10-C8-O7-C6
33	7	804	PTY	O10-C8-O7-C6
35	G	5001	SQD	O49-C7-O47-C45
46	5	803	DGA	OB1-CB1-OG2-CG2
50	8	807	4RF	O23-C22-O21-C20
24	A	1105	CLA	O1D-CGD-O2D-CED
24	3	618	CLA	O1A-CGA-O2A-C1
24	9	609	CLA	O1A-CGA-O2A-C1
24	A	1102	CLA	C3-C5-C6-C7
24	A	1103	CLA	C3-C5-C6-C7
24	A	1106	CLA	C3-C5-C6-C7
24	A	1107	CLA	C3-C5-C6-C7
24	A	1130	CLA	C3-C5-C6-C7
24	B	1204	CLA	C3-C5-C6-C7
24	B	1205	CLA	C3-C5-C6-C7
24	B	1206	CLA	C3-C5-C6-C7
24	B	1208	CLA	C3-C5-C6-C7
24	B	1211	CLA	C3-C5-C6-C7
24	B	1213	CLA	C3-C5-C6-C7
24	B	1215	CLA	C3-C5-C6-C7
24	B	1216	CLA	C3-C5-C6-C7
24	B	1218	CLA	C3-C5-C6-C7
24	B	1237	CLA	C3-C5-C6-C7
24	L	1502	CLA	C3-C5-C6-C7
24	1	604	CLA	C3-C5-C6-C7
24	a	605	CLA	C3-C5-C6-C7
24	3	605	CLA	C3-C5-C6-C7
24	4	612	CLA	C3-C5-C6-C7
24	6	609	CLA	C3-C5-C6-C7
24	7	609	CLA	C3-C5-C6-C7
24	7	610	CLA	C3-C5-C6-C7
24	7	611	CLA	C3-C5-C6-C7
24	8	609	CLA	C3-C5-C6-C7
24	8	610	CLA	C3-C5-C6-C7
24	8	618	CLA	C3-C5-C6-C7
24	2	601	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
24	2	609	CLA	C3-C5-C6-C7
25	B	2002	PQN	C13-C15-C16-C17
41	8	604	CHL	C3-C5-C6-C7
24	K	1401	CLA	O1D-CGD-O2D-CED
24	1	603	CLA	O1D-CGD-O2D-CED
24	A	1102	CLA	CBA-CGA-O2A-C1
24	A	1104	CLA	CBA-CGA-O2A-C1
24	A	1108	CLA	CBA-CGA-O2A-C1
24	A	1119	CLA	CBA-CGA-O2A-C1
24	B	1201	CLA	CBA-CGA-O2A-C1
24	B	1213	CLA	CBA-CGA-O2A-C1
24	B	1219	CLA	CBA-CGA-O2A-C1
24	F	1301	CLA	CBA-CGA-O2A-C1
24	H	1703	CLA	CBA-CGA-O2A-C1
24	L	1501	CLA	CBA-CGA-O2A-C1
24	1	607	CLA	CBA-CGA-O2A-C1
24	a	604	CLA	CBA-CGA-O2A-C1
24	3	604	CLA	CBA-CGA-O2A-C1
24	3	610	CLA	CBA-CGA-O2A-C1
24	4	612	CLA	CBA-CGA-O2A-C1
24	5	612	CLA	CBA-CGA-O2A-C1
24	6	607	CLA	CBA-CGA-O2A-C1
24	7	607	CLA	CBA-CGA-O2A-C1
24	7	610	CLA	CBA-CGA-O2A-C1
24	8	606	CLA	CBA-CGA-O2A-C1
24	8	620	CLA	CBA-CGA-O2A-C1
24	2	605	CLA	CBA-CGA-O2A-C1
24	2	612	CLA	CBA-CGA-O2A-C1
28	F	5002	LHG	C24-C23-O8-C6
30	A	5007	3PH	C32-C31-O31-C3
32	6	803	PCW	C12-C11-O3-C3
33	B	5005	PTY	C31-C30-O4-C1
33	5	802	PTY	C31-C30-O4-C1
34	F	5003	LAP	C2-C1-O1-C13
35	G	5001	SQD	C24-C23-O48-C46
35	7	805	SQD	C24-C23-O48-C46
46	5	803	DGA	CA2-CA1-OG1-CG1
50	8	807	4RF	C15-C16-O18-C19
31	B	5006	LMT	O5'-C5'-C6'-O6'
24	A	1013	CLA	CBD-CGD-O2D-CED
24	A	1101	CLA	CBD-CGD-O2D-CED
24	A	1103	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	A	1106	CLA	CBD-CGD-O2D-CED
24	A	1110	CLA	CBD-CGD-O2D-CED
24	A	1115	CLA	CBD-CGD-O2D-CED
24	A	1127	CLA	CBD-CGD-O2D-CED
24	A	1128	CLA	CBD-CGD-O2D-CED
24	A	1133	CLA	CBD-CGD-O2D-CED
24	B	1201	CLA	CBD-CGD-O2D-CED
24	B	1202	CLA	CBD-CGD-O2D-CED
24	B	1211	CLA	CBD-CGD-O2D-CED
24	B	1212	CLA	CBD-CGD-O2D-CED
24	B	1213	CLA	CBD-CGD-O2D-CED
24	B	1223	CLA	CBD-CGD-O2D-CED
24	B	1227	CLA	CBD-CGD-O2D-CED
24	B	1230	CLA	CBD-CGD-O2D-CED
24	B	1240	CLA	CBD-CGD-O2D-CED
24	G	1602	CLA	CBD-CGD-O2D-CED
24	K	1404	CLA	CBD-CGD-O2D-CED
24	H	1702	CLA	CBD-CGD-O2D-CED
24	6	609	CLA	CBD-CGD-O2D-CED
24	7	607	CLA	CBD-CGD-O2D-CED
24	8	615	CLA	CBD-CGD-O2D-CED
24	2	604	CLA	CBD-CGD-O2D-CED
24	9	601	CLA	CBD-CGD-O2D-CED
28	9	802	LHG	C8-C7-O7-C5
32	B	5004	PCW	C32-C31-O2-C2
33	9	803	PTY	C11-C8-O7-C6
24	A	1123	CLA	O1D-CGD-O2D-CED
24	B	1210	CLA	O1D-CGD-O2D-CED
24	B	1215	CLA	O1D-CGD-O2D-CED
24	B	1216	CLA	O1D-CGD-O2D-CED
24	B	1226	CLA	O1D-CGD-O2D-CED
24	B	1229	CLA	O1D-CGD-O2D-CED
24	F	1302	CLA	O1D-CGD-O2D-CED
24	K	1403	CLA	O1D-CGD-O2D-CED
24	H	1703	CLA	O1D-CGD-O2D-CED
24	a	608	CLA	O1D-CGD-O2D-CED
24	3	603	CLA	O1D-CGD-O2D-CED
24	3	613	CLA	O1D-CGD-O2D-CED
24	4	606	CLA	O1D-CGD-O2D-CED
24	4	612	CLA	O1D-CGD-O2D-CED
24	5	601	CLA	O1D-CGD-O2D-CED
24	5	614	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	6	605	CLA	O1D-CGD-O2D-CED
24	6	608	CLA	O1D-CGD-O2D-CED
24	7	611	CLA	O1D-CGD-O2D-CED
24	8	610	CLA	O1D-CGD-O2D-CED
24	2	606	CLA	O1D-CGD-O2D-CED
24	9	602	CLA	O1D-CGD-O2D-CED
24	9	612	CLA	O1D-CGD-O2D-CED
24	B	1236	CLA	O1A-CGA-O2A-C1
24	8	609	CLA	O1A-CGA-O2A-C1
24	8	610	CLA	O1A-CGA-O2A-C1
24	4	605	CLA	O1A-CGA-O2A-C1
24	A	1107	CLA	O1D-CGD-O2D-CED
24	B	1214	CLA	O1D-CGD-O2D-CED
24	4	605	CLA	O1D-CGD-O2D-CED
24	B	1215	CLA	C4-C3-C5-C6
24	B	1217	CLA	C4-C3-C5-C6
24	B	1228	CLA	C4-C3-C5-C6
24	B	1239	CLA	C4-C3-C5-C6
24	1	604	CLA	C4-C3-C5-C6
24	4	612	CLA	C4-C3-C5-C6
24	5	603	CLA	C4-C3-C5-C6
24	6	601	CLA	C4-C3-C5-C6
24	8	602	CLA	C4-C3-C5-C6
24	B	1215	CLA	C2-C3-C5-C6
24	B	1217	CLA	C2-C3-C5-C6
24	B	1239	CLA	C2-C3-C5-C6
24	1	604	CLA	C2-C3-C5-C6
24	3	616	CLA	C2-C3-C5-C6
24	5	603	CLA	C2-C3-C5-C6
25	B	2002	PQN	C12-C13-C15-C16
41	8	601	CHL	C2-C3-C5-C6
24	3	618	CLA	CBA-CGA-O2A-C1
24	9	609	CLA	CBA-CGA-O2A-C1
24	9	607	CLA	C2-C1-O2A-CGA
24	A	1121	CLA	O1D-CGD-O2D-CED
24	B	1237	CLA	O1D-CGD-O2D-CED
24	3	602	CLA	O1D-CGD-O2D-CED
24	3	604	CLA	O1D-CGD-O2D-CED
24	3	607	CLA	O1D-CGD-O2D-CED
24	5	607	CLA	O1D-CGD-O2D-CED
24	5	617	CLA	O1D-CGD-O2D-CED
24	8	602	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	8	608	CLA	O1D-CGD-O2D-CED
24	A	1101	CLA	C2A-CAA-CBA-CGA
24	8	608	CLA	C3-C5-C6-C7
24	B	1206	CLA	O1A-CGA-O2A-C1
24	A	1110	CLA	C3-C5-C6-C7
24	A	1112	CLA	C3-C5-C6-C7
24	A	1122	CLA	C3-C5-C6-C7
24	B	1021	CLA	C3-C5-C6-C7
24	B	1226	CLA	C3-C5-C6-C7
24	B	1228	CLA	C3-C5-C6-C7
24	3	613	CLA	C3-C5-C6-C7
24	3	616	CLA	C3-C5-C6-C7
24	4	601	CLA	C3-C5-C6-C7
24	4	607	CLA	C3-C5-C6-C7
24	6	601	CLA	C3-C5-C6-C7
24	7	617	CLA	C3-C5-C6-C7
24	8	603	CLA	C3-C5-C6-C7
24	8	606	CLA	C3-C5-C6-C7
24	2	615	CLA	C3-C5-C6-C7
24	9	601	CLA	C3-C5-C6-C7
41	1	609	CHL	C3-C5-C6-C7
41	4	609	CHL	C3-C5-C6-C7
41	5	613	CHL	C3-C5-C6-C7
24	A	1118	CLA	CBA-CGA-O2A-C1
24	A	1120	CLA	CBA-CGA-O2A-C1
24	A	1123	CLA	CBA-CGA-O2A-C1
24	A	1135	CLA	CBA-CGA-O2A-C1
24	B	1204	CLA	CBA-CGA-O2A-C1
24	B	1206	CLA	CBA-CGA-O2A-C1
24	B	1207	CLA	CBA-CGA-O2A-C1
24	B	1209	CLA	CBA-CGA-O2A-C1
24	B	1215	CLA	CBA-CGA-O2A-C1
24	B	1226	CLA	CBA-CGA-O2A-C1
24	B	1230	CLA	CBA-CGA-O2A-C1
24	F	1302	CLA	CBA-CGA-O2A-C1
24	a	611	CLA	CBA-CGA-O2A-C1
24	3	603	CLA	CBA-CGA-O2A-C1
24	3	607	CLA	CBA-CGA-O2A-C1
24	3	612	CLA	CBA-CGA-O2A-C1
24	4	601	CLA	CBA-CGA-O2A-C1
24	4	604	CLA	CBA-CGA-O2A-C1
24	4	606	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	4	608	CLA	CBA-CGA-O2A-C1
24	4	616	CLA	CBA-CGA-O2A-C1
24	5	604	CLA	CBA-CGA-O2A-C1
24	6	603	CLA	CBA-CGA-O2A-C1
24	6	615	CLA	CBA-CGA-O2A-C1
24	7	609	CLA	CBA-CGA-O2A-C1
24	7	615	CLA	CBA-CGA-O2A-C1
24	9	604	CLA	CBA-CGA-O2A-C1
24	9	605	CLA	CBA-CGA-O2A-C1
24	9	606	CLA	CBA-CGA-O2A-C1
24	9	607	CLA	CBA-CGA-O2A-C1
50	8	808	4RF	C15-C16-O18-C19
29	B	5003	DGD	C8A-C9A-CAA-CBA
29	8	802	DGD	CEB-CFB-CGB-CHB
29	B	5003	DGD	CBA-CCA-CDA-CEA
29	8	802	DGD	CEA-CFA-CGA-CHA
27	A	4005	BCR	C19-C20-C21-C22
27	B	4006	BCR	C9-C10-C11-C12
27	F	4001	BCR	C9-C10-C11-C12
27	5	503	BCR	C9-C10-C11-C12
24	A	1108	CLA	O1A-CGA-O2A-C1
24	A	1118	CLA	O1A-CGA-O2A-C1
24	A	1123	CLA	O1A-CGA-O2A-C1
24	A	1135	CLA	O1A-CGA-O2A-C1
24	B	1207	CLA	O1A-CGA-O2A-C1
24	B	1209	CLA	O1A-CGA-O2A-C1
24	B	1212	CLA	O1A-CGA-O2A-C1
24	B	1237	CLA	O1A-CGA-O2A-C1
24	F	1302	CLA	O1A-CGA-O2A-C1
24	a	611	CLA	O1A-CGA-O2A-C1
24	3	604	CLA	O1A-CGA-O2A-C1
24	4	604	CLA	O1A-CGA-O2A-C1
24	4	606	CLA	O1A-CGA-O2A-C1
24	5	603	CLA	O1A-CGA-O2A-C1
24	5	604	CLA	O1A-CGA-O2A-C1
24	5	607	CLA	O1A-CGA-O2A-C1
24	5	617	CLA	O1A-CGA-O2A-C1
24	6	603	CLA	O1A-CGA-O2A-C1
24	6	604	CLA	O1A-CGA-O2A-C1
24	7	603	CLA	O1A-CGA-O2A-C1
24	7	609	CLA	O1A-CGA-O2A-C1
24	2	605	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	a	801	LHG	O9-C7-O7-C5
28	7	803	LHG	O9-C7-O7-C5
24	3	618	CLA	O1D-CGD-O2D-CED
24	4	604	CLA	O1D-CGD-O2D-CED
24	A	1111	CLA	O1D-CGD-O2D-CED
24	A	1125	CLA	O1D-CGD-O2D-CED
24	B	1231	CLA	O1D-CGD-O2D-CED
24	A	1104	CLA	C3-C5-C6-C7
24	A	1114	CLA	C3-C5-C6-C7
24	A	1115	CLA	C3-C5-C6-C7
24	B	1212	CLA	C3-C5-C6-C7
24	K	1402	CLA	C3-C5-C6-C7
24	5	601	CLA	C3-C5-C6-C7
24	5	612	CLA	C3-C5-C6-C7
24	8	612	CLA	CBD-CGD-O2D-CED
24	8	618	CLA	CBD-CGD-O2D-CED
28	F	5002	LHG	C5-C6-O8-C23
28	A	5002	LHG	O2-C2-C3-O3
28	A	5003	LHG	O2-C2-C3-O3
28	B	5001	LHG	O2-C2-C3-O3
28	B	5002	LHG	O2-C2-C3-O3
28	F	5002	LHG	O2-C2-C3-O3
28	1	801	LHG	O2-C2-C3-O3
28	a	801	LHG	O2-C2-C3-O3
28	3	801	LHG	O2-C2-C3-O3
28	4	801	LHG	O2-C2-C3-O3
28	4	802	LHG	O2-C2-C3-O3
28	6	802	LHG	O2-C2-C3-O3
28	7	802	LHG	O2-C2-C3-O3
28	2	801	LHG	O2-C2-C3-O3
28	2	802	LHG	O2-C2-C3-O3
28	9	801	LHG	O2-C2-C3-O3
24	A	1130	CLA	O1D-CGD-O2D-CED
24	A	1132	CLA	O1D-CGD-O2D-CED
24	A	1135	CLA	O1D-CGD-O2D-CED
24	a	604	CLA	O1D-CGD-O2D-CED
24	a	605	CLA	O1D-CGD-O2D-CED
24	6	604	CLA	O1D-CGD-O2D-CED
24	2	608	CLA	O1D-CGD-O2D-CED
24	9	605	CLA	O1D-CGD-O2D-CED
24	A	1117	CLA	CBA-CGA-O2A-C1
24	A	1126	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	A	1139	CLA	CBA-CGA-O2A-C1
24	B	1217	CLA	CBA-CGA-O2A-C1
24	B	1231	CLA	CBA-CGA-O2A-C1
24	B	1236	CLA	CBA-CGA-O2A-C1
24	B	1237	CLA	CBA-CGA-O2A-C1
24	1	603	CLA	CBA-CGA-O2A-C1
24	4	610	CLA	CBA-CGA-O2A-C1
24	5	607	CLA	CBA-CGA-O2A-C1
24	6	604	CLA	CBA-CGA-O2A-C1
24	7	603	CLA	CBA-CGA-O2A-C1
24	7	604	CLA	CBA-CGA-O2A-C1
24	7	612	CLA	CBA-CGA-O2A-C1
24	8	603	CLA	CBA-CGA-O2A-C1
24	8	609	CLA	CBA-CGA-O2A-C1
24	8	610	CLA	CBA-CGA-O2A-C1
24	8	618	CLA	CBA-CGA-O2A-C1
33	9	803	PTY	C31-C30-O4-C1
24	H	1703	CLA	O1A-CGA-O2A-C1
24	5	612	CLA	O1A-CGA-O2A-C1
24	7	607	CLA	O1A-CGA-O2A-C1
24	2	612	CLA	O1A-CGA-O2A-C1
24	9	605	CLA	O1A-CGA-O2A-C1
30	A	5007	3PH	O32-C31-O31-C3
34	F	5003	LAP	O1-C13-C14-O3
24	A	1102	CLA	O1D-CGD-O2D-CED
24	A	1120	CLA	O1D-CGD-O2D-CED
24	A	1134	CLA	O1D-CGD-O2D-CED
24	B	1217	CLA	O1D-CGD-O2D-CED
24	5	606	CLA	O1D-CGD-O2D-CED
24	2	602	CLA	O1D-CGD-O2D-CED
31	A	5008	LMT	C5'-C4'-O1B-C1B
31	B	5006	LMT	C4'-C5'-C6'-O6'
28	B	5002	LHG	C8-C7-O7-C5
28	F	5002	LHG	C8-C7-O7-C5
28	8	801	LHG	C8-C7-O7-C5
33	8	891	PTY	C11-C8-O7-C6
46	8	803	DGA	CB2-CB1-OG2-CG2
24	8	612	CLA	CBA-CGA-O2A-C1
24	6	612	CLA	O1D-CGD-O2D-CED
24	7	604	CLA	O1D-CGD-O2D-CED
24	A	1111	CLA	C3-C5-C6-C7
24	A	1123	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
24	A	1127	CLA	C3-C5-C6-C7
24	A	1136	CLA	C3-C5-C6-C7
24	1	612	CLA	C3-C5-C6-C7
24	4	603	CLA	C3-C5-C6-C7
28	2	802	LHG	C7-C8-C9-C10
23	A	1011	CL0	CBD-CGD-O2D-CED
24	A	1141	CLA	CBD-CGD-O2D-CED
24	L	1502	CLA	CBD-CGD-O2D-CED
24	A	1129	CLA	O1D-CGD-O2D-CED
24	1	604	CLA	O1D-CGD-O2D-CED
24	1	610	CLA	O1D-CGD-O2D-CED
24	1	611	CLA	O1D-CGD-O2D-CED
24	a	601	CLA	O1D-CGD-O2D-CED
24	5	605	CLA	O1D-CGD-O2D-CED
24	B	1212	CLA	CBA-CGA-O2A-C1
24	5	603	CLA	CBA-CGA-O2A-C1
24	5	617	CLA	CBA-CGA-O2A-C1
24	6	612	CLA	CBA-CGA-O2A-C1
24	B	1218	CLA	C4-C3-C5-C6
24	1	612	CLA	C4-C3-C5-C6
24	B	1218	CLA	C2-C3-C5-C6
24	B	1228	CLA	C2-C3-C5-C6
24	4	612	CLA	C2-C3-C5-C6
24	8	602	CLA	C2-C3-C5-C6
24	A	1126	CLA	O1A-CGA-O2A-C1
24	B	1217	CLA	O1A-CGA-O2A-C1
24	B	1230	CLA	O1A-CGA-O2A-C1
24	B	1231	CLA	O1A-CGA-O2A-C1
24	3	607	CLA	O1A-CGA-O2A-C1
24	4	601	CLA	O1A-CGA-O2A-C1
24	4	608	CLA	O1A-CGA-O2A-C1
24	4	610	CLA	O1A-CGA-O2A-C1
24	9	606	CLA	O1A-CGA-O2A-C1
24	9	607	CLA	O1A-CGA-O2A-C1
33	9	803	PTY	O30-C30-O4-C1
33	8	891	PTY	O10-C8-O7-C6
46	8	803	DGA	OB1-CB1-OG2-CG2
24	4	610	CLA	C2C-C3C-CAC-CBC
24	6	615	CLA	O1D-CGD-O2D-CED
32	B	5004	PCW	C2-C1-O3P-P
24	B	1216	CLA	C2A-CAA-CBA-CGA
24	6	606	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
24	6	609	CLA	C2A-CAA-CBA-CGA
24	A	1137	CLA	O1D-CGD-O2D-CED
24	A	1117	CLA	O1A-CGA-O2A-C1
24	A	1120	CLA	O1A-CGA-O2A-C1
24	B	1215	CLA	O1A-CGA-O2A-C1
24	7	604	CLA	O1A-CGA-O2A-C1
24	7	612	CLA	O1A-CGA-O2A-C1
24	8	603	CLA	O1A-CGA-O2A-C1
31	A	5008	LMT	O5'-C1'-O1'-C1
35	H	5001	SQD	O5-C1-O6-C44
28	7	801	LHG	C11-C12-C13-C14
24	A	1130	CLA	CBA-CGA-O2A-C1
24	B	1211	CLA	CBA-CGA-O2A-C1
24	7	606	CLA	CBA-CGA-O2A-C1
24	B	1204	CLA	CBD-CGD-O2D-CED
24	B	1222	CLA	CBD-CGD-O2D-CED
24	5	604	CLA	CBD-CGD-O2D-CED
24	7	601	CLA	CBD-CGD-O2D-CED
24	7	617	CLA	CBD-CGD-O2D-CED
24	8	609	CLA	CBD-CGD-O2D-CED
24	A	1139	CLA	O1A-CGA-O2A-C1
24	8	618	CLA	O1A-CGA-O2A-C1
24	A	1013	CLA	O1D-CGD-O2D-CED
24	B	1238	CLA	O1D-CGD-O2D-CED
24	a	607	CLA	O1D-CGD-O2D-CED
24	7	608	CLA	O1D-CGD-O2D-CED
24	A	1113	CLA	CBD-CGD-O2D-CED
24	A	1117	CLA	CBD-CGD-O2D-CED
24	3	601	CLA	CBD-CGD-O2D-CED
24	2	615	CLA	CBD-CGD-O2D-CED
27	B	4007	BCR	C9-C10-C11-C12
27	H	4001	BCR	C9-C10-C11-C12
27	4	503	BCR	C9-C10-C11-C12
40	1	503	LUT	C29-C30-C31-C32
24	A	1130	CLA	O1A-CGA-O2A-C1
24	A	1137	CLA	O1A-CGA-O2A-C1
24	6	612	CLA	O1A-CGA-O2A-C1
24	7	606	CLA	O1A-CGA-O2A-C1
28	B	5002	LHG	O9-C7-O7-C5
28	F	5002	LHG	O9-C7-O7-C5
28	A	5003	LHG	C1-C2-C3-O3
28	B	5001	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
28	B	5002	LHG	C1-C2-C3-O3
28	6	801	LHG	C1-C2-C3-O3
28	7	802	LHG	C1-C2-C3-O3
28	7	803	LHG	C1-C2-C3-O3
24	A	1106	CLA	CBA-CGA-O2A-C1
24	A	1121	CLA	CBA-CGA-O2A-C1
24	A	1124	CLA	CBA-CGA-O2A-C1
24	A	1131	CLA	CBA-CGA-O2A-C1
24	A	1137	CLA	CBA-CGA-O2A-C1
24	B	1023	CLA	CBA-CGA-O2A-C1
24	B	1202	CLA	CBA-CGA-O2A-C1
24	B	1229	CLA	CBA-CGA-O2A-C1
24	B	1234	CLA	CBA-CGA-O2A-C1
24	H	1701	CLA	CBA-CGA-O2A-C1
24	1	604	CLA	CBA-CGA-O2A-C1
24	1	612	CLA	CBA-CGA-O2A-C1
24	a	602	CLA	CBA-CGA-O2A-C1
24	a	607	CLA	CBA-CGA-O2A-C1
24	3	616	CLA	CBA-CGA-O2A-C1
24	4	611	CLA	CBA-CGA-O2A-C1
24	6	609	CLA	CBA-CGA-O2A-C1
24	7	601	CLA	CBA-CGA-O2A-C1
24	7	617	CLA	CBA-CGA-O2A-C1
24	8	608	CLA	CBA-CGA-O2A-C1
24	8	611	CLA	CBA-CGA-O2A-C1
24	2	615	CLA	CBA-CGA-O2A-C1
34	K	5001	LAP	C2-C1-O1-C13
28	5	801	LHG	C28-C29-C30-C31
28	7	801	LHG	C24-C25-C26-C27
24	B	1205	CLA	O1D-CGD-O2D-CED
24	B	1213	CLA	O1D-CGD-O2D-CED
24	K	1404	CLA	O1D-CGD-O2D-CED
24	L	1503	CLA	O1D-CGD-O2D-CED
24	8	615	CLA	O1D-CGD-O2D-CED
24	B	1211	CLA	O1D-CGD-O2D-CED
24	H	1702	CLA	O1D-CGD-O2D-CED
41	5	610	CHL	C4-C3-C5-C6
24	6	601	CLA	C2-C3-C5-C6
41	5	610	CHL	C2-C3-C5-C6
24	6	607	CLA	C3-C5-C6-C7
24	7	604	CLA	C3-C5-C6-C7
24	8	620	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
24	A	1125	CLA	C14-C13-C15-C16
24	B	1201	CLA	C11-C10-C8-C9
24	B	1209	CLA	C6-C7-C8-C9
24	B	1220	CLA	C11-C10-C8-C9
24	B	1224	CLA	C11-C10-C8-C9
24	B	1226	CLA	C6-C7-C8-C9
24	L	1502	CLA	C11-C10-C8-C9
24	1	605	CLA	C6-C7-C8-C9
24	1	606	CLA	C6-C7-C8-C9
24	3	606	CLA	C14-C13-C15-C16
24	6	601	CLA	C6-C7-C8-C9
24	7	601	CLA	C11-C10-C8-C9
41	8	604	CHL	C11-C12-C13-C14
24	A	1103	CLA	O1D-CGD-O2D-CED
24	A	1115	CLA	O1D-CGD-O2D-CED
24	B	1202	CLA	O1D-CGD-O2D-CED
24	B	1212	CLA	O1D-CGD-O2D-CED
24	B	1240	CLA	O1D-CGD-O2D-CED
24	G	1602	CLA	O1D-CGD-O2D-CED
24	7	607	CLA	O1D-CGD-O2D-CED
24	2	604	CLA	O1D-CGD-O2D-CED
31	A	5008	LMT	C2'-C1'-O1'-C1
31	B	5006	LMT	C2'-C1'-O1'-C1
28	5	801	LHG	C23-C24-C25-C26
28	1	802	LHG	O2-C2-C3-O3
34	B	5007	LAP	O3-C14-C15-O4
24	A	1127	CLA	O1D-CGD-O2D-CED
34	B	5007	LAP	C2-C1-O1-C13
36	G	5002	ERG	C22-C23-C24-C25
29	B	5003	DGD	C9B-CAB-CBB-CCB
24	A	1131	CLA	O1A-CGA-O2A-C1
24	1	612	CLA	O1A-CGA-O2A-C1
24	a	602	CLA	O1A-CGA-O2A-C1
24	a	607	CLA	O1A-CGA-O2A-C1
24	4	611	CLA	O1A-CGA-O2A-C1
24	8	611	CLA	O1A-CGA-O2A-C1
34	K	5001	LAP	O2-C1-O1-C13
24	A	1106	CLA	O1D-CGD-O2D-CED
24	B	1223	CLA	O1D-CGD-O2D-CED
24	B	1230	CLA	O1D-CGD-O2D-CED
27	A	4003	BCR	C36-C18-C19-C20
27	A	4004	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
27	A	4005	BCR	C7-C8-C9-C34
27	A	4005	BCR	C36-C18-C19-C20
27	B	4002	BCR	C37-C22-C23-C24
27	B	4004	BCR	C37-C22-C23-C24
27	B	4005	BCR	C36-C18-C19-C20
27	B	4006	BCR	C37-C22-C23-C24
27	B	4007	BCR	C37-C22-C23-C24
27	K	4002	BCR	C11-C12-C13-C35
27	H	4001	BCR	C37-C22-C23-C24
27	3	504	BCR	C7-C8-C9-C34
27	3	504	BCR	C36-C18-C19-C20
27	3	505	BCR	C36-C18-C19-C20
27	4	503	BCR	C7-C8-C9-C34
27	4	503	BCR	C11-C12-C13-C35
27	4	503	BCR	C36-C18-C19-C20
27	5	504	BCR	C37-C22-C23-C24
27	6	503	BCR	C36-C18-C19-C20
27	6	504	BCR	C36-C18-C19-C20
27	6	504	BCR	C37-C22-C23-C24
37	J	4002	RRX	C36-C18-C19-C20
40	a	503	LUT	C31-C32-C33-C40
40	5	501	LUT	C27-C28-C29-C39
40	5	505	LUT	C7-C8-C9-C19
40	5	505	LUT	C31-C32-C33-C40
40	9	502	LUT	C27-C28-C29-C39
49	7	504	C7Z	C7-C8-C9-C19
27	A	4005	BCR	C17-C18-C19-C20
27	B	4005	BCR	C17-C18-C19-C20
27	3	504	BCR	C7-C8-C9-C10
27	4	503	BCR	C7-C8-C9-C10
27	4	503	BCR	C11-C12-C13-C14
27	6	503	BCR	C17-C18-C19-C20
27	6	504	BCR	C21-C22-C23-C24
37	J	4002	RRX	C17-C18-C19-C20
39	M	4001	ECH	C11-C12-C13-C14
40	5	505	LUT	C7-C8-C9-C10
40	9	502	LUT	C27-C28-C29-C30
49	7	504	C7Z	C7-C8-C9-C10
49	7	504	C7Z	C27-C28-C29-C30
24	A	1125	CLA	C2A-CAA-CBA-CGA
24	A	1141	CLA	C2A-CAA-CBA-CGA
24	F	1302	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
24	6	606	CLA	C3-C5-C6-C7
41	6	619	CHL	C2A-CAA-CBA-CGA
28	A	5002	LHG	C7-C8-C9-C10
28	7	803	LHG	C23-C24-C25-C26
34	F	5003	LAP	C1-C2-C3-C4
24	A	1121	CLA	O1A-CGA-O2A-C1
24	A	1124	CLA	O1A-CGA-O2A-C1
24	B	1202	CLA	O1A-CGA-O2A-C1
24	B	1229	CLA	O1A-CGA-O2A-C1
24	B	1234	CLA	O1A-CGA-O2A-C1
24	6	609	CLA	O1A-CGA-O2A-C1
24	7	617	CLA	O1A-CGA-O2A-C1
24	8	608	CLA	O1A-CGA-O2A-C1
24	2	615	CLA	O1A-CGA-O2A-C1
24	A	1119	CLA	C3-C5-C6-C7
28	A	5001	LHG	O6-C4-C5-O7
24	A	1116	CLA	CBA-CGA-O2A-C1
24	A	1128	CLA	CBA-CGA-O2A-C1
24	1	605	CLA	CBA-CGA-O2A-C1
24	1	606	CLA	CBA-CGA-O2A-C1
24	B	1205	CLA	C15-C16-C17-C18
24	1	607	CLA	C5-C6-C7-C8
24	1	612	CLA	C10-C11-C12-C13
24	3	605	CLA	C15-C16-C17-C18
28	9	802	LHG	C23-C24-C25-C26
50	7	807	4RF	C41-C43-C44-C45
24	A	1108	CLA	C2-C1-O2A-CGA
24	A	1112	CLA	C2-C1-O2A-CGA
24	A	1124	CLA	C2-C1-O2A-CGA
24	A	1125	CLA	C2-C1-O2A-CGA
24	A	1126	CLA	C2-C1-O2A-CGA
24	A	1129	CLA	C2-C1-O2A-CGA
24	A	1130	CLA	C2-C1-O2A-CGA
24	A	1131	CLA	C2-C1-O2A-CGA
24	A	1133	CLA	C2-C1-O2A-CGA
24	B	1022	CLA	C2-C1-O2A-CGA
24	B	1203	CLA	C2-C1-O2A-CGA
24	B	1211	CLA	C2-C1-O2A-CGA
24	B	1216	CLA	C2-C1-O2A-CGA
24	B	1220	CLA	C2-C1-O2A-CGA
24	B	1235	CLA	C2-C1-O2A-CGA
24	B	1236	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
24	1	605	CLA	C2-C1-O2A-CGA
24	1	608	CLA	C2-C1-O2A-CGA
24	1	612	CLA	C2-C1-O2A-CGA
24	a	605	CLA	C2-C1-O2A-CGA
24	3	610	CLA	C2-C1-O2A-CGA
24	4	616	CLA	C2-C1-O2A-CGA
24	5	602	CLA	C2-C1-O2A-CGA
24	5	606	CLA	C2-C1-O2A-CGA
24	6	606	CLA	C2-C1-O2A-CGA
24	6	612	CLA	C2-C1-O2A-CGA
24	7	607	CLA	C2-C1-O2A-CGA
24	7	617	CLA	C2-C1-O2A-CGA
24	8	606	CLA	C2-C1-O2A-CGA
24	8	608	CLA	C2-C1-O2A-CGA
24	8	611	CLA	C2-C1-O2A-CGA
24	8	620	CLA	C2-C1-O2A-CGA
24	B	1201	CLA	O1D-CGD-O2D-CED
24	9	601	CLA	O1D-CGD-O2D-CED
24	A	1013	CLA	C8-C10-C11-C12
24	A	1101	CLA	C8-C10-C11-C12
24	A	1110	CLA	C10-C11-C12-C13
24	A	1117	CLA	C15-C16-C17-C18
24	A	1133	CLA	C8-C10-C11-C12
24	A	1133	CLA	C15-C16-C17-C18
24	B	1023	CLA	C13-C15-C16-C17
24	B	1208	CLA	C5-C6-C7-C8
24	B	1210	CLA	C8-C10-C11-C12
24	B	1224	CLA	C8-C10-C11-C12
24	B	1239	CLA	C5-C6-C7-C8
24	1	612	CLA	C13-C15-C16-C17
24	a	605	CLA	C8-C10-C11-C12
24	4	603	CLA	C5-C6-C7-C8
24	7	601	CLA	C8-C10-C11-C12
28	7	803	LHG	O1-C1-C2-O2
28	8	801	LHG	O1-C1-C2-O2
24	B	1023	CLA	O1A-CGA-O2A-C1
24	1	604	CLA	C13-C15-C16-C17
24	B	1209	CLA	CBD-CGD-O2D-CED
24	A	1102	CLA	C12-C13-C15-C16
24	A	1133	CLA	C12-C13-C15-C16
24	A	1135	CLA	C6-C7-C8-C10
24	B	1203	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
24	B	1214	CLA	C6-C7-C8-C10
41	7	613	CHL	C11-C12-C13-C15
24	A	1101	CLA	O1D-CGD-O2D-CED
24	A	1112	CLA	CBA-CGA-O2A-C1
24	6	606	CLA	CBA-CGA-O2A-C1
28	5	801	LHG	C31-C32-C33-C34
24	A	1132	CLA	C4-C3-C5-C6
41	6	610	CHL	C4-C3-C5-C6
24	A	1116	CLA	C10-C11-C12-C13
24	B	1214	CLA	C8-C10-C11-C12
24	3	606	CLA	C10-C11-C12-C13
33	3	802	PTY	C30-C31-C32-C33
46	8	803	DGA	CB1-CB2-CB3-CB4
27	B	4005	BCR	C19-C20-C21-C22
27	J	4001	BCR	C9-C10-C11-C12
27	K	4002	BCR	C13-C14-C15-C16
27	L	4003	BCR	C13-C14-C15-C16
40	1	502	LUT	C29-C30-C31-C32
40	4	501	LUT	C29-C30-C31-C32
49	7	504	C7Z	C29-C30-C31-C32
24	3	601	CLA	C3-C5-C6-C7
24	4	610	CLA	C3-C5-C6-C7
24	B	1224	CLA	C13-C15-C16-C17
24	1	607	CLA	C10-C11-C12-C13
24	3	606	CLA	C15-C16-C17-C18
24	A	1110	CLA	O1D-CGD-O2D-CED
28	B	5001	LHG	C23-C24-C25-C26
28	F	5001	LHG	C7-C8-C9-C10
28	F	5001	LHG	C23-C24-C25-C26
28	4	802	LHG	C7-C8-C9-C10
28	6	802	LHG	C23-C24-C25-C26
28	7	802	LHG	C7-C8-C9-C10
28	9	801	LHG	C23-C24-C25-C26
50	8	808	4RF	C13-C14-C15-C16
24	1	604	CLA	O1A-CGA-O2A-C1
24	3	616	CLA	O1A-CGA-O2A-C1
35	H	5001	SQD	C8-C7-O47-C45
24	A	1128	CLA	O1D-CGD-O2D-CED
24	6	609	CLA	O1D-CGD-O2D-CED
24	5	606	CLA	CBA-CGA-O2A-C1
24	A	1012	CLA	C5-C6-C7-C8
24	A	1119	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
24	A	1127	CLA	C8-C10-C11-C12
24	A	1135	CLA	C10-C11-C12-C13
24	A	1137	CLA	C8-C10-C11-C12
24	A	1139	CLA	C5-C6-C7-C8
24	B	1202	CLA	C5-C6-C7-C8
24	B	1202	CLA	C15-C16-C17-C18
24	B	1208	CLA	C10-C11-C12-C13
24	B	1219	CLA	C5-C6-C7-C8
24	B	1231	CLA	C5-C6-C7-C8
24	B	1238	CLA	C13-C15-C16-C17
24	L	1502	CLA	C8-C10-C11-C12
24	1	607	CLA	C15-C16-C17-C18
24	7	617	CLA	C5-C6-C7-C8
24	A	1106	CLA	C2A-CAA-CBA-CGA
24	A	1110	CLA	C2A-CAA-CBA-CGA
24	A	1129	CLA	C2A-CAA-CBA-CGA
24	B	1237	CLA	C2A-CAA-CBA-CGA
24	L	1501	CLA	C2A-CAA-CBA-CGA
24	1	610	CLA	C2A-CAA-CBA-CGA
24	a	611	CLA	C2A-CAA-CBA-CGA
24	3	603	CLA	C2A-CAA-CBA-CGA
24	3	610	CLA	C2A-CAA-CBA-CGA
24	4	608	CLA	C2A-CAA-CBA-CGA
24	4	612	CLA	C2A-CAA-CBA-CGA
24	5	603	CLA	C2A-CAA-CBA-CGA
24	5	609	CLA	C2A-CAA-CBA-CGA
24	7	617	CLA	C2A-CAA-CBA-CGA
24	8	618	CLA	C2A-CAA-CBA-CGA
24	2	606	CLA	C2A-CAA-CBA-CGA
41	4	613	CHL	C2A-CAA-CBA-CGA
41	9	610	CHL	C2A-CAA-CBA-CGA
24	4	610	CLA	C4C-C3C-CAC-CBC
24	A	1104	CLA	C8-C10-C11-C12
24	A	1110	CLA	C5-C6-C7-C8
24	A	1119	CLA	C8-C10-C11-C12
24	A	1136	CLA	C10-C11-C12-C13
24	B	1021	CLA	C8-C10-C11-C12
24	B	1203	CLA	C15-C16-C17-C18
24	B	1210	CLA	C15-C16-C17-C18
24	B	1218	CLA	C5-C6-C7-C8
24	B	1221	CLA	C10-C11-C12-C13
24	B	1223	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	B	1235	CLA	C8-C10-C11-C12
24	B	1239	CLA	C13-C15-C16-C17
24	H	1703	CLA	C5-C6-C7-C8
24	3	607	CLA	C10-C11-C12-C13
24	3	613	CLA	C10-C11-C12-C13
24	3	616	CLA	C5-C6-C7-C8
24	5	607	CLA	C5-C6-C7-C8
24	6	601	CLA	C10-C11-C12-C13
24	6	609	CLA	C15-C16-C17-C18
24	6	615	CLA	C8-C10-C11-C12
24	2	601	CLA	C10-C11-C12-C13
24	9	605	CLA	C10-C11-C12-C13
28	A	5002	LHG	C23-C24-C25-C26
28	F	5002	LHG	C7-C8-C9-C10
28	1	802	LHG	C23-C24-C25-C26
28	7	801	LHG	C23-C24-C25-C26
28	7	802	LHG	C23-C24-C25-C26
28	2	802	LHG	C23-C24-C25-C26
33	9	803	PTY	C8-C11-C12-C13
50	8	807	4RF	C41-C43-C44-C45
24	A	1106	CLA	O1A-CGA-O2A-C1
24	H	1701	CLA	O1A-CGA-O2A-C1
24	A	1125	CLA	C3-C5-C6-C7
31	1	804	LMT	O5'-C1'-O1'-C1
24	B	1227	CLA	O1D-CGD-O2D-CED
24	A	1103	CLA	C8-C10-C11-C12
24	A	1103	CLA	C10-C11-C12-C13
24	A	1123	CLA	C10-C11-C12-C13
24	A	1128	CLA	C8-C10-C11-C12
24	B	1021	CLA	C13-C15-C16-C17
24	B	1023	CLA	C8-C10-C11-C12
24	B	1210	CLA	C10-C11-C12-C13
24	B	1212	CLA	C10-C11-C12-C13
24	B	1224	CLA	C10-C11-C12-C13
24	B	1228	CLA	C13-C15-C16-C17
24	B	1235	CLA	C5-C6-C7-C8
24	B	1238	CLA	C15-C16-C17-C18
24	a	603	CLA	C10-C11-C12-C13
24	a	604	CLA	C13-C15-C16-C17
24	4	610	CLA	C8-C10-C11-C12
24	4	612	CLA	C8-C10-C11-C12
24	6	604	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	6	607	CLA	C5-C6-C7-C8
24	7	603	CLA	C13-C15-C16-C17
24	7	607	CLA	C8-C10-C11-C12
24	7	611	CLA	C5-C6-C7-C8
24	8	620	CLA	C15-C16-C17-C18
24	9	605	CLA	C8-C10-C11-C12
28	5	801	LHG	O2-C2-C3-O3
28	7	803	LHG	O2-C2-C3-O3
38	J	5001	LPX	O1-C3-C4-O5
28	2	802	LHG	C24-C23-O8-C6
24	4	612	CLA	C13-C15-C16-C17
28	8	801	LHG	C23-C24-C25-C26
24	B	1203	CLA	C8-C10-C11-C12
24	B	1209	CLA	C15-C16-C17-C18
24	B	1212	CLA	C8-C10-C11-C12
24	B	1220	CLA	C5-C6-C7-C8
24	B	1226	CLA	C15-C16-C17-C18
24	a	612	CLA	C5-C6-C7-C8
24	5	612	CLA	C10-C11-C12-C13
24	7	615	CLA	C5-C6-C7-C8
24	9	612	CLA	C15-C16-C17-C18
28	8	801	LHG	O9-C7-O7-C5
24	9	602	CLA	CBA-CGA-O2A-C1
29	A	5005	DGD	C8B-C9B-CAB-CBB
24	8	612	CLA	O1D-CGD-O2D-CED
24	8	618	CLA	O1D-CGD-O2D-CED
24	A	1101	CLA	C15-C16-C17-C18
24	A	1102	CLA	C8-C10-C11-C12
24	A	1104	CLA	C13-C15-C16-C17
24	A	1136	CLA	C8-C10-C11-C12
24	B	1209	CLA	C5-C6-C7-C8
24	B	1216	CLA	C5-C6-C7-C8
24	B	1228	CLA	C8-C10-C11-C12
24	1	605	CLA	C10-C11-C12-C13
24	3	612	CLA	C15-C16-C17-C18
24	4	601	CLA	C5-C6-C7-C8
24	8	610	CLA	C5-C6-C7-C8
24	7	601	CLA	O1A-CGA-O2A-C1
34	B	5007	LAP	O2-C1-O1-C13
24	A	1132	CLA	C2-C3-C5-C6
28	A	5001	LHG	C23-C24-C25-C26
28	4	801	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
32	B	5004	PCW	C11-C12-C13-C14
33	7	804	PTY	C8-C11-C12-C13
50	8	807	4RF	C13-C14-C15-C16
24	A	1133	CLA	O1D-CGD-O2D-CED
24	8	612	CLA	O1A-CGA-O2A-C1
24	A	1114	CLA	C5-C6-C7-C8
24	B	1022	CLA	C13-C15-C16-C17
24	B	1201	CLA	C5-C6-C7-C8
24	1	603	CLA	C10-C11-C12-C13
24	3	605	CLA	C5-C6-C7-C8
24	7	603	CLA	C5-C6-C7-C8
24	8	618	CLA	C5-C6-C7-C8
24	9	603	CLA	C10-C11-C12-C13
24	9	606	CLA	C5-C6-C7-C8
24	A	1125	CLA	CBA-CGA-O2A-C1
24	A	1133	CLA	CBA-CGA-O2A-C1
24	4	603	CLA	CBA-CGA-O2A-C1
24	5	609	CLA	CBA-CGA-O2A-C1
28	A	5002	LHG	C8-C7-O7-C5
28	6	801	LHG	C8-C7-O7-C5
24	A	1116	CLA	O1A-CGA-O2A-C1
24	B	1211	CLA	O1A-CGA-O2A-C1
24	5	605	CLA	CBA-CGA-O2A-C1
24	A	1013	CLA	C3-C5-C6-C7
24	B	1236	CLA	C3-C5-C6-C7
24	4	611	CLA	C3-C5-C6-C7
24	4	615	CLA	C3-C5-C6-C7
24	2	604	CLA	C3-C5-C6-C7
24	2	615	CLA	C8-C10-C11-C12
27	B	4004	BCR	C9-C10-C11-C12
27	B	4006	BCR	C15-C16-C17-C18
27	K	4002	BCR	C9-C10-C11-C12
40	a	501	LUT	C29-C30-C31-C32
24	A	1115	CLA	C8-C10-C11-C12
24	B	1212	CLA	C5-C6-C7-C8
24	3	613	CLA	C8-C10-C11-C12
24	1	606	CLA	O1A-CGA-O2A-C1
28	A	5002	LHG	O9-C7-O7-C5
28	6	801	LHG	O9-C7-O7-C5
35	H	5001	SQD	O49-C7-O47-C45
28	F	5002	LHG	C1-C2-C3-O3
28	1	801	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
28	4	802	LHG	C1-C2-C3-O3
38	J	5001	LPX	O1-C3-C4-C5
24	A	1139	CLA	C2A-CAA-CBA-CGA
24	3	604	CLA	C2A-CAA-CBA-CGA
24	7	604	CLA	C2A-CAA-CBA-CGA
24	8	603	CLA	C2A-CAA-CBA-CGA
24	A	1013	CLA	CBA-CGA-O2A-C1
28	A	5002	LHG	C24-C23-O8-C6
52	9	504	A8S	O11-C1-C2-C3
24	A	1013	CLA	C5-C6-C7-C8
24	A	1102	CLA	C13-C15-C16-C17
24	B	1213	CLA	C10-C11-C12-C13
24	B	1214	CLA	C5-C6-C7-C8
24	B	1215	CLA	C5-C6-C7-C8
24	B	1240	CLA	C5-C6-C7-C8
24	a	604	CLA	C8-C10-C11-C12
24	a	605	CLA	C5-C6-C7-C8
24	4	612	CLA	C10-C11-C12-C13
24	5	612	CLA	C8-C10-C11-C12
24	7	604	CLA	C10-C11-C12-C13
24	7	609	CLA	C10-C11-C12-C13
41	7	613	CHL	C5-C6-C7-C8
24	A	1109	CLA	C3-C5-C6-C7
24	5	603	CLA	C3-C5-C6-C7
33	B	5005	PTY	C30-C31-C32-C33
24	A	1101	CLA	C5-C6-C7-C8
24	A	1112	CLA	C5-C6-C7-C8
24	A	1122	CLA	C10-C11-C12-C13
24	A	1122	CLA	C15-C16-C17-C18
24	A	1132	CLA	C5-C6-C7-C8
24	B	1021	CLA	C10-C11-C12-C13
24	B	1202	CLA	C10-C11-C12-C13
24	B	1204	CLA	C15-C16-C17-C18
24	3	610	CLA	C10-C11-C12-C13
24	4	601	CLA	C10-C11-C12-C13
24	6	604	CLA	C15-C16-C17-C18
24	A	1128	CLA	C10-C11-C12-C13
24	B	1201	CLA	C13-C15-C16-C17
24	B	1226	CLA	C13-C15-C16-C17
24	1	604	CLA	C15-C16-C17-C18
24	1	608	CLA	C10-C11-C12-C13
24	3	605	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
24	8	603	CLA	C5-C6-C7-C8
24	8	606	CLA	C5-C6-C7-C8
41	4	609	CHL	C5-C6-C7-C8
24	A	1113	CLA	CBA-CGA-O2A-C1
24	A	1127	CLA	CBA-CGA-O2A-C1
24	L	1502	CLA	CBA-CGA-O2A-C1
24	1	606	CLA	C8-C10-C11-C12
24	8	606	CLA	C8-C10-C11-C12
24	2	604	CLA	C4-C3-C5-C6
24	1	612	CLA	C2-C3-C5-C6
24	A	1141	CLA	O1D-CGD-O2D-CED
24	L	1502	CLA	O1D-CGD-O2D-CED
24	7	601	CLA	O1D-CGD-O2D-CED
24	A	1111	CLA	C10-C11-C12-C13
24	A	1131	CLA	C15-C16-C17-C18
24	K	1402	CLA	C8-C10-C11-C12
24	8	609	CLA	C5-C6-C7-C8
36	G	5002	ERG	C13-C17-C20-C22
32	6	803	PCW	C32-C31-O2-C2
28	6	801	LHG	C25-C26-C27-C28
32	6	803	PCW	O31-C31-O2-C2
29	8	802	DGD	C2E-C1E-O5D-C6D
35	7	805	SQD	C2-C1-O6-C44
24	a	603	CLA	C13-C15-C16-C17
28	A	5003	LHG	C7-C8-C9-C10
24	A	1134	CLA	CBA-CGA-O2A-C1
24	B	1210	CLA	CBA-CGA-O2A-C1
24	a	605	CLA	CBA-CGA-O2A-C1
24	9	603	CLA	CBA-CGA-O2A-C1
24	A	1111	CLA	C16-C17-C18-C20
24	A	1126	CLA	C16-C17-C18-C19
24	A	1128	CLA	C16-C17-C18-C19
24	A	1140	CLA	C6-C7-C8-C9
24	a	608	CLA	C6-C7-C8-C10
24	4	611	CLA	C5-C6-C7-C8
24	A	1128	CLA	O1A-CGA-O2A-C1
24	4	603	CLA	O1A-CGA-O2A-C1
24	6	606	CLA	O1A-CGA-O2A-C1
28	7	801	LHG	C7-C8-C9-C10
24	7	609	CLA	CBD-CGD-O2D-CED
24	A	1110	CLA	C8-C10-C11-C12
24	B	1228	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
27	F	4001	BCR	C37-C22-C23-C24
27	G	4001	BCR	C37-C22-C23-C24
27	5	504	BCR	C11-C12-C13-C35
28	7	802	LHG	C2-C3-O3-P
37	J	4002	RRX	C37-C22-C23-C24
40	a	501	LUT	C27-C28-C29-C39
40	6	502	LUT	C27-C28-C29-C39
49	7	504	C7Z	C27-C28-C29-C39
51	8	806	P5S	C2-C3-O16-P12
28	3	801	LHG	C25-C26-C27-C28
24	a	612	CLA	C8-C10-C11-C12
27	B	4007	BCR	C21-C22-C23-C24
27	G	4001	BCR	C21-C22-C23-C24
27	5	504	BCR	C21-C22-C23-C24
37	J	4002	RRX	C7-C8-C9-C10
40	5	501	LUT	C27-C28-C29-C30
40	6	502	LUT	C27-C28-C29-C30
24	A	1104	CLA	C2A-CAA-CBA-CGA
24	A	1118	CLA	C2A-CAA-CBA-CGA
24	A	1131	CLA	C2A-CAA-CBA-CGA
24	A	1134	CLA	C2A-CAA-CBA-CGA
24	B	1201	CLA	C2A-CAA-CBA-CGA
24	B	1204	CLA	C2A-CAA-CBA-CGA
24	B	1209	CLA	C2A-CAA-CBA-CGA
24	B	1239	CLA	C2A-CAA-CBA-CGA
24	G	1601	CLA	C2A-CAA-CBA-CGA
24	G	1602	CLA	C2A-CAA-CBA-CGA
24	1	603	CLA	C2A-CAA-CBA-CGA
24	1	606	CLA	C2A-CAA-CBA-CGA
24	1	612	CLA	C2A-CAA-CBA-CGA
24	5	604	CLA	C2A-CAA-CBA-CGA
24	5	607	CLA	C2A-CAA-CBA-CGA
24	6	603	CLA	C2A-CAA-CBA-CGA
24	7	606	CLA	C2A-CAA-CBA-CGA
24	7	615	CLA	C2A-CAA-CBA-CGA
24	8	611	CLA	C2A-CAA-CBA-CGA
24	2	615	CLA	C2A-CAA-CBA-CGA
41	1	609	CHL	C2A-CAA-CBA-CGA
41	4	618	CHL	C2A-CAA-CBA-CGA
24	3	601	CLA	C10-C11-C12-C13
24	6	604	CLA	C13-C15-C16-C17
24	7	606	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
28	A	5003	LHG	O1-C1-C2-C3
28	B	5001	LHG	O1-C1-C2-C3
28	F	5001	LHG	O1-C1-C2-C3
28	F	5002	LHG	O1-C1-C2-C3
28	1	801	LHG	O1-C1-C2-C3
28	6	802	LHG	O1-C1-C2-C3
28	7	802	LHG	O1-C1-C2-C3
28	7	803	LHG	O1-C1-C2-C3
28	8	801	LHG	O1-C1-C2-C3
28	2	801	LHG	O1-C1-C2-C3
28	2	802	LHG	O1-C1-C2-C3
35	G	5001	SQD	C44-C45-O47-C7
24	A	1108	CLA	C16-C17-C18-C19
24	A	1116	CLA	C11-C12-C13-C15
24	F	1302	CLA	C6-C7-C8-C10
24	a	603	CLA	C16-C17-C18-C19
24	3	604	CLA	C11-C12-C13-C15
24	4	607	CLA	C6-C7-C8-C10
24	6	601	CLA	C11-C12-C13-C15
24	6	603	CLA	C16-C17-C18-C19
24	8	620	CLA	C16-C17-C18-C20
23	A	1011	CL0	O1D-CGD-O2D-CED
24	A	1112	CLA	O1A-CGA-O2A-C1
24	A	1125	CLA	O1A-CGA-O2A-C1
24	A	1133	CLA	O1A-CGA-O2A-C1
24	1	605	CLA	O1A-CGA-O2A-C1
24	5	606	CLA	O1A-CGA-O2A-C1
24	5	609	CLA	O1A-CGA-O2A-C1
41	3	611	CHL	C3-C5-C6-C7
24	5	612	CLA	C15-C16-C17-C18
29	8	802	DGD	O6E-C1E-O5D-C6D
35	7	805	SQD	O5-C1-O6-C44
28	1	801	LHG	C8-C7-O7-C5
28	5	801	LHG	C8-C7-O7-C5
28	A	5003	LHG	C23-C24-C25-C26
33	3	802	PTY	O4-C1-C6-O7
24	a	601	CLA	CBA-CGA-O2A-C1
24	8	602	CLA	CBA-CGA-O2A-C1
24	2	621	CLA	CBA-CGA-O2A-C1
24	A	1133	CLA	C5-C6-C7-C8
24	B	1203	CLA	C10-C11-C12-C13
24	8	603	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
24	8	609	CLA	C8-C10-C11-C12
28	4	801	LHG	C23-C24-C25-C26
24	B	1229	CLA	C3-C5-C6-C7
24	B	1204	CLA	O1D-CGD-O2D-CED
24	5	604	CLA	O1D-CGD-O2D-CED
24	A	1012	CLA	C2-C1-O2A-CGA
24	A	1105	CLA	C2-C1-O2A-CGA
24	A	1111	CLA	C2-C1-O2A-CGA
24	A	1114	CLA	C2-C1-O2A-CGA
24	A	1118	CLA	C2-C1-O2A-CGA
24	A	1127	CLA	C2-C1-O2A-CGA
24	A	1139	CLA	C2-C1-O2A-CGA
24	B	1202	CLA	C2-C1-O2A-CGA
24	B	1215	CLA	C2-C1-O2A-CGA
24	B	1228	CLA	C2-C1-O2A-CGA
24	B	1230	CLA	C2-C1-O2A-CGA
24	B	1240	CLA	C2-C1-O2A-CGA
24	F	1301	CLA	C2-C1-O2A-CGA
24	G	1601	CLA	C2-C1-O2A-CGA
24	L	1501	CLA	C2-C1-O2A-CGA
24	1	611	CLA	C2-C1-O2A-CGA
24	a	602	CLA	C2-C1-O2A-CGA
24	a	608	CLA	C2-C1-O2A-CGA
24	3	605	CLA	C2-C1-O2A-CGA
24	3	607	CLA	C2-C1-O2A-CGA
24	3	613	CLA	C2-C1-O2A-CGA
24	5	607	CLA	C2-C1-O2A-CGA
24	5	609	CLA	C2-C1-O2A-CGA
24	5	612	CLA	C2-C1-O2A-CGA
24	6	607	CLA	C2-C1-O2A-CGA
24	7	606	CLA	C2-C1-O2A-CGA
24	7	611	CLA	C2-C1-O2A-CGA
24	2	612	CLA	C2-C1-O2A-CGA
24	2	615	CLA	C2-C1-O2A-CGA
24	9	601	CLA	C2-C1-O2A-CGA
24	9	605	CLA	C2-C1-O2A-CGA
24	9	612	CLA	C2-C1-O2A-CGA
41	3	611	CHL	C2-C1-O2A-CGA
23	A	1011	CL0	C16-C17-C18-C19
24	A	1107	CLA	C6-C7-C8-C10
24	A	1108	CLA	C16-C17-C18-C20
24	A	1111	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
24	A	1126	CLA	C16-C17-C18-C20
24	A	1128	CLA	C16-C17-C18-C20
24	A	1136	CLA	C16-C17-C18-C20
24	B	1022	CLA	C16-C17-C18-C19
24	B	1223	CLA	C16-C17-C18-C19
24	F	1302	CLA	C6-C7-C8-C9
24	1	605	CLA	C16-C17-C18-C20
24	a	603	CLA	C16-C17-C18-C20
24	a	608	CLA	C6-C7-C8-C9
24	4	615	CLA	C11-C12-C13-C15
24	6	615	CLA	C16-C17-C18-C19
24	8	603	CLA	C16-C17-C18-C20
24	9	605	CLA	C11-C12-C13-C15
25	A	2001	PQN	C26-C27-C28-C30
24	B	1210	CLA	C5-C6-C7-C8
24	B	1231	CLA	C10-C11-C12-C13
24	B	1240	CLA	C10-C11-C12-C13
28	4	802	LHG	C11-C12-C13-C14
28	7	801	LHG	C11-C10-C9-C8
24	B	1208	CLA	CBD-CGD-O2D-CED
28	A	5002	LHG	C34-C35-C36-C37
28	1	802	LHG	C11-C12-C13-C14
28	4	801	LHG	C13-C14-C15-C16
28	2	801	LHG	C28-C29-C30-C31
33	8	891	PTY	C12-C13-C14-C15
24	3	612	CLA	C5-C6-C7-C8
28	F	5001	LHG	C11-C12-C13-C14
28	4	802	LHG	C9-C10-C11-C12
28	6	801	LHG	C11-C12-C13-C14
28	7	801	LHG	C26-C27-C28-C29
28	7	802	LHG	C11-C12-C13-C14
46	8	803	DGA	CB3-CB4-CB5-CB6
24	B	1219	CLA	C10-C11-C12-C13
28	5	801	LHG	C11-C12-C13-C14
28	8	801	LHG	C26-C27-C28-C29
33	B	5005	PTY	C13-C14-C15-C16
33	9	803	PTY	C33-C34-C35-C36
35	7	805	SQD	C10-C11-C12-C13
28	A	5002	LHG	O1-C1-C2-O2
28	A	5003	LHG	O1-C1-C2-O2
28	B	5002	LHG	O1-C1-C2-O2
28	F	5001	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
28	F	5002	LHG	O1-C1-C2-O2
28	1	801	LHG	O1-C1-C2-O2
28	1	802	LHG	O1-C1-C2-O2
28	a	801	LHG	O1-C1-C2-O2
28	3	801	LHG	O1-C1-C2-O2
28	4	801	LHG	O1-C1-C2-O2
28	4	802	LHG	O1-C1-C2-O2
28	6	801	LHG	O1-C1-C2-O2
28	7	802	LHG	O1-C1-C2-O2
28	2	802	LHG	O1-C1-C2-O2
28	9	801	LHG	O1-C1-C2-O2
31	2	804	LMT	C2-C1-O1'-C1'
35	7	805	SQD	C13-C14-C15-C16
42	8	809	OLA	C3-C4-C5-C6
47	6	806	SPH	C11-C12-C13-C14
24	6	603	CLA	C5-C6-C7-C8
24	A	1012	CLA	C4B-C3B-CAB-CBB
24	A	1109	CLA	C4B-C3B-CAB-CBB
24	A	1120	CLA	C4B-C3B-CAB-CBB
24	A	1139	CLA	C4B-C3B-CAB-CBB
24	B	1220	CLA	C4B-C3B-CAB-CBB
24	B	1230	CLA	C4B-C3B-CAB-CBB
24	B	1237	CLA	C4B-C3B-CAB-CBB
24	B	1238	CLA	C4B-C3B-CAB-CBB
24	K	1403	CLA	C4B-C3B-CAB-CBB
24	K	1404	CLA	C4B-C3B-CAB-CBB
24	H	1701	CLA	C4B-C3B-CAB-CBB
24	H	1702	CLA	C4B-C3B-CAB-CBB
24	L	1502	CLA	C4B-C3B-CAB-CBB
24	a	602	CLA	C4B-C3B-CAB-CBB
24	a	603	CLA	C4B-C3B-CAB-CBB
24	a	608	CLA	C4B-C3B-CAB-CBB
24	3	618	CLA	C4B-C3B-CAB-CBB
24	4	605	CLA	C4B-C3B-CAB-CBB
24	4	607	CLA	C4B-C3B-CAB-CBB
24	4	616	CLA	C4B-C3B-CAB-CBB
24	5	607	CLA	C4B-C3B-CAB-CBB
24	5	614	CLA	C4B-C3B-CAB-CBB
24	5	616	CLA	C4B-C3B-CAB-CBB
24	6	603	CLA	C4B-C3B-CAB-CBB
24	7	602	CLA	C4B-C3B-CAB-CBB
24	7	603	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	8	608	CLA	C4B-C3B-CAB-CBB
24	8	610	CLA	C4B-C3B-CAB-CBB
24	8	615	CLA	C4B-C3B-CAB-CBB
24	8	618	CLA	C4B-C3B-CAB-CBB
24	2	604	CLA	C4B-C3B-CAB-CBB
24	2	606	CLA	C4B-C3B-CAB-CBB
24	2	607	CLA	C4B-C3B-CAB-CBB
24	2	612	CLA	C4B-C3B-CAB-CBB
24	2	621	CLA	C4B-C3B-CAB-CBB
33	8	891	PTY	C30-C31-C32-C33
28	B	5002	LHG	C31-C32-C33-C34
28	6	801	LHG	C28-C29-C30-C31
28	8	801	LHG	C11-C12-C13-C14
24	A	1116	CLA	C11-C12-C13-C14
24	B	1021	CLA	C16-C17-C18-C19
24	B	1211	CLA	C6-C7-C8-C10
24	H	1703	CLA	C6-C7-C8-C9
24	1	612	CLA	C16-C17-C18-C19
24	1	612	CLA	C16-C17-C18-C20
24	a	604	CLA	C16-C17-C18-C20
24	3	604	CLA	C11-C12-C13-C14
24	6	601	CLA	C11-C12-C13-C14
24	8	620	CLA	C16-C17-C18-C19
24	9	612	CLA	C16-C17-C18-C19
24	9	612	CLA	C16-C17-C18-C20
24	7	617	CLA	O1D-CGD-O2D-CED
24	A	1114	CLA	C2A-CAA-CBA-CGA
24	A	1116	CLA	C2A-CAA-CBA-CGA
24	B	1023	CLA	C2A-CAA-CBA-CGA
24	B	1212	CLA	C2A-CAA-CBA-CGA
24	B	1225	CLA	C2A-CAA-CBA-CGA
24	K	1404	CLA	C2A-CAA-CBA-CGA
24	H	1702	CLA	C2A-CAA-CBA-CGA
24	4	604	CLA	C2A-CAA-CBA-CGA
24	4	610	CLA	C2A-CAA-CBA-CGA
24	5	616	CLA	C2A-CAA-CBA-CGA
24	6	604	CLA	C2A-CAA-CBA-CGA
28	9	802	LHG	C28-C29-C30-C31
24	A	1108	CLA	C10-C11-C12-C13
24	A	1127	CLA	C5-C6-C7-C8
24	A	1132	CLA	C13-C15-C16-C17
24	B	1209	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	B	1216	CLA	C10-C11-C12-C13
24	9	604	CLA	C10-C11-C12-C13
28	5	801	LHG	C13-C14-C15-C16
28	6	802	LHG	C25-C26-C27-C28
28	1	801	LHG	C23-C24-C25-C26
24	6	601	CLA	CBA-CGA-O2A-C1
28	2	801	LHG	C24-C23-O8-C6
28	A	5002	LHG	C10-C11-C12-C13
28	B	5001	LHG	C13-C14-C15-C16
28	B	5001	LHG	C33-C34-C35-C36
28	7	803	LHG	C9-C10-C11-C12
28	2	801	LHG	C11-C12-C13-C14
31	B	5006	LMT	C11-C10-C9-C8
51	8	806	P5S	C41-C42-C43-C44
24	a	605	CLA	O1A-CGA-O2A-C1
28	A	5002	LHG	O10-C23-O8-C6
28	2	802	LHG	O10-C23-O8-C6
24	A	1133	CLA	C3-C5-C6-C7
24	A	1101	CLA	C3A-C2A-CAA-CBA
24	A	1104	CLA	C3A-C2A-CAA-CBA
24	A	1109	CLA	C3A-C2A-CAA-CBA
24	A	1111	CLA	C3A-C2A-CAA-CBA
24	A	1121	CLA	C4-C3-C5-C6
24	A	1123	CLA	C3A-C2A-CAA-CBA
24	A	1131	CLA	C3A-C2A-CAA-CBA
24	B	1206	CLA	C3A-C2A-CAA-CBA
24	B	1207	CLA	C3A-C2A-CAA-CBA
24	B	1224	CLA	C3A-C2A-CAA-CBA
24	H	1701	CLA	C3A-C2A-CAA-CBA
24	1	602	CLA	C3A-C2A-CAA-CBA
24	1	605	CLA	C3A-C2A-CAA-CBA
24	a	602	CLA	C3A-C2A-CAA-CBA
24	4	610	CLA	C3A-C2A-CAA-CBA
24	7	602	CLA	C3A-C2A-CAA-CBA
24	9	603	CLA	C3A-C2A-CAA-CBA
41	1	613	CHL	C3A-C2A-CAA-CBA
41	6	619	CHL	C3A-C2A-CAA-CBA
28	7	801	LHG	C34-C35-C36-C37
28	7	802	LHG	C26-C27-C28-C29
31	1	804	LMT	C3-C4-C5-C6
28	6	801	LHG	C11-C10-C9-C8
24	A	1111	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
24	K	1402	CLA	C5-C6-C7-C8
24	4	610	CLA	C10-C11-C12-C13
24	5	601	CLA	C8-C10-C11-C12
24	8	618	CLA	C8-C10-C11-C12
28	4	802	LHG	C23-C24-C25-C26
24	B	1222	CLA	O1D-CGD-O2D-CED
24	8	609	CLA	O1D-CGD-O2D-CED
29	8	802	DGD	C9B-CAB-CBB-CCB
27	A	4002	BCR	C9-C10-C11-C12
27	A	4004	BCR	C13-C14-C15-C16
27	B	4005	BCR	C13-C14-C15-C16
27	L	4001	BCR	C13-C14-C15-C16
27	L	4003	BCR	C19-C20-C21-C22
27	7	503	BCR	C9-C10-C11-C12
40	3	501	LUT	C29-C30-C31-C32
40	3	502	LUT	C29-C30-C31-C32
40	6	502	LUT	C29-C30-C31-C32
24	A	1107	CLA	C6-C7-C8-C9
24	B	1211	CLA	C6-C7-C8-C9
24	H	1703	CLA	C6-C7-C8-C10
24	4	607	CLA	C6-C7-C8-C9
24	7	603	CLA	C16-C17-C18-C19
24	8	618	CLA	C11-C12-C13-C14
24	9	605	CLA	C11-C12-C13-C14
25	A	2001	PQN	C26-C27-C28-C29
31	A	5008	LMT	C3'-C4'-O1B-C1B
24	L	1502	CLA	O1A-CGA-O2A-C1
24	B	1021	CLA	C5-C6-C7-C8
28	B	5002	LHG	C33-C34-C35-C36
23	A	1011	CL0	CBA-CGA-O2A-C1
24	B	1221	CLA	CBA-CGA-O2A-C1
28	F	5001	LHG	C28-C29-C30-C31
28	F	5002	LHG	C9-C10-C11-C12
28	4	801	LHG	C31-C32-C33-C34
28	4	802	LHG	C13-C14-C15-C16
28	2	801	LHG	C10-C11-C12-C13
28	2	802	LHG	C9-C10-C11-C12
33	B	5005	PTY	C21-C22-C23-C24
33	9	803	PTY	C38-C39-C40-C41
24	H	1701	CLA	C3-C5-C6-C7
24	5	607	CLA	C3-C5-C6-C7
28	6	802	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
28	7	803	LHG	C7-C8-C9-C10
28	8	801	LHG	C7-C8-C9-C10
24	A	1126	CLA	C8-C10-C11-C12
24	A	1133	CLA	C13-C15-C16-C17
24	a	605	CLA	C15-C16-C17-C18
24	3	601	CLA	O1D-CGD-O2D-CED
28	A	5003	LHG	C11-C10-C9-C8
28	F	5001	LHG	C9-C10-C11-C12
28	F	5001	LHG	C16-C17-C18-C19
28	7	801	LHG	C31-C32-C33-C34
28	2	802	LHG	C11-C10-C9-C8
32	6	803	PCW	C12-C13-C14-C15
24	A	1013	CLA	O1A-CGA-O2A-C1
24	A	1113	CLA	O1A-CGA-O2A-C1
24	A	1127	CLA	O1A-CGA-O2A-C1
24	B	1210	CLA	O1A-CGA-O2A-C1
28	B	5002	LHG	C26-C27-C28-C29
28	4	801	LHG	C34-C35-C36-C37
24	A	1117	CLA	O1D-CGD-O2D-CED
28	6	802	LHG	C11-C12-C13-C14
30	A	5007	3PH	C34-C35-C36-C37
24	A	1113	CLA	O1D-CGD-O2D-CED
31	1	804	LMT	C7-C8-C9-C10
47	6	806	SPH	C10-C11-C12-C13
50	7	807	4RF	C24-C25-C26-C27
24	A	1109	CLA	C16-C17-C18-C19
24	4	615	CLA	C11-C12-C13-C14
28	3	801	LHG	C7-C8-C9-C10
33	8	891	PTY	C8-C11-C12-C13
24	a	601	CLA	O1A-CGA-O2A-C1
24	A	1104	CLA	C2B-C3B-CAB-CBB
24	A	1120	CLA	C2B-C3B-CAB-CBB
24	A	1122	CLA	C2B-C3B-CAB-CBB
24	A	1139	CLA	C2B-C3B-CAB-CBB
24	G	1602	CLA	C2B-C3B-CAB-CBB
24	K	1402	CLA	C2B-C3B-CAB-CBB
24	K	1404	CLA	C2B-C3B-CAB-CBB
24	H	1703	CLA	C2B-C3B-CAB-CBB
24	a	601	CLA	C2B-C3B-CAB-CBB
24	a	603	CLA	C2B-C3B-CAB-CBB
24	a	608	CLA	C2B-C3B-CAB-CBB
24	3	618	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	4	605	CLA	C2B-C3B-CAB-CBB
24	4	617	CLA	C2B-C3B-CAB-CBB
24	5	607	CLA	C2B-C3B-CAB-CBB
24	5	614	CLA	C2B-C3B-CAB-CBB
24	5	616	CLA	C2B-C3B-CAB-CBB
24	5	617	CLA	C2B-C3B-CAB-CBB
24	6	603	CLA	C2B-C3B-CAB-CBB
24	6	618	CLA	C2B-C3B-CAB-CBB
24	7	602	CLA	C2B-C3B-CAB-CBB
24	7	603	CLA	C2B-C3B-CAB-CBB
24	8	608	CLA	C2B-C3B-CAB-CBB
24	8	615	CLA	C2B-C3B-CAB-CBB
24	8	618	CLA	C2B-C3B-CAB-CBB
24	2	607	CLA	C2B-C3B-CAB-CBB
24	2	612	CLA	C2B-C3B-CAB-CBB
24	2	621	CLA	C2B-C3B-CAB-CBB
27	A	4004	BCR	C1-C6-C7-C8
27	A	4004	BCR	C5-C6-C7-C8
27	A	4005	BCR	C1-C6-C7-C8
27	B	4002	BCR	C1-C6-C7-C8
27	B	4004	BCR	C23-C24-C25-C26
27	B	4004	BCR	C23-C24-C25-C30
27	F	4001	BCR	C23-C24-C25-C26
27	F	4001	BCR	C23-C24-C25-C30
27	I	4001	BCR	C1-C6-C7-C8
27	I	4001	BCR	C5-C6-C7-C8
27	H	4001	BCR	C1-C6-C7-C8
27	H	4001	BCR	C5-C6-C7-C8
27	L	4001	BCR	C1-C6-C7-C8
27	L	4001	BCR	C5-C6-C7-C8
27	L	4001	BCR	C23-C24-C25-C30
27	L	4002	BCR	C1-C6-C7-C8
27	L	4002	BCR	C5-C6-C7-C8
27	L	4003	BCR	C1-C6-C7-C8
27	L	4003	BCR	C5-C6-C7-C8
27	4	503	BCR	C23-C24-C25-C26
27	4	503	BCR	C23-C24-C25-C30
27	5	503	BCR	C1-C6-C7-C8
27	5	504	BCR	C23-C24-C25-C26
27	5	504	BCR	C23-C24-C25-C30
27	6	503	BCR	C1-C6-C7-C8
27	6	503	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
27	6	504	BCR	C23-C24-C25-C26
27	6	504	BCR	C23-C24-C25-C30
27	7	503	BCR	C1-C6-C7-C8
27	7	503	BCR	C5-C6-C7-C8
37	J	4002	RRX	C5-C6-C7-C8
39	M	4001	ECH	C23-C24-C25-C26
40	1	501	LUT	C1-C6-C7-C8
40	1	501	LUT	C5-C6-C7-C8
40	a	501	LUT	C1-C6-C7-C8
28	B	5001	LHG	C30-C31-C32-C33
28	6	801	LHG	C33-C34-C35-C36
24	B	1222	CLA	C8-C10-C11-C12
24	1	604	CLA	C8-C10-C11-C12
28	A	5002	LHG	C13-C14-C15-C16
28	A	5003	LHG	C11-C12-C13-C14
28	A	5003	LHG	C16-C17-C18-C19
33	9	803	PTY	C17-C18-C19-C20
24	A	1113	CLA	C2A-CAA-CBA-CGA
24	B	1214	CLA	C2A-CAA-CBA-CGA
24	K	1404	CLA	C3-C5-C6-C7
24	4	601	CLA	C2A-CAA-CBA-CGA
24	9	604	CLA	C2A-CAA-CBA-CGA
28	2	801	LHG	C23-C24-C25-C26
24	B	1215	CLA	C8-C10-C11-C12
24	8	603	CLA	C15-C16-C17-C18
24	A	1134	CLA	O1A-CGA-O2A-C1
24	B	1221	CLA	O1A-CGA-O2A-C1
24	8	602	CLA	O1A-CGA-O2A-C1
24	2	621	CLA	O1A-CGA-O2A-C1
24	9	603	CLA	O1A-CGA-O2A-C1
28	7	803	LHG	C11-C12-C13-C14
28	1	801	LHG	O9-C7-O7-C5
28	5	801	LHG	O9-C7-O7-C5
24	B	1208	CLA	C4-C3-C5-C6
24	B	1213	CLA	C4-C3-C5-C6
24	a	605	CLA	C4-C3-C5-C6
24	7	610	CLA	C4-C3-C5-C6
28	3	801	LHG	C13-C14-C15-C16
27	A	4004	BCR	C10-C11-C12-C13
27	B	4003	BCR	C10-C11-C12-C13
27	5	504	BCR	C10-C11-C12-C13
48	7	502	XAT	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	1	605	CLA	C5-C6-C7-C8
24	A	1121	CLA	C2-C3-C5-C6
24	7	610	CLA	C2-C3-C5-C6
24	2	604	CLA	C2-C3-C5-C6
41	6	610	CHL	C2-C3-C5-C6
24	1	605	CLA	C16-C17-C18-C19
28	B	5002	LHG	C13-C14-C15-C16
28	7	801	LHG	C33-C34-C35-C36
50	8	807	4RF	C10-C11-C12-C13
28	B	5002	LHG	C7-C8-C9-C10
33	5	802	PTY	C8-C11-C12-C13
24	5	602	CLA	CBA-CGA-O2A-C1
28	3	801	LHG	C24-C23-O8-C6
38	J	5001	LPX	C7-C6-O6-C5
46	8	803	DGA	CA2-CA1-OG1-CG1
24	6	601	CLA	O1A-CGA-O2A-C1
41	4	618	CHL	C3-C5-C6-C7
24	a	612	CLA	C6-C7-C8-C9
24	6	609	CLA	C6-C7-C8-C9
28	B	5002	LHG	C34-C35-C36-C37
28	a	801	LHG	C28-C29-C30-C31
31	B	5006	LMT	C2-C3-C4-C5
46	8	803	DGA	CAB-CBB-CCB-CDB
24	B	1220	CLA	C8-C10-C11-C12
24	B	1229	CLA	C8-C10-C11-C12
28	F	5002	LHG	C11-C10-C9-C8
28	6	802	LHG	C28-C29-C30-C31
28	7	801	LHG	C25-C26-C27-C28
28	7	802	LHG	C28-C29-C30-C31
29	B	5003	DGD	CAA-CBA-CCA-CDA
28	2	801	LHG	C11-C10-C9-C8
28	2	802	LHG	C11-C12-C13-C14
50	8	807	4RF	C27-C28-C29-C30
24	B	1239	CLA	C10-C11-C12-C13
24	a	603	CLA	C5-C6-C7-C8
24	7	612	CLA	C10-C11-C12-C13
23	A	1011	CL0	O1A-CGA-O2A-C1
28	1	802	LHG	C13-C14-C15-C16
28	7	801	LHG	C28-C29-C30-C31
28	2	802	LHG	C25-C26-C27-C28
28	9	802	LHG	C13-C14-C15-C16
28	B	5002	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
28	1	801	LHG	C28-C29-C30-C31
28	2	802	LHG	C13-C14-C15-C16
34	F	5003	LAP	C2-C3-C4-C5
30	A	5007	3PH	C32-C33-C34-C35
27	I	4001	BCR	C19-C20-C21-C22
23	A	1011	CL0	C16-C17-C18-C20
24	A	1136	CLA	C16-C17-C18-C19
24	A	1140	CLA	C6-C7-C8-C10
24	B	1223	CLA	C16-C17-C18-C20
24	6	603	CLA	C16-C17-C18-C20
24	8	603	CLA	C16-C17-C18-C19
36	G	5002	ERG	C17-C20-C22-C23
28	2	802	LHG	C8-C7-O7-C5
29	A	5005	DGD	C2B-C1B-O2G-C2G
51	8	806	P5S	C39-C38-O37-C2
28	F	5002	LHG	C23-C24-C25-C26
32	B	5004	PCW	C31-C32-C33-C34
28	A	5003	LHG	C18-C19-C20-C21
28	6	802	LHG	C29-C30-C31-C32
24	A	1130	CLA	C5-C6-C7-C8
24	a	601	CLA	C5-C6-C7-C8
28	1	802	LHG	C15-C16-C17-C18
29	B	5003	DGD	C9A-CAA-CBA-CCA
33	B	5005	PTY	C23-C24-C25-C26
28	2	802	LHG	C35-C36-C37-C38
24	A	1102	CLA	C5-C6-C7-C8
24	1	606	CLA	C5-C6-C7-C8
27	A	4001	BCR	C11-C12-C13-C35
27	F	4001	BCR	C36-C18-C19-C20
27	L	4002	BCR	C37-C22-C23-C24
27	L	4003	BCR	C11-C12-C13-C35
28	3	801	LHG	C31-C32-C33-C34
28	7	801	LHG	C30-C31-C32-C33
28	a	801	LHG	C7-C8-C9-C10
28	1	801	LHG	C30-C31-C32-C33
33	B	5005	PTY	C32-C33-C34-C35
33	5	802	PTY	C34-C35-C36-C37
27	A	4004	BCR	C17-C18-C19-C20
27	L	4002	BCR	C21-C22-C23-C24
24	B	1224	CLA	CBA-CGA-O2A-C1
24	9	602	CLA	O1A-CGA-O2A-C1
28	B	5001	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
24	A	1127	CLA	C2A-CAA-CBA-CGA
24	B	1220	CLA	C2A-CAA-CBA-CGA
24	B	1224	CLA	C2A-CAA-CBA-CGA
24	B	1227	CLA	C2A-CAA-CBA-CGA
24	7	609	CLA	C2A-CAA-CBA-CGA
24	8	609	CLA	C2A-CAA-CBA-CGA
41	8	604	CHL	C2A-CAA-CBA-CGA
24	B	1216	CLA	C14-C13-C15-C16
24	A	1109	CLA	C16-C17-C18-C20
24	A	1125	CLA	C16-C17-C18-C19
24	a	604	CLA	C16-C17-C18-C19
24	6	615	CLA	C16-C17-C18-C20
24	7	603	CLA	C16-C17-C18-C20
24	8	618	CLA	C11-C12-C13-C15
24	9	604	CLA	C11-C12-C13-C14
24	9	604	CLA	C11-C12-C13-C15
28	3	801	LHG	C11-C12-C13-C14
29	A	5005	DGD	C4B-C5B-C6B-C7B
28	2	801	LHG	O10-C23-O8-C6
24	a	605	CLA	C2-C3-C5-C6
28	4	801	LHG	C18-C19-C20-C21
28	2	801	LHG	C13-C14-C15-C16
28	9	802	LHG	C31-C32-C33-C34
25	A	2001	PQN	C25-C26-C27-C28
28	F	5002	LHG	C11-C12-C13-C14
29	B	5003	DGD	C4B-C5B-C6B-C7B
24	B	1202	CLA	C3-C5-C6-C7
24	9	605	CLA	C3-C5-C6-C7
24	B	1204	CLA	C13-C15-C16-C17
24	5	604	CLA	C10-C11-C12-C13
29	B	5003	DGD	CCA-CDA-CEA-CFA
24	B	1214	CLA	CBA-CGA-O2A-C1
28	a	801	LHG	O6-C4-C5-O7
24	2	615	CLA	O1D-CGD-O2D-CED
28	B	5001	LHG	C29-C30-C31-C32
29	B	5003	DGD	C2G-C1G-O1G-C1A
24	A	1012	CLA	C8-C10-C11-C12
24	A	1135	CLA	C16-C17-C18-C19
28	B	5001	LHG	C11-C12-C13-C14
28	7	803	LHG	C13-C14-C15-C16
28	2	801	LHG	C34-C35-C36-C37
31	A	5008	LMT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
28	9	801	LHG	C7-C8-C9-C10
24	1	605	CLA	C13-C15-C16-C17
28	9	802	LHG	C33-C34-C35-C36
33	5	802	PTY	C15-C16-C17-C18
28	7	802	LHG	O7-C5-C6-O8
28	4	801	LHG	C28-C29-C30-C31
28	9	802	LHG	C29-C30-C31-C32
28	8	801	LHG	C24-C25-C26-C27
34	B	5007	LAP	C4-C5-C6-C7
34	K	5001	LAP	C2-C3-C4-C5
24	1	612	CLA	C8-C10-C11-C12
28	3	801	LHG	C29-C30-C31-C32
33	8	891	PTY	C13-C14-C15-C16
24	A	1109	CLA	C2-C1-O2A-CGA
24	A	1132	CLA	C2-C1-O2A-CGA
24	B	1212	CLA	C2-C1-O2A-CGA
24	4	610	CLA	C2-C1-O2A-CGA
24	4	615	CLA	C2-C1-O2A-CGA
41	3	608	CHL	C3A-C2A-CAA-CBA
28	4	801	LHG	C2-C3-O3-P
33	5	802	PTY	C33-C34-C35-C36
33	9	803	PTY	C22-C23-C24-C25
29	B	5003	DGD	C3A-C4A-C5A-C6A
24	A	1111	CLA	C4-C3-C5-C6
24	1	608	CLA	C4-C3-C5-C6
24	B	1209	CLA	C3-C5-C6-C7
24	B	1240	CLA	C3-C5-C6-C7
29	A	5005	DGD	O1B-C1B-O2G-C2G
51	8	806	P5S	O47-C38-O37-C2
31	B	5006	LMT	C5'-C4'-O1B-C1B
28	2	802	LHG	C1-C2-C3-O3
34	B	5007	LAP	C13-C14-C15-O4
24	A	1126	CLA	C10-C11-C12-C13
31	2	804	LMT	C5-C6-C7-C8
33	8	891	PTY	C31-C32-C33-C34
34	F	5003	LAP	C7-C8-C9-C10
24	A	1135	CLA	C2A-CAA-CBA-CGA
24	B	1206	CLA	C2A-CAA-CBA-CGA
24	B	1213	CLA	C2A-CAA-CBA-CGA
24	3	606	CLA	C2A-CAA-CBA-CGA
24	6	601	CLA	C2A-CAA-CBA-CGA
24	7	603	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
24	2	604	CLA	C2A-CAA-CBA-CGA
29	8	802	DGD	C2A-C1A-O1G-C1G
28	A	5003	LHG	C17-C18-C19-C20
28	F	5001	LHG	C11-C10-C9-C8
24	B	1209	CLA	O1D-CGD-O2D-CED
24	A	1128	CLA	C15-C16-C17-C18
24	3	604	CLA	C10-C11-C12-C13
24	2	601	CLA	C8-C10-C11-C12
29	8	802	DGD	C1A-C2A-C3A-C4A
46	8	803	DGA	CA4-CA5-CA6-CA7
24	B	1204	CLA	C16-C17-C18-C20
28	7	801	LHG	O1-C1-C2-O2
28	9	802	LHG	O1-C1-C2-O2
46	8	803	DGA	OA1-CA1-OG1-CG1
24	A	1131	CLA	C3-C5-C6-C7
24	1	608	CLA	C3-C5-C6-C7
31	2	804	LMT	C1-C2-C3-C4
28	4	801	LHG	C16-C17-C18-C19
28	6	801	LHG	C13-C14-C15-C16
28	2	802	LHG	C34-C35-C36-C37
24	A	1101	CLA	C1A-C2A-CAA-CBA
24	A	1103	CLA	C1A-C2A-CAA-CBA
24	A	1104	CLA	C1A-C2A-CAA-CBA
24	A	1106	CLA	C1A-C2A-CAA-CBA
24	A	1107	CLA	C1A-C2A-CAA-CBA
24	A	1108	CLA	C1A-C2A-CAA-CBA
24	A	1116	CLA	C1A-C2A-CAA-CBA
24	A	1118	CLA	C1A-C2A-CAA-CBA
24	A	1121	CLA	C1A-C2A-CAA-CBA
24	A	1129	CLA	C1A-C2A-CAA-CBA
24	A	1131	CLA	C1A-C2A-CAA-CBA
24	A	1132	CLA	C1A-C2A-CAA-CBA
24	A	1141	CLA	C1A-C2A-CAA-CBA
24	B	1206	CLA	C1A-C2A-CAA-CBA
24	B	1207	CLA	C1A-C2A-CAA-CBA
24	B	1211	CLA	C1A-C2A-CAA-CBA
24	B	1212	CLA	C1A-C2A-CAA-CBA
24	B	1214	CLA	C1A-C2A-CAA-CBA
24	B	1216	CLA	C1A-C2A-CAA-CBA
24	B	1217	CLA	C1A-C2A-CAA-CBA
24	B	1219	CLA	C1A-C2A-CAA-CBA
24	B	1220	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	B	1229	CLA	C1A-C2A-CAA-CBA
24	B	1239	CLA	C1A-C2A-CAA-CBA
24	K	1402	CLA	C1A-C2A-CAA-CBA
24	H	1701	CLA	C1A-C2A-CAA-CBA
24	1	601	CLA	C1A-C2A-CAA-CBA
24	1	602	CLA	C1A-C2A-CAA-CBA
24	1	604	CLA	C1A-C2A-CAA-CBA
24	1	607	CLA	C1A-C2A-CAA-CBA
24	1	608	CLA	C1A-C2A-CAA-CBA
24	1	611	CLA	C1A-C2A-CAA-CBA
24	a	601	CLA	C1A-C2A-CAA-CBA
24	a	602	CLA	C1A-C2A-CAA-CBA
24	a	607	CLA	C1A-C2A-CAA-CBA
24	a	611	CLA	C1A-C2A-CAA-CBA
24	3	601	CLA	C1A-C2A-CAA-CBA
24	3	610	CLA	C1A-C2A-CAA-CBA
24	3	618	CLA	C1A-C2A-CAA-CBA
24	4	606	CLA	C1A-C2A-CAA-CBA
24	4	607	CLA	C1A-C2A-CAA-CBA
24	4	610	CLA	C1A-C2A-CAA-CBA
24	4	616	CLA	C1A-C2A-CAA-CBA
24	4	617	CLA	C1A-C2A-CAA-CBA
24	5	601	CLA	C1A-C2A-CAA-CBA
24	5	608	CLA	C1A-C2A-CAA-CBA
24	6	601	CLA	C1A-C2A-CAA-CBA
24	6	606	CLA	C1A-C2A-CAA-CBA
24	6	607	CLA	C1A-C2A-CAA-CBA
24	7	602	CLA	C1A-C2A-CAA-CBA
24	7	610	CLA	C1A-C2A-CAA-CBA
24	8	610	CLA	C1A-C2A-CAA-CBA
24	8	612	CLA	C1A-C2A-CAA-CBA
24	2	603	CLA	C1A-C2A-CAA-CBA
24	2	606	CLA	C1A-C2A-CAA-CBA
24	2	610	CLA	C1A-C2A-CAA-CBA
24	2	621	CLA	C1A-C2A-CAA-CBA
24	9	603	CLA	C1A-C2A-CAA-CBA
24	9	606	CLA	C1A-C2A-CAA-CBA
24	a	601	CLA	C8-C10-C11-C12
28	3	801	LHG	C35-C36-C37-C38
50	8	808	4RF	C02-C03-C04-C05
38	J	5001	LPX	O7-C6-O6-C5
28	A	5001	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
28	B	5002	LHG	O6-C4-C5-C6
28	1	802	LHG	O6-C4-C5-C6
28	3	801	LHG	O6-C4-C5-C6
28	7	802	LHG	O6-C4-C5-C6
28	2	801	LHG	O6-C4-C5-C6
33	B	5005	PTY	O14-C5-C6-C1
28	2	802	LHG	O9-C7-O7-C5
28	4	801	LHG	C11-C12-C13-C14
24	A	1012	CLA	C11-C10-C8-C7
24	A	1101	CLA	C11-C12-C13-C15
24	A	1103	CLA	C6-C7-C8-C10
24	A	1117	CLA	C6-C7-C8-C10
24	A	1122	CLA	C12-C13-C15-C16
24	A	1126	CLA	C11-C12-C13-C15
24	A	1127	CLA	C12-C13-C15-C16
24	A	1135	CLA	C11-C10-C8-C7
24	A	1136	CLA	C6-C7-C8-C10
24	A	1138	CLA	C11-C10-C8-C7
24	B	1203	CLA	C11-C12-C13-C15
24	B	1204	CLA	C6-C7-C8-C10
24	B	1215	CLA	C11-C10-C8-C7
24	B	1221	CLA	C11-C10-C8-C7
24	B	1223	CLA	C11-C12-C13-C15
24	B	1224	CLA	C6-C7-C8-C10
24	B	1229	CLA	C6-C7-C8-C10
24	B	1229	CLA	C11-C10-C8-C7
24	1	604	CLA	C12-C13-C15-C16
24	1	605	CLA	C6-C7-C8-C10
24	1	606	CLA	C6-C7-C8-C10
24	a	605	CLA	C12-C13-C15-C16
24	a	607	CLA	C11-C10-C8-C7
24	3	613	CLA	C11-C12-C13-C15
24	4	610	CLA	C6-C7-C8-C10
24	5	601	CLA	C11-C10-C8-C7
24	6	604	CLA	C11-C10-C8-C7
24	7	609	CLA	C11-C10-C8-C7
24	7	611	CLA	C6-C7-C8-C10
24	7	611	CLA	C11-C10-C8-C7
24	8	609	CLA	C11-C10-C8-C7
41	1	609	CHL	C12-C13-C15-C16
41	6	619	CHL	C11-C12-C13-C15
41	8	604	CHL	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
24	A	1125	CLA	C16-C17-C18-C20
24	A	1123	CLA	C15-C16-C17-C18
31	1	804	LMT	C4B-C5B-C6B-O6B
24	B	1224	CLA	C15-C16-C17-C18
28	2	801	LHG	C7-C8-C9-C10
45	6	804	PLM	C1-C2-C3-C4
34	K	5001	LAP	C6-C7-C8-C9
24	A	1123	CLA	C4-C3-C5-C6
24	A	1103	CLA	C2-C3-C5-C6
24	A	1123	CLA	C2-C3-C5-C6
24	A	1125	CLA	C2-C3-C5-C6
24	5	602	CLA	O1A-CGA-O2A-C1
24	A	1117	CLA	C13-C15-C16-C17
24	K	1402	CLA	C10-C11-C12-C13
24	1	604	CLA	C10-C11-C12-C13
24	4	604	CLA	C8-C10-C11-C12
28	A	5001	LHG	C8-C7-O7-C5
24	A	1012	CLA	C2A-CAA-CBA-CGA
24	A	1013	CLA	C2A-CAA-CBA-CGA
24	B	1217	CLA	C2A-CAA-CBA-CGA
24	8	612	CLA	C2A-CAA-CBA-CGA
24	A	1012	CLA	C11-C10-C8-C9
24	A	1102	CLA	C14-C13-C15-C16
24	A	1109	CLA	C11-C12-C13-C14
24	A	1114	CLA	C11-C10-C8-C9
24	A	1117	CLA	C6-C7-C8-C9
24	A	1127	CLA	C14-C13-C15-C16
24	A	1135	CLA	C6-C7-C8-C9
24	A	1135	CLA	C11-C10-C8-C9
24	B	1202	CLA	C11-C12-C13-C14
24	B	1204	CLA	C6-C7-C8-C9
24	B	1207	CLA	C6-C7-C8-C9
24	B	1213	CLA	C11-C10-C8-C9
24	B	1214	CLA	C14-C13-C15-C16
24	B	1223	CLA	C11-C12-C13-C14
24	B	1229	CLA	C6-C7-C8-C9
24	B	1229	CLA	C11-C10-C8-C9
24	B	1230	CLA	C6-C7-C8-C9
24	B	1237	CLA	C6-C7-C8-C9
24	1	605	CLA	C14-C13-C15-C16
24	a	605	CLA	C14-C13-C15-C16
24	3	606	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
24	3	613	CLA	C11-C12-C13-C14
24	4	610	CLA	C14-C13-C15-C16
24	4	611	CLA	C6-C7-C8-C9
24	7	603	CLA	C11-C10-C8-C9
24	7	604	CLA	C11-C10-C8-C9
24	7	611	CLA	C11-C10-C8-C9
24	2	605	CLA	C11-C10-C8-C9
24	9	601	CLA	C6-C7-C8-C9
28	7	801	LHG	C13-C14-C15-C16
31	2	804	LMT	O5B-C5B-C6B-O6B
40	5	501	LUT	C29-C30-C31-C32
28	F	5002	LHG	C28-C29-C30-C31
46	8	803	DGA	CB5-CB6-CB7-CB8
29	B	5003	DGD	C2A-C1A-O1G-C1G
24	5	605	CLA	O1A-CGA-O2A-C1
33	B	5005	PTY	C22-C23-C24-C25
28	A	5003	LHG	C4-C5-C6-O8
28	a	801	LHG	C4-C5-C6-O8
28	4	802	LHG	C4-C5-C6-O8
28	6	801	LHG	C4-C5-C6-O8
28	8	801	LHG	C4-C5-C6-O8
28	2	801	LHG	C4-C5-C6-O8
28	9	802	LHG	C4-C5-C6-O8
30	A	5007	3PH	C1-C2-C3-O31
33	5	802	PTY	O4-C1-C6-C5
33	9	803	PTY	O4-C1-C6-C5
35	G	5001	SQD	C44-C45-C46-O48
35	H	5001	SQD	O6-C44-C45-C46
50	8	808	4RF	O18-C19-C20-C39
28	7	802	LHG	C11-C10-C9-C8
24	A	1118	CLA	C3-C5-C6-C7
31	A	5008	LMT	O5'-C5'-C6'-O6'
28	1	802	LHG	C14-C15-C16-C17
24	A	1135	CLA	C13-C15-C16-C17
24	B	1201	CLA	C15-C16-C17-C18
31	B	5006	LMT	C4B-C5B-C6B-O6B
28	A	5002	LHG	C27-C28-C29-C30
28	F	5001	LHG	C25-C26-C27-C28
28	2	802	LHG	C26-C27-C28-C29
24	A	1129	CLA	CBA-CGA-O2A-C1
24	B	1209	CLA	C16-C17-C18-C20
24	6	607	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
33	5	802	PTY	C11-C12-C13-C14
24	A	1138	CLA	C8-C10-C11-C12
24	3	605	CLA	C8-C10-C11-C12
24	B	1214	CLA	O1A-CGA-O2A-C1
28	A	5002	LHG	C30-C31-C32-C33
28	5	801	LHG	C10-C11-C12-C13
28	2	802	LHG	C29-C30-C31-C32
41	a	610	CHL	CHA-CBD-CGD-O1D
41	a	610	CHL	CHA-CBD-CGD-O2D
41	3	611	CHL	CHA-CBD-CGD-O2D
41	5	610	CHL	CHA-CBD-CGD-O2D
41	9	610	CHL	CHA-CBD-CGD-O2D
24	B	1231	CLA	C13-C15-C16-C17
33	B	5005	PTY	C8-C11-C12-C13
33	5	802	PTY	C30-C31-C32-C33
28	3	801	LHG	O10-C23-O8-C6
28	9	801	LHG	C26-C27-C28-C29
33	B	5005	PTY	C24-C25-C26-C27
24	A	1103	CLA	C4-C3-C5-C6
24	2	601	CLA	C4-C3-C5-C6
24	B	1204	CLA	C2-C3-C5-C6
24	B	1213	CLA	C2-C3-C5-C6
24	1	608	CLA	C2-C3-C5-C6
31	B	5006	LMT	C6-C7-C8-C9
24	B	1221	CLA	C15-C16-C17-C18
27	A	4003	BCR	C7-C8-C9-C34
27	L	4001	BCR	C37-C22-C23-C24
27	3	503	BCR	C37-C22-C23-C24
39	M	4001	ECH	C37-C22-C23-C24
28	B	5002	LHG	C28-C29-C30-C31
27	3	503	BCR	C21-C22-C23-C24
40	a	501	LUT	C27-C28-C29-C30
40	5	505	LUT	C31-C32-C33-C34
24	B	1224	CLA	O1A-CGA-O2A-C1
29	8	802	DGD	O1A-C1A-O1G-C1G
24	A	1136	CLA	C15-C16-C17-C18
24	3	606	CLA	C13-C15-C16-C17
28	2	802	LHG	C24-C25-C26-C27
24	G	1603	CLA	C2A-CAA-CBA-CGA
24	a	608	CLA	C2A-CAA-CBA-CGA
28	9	802	LHG	C25-C26-C27-C28
24	B	1237	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	B	1238	CLA	C5-C6-C7-C8
28	9	802	LHG	C7-C8-C9-C10
29	B	5003	DGD	O1A-C1A-O1G-C1G
24	A	1115	CLA	CBA-CGA-O2A-C1
24	B	1203	CLA	CBA-CGA-O2A-C1
28	2	801	LHG	C6-C5-O7-C7
33	5	802	PTY	C1-C6-O7-C8
33	7	804	PTY	C1-C6-O7-C8
50	8	807	4RF	C39-C20-O21-C22
50	8	808	4RF	C39-C20-O21-C22
28	7	803	LHG	C28-C29-C30-C31
29	B	5003	DGD	C2B-C3B-C4B-C5B
24	A	1125	CLA	C13-C15-C16-C17
24	2	605	CLA	C8-C10-C11-C12
28	F	5001	LHG	C26-C27-C28-C29
33	3	802	PTY	C12-C13-C14-C15
33	5	802	PTY	C36-C37-C38-C39
27	L	4001	BCR	C9-C10-C11-C12
40	1	501	LUT	C29-C30-C31-C32
40	8	502	LUT	C29-C30-C31-C32
40	9	501	LUT	C29-C30-C31-C32
24	A	1135	CLA	C16-C17-C18-C20
28	6	802	LHG	C11-C10-C9-C8
28	6	801	LHG	C35-C36-C37-C38
28	7	803	LHG	O6-C4-C5-O7
28	2	801	LHG	C25-C26-C27-C28
24	B	1021	CLA	CBA-CGA-O2A-C1
24	B	1235	CLA	CBA-CGA-O2A-C1
24	B	1238	CLA	CBA-CGA-O2A-C1
24	1	608	CLA	CBA-CGA-O2A-C1
24	3	606	CLA	CBA-CGA-O2A-C1
24	9	601	CLA	CBA-CGA-O2A-C1
28	8	801	LHG	C30-C31-C32-C33
47	6	806	SPH	C6-C7-C8-C9
24	B	1240	CLA	C4-C3-C5-C6
24	B	1208	CLA	C2-C3-C5-C6
24	9	612	CLA	C2-C3-C5-C6
28	A	5002	LHG	C16-C17-C18-C19
28	B	5001	LHG	C31-C32-C33-C34
32	B	5004	PCW	C12-C13-C14-C15
24	1	604	CLA	C16-C17-C18-C20
28	9	802	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
50	8	807	4RF	C32-C33-C34-C35
28	A	5001	LHG	O7-C5-C6-O8
28	A	5002	LHG	O7-C5-C6-O8
28	8	801	LHG	O7-C5-C6-O8
28	9	801	LHG	C11-C12-C13-C14
28	6	801	LHG	C12-C13-C14-C15
28	9	801	LHG	C11-C10-C9-C8
33	3	802	PTY	C33-C34-C35-C36
51	8	806	P5S	C42-C43-C44-C45
24	7	601	CLA	C2A-CAA-CBA-CGA
24	A	1114	CLA	C13-C15-C16-C17
28	4	802	LHG	C11-C10-C9-C8
42	1	803	OLA	C10-C11-C12-C13
42	8	809	OLA	C10-C11-C12-C13
28	1	802	LHG	C28-C29-C30-C31
24	4	615	CLA	C5-C6-C7-C8
24	A	1136	CLA	CBA-CGA-O2A-C1
50	8	808	4RF	C31-C32-C33-C34
28	9	802	LHG	C10-C11-C12-C13
45	4	803	PLM	C4-C5-C6-C7
24	3	607	CLA	C13-C15-C16-C17
24	3	607	CLA	C15-C16-C17-C18
24	A	1129	CLA	O1A-CGA-O2A-C1
24	B	1208	CLA	O1D-CGD-O2D-CED
24	7	609	CLA	O1D-CGD-O2D-CED
28	3	801	LHG	C23-C24-C25-C26
35	7	805	SQD	C7-C8-C9-C10
28	A	5002	LHG	C11-C12-C13-C14
24	B	1226	CLA	C5-C6-C7-C8
24	5	603	CLA	C11-C10-C8-C9
24	A	1137	CLA	C11-C12-C13-C14
24	B	1204	CLA	C16-C17-C18-C19
24	B	1212	CLA	C16-C17-C18-C20
41	8	601	CHL	C11-C12-C13-C15
24	A	1126	CLA	C4-C3-C5-C6
24	B	1204	CLA	C4-C3-C5-C6
24	B	1205	CLA	C4-C3-C5-C6
24	B	1220	CLA	C4-C3-C5-C6
24	8	603	CLA	C4-C3-C5-C6
24	4	610	CLA	C2-C3-C5-C6
24	7	603	CLA	C8-C10-C11-C12
28	4	801	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
28	6	802	LHG	O1-C1-C2-O2
24	A	1101	CLA	C11-C12-C13-C14
24	A	1103	CLA	C6-C7-C8-C9
24	A	1117	CLA	C11-C10-C8-C9
24	A	1119	CLA	C11-C12-C13-C14
24	A	1122	CLA	C14-C13-C15-C16
24	A	1126	CLA	C11-C10-C8-C9
24	A	1126	CLA	C11-C12-C13-C14
24	A	1138	CLA	C11-C10-C8-C9
24	B	1215	CLA	C11-C10-C8-C9
24	B	1217	CLA	C6-C7-C8-C9
24	B	1221	CLA	C11-C10-C8-C9
24	B	1223	CLA	C6-C7-C8-C9
24	B	1224	CLA	C6-C7-C8-C9
24	1	604	CLA	C14-C13-C15-C16
24	a	604	CLA	C11-C10-C8-C9
24	3	601	CLA	C11-C10-C8-C9
24	4	610	CLA	C6-C7-C8-C9
24	4	612	CLA	C11-C10-C8-C9
24	5	601	CLA	C11-C10-C8-C9
24	5	604	CLA	C14-C13-C15-C16
24	6	604	CLA	C11-C10-C8-C9
24	7	609	CLA	C11-C10-C8-C9
24	7	611	CLA	C6-C7-C8-C9
24	7	612	CLA	C11-C10-C8-C9
24	8	609	CLA	C11-C10-C8-C9
25	A	2001	PQN	C21-C22-C23-C24
41	1	609	CHL	C14-C13-C15-C16
41	4	609	CHL	C11-C10-C8-C9
41	8	604	CHL	C11-C10-C8-C9
24	A	1122	CLA	C8-C10-C11-C12
24	B	1023	CLA	C10-C11-C12-C13
24	9	612	CLA	C8-C10-C11-C12
41	1	609	CHL	C5-C6-C7-C8
28	7	801	LHG	C2-C3-O3-P
24	A	1112	CLA	C4B-C3B-CAB-CBB
24	A	1115	CLA	C4B-C3B-CAB-CBB
24	A	1118	CLA	C4B-C3B-CAB-CBB
24	A	1119	CLA	C4B-C3B-CAB-CBB
24	A	1121	CLA	C4B-C3B-CAB-CBB
24	A	1124	CLA	C4B-C3B-CAB-CBB
24	A	1126	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	A	1129	CLA	C4B-C3B-CAB-CBB
24	A	1131	CLA	C4B-C3B-CAB-CBB
24	A	1132	CLA	C4B-C3B-CAB-CBB
24	A	1133	CLA	C4B-C3B-CAB-CBB
24	A	1141	CLA	C4B-C3B-CAB-CBB
24	B	1023	CLA	C4B-C3B-CAB-CBB
24	B	1204	CLA	C4B-C3B-CAB-CBB
24	B	1212	CLA	C4B-C3B-CAB-CBB
24	B	1214	CLA	C4B-C3B-CAB-CBB
24	B	1218	CLA	C4B-C3B-CAB-CBB
24	B	1224	CLA	C4B-C3B-CAB-CBB
24	B	1235	CLA	C4B-C3B-CAB-CBB
24	F	1301	CLA	C4B-C3B-CAB-CBB
24	H	1703	CLA	C4B-C3B-CAB-CBB
24	L	1501	CLA	C4B-C3B-CAB-CBB
24	1	602	CLA	C4B-C3B-CAB-CBB
24	1	603	CLA	C4B-C3B-CAB-CBB
24	1	608	CLA	C4B-C3B-CAB-CBB
24	1	612	CLA	C4B-C3B-CAB-CBB
24	1	615	CLA	C4B-C3B-CAB-CBB
24	a	605	CLA	C4B-C3B-CAB-CBB
24	a	607	CLA	C4B-C3B-CAB-CBB
24	a	611	CLA	C4B-C3B-CAB-CBB
24	a	612	CLA	C4B-C3B-CAB-CBB
24	a	615	CLA	C4B-C3B-CAB-CBB
24	3	616	CLA	C4B-C3B-CAB-CBB
24	4	602	CLA	C4B-C3B-CAB-CBB
24	4	612	CLA	C4B-C3B-CAB-CBB
24	4	615	CLA	C4B-C3B-CAB-CBB
24	4	617	CLA	C4B-C3B-CAB-CBB
24	5	601	CLA	C4B-C3B-CAB-CBB
24	5	603	CLA	C4B-C3B-CAB-CBB
24	5	608	CLA	C4B-C3B-CAB-CBB
24	5	609	CLA	C4B-C3B-CAB-CBB
24	5	617	CLA	C4B-C3B-CAB-CBB
24	6	602	CLA	C4B-C3B-CAB-CBB
24	6	607	CLA	C4B-C3B-CAB-CBB
24	6	608	CLA	C4B-C3B-CAB-CBB
24	6	612	CLA	C4B-C3B-CAB-CBB
24	6	615	CLA	C4B-C3B-CAB-CBB
24	6	618	CLA	C4B-C3B-CAB-CBB
24	7	606	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	7	610	CLA	C4B-C3B-CAB-CBB
24	7	615	CLA	C4B-C3B-CAB-CBB
24	8	602	CLA	C4B-C3B-CAB-CBB
24	8	605	CLA	C4B-C3B-CAB-CBB
24	8	607	CLA	C4B-C3B-CAB-CBB
24	8	611	CLA	C4B-C3B-CAB-CBB
24	8	612	CLA	C4B-C3B-CAB-CBB
24	2	602	CLA	C4B-C3B-CAB-CBB
24	2	603	CLA	C4B-C3B-CAB-CBB
24	2	608	CLA	C4B-C3B-CAB-CBB
24	2	610	CLA	C4B-C3B-CAB-CBB
24	9	603	CLA	C4B-C3B-CAB-CBB
24	9	605	CLA	C4B-C3B-CAB-CBB
24	9	607	CLA	C4B-C3B-CAB-CBB
24	9	608	CLA	C4B-C3B-CAB-CBB
28	A	5002	LHG	C28-C29-C30-C31
28	F	5001	LHG	C13-C14-C15-C16
28	1	802	LHG	O8-C23-C24-C25
24	2	621	CLA	C2A-CAA-CBA-CGA
29	A	5005	DGD	C2D-C1D-O3G-C3G
41	6	619	CHL	C10-C11-C12-C13
33	B	5005	PTY	C18-C19-C20-C21
24	A	1108	CLA	C3-C5-C6-C7
24	a	603	CLA	C3-C5-C6-C7
28	F	5001	LHG	O6-C4-C5-C6
28	a	801	LHG	O6-C4-C5-C6
28	4	801	LHG	O6-C4-C5-C6
28	8	801	LHG	O6-C4-C5-C6
28	2	802	LHG	O6-C4-C5-C6
24	A	1108	CLA	C11-C12-C13-C15
24	A	1109	CLA	C11-C12-C13-C15
24	A	1114	CLA	C11-C10-C8-C7
24	A	1115	CLA	C11-C10-C8-C7
24	A	1117	CLA	C11-C10-C8-C7
24	A	1117	CLA	C11-C12-C13-C15
24	A	1119	CLA	C11-C12-C13-C15
24	A	1126	CLA	C11-C10-C8-C7
24	B	1201	CLA	C11-C10-C8-C7
24	B	1202	CLA	C11-C12-C13-C15
24	B	1207	CLA	C6-C7-C8-C10
24	B	1213	CLA	C11-C10-C8-C7
24	B	1214	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	B	1215	CLA	C6-C7-C8-C10
24	B	1217	CLA	C6-C7-C8-C10
24	B	1219	CLA	C6-C7-C8-C10
24	B	1220	CLA	C11-C10-C8-C7
24	B	1223	CLA	C6-C7-C8-C10
24	B	1225	CLA	C11-C12-C13-C15
24	B	1230	CLA	C6-C7-C8-C10
24	B	1237	CLA	C6-C7-C8-C10
24	1	605	CLA	C12-C13-C15-C16
24	1	612	CLA	C11-C10-C8-C7
24	a	604	CLA	C11-C10-C8-C7
24	a	605	CLA	C11-C12-C13-C15
24	3	601	CLA	C11-C10-C8-C7
24	3	606	CLA	C6-C7-C8-C10
24	3	612	CLA	C11-C10-C8-C7
24	4	612	CLA	C6-C7-C8-C10
24	4	612	CLA	C11-C10-C8-C7
24	5	604	CLA	C12-C13-C15-C16
24	7	601	CLA	C11-C10-C8-C7
24	7	603	CLA	C11-C10-C8-C7
24	7	604	CLA	C11-C10-C8-C7
24	8	606	CLA	C11-C10-C8-C7
24	8	620	CLA	C12-C13-C15-C16
24	2	605	CLA	C11-C10-C8-C7
24	9	601	CLA	C6-C7-C8-C10
25	A	2001	PQN	C21-C22-C23-C25
41	4	609	CHL	C11-C10-C8-C7
41	5	610	CHL	C11-C10-C8-C7
41	8	604	CHL	C11-C10-C8-C7
24	a	604	CLA	C10-C11-C12-C13
28	1	801	LHG	C31-C32-C33-C34
28	4	801	LHG	C19-C20-C21-C22
28	9	802	LHG	C30-C31-C32-C33
24	6	607	CLA	C6-C7-C8-C9
28	A	5003	LHG	C28-C29-C30-C31
24	A	1102	CLA	C3A-C2A-CAA-CBA
24	A	1109	CLA	C4-C3-C5-C6
24	A	1124	CLA	C3A-C2A-CAA-CBA
24	A	1125	CLA	C4-C3-C5-C6
24	A	1134	CLA	C3A-C2A-CAA-CBA
24	B	1022	CLA	C4-C3-C5-C6
24	B	1212	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	B	1214	CLA	C3A-C2A-CAA-CBA
24	B	1231	CLA	C3A-C2A-CAA-CBA
24	B	1231	CLA	C4-C3-C5-C6
24	B	1235	CLA	C3A-C2A-CAA-CBA
24	B	1239	CLA	C3A-C2A-CAA-CBA
24	L	1502	CLA	C3A-C2A-CAA-CBA
24	a	603	CLA	C3A-C2A-CAA-CBA
24	3	606	CLA	C3A-C2A-CAA-CBA
24	5	608	CLA	C3A-C2A-CAA-CBA
24	5	618	CLA	C3A-C2A-CAA-CBA
24	6	603	CLA	C4-C3-C5-C6
24	6	609	CLA	C3A-C2A-CAA-CBA
24	6	612	CLA	C3A-C2A-CAA-CBA
24	2	604	CLA	C3A-C2A-CAA-CBA
24	2	605	CLA	C3A-C2A-CAA-CBA
24	4	615	CLA	C8-C10-C11-C12
24	A	1116	CLA	CAA-CBA-CGA-O2A
24	6	603	CLA	C2-C3-C5-C6
24	9	601	CLA	O1A-CGA-O2A-C1
27	A	4001	BCR	C19-C20-C21-C22
27	B	4003	BCR	C19-C20-C21-C22
27	B	4004	BCR	C13-C14-C15-C16
27	B	4007	BCR	C19-C20-C21-C22
27	I	4001	BCR	C13-C14-C15-C16
27	L	4002	BCR	C13-C14-C15-C16
27	L	4003	BCR	C9-C10-C11-C12
27	3	503	BCR	C13-C14-C15-C16
27	7	503	BCR	C19-C20-C21-C22
40	a	502	LUT	C29-C30-C31-C32
40	a	503	LUT	C29-C30-C31-C32
24	2	605	CLA	C10-C11-C12-C13
27	B	4003	BCR	C36-C18-C19-C20
28	5	801	LHG	C34-C35-C36-C37
31	B	5006	LMT	C3'-C4'-O1B-C1B
32	B	5004	PCW	C14-C15-C16-C17
43	3	506	QTB	C09-C10-C11-C17
24	B	1203	CLA	O1A-CGA-O2A-C1
28	2	801	LHG	C9-C10-C11-C12
46	8	803	DGA	CBB-CCB-CDB-CEB
24	7	603	CLA	C15-C16-C17-C18
28	A	5001	LHG	C7-C8-C9-C10
28	1	802	LHG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
28	3	801	LHG	C26-C27-C28-C29
24	A	1119	CLA	C2A-CAA-CBA-CGA
24	3	612	CLA	C2A-CAA-CBA-CGA
24	4	617	CLA	C2A-CAA-CBA-CGA
24	7	612	CLA	C2A-CAA-CBA-CGA
46	8	803	DGA	CA2-CA3-CA4-CA5
28	A	5001	LHG	C4-C5-C6-O8
28	A	5002	LHG	C4-C5-C6-O8
28	F	5001	LHG	C4-C5-C6-O8
28	F	5002	LHG	C4-C5-C6-O8
28	1	801	LHG	C4-C5-C6-O8
28	1	802	LHG	C4-C5-C6-O8
28	3	801	LHG	C4-C5-C6-O8
28	6	802	LHG	C4-C5-C6-O8
28	7	802	LHG	C4-C5-C6-O8
29	A	5005	DGD	C1G-C2G-C3G-O3G
33	3	802	PTY	O4-C1-C6-C5
35	G	5001	SQD	O6-C44-C45-C46
50	8	807	4RF	O18-C19-C20-C39
28	1	801	LHG	C9-C10-C11-C12
24	B	1210	CLA	C3-C5-C6-C7
52	9	504	A8S	O12-C1-C2-C3
24	A	1105	CLA	C8-C10-C11-C12
28	9	802	LHG	C11-C12-C13-C14
28	6	802	LHG	C30-C31-C32-C33
28	B	5001	LHG	C11-C10-C9-C8
28	8	801	LHG	C25-C26-C27-C28
50	8	807	4RF	C28-C29-C30-C31
41	8	604	CHL	C1A-C2A-CAA-CBA
33	3	802	PTY	C11-C12-C13-C14
33	5	802	PTY	C16-C17-C18-C19
33	8	891	PTY	C11-C12-C13-C14
42	8	809	OLA	C5-C6-C7-C8
29	8	802	DGD	C2G-C1G-O1G-C1A
24	4	610	CLA	C4-C3-C5-C6
24	9	612	CLA	C4-C3-C5-C6
28	2	801	LHG	C26-C27-C28-C29
24	A	1127	CLA	CAA-CBA-CGA-O2A
24	A	1109	CLA	C2-C3-C5-C6
24	A	1126	CLA	C2-C3-C5-C6
24	B	1022	CLA	C2-C3-C5-C6
24	B	1205	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	8	603	CLA	C2-C3-C5-C6
24	A	1134	CLA	C3-C5-C6-C7
24	8	609	CLA	C11-C12-C13-C15
24	7	610	CLA	C5-C6-C7-C8
28	F	5001	LHG	O6-C4-C5-O7
28	1	802	LHG	O6-C4-C5-O7
28	3	801	LHG	O6-C4-C5-O7
28	8	801	LHG	O6-C4-C5-O7
28	2	802	LHG	O6-C4-C5-O7
28	9	802	LHG	O6-C4-C5-O7
28	A	5003	LHG	C26-C27-C28-C29
50	8	808	4RF	C12-C13-C14-C15
24	1	608	CLA	O1A-CGA-O2A-C1
24	A	1115	CLA	C2B-C3B-CAB-CBB
24	A	1118	CLA	C2B-C3B-CAB-CBB
24	B	1214	CLA	C2B-C3B-CAB-CBB
24	1	602	CLA	C2B-C3B-CAB-CBB
24	3	616	CLA	C2B-C3B-CAB-CBB
24	4	602	CLA	C2B-C3B-CAB-CBB
24	7	610	CLA	C2B-C3B-CAB-CBB
24	8	602	CLA	C2B-C3B-CAB-CBB
24	2	602	CLA	C2B-C3B-CAB-CBB
24	9	603	CLA	C2B-C3B-CAB-CBB
27	A	4003	BCR	C1-C6-C7-C8
27	A	4005	BCR	C5-C6-C7-C8
27	B	4002	BCR	C5-C6-C7-C8
27	F	4001	BCR	C1-C6-C7-C8
27	G	4001	BCR	C23-C24-C25-C30
27	L	4003	BCR	C23-C24-C25-C30
27	7	503	BCR	C23-C24-C25-C30
31	B	5006	LMT	C3-C4-C5-C6
46	5	803	DGA	CA4-CA5-CA6-CA7
28	8	801	LHG	C11-C10-C9-C8
28	3	801	LHG	C11-C10-C9-C8
32	6	803	PCW	C32-C33-C34-C35
28	6	801	LHG	C26-C27-C28-C29
24	A	1102	CLA	C15-C16-C17-C18
24	A	1116	CLA	C8-C10-C11-C12
29	8	802	DGD	O6D-C5D-C6D-O5D
28	2	802	LHG	C28-C29-C30-C31
28	4	801	LHG	C11-C10-C9-C8
24	B	1209	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
24	A	1103	CLA	CAA-CBA-CGA-O2A
24	G	1601	CLA	CAA-CBA-CGA-O2A
24	A	1107	CLA	C2A-CAA-CBA-CGA
24	5	608	CLA	C2A-CAA-CBA-CGA
24	5	604	CLA	C15-C16-C17-C18
24	7	612	CLA	C8-C10-C11-C12
28	F	5002	LHG	O7-C5-C6-O8
28	a	801	LHG	O7-C5-C6-O8
28	4	802	LHG	O7-C5-C6-O8
28	6	802	LHG	O7-C5-C6-O8
33	9	803	PTY	O4-C1-C6-O7
35	H	5001	SQD	O6-C44-C45-O47
35	7	805	SQD	O47-C45-C46-O48
50	8	807	4RF	O18-C19-C20-O21
24	5	603	CLA	C11-C10-C8-C7
28	B	5001	LHG	C16-C17-C18-C19
24	A	1115	CLA	O1A-CGA-O2A-C1
24	B	1021	CLA	O1A-CGA-O2A-C1
24	B	1215	CLA	C10-C11-C12-C13
28	5	801	LHG	C19-C20-C21-C22
24	6	602	CLA	C2-C1-O2A-CGA
24	A	1137	CLA	C11-C12-C13-C15
24	B	1212	CLA	C16-C17-C18-C19
24	B	1228	CLA	C5-C6-C7-C8
33	B	5005	PTY	C11-C8-O7-C6
24	A	1108	CLA	C11-C12-C13-C14
24	A	1136	CLA	C6-C7-C8-C9
24	B	1203	CLA	C11-C12-C13-C14
24	B	1240	CLA	C6-C7-C8-C9
24	a	607	CLA	C11-C10-C8-C9
24	5	603	CLA	C6-C7-C8-C9
24	8	609	CLA	C6-C7-C8-C9
24	8	620	CLA	C14-C13-C15-C16
41	5	610	CHL	C11-C10-C8-C9
41	6	619	CHL	C6-C7-C8-C9
41	6	619	CHL	C11-C10-C8-C9
24	A	1126	CLA	C15-C16-C17-C18
28	7	803	LHG	C17-C18-C19-C20
47	6	806	SPH	O1-C1-C2-C3
28	A	5002	LHG	C9-C10-C11-C12
24	B	1021	CLA	C16-C17-C18-C20
24	B	1230	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
50	8	808	4RF	C05-C06-C07-C08
28	B	5002	LHG	C11-C10-C9-C8
24	7	608	CLA	C1A-C2A-CAA-CBA
28	5	801	LHG	C26-C27-C28-C29
28	8	801	LHG	C29-C30-C31-C32
33	5	802	PTY	C31-C32-C33-C34
28	A	5001	LHG	O1-C1-C2-O2
27	A	4001	BCR	C9-C10-C11-C12
27	A	4003	BCR	C19-C20-C21-C22
27	B	4006	BCR	C19-C20-C21-C22
40	2	501	LUT	C29-C30-C31-C32
24	B	1022	CLA	C16-C17-C18-C20
24	3	612	CLA	CBD-CGD-O2D-CED
28	A	5003	LHG	C15-C16-C17-C18
28	5	801	LHG	C35-C36-C37-C38
24	7	609	CLA	C5-C6-C7-C8
28	3	801	LHG	C1-C2-C3-O3
28	3	801	LHG	C16-C17-C18-C19
33	8	891	PTY	C16-C17-C18-C19
50	8	807	4RF	C26-C27-C28-C29
41	6	610	CHL	CAA-CBA-CGA-O2A
50	7	807	4RF	C15-C16-O18-C19
24	A	1105	CLA	C5-C6-C7-C8
24	6	615	CLA	C15-C16-C17-C18
32	B	5004	PCW	O3P-C1-C2-C3
33	7	804	PTY	O14-C5-C6-C1
24	A	1122	CLA	C13-C15-C16-C17
24	B	1210	CLA	C13-C15-C16-C17
24	B	1223	CLA	C13-C15-C16-C17
27	A	4001	BCR	C36-C18-C19-C20
24	A	1012	CLA	C12-C13-C15-C16
24	A	1115	CLA	C6-C7-C8-C10
24	B	1021	CLA	C6-C7-C8-C10
24	B	1240	CLA	C6-C7-C8-C10
24	3	601	CLA	C12-C13-C15-C16
24	3	605	CLA	C11-C10-C8-C7
24	3	605	CLA	C12-C13-C15-C16
24	4	610	CLA	C12-C13-C15-C16
24	5	603	CLA	C6-C7-C8-C10
24	7	601	CLA	C6-C7-C8-C10
24	9	603	CLA	C11-C12-C13-C15
41	4	609	CHL	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
41	5	610	CHL	C12-C13-C15-C16
41	6	619	CHL	C11-C10-C8-C7
24	B	1225	CLA	C8-C10-C11-C12
24	B	1229	CLA	C13-C15-C16-C17
27	A	4001	BCR	C11-C12-C13-C14
27	L	4003	BCR	C11-C12-C13-C14
27	5	504	BCR	C11-C12-C13-C14
39	M	4001	ECH	C21-C22-C23-C24
24	B	1235	CLA	O1A-CGA-O2A-C1
24	B	1238	CLA	O1A-CGA-O2A-C1
24	3	606	CLA	O1A-CGA-O2A-C1
29	8	802	DGD	C2G-C3G-O3G-C1D
28	2	801	LHG	C31-C32-C33-C34
24	A	1132	CLA	C2A-CAA-CBA-CGA
24	B	1228	CLA	C2A-CAA-CBA-CGA
24	6	602	CLA	C3-C5-C6-C7
24	2	605	CLA	C2A-CAA-CBA-CGA
33	B	5005	PTY	C33-C34-C35-C36
24	A	1134	CLA	C11-C12-C13-C15
24	B	1202	CLA	C16-C17-C18-C20
24	8	609	CLA	C11-C12-C13-C14
28	9	801	LHG	C8-C7-O7-C5
28	A	5001	LHG	O9-C7-O7-C5
24	A	1119	CLA	C4-C3-C5-C6
24	B	1206	CLA	C4-C3-C5-C6
24	L	1502	CLA	C4-C3-C5-C6
24	9	601	CLA	C4-C3-C5-C6
24	B	1231	CLA	C2-C3-C5-C6
24	B	1207	CLA	C3-C5-C6-C7
30	A	5007	3PH	C36-C37-C38-C39
24	8	620	CLA	C10-C11-C12-C13
32	B	5004	PCW	C3-C2-O2-C31
46	8	803	DGA	CG1-CG2-OG2-CB1
28	B	5002	LHG	C27-C28-C29-C30
27	5	503	BCR	C19-C20-C21-C22
27	5	504	BCR	C15-C16-C17-C18
27	6	503	BCR	C19-C20-C21-C22
40	9	502	LUT	C29-C30-C31-C32
28	1	802	LHG	C9-C10-C11-C12
28	F	5002	LHG	C24-C25-C26-C27
28	B	5002	LHG	O6-C4-C5-O7
28	4	801	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
28	4	802	LHG	O6-C4-C5-O7
32	6	803	PCW	O3P-C1-C2-O2
28	B	5001	LHG	C4-C5-C6-O8
35	7	805	SQD	C44-C45-C46-O48
50	7	807	4RF	O18-C19-C20-C39
51	8	806	P5S	O19-C1-C2-C3
24	5	604	CLA	C16-C17-C18-C20
24	A	1136	CLA	O1A-CGA-O2A-C1
24	A	1107	CLA	C4-C3-C5-C6
24	8	610	CLA	C2A-CAA-CBA-CGA
24	2	609	CLA	C2A-CAA-CBA-CGA
24	B	1240	CLA	C2-C3-C5-C6
28	3	801	LHG	O7-C5-C6-O8
28	6	801	LHG	O7-C5-C6-O8
29	A	5005	DGD	O2G-C2G-C3G-O3G
33	B	5005	PTY	O4-C1-C6-O7
35	G	5001	SQD	O6-C44-C45-O47
35	G	5001	SQD	O47-C45-C46-O48
50	8	808	4RF	O18-C19-C20-O21
50	8	808	4RF	O21-C20-C39-O40
51	8	806	P5S	O19-C1-C2-O37
24	B	1220	CLA	C10-C11-C12-C13
24	9	603	CLA	C15-C16-C17-C18
24	A	1115	CLA	C6-C7-C8-C9
24	B	1219	CLA	C6-C7-C8-C9
24	1	606	CLA	C11-C10-C8-C9
24	3	601	CLA	C14-C13-C15-C16
24	3	605	CLA	C14-C13-C15-C16
30	A	5007	3PH	C24-C25-C26-C27
28	3	801	LHG	C30-C31-C32-C33
34	B	5007	LAP	C3-C4-C5-C6
34	K	5001	LAP	C5-C6-C7-C8
24	A	1131	CLA	C5-C6-C7-C8
28	6	801	LHG	C10-C11-C12-C13
50	8	807	4RF	C31-C32-C33-C34
28	B	5001	LHG	C7-C8-C9-C10
28	1	801	LHG	C25-C26-C27-C28
24	A	1107	CLA	C5-C6-C7-C8
24	4	604	CLA	C5-C6-C7-C8
24	B	1223	CLA	C2-C1-O2A-CGA
24	4	606	CLA	C2-C1-O2A-CGA
24	5	603	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
24	1	604	CLA	C16-C17-C18-C19
24	7	607	CLA	C11-C12-C13-C14
28	A	5002	LHG	C19-C20-C21-C22
33	B	5005	PTY	C31-C32-C33-C34
32	B	5004	PCW	O4P-C4-C5-N
34	B	5007	LAP	O6-C16-C17-N8
34	F	5003	LAP	O6-C16-C17-N8
24	B	1220	CLA	C3-C5-C6-C7
24	A	1134	CLA	C10-C11-C12-C13
50	8	807	4RF	C46-C47-C48-C49
24	A	1113	CLA	C3-C5-C6-C7
24	A	1139	CLA	C6-C7-C8-C10
24	1	603	CLA	C16-C17-C18-C20
29	B	5003	DGD	C1B-C2B-C3B-C4B
50	7	807	4RF	O17-C16-O18-C19
46	5	803	DGA	CA6-CA7-CA8-CA9
41	8	604	CHL	C14-C13-C15-C16
45	4	803	PLM	C1-C2-C3-C4
51	8	806	P5S	CA-CB-OG-P12
28	B	5002	LHG	C25-C26-C27-C28
27	5	504	BCR	C7-C8-C9-C34
40	1	501	LUT	C27-C28-C29-C39
28	a	801	LHG	C31-C32-C33-C34
24	A	1108	CLA	C4B-C3B-CAB-CBB
24	A	1130	CLA	C4B-C3B-CAB-CBB
24	A	1133	CLA	C1A-C2A-CAA-CBA
24	A	1134	CLA	C4B-C3B-CAB-CBB
24	A	1135	CLA	C4B-C3B-CAB-CBB
24	A	1136	CLA	C4B-C3B-CAB-CBB
24	B	1205	CLA	C4B-C3B-CAB-CBB
24	B	1217	CLA	C4B-C3B-CAB-CBB
24	B	1218	CLA	C1A-C2A-CAA-CBA
24	B	1223	CLA	C4B-C3B-CAB-CBB
24	B	1232	CLA	C4B-C3B-CAB-CBB
24	B	1239	CLA	C4B-C3B-CAB-CBB
24	F	1302	CLA	C1A-C2A-CAA-CBA
24	J	1901	CLA	C4B-C3B-CAB-CBB
24	K	1401	CLA	C4B-C3B-CAB-CBB
24	4	603	CLA	C4B-C3B-CAB-CBB
24	4	610	CLA	C4B-C3B-CAB-CBB
24	5	602	CLA	C4B-C3B-CAB-CBB
24	5	605	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	5	618	CLA	C1A-C2A-CAA-CBA
24	6	609	CLA	C1A-C2A-CAA-CBA
24	7	608	CLA	C4B-C3B-CAB-CBB
24	7	609	CLA	C4B-C3B-CAB-CBB
24	7	617	CLA	C4B-C3B-CAB-CBB
24	2	605	CLA	C1A-C2A-CAA-CBA
24	2	615	CLA	C4B-C3B-CAB-CBB
24	9	612	CLA	CBA-CGA-O2A-C1
29	8	802	DGD	C6A-C7A-C8A-C9A
24	B	1216	CLA	C4-C3-C5-C6
24	B	1234	CLA	C4-C3-C5-C6
24	1	603	CLA	C4-C3-C5-C6
24	9	603	CLA	C4-C3-C5-C6
28	A	5002	LHG	C33-C34-C35-C36
24	L	1502	CLA	C2-C3-C5-C6
27	A	4001	BCR	C17-C18-C19-C20
27	A	4003	BCR	C7-C8-C9-C10
27	B	4003	BCR	C17-C18-C19-C20
27	F	4001	BCR	C17-C18-C19-C20
27	L	4001	BCR	C21-C22-C23-C24
27	F	4001	BCR	C13-C14-C15-C16
27	K	4001	BCR	C13-C14-C15-C16
27	3	503	BCR	C19-C20-C21-C22
27	3	505	BCR	C19-C20-C21-C22
28	1	802	LHG	C26-C27-C28-C29
24	A	1135	CLA	C3-C5-C6-C7
24	B	1235	CLA	C2A-CAA-CBA-CGA
24	a	601	CLA	C2A-CAA-CBA-CGA
24	5	601	CLA	C2A-CAA-CBA-CGA
28	5	801	LHG	C15-C16-C17-C18
50	7	807	4RF	C44-C45-C46-C47
28	A	5002	LHG	O6-C4-C5-C6
28	B	5001	LHG	O6-C4-C5-C6
28	F	5002	LHG	O6-C4-C5-C6
28	1	801	LHG	O6-C4-C5-C6
28	6	802	LHG	O6-C4-C5-C6
28	7	803	LHG	O6-C4-C5-C6
33	3	802	PTY	O14-C5-C6-C1
33	B	5005	PTY	O10-C8-O7-C6
24	A	1110	CLA	C11-C10-C8-C7
24	A	1114	CLA	C11-C12-C13-C15
24	A	1132	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
24	A	1136	CLA	C12-C13-C15-C16
24	B	1216	CLA	C6-C7-C8-C10
24	B	1220	CLA	C6-C7-C8-C10
24	B	1223	CLA	C12-C13-C15-C16
24	B	1228	CLA	C6-C7-C8-C10
24	K	1402	CLA	C6-C7-C8-C10
24	1	603	CLA	C11-C10-C8-C7
24	3	603	CLA	C11-C12-C13-C15
24	3	610	CLA	C11-C10-C8-C7
24	6	601	CLA	C6-C7-C8-C10
24	2	601	CLA	C11-C10-C8-C7
24	9	612	CLA	C12-C13-C15-C16
46	5	803	DGA	CB3-CB4-CB5-CB6
28	1	802	LHG	C11-C10-C9-C8
24	B	1202	CLA	C16-C17-C18-C19
24	7	610	CLA	C6-C7-C8-C10
24	B	1216	CLA	CBA-CGA-O2A-C1
28	4	802	LHG	C24-C23-O8-C6
28	F	5002	LHG	C26-C27-C28-C29
33	9	803	PTY	C21-C22-C23-C24
24	B	1207	CLA	C5-C6-C7-C8
33	7	804	PTY	C31-C32-C33-C34
24	2	603	CLA	C3-C5-C6-C7
28	F	5002	LHG	C2-C3-O3-P
28	a	801	LHG	C2-C3-O3-P
28	6	801	LHG	C2-C3-O3-P
33	7	804	PTY	C6-C5-O14-P1
41	4	618	CHL	C3A-C2A-CAA-CBA
24	A	1013	CLA	C13-C15-C16-C17
28	9	801	LHG	O9-C7-O7-C5
28	A	5002	LHG	O6-C4-C5-O7
28	B	5001	LHG	O6-C4-C5-O7
28	F	5002	LHG	O6-C4-C5-O7
28	1	801	LHG	O6-C4-C5-O7
28	6	801	LHG	O6-C4-C5-O7
28	6	802	LHG	O6-C4-C5-O7
32	B	5004	PCW	O3P-C1-C2-O2
33	9	803	PTY	O14-C5-C6-O7
28	9	802	LHG	C9-C10-C11-C12
28	4	801	LHG	C8-C7-O7-C5
24	B	1022	CLA	C2A-CAA-CBA-CGA
24	a	604	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
24	A	1012	CLA	C14-C13-C15-C16
24	A	1133	CLA	C14-C13-C15-C16
24	B	1021	CLA	C6-C7-C8-C9
24	B	1214	CLA	C6-C7-C8-C9
24	B	1225	CLA	C11-C12-C13-C14
24	3	612	CLA	C6-C7-C8-C9
24	3	612	CLA	C11-C10-C8-C9
24	7	601	CLA	C6-C7-C8-C9
24	9	603	CLA	C11-C12-C13-C14
33	9	803	PTY	C37-C38-C39-C40
27	K	4001	BCR	C9-C10-C11-C12
40	4	502	LUT	C29-C30-C31-C32
49	7	504	C7Z	C13-C14-C15-C35
28	2	801	LHG	C24-C25-C26-C27
24	4	604	CLA	C10-C11-C12-C13
28	6	801	LHG	C31-C32-C33-C34
24	A	1120	CLA	C1-C2-C3-C4
38	a	804	LPX	C13-C14-C15-C16
50	8	808	4RF	C50-C51-C52-C53
28	A	5003	LHG	O7-C5-C6-O8
28	F	5001	LHG	O7-C5-C6-O8
28	2	801	LHG	O7-C5-C6-O8
50	8	807	4RF	O21-C20-C39-O40
28	B	5001	LHG	C34-C35-C36-C37
24	A	1134	CLA	C11-C12-C13-C14
33	B	5005	PTY	O4-C1-C6-C5
50	8	807	4RF	C19-C20-C39-O40
24	B	1224	CLA	C4-C3-C5-C6
24	4	610	CLA	C13-C15-C16-C17
24	2	604	CLA	CAA-CBA-CGA-O2A
51	8	806	P5S	O37-C38-C39-C40
24	5	601	CLA	O1A-CGA-O2A-C1
24	A	1119	CLA	C2-C3-C5-C6
24	A	1121	CLA	C3-C5-C6-C7
50	8	807	4RF	C11-C12-C13-C14
24	A	1121	CLA	C8-C10-C11-C12
24	B	1214	CLA	C13-C15-C16-C17
24	A	1102	CLA	CAD-CBD-CGD-O2D
24	A	1111	CLA	CAD-CBD-CGD-O2D
24	A	1136	CLA	CAD-CBD-CGD-O2D
24	B	1207	CLA	CAD-CBD-CGD-O2D
24	B	1210	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	B	1217	CLA	CAD-CBD-CGD-O2D
24	B	1223	CLA	CAD-CBD-CGD-O2D
24	B	1227	CLA	CAD-CBD-CGD-O2D
24	6	609	CLA	CAD-CBD-CGD-O2D
24	2	605	CLA	CAD-CBD-CGD-O2D
41	a	609	CHL	CAD-CBD-CGD-O2D
41	8	613	CHL	CAD-CBD-CGD-O2D
24	A	1133	CLA	C10-C11-C12-C13
50	8	808	4RF	C45-C46-C47-C48
24	5	601	CLA	CBA-CGA-O2A-C1
24	B	1234	CLA	C2A-CAA-CBA-CGA
24	B	1220	CLA	O1A-CGA-O2A-C1
46	5	803	DGA	CA2-CA3-CA4-CA5
28	4	802	LHG	O10-C23-O8-C6
23	A	1011	CL0	CHA-CBD-CGD-O1D
23	A	1011	CL0	CHA-CBD-CGD-O2D
24	A	1102	CLA	CAD-CBD-CGD-O1D
24	A	1111	CLA	CAD-CBD-CGD-O1D
24	A	1123	CLA	CAD-CBD-CGD-O1D
24	A	1125	CLA	CAD-CBD-CGD-O1D
24	A	1133	CLA	CHA-CBD-CGD-O1D
24	A	1135	CLA	CHA-CBD-CGD-O1D
24	A	1135	CLA	CHA-CBD-CGD-O2D
24	A	1136	CLA	CAD-CBD-CGD-O1D
24	B	1207	CLA	CAD-CBD-CGD-O1D
24	B	1210	CLA	CAD-CBD-CGD-O1D
24	B	1212	CLA	CHA-CBD-CGD-O1D
24	B	1212	CLA	CHA-CBD-CGD-O2D
24	B	1217	CLA	CAD-CBD-CGD-O1D
24	B	1223	CLA	CAD-CBD-CGD-O1D
24	B	1227	CLA	CAD-CBD-CGD-O1D
24	B	1235	CLA	CAD-CBD-CGD-O1D
24	1	604	CLA	CHA-CBD-CGD-O1D
24	1	604	CLA	CHA-CBD-CGD-O2D
24	a	604	CLA	CHA-CBD-CGD-O1D
24	a	604	CLA	CHA-CBD-CGD-O2D
24	3	604	CLA	CHA-CBD-CGD-O1D
24	3	604	CLA	CHA-CBD-CGD-O2D
24	5	608	CLA	CHA-CBD-CGD-O1D
24	6	609	CLA	CAD-CBD-CGD-O1D
24	7	604	CLA	CHA-CBD-CGD-O1D
24	7	604	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	7	617	CLA	CAD-CBD-CGD-O1D
24	2	605	CLA	CAD-CBD-CGD-O1D
24	9	605	CLA	CHA-CBD-CGD-O1D
24	9	605	CLA	CHA-CBD-CGD-O2D
27	A	4002	BCR	C19-C20-C21-C22
27	G	4001	BCR	C9-C10-C11-C12
27	G	4001	BCR	C13-C14-C15-C16
27	I	4001	BCR	C15-C16-C17-C18
28	B	5002	LHG	C3-O3-P-O5
28	1	802	LHG	C3-O3-P-O5
28	a	801	LHG	C4-O6-P-O5
28	3	801	LHG	C3-O3-P-O5
28	3	801	LHG	C4-O6-P-O5
28	4	802	LHG	C4-O6-P-O4
28	6	801	LHG	C4-O6-P-O5
28	6	802	LHG	C4-O6-P-O5
28	9	801	LHG	C3-O3-P-O5
32	B	5004	PCW	C1-O3P-P-O2P
32	B	5004	PCW	C4-O4P-P-O2P
32	B	5004	PCW	C4-O4P-P-O3P
33	5	802	PTY	N1-C2-C3-O11
33	7	804	PTY	C3-O11-P1-O13
33	7	804	PTY	C3-O11-P1-O14
33	7	804	PTY	C5-O14-P1-O11
33	7	804	PTY	C5-O14-P1-O12
33	7	804	PTY	C5-O14-P1-O13
33	9	803	PTY	N1-C2-C3-O11
33	9	803	PTY	C3-O11-P1-O13
34	B	5007	LAP	C15-O4-P9-O5
34	B	5007	LAP	C16-O6-P9-O5
34	F	5003	LAP	C15-O4-P9-O5
34	F	5003	LAP	C16-O6-P9-O5
34	K	5001	LAP	C16-O6-P9-O7
38	J	5001	LPX	C1-O2-P1-O1
38	J	5001	LPX	C1-O2-P1-O4
38	a	804	LPX	C1-O2-P1-O4
40	a	501	LUT	C25-C26-C27-C28
40	9	501	LUT	C25-C26-C27-C28
40	9	502	LUT	C25-C26-C27-C28
41	a	609	CHL	CAD-CBD-CGD-O1D
41	5	610	CHL	CHA-CBD-CGD-O1D
41	5	611	CHL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
41	8	613	CHL	CAD-CBD-CGD-O1D
24	B	1203	CLA	C3-C5-C6-C7
24	B	1231	CLA	C3-C5-C6-C7
24	A	1012	CLA	C2B-C3B-CAB-CBB
24	A	1108	CLA	C2B-C3B-CAB-CBB
24	A	1109	CLA	C2B-C3B-CAB-CBB
24	A	1133	CLA	C2B-C3B-CAB-CBB
24	A	1135	CLA	C2B-C3B-CAB-CBB
24	B	1205	CLA	C2B-C3B-CAB-CBB
24	B	1217	CLA	C2B-C3B-CAB-CBB
24	B	1220	CLA	C2B-C3B-CAB-CBB
24	B	1230	CLA	C2B-C3B-CAB-CBB
24	B	1237	CLA	C2B-C3B-CAB-CBB
24	B	1238	CLA	C2B-C3B-CAB-CBB
24	F	1301	CLA	C2B-C3B-CAB-CBB
24	J	1901	CLA	C2B-C3B-CAB-CBB
24	K	1401	CLA	C2B-C3B-CAB-CBB
24	K	1403	CLA	C2B-C3B-CAB-CBB
24	H	1701	CLA	C2B-C3B-CAB-CBB
24	H	1702	CLA	C2B-C3B-CAB-CBB
24	L	1502	CLA	C2B-C3B-CAB-CBB
24	a	602	CLA	C2B-C3B-CAB-CBB
24	a	605	CLA	C2B-C3B-CAB-CBB
24	4	603	CLA	C2B-C3B-CAB-CBB
24	4	607	CLA	C2B-C3B-CAB-CBB
24	4	610	CLA	C2B-C3B-CAB-CBB
24	4	615	CLA	C2B-C3B-CAB-CBB
24	4	616	CLA	C2B-C3B-CAB-CBB
24	7	617	CLA	C2B-C3B-CAB-CBB
24	8	605	CLA	C2B-C3B-CAB-CBB
24	8	610	CLA	C2B-C3B-CAB-CBB
24	2	604	CLA	C2B-C3B-CAB-CBB
24	2	606	CLA	C2B-C3B-CAB-CBB
24	2	610	CLA	C2B-C3B-CAB-CBB
40	6	502	LUT	C1-C6-C7-C8
24	A	1107	CLA	C2-C3-C5-C6
24	3	613	CLA	C5-C6-C7-C8
28	A	5002	LHG	C2-C3-O3-P
28	A	5003	LHG	C2-C3-O3-P
28	B	5002	LHG	C2-C3-O3-P
28	F	5001	LHG	C2-C3-O3-P
28	6	802	LHG	C2-C3-O3-P

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Mol	Chain	Res	Type	Atoms
28	9	802	LHG	C2-C3-O3-P
38	a	804	LPX	C4-C3-O1-P1
40	5	505	LUT	C27-C28-C29-C39
28	F	5001	LHG	C29-C30-C31-C32
46	8	803	DGA	CA5-CA6-CA7-CA8
28	a	801	LHG	C30-C31-C32-C33
33	3	802	PTY	C15-C16-C17-C18
35	H	5001	SQD	C12-C13-C14-C15
28	a	801	LHG	C23-C24-C25-C26
42	8	809	OLA	C1-C2-C3-C4
41	6	619	CHL	C8-C10-C11-C12
24	2	604	CLA	C11-C10-C8-C7
29	8	802	DGD	C3G-C2G-O2G-C1B
29	A	5005	DGD	C7B-C8B-C9B-CAB
50	8	808	4RF	C44-C45-C46-C47
27	H	4001	BCR	C18-C19-C20-C21
27	6	503	BCR	C18-C19-C20-C21
24	A	1111	CLA	C2-C3-C5-C6
24	B	1206	CLA	C2-C3-C5-C6
42	1	803	OLA	C1-C2-C3-C4
28	A	5003	LHG	C14-C15-C16-C17
28	7	801	LHG	C32-C33-C34-C35
28	8	801	LHG	C27-C28-C29-C30
27	B	4004	BCR	C19-C20-C21-C22
24	A	1117	CLA	C16-C17-C18-C20
28	9	802	LHG	O6-C4-C5-C6
32	6	803	PCW	O3P-C1-C2-C3
33	9	803	PTY	O14-C5-C6-C1
24	B	1220	CLA	CBA-CGA-O2A-C1
24	B	1216	CLA	O1A-CGA-O2A-C1
24	3	603	CLA	C10-C11-C12-C13
24	A	1013	CLA	C14-C13-C15-C16
24	A	1103	CLA	C14-C13-C15-C16
24	A	1105	CLA	C6-C7-C8-C9
24	A	1115	CLA	C11-C10-C8-C9
24	A	1117	CLA	C11-C12-C13-C14
24	A	1119	CLA	C6-C7-C8-C9
24	B	1228	CLA	C6-C7-C8-C9
24	B	1231	CLA	C11-C10-C8-C9
24	B	1237	CLA	C11-C10-C8-C9
24	1	603	CLA	C11-C10-C8-C9
24	1	612	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	a	605	CLA	C11-C12-C13-C14
24	3	601	CLA	C6-C7-C8-C9
24	3	605	CLA	C11-C10-C8-C9
24	4	612	CLA	C6-C7-C8-C9
24	5	604	CLA	C11-C10-C8-C9
24	7	603	CLA	C11-C12-C13-C14
24	8	606	CLA	C11-C10-C8-C9
41	1	609	CHL	C11-C10-C8-C9
24	A	1103	CLA	C12-C13-C15-C16
24	A	1105	CLA	C6-C7-C8-C10
24	A	1119	CLA	C6-C7-C8-C10
24	A	1125	CLA	C11-C10-C8-C7
24	B	1212	CLA	C6-C7-C8-C10
24	B	1231	CLA	C11-C10-C8-C7
24	B	1237	CLA	C11-C10-C8-C7
24	3	601	CLA	C6-C7-C8-C10
24	5	604	CLA	C11-C10-C8-C7
28	4	802	LHG	C10-C11-C12-C13
28	7	802	LHG	O6-C4-C5-O7
28	2	801	LHG	O6-C4-C5-O7
33	B	5005	PTY	O14-C5-C6-O7
33	3	802	PTY	O14-C5-C6-O7
33	7	804	PTY	O14-C5-C6-O7
24	5	604	CLA	C16-C17-C18-C19
24	2	603	CLA	C8-C10-C11-C12
24	B	1224	CLA	CAA-CBA-CGA-O2A
24	1	605	CLA	CAA-CBA-CGA-O2A
28	6	801	LHG	C19-C20-C21-C22
24	6	615	CLA	C10-C11-C12-C13
29	8	802	DGD	C4D-C5D-C6D-O5D
24	B	1214	CLA	C4-C3-C5-C6
24	2	605	CLA	CAA-CBA-CGA-O2A
24	A	1109	CLA	CBA-CGA-O2A-C1
24	A	1139	CLA	C6-C7-C8-C9
24	1	603	CLA	C16-C17-C18-C19
24	7	607	CLA	C11-C12-C13-C15
24	6	601	CLA	C5-C6-C7-C8
31	A	5008	LMT	C1-C2-C3-C4
31	B	5006	LMT	C5-C6-C7-C8
32	B	5004	PCW	C13-C14-C15-C16
28	B	5001	LHG	O7-C5-C6-O8
28	9	802	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
30	A	5007	3PH	O21-C2-C3-O31
33	5	802	PTY	O4-C1-C6-O7
24	1	604	CLA	C5-C6-C7-C8
27	7	503	BCR	C13-C14-C15-C16
24	A	1112	CLA	C6-C7-C8-C10
42	8	809	OLA	C13-C14-C15-C16
28	2	802	LHG	C16-C17-C18-C19
24	3	602	CLA	CAA-CBA-CGA-O2A
30	A	5007	3PH	C22-C23-C24-C25
50	8	808	4RF	C33-C34-C35-C36
28	4	801	LHG	O9-C7-O7-C5
24	A	1103	CLA	C2-C1-O2A-CGA
24	A	1106	CLA	C2-C1-O2A-CGA
24	4	602	CLA	C2-C1-O2A-CGA
24	8	610	CLA	C2-C1-O2A-CGA
41	a	609	CHL	C4-C3-C5-C6
24	A	1118	CLA	C6-C7-C8-C9
24	A	1114	CLA	C8-C10-C11-C12
28	3	801	LHG	C34-C35-C36-C37
24	1	608	CLA	C5-C6-C7-C8
28	5	801	LHG	C33-C34-C35-C36
24	A	1117	CLA	C3-C5-C6-C7
28	9	801	LHG	C24-C25-C26-C27
33	5	802	PTY	C32-C33-C34-C35
24	3	613	CLA	CAA-CBA-CGA-O2A
29	8	802	DGD	C5D-C6D-O5D-C1E
24	A	1108	CLA	C2A-CAA-CBA-CGA
24	3	616	CLA	C2A-CAA-CBA-CGA
27	B	4007	BCR	C15-C16-C17-C18
40	5	502	LUT	C29-C30-C31-C32
24	B	1221	CLA	C16-C17-C18-C19
28	1	801	LHG	C11-C10-C9-C8
32	6	803	PCW	C16-C17-C18-C19
24	A	1117	CLA	C4-C3-C5-C6
24	A	1110	CLA	C11-C10-C8-C9
24	B	1226	CLA	C11-C10-C8-C9
24	K	1402	CLA	C6-C7-C8-C9
24	2	601	CLA	C11-C10-C8-C9
24	9	612	CLA	C14-C13-C15-C16
41	4	609	CHL	C14-C13-C15-C16
41	6	619	CHL	C11-C12-C13-C14
28	1	802	LHG	C2-C3-O3-P

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Mol	Chain	Res	Type	Atoms
24	3	605	CLA	C4B-C3B-CAB-CBB
24	3	606	CLA	C4B-C3B-CAB-CBB
24	3	607	CLA	C4B-C3B-CAB-CBB
24	6	605	CLA	C4B-C3B-CAB-CBB
24	7	601	CLA	C4B-C3B-CAB-CBB
24	8	603	CLA	C4B-C3B-CAB-CBB
24	B	1230	CLA	C10-C11-C12-C13
24	A	1104	CLA	C5-C6-C7-C8
24	B	1208	CLA	CBA-CGA-O2A-C1
28	9	801	LHG	C24-C23-O8-C6
24	B	1240	CLA	C15-C16-C17-C18
24	9	608	CLA	O1D-CGD-O2D-CED
24	B	1226	CLA	C2A-CAA-CBA-CGA
24	1	611	CLA	C4-C3-C5-C6
24	7	603	CLA	C4-C3-C5-C6
24	7	606	CLA	C4-C3-C5-C6
24	8	610	CLA	C4-C3-C5-C6
24	B	1214	CLA	C2-C3-C5-C6
24	9	603	CLA	C2-C3-C5-C6
41	a	609	CHL	C2-C3-C5-C6
33	9	803	PTY	C32-C33-C34-C35
24	9	612	CLA	O1A-CGA-O2A-C1
27	G	4001	BCR	C15-C16-C17-C18
27	L	4001	BCR	C19-C20-C21-C22
40	a	503	LUT	C13-C14-C15-C35
24	3	610	CLA	O1D-CGD-O2D-CED
24	B	1226	CLA	C11-C10-C8-C7
24	a	605	CLA	C6-C7-C8-C10
24	3	613	CLA	C6-C7-C8-C10
24	3	612	CLA	O1D-CGD-O2D-CED
24	A	1109	CLA	O1A-CGA-O2A-C1
24	B	1206	CLA	C2C-C3C-CAC-CBC
24	A	1112	CLA	C6-C7-C8-C9
41	8	601	CHL	C11-C12-C13-C14
24	A	1131	CLA	C13-C15-C16-C17
28	4	801	LHG	O7-C5-C6-O8
28	F	5002	LHG	C29-C30-C31-C32
24	3	605	CLA	C4-C3-C5-C6
24	7	615	CLA	C3A-C2A-CAA-CBA
41	4	609	CHL	C3A-C2A-CAA-CBA
33	B	5005	PTY	C25-C26-C27-C28
24	B	1220	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	B	1232	CLA	C2A-CAA-CBA-CGA
24	8	615	CLA	C2A-CAA-CBA-CGA
32	6	803	PCW	C33-C34-C35-C36
27	A	4005	BCR	C16-C17-C18-C36
27	B	4003	BCR	C11-C10-C9-C34
27	B	4003	BCR	C20-C21-C22-C37
27	F	4001	BCR	C35-C13-C14-C15
40	6	501	LUT	C40-C33-C34-C35
24	B	1206	CLA	C4C-C3C-CAC-CBC
24	3	607	CLA	C3-C5-C6-C7
24	2	604	CLA	C11-C10-C8-C9
34	F	5003	LAP	C5-C6-C7-C8
24	1	602	CLA	CAA-CBA-CGA-O1A
24	A	1119	CLA	C15-C16-C17-C18
24	1	603	CLA	C8-C10-C11-C12
24	A	1116	CLA	C2-C1-O2A-CGA
24	B	1224	CLA	C2-C1-O2A-CGA
24	F	1302	CLA	C2-C1-O2A-CGA
24	2	601	CLA	C2-C1-O2A-CGA
27	F	4001	BCR	C19-C20-C21-C22
27	K	4001	BCR	C19-C20-C21-C22
27	5	504	BCR	C19-C20-C21-C22
27	8	503	BCR	C19-C20-C21-C22
41	a	606	CHL	C2-C1-O2A-CGA
35	G	5001	SQD	C25-C26-C27-C28
24	B	1237	CLA	C5-C6-C7-C8
27	5	503	BCR	C36-C18-C19-C20
30	A	5007	3PH	C2-C1-O11-P
28	B	5001	LHG	C25-C26-C27-C28
24	5	612	CLA	C5-C6-C7-C8
28	9	801	LHG	C25-C26-C27-C28
24	B	1221	CLA	C4-C3-C5-C6
35	G	5001	SQD	C12-C13-C14-C15
24	B	1224	CLA	C2-C3-C5-C6
24	B	1234	CLA	C2-C3-C5-C6
24	A	1117	CLA	C16-C17-C18-C19
24	B	1022	CLA	C10-C11-C12-C13
42	8	809	OLA	O1-C1-C2-C3
29	B	5003	DGD	O1G-C1G-C2G-C3G
24	B	1206	CLA	C5-C6-C7-C8
28	2	801	LHG	C30-C31-C32-C33
24	A	1111	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	A	1114	CLA	C11-C12-C13-C14
24	A	1123	CLA	C11-C10-C8-C9
24	B	1216	CLA	C6-C7-C8-C9
24	B	1223	CLA	C14-C13-C15-C16
24	1	605	CLA	C11-C10-C8-C9
24	3	606	CLA	C11-C12-C13-C14
24	8	606	CLA	C6-C7-C8-C9
24	4	610	CLA	C16-C17-C18-C19
24	7	601	CLA	C11-C12-C13-C15
24	7	611	CLA	C10-C11-C12-C13
51	8	806	P5S	C22-C23-C24-C25
28	B	5001	LHG	C10-C11-C12-C13
29	8	802	DGD	O1G-C1A-C2A-C3A
24	A	1123	CLA	C13-C15-C16-C17
24	B	1211	CLA	C5-C6-C7-C8
24	9	612	CLA	C5-C6-C7-C8
28	9	802	LHG	C26-C27-C28-C29
24	1	603	CLA	C3-C5-C6-C7
41	4	618	CHL	C1A-C2A-CAA-CBA
27	B	4002	BCR	C15-C16-C17-C18
43	a	504	QTB	C02-C03-C04-C05
24	3	610	CLA	C4-C3-C5-C6
28	9	802	LHG	C19-C20-C21-C22
24	B	1221	CLA	C2-C3-C5-C6
24	3	605	CLA	C2-C3-C5-C6
50	7	807	4RF	C07-C08-C09-C10
24	A	1103	CLA	C2A-CAA-CBA-CGA
24	9	609	CLA	C2A-CAA-CBA-CGA
24	3	618	CLA	CAA-CBA-CGA-O2A
24	9	609	CLA	CAA-CBA-CGA-O2A
24	A	1102	CLA	C1A-C2A-CAA-CBA
24	A	1134	CLA	C1A-C2A-CAA-CBA
24	B	1021	CLA	C1A-C2A-CAA-CBA
24	B	1209	CLA	C1A-C2A-CAA-CBA
24	B	1231	CLA	C1A-C2A-CAA-CBA
24	B	1236	CLA	C1A-C2A-CAA-CBA
24	K	1403	CLA	C1A-C2A-CAA-CBA
24	3	607	CLA	C1A-C2A-CAA-CBA
24	4	612	CLA	C1A-C2A-CAA-CBA
24	6	608	CLA	C1A-C2A-CAA-CBA
24	6	612	CLA	C1A-C2A-CAA-CBA
24	6	618	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	7	607	CLA	C1A-C2A-CAA-CBA
24	7	615	CLA	C1A-C2A-CAA-CBA
24	8	608	CLA	C1A-C2A-CAA-CBA
24	2	608	CLA	C1A-C2A-CAA-CBA
24	2	609	CLA	C1A-C2A-CAA-CBA
27	A	4005	BCR	C16-C17-C18-C19
27	B	4003	BCR	C11-C10-C9-C8
27	B	4003	BCR	C20-C21-C22-C23
27	F	4001	BCR	C12-C13-C14-C15
40	6	501	LUT	C32-C33-C34-C35
51	8	806	P5S	C39-C40-C41-C42
24	1	611	CLA	C6-C7-C8-C9
24	G	1603	CLA	CAA-CBA-CGA-O1A
34	B	5007	LAP	C1-C2-C3-C4
28	5	801	LHG	C9-C10-C11-C12
24	A	1114	CLA	C10-C11-C12-C13
24	A	1117	CLA	C2B-C3B-CAB-CBB
24	A	1124	CLA	C2B-C3B-CAB-CBB
24	A	1129	CLA	C2B-C3B-CAB-CBB
24	A	1130	CLA	C2B-C3B-CAB-CBB
24	A	1131	CLA	C2B-C3B-CAB-CBB
24	A	1134	CLA	C2B-C3B-CAB-CBB
24	A	1136	CLA	C2B-C3B-CAB-CBB
24	A	1138	CLA	C2B-C3B-CAB-CBB
24	B	1023	CLA	C2B-C3B-CAB-CBB
24	B	1218	CLA	C2B-C3B-CAB-CBB
24	B	1223	CLA	C2B-C3B-CAB-CBB
24	B	1224	CLA	C2B-C3B-CAB-CBB
24	B	1232	CLA	C2B-C3B-CAB-CBB
24	B	1239	CLA	C2B-C3B-CAB-CBB
24	G	1601	CLA	C2B-C3B-CAB-CBB
24	1	603	CLA	C2B-C3B-CAB-CBB
24	1	608	CLA	C2B-C3B-CAB-CBB
24	1	615	CLA	C2B-C3B-CAB-CBB
24	a	607	CLA	C2B-C3B-CAB-CBB
24	a	611	CLA	C2B-C3B-CAB-CBB
24	a	615	CLA	C2B-C3B-CAB-CBB
24	3	605	CLA	C2B-C3B-CAB-CBB
24	3	606	CLA	C2B-C3B-CAB-CBB
24	3	607	CLA	C2B-C3B-CAB-CBB
24	5	602	CLA	C2B-C3B-CAB-CBB
24	5	603	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	5	605	CLA	C2B-C3B-CAB-CBB
24	5	608	CLA	C2B-C3B-CAB-CBB
24	6	605	CLA	C2B-C3B-CAB-CBB
24	6	608	CLA	C2B-C3B-CAB-CBB
24	6	612	CLA	C2B-C3B-CAB-CBB
24	6	615	CLA	C2B-C3B-CAB-CBB
24	7	601	CLA	C2B-C3B-CAB-CBB
24	7	608	CLA	C2B-C3B-CAB-CBB
24	7	609	CLA	C2B-C3B-CAB-CBB
24	8	603	CLA	C2B-C3B-CAB-CBB
24	2	603	CLA	C2B-C3B-CAB-CBB
24	2	608	CLA	C2B-C3B-CAB-CBB
24	2	613	CLA	C2B-C3B-CAB-CBB
24	2	615	CLA	C2B-C3B-CAB-CBB
24	9	607	CLA	C2B-C3B-CAB-CBB
24	9	608	CLA	C2B-C3B-CAB-CBB
24	9	609	CLA	C2B-C3B-CAB-CBB
27	A	4003	BCR	C5-C6-C7-C8
27	B	4001	BCR	C1-C6-C7-C8
27	B	4007	BCR	C1-C6-C7-C8
27	B	4007	BCR	C23-C24-C25-C30
27	F	4001	BCR	C5-C6-C7-C8
27	L	4003	BCR	C23-C24-C25-C26
27	7	503	BCR	C23-C24-C25-C26
37	J	4002	RRX	C23-C24-C25-C26
40	4	502	LUT	C1-C6-C7-C8
40	5	502	LUT	C1-C6-C7-C8
40	6	502	LUT	C5-C6-C7-C8
40	8	501	LUT	C1-C6-C7-C8
49	7	504	C7Z	C5-C6-C7-C8
28	2	802	LHG	C15-C16-C17-C18
24	1	602	CLA	CAA-CBA-CGA-O2A
42	8	809	OLA	O2-C1-C2-C3
28	3	801	LHG	C2-C3-O3-P
24	A	1112	CLA	C4-C3-C5-C6
24	A	1128	CLA	C4-C3-C5-C6
24	B	1202	CLA	C4-C3-C5-C6
35	H	5001	SQD	C13-C14-C15-C16
24	1	611	CLA	C2-C3-C5-C6
24	9	601	CLA	C2-C3-C5-C6
28	1	802	LHG	O10-C23-C24-C25
41	3	611	CHL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
50	8	808	4RF	C48-C49-C50-C51
24	G	1603	CLA	CAA-CBA-CGA-O2A
24	A	1102	CLA	C10-C11-C12-C13
24	A	1104	CLA	C11-C10-C8-C7
24	A	1105	CLA	C11-C10-C8-C7
24	A	1123	CLA	C11-C10-C8-C7
24	A	1125	CLA	C12-C13-C15-C16
24	B	1224	CLA	C11-C10-C8-C7
24	B	1226	CLA	C6-C7-C8-C10
24	B	1237	CLA	C12-C13-C15-C16
24	L	1502	CLA	C11-C10-C8-C7
24	1	601	CLA	C11-C10-C8-C7
24	1	606	CLA	C11-C10-C8-C7
24	3	610	CLA	C6-C7-C8-C10
24	4	604	CLA	C6-C7-C8-C10
24	7	603	CLA	C11-C12-C13-C15
24	7	607	CLA	C11-C10-C8-C7
24	8	606	CLA	C6-C7-C8-C10
24	9	605	CLA	C11-C10-C8-C7
24	A	1109	CLA	C2A-CAA-CBA-CGA
24	3	601	CLA	C2A-CAA-CBA-CGA
24	6	605	CLA	C2A-CAA-CBA-CGA
28	a	801	LHG	C29-C30-C31-C32
50	8	807	4RF	C33-C34-C35-C36
28	9	802	LHG	C35-C36-C37-C38
24	A	1118	CLA	C6-C7-C8-C10
24	B	1220	CLA	C11-C12-C13-C14
24	B	1216	CLA	C12-C13-C15-C16
24	4	611	CLA	C11-C10-C8-C7
41	8	604	CHL	C12-C13-C15-C16
24	B	1208	CLA	O1A-CGA-O2A-C1
24	8	605	CLA	CAA-CBA-CGA-O2A
24	A	1138	CLA	C4-C3-C5-C6
24	1	606	CLA	C4-C3-C5-C6
24	A	1138	CLA	CAA-CBA-CGA-O2A
24	A	1117	CLA	C2-C3-C5-C6
24	7	603	CLA	C2-C3-C5-C6
24	7	606	CLA	C2-C3-C5-C6
24	8	610	CLA	C2-C3-C5-C6
24	a	604	CLA	C5-C6-C7-C8
24	L	1503	CLA	CAA-CBA-CGA-O2A
40	1	501	LUT	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
24	B	1225	CLA	C16-C17-C18-C19
24	K	1402	CLA	C11-C12-C13-C14
41	1	613	CHL	C2-C1-O2A-CGA
38	a	804	LPX	C6-C7-C8-C9
28	B	5001	LHG	C27-C28-C29-C30
29	8	802	DGD	C3B-C4B-C5B-C6B
24	B	1238	CLA	C2A-CAA-CBA-CGA
24	A	1141	CLA	CAA-CBA-CGA-O2A
25	A	2001	PQN	C19-C18-C20-C21
24	8	618	CLA	C10-C11-C12-C13
45	6	804	PLM	CA-CB-CC-CD
40	5	502	LUT	C9-C10-C11-C12
31	B	5006	LMT	O5B-C5B-C6B-O6B
24	B	1203	CLA	C4-C3-C5-C6
24	a	601	CLA	C4-C3-C5-C6
24	3	607	CLA	C4-C3-C5-C6
24	4	615	CLA	C4-C3-C5-C6
24	6	609	CLA	C4-C3-C5-C6
28	B	5001	LHG	C2-C3-O3-P
33	9	803	PTY	C6-C5-O14-P1
24	B	1216	CLA	C2-C3-C5-C6
24	1	603	CLA	C2-C3-C5-C6
24	4	615	CLA	C2-C3-C5-C6
28	9	801	LHG	C10-C11-C12-C13
28	9	801	LHG	O10-C23-O8-C6
24	A	1012	CLA	C15-C16-C17-C18
28	4	801	LHG	C27-C28-C29-C30
24	9	608	CLA	CAA-CBA-CGA-O2A
24	A	1125	CLA	C8-C10-C11-C12
33	9	803	PTY	C39-C40-C41-C42
35	7	805	SQD	C14-C15-C16-C17
50	8	807	4RF	C08-C09-C10-C11
50	8	808	4RF	C19-C20-C39-O40
50	8	807	4RF	C24-C25-C26-C27
28	2	801	LHG	C35-C36-C37-C38
24	1	602	CLA	C2A-CAA-CBA-CGA
41	5	610	CHL	C2A-CAA-CBA-CGA
24	1	601	CLA	C11-C12-C13-C15
41	a	613	CHL	CAA-CBA-CGA-O1A
41	a	613	CHL	CAA-CBA-CGA-O2A
46	5	803	DGA	CB2-CB3-CB4-CB5
28	B	5001	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
24	A	1130	CLA	C4-C3-C5-C6
24	a	603	CLA	C4-C3-C5-C6
24	4	603	CLA	C4-C3-C5-C6
24	4	607	CLA	C4-C3-C5-C6
24	8	609	CLA	C4-C3-C5-C6
29	A	5005	DGD	C6B-C7B-C8B-C9B
27	A	4004	BCR	C9-C10-C11-C12
24	A	1116	CLA	CAA-CBA-CGA-O1A
28	B	5002	LHG	O8-C23-C24-C25
24	3	607	CLA	C2-C3-C5-C6
28	B	5002	LHG	C16-C17-C18-C19
24	A	1116	CLA	C4B-C3B-CAB-CBB
24	A	1117	CLA	C4B-C3B-CAB-CBB
24	A	1138	CLA	C4B-C3B-CAB-CBB
24	G	1601	CLA	C4B-C3B-CAB-CBB
24	a	604	CLA	C4B-C3B-CAB-CBB
24	3	603	CLA	C4B-C3B-CAB-CBB
24	7	605	CLA	C4B-C3B-CAB-CBB
24	7	612	CLA	C4B-C3B-CAB-CBB
24	2	613	CLA	C4B-C3B-CAB-CBB
24	9	606	CLA	C4B-C3B-CAB-CBB
24	9	609	CLA	C4B-C3B-CAB-CBB
24	7	607	CLA	C2-C3-C5-C6
24	A	1111	CLA	CAA-CBA-CGA-O2A
24	a	608	CLA	CAA-CBA-CGA-O2A
31	1	804	LMT	C2-C3-C4-C5
33	3	802	PTY	C13-C14-C15-C16
24	1	610	CLA	CAA-CBA-CGA-O2A
24	6	604	CLA	C16-C17-C18-C19
35	H	5001	SQD	C16-C17-C18-C19
41	8	604	CHL	CHA-CBD-CGD-O1D
24	B	1021	CLA	CAA-CBA-CGA-O2A
24	2	609	CLA	CAA-CBA-CGA-O2A
24	L	1503	CLA	CAA-CBA-CGA-O1A
24	A	1118	CLA	C4-C3-C5-C6
28	7	803	LHG	O7-C5-C6-O8
24	8	605	CLA	CAA-CBA-CGA-O1A
24	A	1127	CLA	CAA-CBA-CGA-O1A
28	2	801	LHG	C2-C3-O3-P
32	6	803	PCW	C2-C1-O3P-P
28	B	5001	LHG	C35-C36-C37-C38
24	A	1122	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
24	3	606	CLA	C11-C12-C13-C15
24	B	1232	CLA	CAA-CBA-CGA-O2A
28	5	801	LHG	C29-C30-C31-C32
24	A	1111	CLA	C6-C7-C8-C9
24	A	1132	CLA	C6-C7-C8-C9
33	7	804	PTY	C14-C15-C16-C17
28	B	5002	LHG	C30-C31-C32-C33
29	A	5005	DGD	C2G-C3G-O3G-C1D
24	A	1126	CLA	CAA-CBA-CGA-O2A
24	G	1601	CLA	CAA-CBA-CGA-O1A
42	8	809	OLA	C9-C10-C11-C12
24	B	1208	CLA	C2-C1-O2A-CGA
24	B	1239	CLA	C2-C1-O2A-CGA
24	4	604	CLA	C2-C1-O2A-CGA
24	2	602	CLA	C2-C1-O2A-CGA
24	9	604	CLA	C2-C1-O2A-CGA
31	B	5006	LMT	C9-C10-C11-C12
33	7	804	PTY	C13-C14-C15-C16
24	B	1021	CLA	C3A-C2A-CAA-CBA
24	6	615	CLA	C3A-C2A-CAA-CBA
24	2	612	CLA	C3A-C2A-CAA-CBA
24	9	607	CLA	C3A-C2A-CAA-CBA
24	A	1141	CLA	CAA-CBA-CGA-O1A
24	9	608	CLA	CAA-CBA-CGA-O1A
24	A	1103	CLA	CAA-CBA-CGA-O1A
24	1	610	CLA	CAA-CBA-CGA-O1A
27	I	4001	BCR	C10-C11-C12-C13
42	8	809	OLA	C12-C13-C14-C15
28	B	5002	LHG	C35-C36-C37-C38
24	4	602	CLA	C2A-CAA-CBA-CGA
31	1	804	LMT	C6-C7-C8-C9
24	1	611	CLA	C3-C5-C6-C7
50	8	808	4RF	C41-C43-C44-C45
24	B	1232	CLA	CAA-CBA-CGA-O1A
35	7	805	SQD	O49-C7-O47-C45
28	8	801	LHG	C2-C3-O3-P
28	2	802	LHG	C2-C3-O3-P
28	9	801	LHG	O6-C4-C5-O7
24	A	1106	CLA	C5-C6-C7-C8
29	B	5003	DGD	C5A-C6A-C7A-C8A
38	a	804	LPX	C12-C13-C14-C15
28	7	803	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
24	A	1127	CLA	C10-C11-C12-C13
24	1	607	CLA	C8-C10-C11-C12
42	1	803	OLA	C14-C15-C16-C17
28	7	802	LHG	C27-C28-C29-C30
24	B	1212	CLA	C4-C3-C5-C6
24	A	1130	CLA	C2A-CAA-CBA-CGA
24	6	615	CLA	C2A-CAA-CBA-CGA
41	7	613	CHL	C2A-CAA-CBA-CGA
27	K	4002	BCR	C19-C20-C21-C22
27	6	504	BCR	C19-C20-C21-C22
24	B	1221	CLA	C16-C17-C18-C20
24	7	601	CLA	C11-C12-C13-C14
31	A	5008	LMT	C3-C4-C5-C6
24	B	1218	CLA	O1D-CGD-O2D-CED
28	2	802	LHG	O7-C5-C6-O8
24	A	1123	CLA	C6-C7-C8-C9
24	A	1125	CLA	C11-C10-C8-C9
24	A	1136	CLA	C14-C13-C15-C16
24	B	1210	CLA	C11-C12-C13-C14
24	B	1220	CLA	C6-C7-C8-C9
24	3	603	CLA	C11-C12-C13-C14
24	3	605	CLA	C6-C7-C8-C9
41	5	610	CHL	C14-C13-C15-C16
36	G	5002	ERG	C22-C23-C24-C28
24	A	1121	CLA	CAA-CBA-CGA-O2A
28	2	801	LHG	C19-C20-C21-C22
28	6	801	LHG	O6-C4-C5-C6
28	9	801	LHG	O6-C4-C5-C6
34	F	5003	LAP	C11-C10-C9-C8
40	5	505	LUT	C27-C28-C29-C30
28	3	801	LHG	C17-C18-C19-C20
35	G	5001	SQD	C11-C12-C13-C14
24	5	603	CLA	CAA-CBA-CGA-O2A
28	2	802	LHG	O7-C7-C8-C9
33	B	5005	PTY	C12-C11-C8-O7
41	5	611	CHL	CAA-CBA-CGA-O2A
24	1	606	CLA	C2-C3-C5-C6
24	A	1101	CLA	C6-C7-C8-C10
24	A	1111	CLA	C6-C7-C8-C10
24	B	1021	CLA	C12-C13-C15-C16
24	B	1209	CLA	C6-C7-C8-C10
25	A	2001	PQN	C17-C18-C20-C21

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Mol	Chain	Res	Type	Atoms
24	B	1221	CLA	C3-C5-C6-C7
24	A	1110	CLA	C2B-C3B-CAB-CBB
24	A	1112	CLA	C2B-C3B-CAB-CBB
24	A	1116	CLA	C2B-C3B-CAB-CBB
24	A	1119	CLA	C2B-C3B-CAB-CBB
24	A	1121	CLA	C2B-C3B-CAB-CBB
24	A	1126	CLA	C2B-C3B-CAB-CBB
24	A	1132	CLA	C2B-C3B-CAB-CBB
24	A	1141	CLA	C2B-C3B-CAB-CBB
24	B	1204	CLA	C2B-C3B-CAB-CBB
24	B	1212	CLA	C2B-C3B-CAB-CBB
24	B	1235	CLA	C2B-C3B-CAB-CBB
24	L	1501	CLA	C2B-C3B-CAB-CBB
24	1	612	CLA	C2B-C3B-CAB-CBB
24	a	604	CLA	C2B-C3B-CAB-CBB
24	a	612	CLA	C2B-C3B-CAB-CBB
24	4	612	CLA	C2B-C3B-CAB-CBB
24	5	601	CLA	C2B-C3B-CAB-CBB
24	5	609	CLA	C2B-C3B-CAB-CBB
24	6	601	CLA	C2B-C3B-CAB-CBB
24	6	602	CLA	C2B-C3B-CAB-CBB
24	6	604	CLA	C2B-C3B-CAB-CBB
24	6	606	CLA	C2B-C3B-CAB-CBB
24	6	607	CLA	C2B-C3B-CAB-CBB
24	7	604	CLA	C2B-C3B-CAB-CBB
24	7	605	CLA	C2B-C3B-CAB-CBB
24	7	606	CLA	C2B-C3B-CAB-CBB
24	7	615	CLA	C2B-C3B-CAB-CBB
24	8	606	CLA	C2B-C3B-CAB-CBB
24	8	607	CLA	C2B-C3B-CAB-CBB
24	8	611	CLA	C2B-C3B-CAB-CBB
24	8	612	CLA	C2B-C3B-CAB-CBB
24	9	602	CLA	C2B-C3B-CAB-CBB
24	9	605	CLA	C2B-C3B-CAB-CBB
27	B	4001	BCR	C5-C6-C7-C8
27	B	4007	BCR	C5-C6-C7-C8
27	G	4001	BCR	C1-C6-C7-C8
27	G	4001	BCR	C5-C6-C7-C8
27	G	4001	BCR	C23-C24-C25-C26
40	3	501	LUT	C1-C6-C7-C8
40	3	501	LUT	C5-C6-C7-C8
40	4	502	LUT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
40	5	502	LUT	C5-C6-C7-C8
40	7	501	LUT	C1-C6-C7-C8
40	7	501	LUT	C5-C6-C7-C8
40	8	501	LUT	C5-C6-C7-C8
40	9	502	LUT	C1-C6-C7-C8
40	9	502	LUT	C5-C6-C7-C8
31	B	5006	LMT	C7-C8-C9-C10
50	8	808	4RF	C03-C04-C05-C06
24	B	1210	CLA	C2-C1-O2A-CGA
24	1	603	CLA	C2-C1-O2A-CGA
24	a	607	CLA	C2-C1-O2A-CGA
24	4	608	CLA	C2-C1-O2A-CGA
24	5	604	CLA	C2-C1-O2A-CGA
24	6	604	CLA	C2-C1-O2A-CGA
24	7	604	CLA	C2-C1-O2A-CGA
24	2	621	CLA	C2-C1-O2A-CGA
24	A	1111	CLA	C13-C15-C16-C17
28	a	801	LHG	C9-C10-C11-C12
24	1	601	CLA	C10-C11-C12-C13
28	F	5002	LHG	C10-C11-C12-C13
28	1	802	LHG	C16-C17-C18-C19
24	6	604	CLA	C16-C17-C18-C20
24	7	615	CLA	C3-C5-C6-C7
24	B	1210	CLA	CAA-CBA-CGA-O2A
24	7	607	CLA	CAA-CBA-CGA-O2A
24	B	1202	CLA	C2-C3-C5-C6
24	5	612	CLA	C2-C3-C5-C6
45	6	804	PLM	O2-C1-C2-C3
24	A	1137	CLA	C2A-CAA-CBA-CGA
24	B	1210	CLA	C2A-CAA-CBA-CGA
24	4	603	CLA	C2A-CAA-CBA-CGA
35	7	805	SQD	C8-C7-O47-C45
24	B	1222	CLA	C10-C11-C12-C13
24	B	1239	CLA	C8-C10-C11-C12
24	6	609	CLA	CAA-CBA-CGA-O2A
30	A	5007	3PH	O21-C21-C22-C23
35	7	805	SQD	O47-C7-C8-C9
24	A	1108	CLA	C5-C6-C7-C8
28	A	5002	LHG	C35-C36-C37-C38
24	B	1227	CLA	CAA-CBA-CGA-O2A
24	B	1238	CLA	CAA-CBA-CGA-O2A
24	3	616	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	8	612	CLA	CAA-CBA-CGA-O2A
24	2	606	CLA	CAA-CBA-CGA-O2A
28	5	801	LHG	O7-C7-C8-C9
28	6	801	LHG	O8-C23-C24-C25
24	1	611	CLA	C6-C7-C8-C10
24	a	607	CLA	C4-C3-C5-C6
28	9	802	LHG	C11-C10-C9-C8
24	A	1131	CLA	CAA-CBA-CGA-O2A
24	a	607	CLA	CAA-CBA-CGA-O2A
24	3	601	CLA	CAA-CBA-CGA-O2A
24	3	607	CLA	CAA-CBA-CGA-O2A
41	3	611	CHL	CAA-CBA-CGA-O2A
24	A	1128	CLA	C2-C3-C5-C6
24	4	617	CLA	CAA-CBA-CGA-O2A
24	a	608	CLA	O1A-CGA-O2A-C1
24	1	604	CLA	C2A-CAA-CBA-CGA
28	7	801	LHG	C9-C10-C11-C12
42	1	803	OLA	C12-C13-C14-C15
24	K	1402	CLA	CAA-CBA-CGA-O2A
24	2	610	CLA	CAA-CBA-CGA-O2A
30	A	5007	3PH	C28-C29-C2A-C2B
28	5	801	LHG	C16-C17-C18-C19
24	G	1602	CLA	CBA-CGA-O2A-C1
24	1	611	CLA	C5-C6-C7-C8
24	4	610	CLA	C5-C6-C7-C8
28	1	802	LHG	C24-C25-C26-C27
24	A	1104	CLA	C11-C10-C8-C9
24	A	1105	CLA	C11-C10-C8-C9
24	A	1134	CLA	C6-C7-C8-C9
24	B	1203	CLA	C11-C10-C8-C9
24	1	601	CLA	C11-C10-C8-C9
24	9	605	CLA	C11-C10-C8-C9
24	B	1208	CLA	CAA-CBA-CGA-O2A
24	5	602	CLA	CAA-CBA-CGA-O2A
24	5	612	CLA	CAA-CBA-CGA-O2A
24	6	603	CLA	CAA-CBA-CGA-O2A
24	7	606	CLA	CAA-CBA-CGA-O2A
24	7	617	CLA	CAA-CBA-CGA-O2A
24	2	601	CLA	CAA-CBA-CGA-O2A
24	2	603	CLA	CAA-CBA-CGA-O2A
24	9	607	CLA	CAA-CBA-CGA-O2A
41	7	613	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	B	1220	CLA	C11-C12-C13-C15
24	1	601	CLA	C11-C12-C13-C14
24	A	1126	CLA	C5-C6-C7-C8
24	A	1134	CLA	C5-C6-C7-C8
24	9	612	CLA	C13-C15-C16-C17
24	A	1110	CLA	C4B-C3B-CAB-CBB
24	A	1140	CLA	C1A-C2A-CAA-CBA
24	B	1227	CLA	C1A-C2A-CAA-CBA
24	B	1235	CLA	C1A-C2A-CAA-CBA
24	a	603	CLA	C1A-C2A-CAA-CBA
24	3	610	CLA	C4B-C3B-CAB-CBB
24	6	601	CLA	C4B-C3B-CAB-CBB
24	6	604	CLA	C4B-C3B-CAB-CBB
24	6	606	CLA	C4B-C3B-CAB-CBB
24	6	615	CLA	C1A-C2A-CAA-CBA
24	6	617	CLA	C4B-C3B-CAB-CBB
24	7	604	CLA	C4B-C3B-CAB-CBB
24	7	611	CLA	C1A-C2A-CAA-CBA
24	8	606	CLA	C4B-C3B-CAB-CBB
24	8	609	CLA	C4B-C3B-CAB-CBB
24	9	602	CLA	C4B-C3B-CAB-CBB
24	A	1104	CLA	CAA-CBA-CGA-O2A
24	B	1211	CLA	CAA-CBA-CGA-O2A
24	a	603	CLA	CAA-CBA-CGA-O2A
24	8	603	CLA	CAA-CBA-CGA-O2A
24	8	609	CLA	CAA-CBA-CGA-O2A
24	2	602	CLA	CAA-CBA-CGA-O2A
28	2	801	LHG	O8-C23-C24-C25
24	A	1112	CLA	C2-C3-C5-C6
24	3	610	CLA	C2-C3-C5-C6
27	5	504	BCR	C7-C8-C9-C10
40	6	502	LUT	C33-C34-C35-C15
41	6	610	CHL	CAA-CBA-CGA-O1A
24	A	1137	CLA	CAA-CBA-CGA-O2A
24	L	1502	CLA	CAA-CBA-CGA-O2A
24	4	603	CLA	CAA-CBA-CGA-O2A
24	4	615	CLA	CAA-CBA-CGA-O2A
24	6	615	CLA	CAA-CBA-CGA-O2A
24	7	612	CLA	CAA-CBA-CGA-O2A
28	1	801	LHG	O8-C23-C24-C25
28	7	803	LHG	O7-C7-C8-C9
41	8	604	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
46	5	803	DGA	OG2-CB1-CB2-CB3
29	B	5003	DGD	C2A-C3A-C4A-C5A
28	B	5002	LHG	C12-C13-C14-C15
24	K	1402	CLA	C11-C12-C13-C15
28	4	802	LHG	O6-C4-C5-C6
24	8	610	CLA	CAA-CBA-CGA-O2A
28	5	801	LHG	O8-C23-C24-C25
46	8	803	DGA	OG2-CB1-CB2-CB3
46	5	803	DGA	CA5-CA6-CA7-CA8
28	7	802	LHG	C9-C10-C11-C12
24	5	603	CLA	C5-C6-C7-C8
24	5	612	CLA	C4-C3-C5-C6
42	8	809	OLA	C7-C8-C9-C10
24	1	606	CLA	C2-C1-O2A-CGA
41	6	611	CHL	C2-C1-O2A-CGA
24	A	1103	CLA	C11-C12-C13-C15
24	A	1106	CLA	C11-C10-C8-C7
24	B	1208	CLA	C6-C7-C8-C10
24	1	604	CLA	C11-C10-C8-C7
24	2	615	CLA	C6-C7-C8-C10
24	B	1239	CLA	C16-C17-C18-C20
25	A	2001	PQN	C15-C16-C17-C18
24	A	1112	CLA	CAA-CBA-CGA-O2A
24	B	1209	CLA	CAA-CBA-CGA-O2A
28	8	801	LHG	O8-C23-C24-C25
24	H	1703	CLA	C2A-CAA-CBA-CGA
24	a	612	CLA	C2A-CAA-CBA-CGA
24	8	602	CLA	C2A-CAA-CBA-CGA
24	9	603	CLA	C8-C10-C11-C12
33	3	802	PTY	O4-C30-C31-C32
33	9	803	PTY	O4-C30-C31-C32
28	9	801	LHG	C2-C3-O3-P
33	8	891	PTY	C34-C35-C36-C37
24	A	1140	CLA	C3A-C2A-CAA-CBA
24	B	1201	CLA	C3A-C2A-CAA-CBA
24	7	606	CLA	C3A-C2A-CAA-CBA
24	2	601	CLA	C3A-C2A-CAA-CBA
24	2	603	CLA	C3A-C2A-CAA-CBA
41	a	610	CHL	C3A-C2A-CAA-CBA
41	6	613	CHL	C3A-C2A-CAA-CBA
41	8	601	CHL	C3A-C2A-CAA-CBA
24	5	603	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
24	A	1140	CLA	CAA-CBA-CGA-O2A
32	6	803	PCW	O3-C11-C12-C13
24	4	617	CLA	CAA-CBA-CGA-O1A
34	F	5003	LAP	C14-C13-O1-C1
31	2	804	LMT	C3-C4-C5-C6
33	5	802	PTY	C14-C15-C16-C17
24	B	1238	CLA	CAA-CBA-CGA-O1A
41	5	611	CHL	CAA-CBA-CGA-O1A
33	9	803	PTY	C16-C17-C18-C19
24	A	1103	CLA	CBA-CGA-O2A-C1
28	1	801	LHG	O7-C7-C8-C9
24	A	1121	CLA	CAA-CBA-CGA-O1A
24	B	1211	CLA	CAA-CBA-CGA-O1A
24	B	1227	CLA	CAA-CBA-CGA-O1A
45	6	804	PLM	O1-C1-C2-C3
24	A	1122	CLA	C6-C7-C8-C9
24	B	1212	CLA	C6-C7-C8-C9
24	B	1237	CLA	C14-C13-C15-C16
24	3	610	CLA	C11-C10-C8-C9
24	4	604	CLA	C6-C7-C8-C9
24	6	609	CLA	C11-C10-C8-C9
24	7	607	CLA	C11-C10-C8-C9
34	F	5003	LAP	O1-C13-C14-C15
24	A	1108	CLA	CAA-CBA-CGA-O2A
24	A	1115	CLA	CAA-CBA-CGA-O2A
24	1	603	CLA	CAA-CBA-CGA-O2A
24	2	604	CLA	CAA-CBA-CGA-O1A
24	B	1240	CLA	C8-C10-C11-C12
24	2	603	CLA	C10-C11-C12-C13
24	A	1112	CLA	CAA-CBA-CGA-O1A
24	B	1208	CLA	CAA-CBA-CGA-O1A
24	5	602	CLA	CAA-CBA-CGA-O1A
24	6	609	CLA	CAA-CBA-CGA-O1A
24	7	617	CLA	CAA-CBA-CGA-O1A
24	8	612	CLA	CAA-CBA-CGA-O1A
24	A	1105	CLA	CBA-CGA-O2A-C1
24	1	612	CLA	CAA-CBA-CGA-O2A
24	2	615	CLA	CAA-CBA-CGA-O2A
24	5	609	CLA	C4-C3-C5-C6
40	8	501	LUT	C21-C26-C27-C28
24	A	1103	CLA	O1A-CGA-O2A-C1
24	A	1137	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
24	3	616	CLA	CAA-CBA-CGA-O1A
24	4	615	CLA	CAA-CBA-CGA-O1A
24	6	603	CLA	CAA-CBA-CGA-O1A
24	8	609	CLA	CAA-CBA-CGA-O1A
28	6	801	LHG	O10-C23-C24-C25
28	7	803	LHG	O9-C7-C8-C9
41	7	613	CHL	CAA-CBA-CGA-O1A
33	B	5005	PTY	C15-C16-C17-C18
28	A	5002	LHG	C24-C25-C26-C27
24	A	1105	CLA	O1A-CGA-O2A-C1
24	A	1128	CLA	CAA-CBA-CGA-O2A
24	A	1130	CLA	CAA-CBA-CGA-O2A
34	F	5003	LAP	O1-C1-C2-C3
24	4	610	CLA	C16-C17-C18-C20
24	6	617	CLA	CAA-CBA-CGA-O2A
42	1	803	OLA	O2-C1-C2-C3
24	9	608	CLA	CBD-CGD-O2D-CED
27	5	503	BCR	C17-C18-C19-C20
24	K	1402	CLA	CAA-CBA-CGA-O1A
24	3	607	CLA	CAA-CBA-CGA-O1A
28	5	801	LHG	O9-C7-C8-C9
28	2	801	LHG	O10-C23-C24-C25
24	L	1502	CLA	C5-C6-C7-C8
24	2	609	CLA	C5-C6-C7-C8
46	8	803	DGA	CB9-CAB-CBB-CCB
24	7	606	CLA	CAA-CBA-CGA-O1A
24	8	603	CLA	CAA-CBA-CGA-O1A
24	2	606	CLA	CAA-CBA-CGA-O1A
24	2	610	CLA	CAA-CBA-CGA-O1A
28	1	801	LHG	O10-C23-C24-C25
28	5	801	LHG	O10-C23-C24-C25
33	B	5005	PTY	C12-C11-C8-O10
35	7	805	SQD	O49-C7-C8-C9
24	A	1129	CLA	CAA-CBA-CGA-O2A
28	F	5001	LHG	O8-C23-C24-C25
28	7	803	LHG	O8-C23-C24-C25
28	8	801	LHG	O7-C7-C8-C9
41	1	613	CHL	C2A-CAA-CBA-CGA
28	8	801	LHG	C28-C29-C30-C31
35	G	5001	SQD	C30-C31-C32-C33
28	2	802	LHG	C4-C5-C6-O8
24	A	1104	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
24	A	1131	CLA	CAA-CBA-CGA-O1A
24	5	612	CLA	CAA-CBA-CGA-O1A
28	2	802	LHG	O9-C7-C8-C9
41	8	604	CHL	CAA-CBA-CGA-O1A
33	9	803	PTY	C30-C31-C32-C33
24	A	1123	CLA	C5-C6-C7-C8
24	B	1214	CLA	CAA-CBA-CGA-O2A
24	3	603	CLA	CAA-CBA-CGA-O2A
24	5	609	CLA	CAA-CBA-CGA-O2A
24	7	603	CLA	CAA-CBA-CGA-O2A
46	5	803	DGA	OB1-CB1-CB2-CB3
24	a	608	CLA	CBA-CGA-O2A-C1
50	8	808	4RF	C22-C24-C25-C26
24	3	604	CLA	CAD-CBD-CGD-O2D
24	4	604	CLA	CAD-CBD-CGD-O2D
24	6	617	CLA	CAD-CBD-CGD-O2D
24	F	1302	CLA	CAA-CBA-CGA-O2A
24	6	618	CLA	CAA-CBA-CGA-O2A
24	a	603	CLA	CAA-CBA-CGA-O1A
24	7	612	CLA	CAA-CBA-CGA-O1A
24	8	610	CLA	CAA-CBA-CGA-O1A
31	2	804	LMT	O1'-C1-C2-C3
24	3	603	CLA	C13-C15-C16-C17
24	A	1013	CLA	C2-C1-O2A-CGA
24	A	1102	CLA	C2-C1-O2A-CGA
24	A	1138	CLA	C2-C1-O2A-CGA
24	B	1204	CLA	C2-C1-O2A-CGA
24	5	601	CLA	C2-C1-O2A-CGA
24	B	1210	CLA	CAA-CBA-CGA-O1A
24	3	601	CLA	CAA-CBA-CGA-O1A
24	7	607	CLA	CAA-CBA-CGA-O1A
24	9	607	CLA	CAA-CBA-CGA-O1A
41	3	611	CHL	CAA-CBA-CGA-O1A
24	6	606	CLA	CAA-CBA-CGA-O2A
41	6	613	CHL	C1A-C2A-CAA-CBA
24	1	606	CLA	C3-C5-C6-C7
24	A	1115	CLA	C2A-CAA-CBA-CGA
24	B	1215	CLA	C2A-CAA-CBA-CGA
24	2	603	CLA	C2A-CAA-CBA-CGA
31	2	804	LMT	C11-C10-C9-C8
24	B	1237	CLA	CAA-CBA-CGA-O1A
24	a	607	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
24	2	602	CLA	CAA-CBA-CGA-O1A
34	F	5003	LAP	O2-C1-C2-C3
46	8	803	DGA	OB1-CB1-CB2-CB3
24	8	618	CLA	CAA-CBA-CGA-O2A
24	8	620	CLA	CAA-CBA-CGA-O2A
41	9	610	CHL	CAA-CBA-CGA-O2A
24	B	1218	CLA	CBD-CGD-O2D-CED
24	B	1209	CLA	CAA-CBA-CGA-O1A
24	4	603	CLA	CAA-CBA-CGA-O1A
24	2	601	CLA	CAA-CBA-CGA-O1A
28	8	801	LHG	O10-C23-C24-C25
32	6	803	PCW	O11-C11-C12-C13
28	7	801	LHG	C35-C36-C37-C38
24	B	1204	CLA	CAA-CBA-CGA-O2A
24	9	601	CLA	CAA-CBA-CGA-O2A
41	4	618	CHL	CAA-CBA-CGA-O2A
32	6	803	PCW	C14-C15-C16-C17
33	9	803	PTY	C36-C37-C38-C39
24	1	612	CLA	CAA-CBA-CGA-O1A
24	6	615	CLA	CAA-CBA-CGA-O1A
24	2	603	CLA	CAA-CBA-CGA-O1A
24	2	615	CLA	CAA-CBA-CGA-O1A
33	9	803	PTY	O30-C30-C31-C32

There are no ring outliers.

341 monomers are involved in 915 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	4	801	LHG	3	0
27	5	504	BCR	4	0
29	B	5003	DGD	10	0
27	A	4001	BCR	5	0
28	7	801	LHG	4	0
24	8	620	CLA	1	0
24	B	1220	CLA	8	0
24	A	1130	CLA	2	0
41	4	609	CHL	6	0
40	1	503	LUT	3	0
38	J	5001	LPX	1	0
41	5	610	CHL	10	0
24	A	1124	CLA	3	0
24	B	1237	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	a	606	CHL	7	0
40	6	502	LUT	5	0
24	3	610	CLA	2	0
24	B	1208	CLA	1	0
24	6	617	CLA	1	0
24	L	1501	CLA	3	0
24	B	1240	CLA	5	0
24	A	1120	CLA	4	0
24	K	1404	CLA	2	0
24	1	607	CLA	2	0
27	6	503	BCR	1	0
24	1	605	CLA	4	0
24	9	606	CLA	2	0
24	A	1108	CLA	4	0
37	J	4002	RRX	6	0
24	5	605	CLA	1	0
41	3	611	CHL	4	0
24	H	1701	CLA	3	0
27	B	4001	BCR	5	0
24	A	1116	CLA	9	0
24	A	1111	CLA	5	0
24	A	1127	CLA	7	0
24	A	1104	CLA	3	0
27	3	504	BCR	3	0
24	5	602	CLA	1	0
24	5	606	CLA	2	0
24	4	603	CLA	3	0
34	F	5003	LAP	3	0
24	1	604	CLA	7	0
24	2	603	CLA	6	0
24	A	1106	CLA	5	0
23	A	1011	CL0	6	0
24	2	608	CLA	1	0
41	5	611	CHL	2	0
28	3	801	LHG	5	0
24	A	1122	CLA	6	0
24	7	604	CLA	6	0
40	7	501	LUT	3	0
24	A	1119	CLA	6	0
24	3	605	CLA	4	0
24	A	1103	CLA	6	0
24	B	1212	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	1	608	CLA	6	0
27	B	4002	BCR	4	0
24	a	607	CLA	3	0
24	A	1112	CLA	2	0
27	B	4007	BCR	2	0
24	9	608	CLA	1	0
35	G	5001	SQD	2	0
28	F	5002	LHG	2	0
24	8	611	CLA	1	0
24	7	612	CLA	6	0
24	9	612	CLA	7	0
41	4	618	CHL	3	0
28	9	802	LHG	3	0
24	A	1129	CLA	2	0
24	6	609	CLA	4	0
24	a	602	CLA	1	0
24	2	612	CLA	4	0
24	A	1140	CLA	2	0
40	6	501	LUT	7	0
24	A	1109	CLA	5	0
40	4	502	LUT	4	0
24	B	1206	CLA	1	0
24	2	601	CLA	4	0
26	C	3003	SF4	1	0
28	A	5001	LHG	3	0
27	4	503	BCR	1	0
24	B	1223	CLA	2	0
24	A	1105	CLA	1	0
40	a	503	LUT	3	0
52	9	504	A8S	1	0
24	1	610	CLA	1	0
24	8	615	CLA	1	0
27	J	4001	BCR	4	0
28	F	5001	LHG	3	0
24	2	605	CLA	2	0
41	9	610	CHL	2	0
28	A	5002	LHG	2	0
24	1	601	CLA	3	0
24	9	603	CLA	5	0
24	A	1135	CLA	5	0
24	7	615	CLA	1	0
29	A	5005	DGD	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	a	611	CLA	1	0
24	2	615	CLA	4	0
45	4	803	PLM	1	0
41	6	613	CHL	2	0
24	5	603	CLA	1	0
45	6	804	PLM	2	0
41	3	608	CHL	3	0
40	2	502	LUT	9	0
27	A	4004	BCR	6	0
24	a	612	CLA	6	0
24	A	1115	CLA	2	0
24	1	602	CLA	1	0
27	L	4001	BCR	5	0
50	7	807	4RF	1	0
24	A	1101	CLA	5	0
27	G	4001	BCR	3	0
27	5	503	BCR	2	0
24	3	603	CLA	6	0
50	8	807	4RF	1	0
28	A	5003	LHG	5	0
27	I	4001	BCR	6	0
24	B	1224	CLA	7	0
28	6	802	LHG	1	0
24	6	615	CLA	5	0
27	B	4006	BCR	8	0
46	8	803	DGA	2	0
24	A	1102	CLA	6	0
24	4	607	CLA	1	0
24	3	613	CLA	3	0
28	2	801	LHG	4	0
24	1	611	CLA	2	0
24	A	1132	CLA	3	0
24	a	601	CLA	4	0
27	B	4005	BCR	1	0
41	8	604	CHL	4	0
40	9	502	LUT	7	0
24	6	612	CLA	3	0
27	K	4002	BCR	1	0
41	8	613	CHL	3	0
24	B	1207	CLA	13	0
28	1	801	LHG	4	0
24	B	1234	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	9	604	CLA	4	0
40	3	501	LUT	6	0
24	B	1216	CLA	3	0
40	8	501	LUT	4	0
29	8	802	DGD	8	0
24	B	1022	CLA	4	0
31	B	5006	LMT	5	0
32	B	5004	PCW	2	0
24	4	611	CLA	5	0
28	9	801	LHG	3	0
24	B	1217	CLA	3	0
24	2	609	CLA	3	0
27	A	4003	BCR	5	0
24	B	1210	CLA	4	0
27	3	503	BCR	4	0
24	A	1012	CLA	4	0
27	K	4001	BCR	7	0
24	7	601	CLA	5	0
24	A	1117	CLA	11	0
24	8	612	CLA	2	0
24	A	1121	CLA	4	0
24	K	1403	CLA	1	0
27	L	4002	BCR	3	0
24	3	601	CLA	3	0
24	B	1213	CLA	1	0
35	7	805	SQD	1	0
24	B	1215	CLA	4	0
24	8	605	CLA	1	0
40	a	501	LUT	2	0
24	5	608	CLA	1	0
24	2	604	CLA	10	0
24	8	608	CLA	1	0
24	A	1136	CLA	6	0
24	7	605	CLA	2	0
24	G	1603	CLA	2	0
24	A	1110	CLA	3	0
27	L	4003	BCR	2	0
24	L	1502	CLA	2	0
24	6	603	CLA	3	0
24	7	608	CLA	5	0
33	B	5005	PTY	2	0
28	B	5002	LHG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1113	CLA	1	0
24	A	1133	CLA	9	0
24	B	1023	CLA	9	0
24	B	1230	CLA	2	0
33	8	891	PTY	2	0
27	A	4005	BCR	6	0
24	A	1114	CLA	3	0
24	G	1602	CLA	1	0
27	7	503	BCR	2	0
24	a	605	CLA	5	0
24	5	616	CLA	1	0
24	7	607	CLA	2	0
24	7	611	CLA	2	0
40	1	502	LUT	4	0
40	a	502	LUT	5	0
41	1	613	CHL	2	0
24	F	1302	CLA	3	0
27	6	504	BCR	3	0
24	6	604	CLA	3	0
27	B	4004	BCR	6	0
41	6	610	CHL	3	0
24	6	605	CLA	1	0
24	8	610	CLA	5	0
33	7	804	PTY	1	0
41	4	613	CHL	1	0
24	1	603	CLA	7	0
28	6	801	LHG	6	0
24	8	606	CLA	3	0
27	F	4001	BCR	7	0
27	H	4001	BCR	2	0
24	B	1218	CLA	2	0
24	A	1107	CLA	3	0
24	8	618	CLA	2	0
24	6	602	CLA	3	0
28	1	802	LHG	2	0
24	5	607	CLA	1	0
24	K	1401	CLA	4	0
24	1	615	CLA	2	0
24	3	607	CLA	2	0
28	5	801	LHG	1	0
24	8	607	CLA	2	0
24	1	612	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	K	5001	LAP	2	0
24	B	1236	CLA	2	0
24	3	616	CLA	5	0
24	A	1134	CLA	3	0
24	8	602	CLA	1	0
24	B	1227	CLA	3	0
24	B	1226	CLA	3	0
24	B	1204	CLA	7	0
24	B	1211	CLA	1	0
24	6	601	CLA	9	0
24	4	601	CLA	7	0
24	7	617	CLA	4	0
24	B	1238	CLA	3	0
41	a	609	CHL	3	0
24	8	609	CLA	5	0
24	2	621	CLA	4	0
46	5	803	DGA	1	0
28	a	801	LHG	2	0
24	A	1137	CLA	4	0
24	A	1128	CLA	6	0
24	B	1202	CLA	7	0
24	B	1219	CLA	3	0
41	6	611	CHL	2	0
24	B	1021	CLA	5	0
24	7	609	CLA	3	0
24	a	604	CLA	3	0
41	7	613	CHL	4	0
24	5	617	CLA	4	0
24	9	609	CLA	1	0
24	4	610	CLA	3	0
24	H	1703	CLA	3	0
24	4	608	CLA	1	0
24	4	615	CLA	2	0
24	5	612	CLA	6	0
47	6	806	SPH	1	0
27	A	4002	BCR	4	0
24	A	1118	CLA	4	0
41	1	609	CHL	6	0
24	1	606	CLA	2	0
24	9	601	CLA	5	0
27	B	4003	BCR	4	0
40	5	502	LUT	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	3	502	LUT	4	0
24	J	1901	CLA	1	0
24	A	1138	CLA	3	0
40	8	502	LUT	11	0
41	5	613	CHL	1	0
24	8	603	CLA	2	0
32	6	803	PCW	2	0
24	A	1131	CLA	4	0
24	A	1126	CLA	12	0
40	2	501	LUT	4	0
25	B	2002	PQN	7	0
40	4	501	LUT	9	0
24	B	1225	CLA	7	0
25	A	2001	PQN	5	0
31	2	804	LMT	1	0
24	B	1209	CLA	5	0
24	B	1228	CLA	6	0
24	B	1229	CLA	4	0
24	5	601	CLA	5	0
50	8	808	4RF	2	0
24	5	604	CLA	1	0
24	3	604	CLA	2	0
40	5	505	LUT	8	0
24	A	1141	CLA	2	0
24	A	1123	CLA	6	0
24	6	618	CLA	2	0
24	B	1214	CLA	6	0
31	A	5008	LMT	3	0
35	H	5001	SQD	6	0
24	a	603	CLA	2	0
24	4	605	CLA	1	0
41	8	601	CHL	5	0
39	M	4001	ECH	4	0
28	2	802	LHG	2	0
33	5	802	PTY	3	0
24	B	1231	CLA	6	0
24	B	1222	CLA	5	0
40	9	501	LUT	4	0
24	7	610	CLA	1	0
41	6	619	CHL	2	0
24	A	1139	CLA	3	0
24	4	604	CLA	5	0

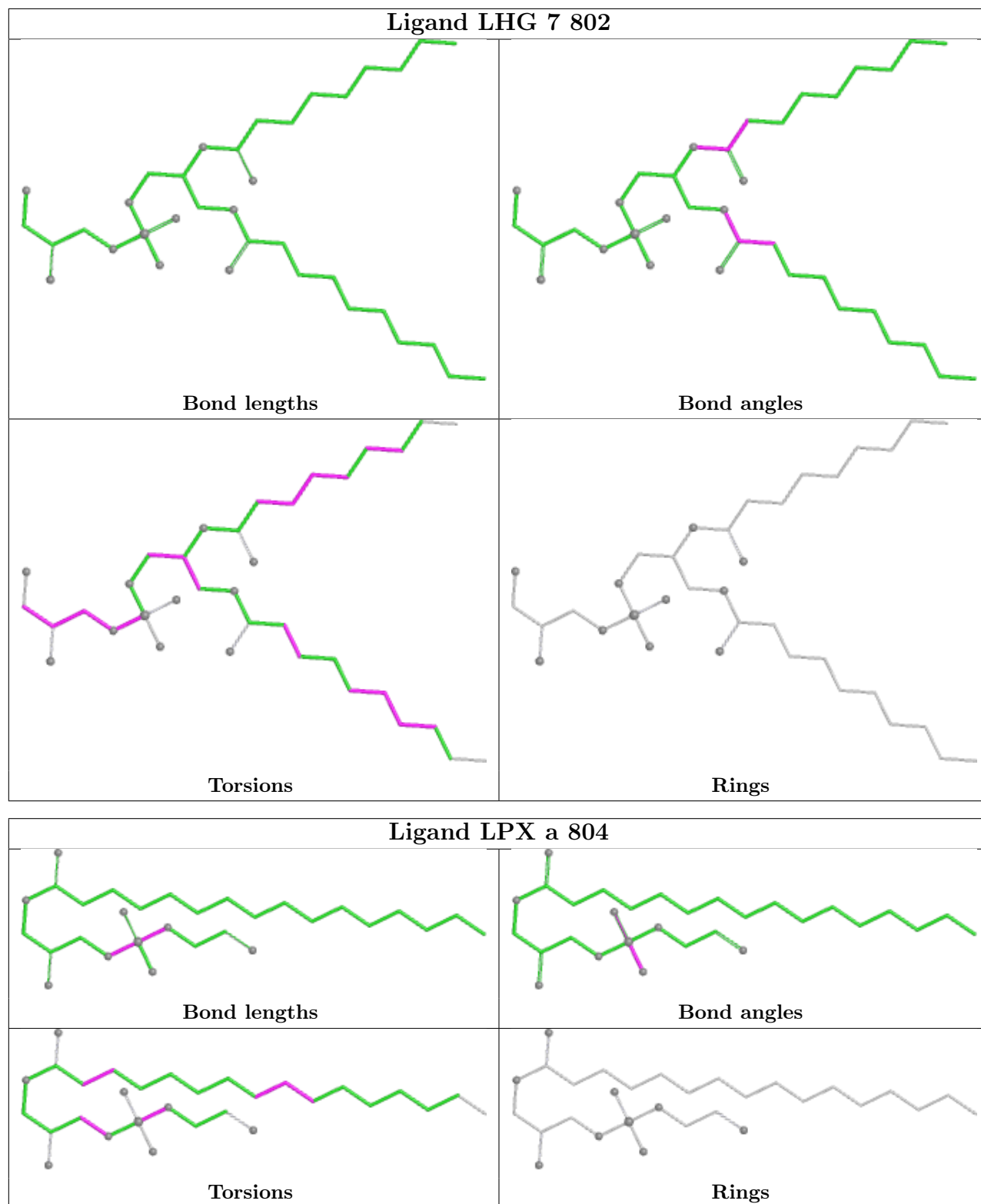
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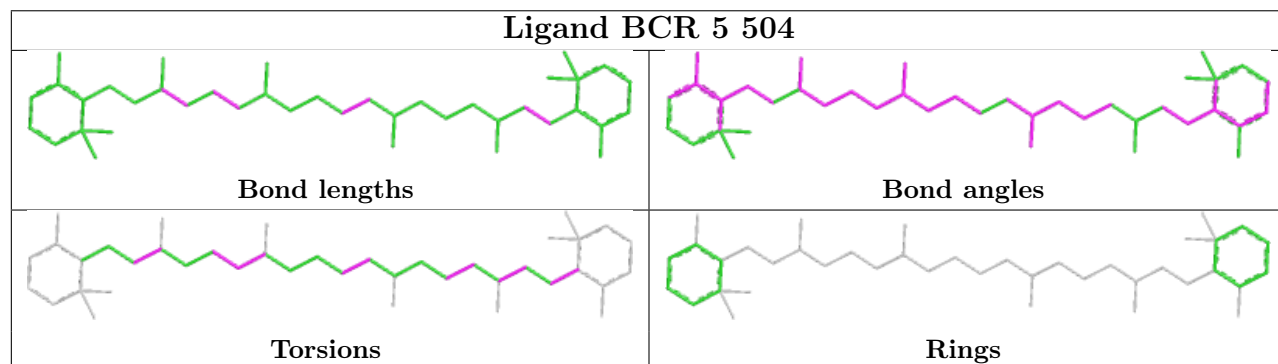
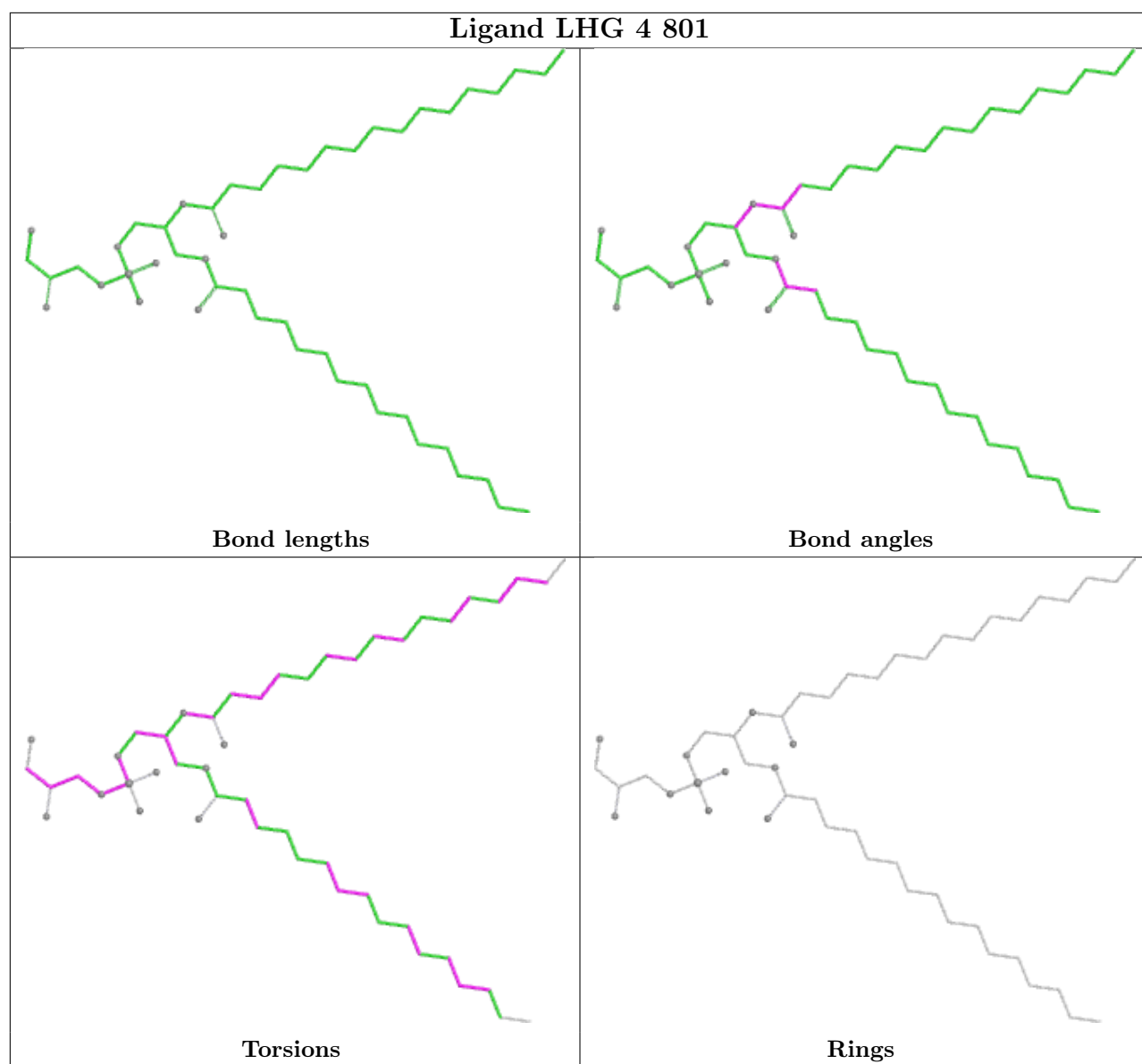
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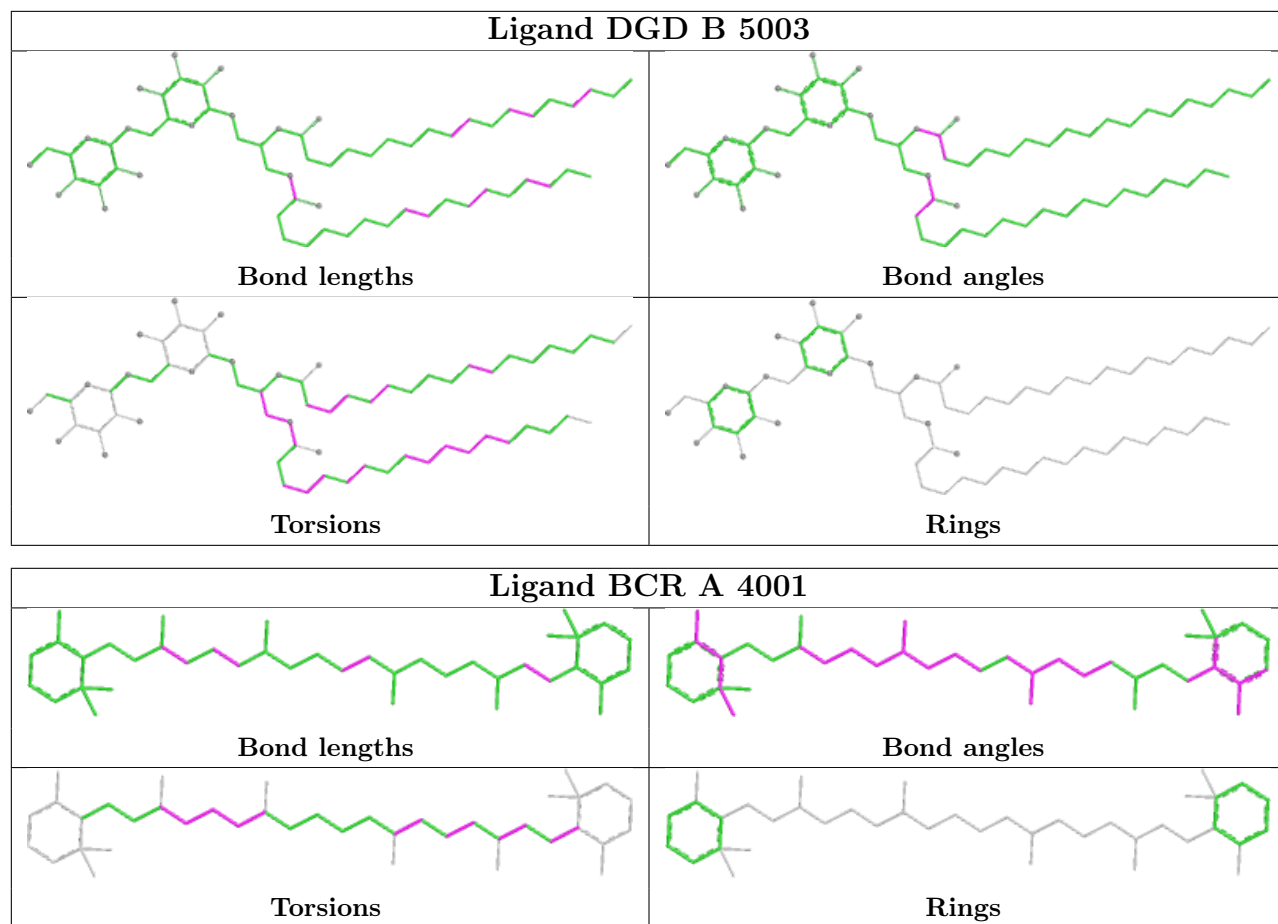
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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40	1	501	LUT	5	0
24	3	612	CLA	6	0
48	7	502	XAT	3	0
24	H	1702	CLA	2	0
24	7	606	CLA	1	0
41	a	610	CHL	1	0
40	5	501	LUT	3	0
24	B	1203	CLA	3	0
24	7	603	CLA	2	0
24	2	607	CLA	1	0
42	1	803	OLA	2	0
27	3	505	BCR	3	0
24	B	1235	CLA	5	0
24	B	1205	CLA	4	0
24	B	1201	CLA	4	0
24	A	1125	CLA	4	0
24	B	1239	CLA	4	0
27	8	503	BCR	1	0
33	9	803	PTY	2	0
33	3	802	PTY	1	0
24	B	1221	CLA	4	0
42	8	809	OLA	3	0
24	3	606	CLA	4	0
24	A	1013	CLA	8	0
28	B	5001	LHG	3	0
24	5	618	CLA	1	0
24	F	1301	CLA	3	0
28	8	801	LHG	1	0
41	a	613	CHL	2	0
24	B	1232	CLA	2	0
36	G	5002	ERG	6	0
24	4	612	CLA	4	0

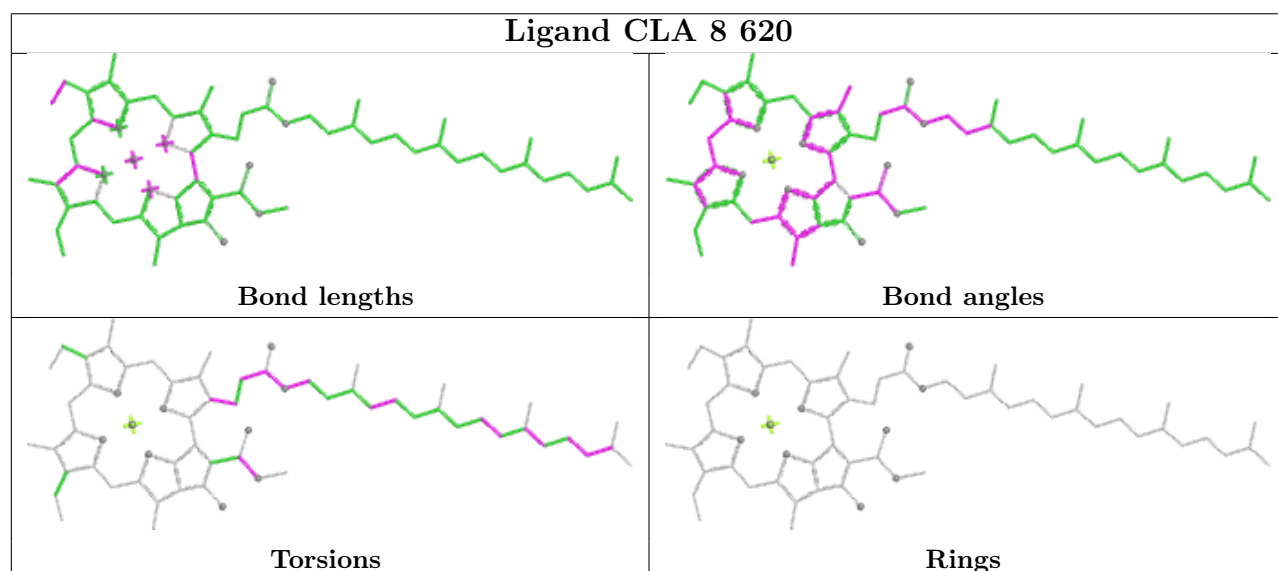
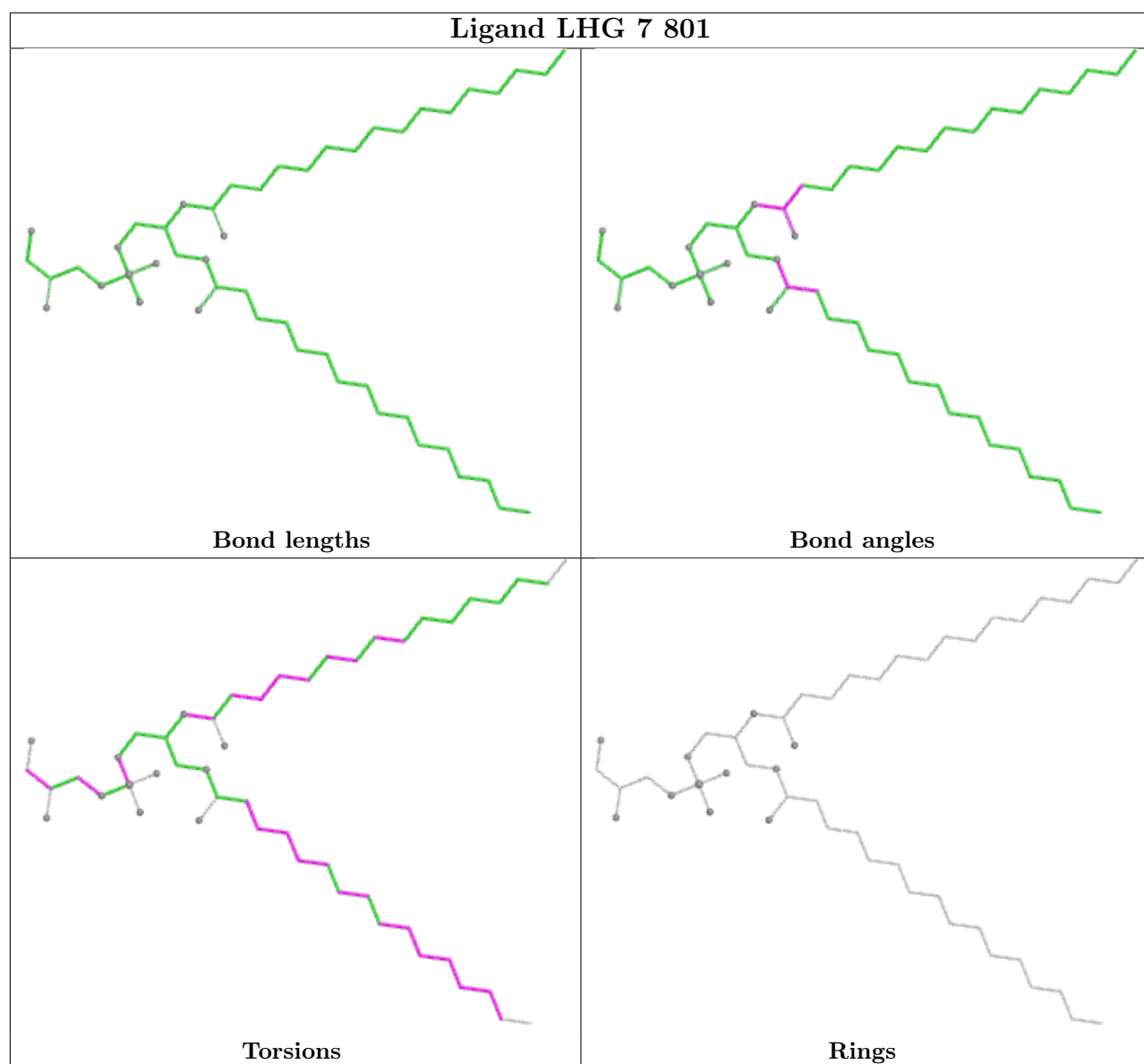
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

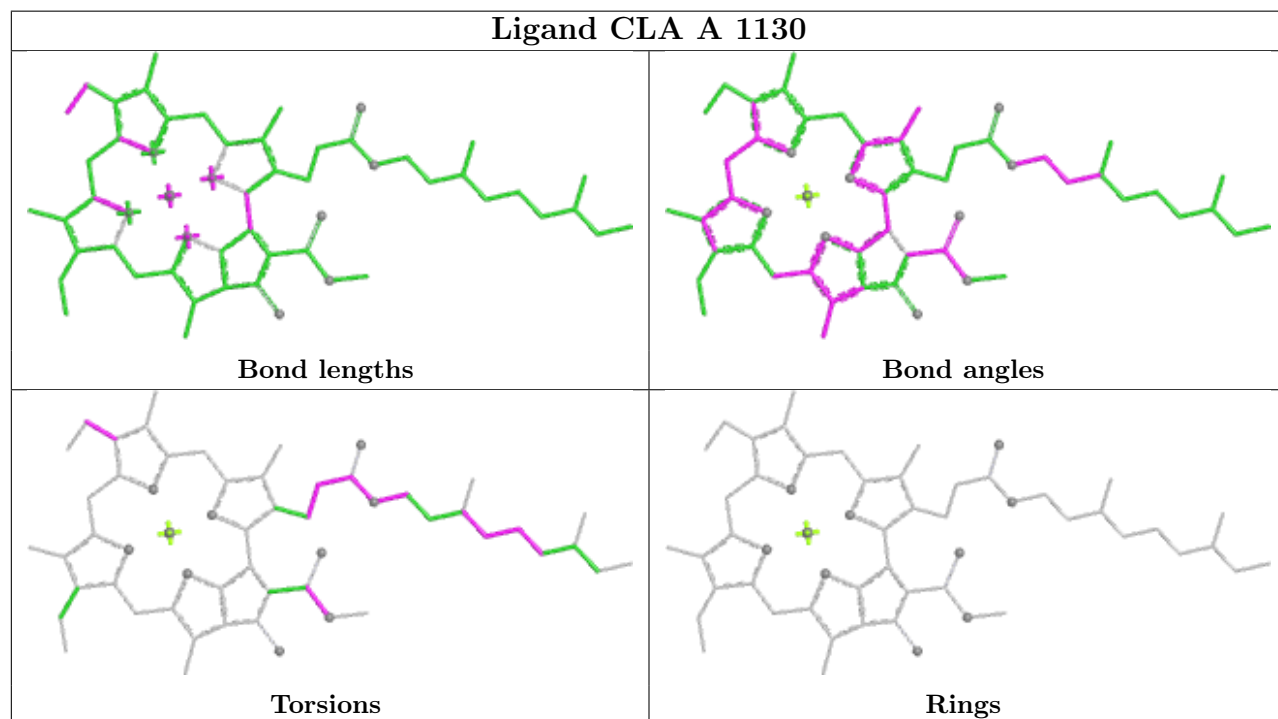
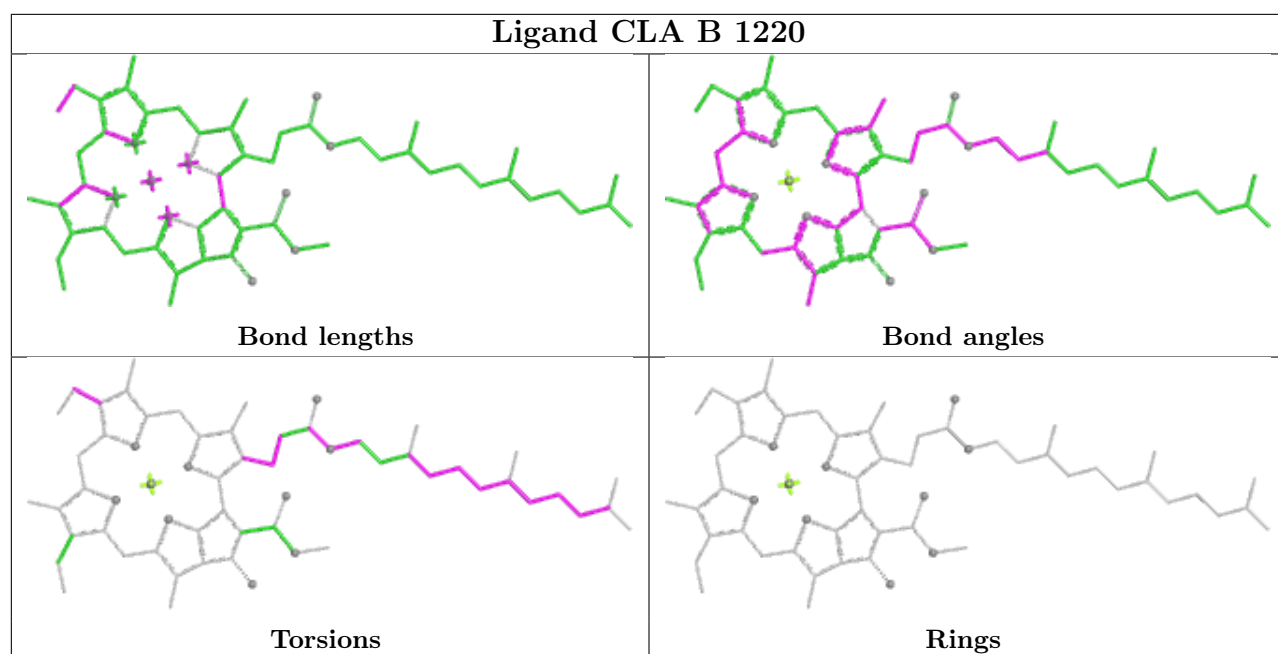
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

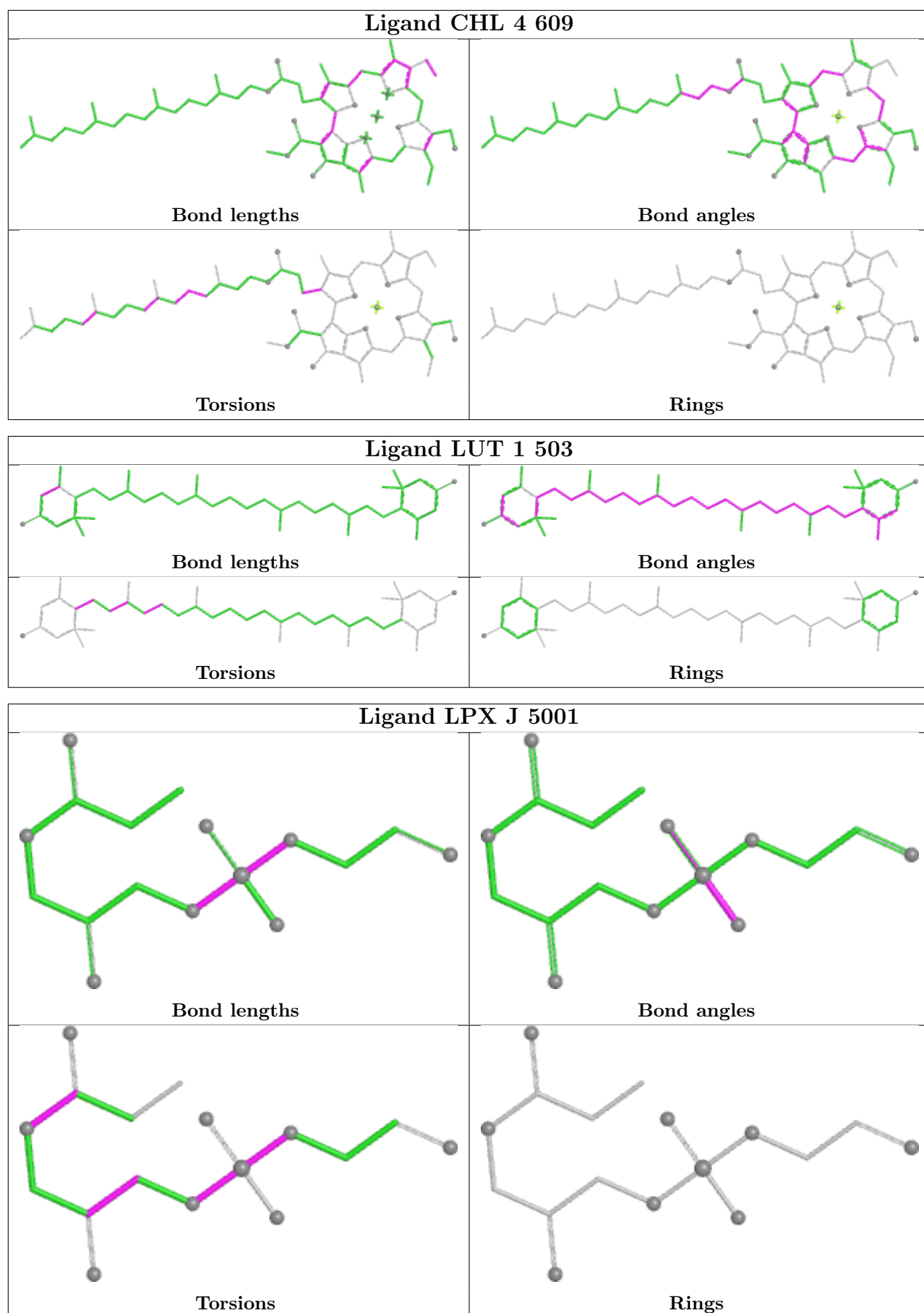


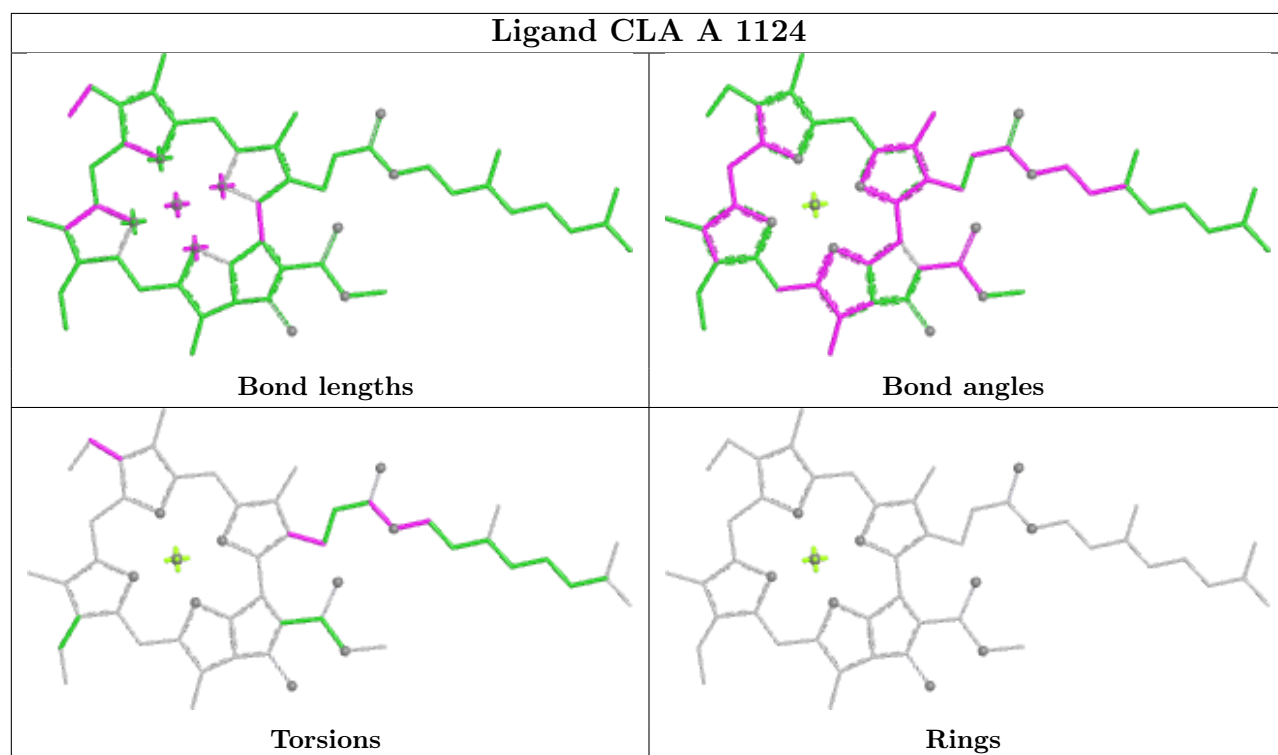
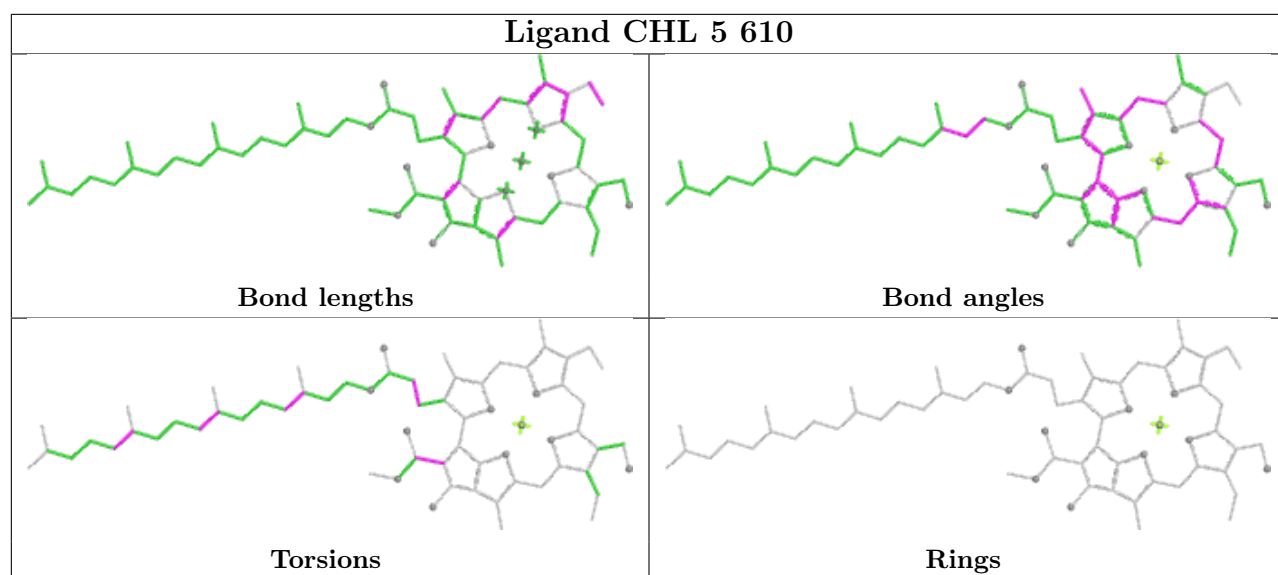


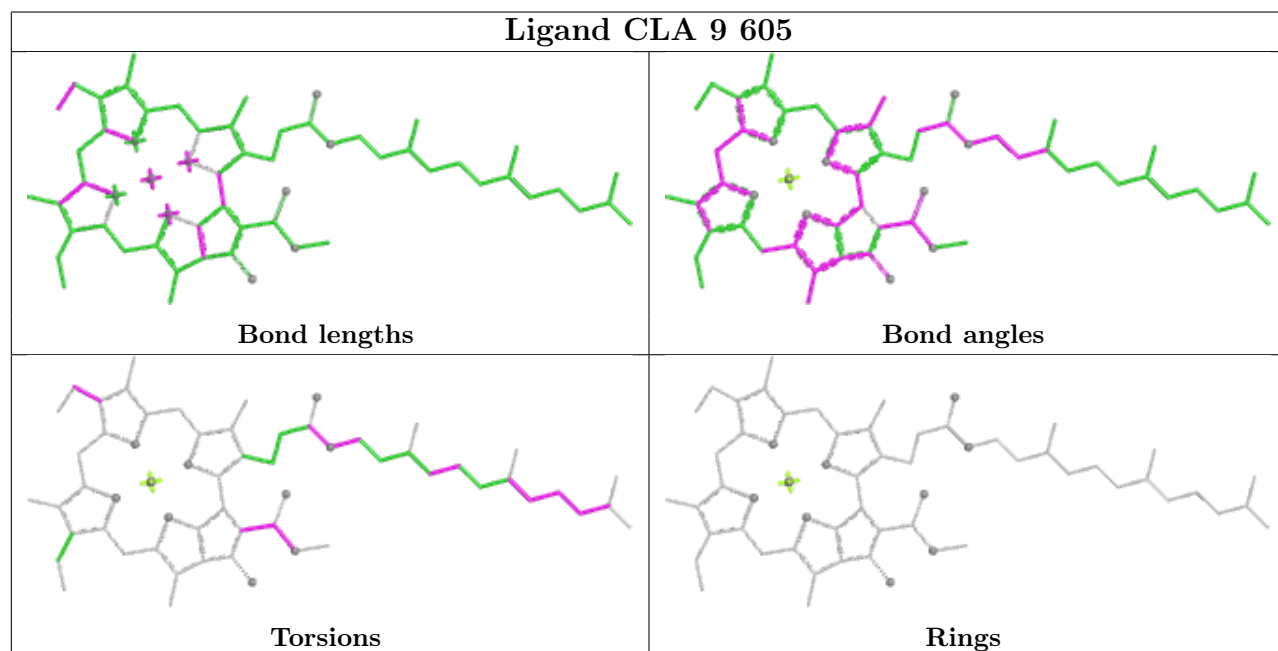
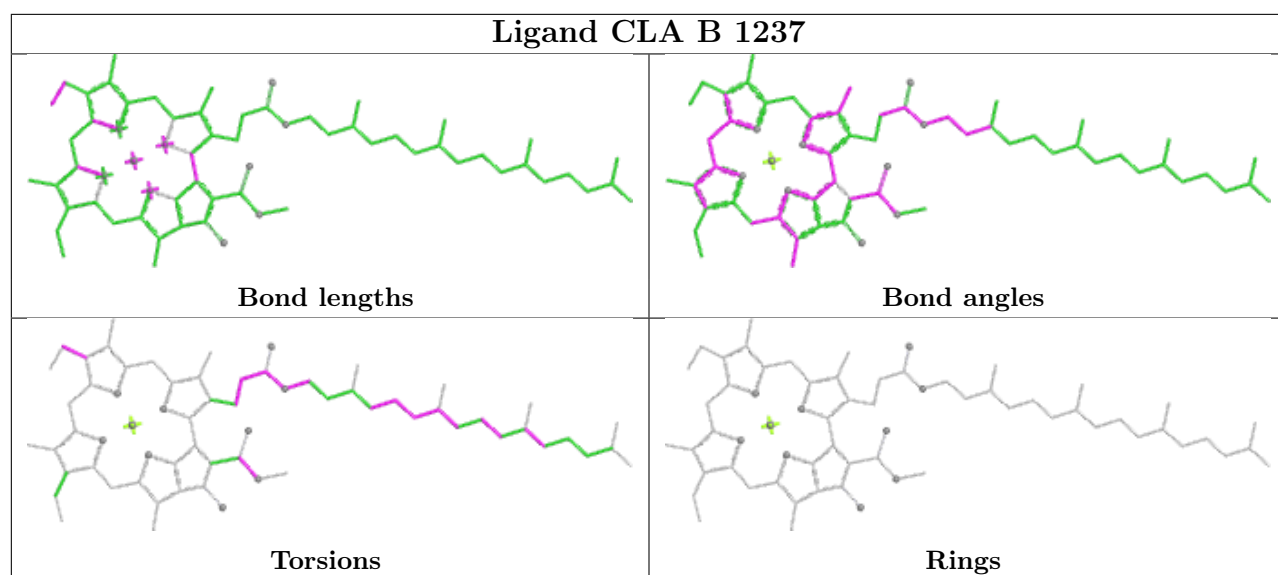


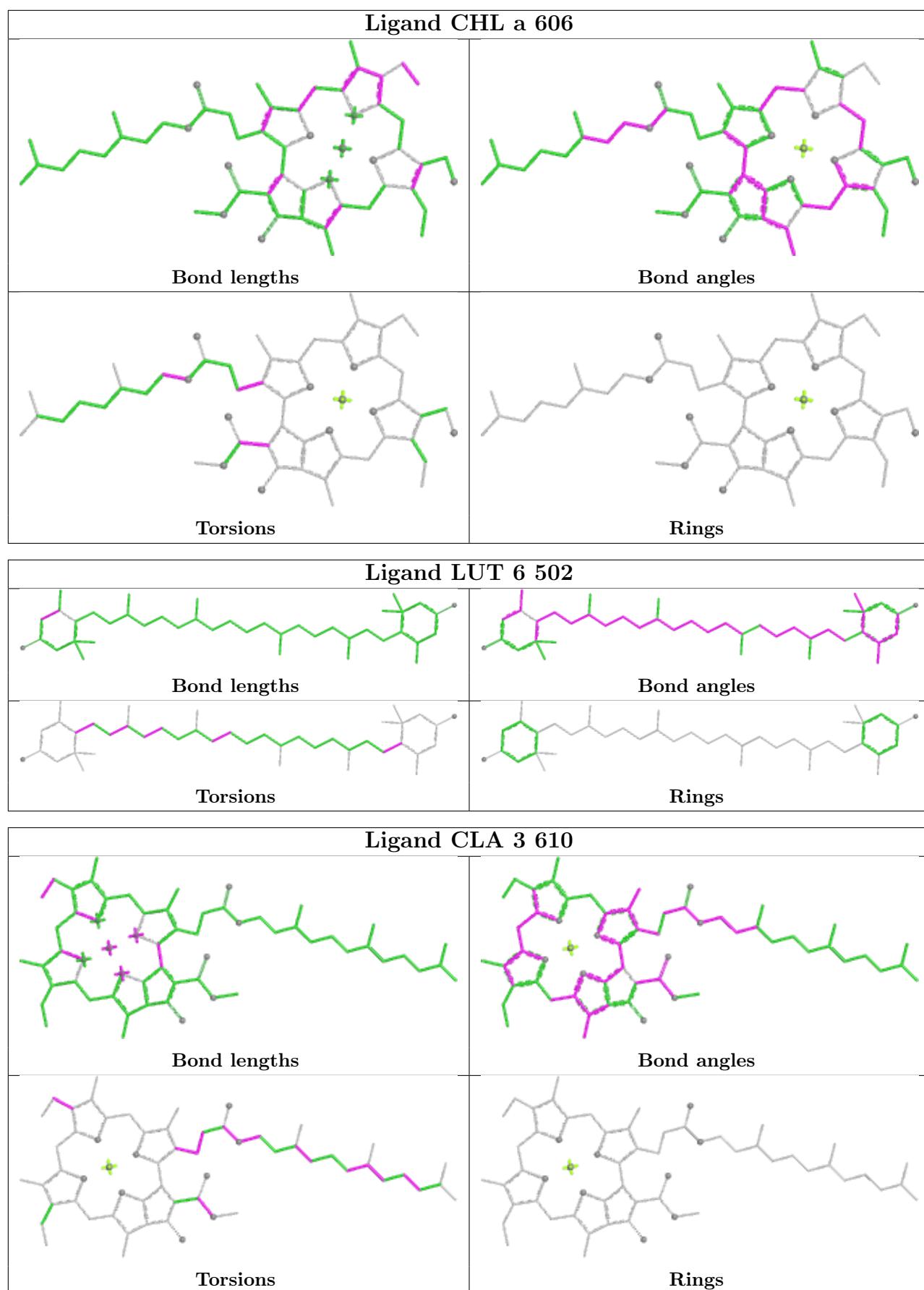




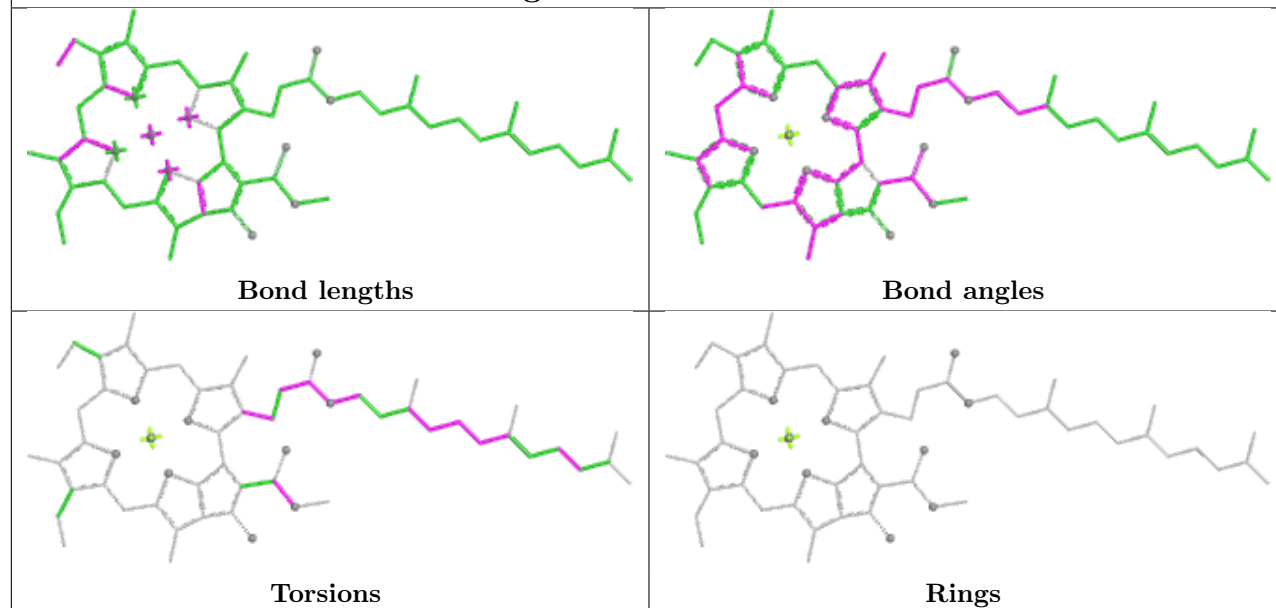




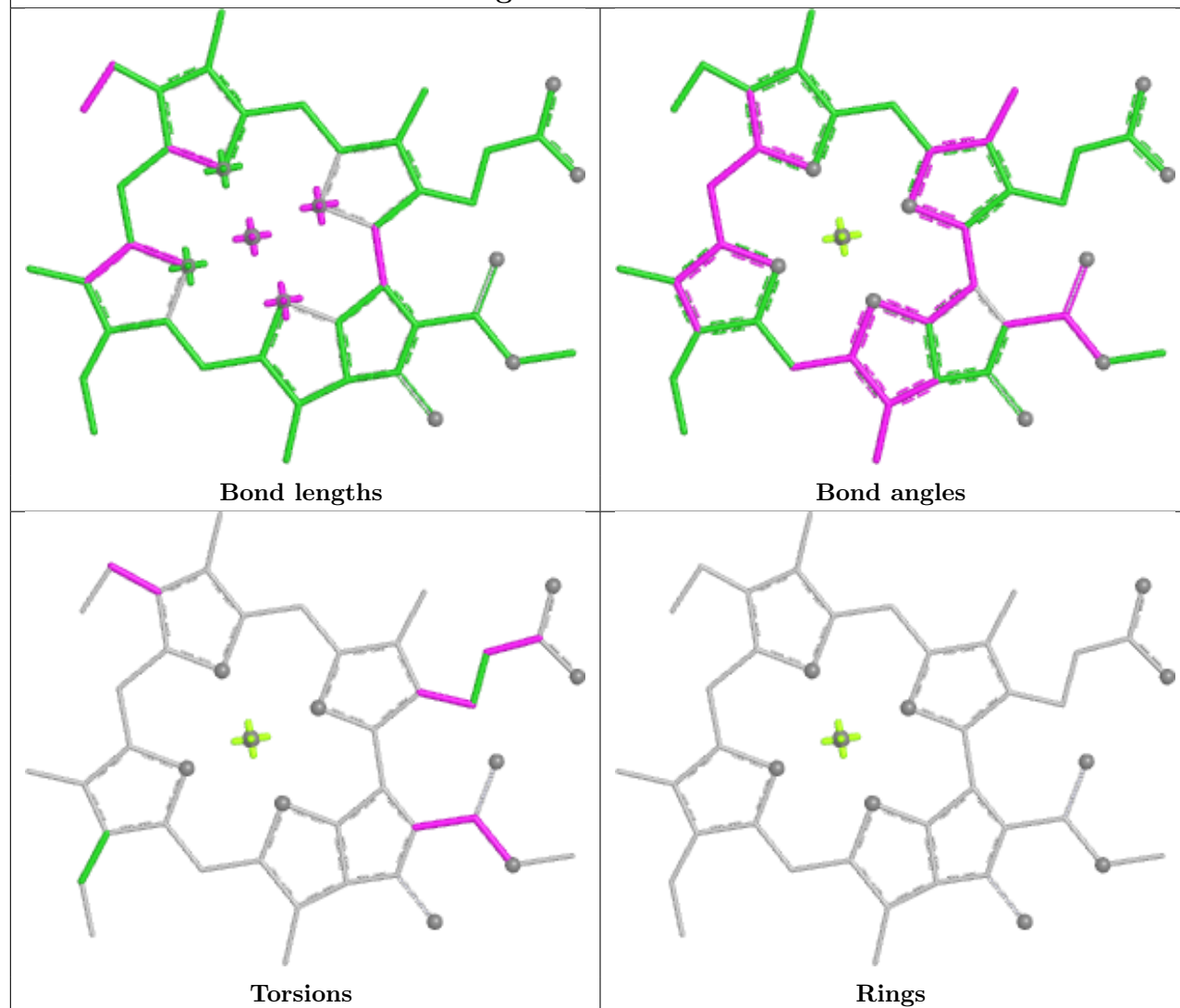




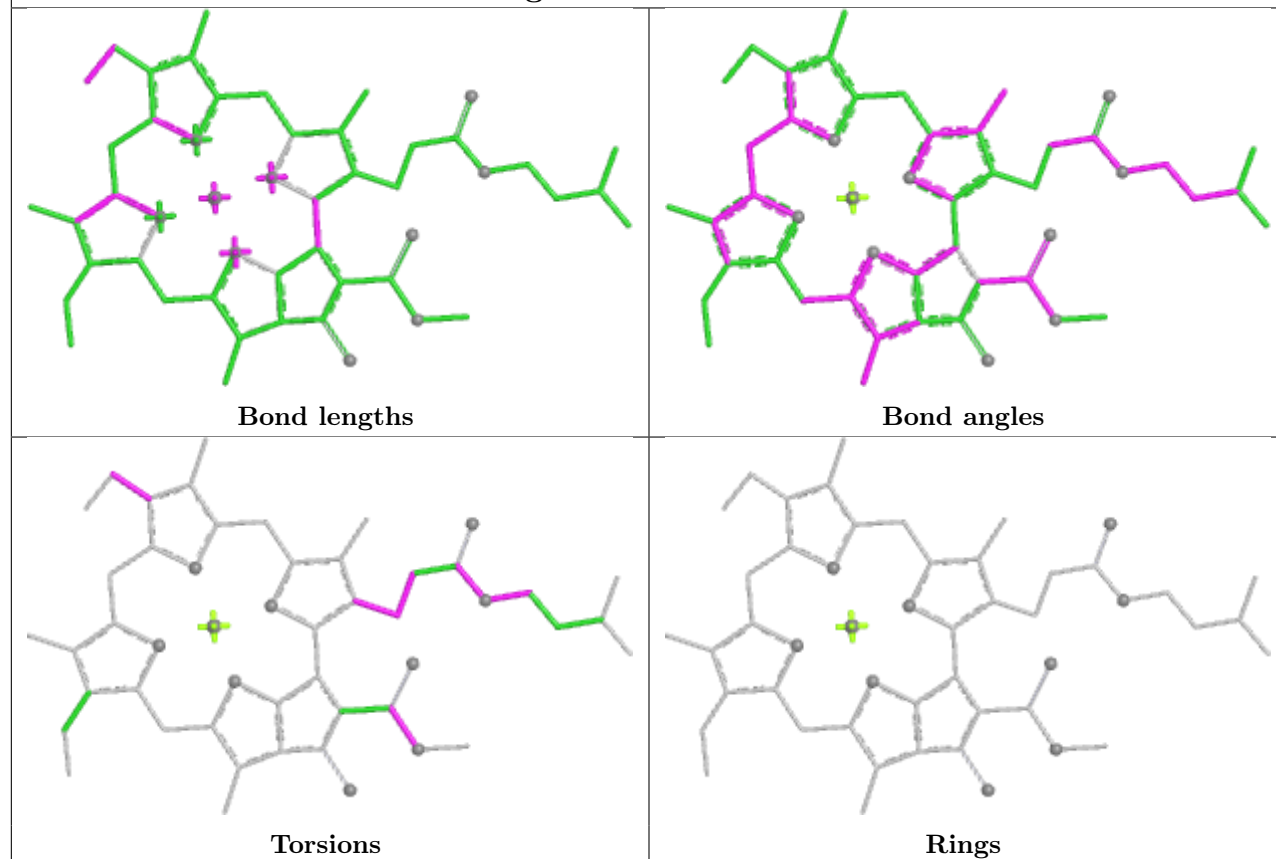
Ligand CLA B 1208



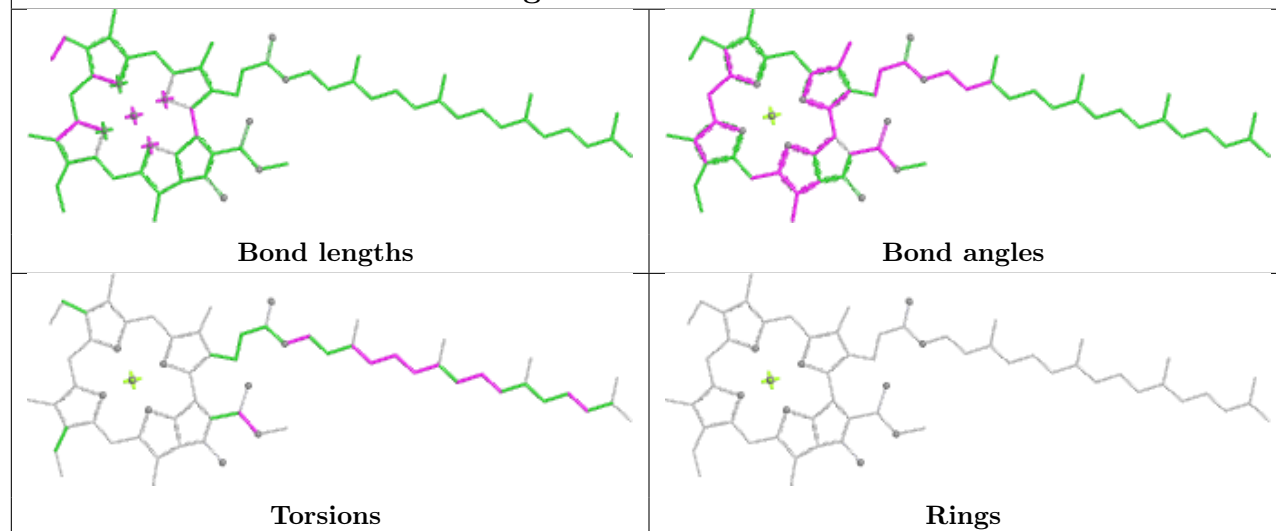
Ligand CLA 6 617



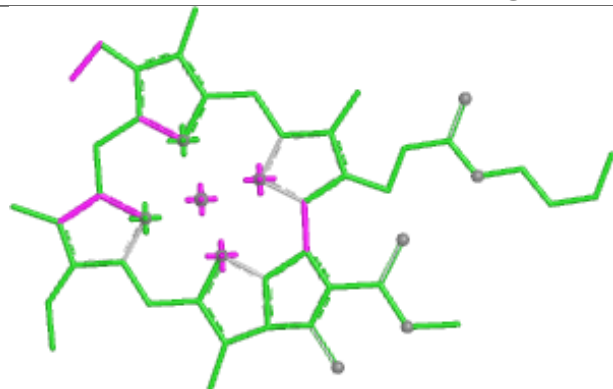
Ligand CLA L 1501



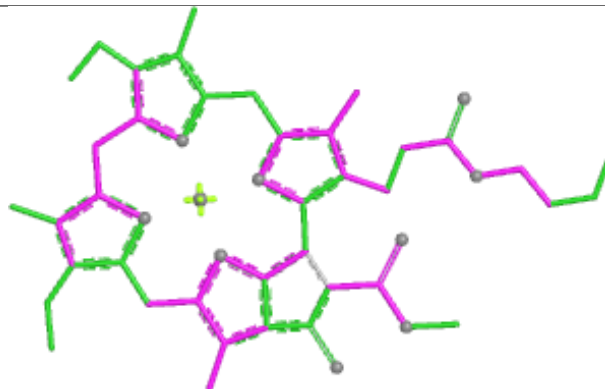
Ligand CLA B 1240



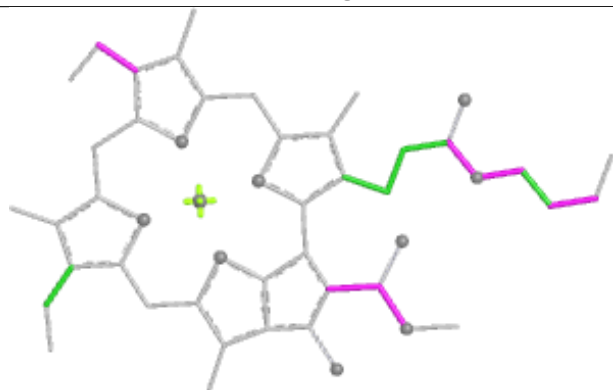
Ligand CLA A 1120



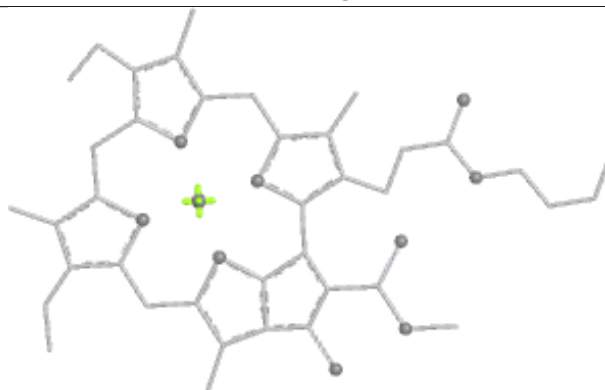
Bond lengths



Bond angles

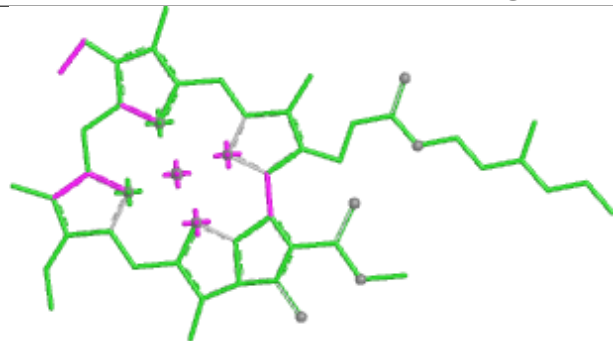


Torsions

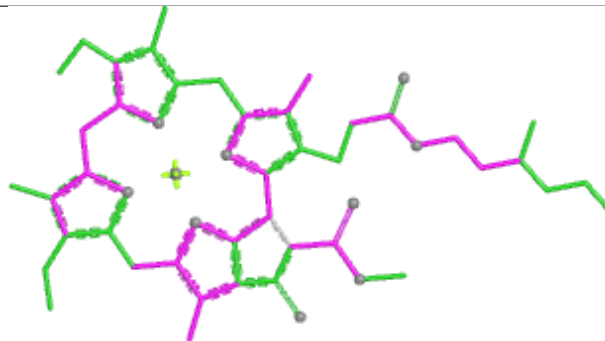


Rings

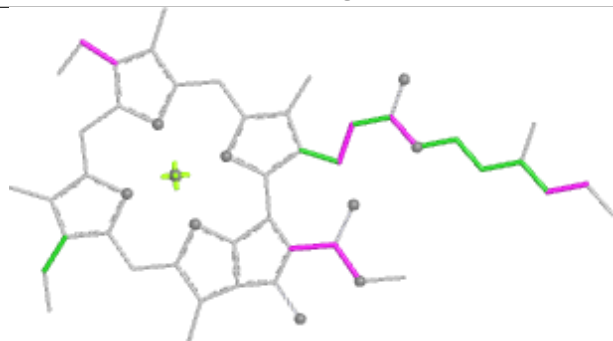
Ligand CLA K 1404



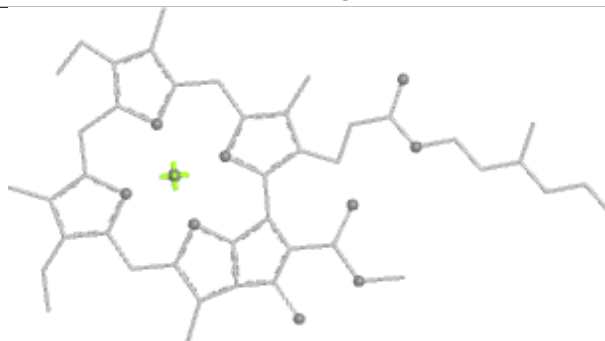
Bond lengths



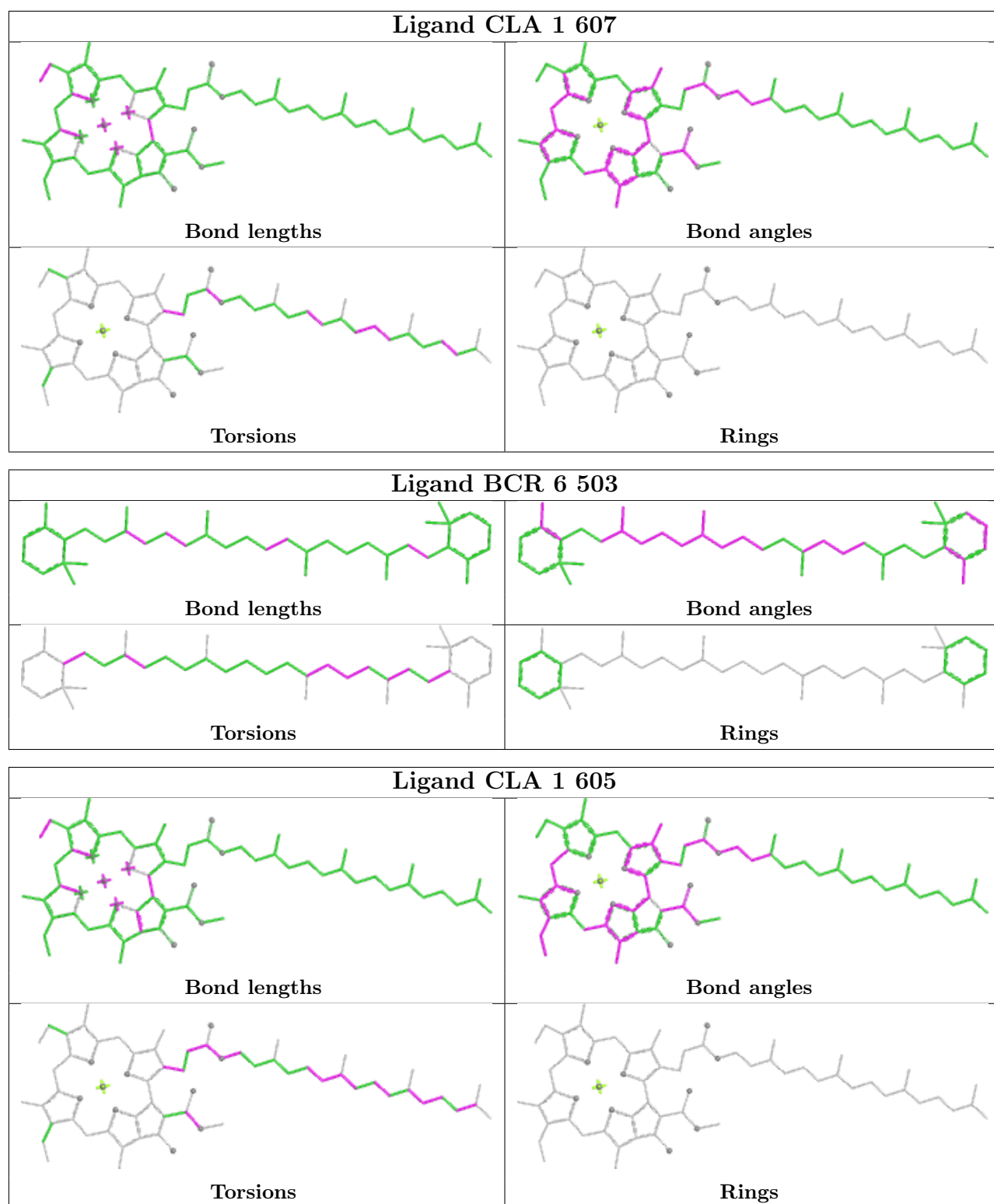
Bond angles



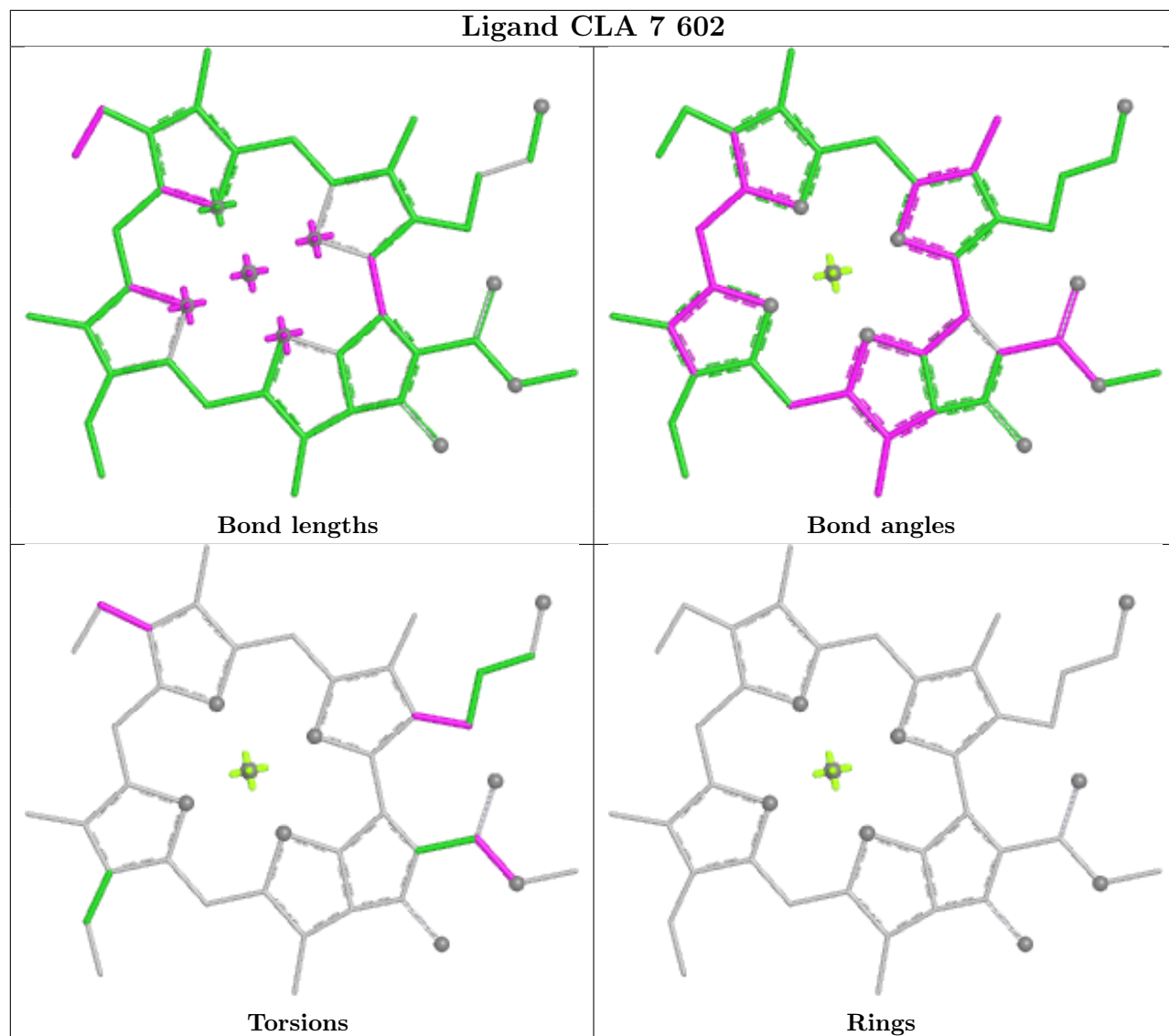
Torsions



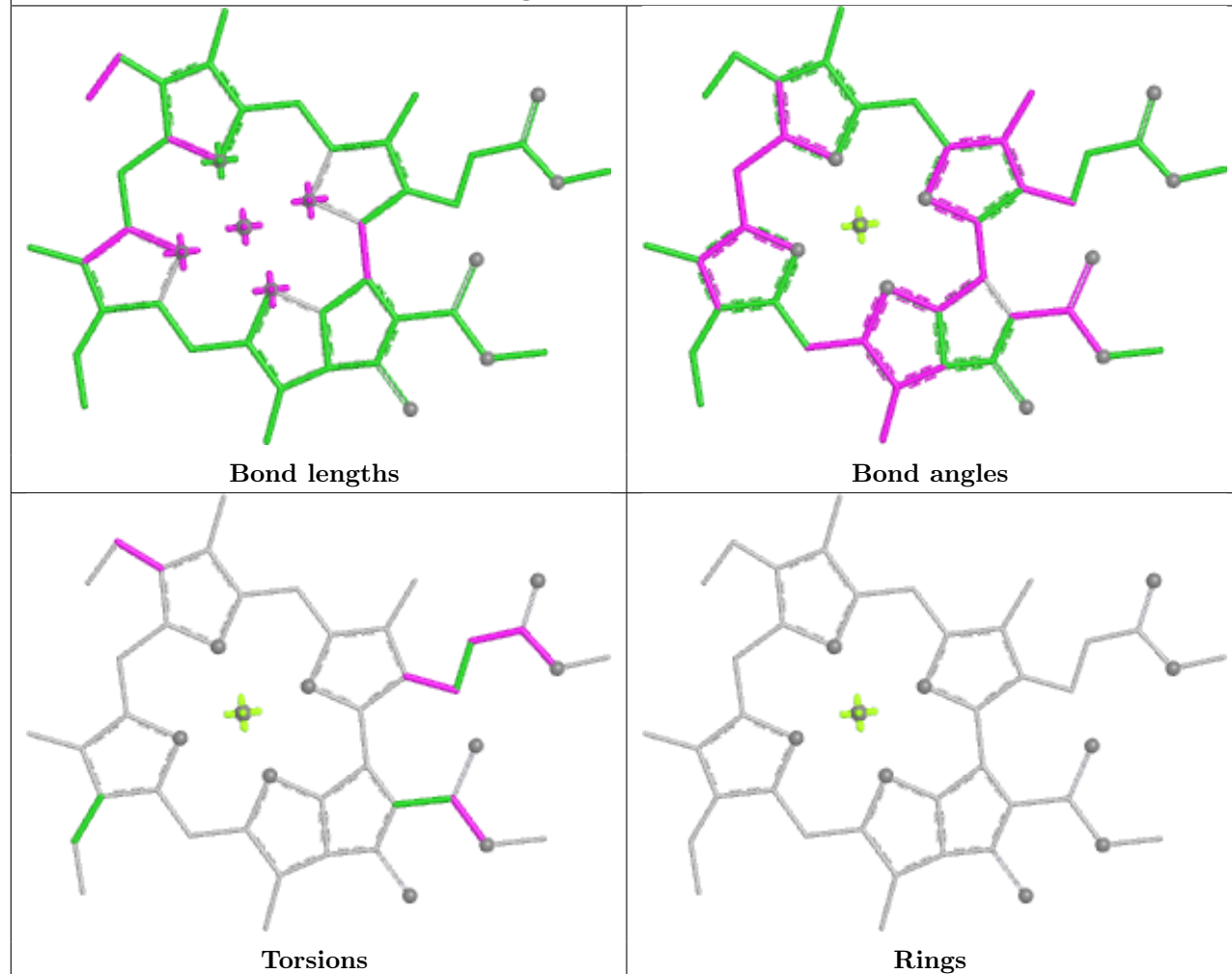
Rings



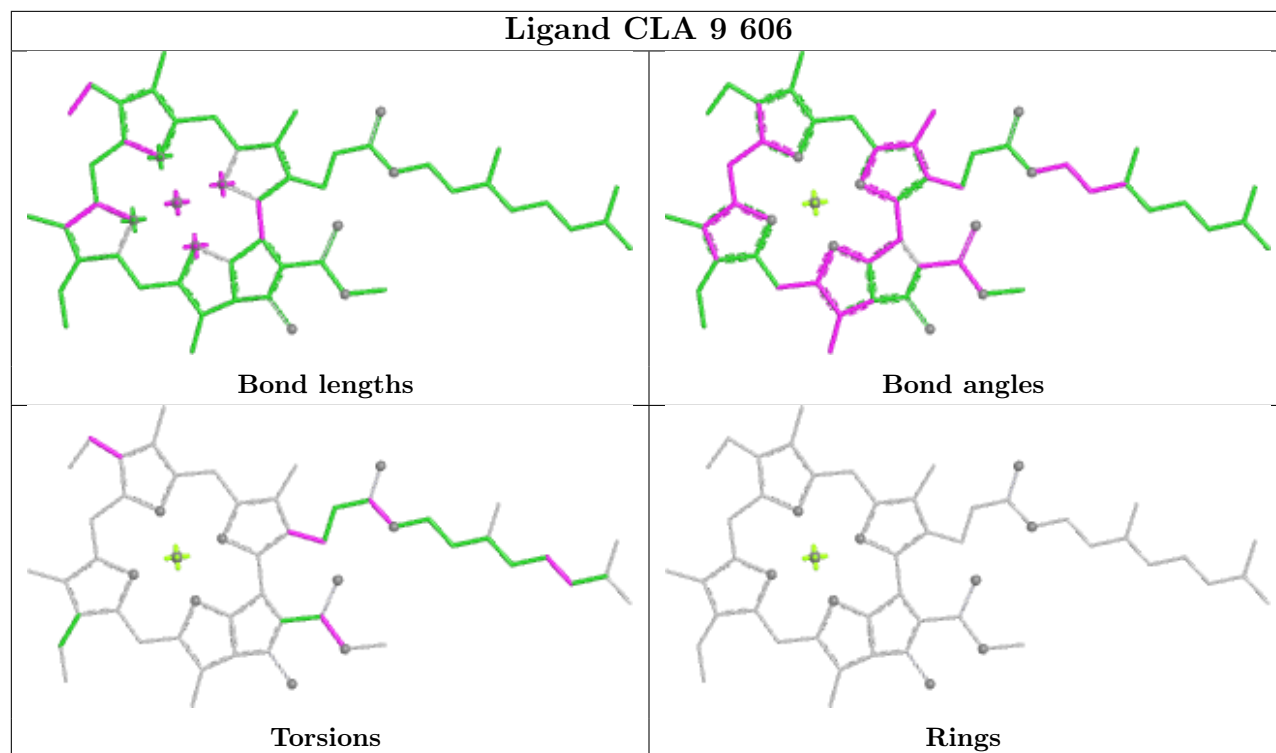
Ligand CLA 7 602



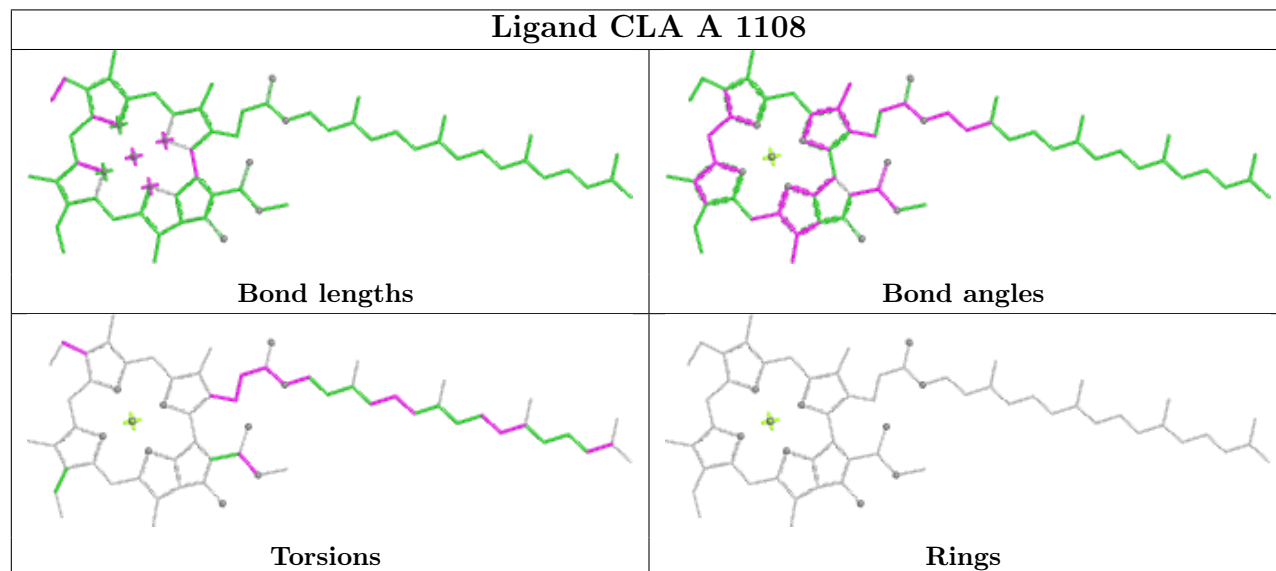
Ligand CLA 3 618



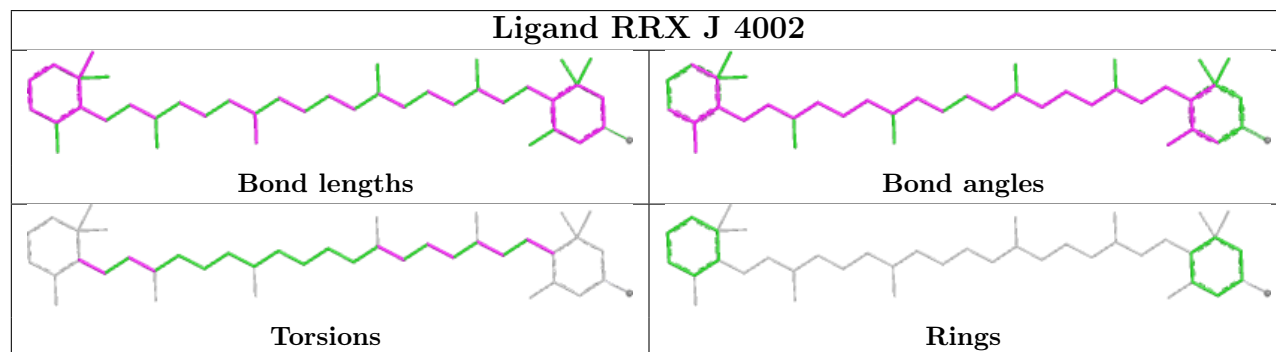
Ligand CLA 9 606

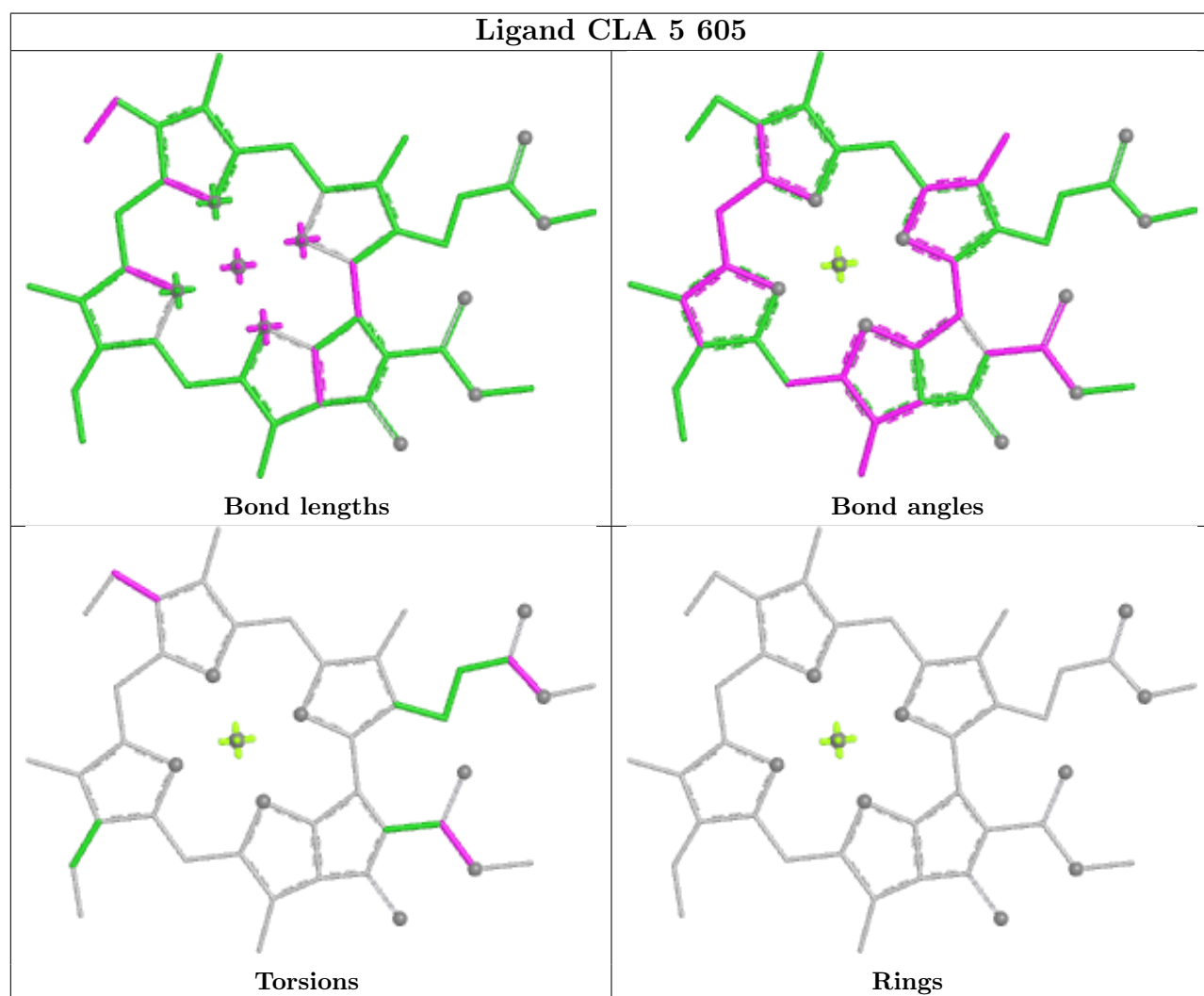
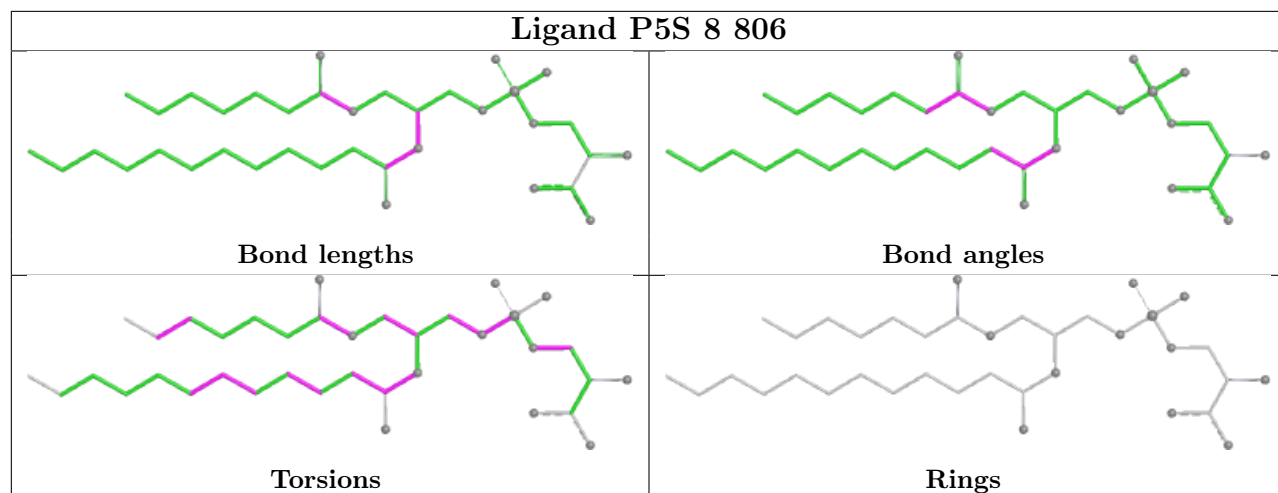


Ligand CLA A 1108

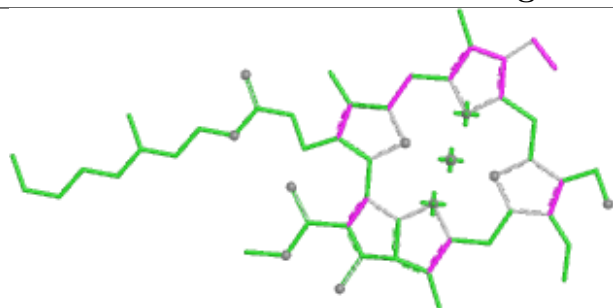


Ligand RRX J 4002

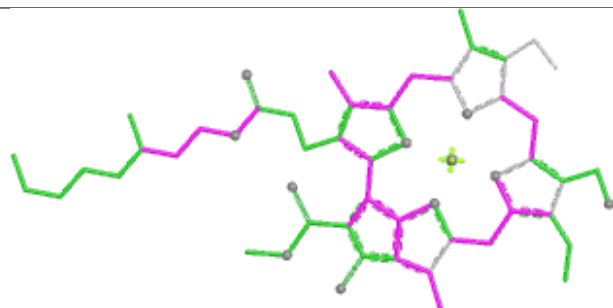




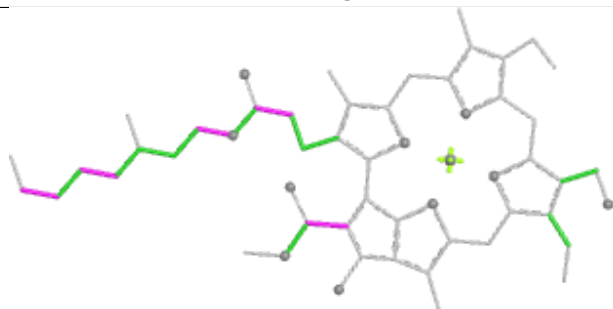
Ligand CHL 3 611



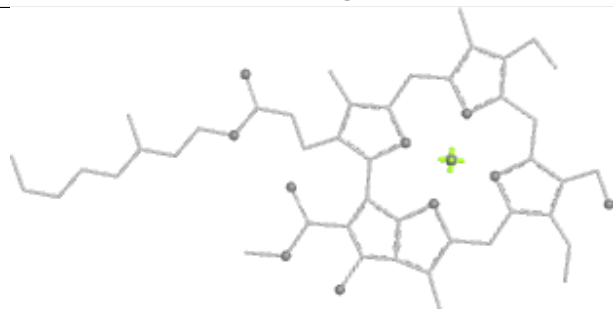
Bond lengths



Bond angles

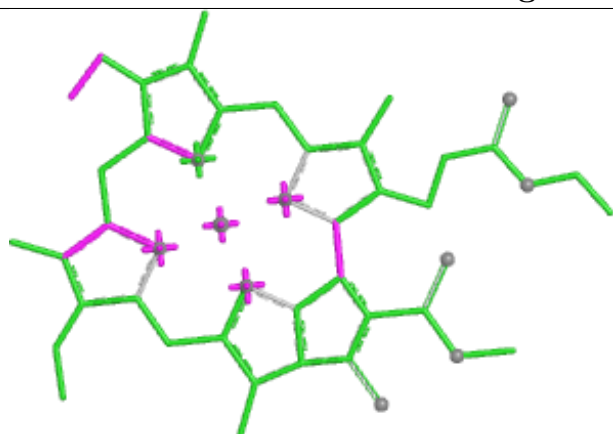


Torsions

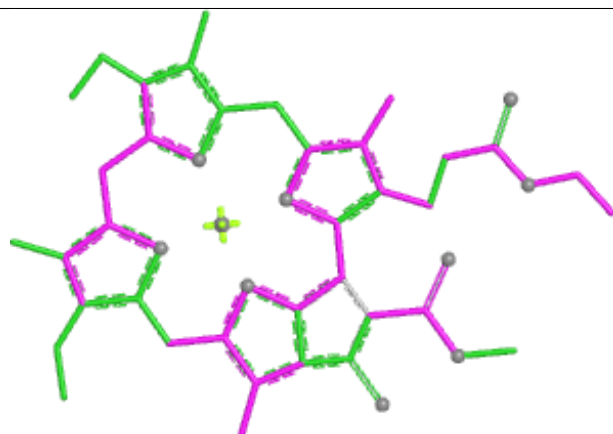


Rings

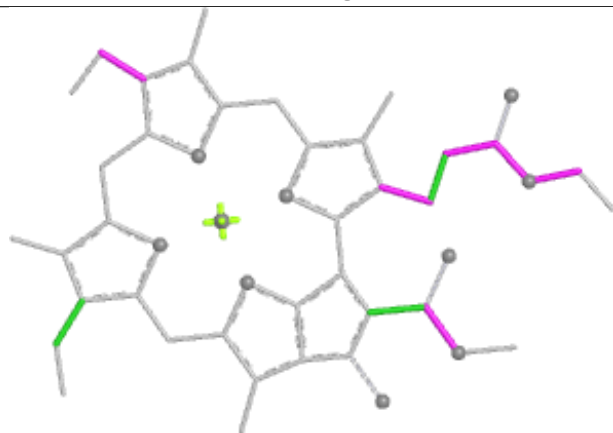
Ligand CLA 9 607



Bond lengths



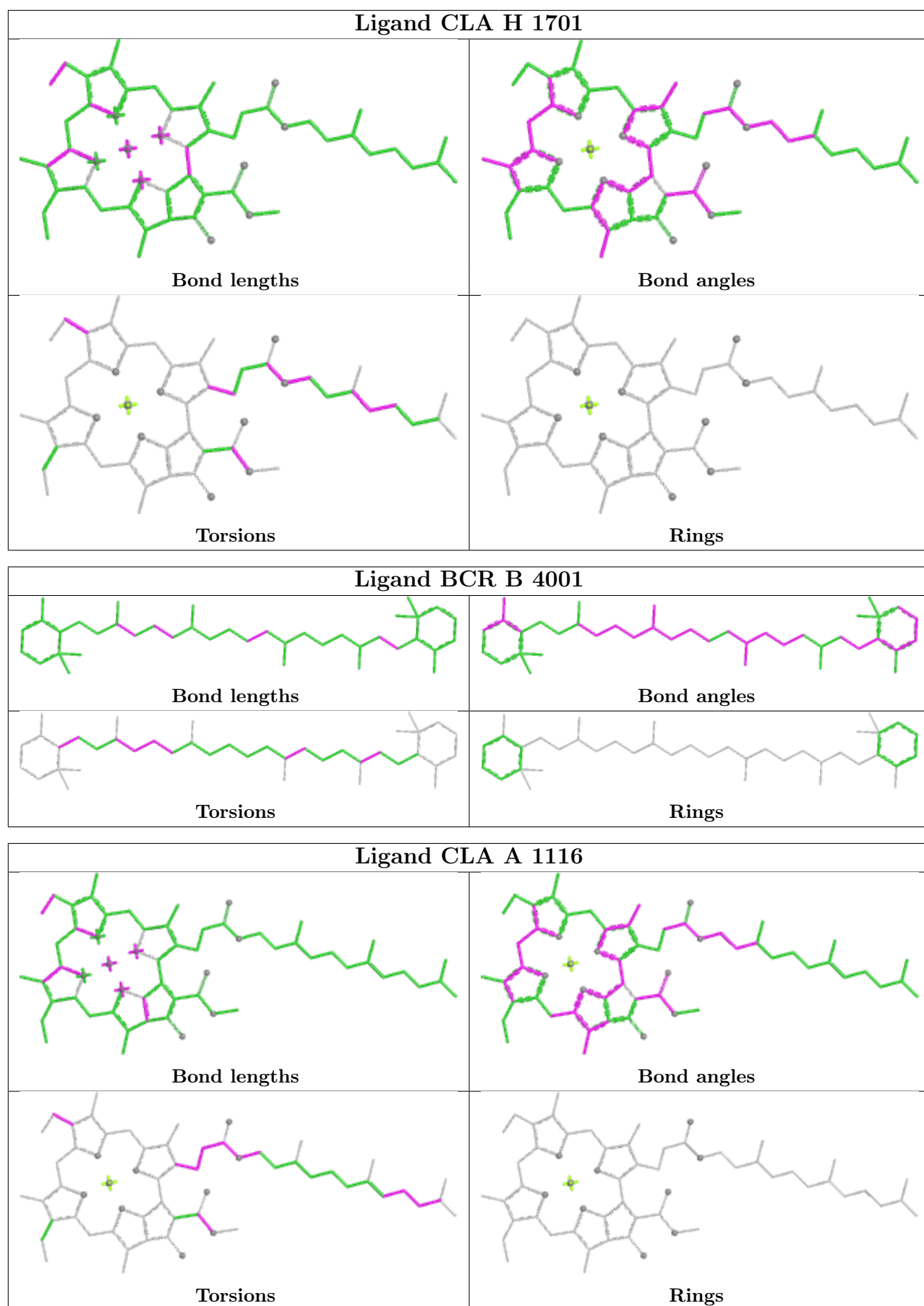
Bond angles

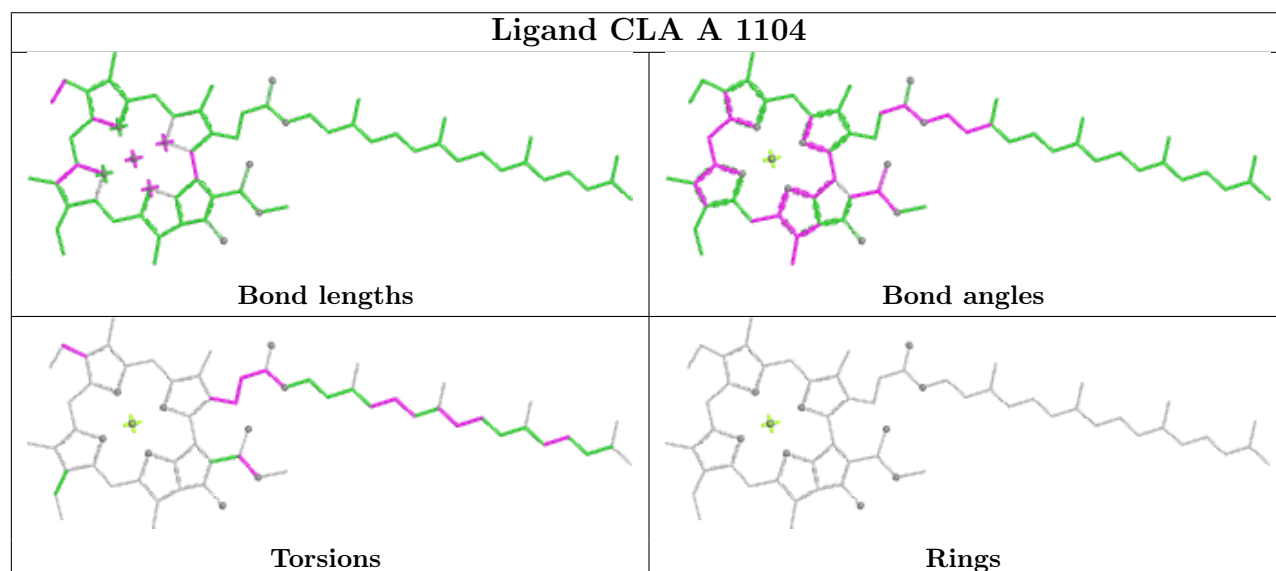
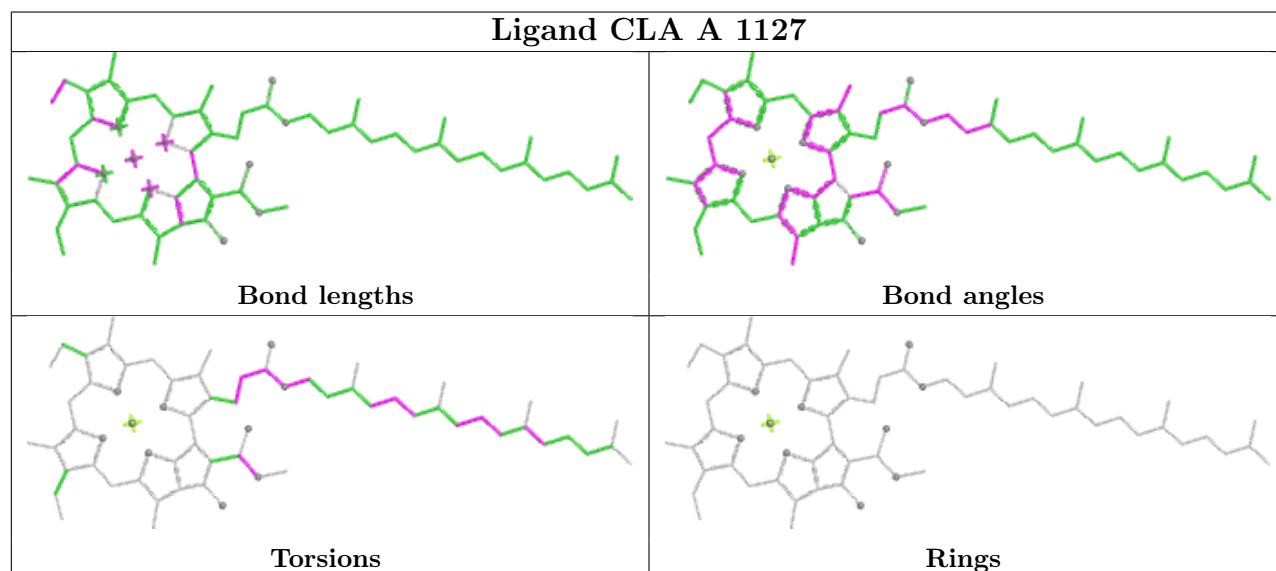
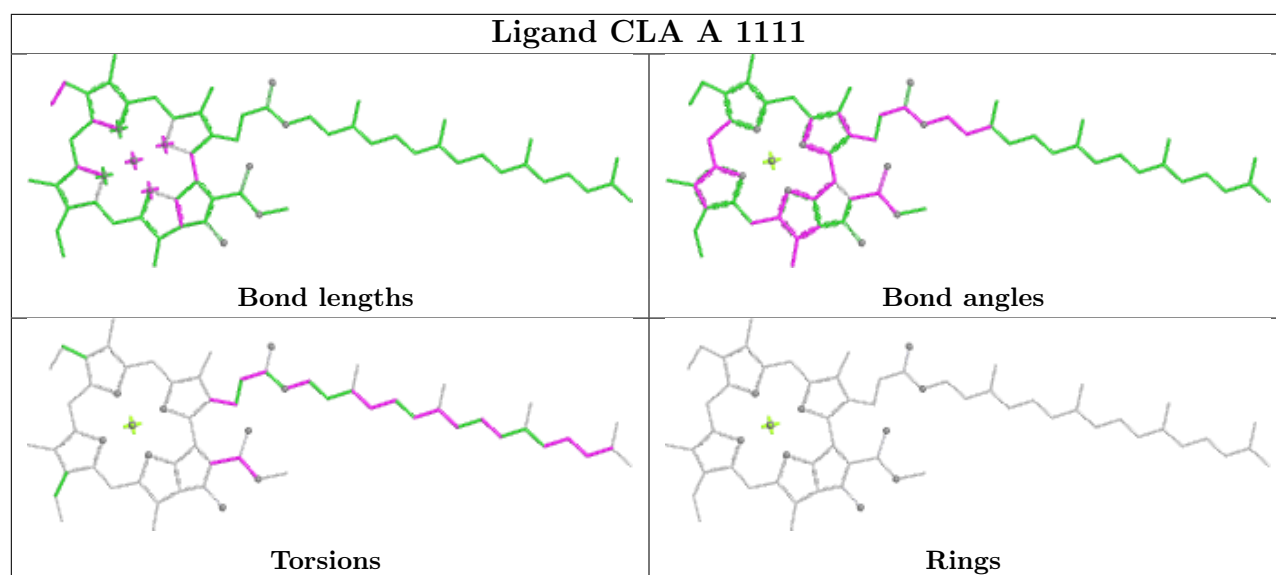


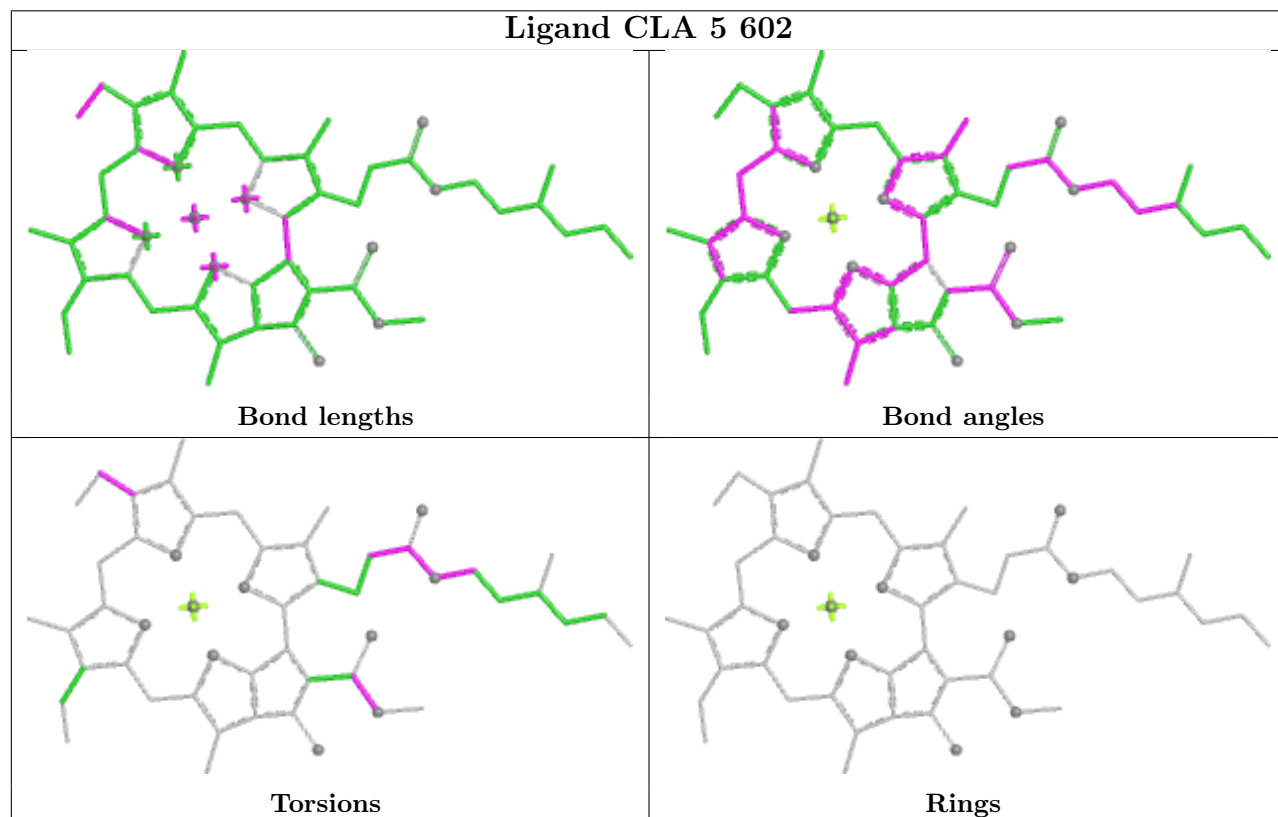
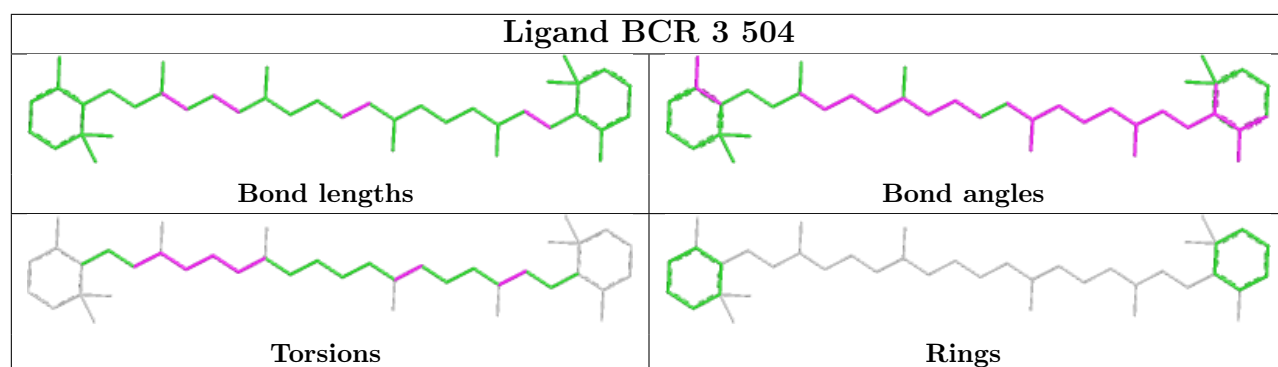
Torsions



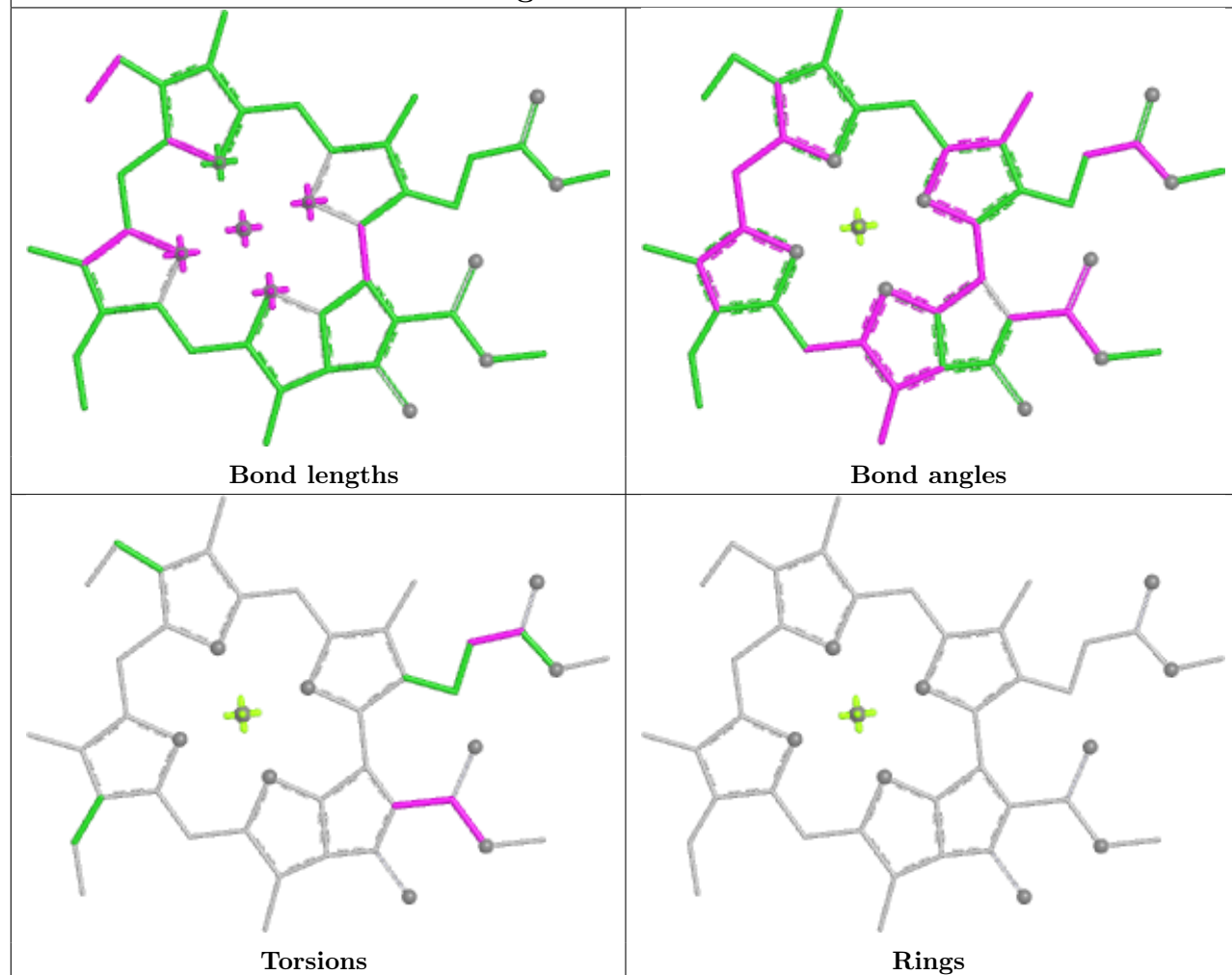
Rings



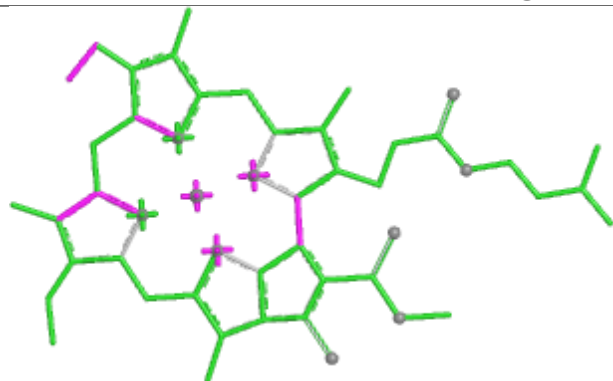




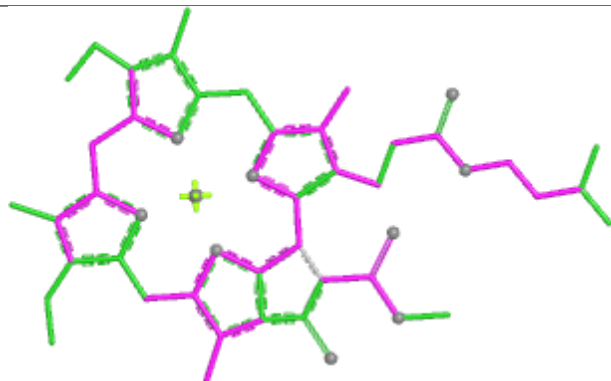
Ligand CLA 3 602



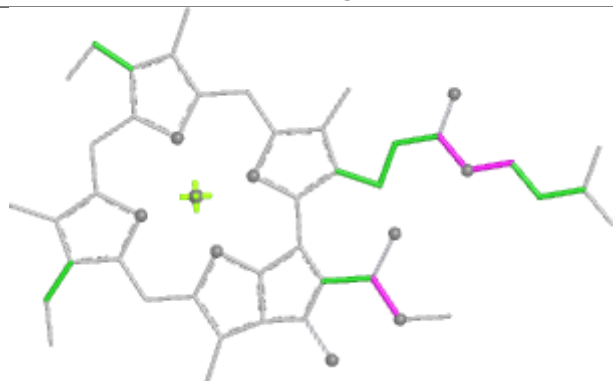
Ligand CLA 5 606



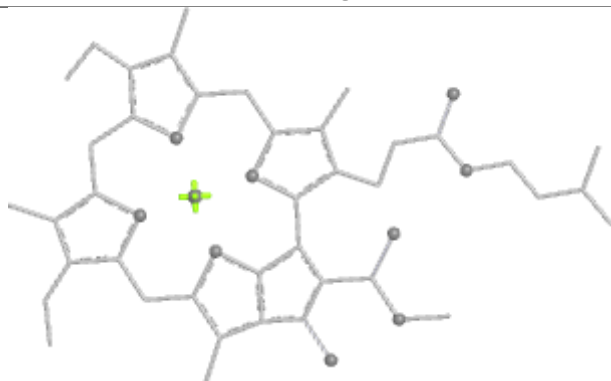
Bond lengths



Bond angles

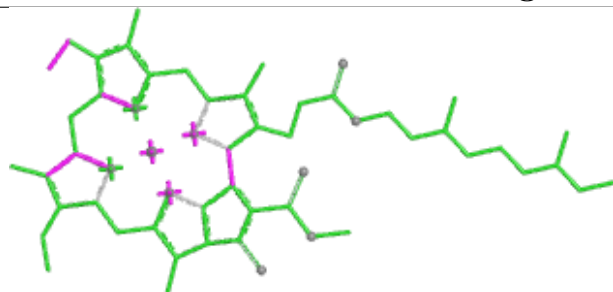


Torsions

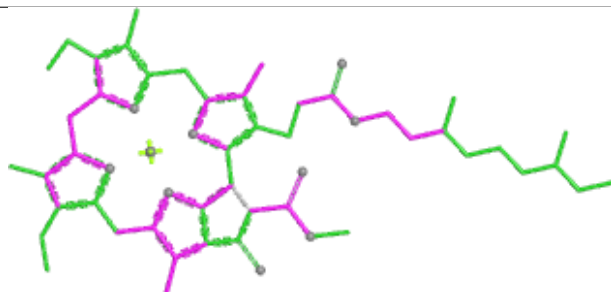


Rings

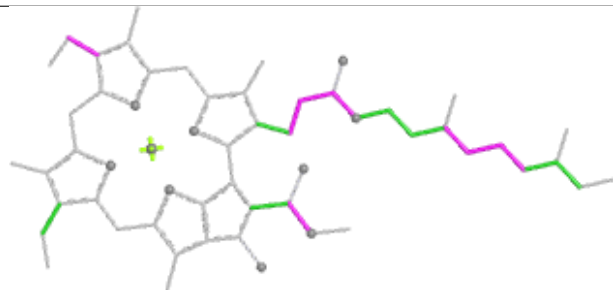
Ligand CLA 4 603



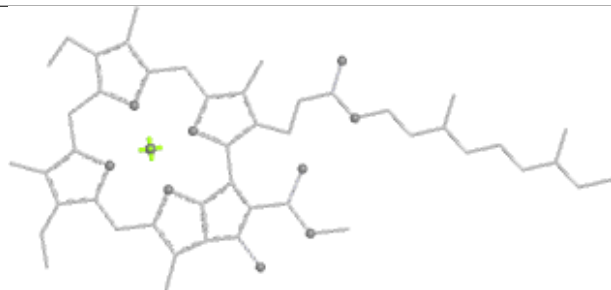
Bond lengths



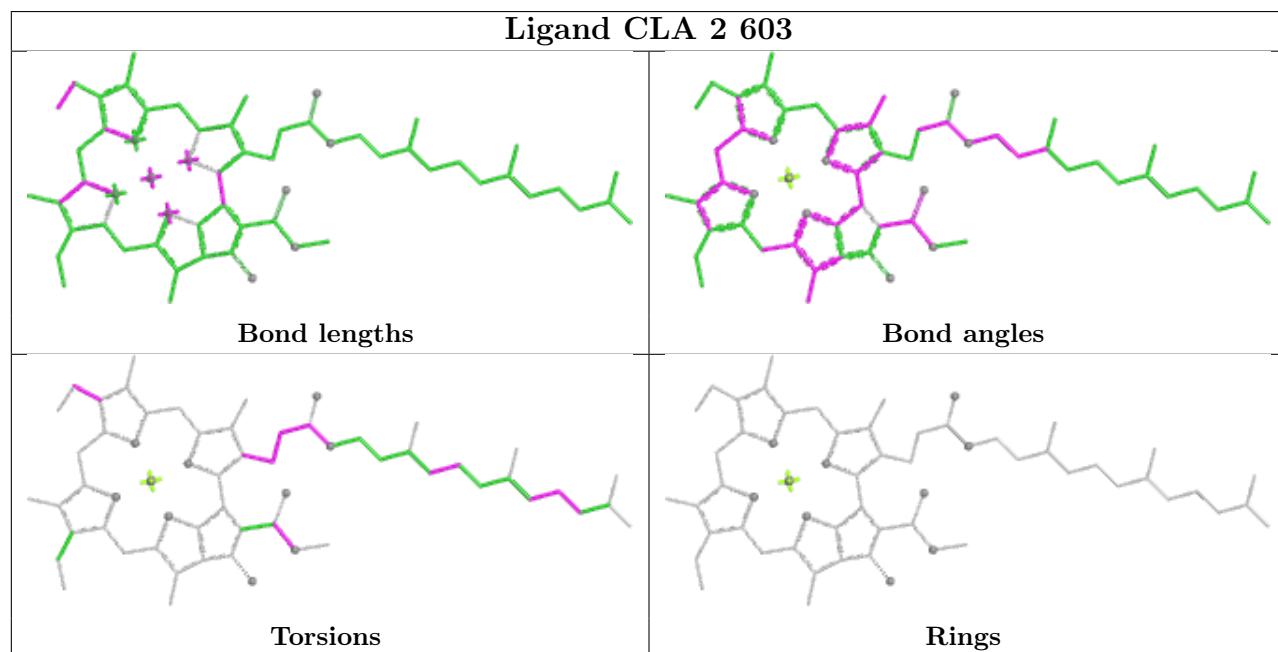
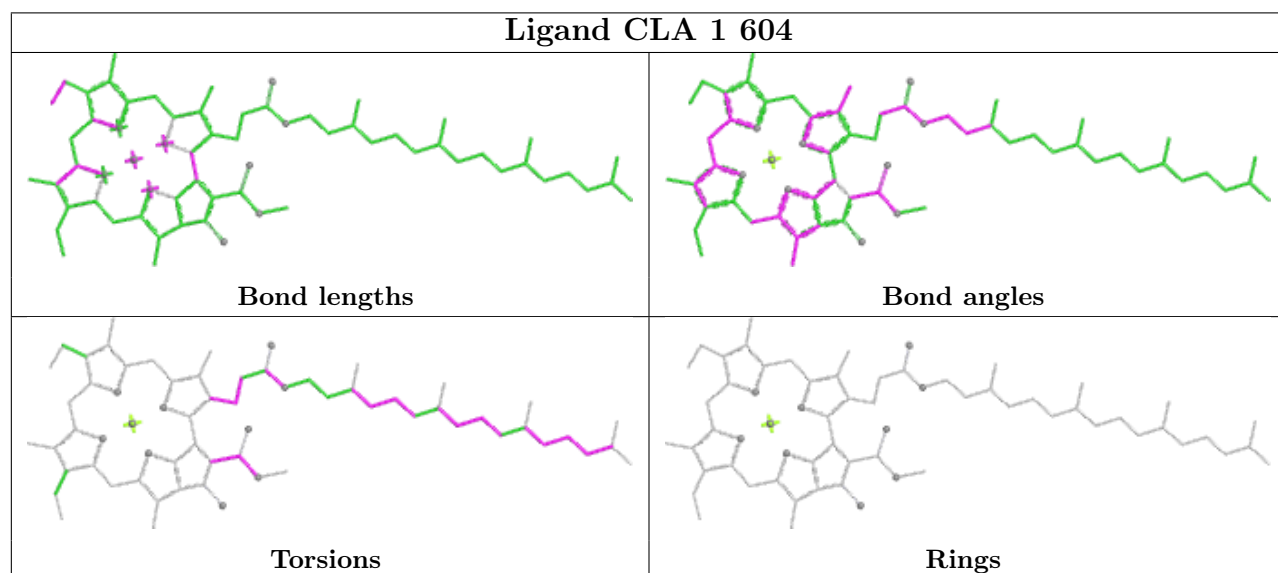
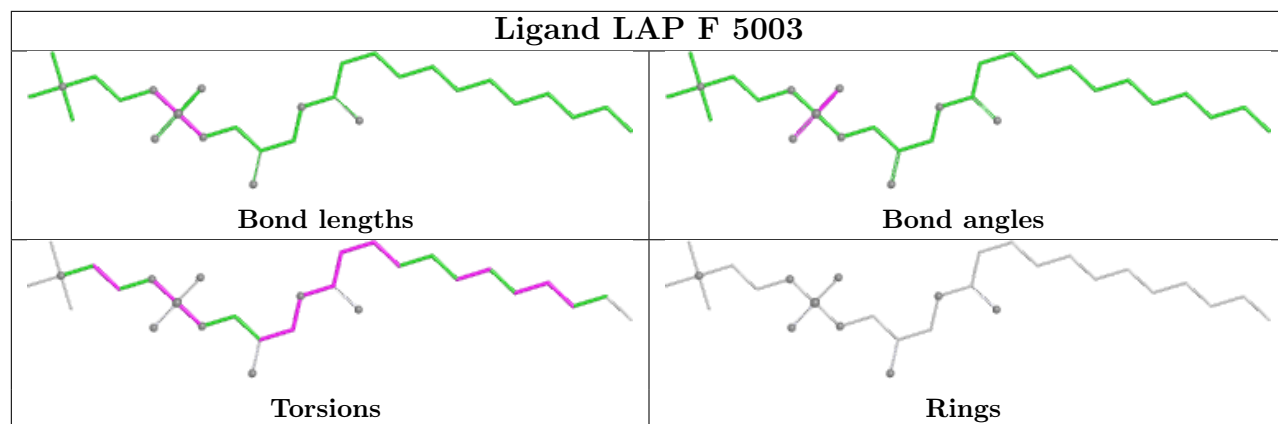
Bond angles

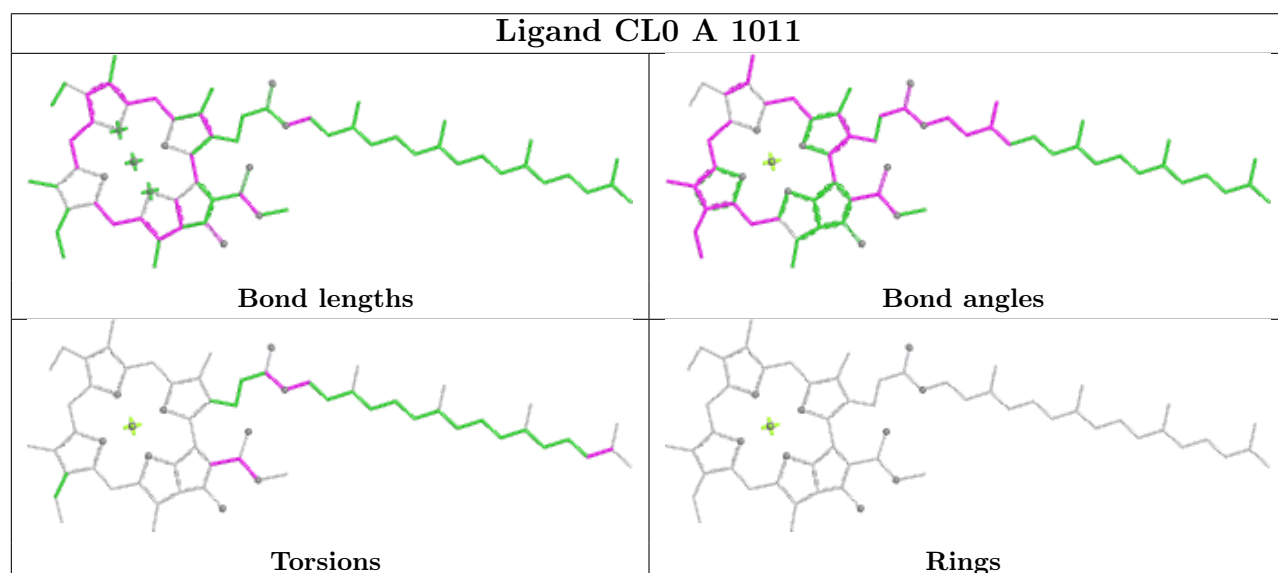
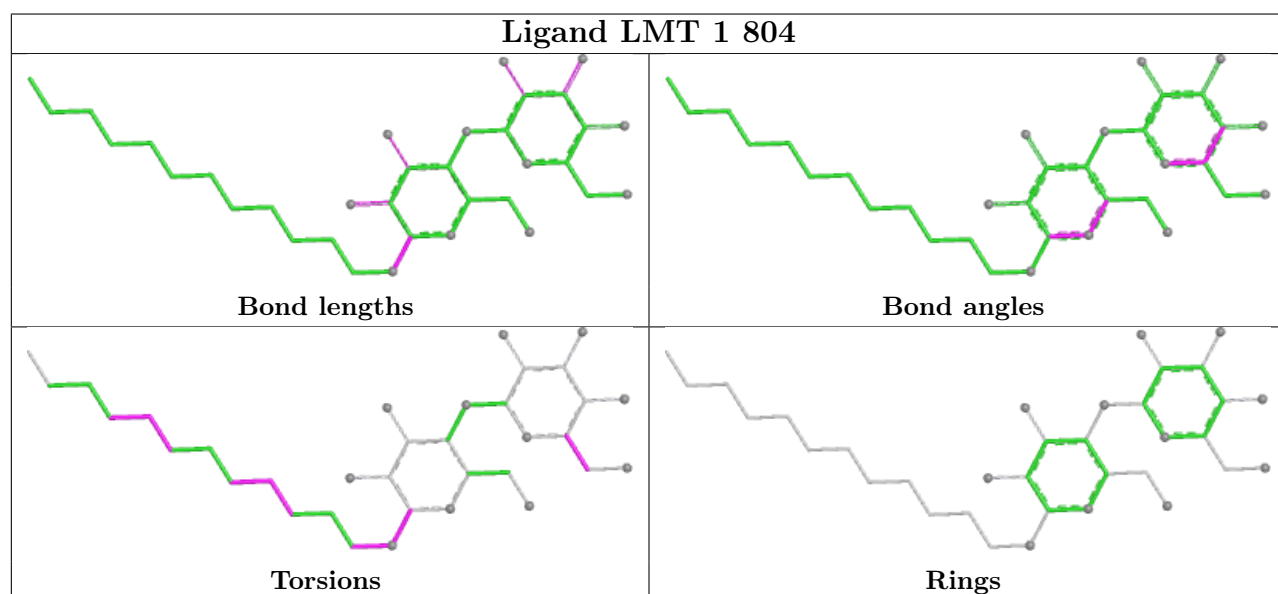
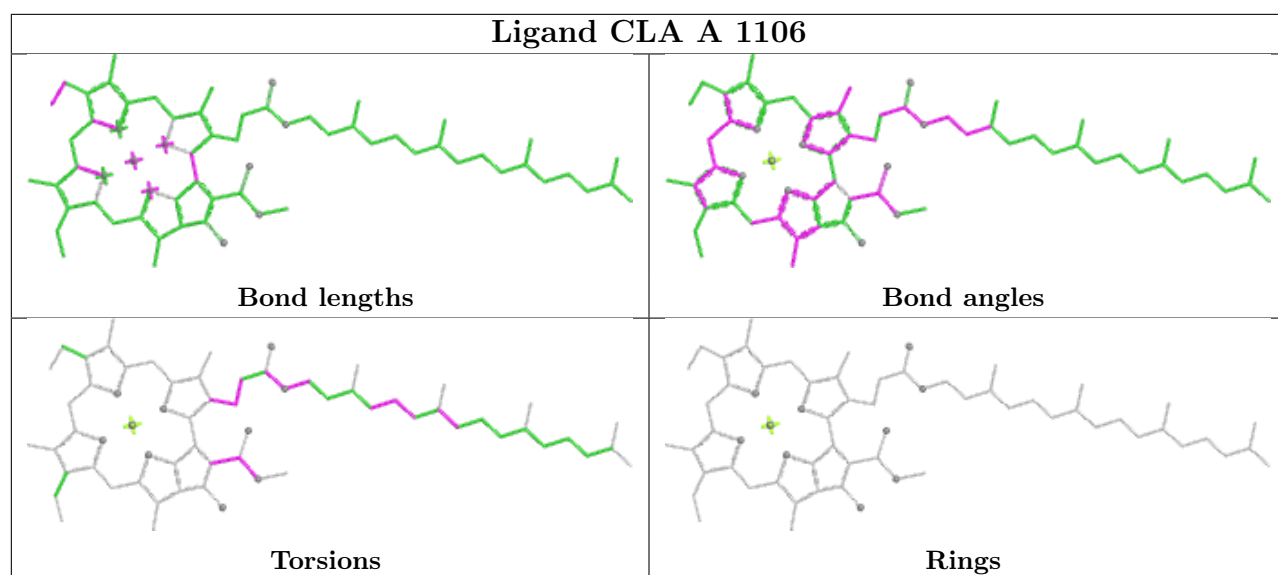


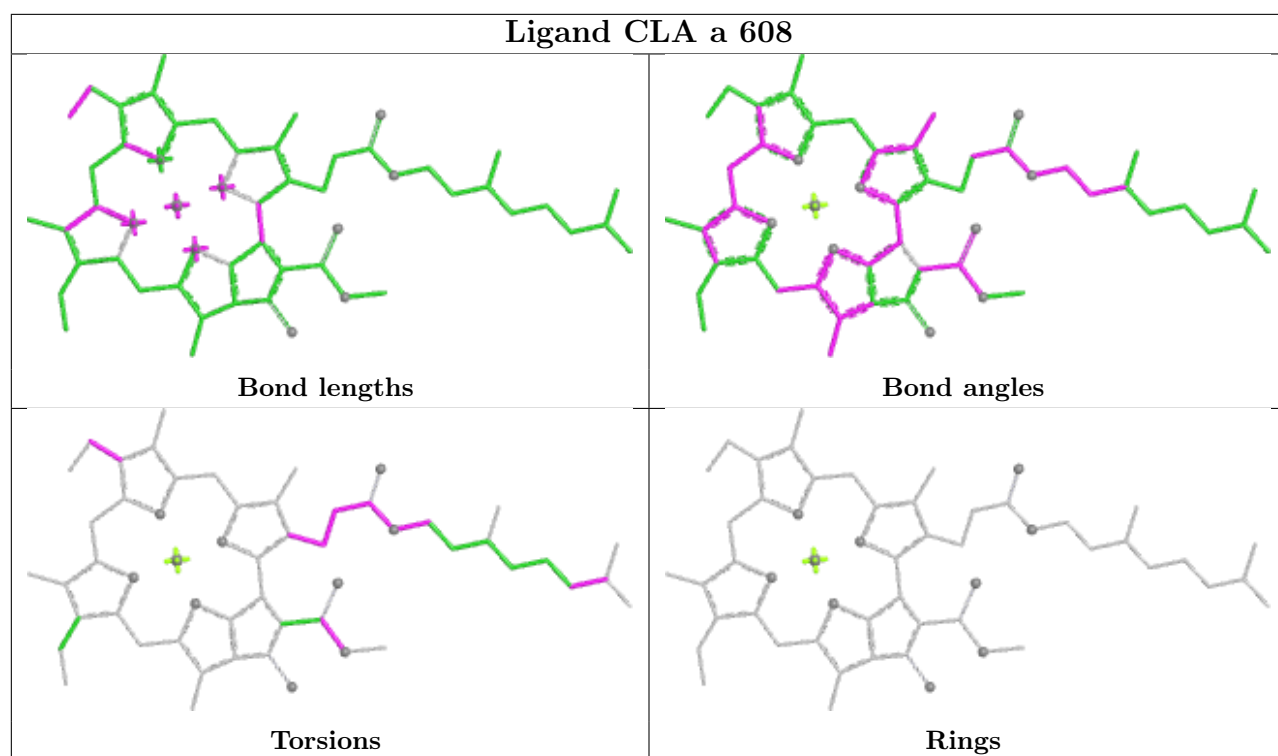
Torsions



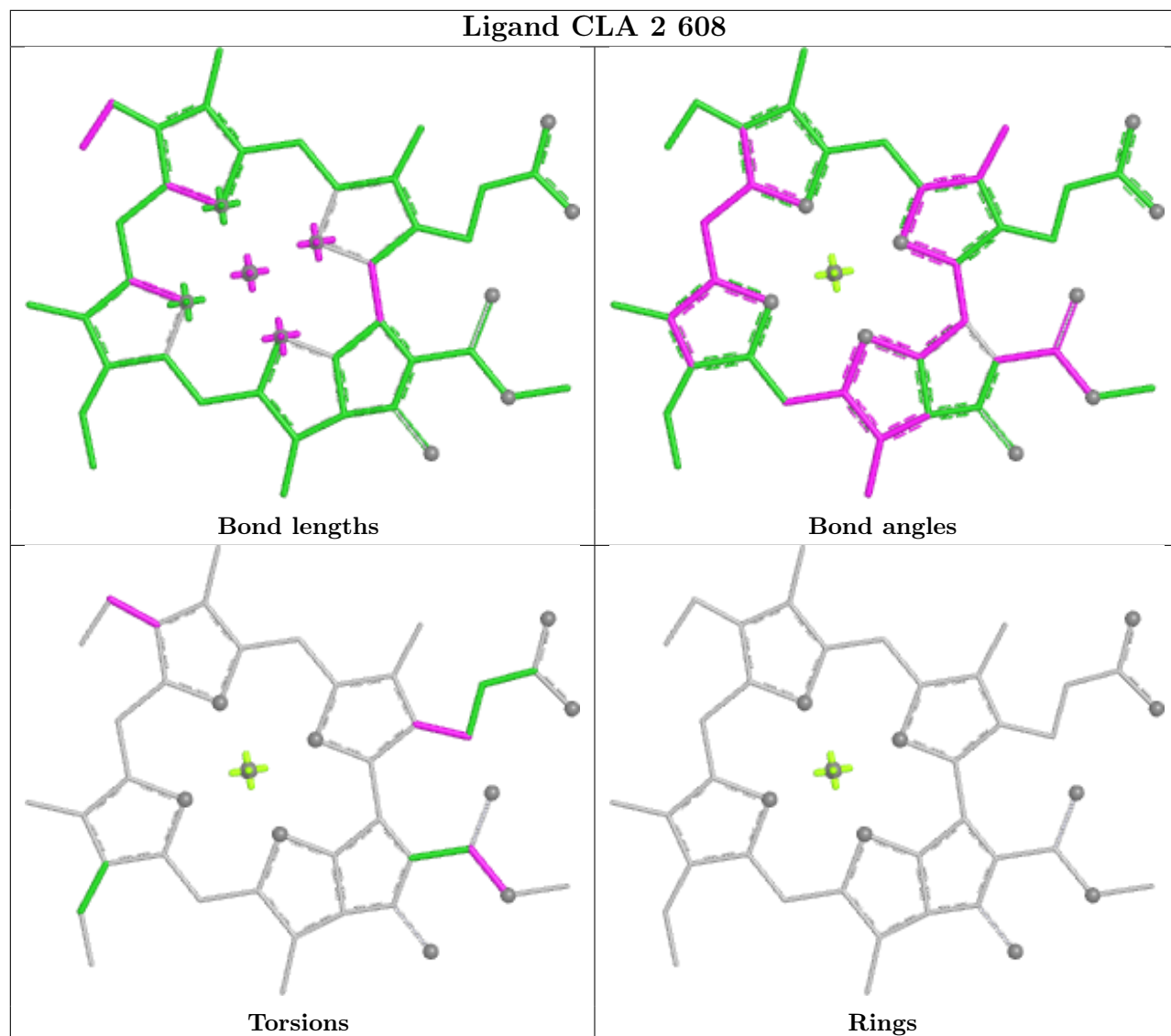
Rings

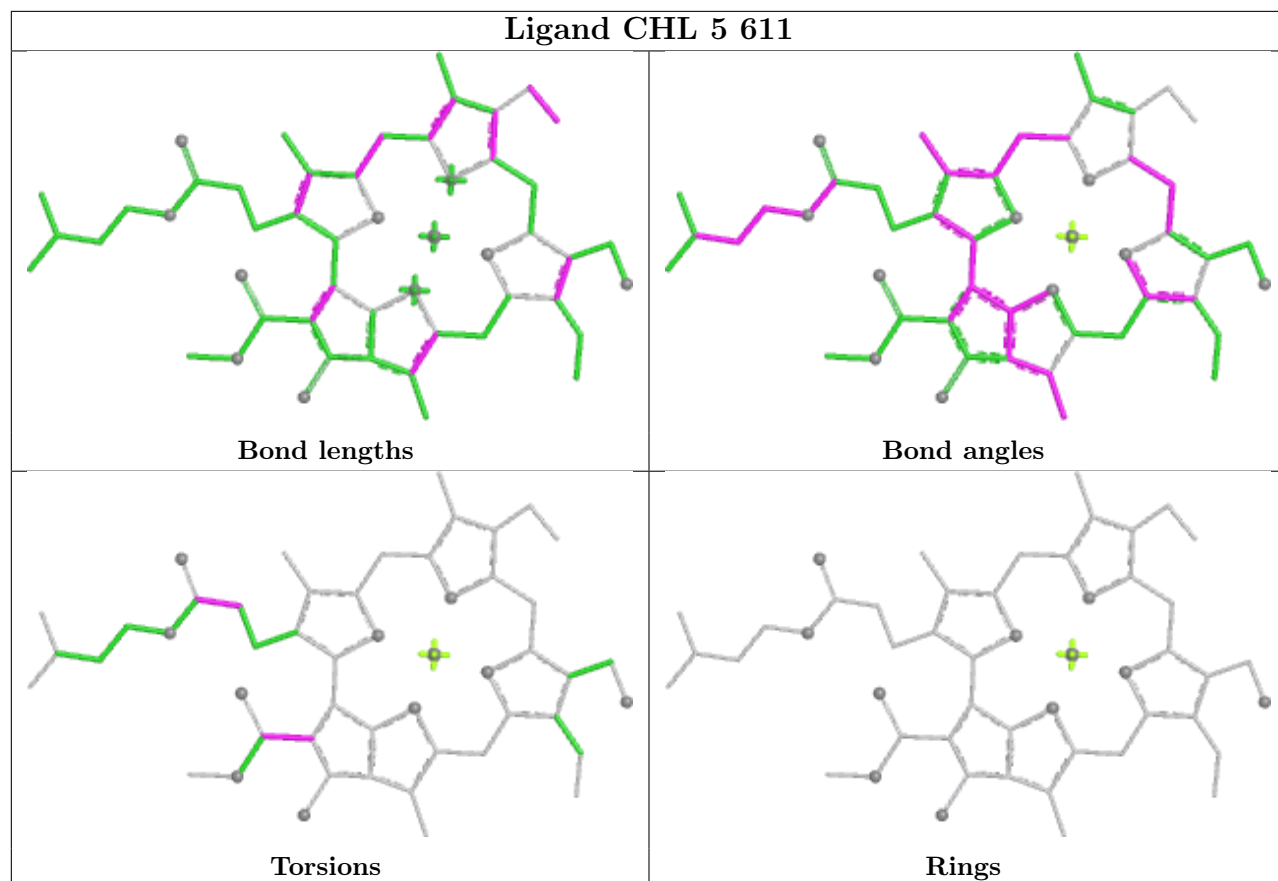


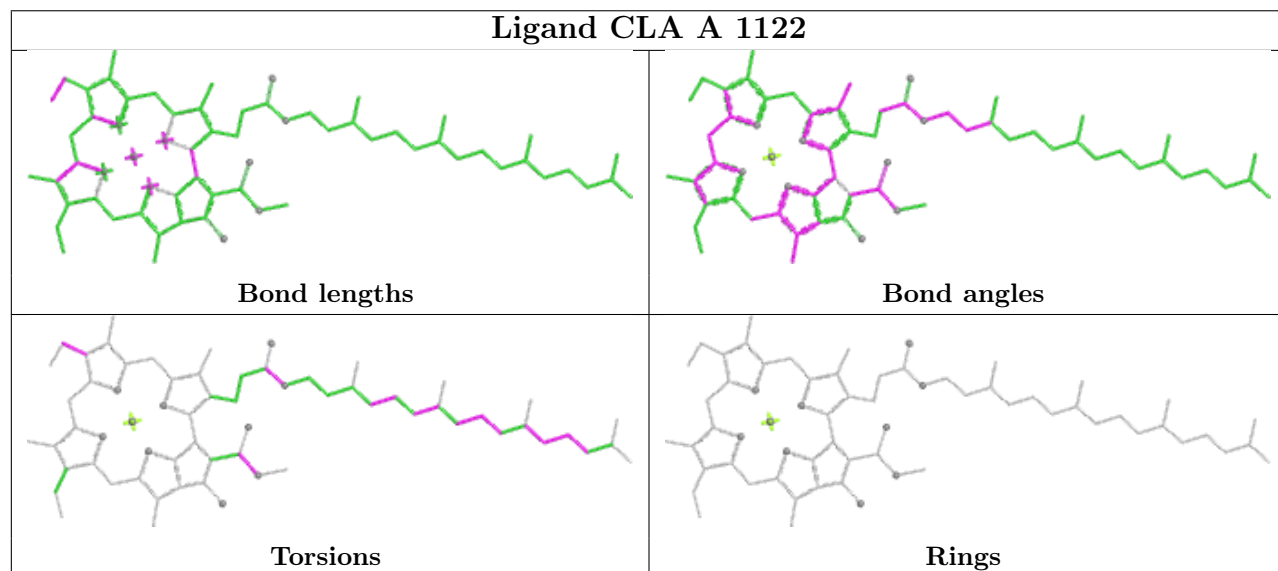
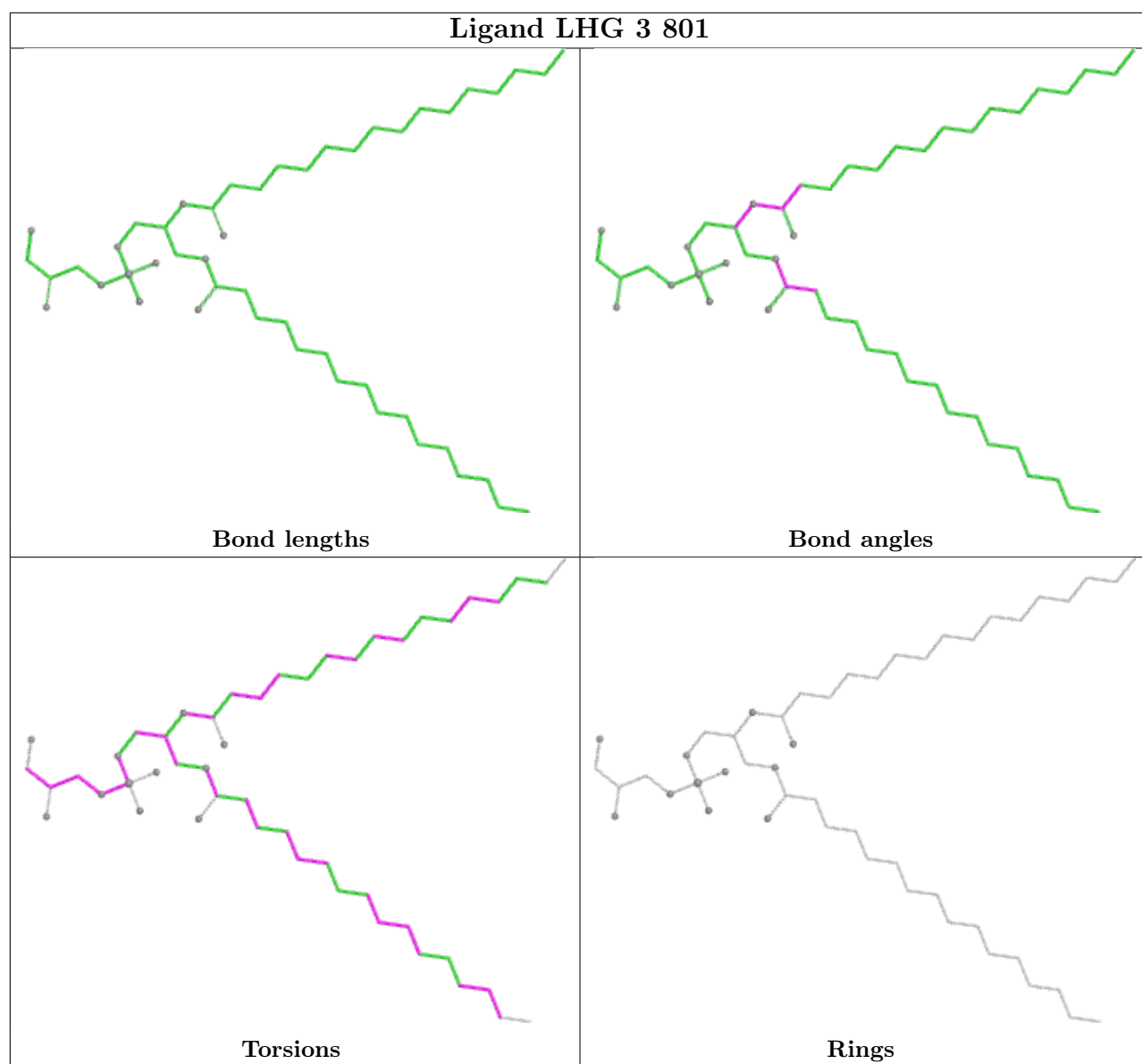


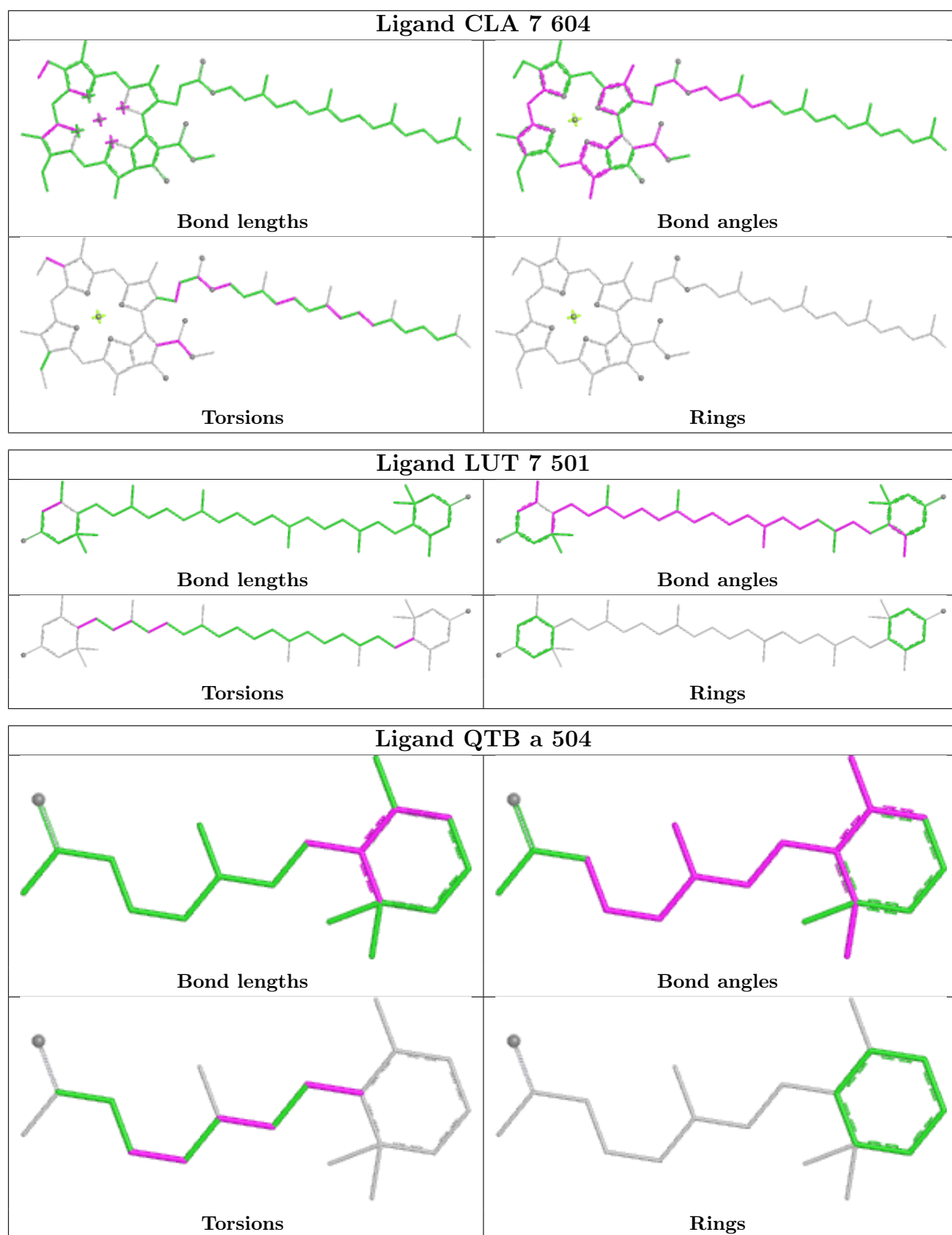


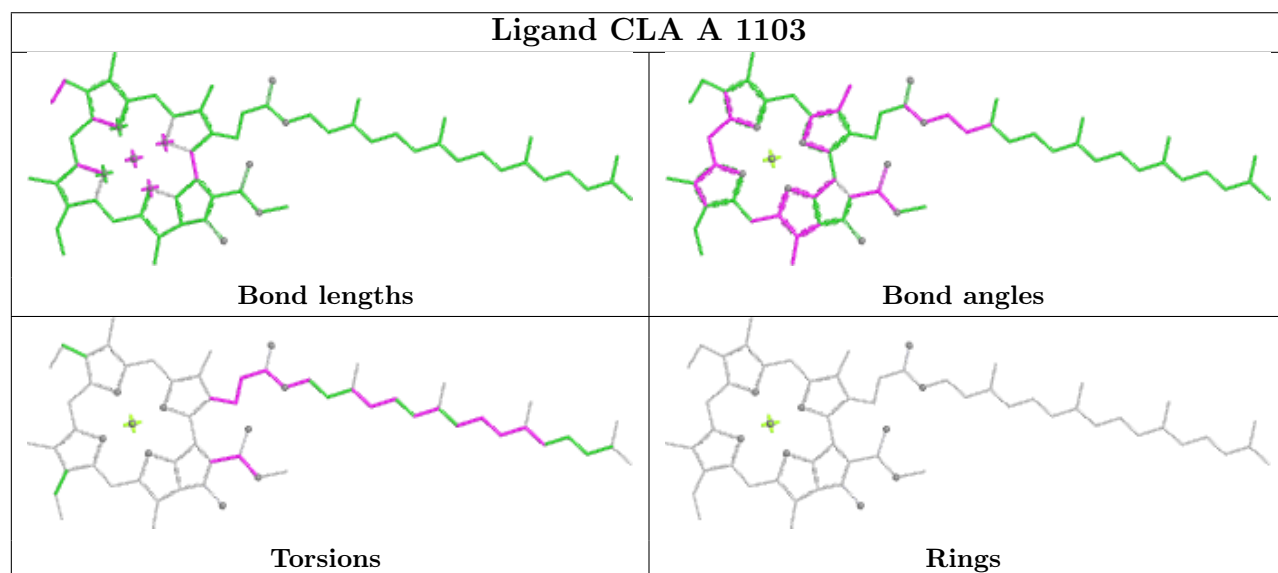
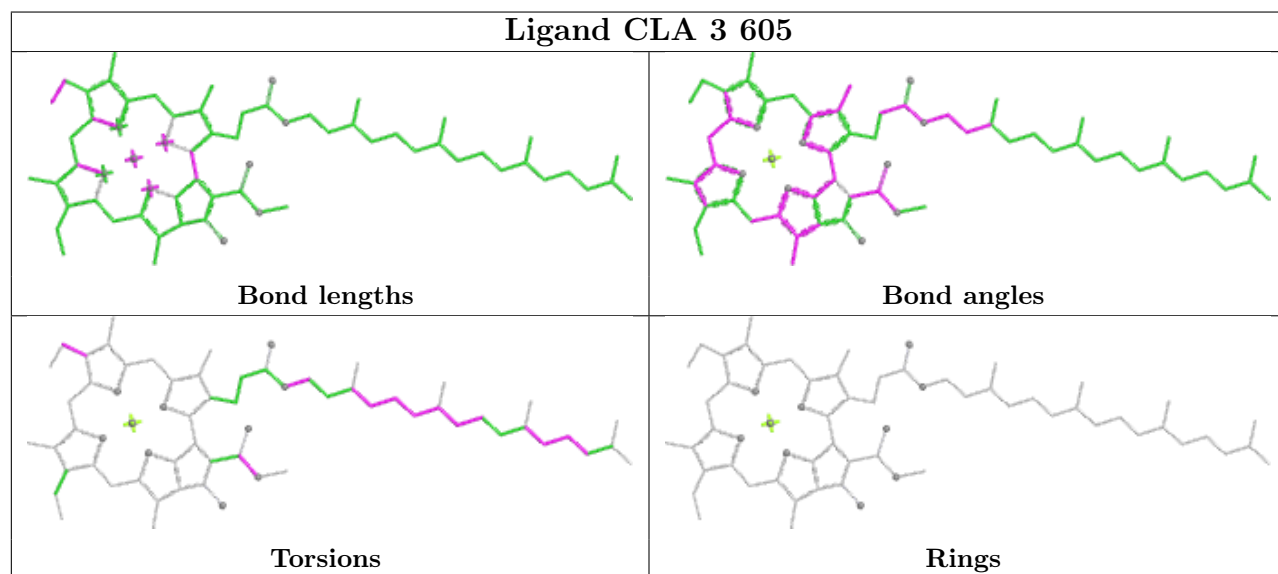
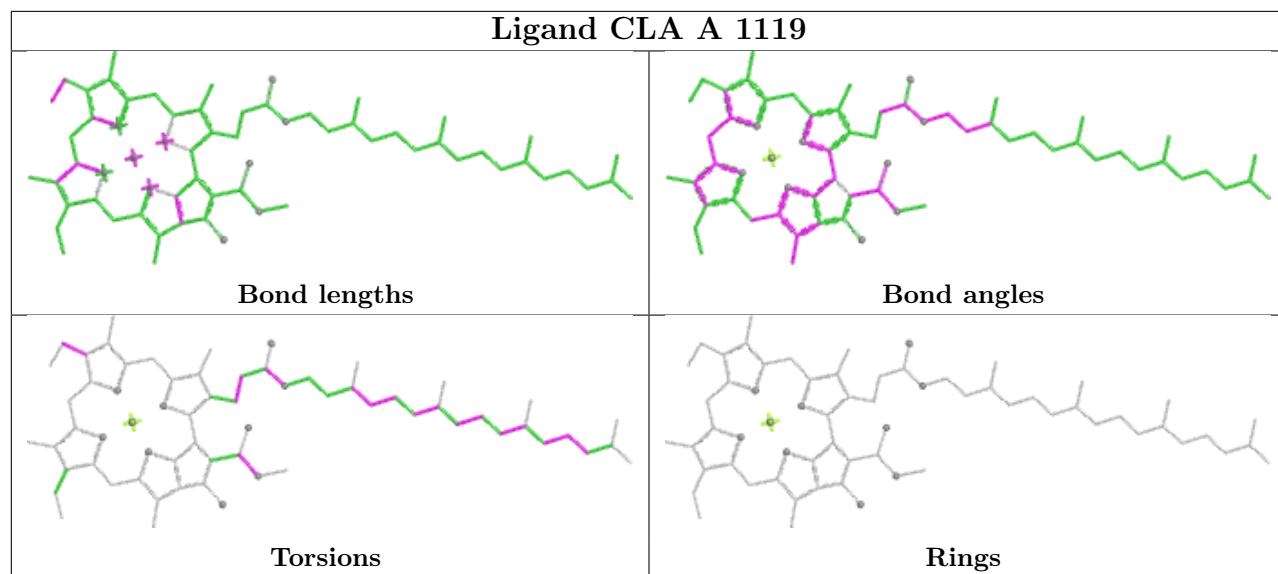
Ligand CLA 2 608

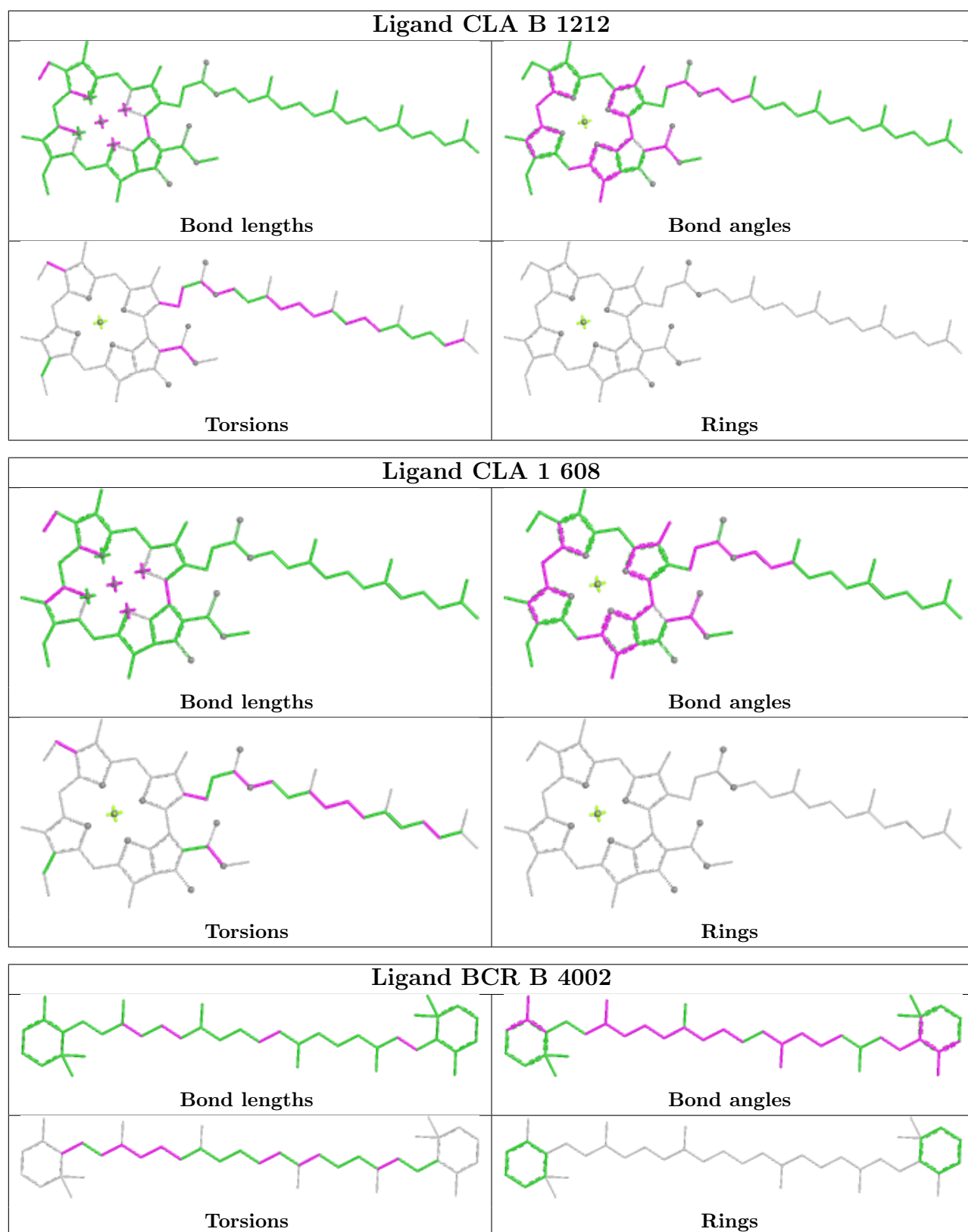




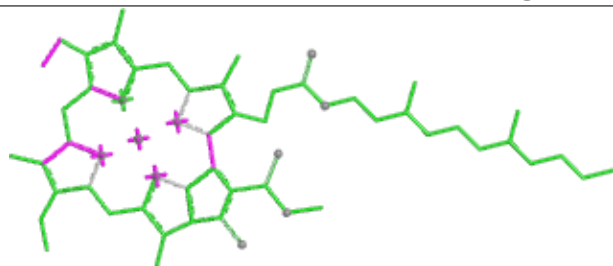




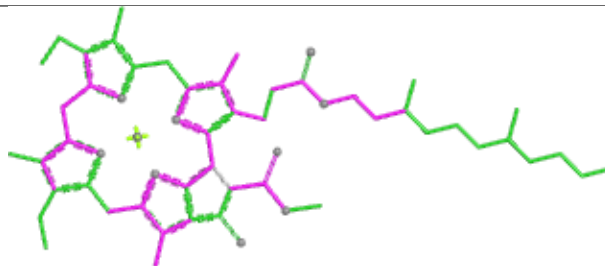




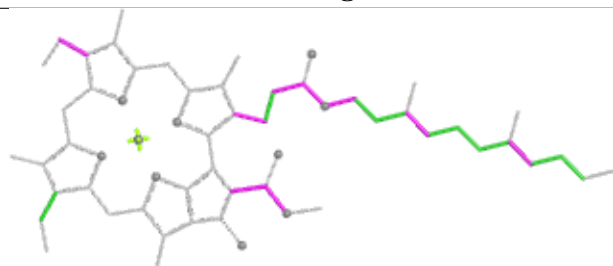
Ligand CLA a 607



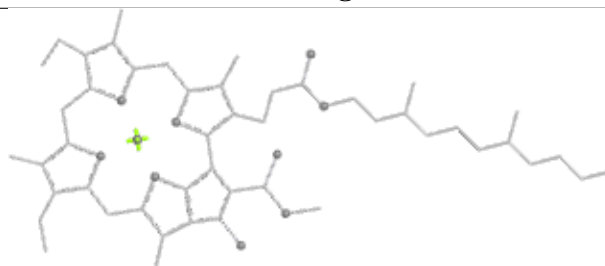
Bond lengths



Bond angles

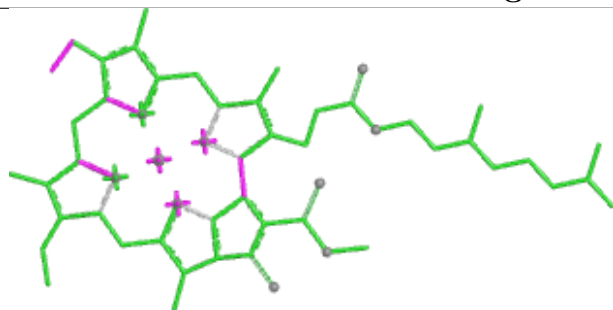


Torsions

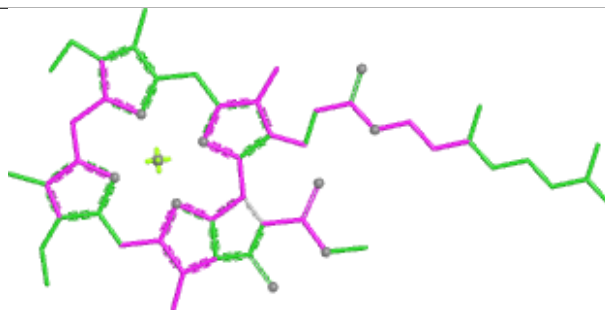


Rings

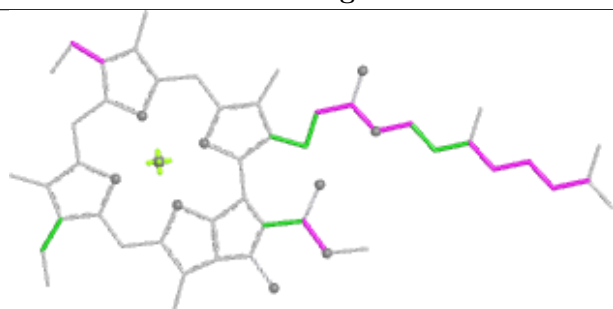
Ligand CLA A 1112



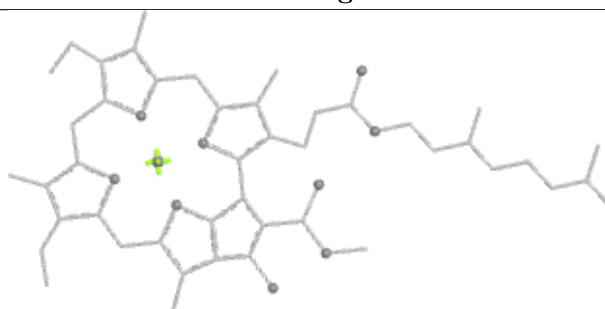
Bond lengths



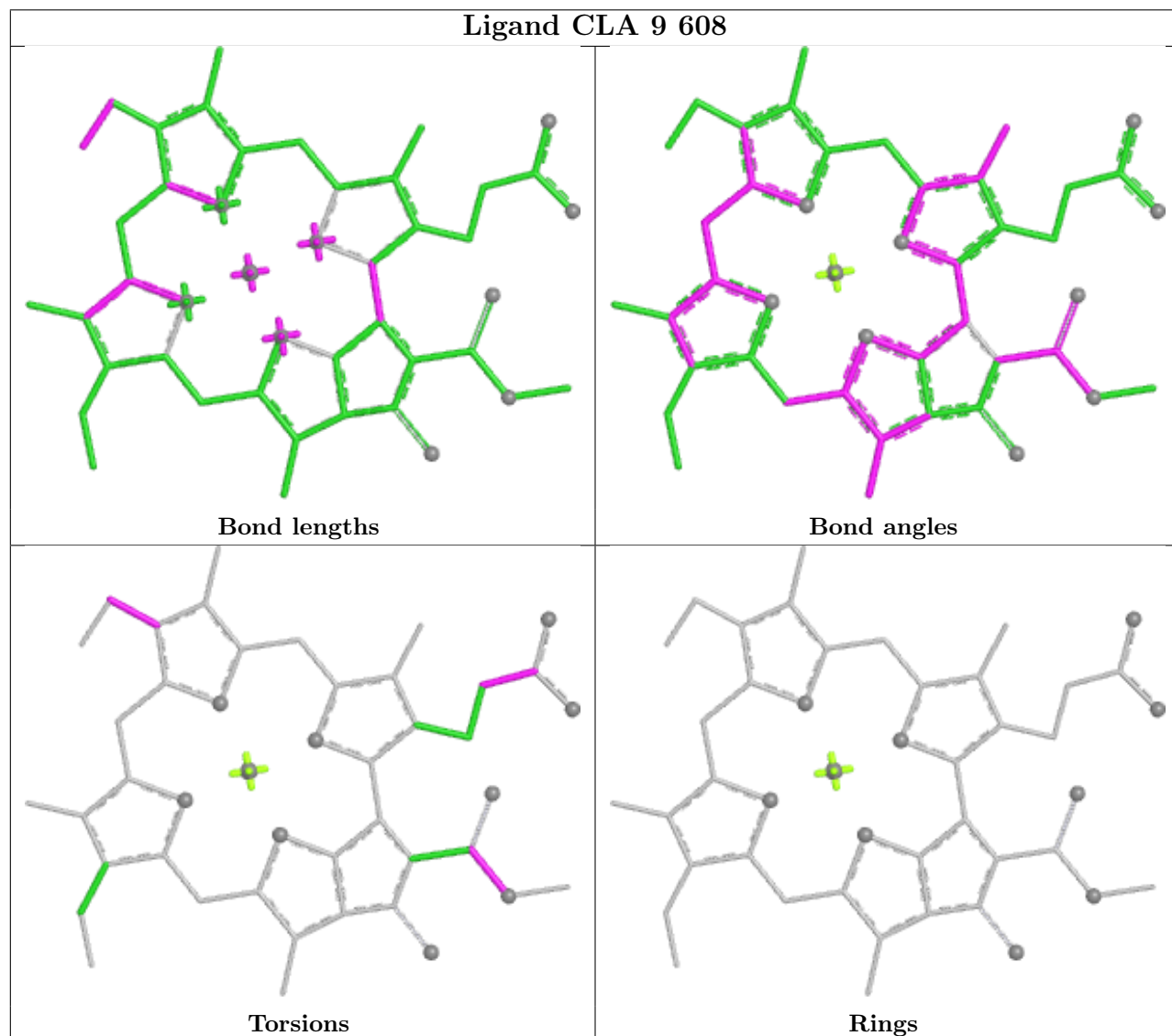
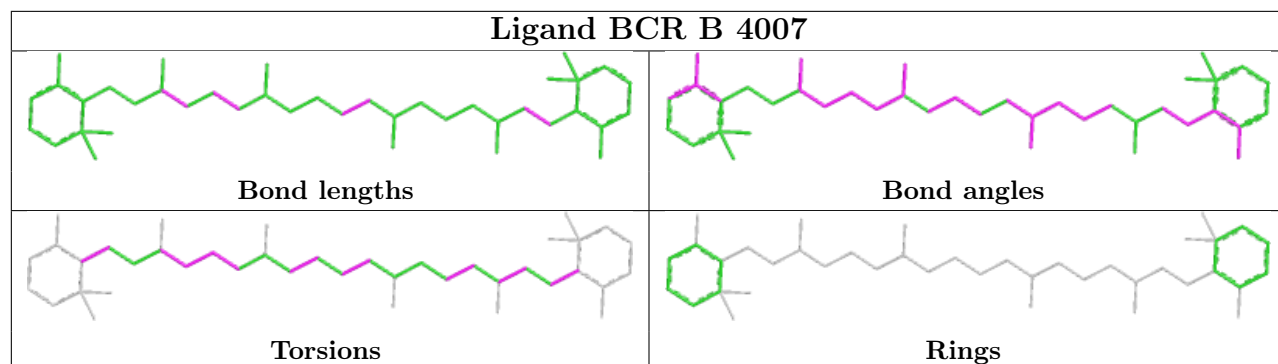
Bond angles

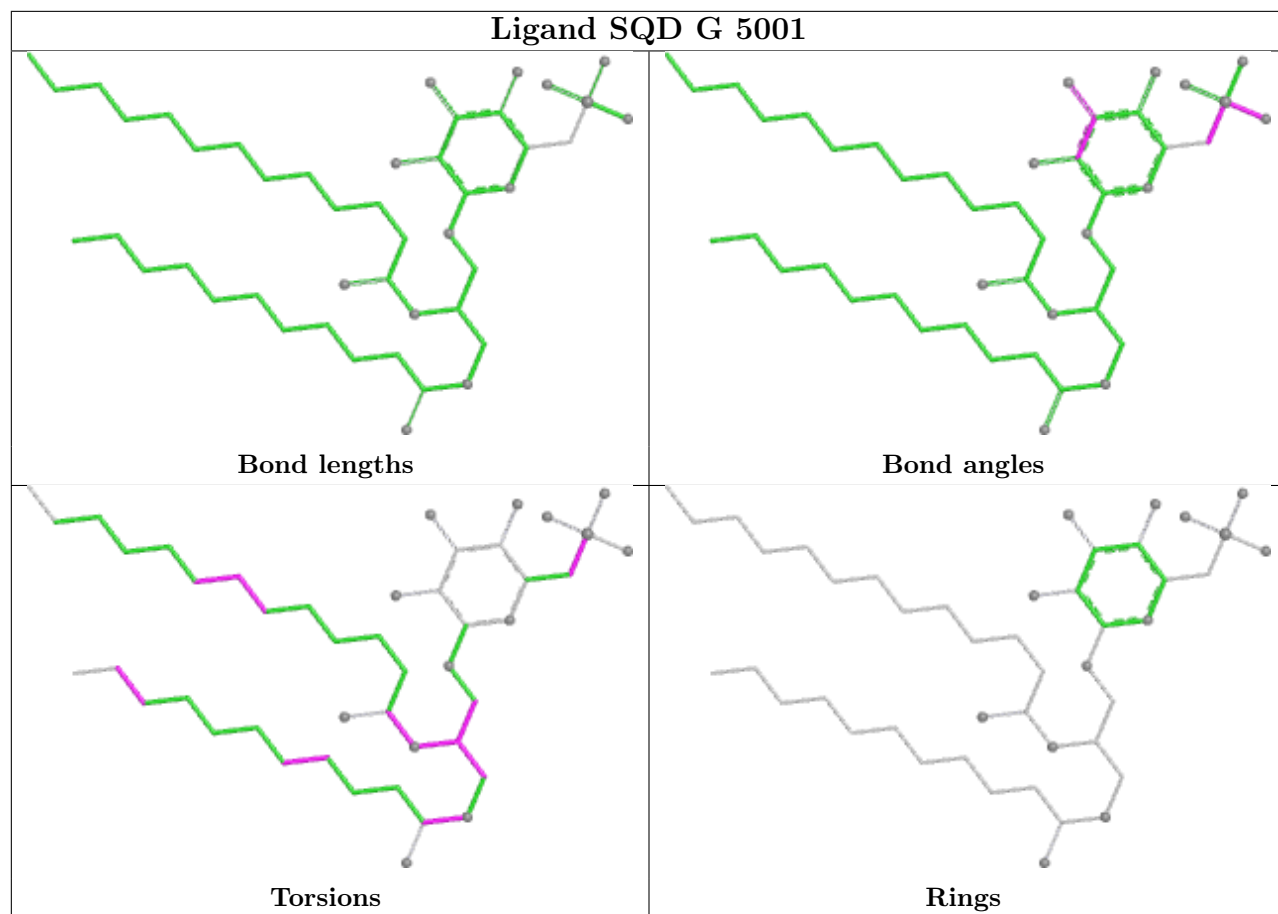


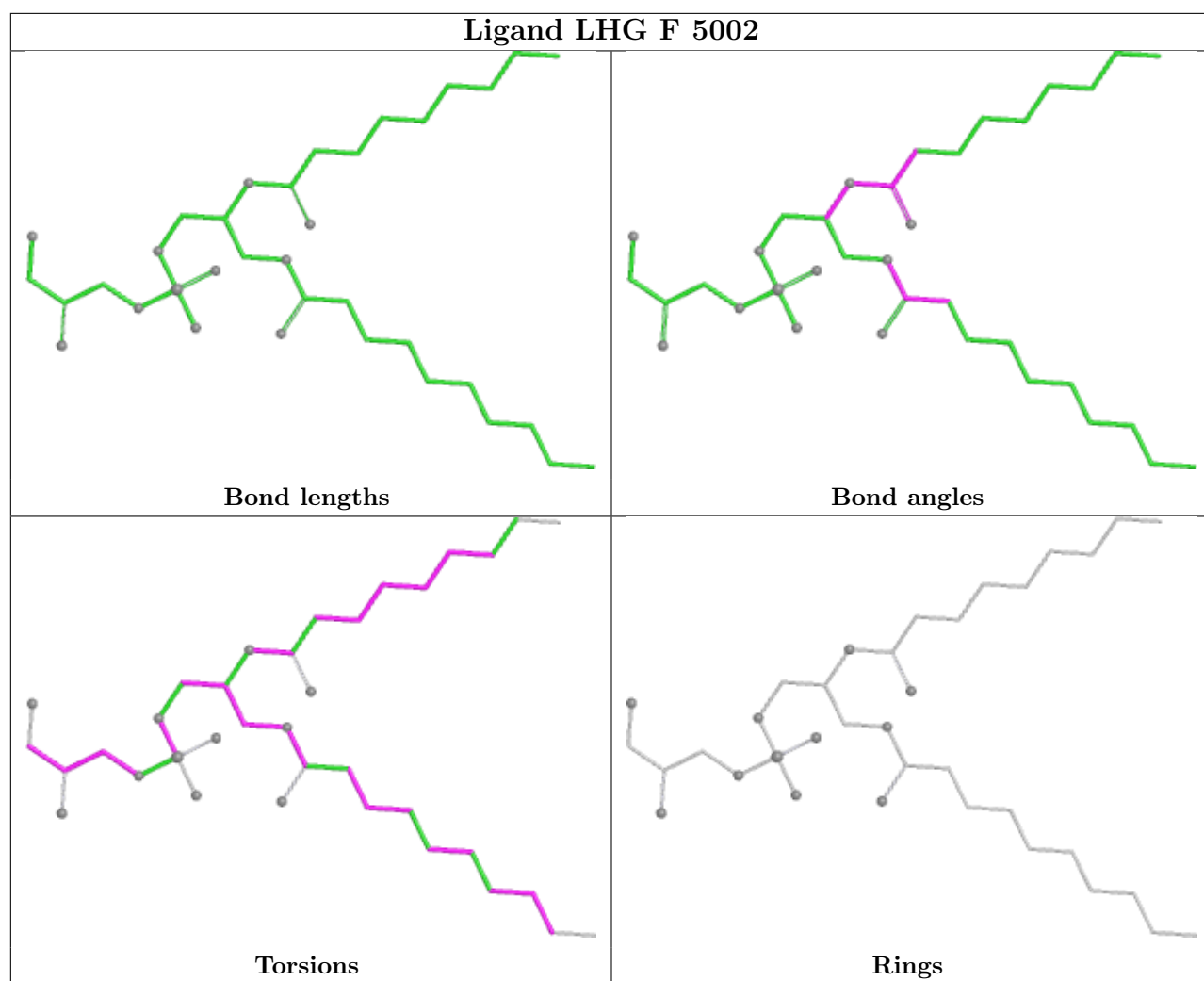
Torsions



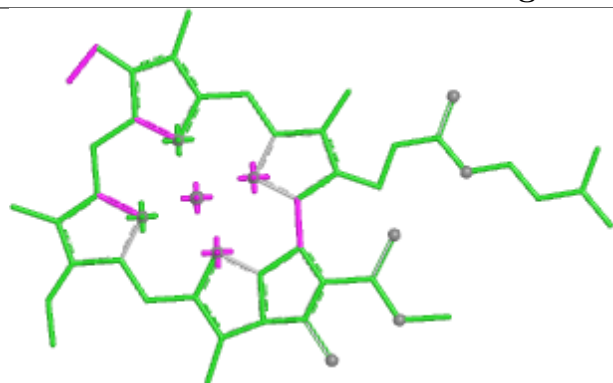
Rings



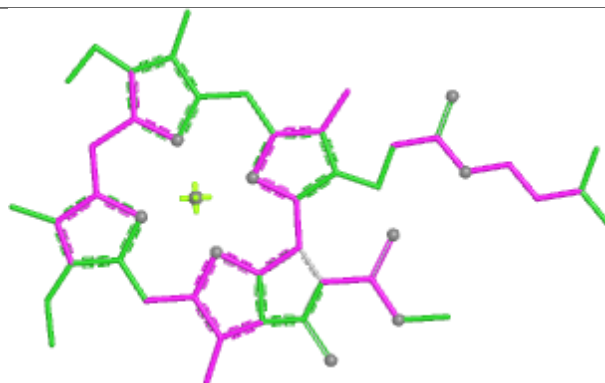




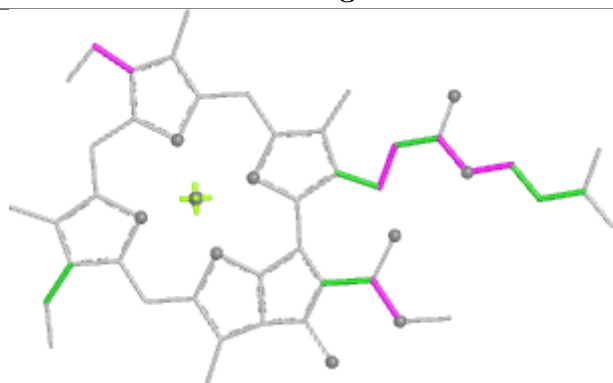
Ligand CLA 8 611



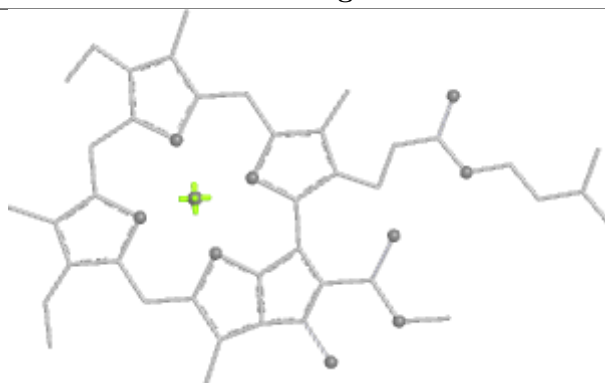
Bond lengths



Bond angles

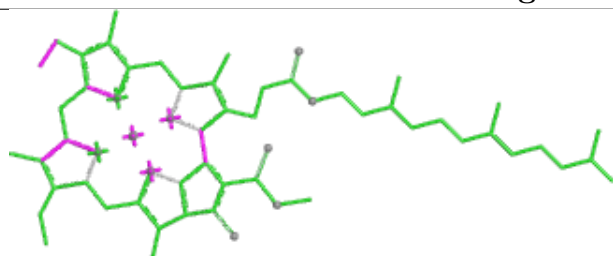


Torsions

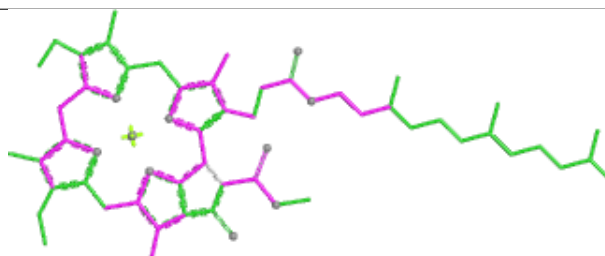


Rings

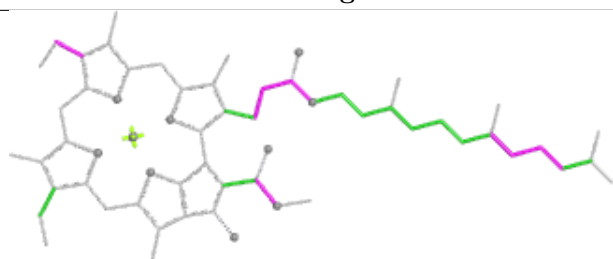
Ligand CLA 7 612



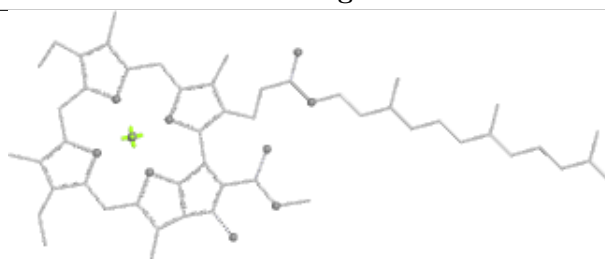
Bond lengths



Bond angles

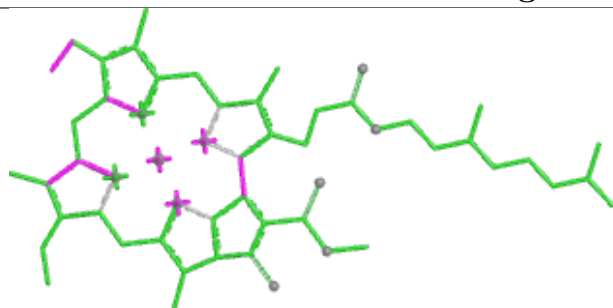


Torsions

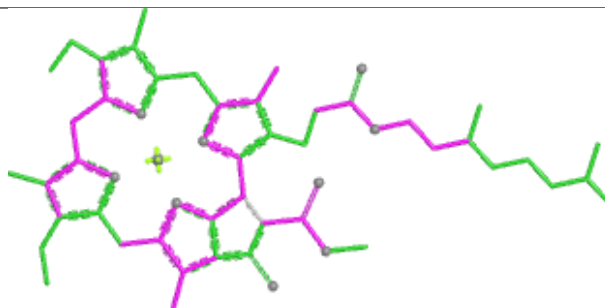


Rings

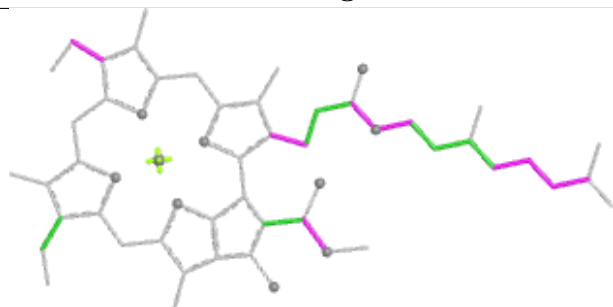
Ligand CLA 6 607



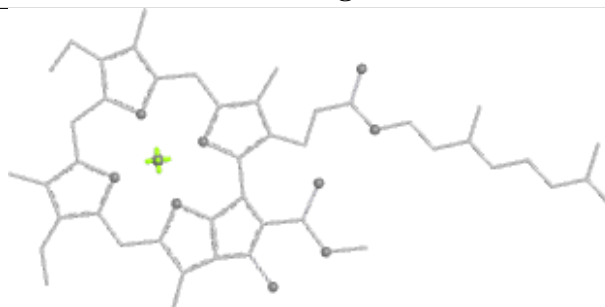
Bond lengths



Bond angles

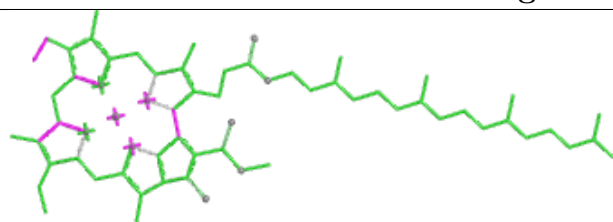


Torsions

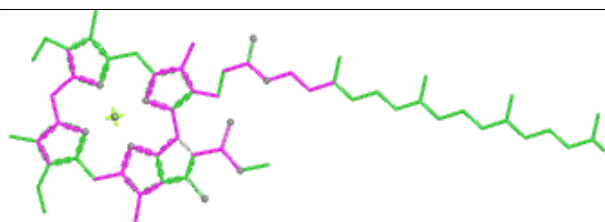


Rings

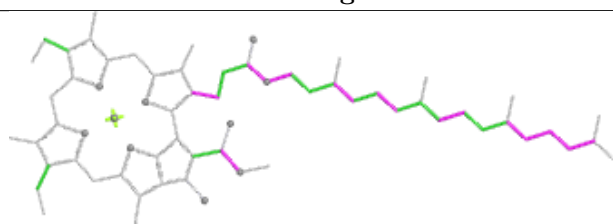
Ligand CLA 9 612



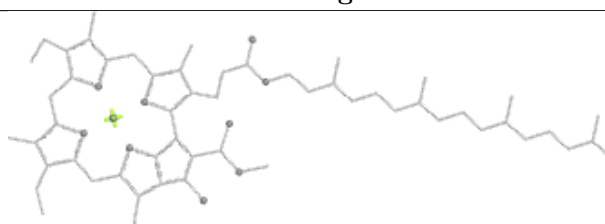
Bond lengths



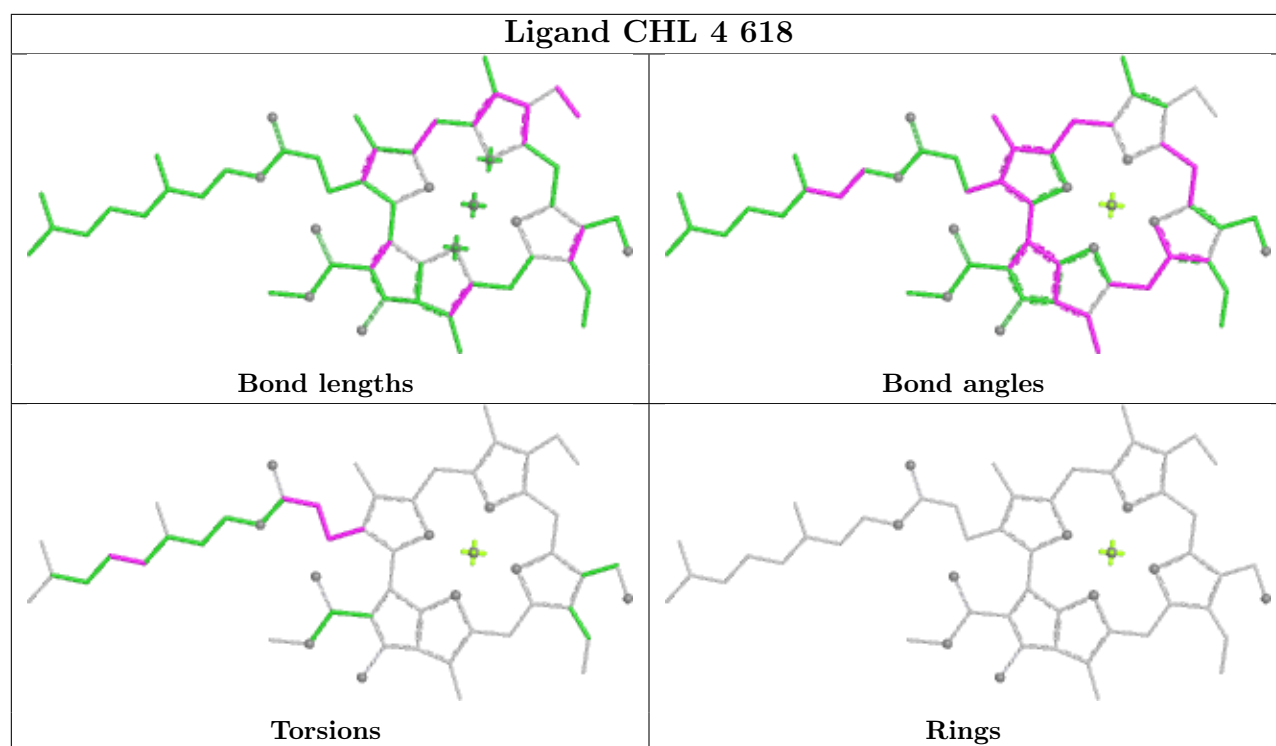
Bond angles

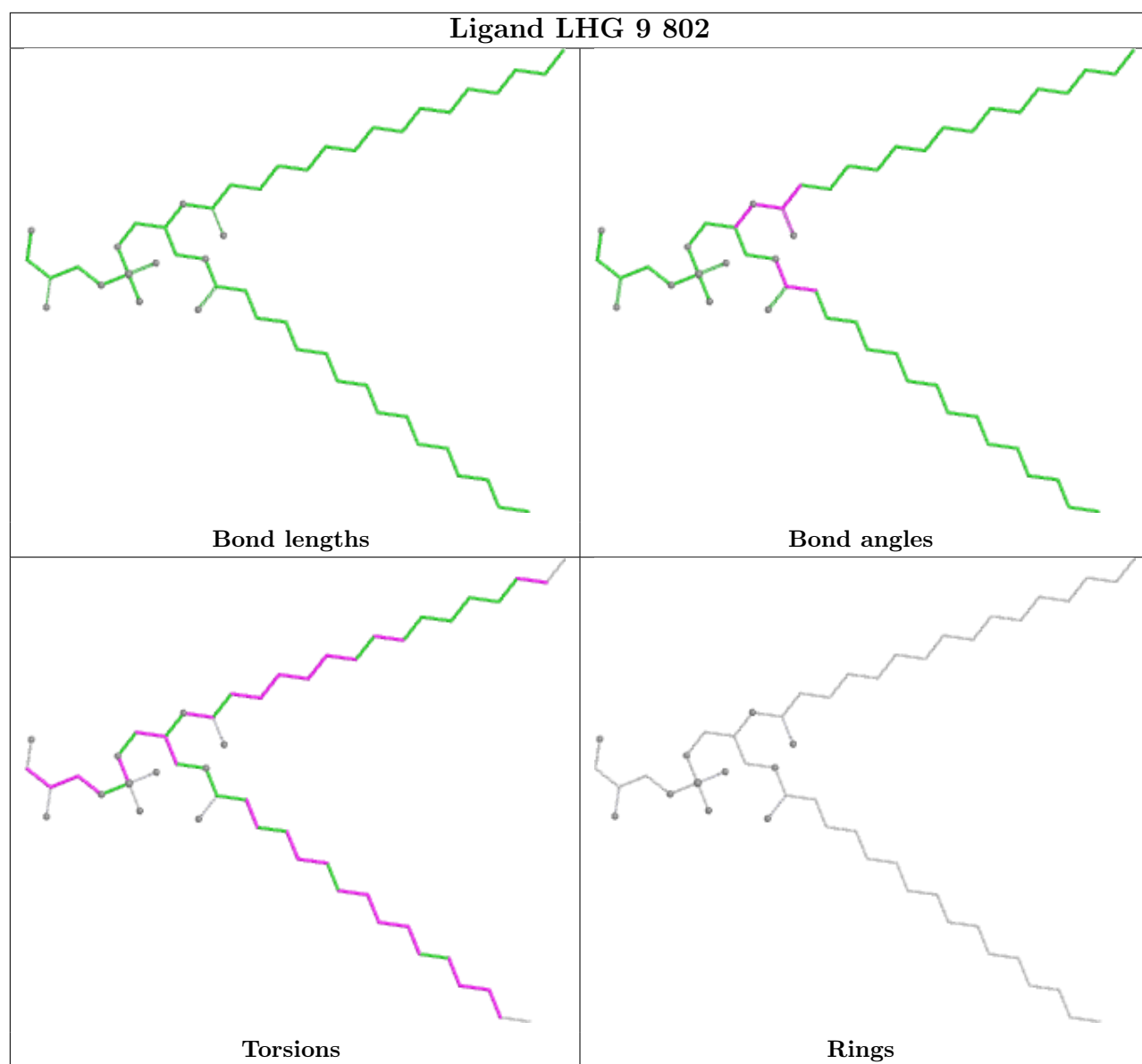


Torsions

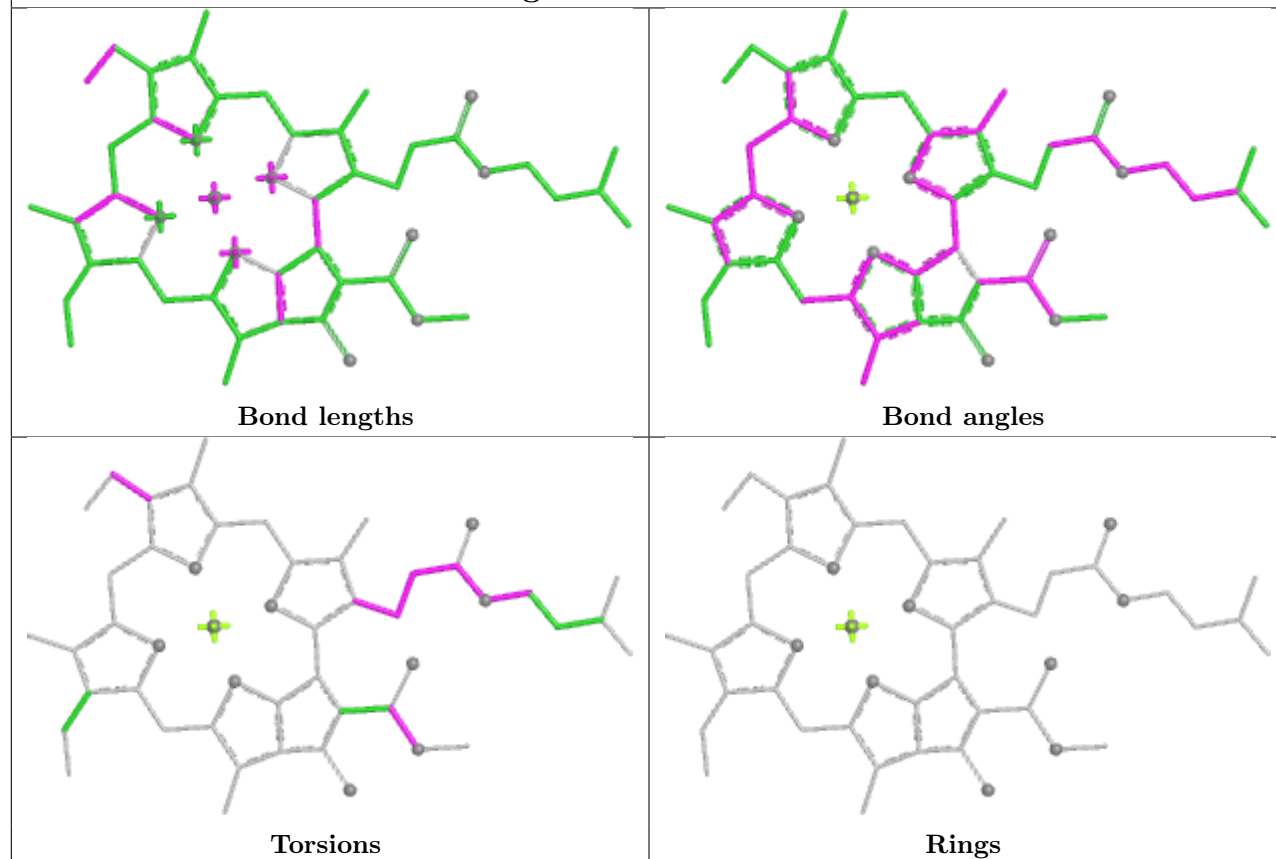


Rings

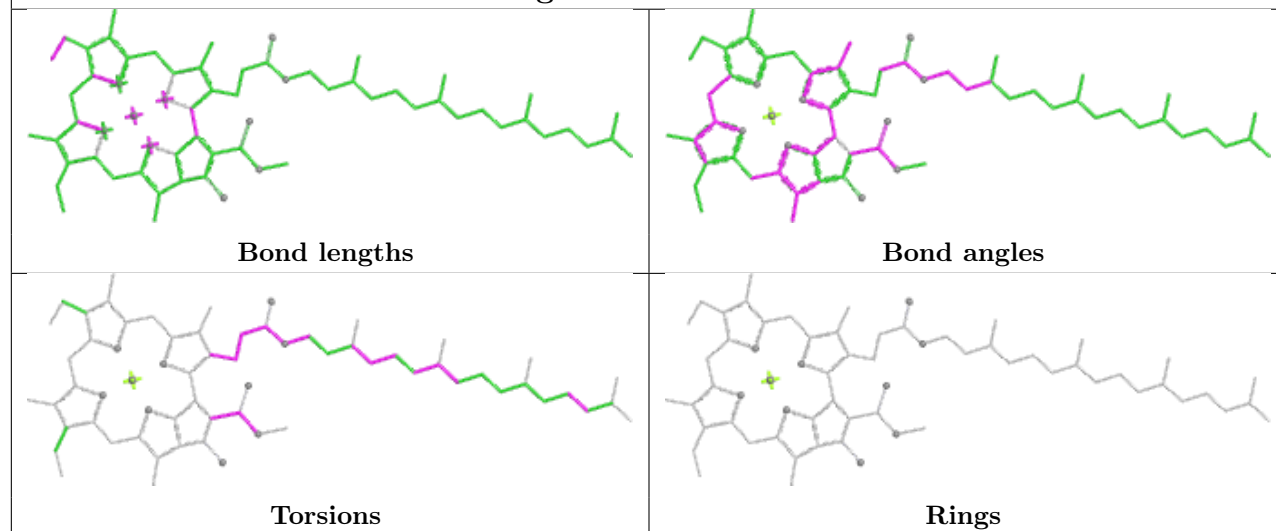


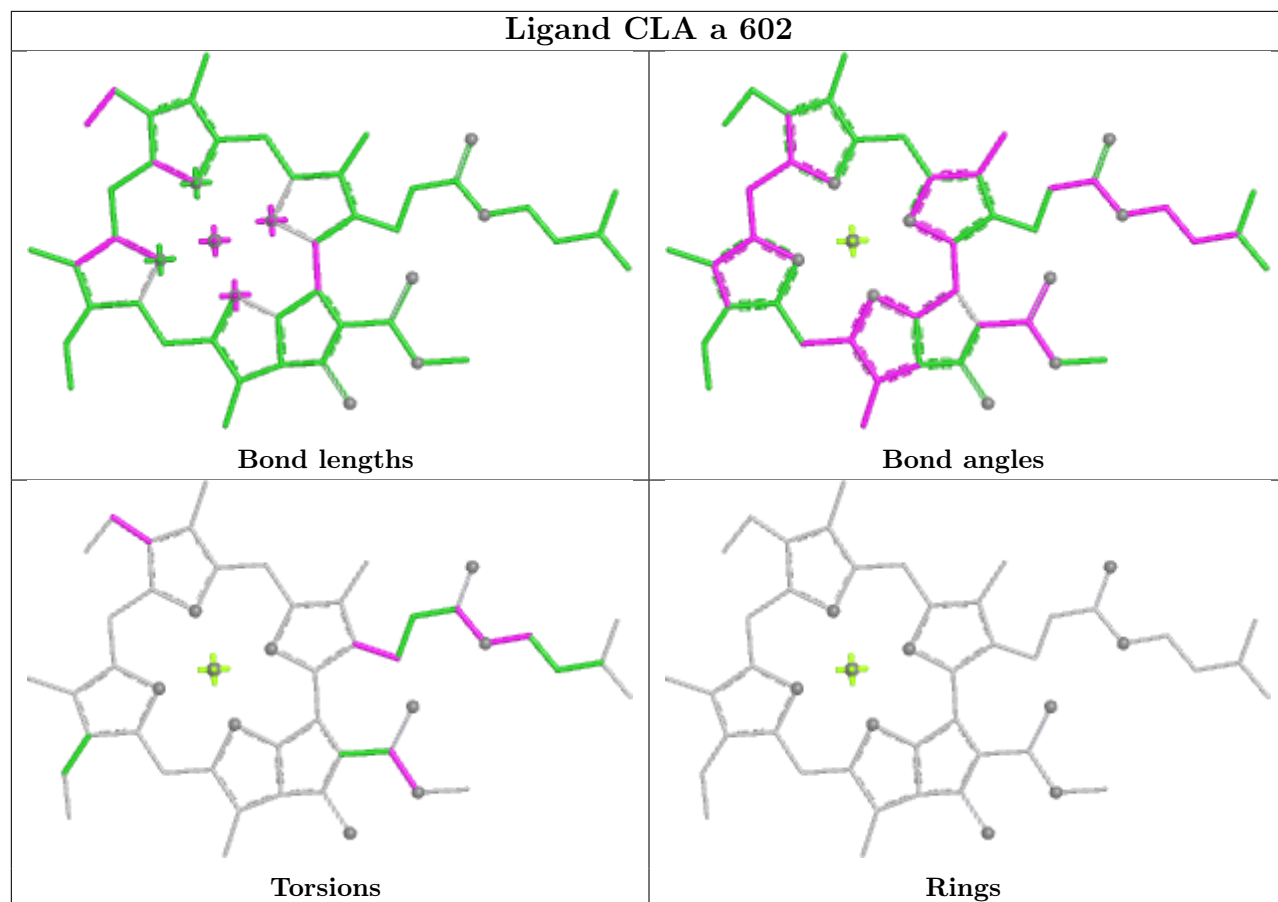


Ligand CLA A 1129

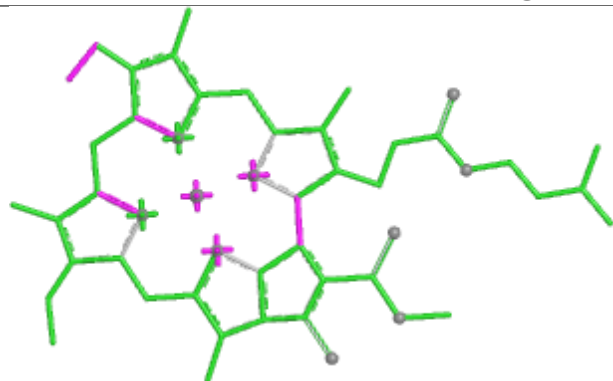


Ligand CLA 6 609

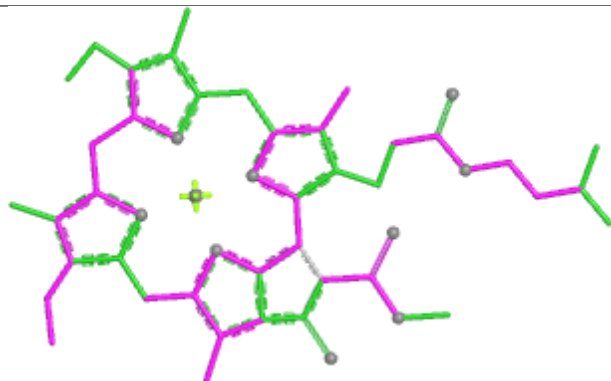




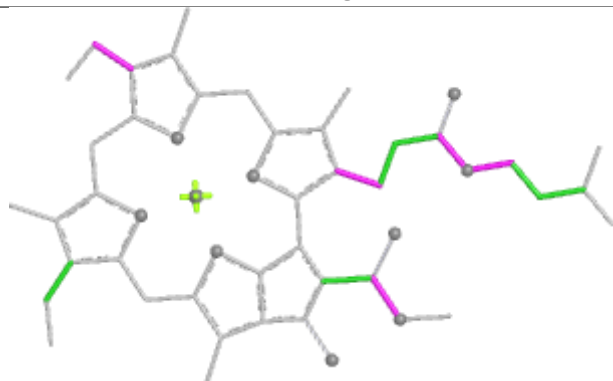
Ligand CLA 2 612



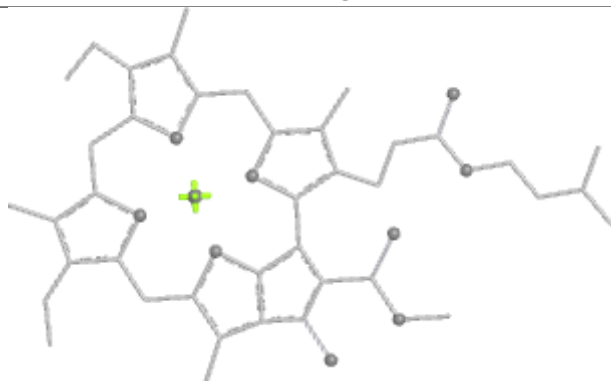
Bond lengths



Bond angles

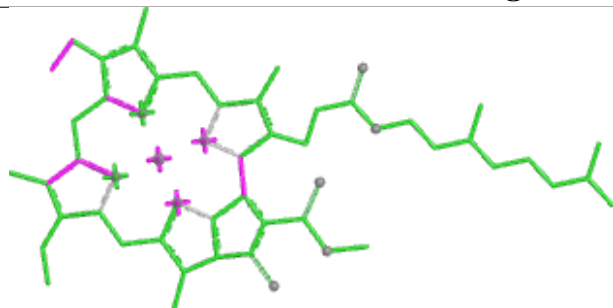


Torsions

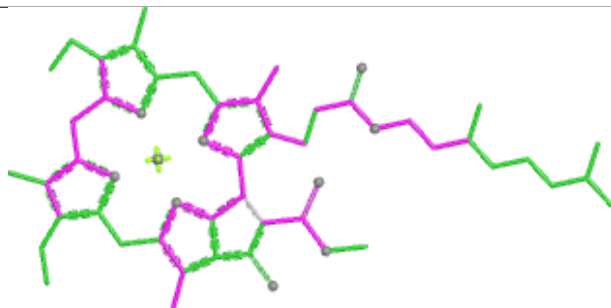


Rings

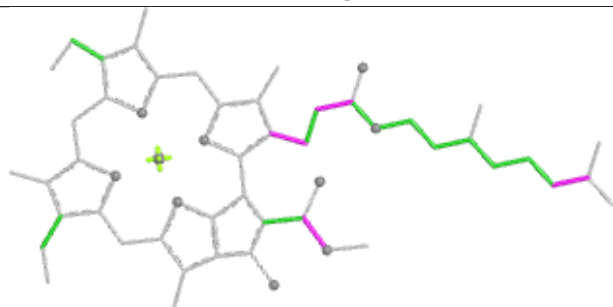
Ligand CLA A 1140



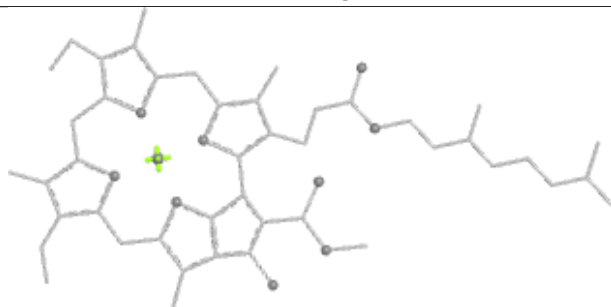
Bond lengths



Bond angles

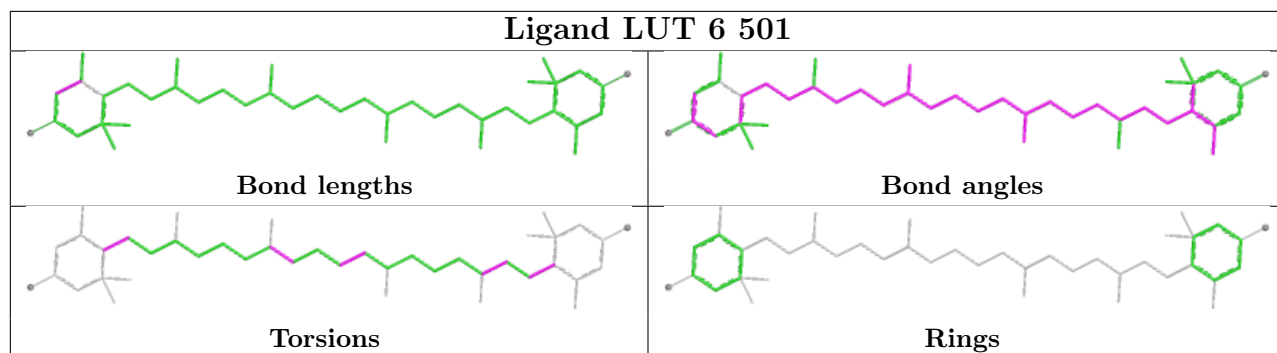


Torsions

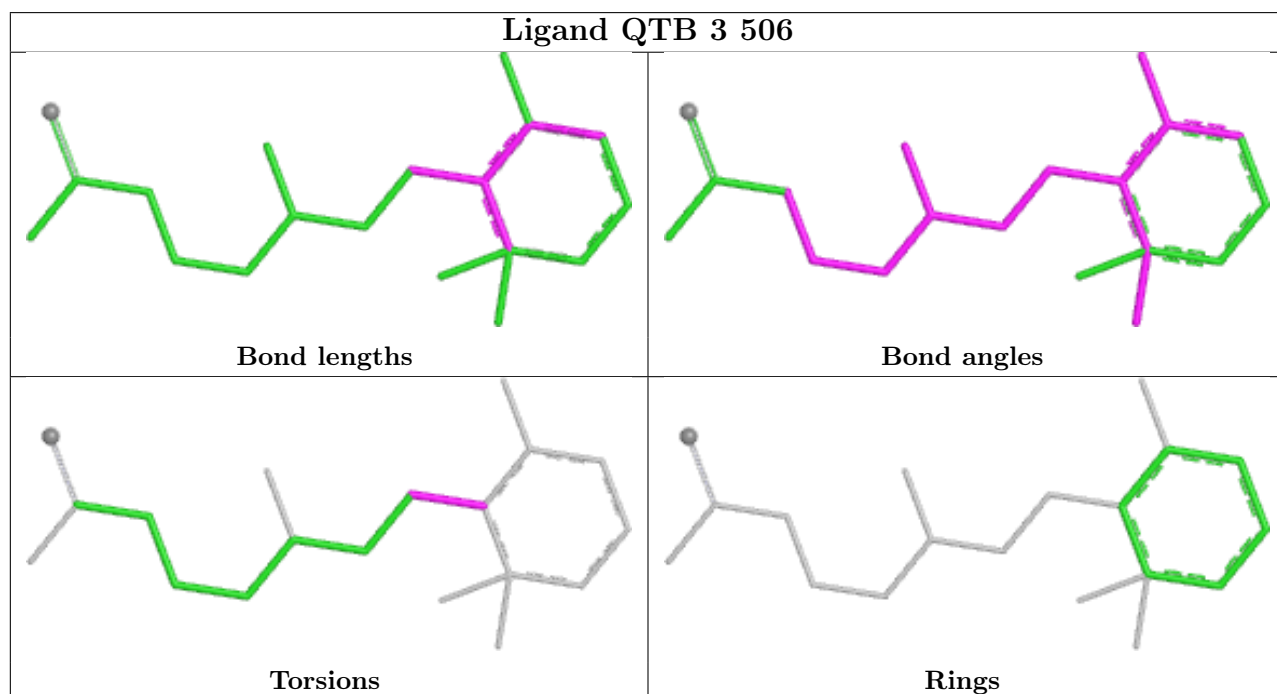


Rings

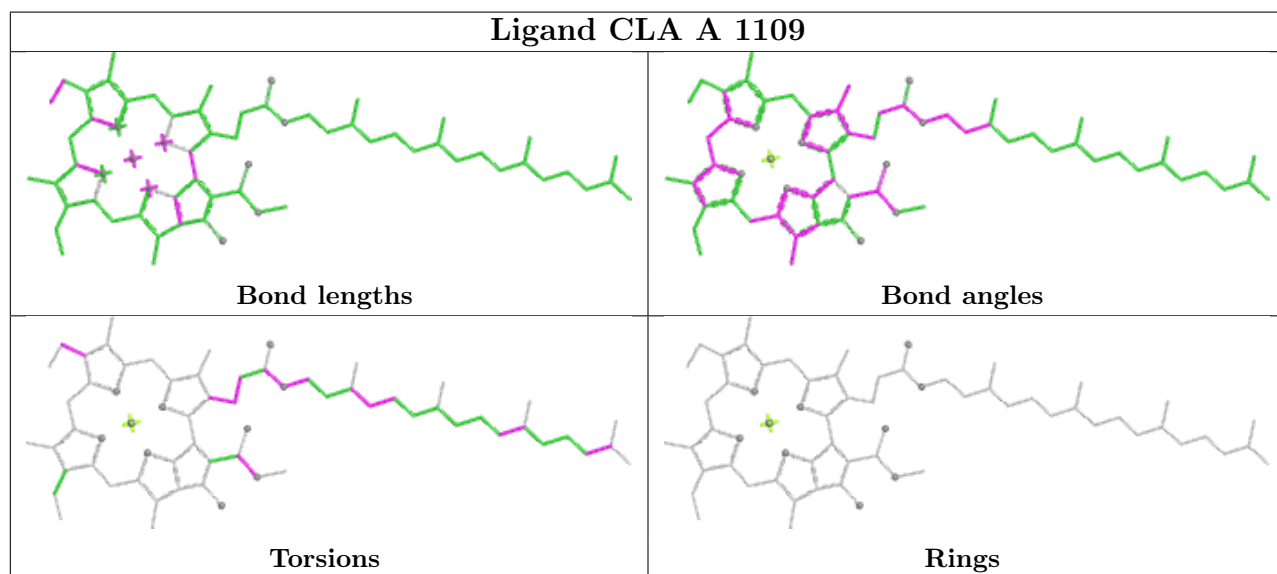
Ligand LUT 6 501



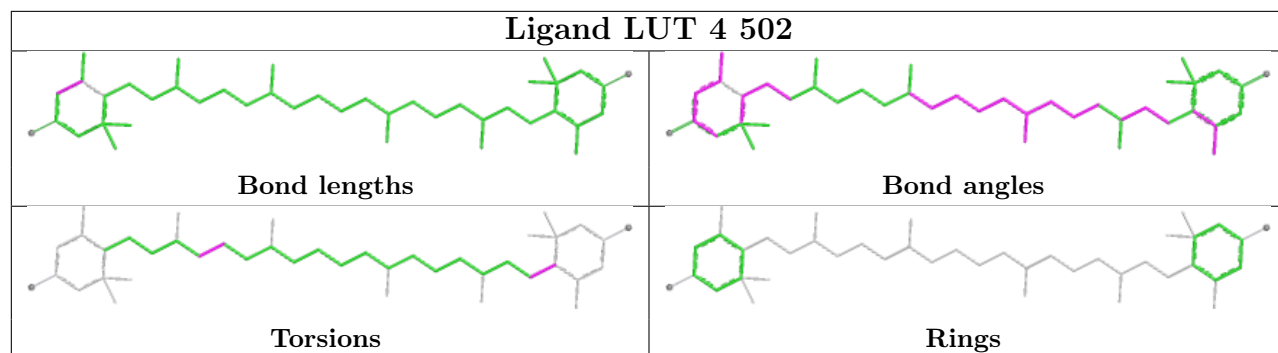
Ligand QTB 3 506



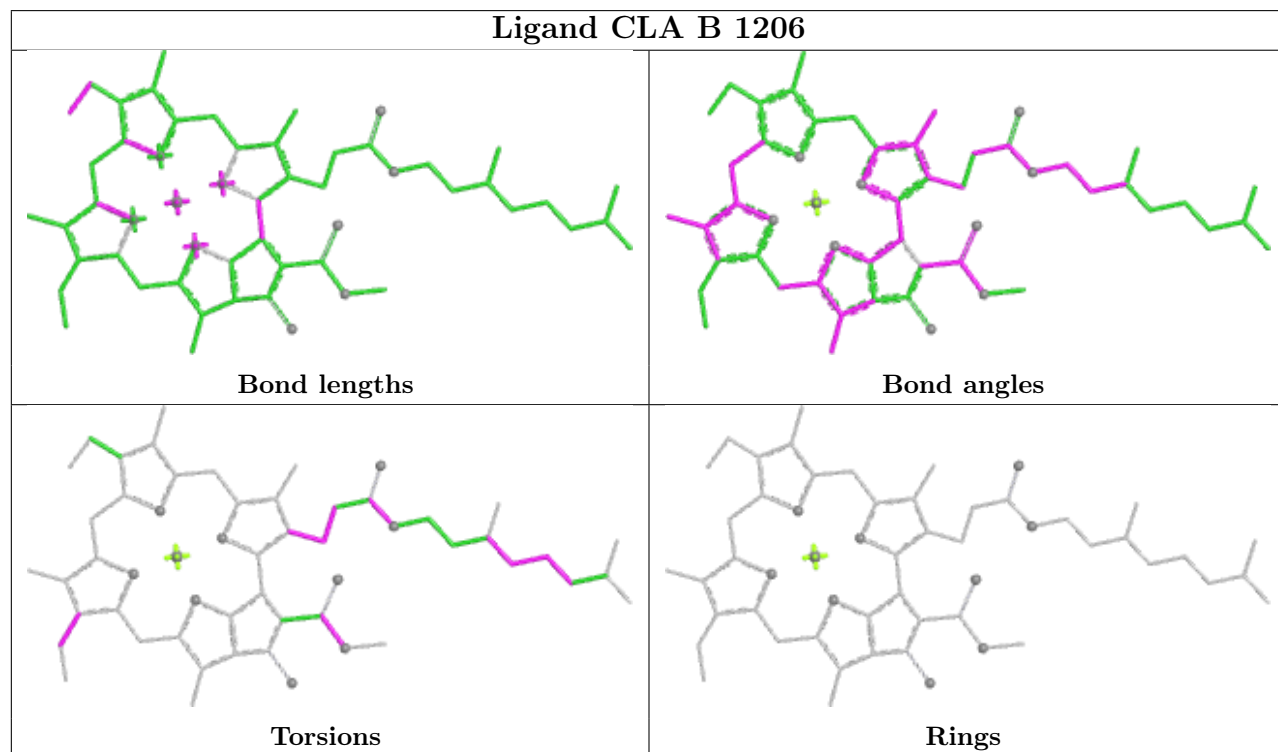
Ligand CLA A 1109



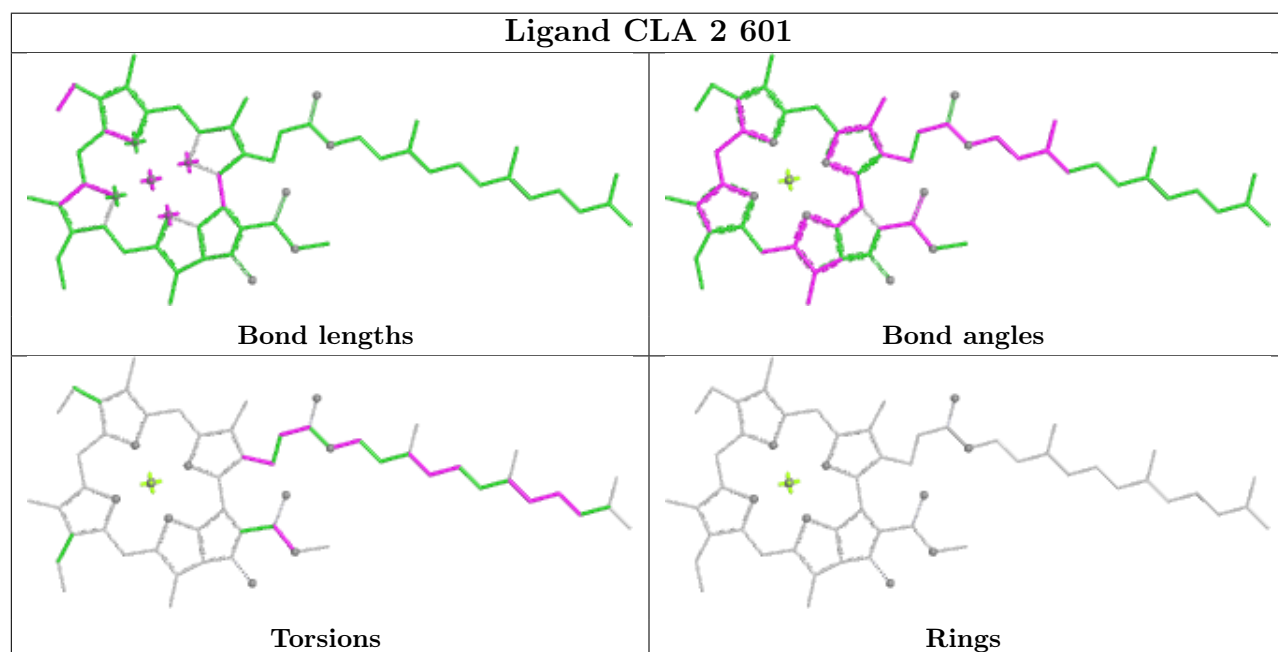
Ligand LUT 4 502

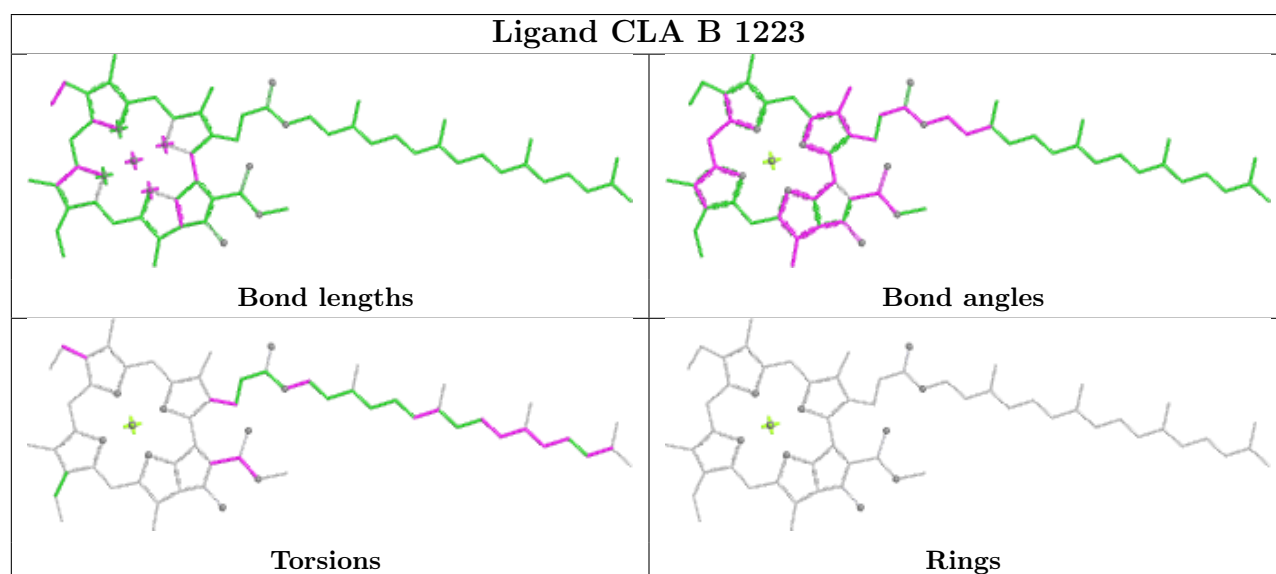
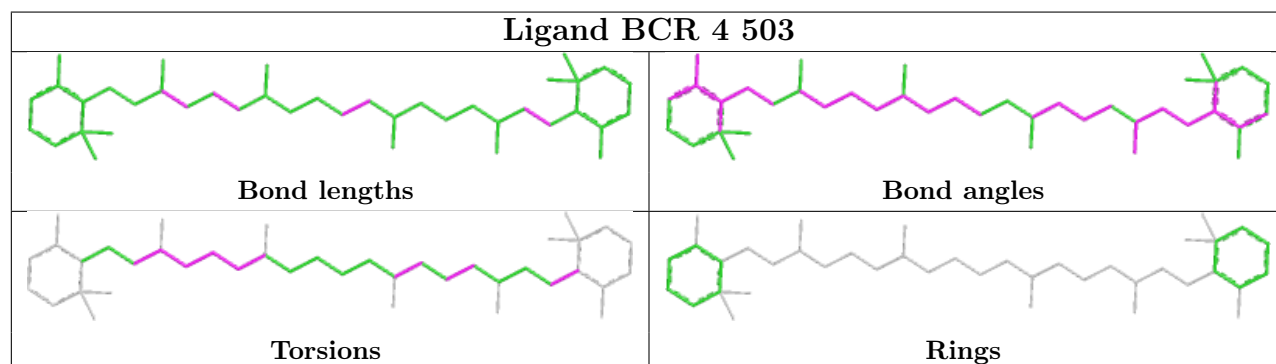
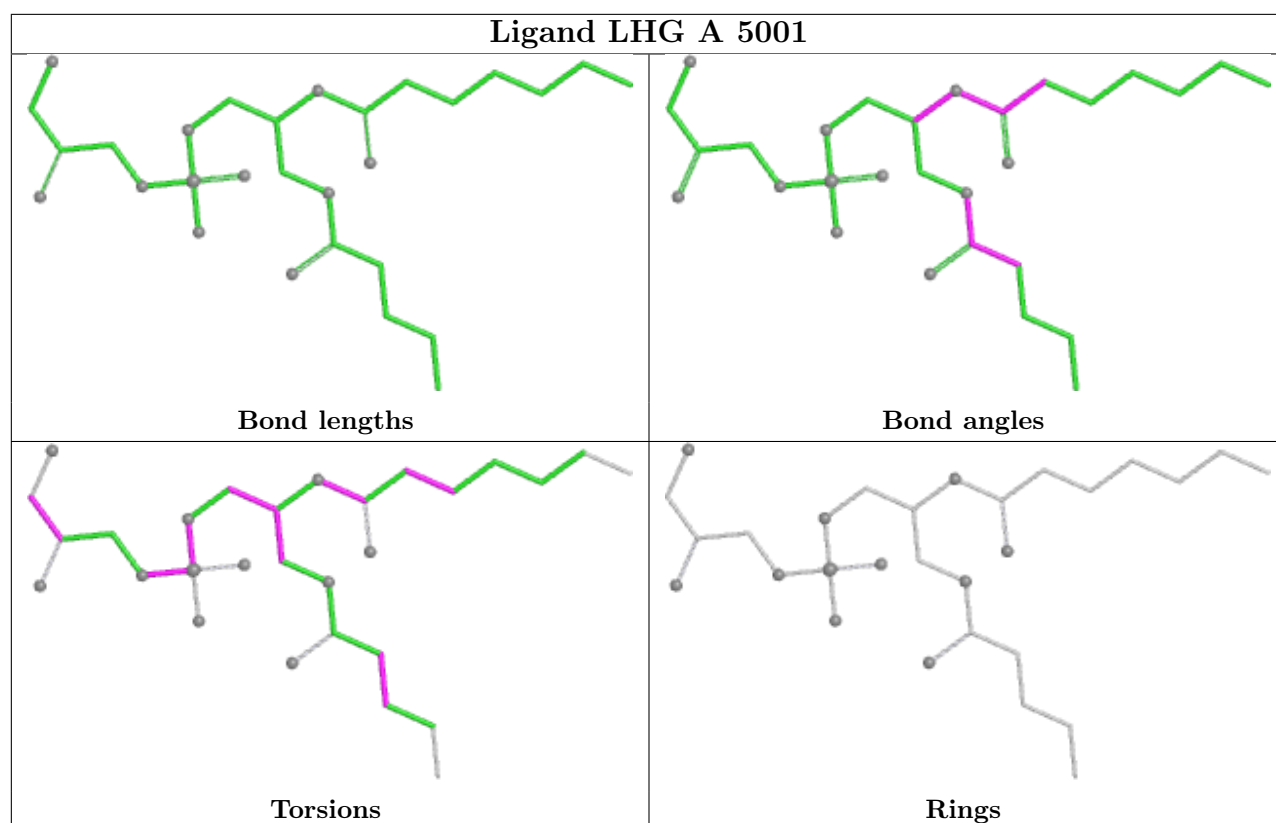


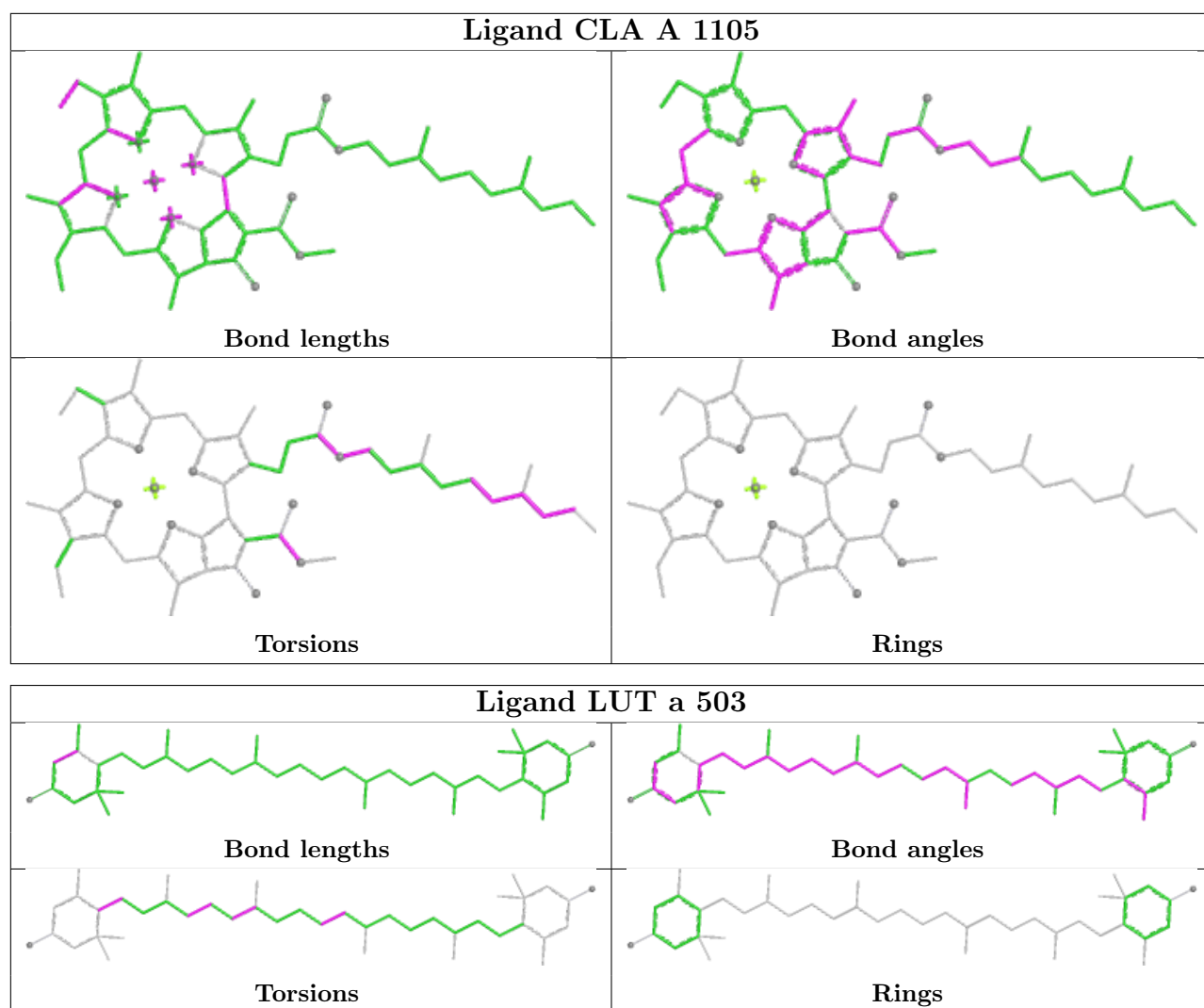
Ligand CLA B 1206

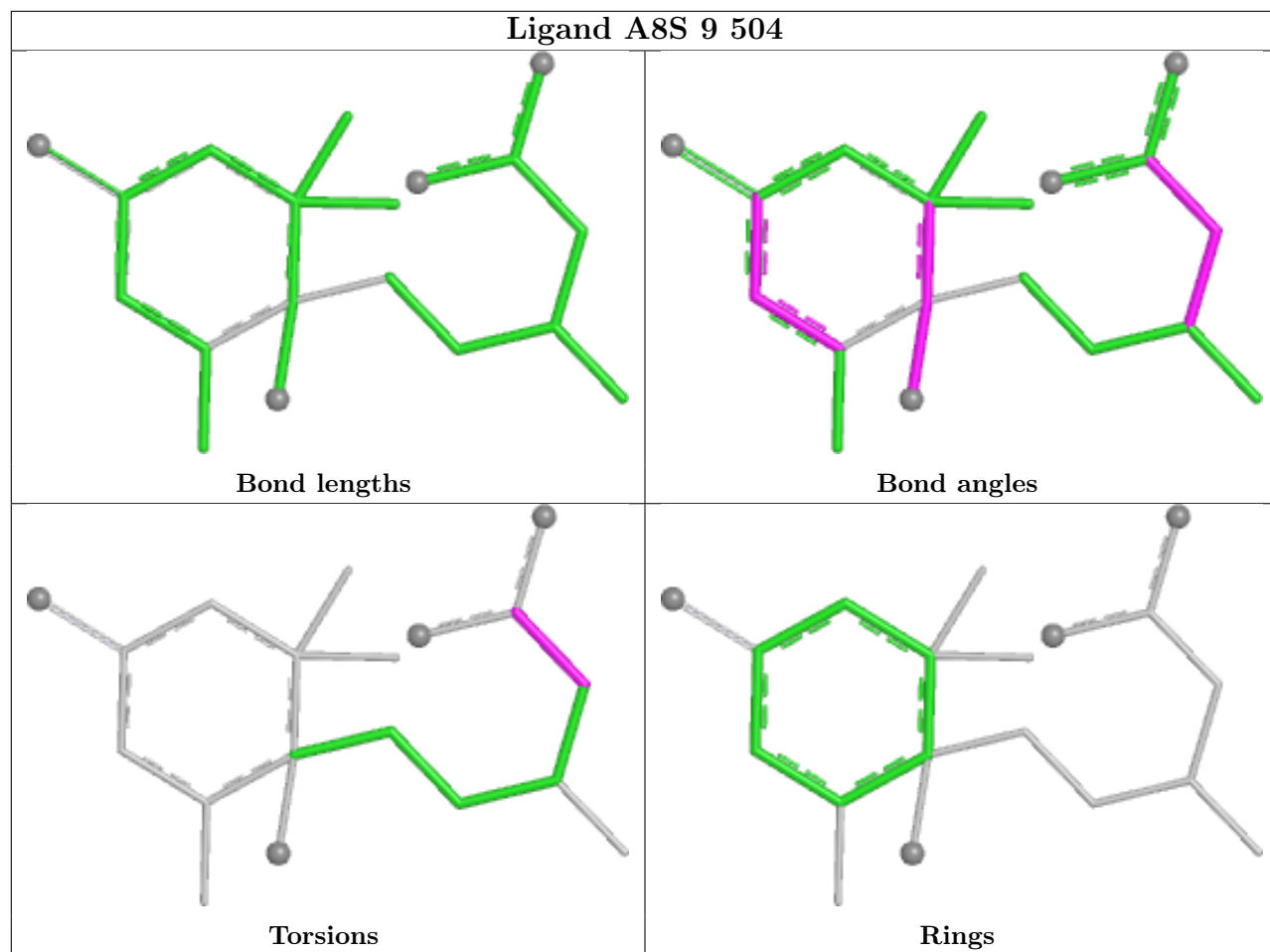


Ligand CLA 2 601

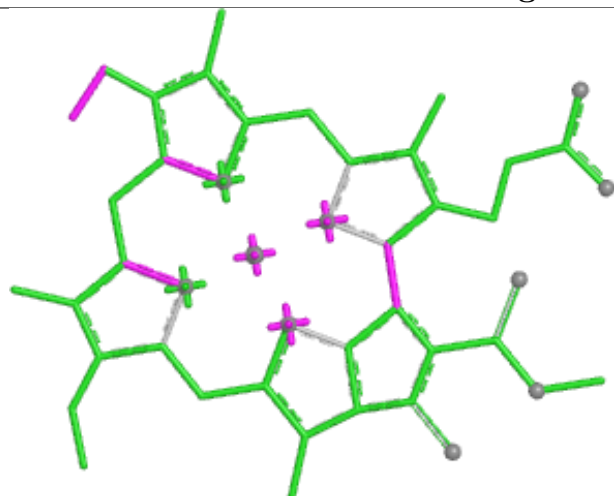




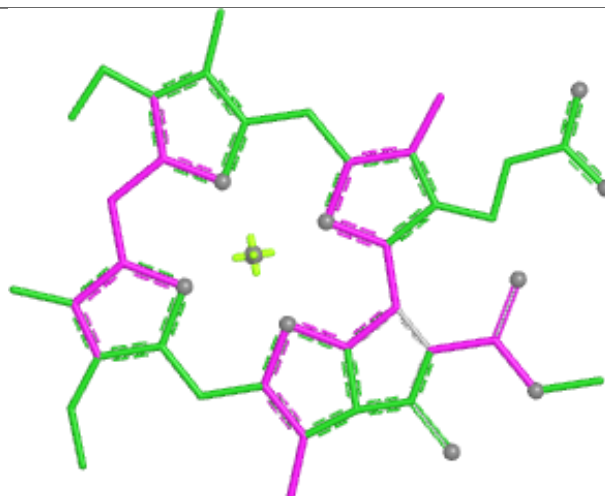




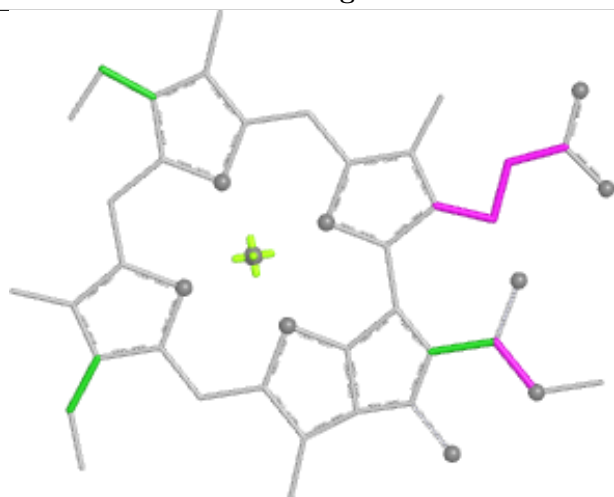
Ligand CLA 1 610



Bond lengths



Bond angles

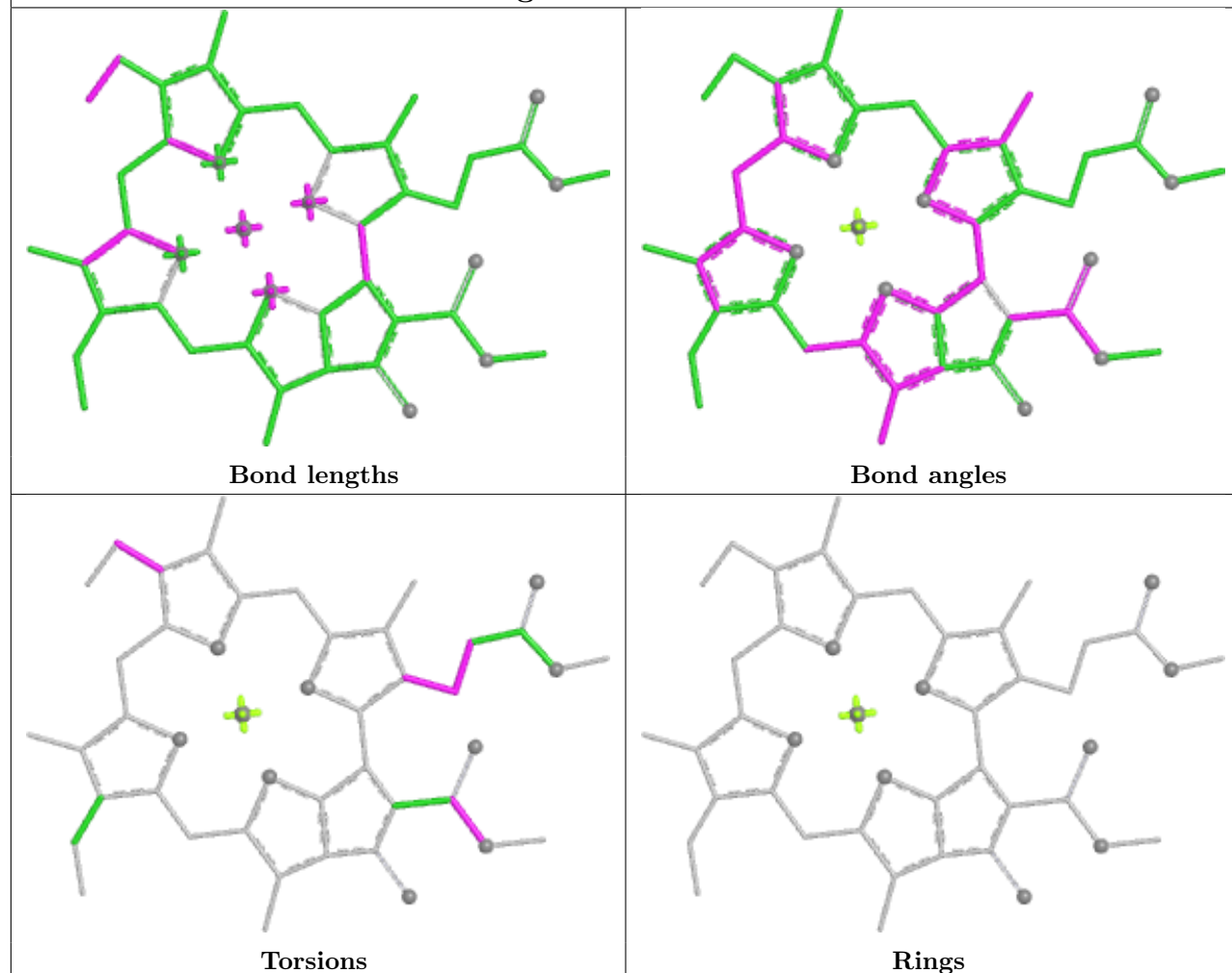


Torsions

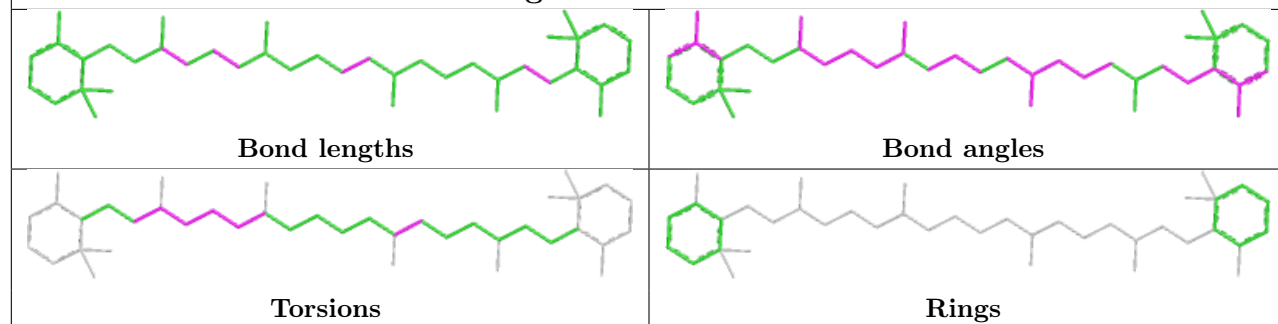


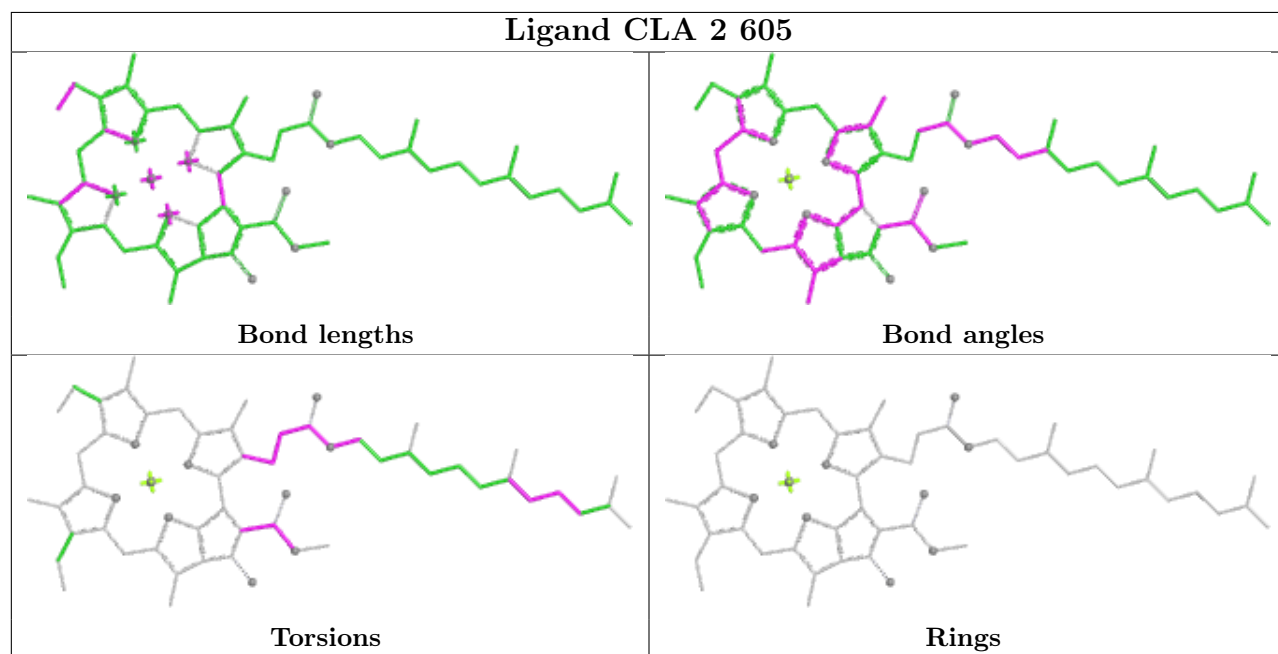
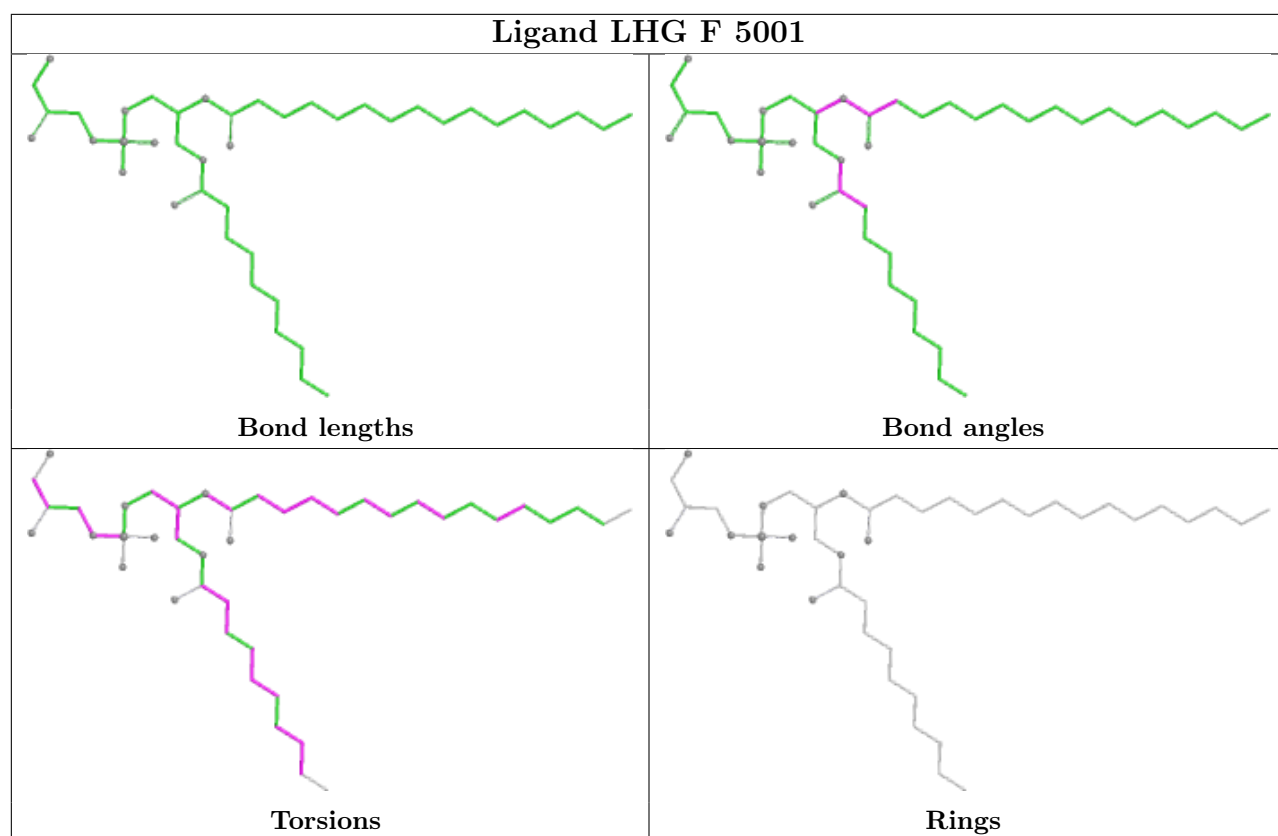
Rings

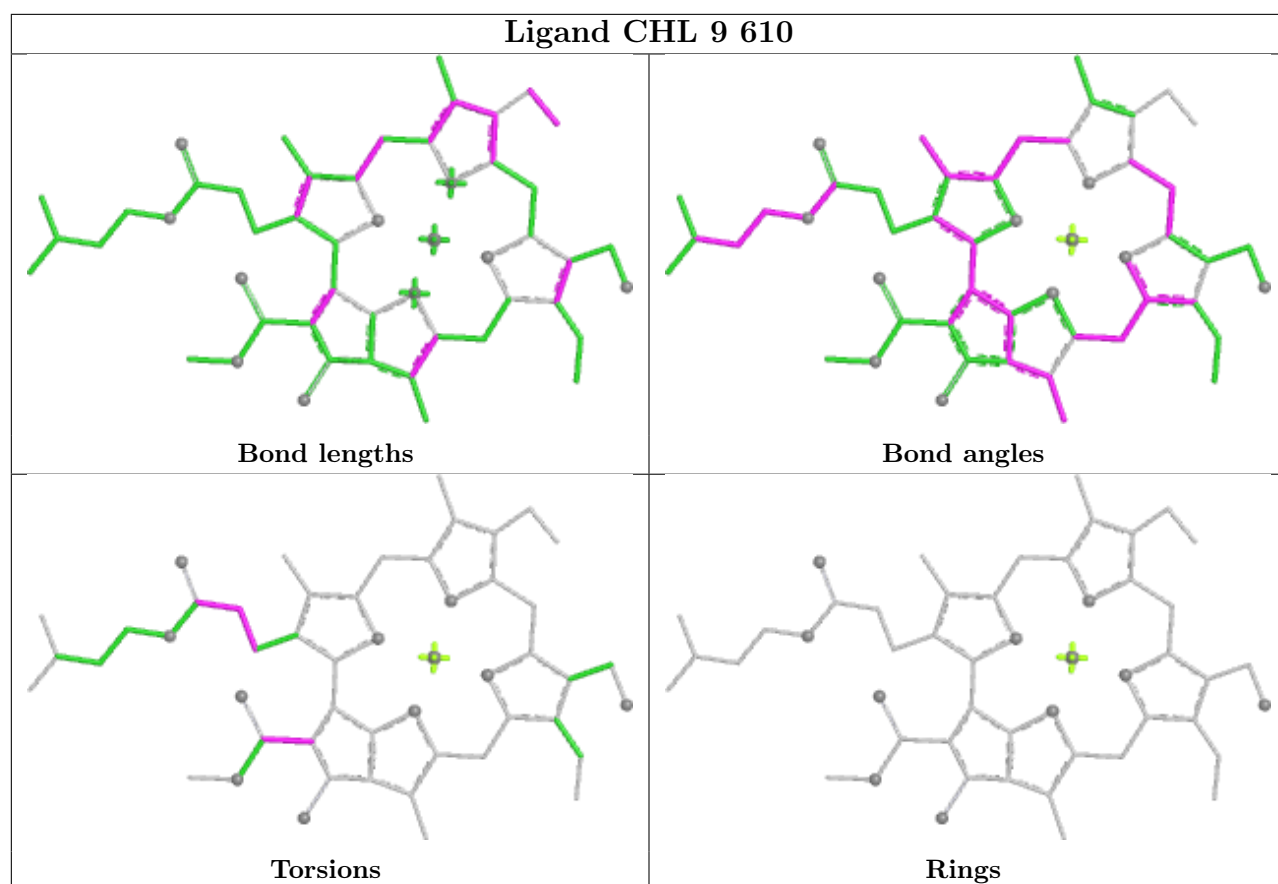
Ligand CLA 8 615

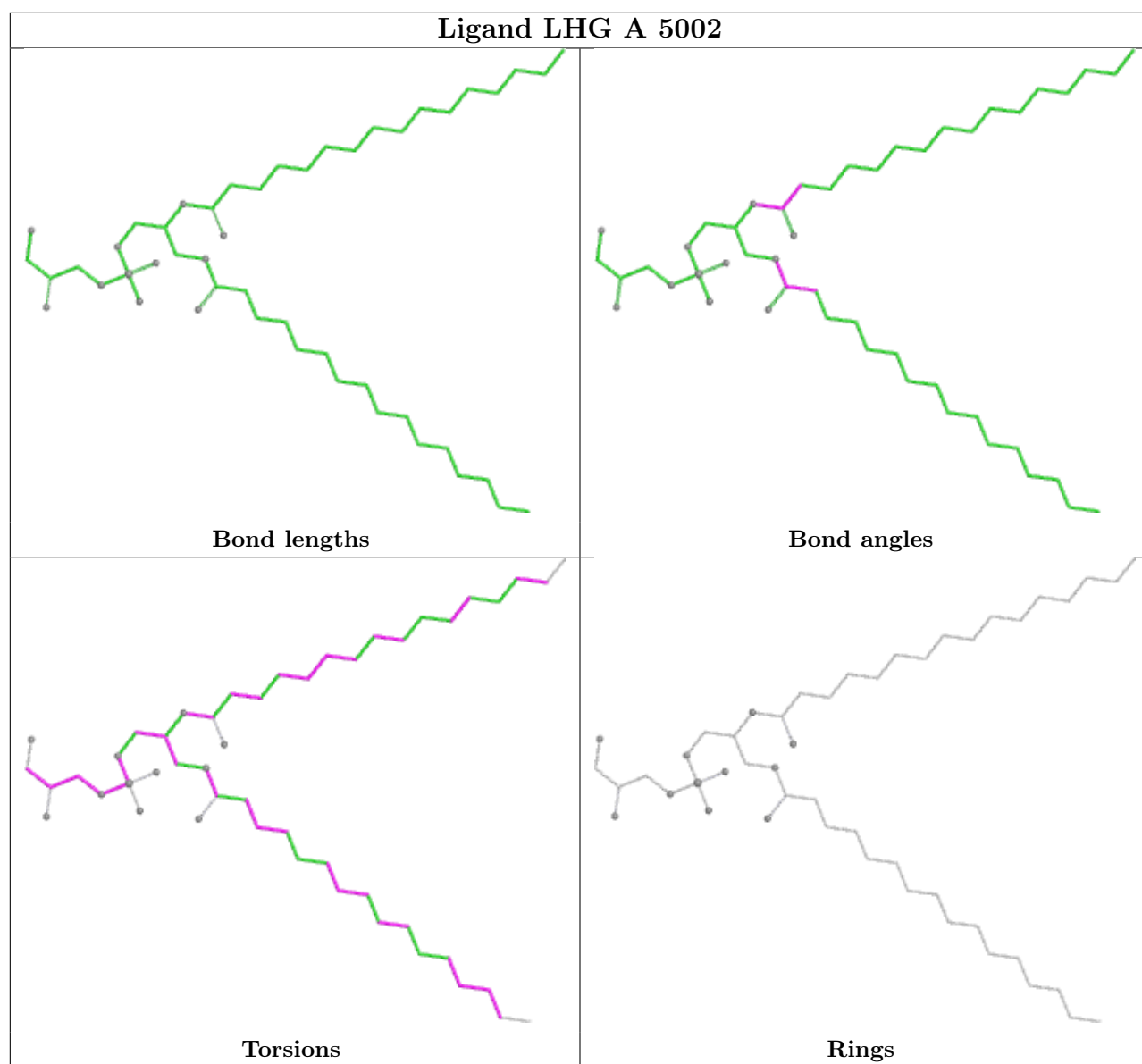


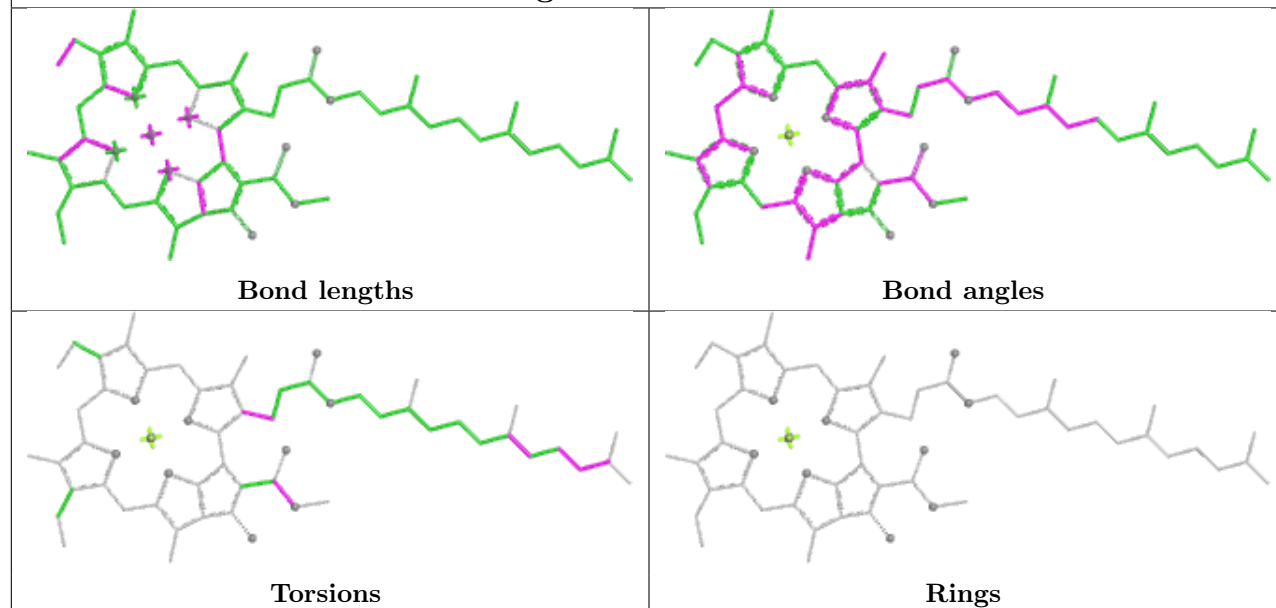
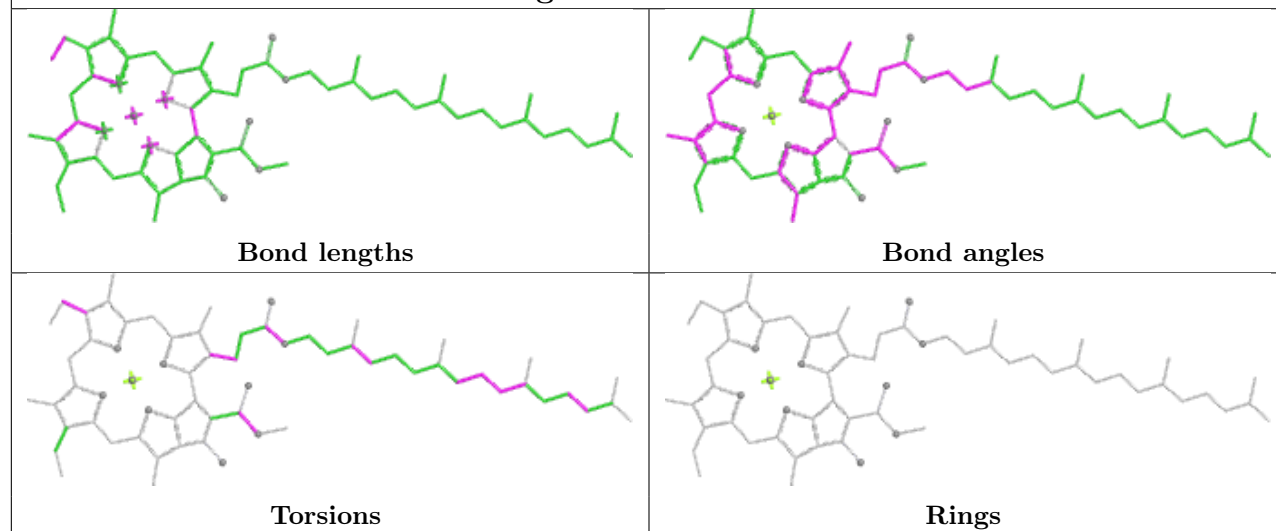
Ligand BCR J 4001

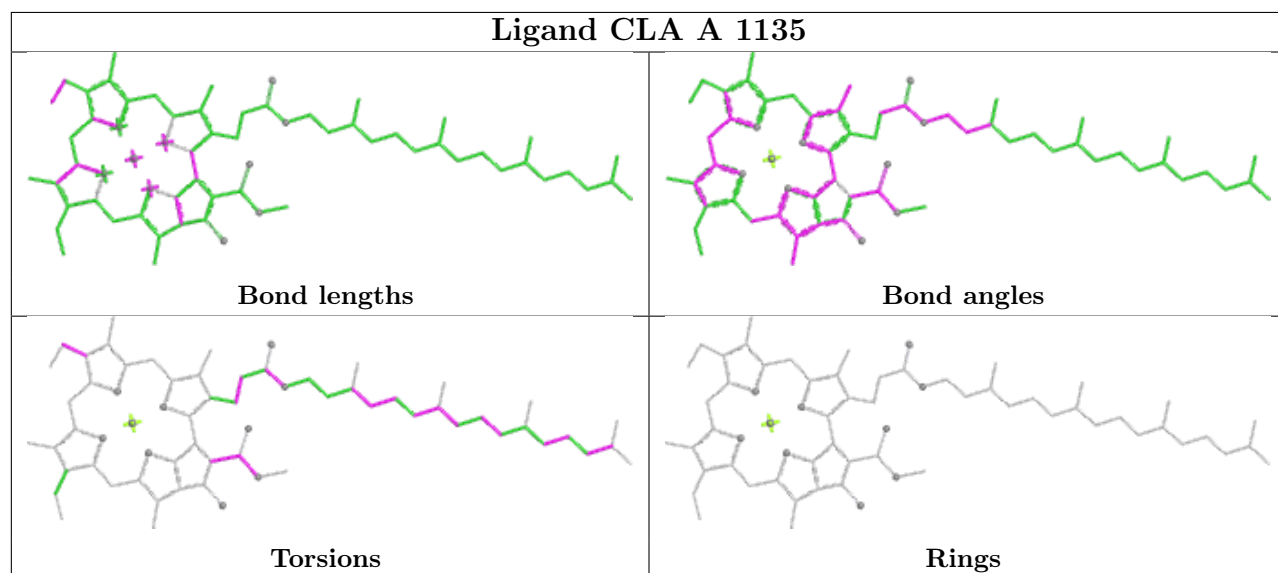
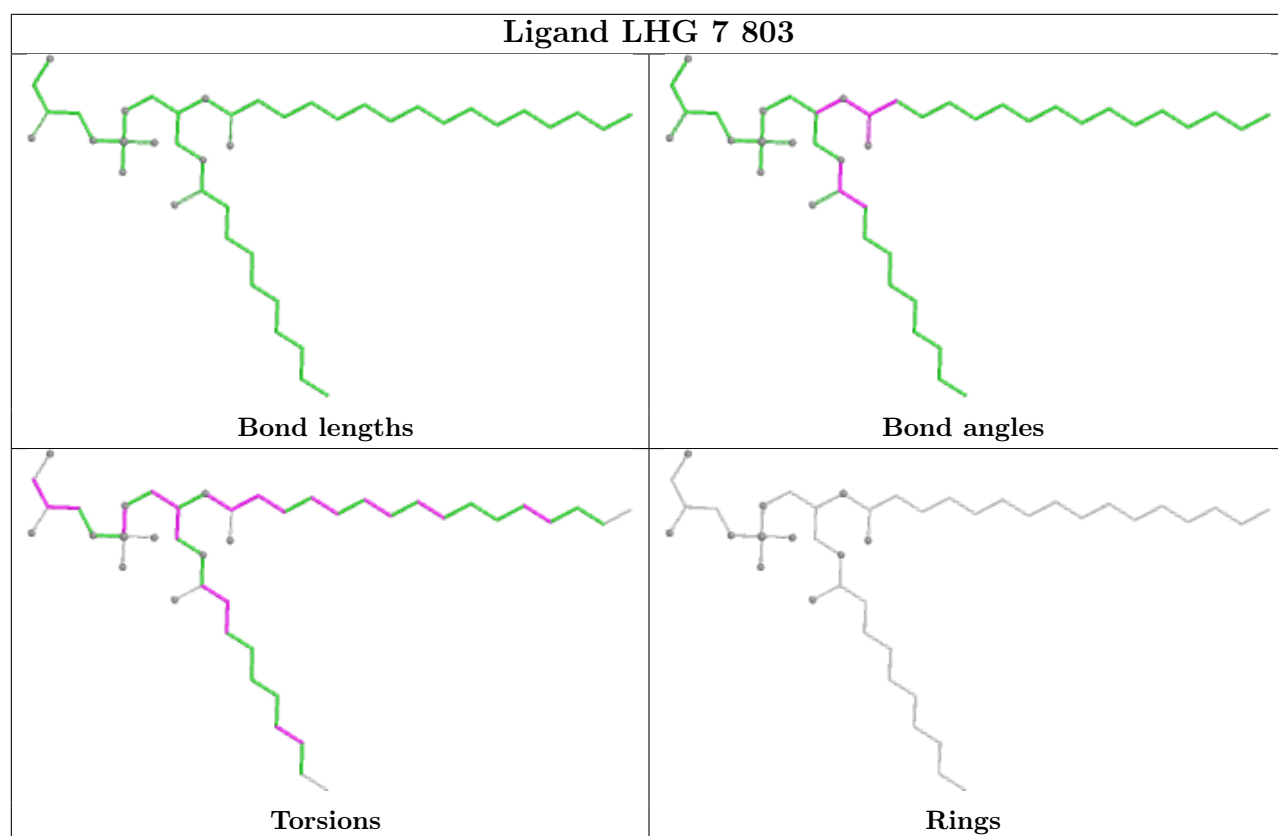


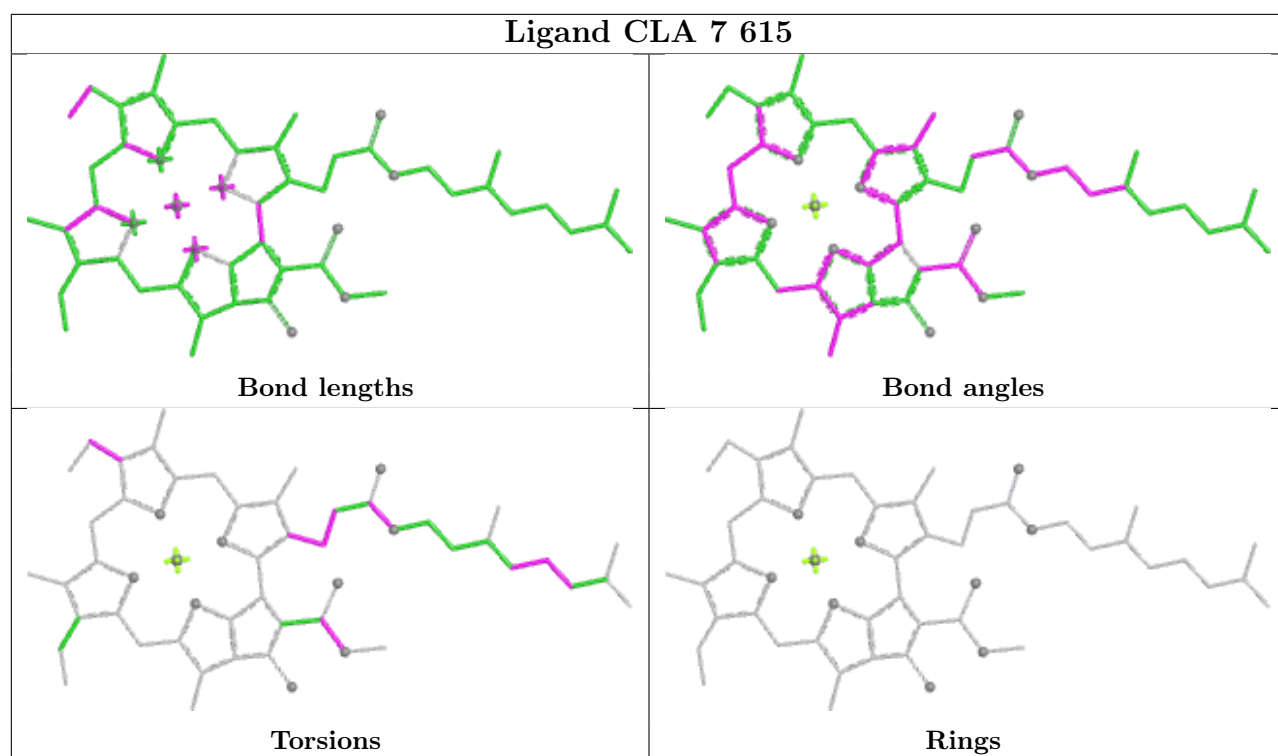




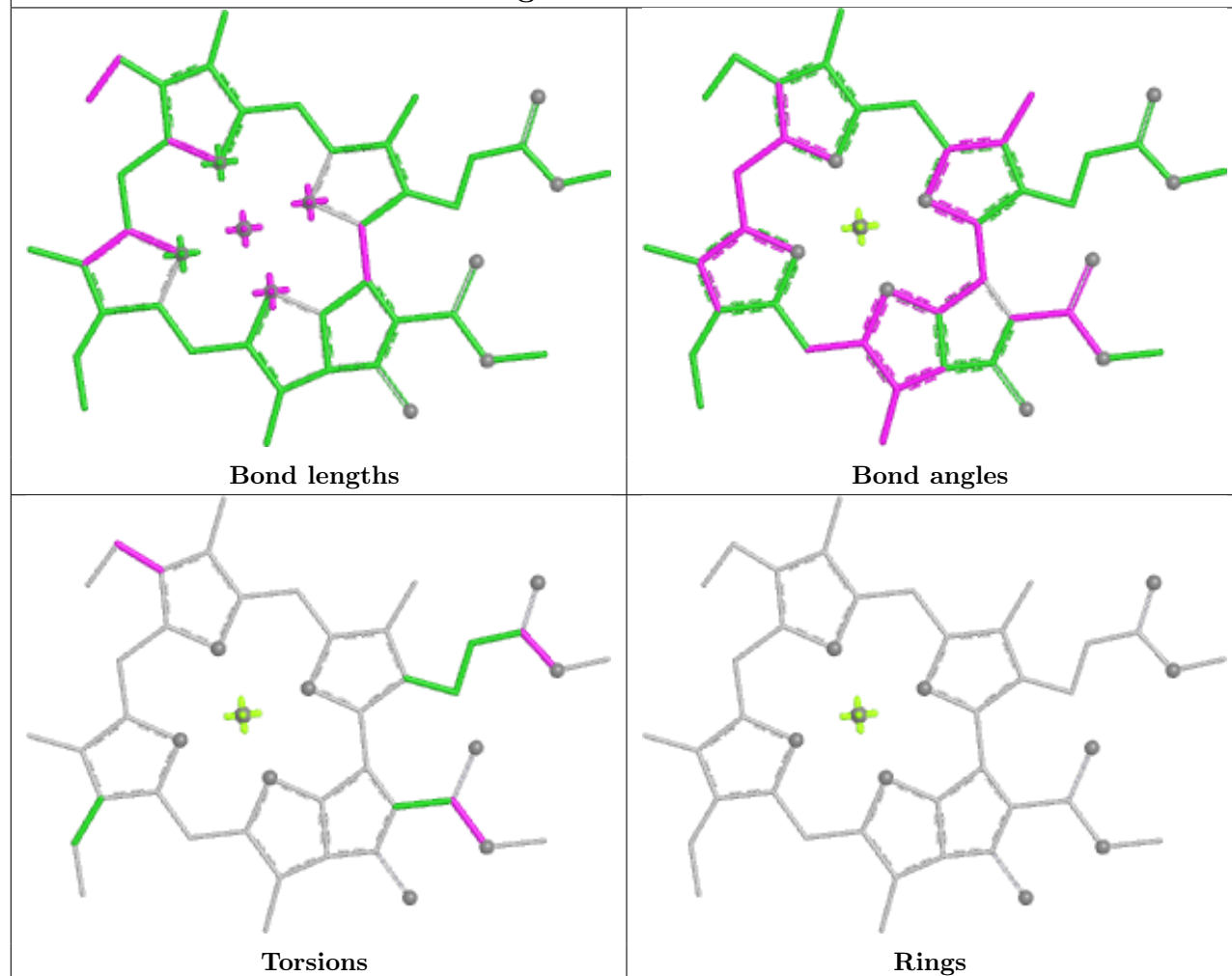


Ligand CLA 1 601**Ligand CLA 9 603**

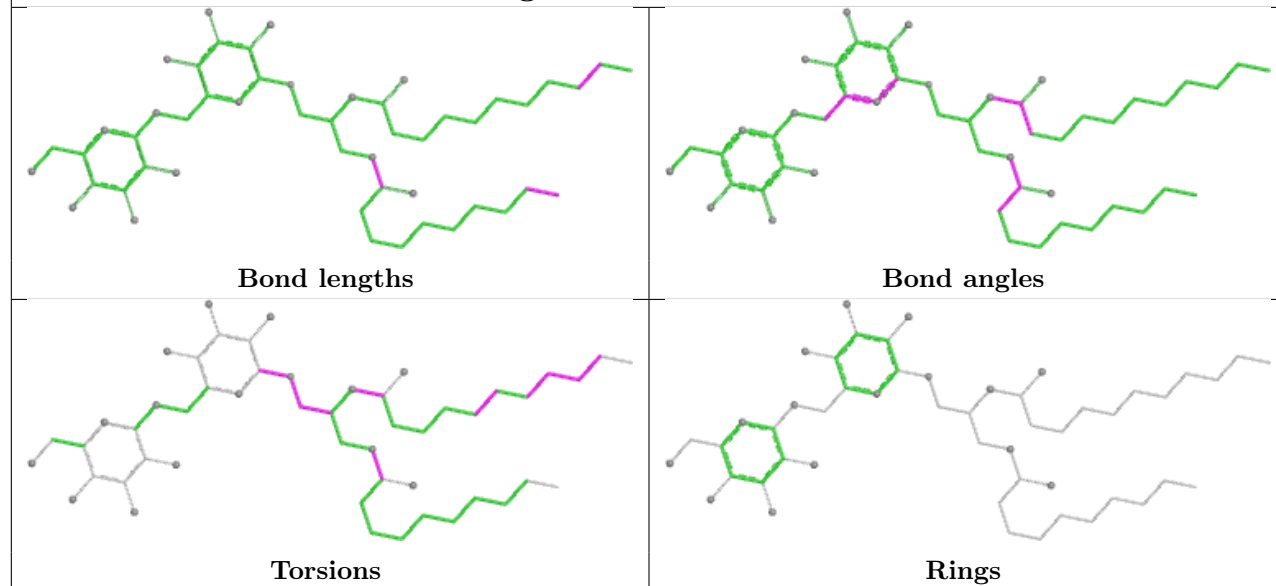




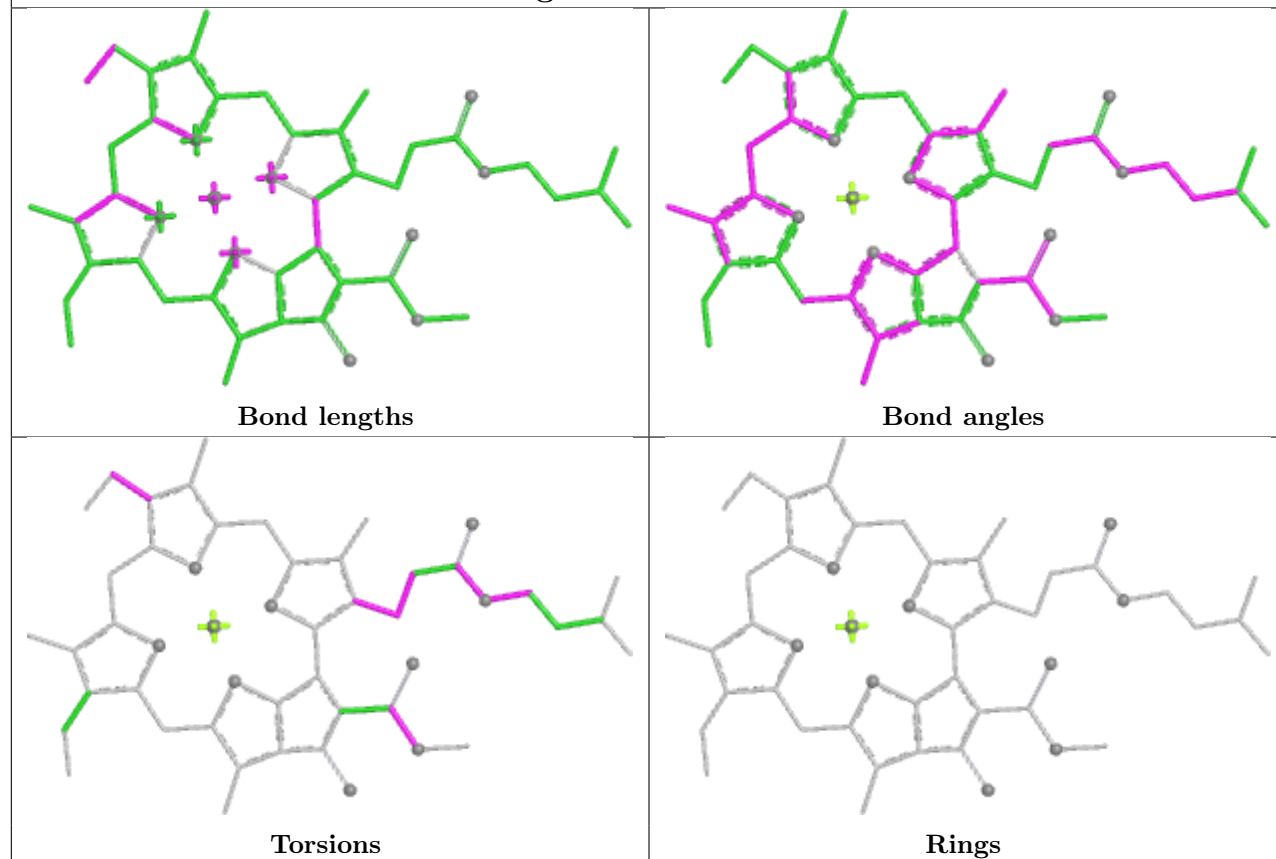
Ligand CLA 5 614



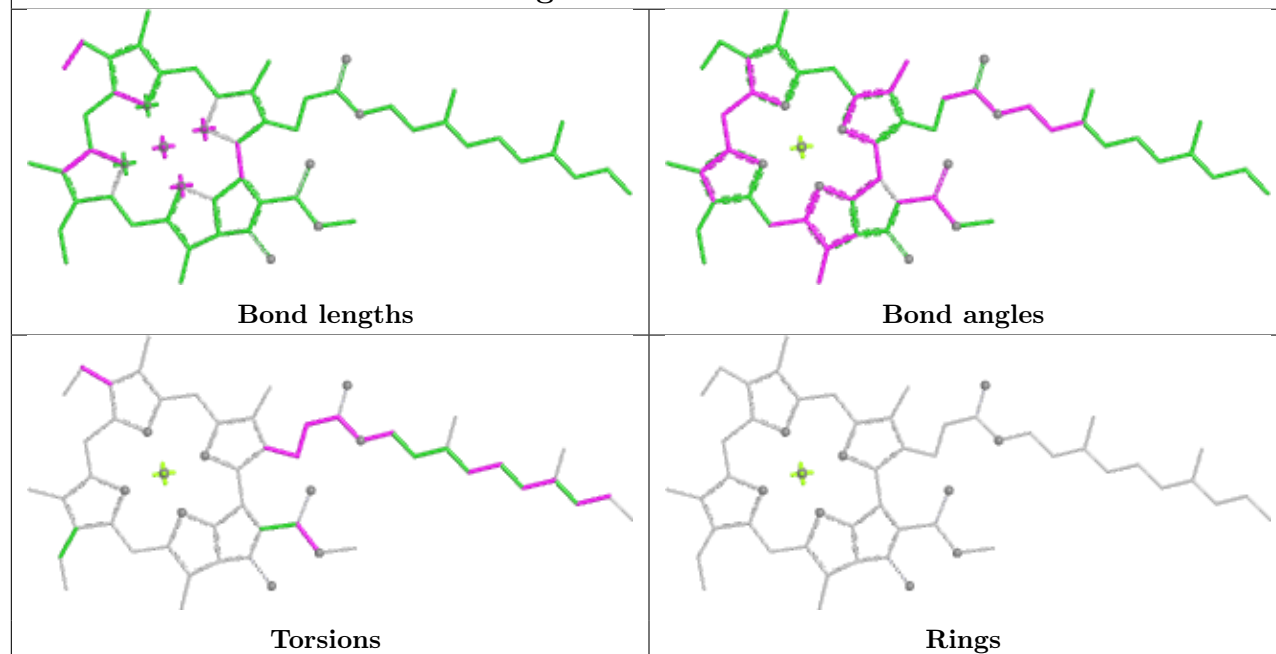
Ligand DGD A 5005

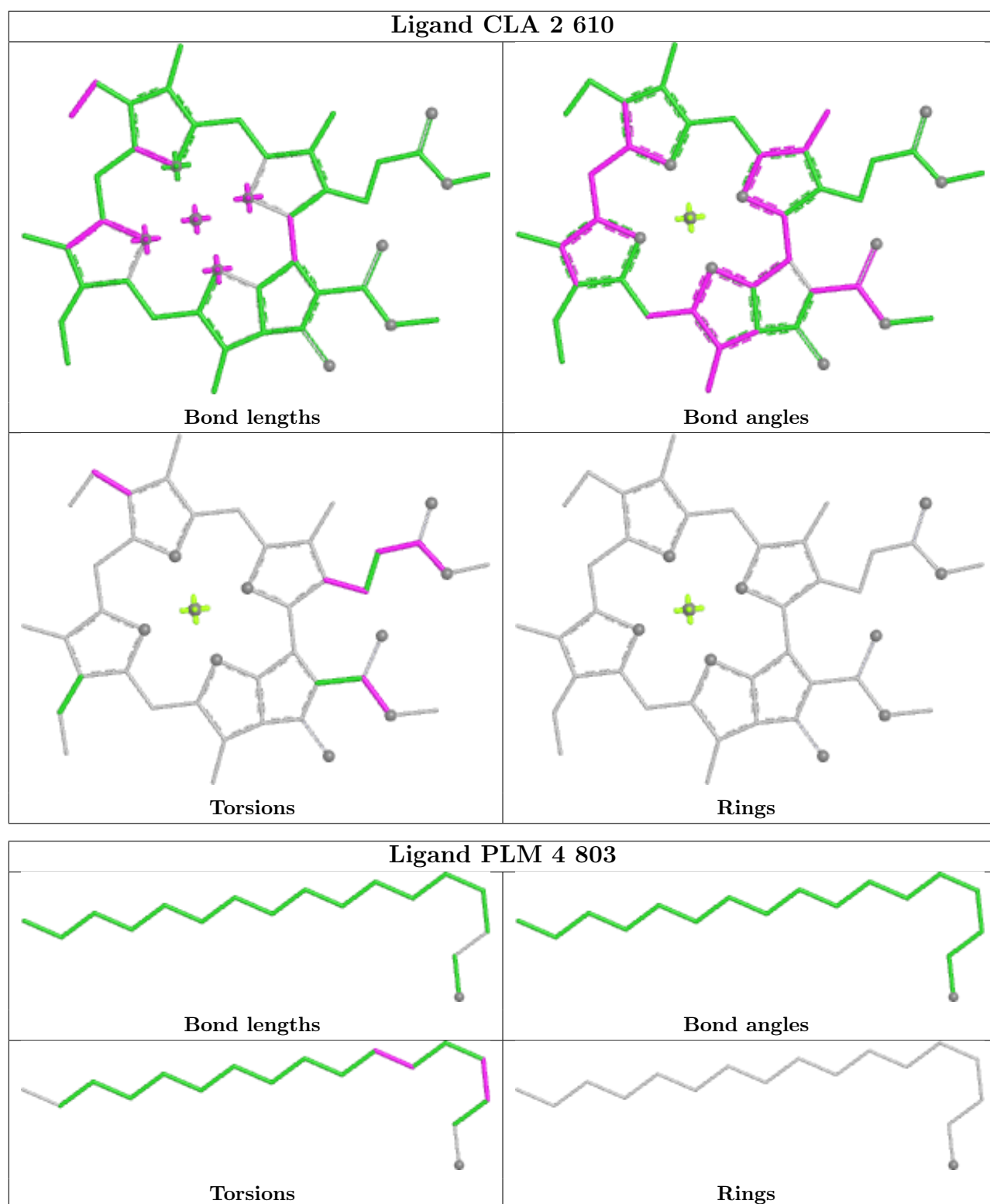


Ligand CLA a 611

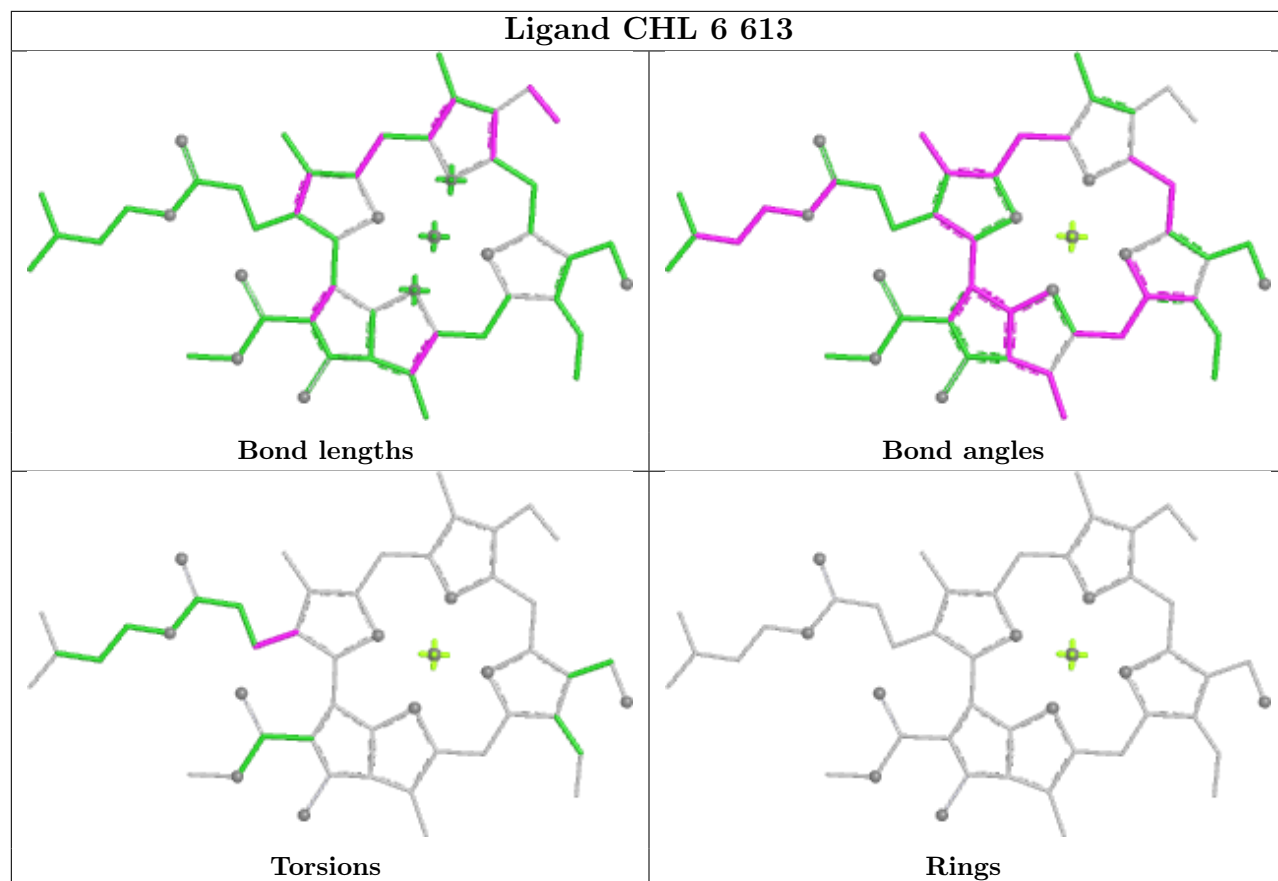


Ligand CLA 2 615

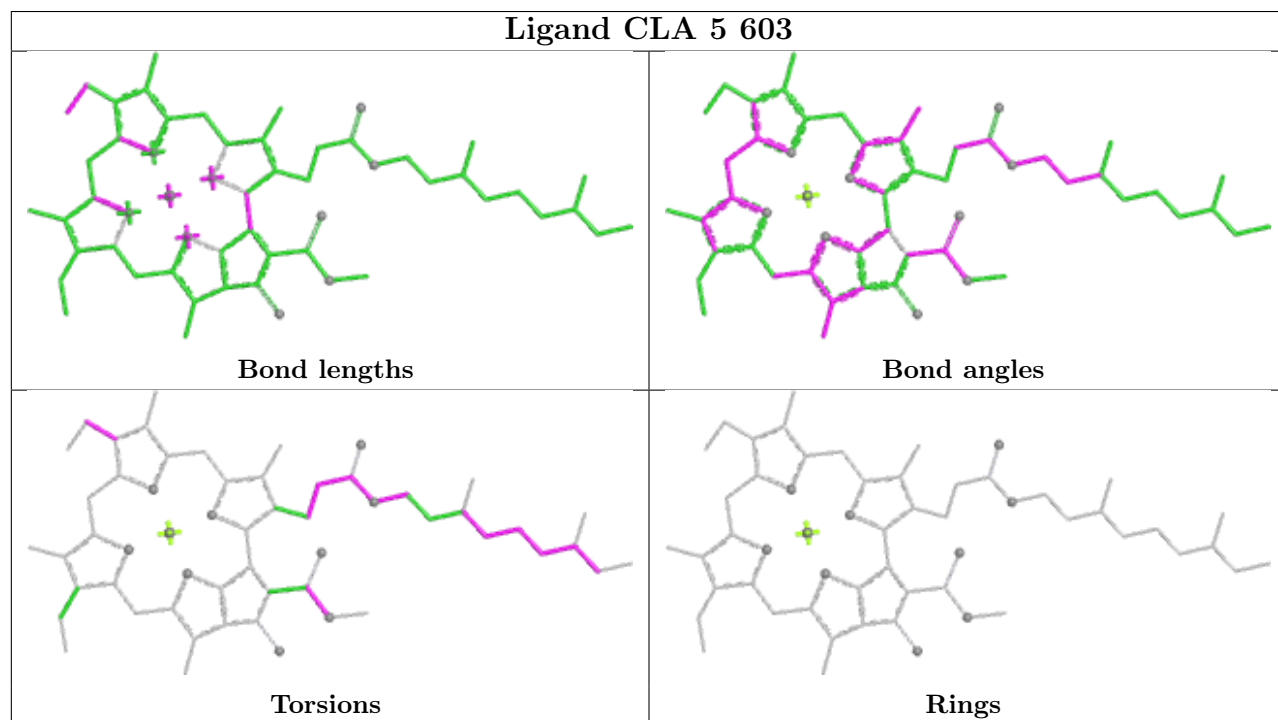


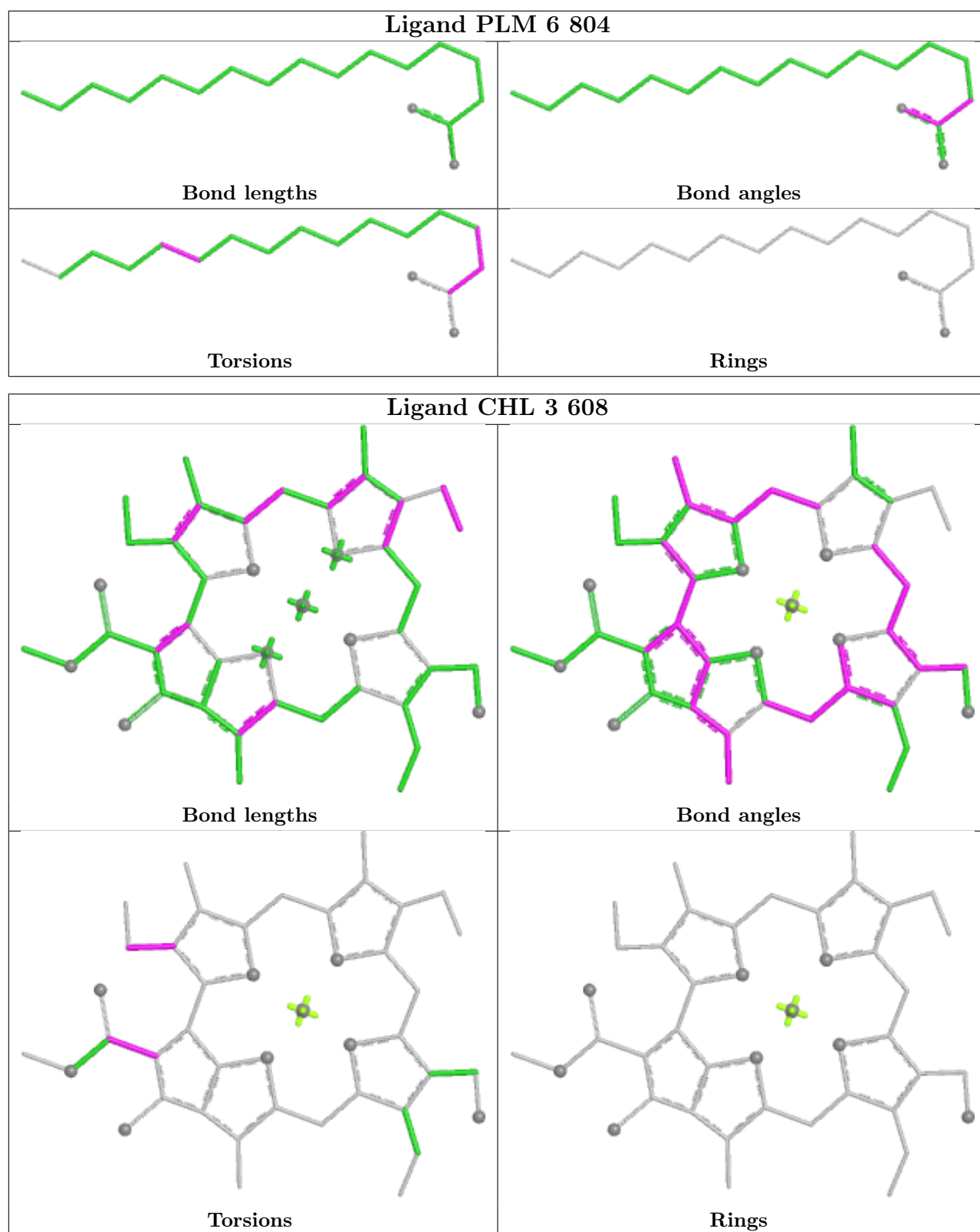


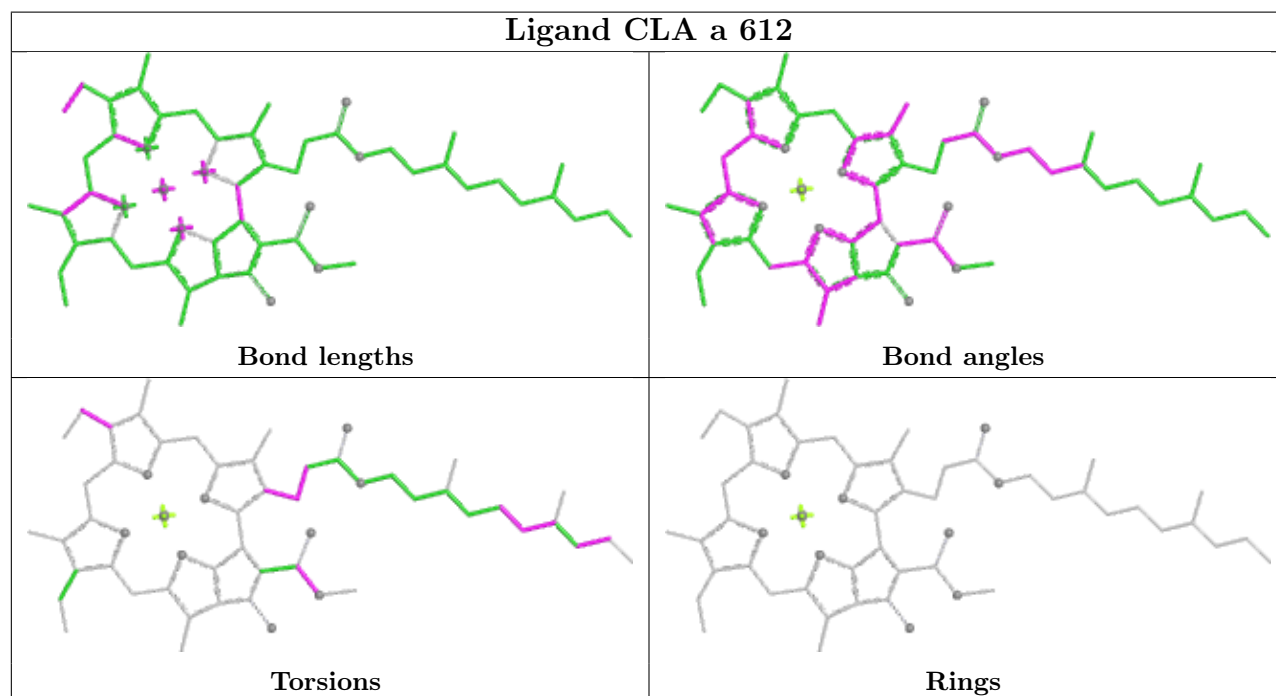
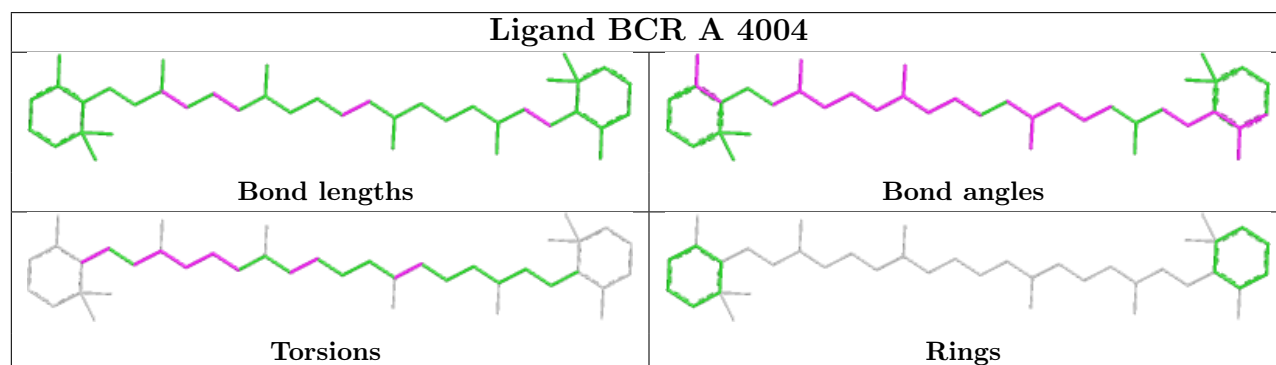
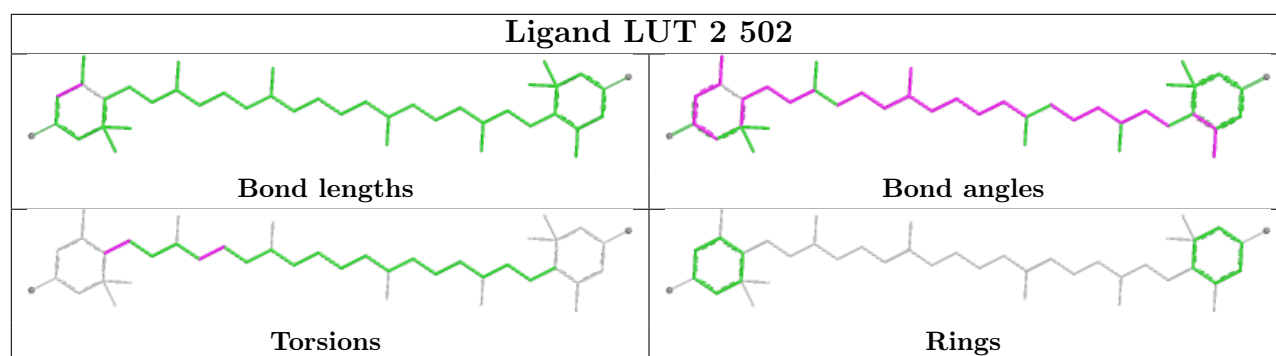
Ligand CHL 6 613



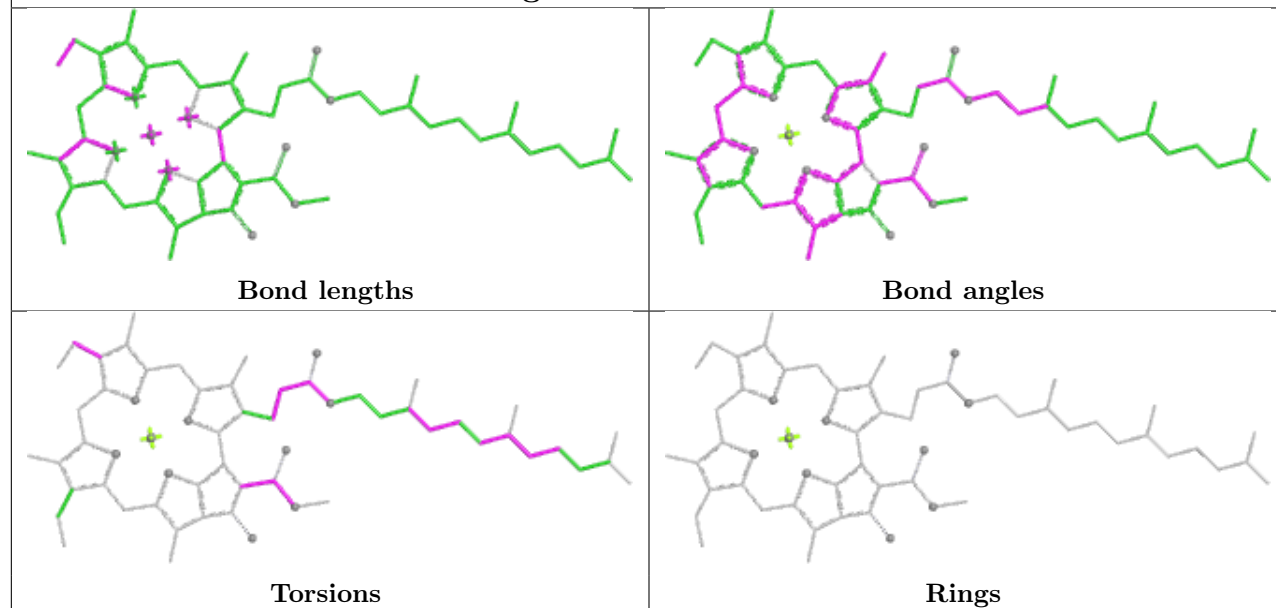
Ligand CLA 5 603



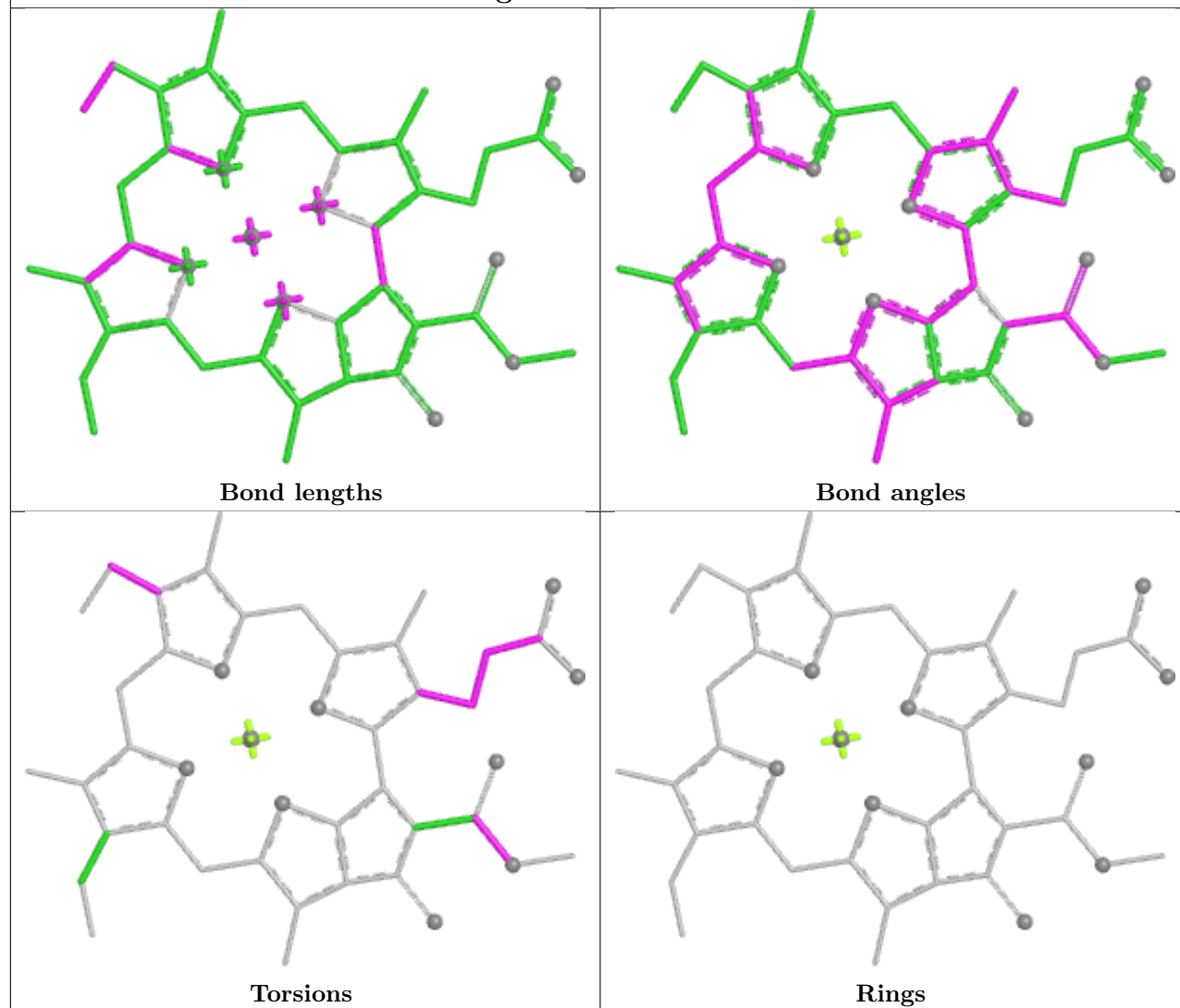


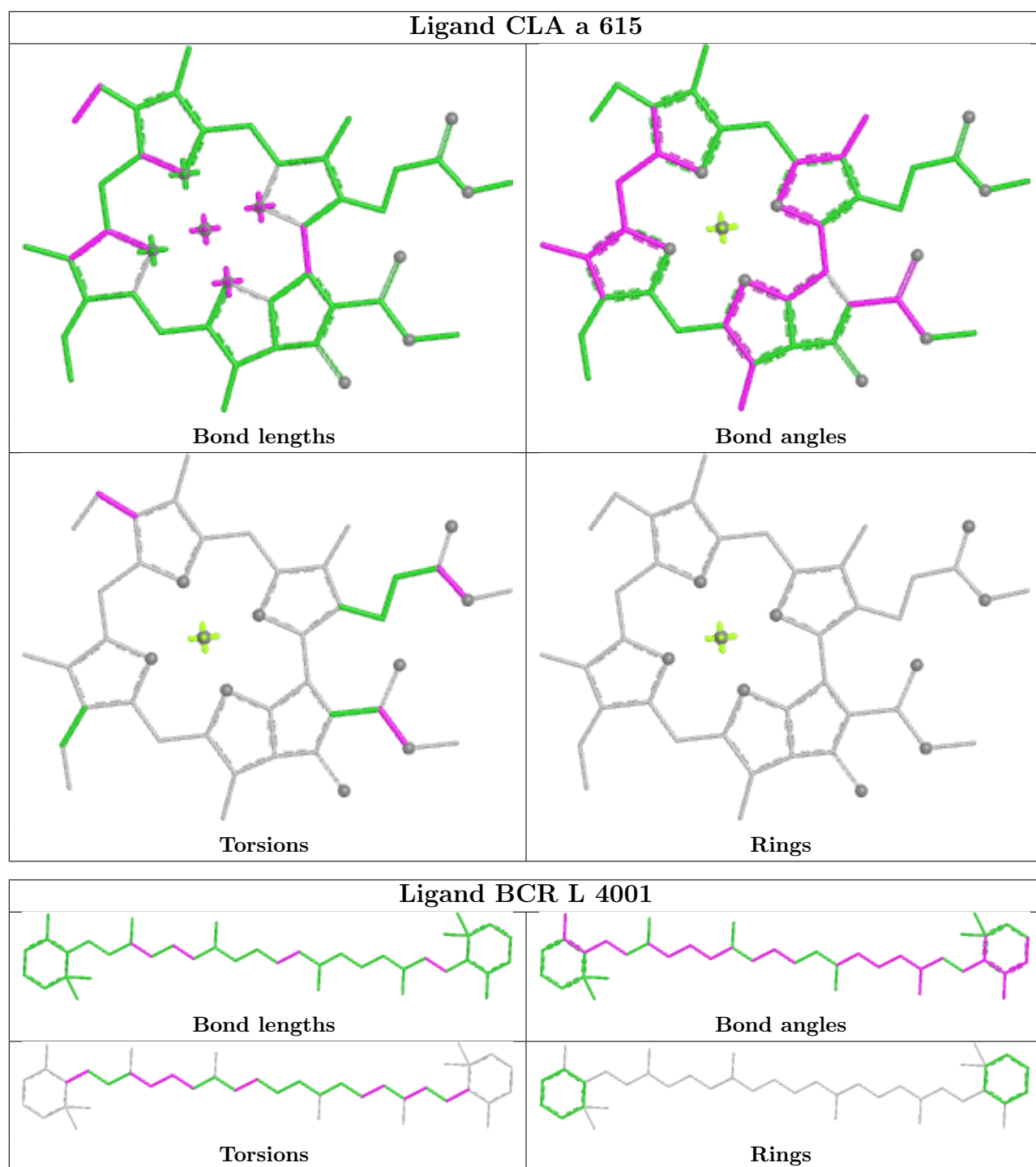


Ligand CLA A 1115

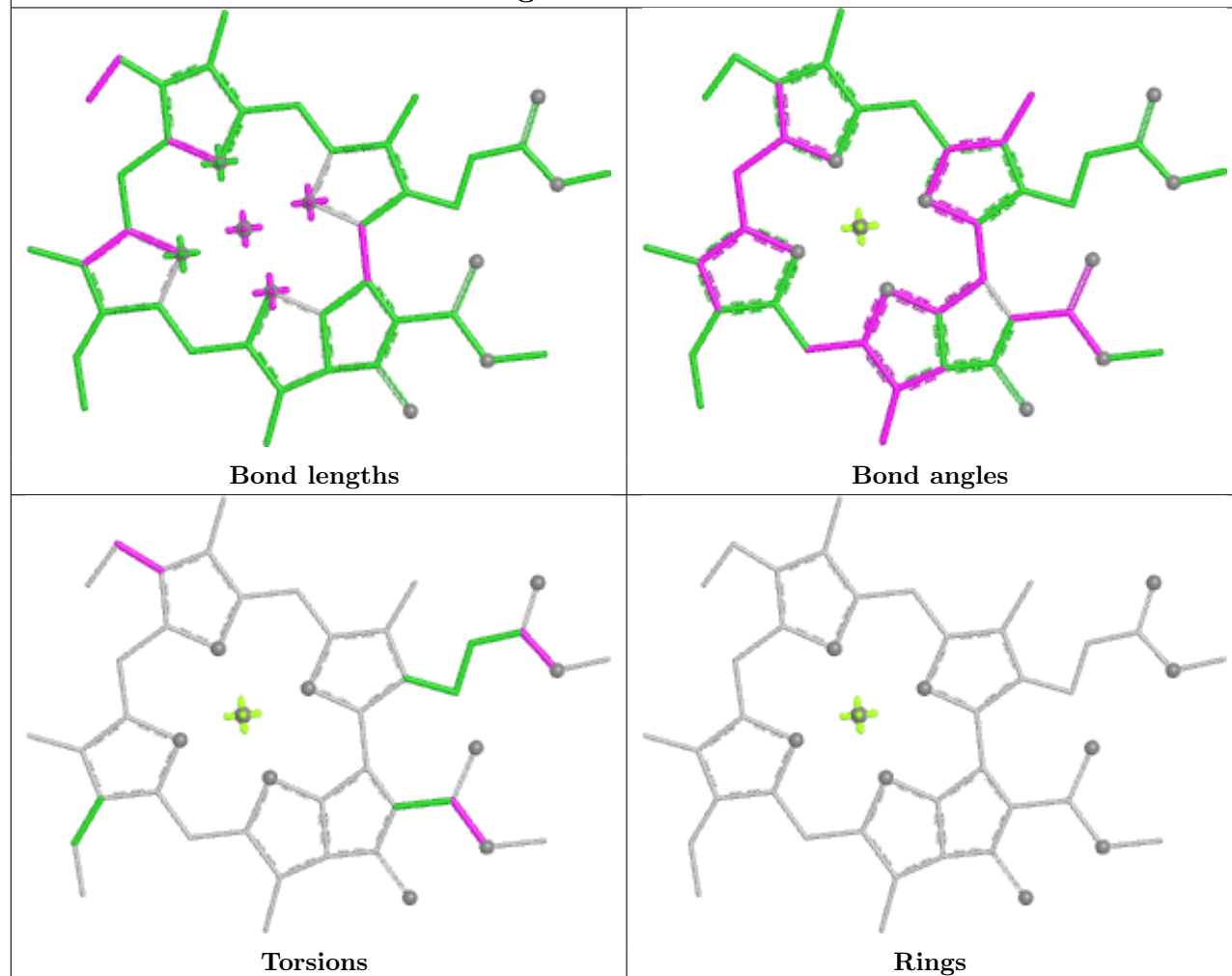


Ligand CLA 1 602

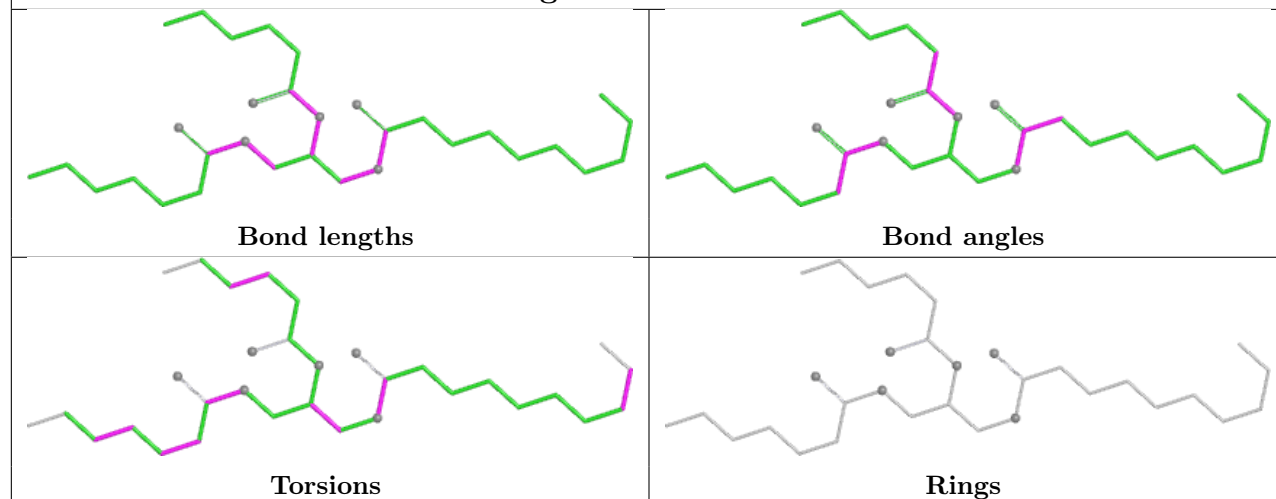


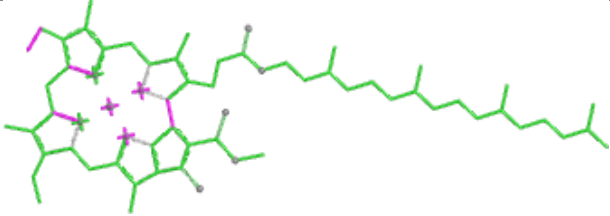
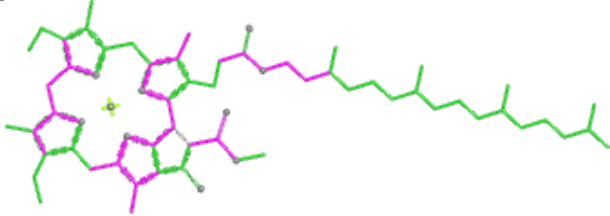
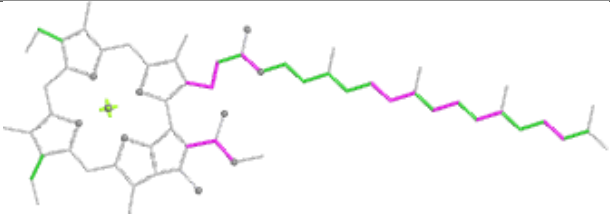
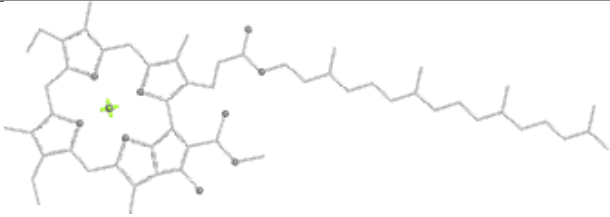
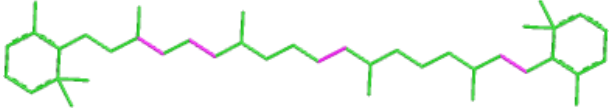
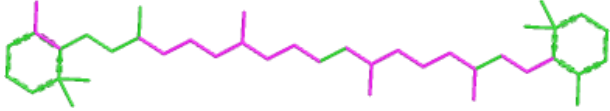
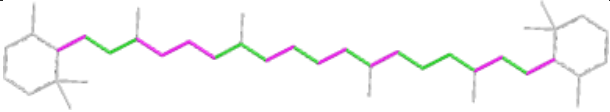
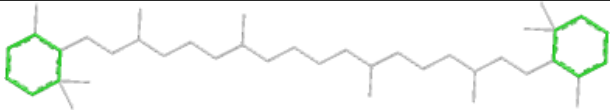
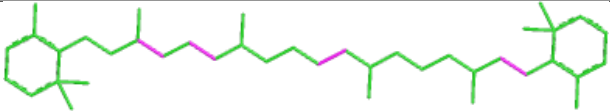
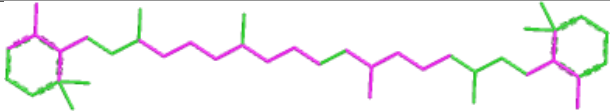
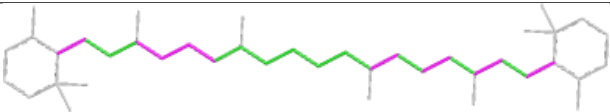
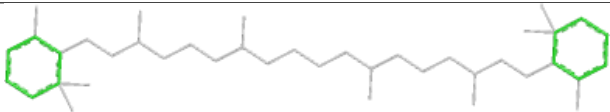


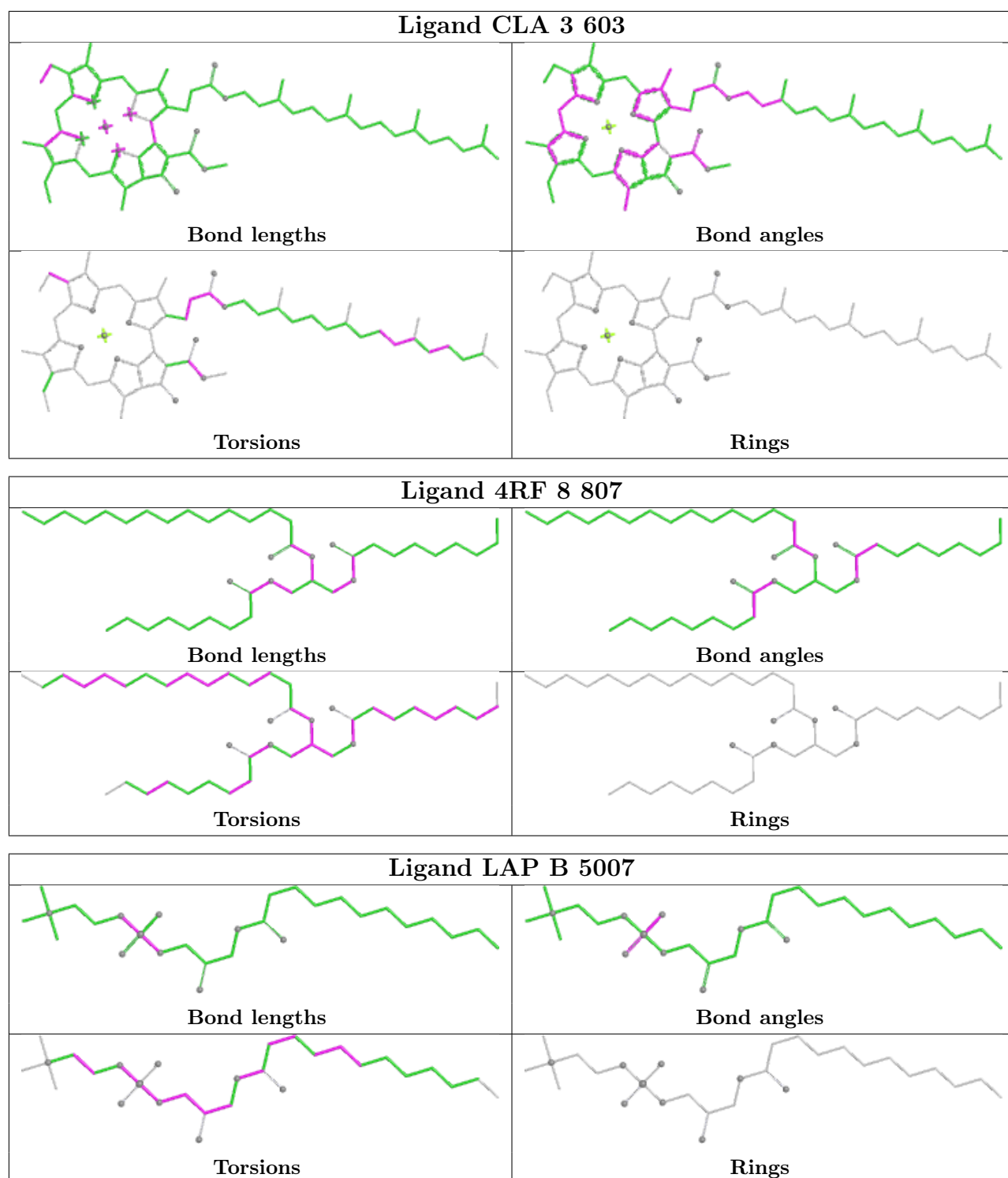
Ligand CLA 9 602

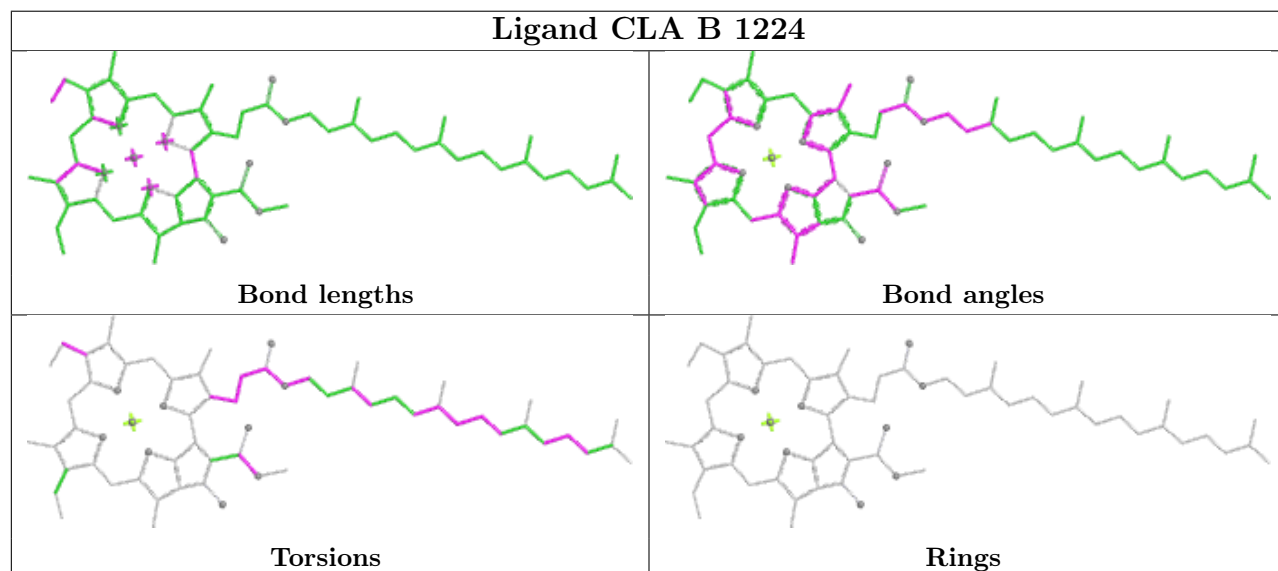
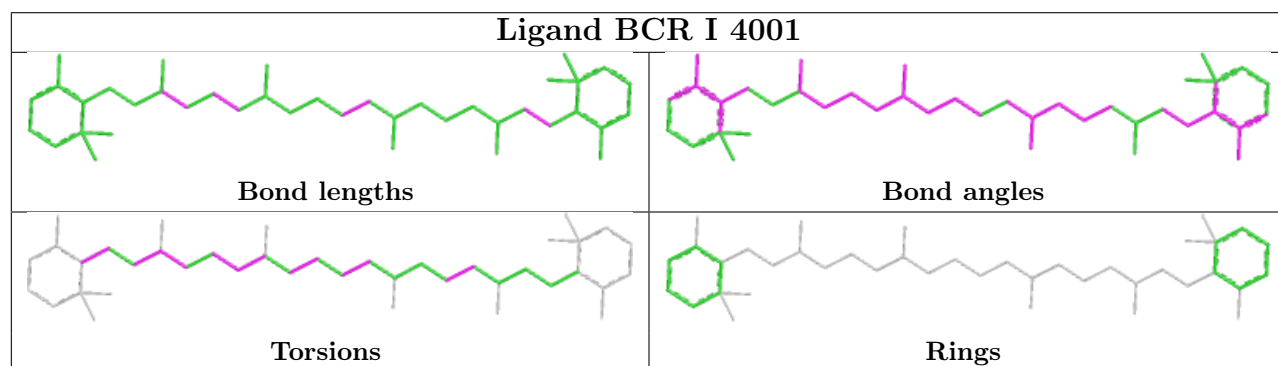
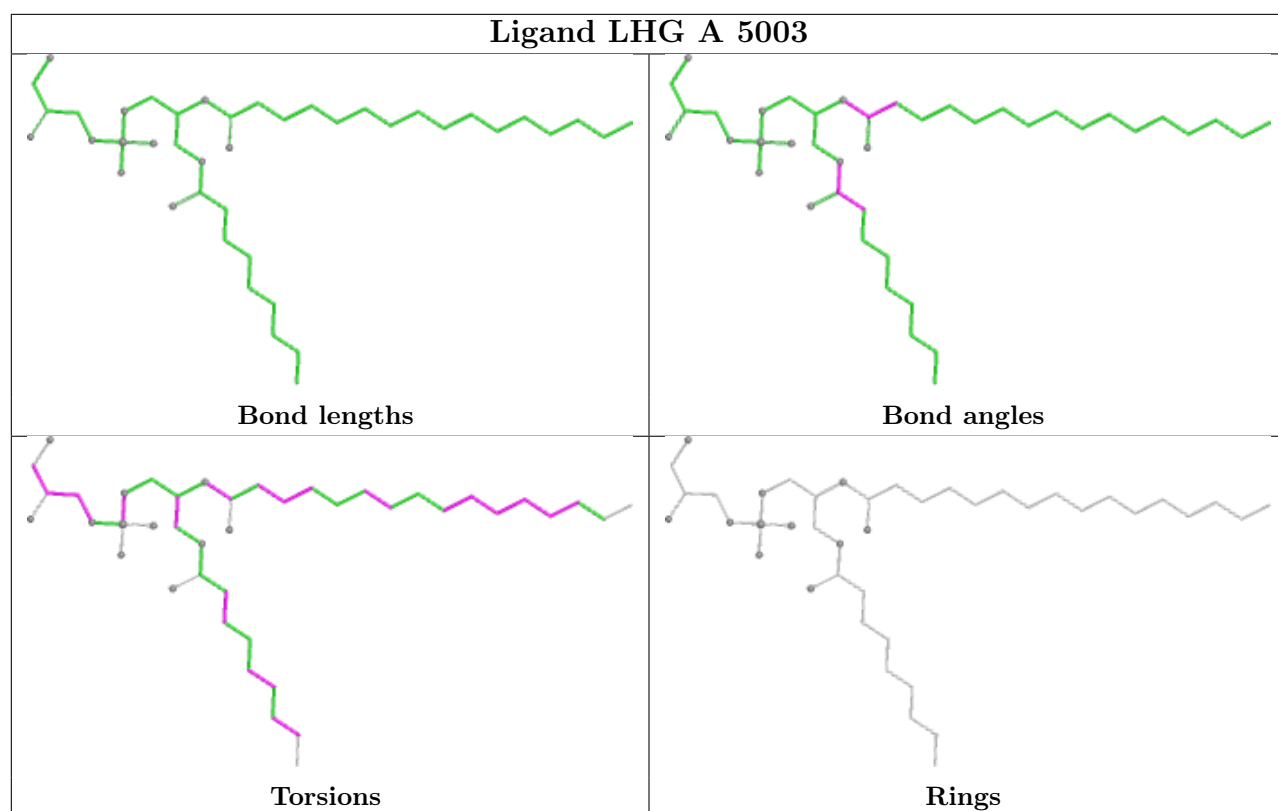


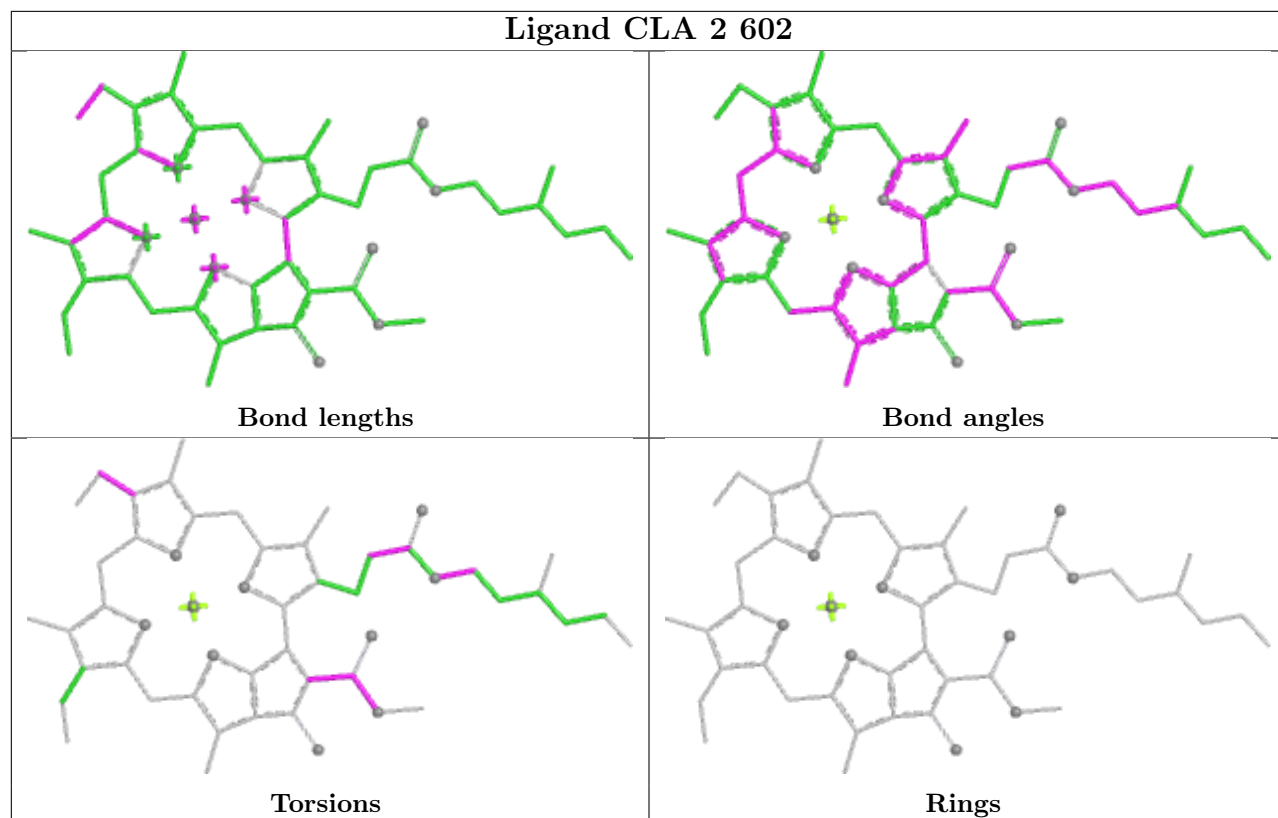
Ligand 4RF 7 807

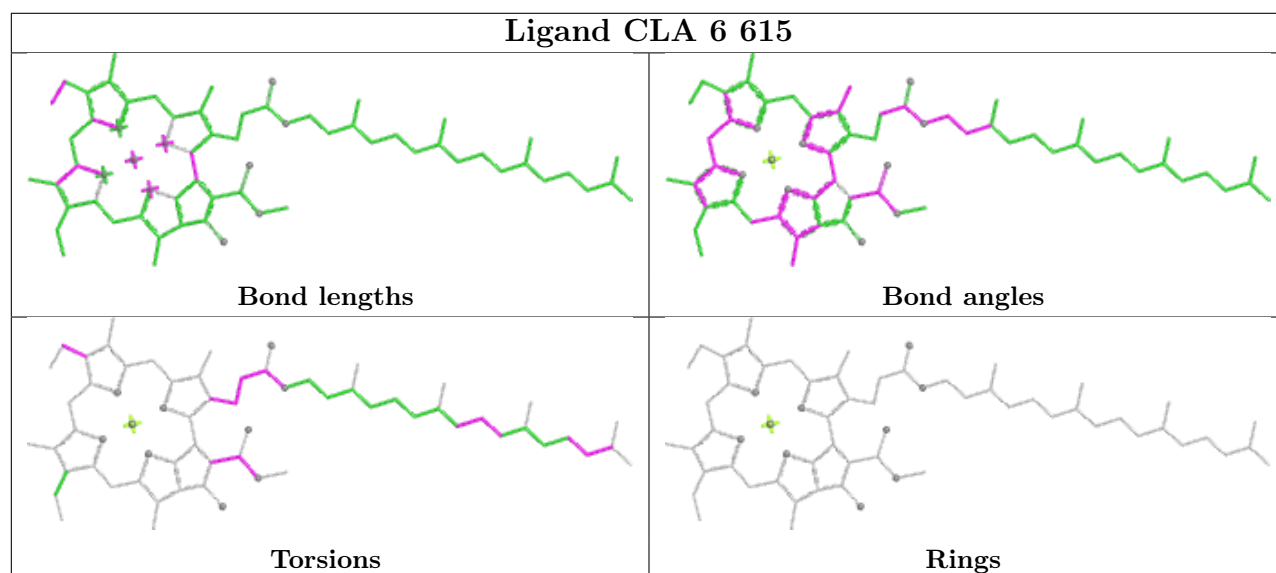
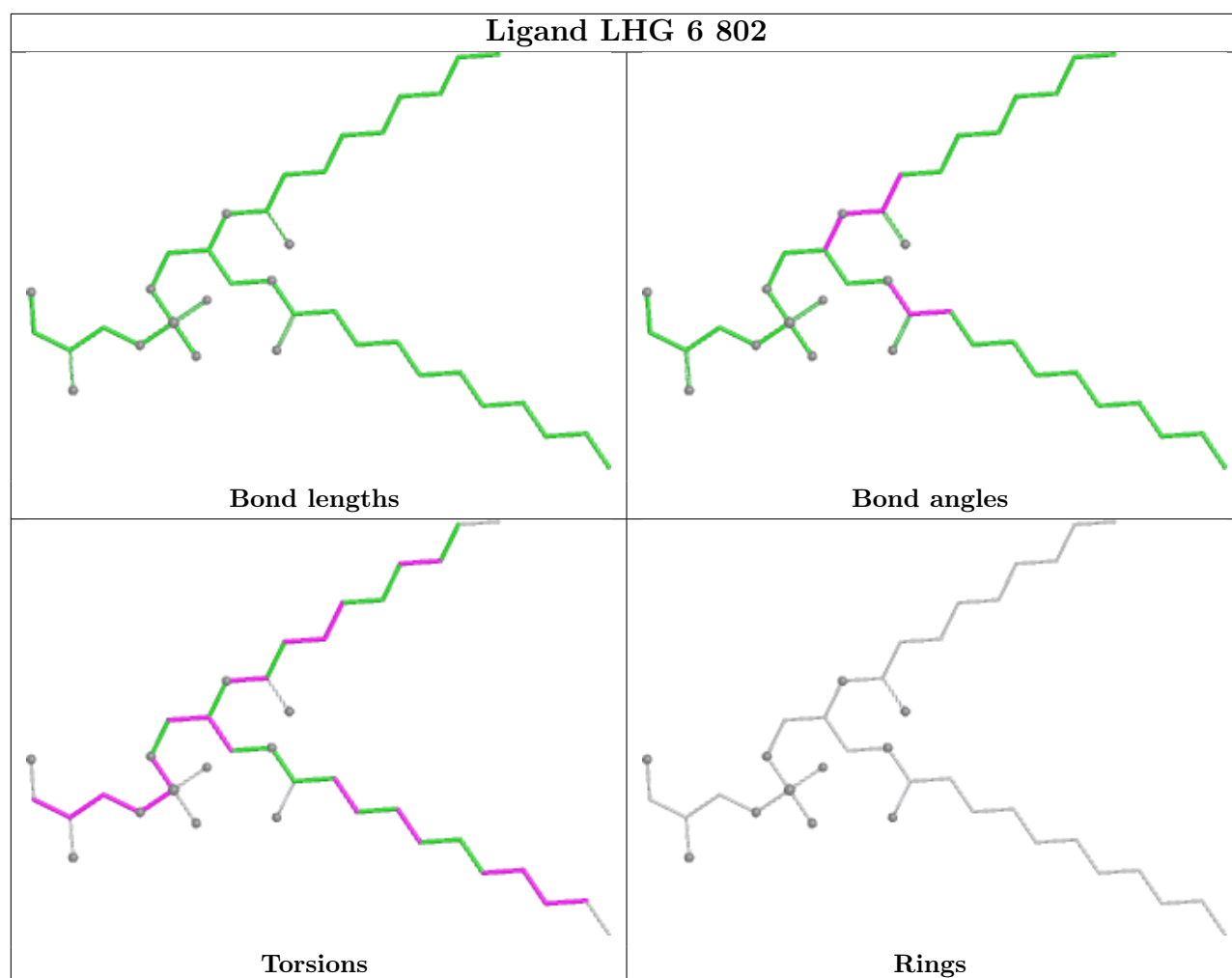


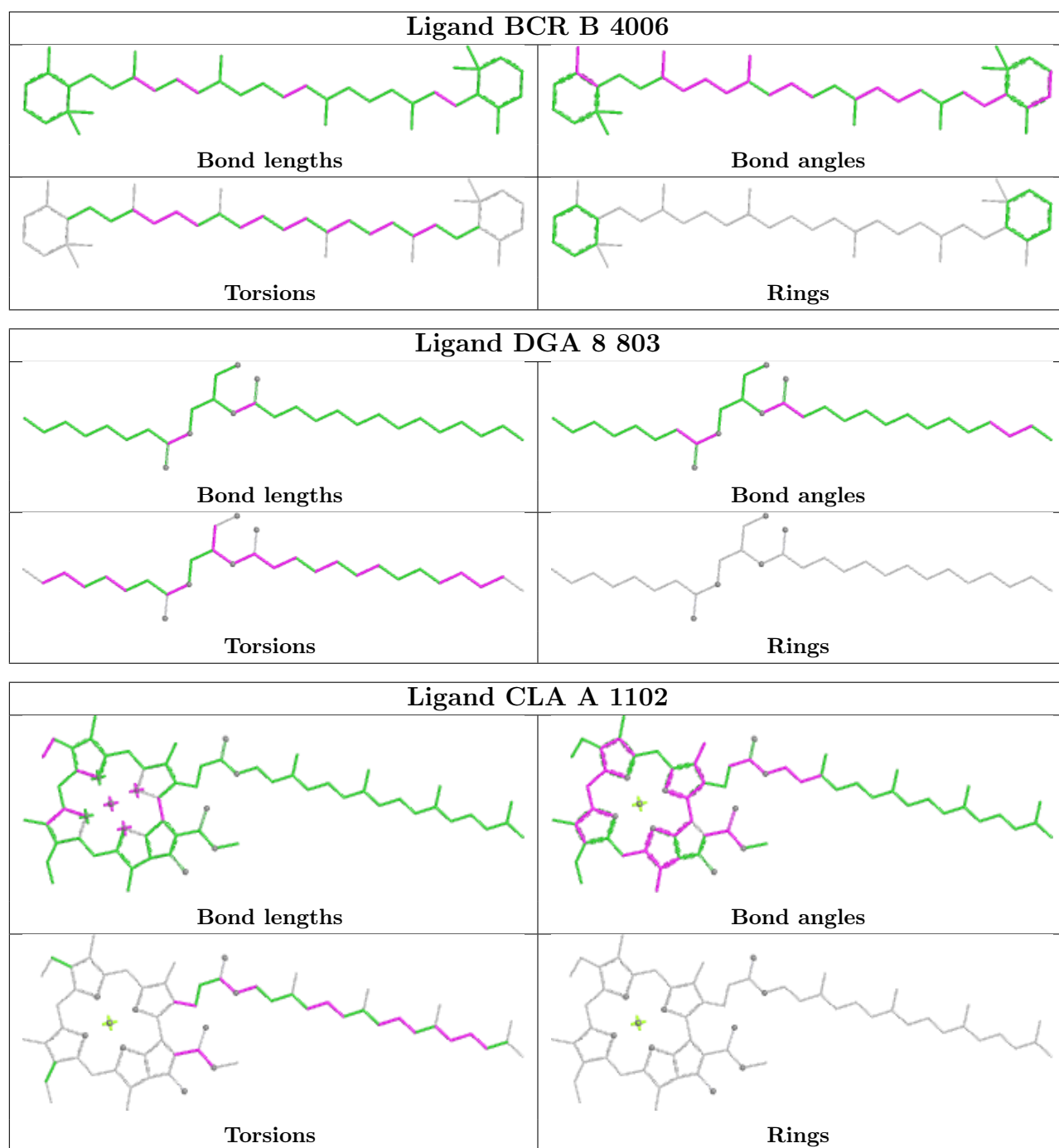
Ligand CLA A 1101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR G 4001	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR 5 503	
 Bond lengths	 Bond angles
 Torsions	 Rings



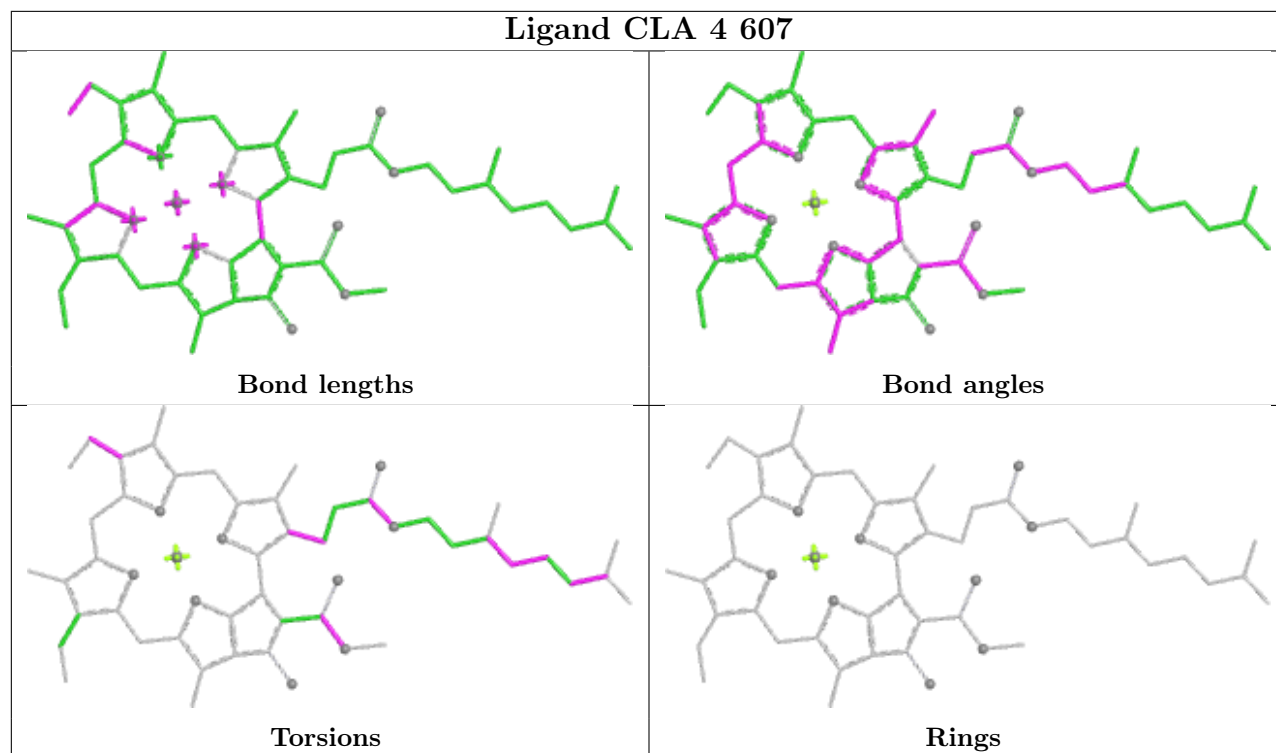




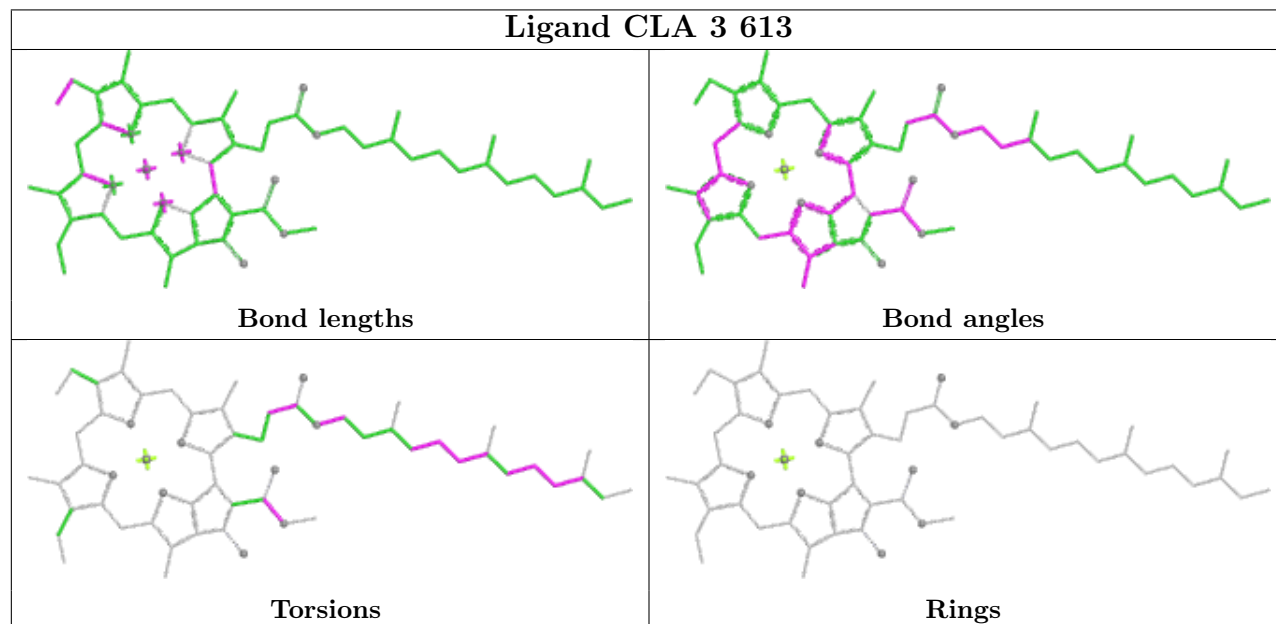


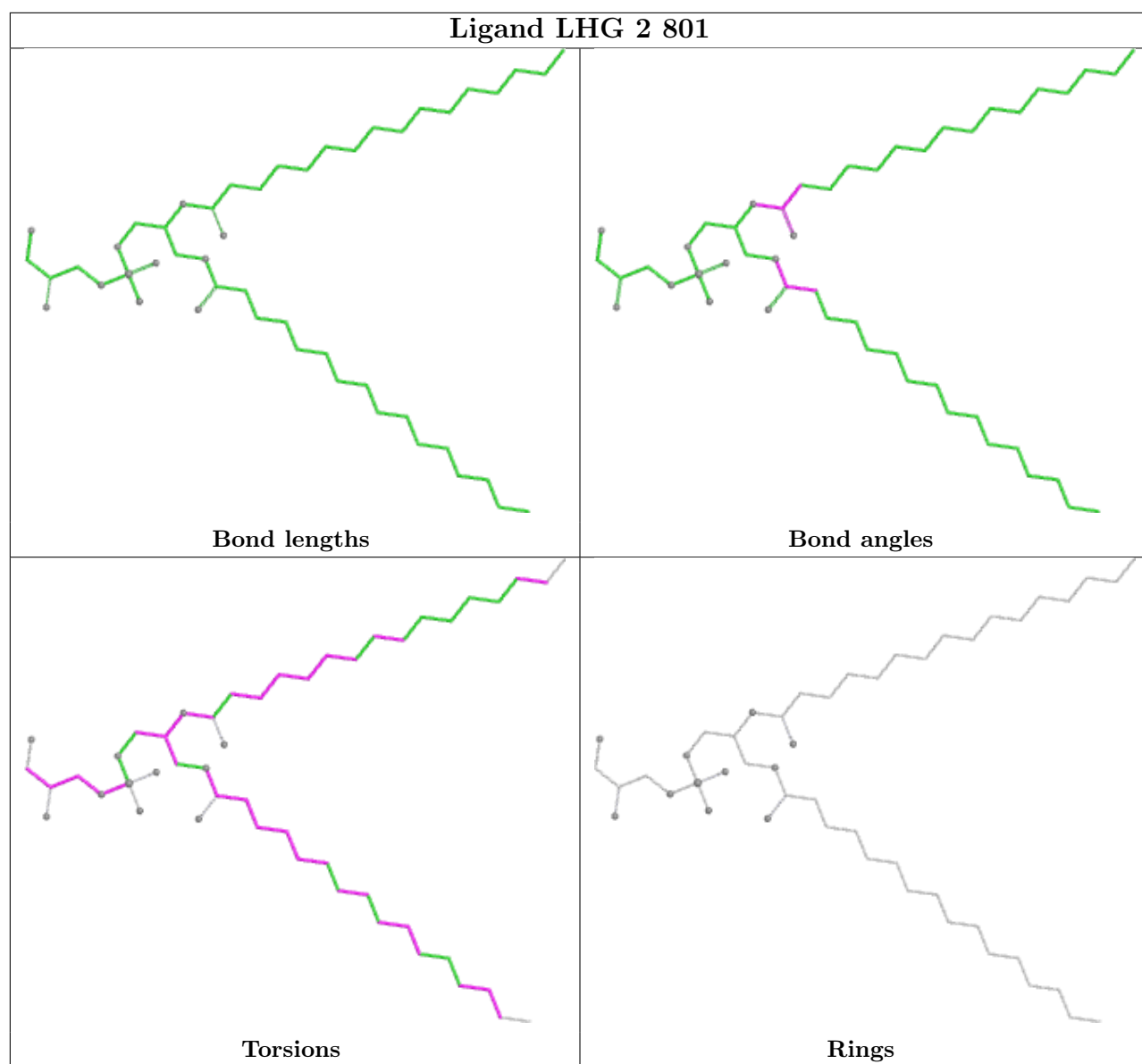


Ligand CLA 4 607

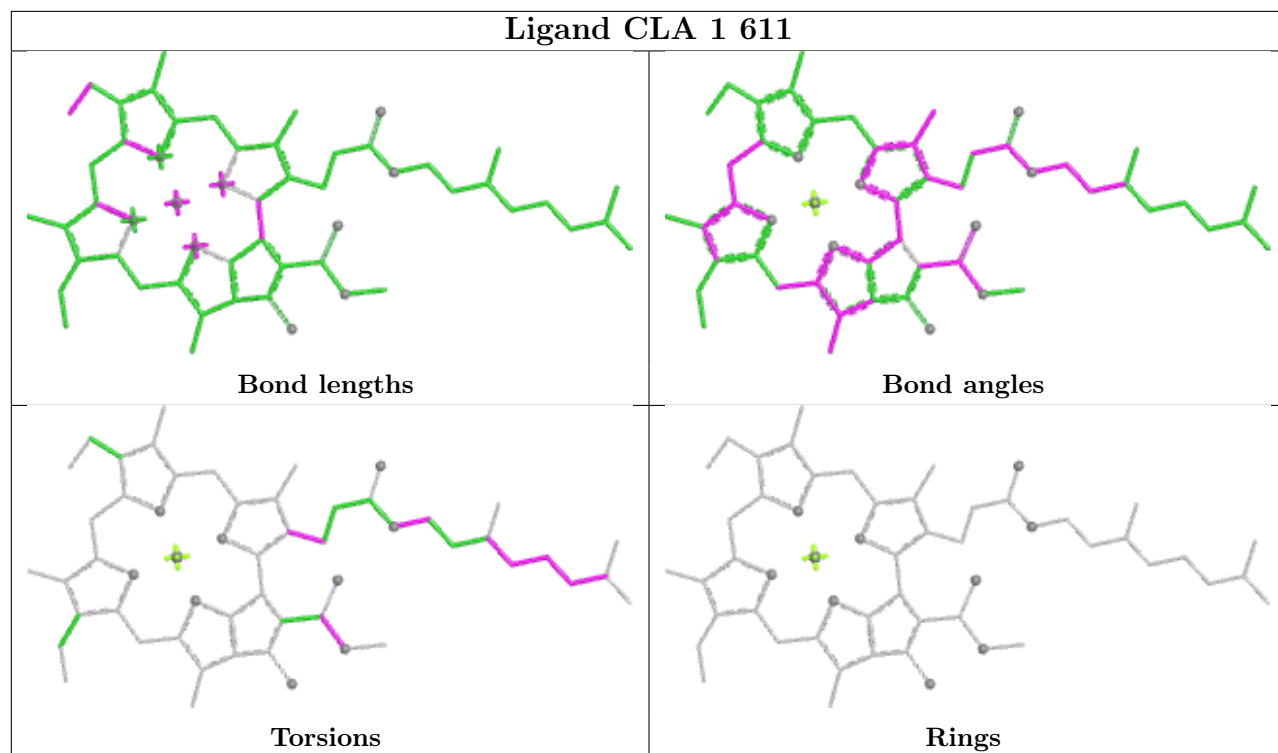


Ligand CLA 3 613

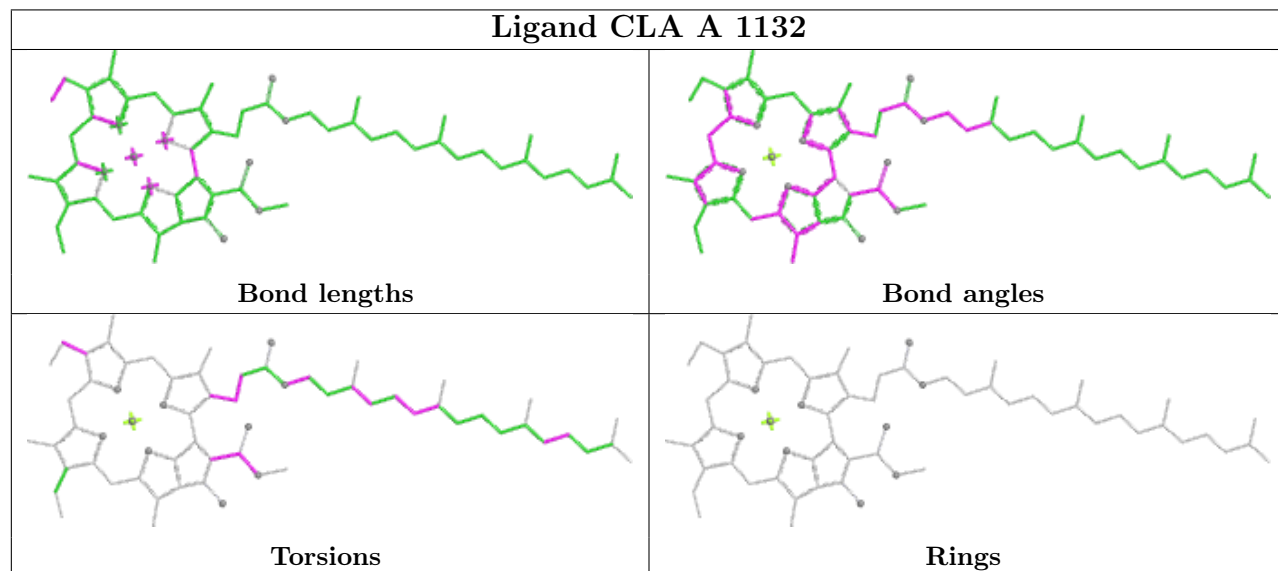


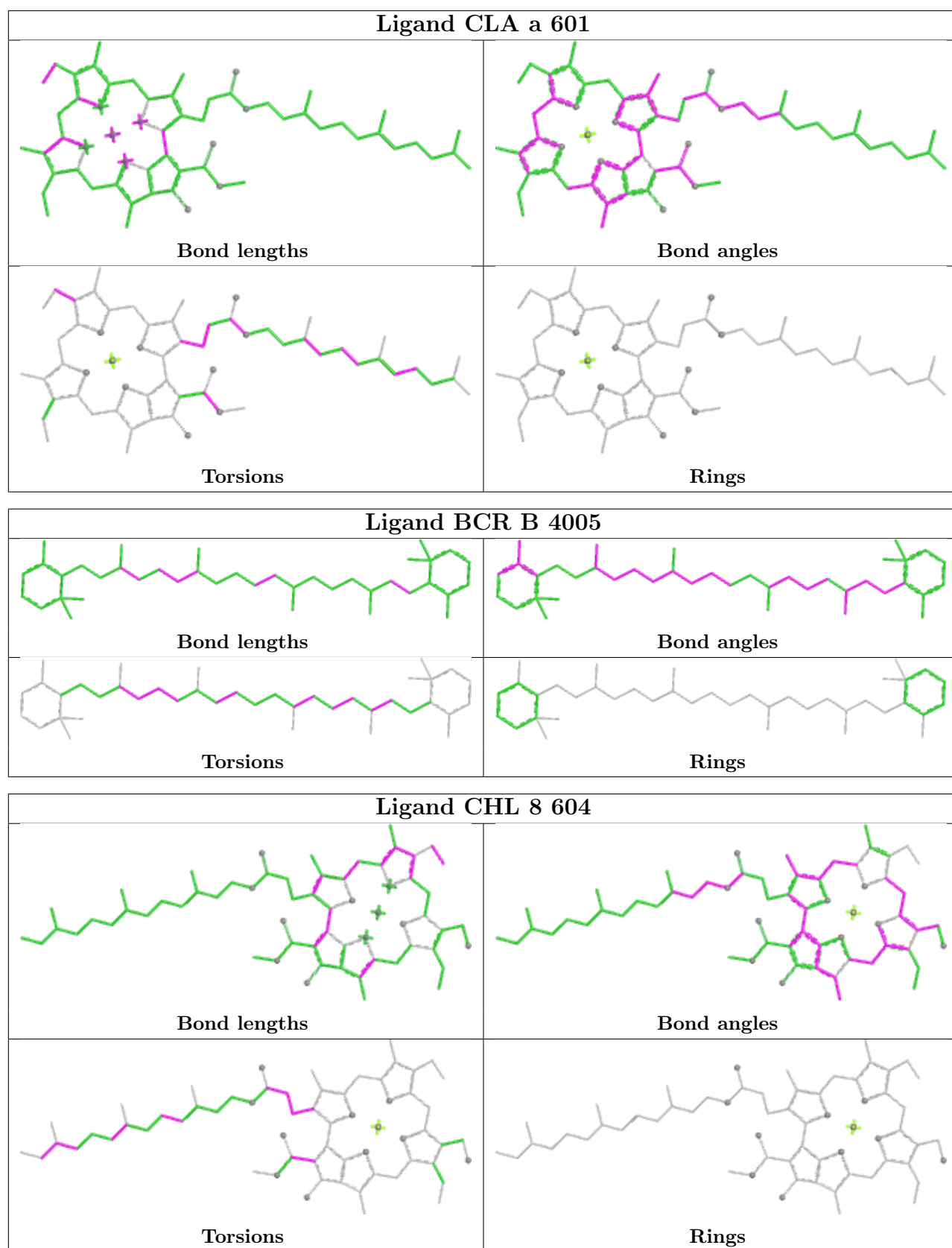


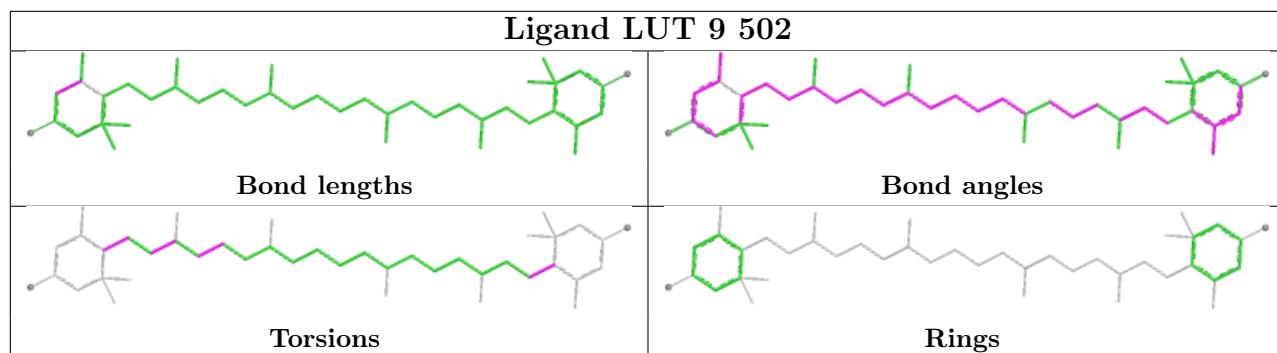
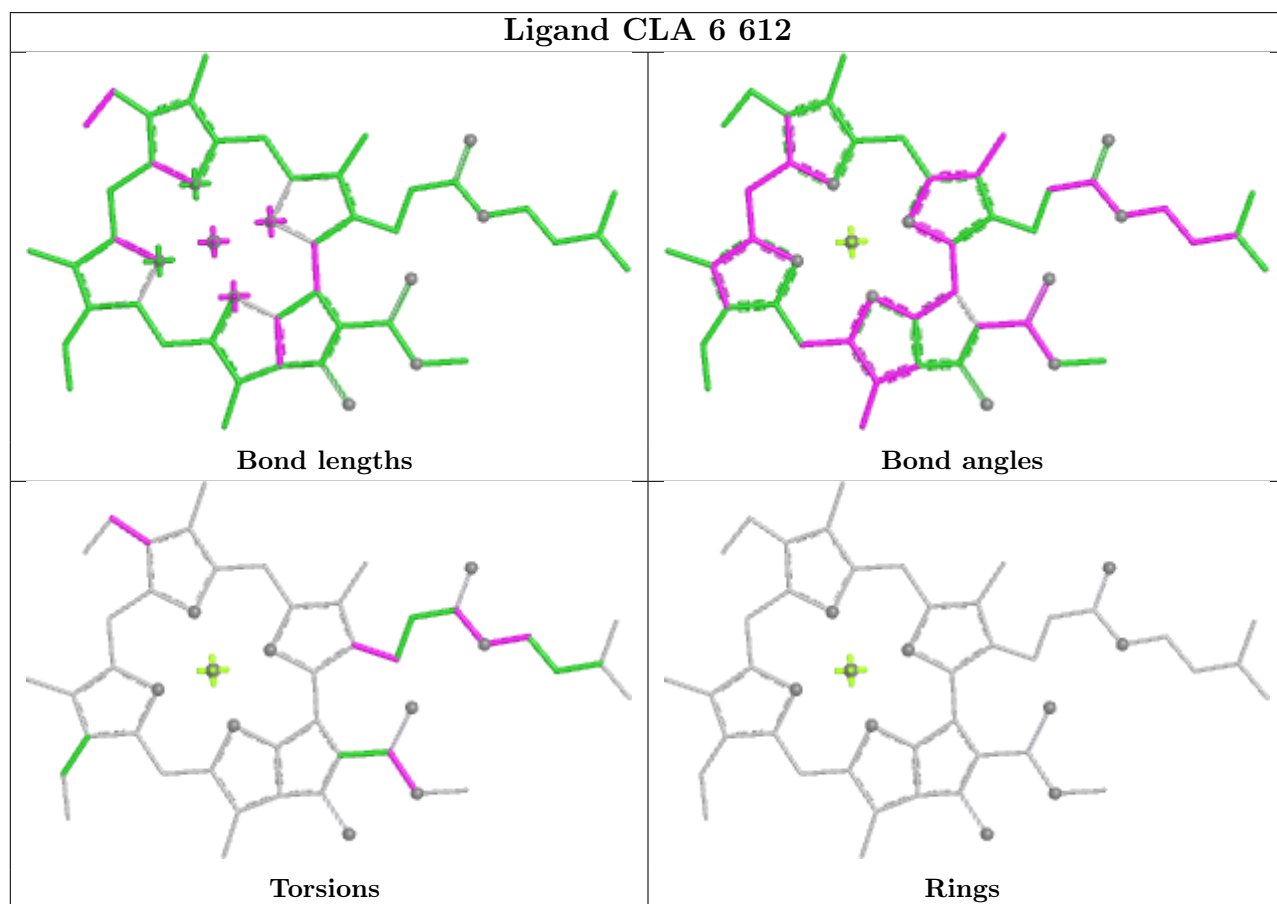
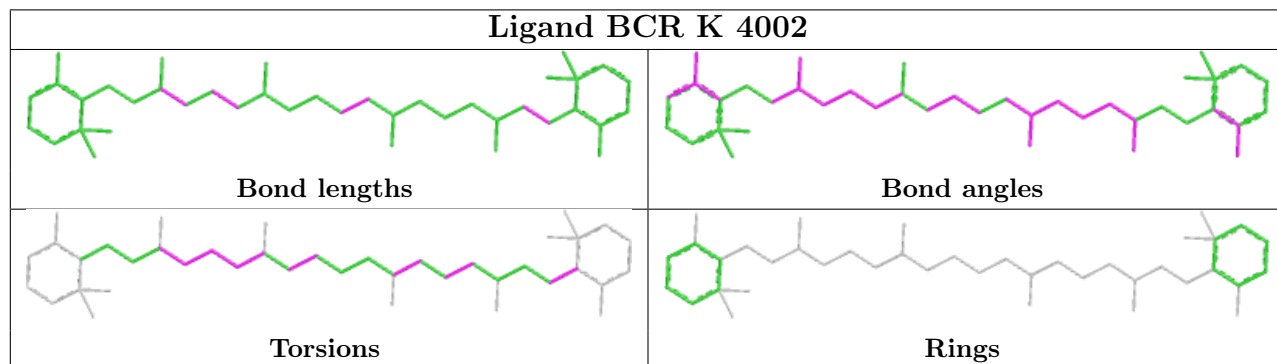
Ligand CLA 1 611



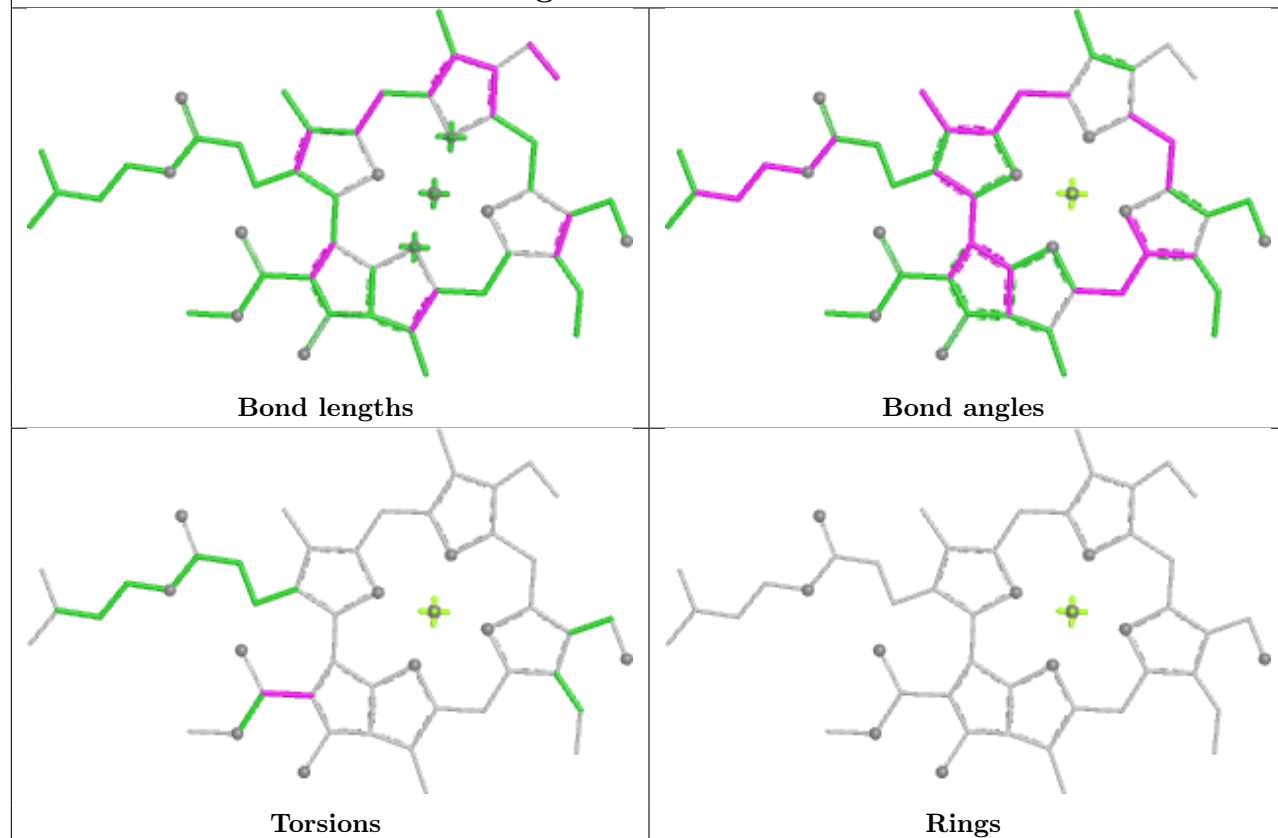
Ligand CLA A 1132



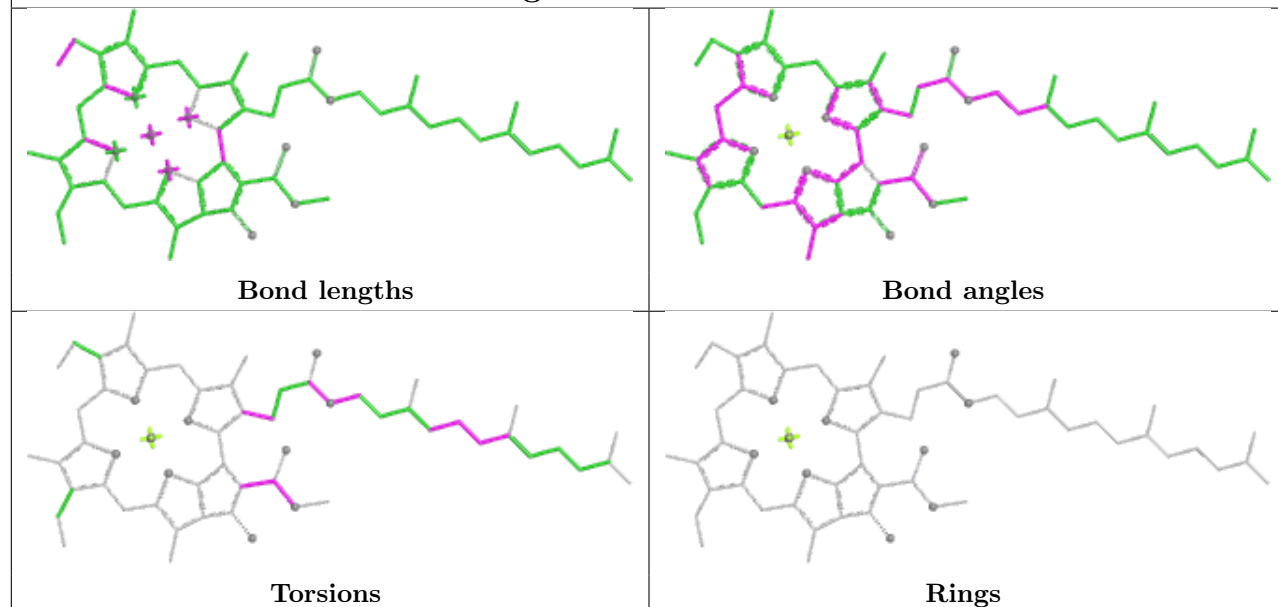


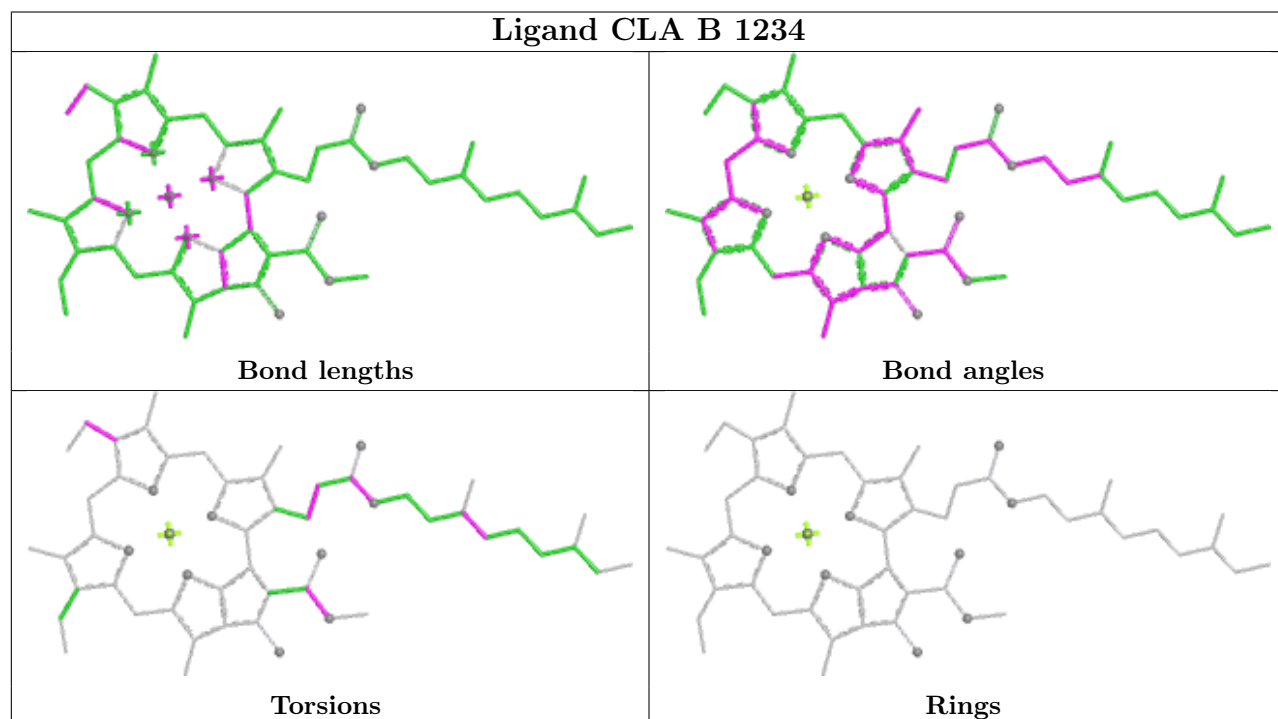
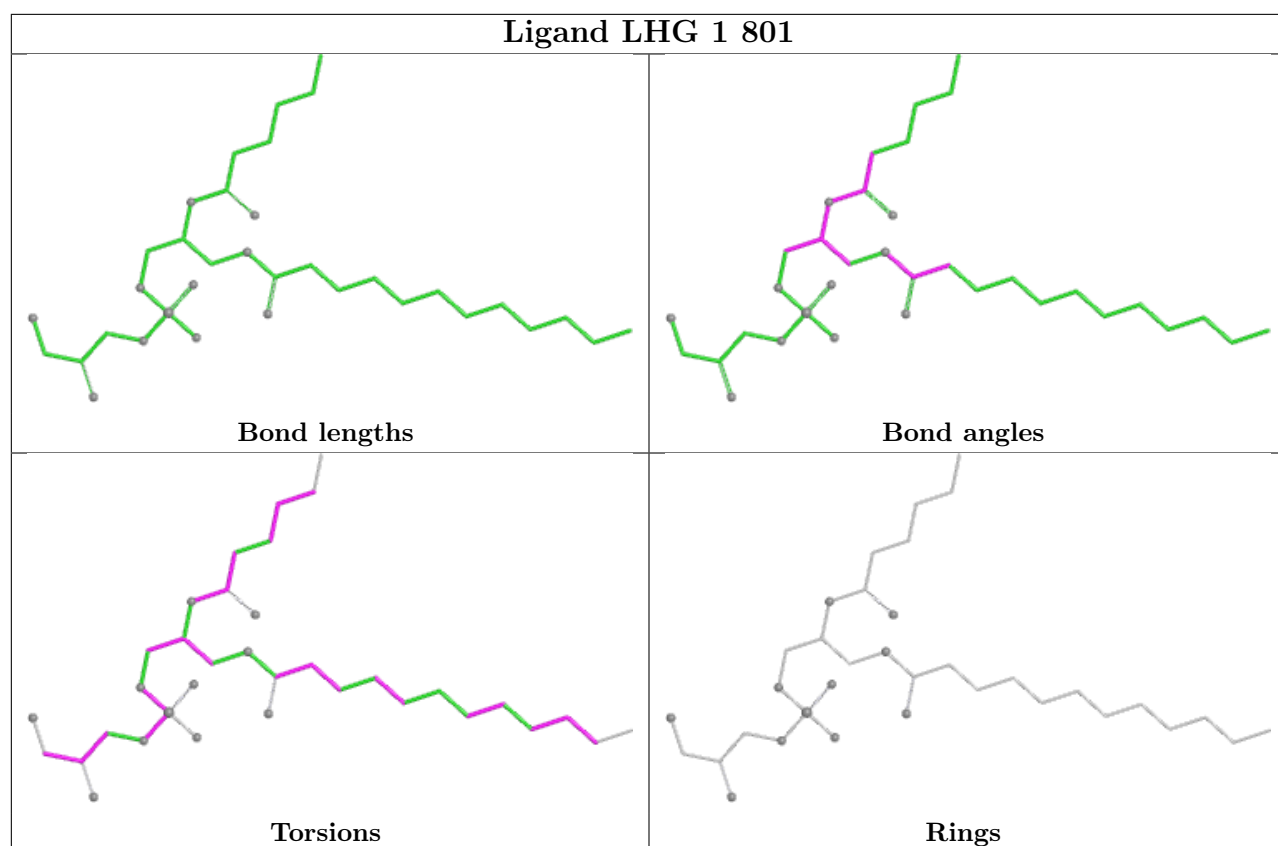
Ligand LUT 9 502**Ligand CLA 6 612****Ligand BCR K 4002**

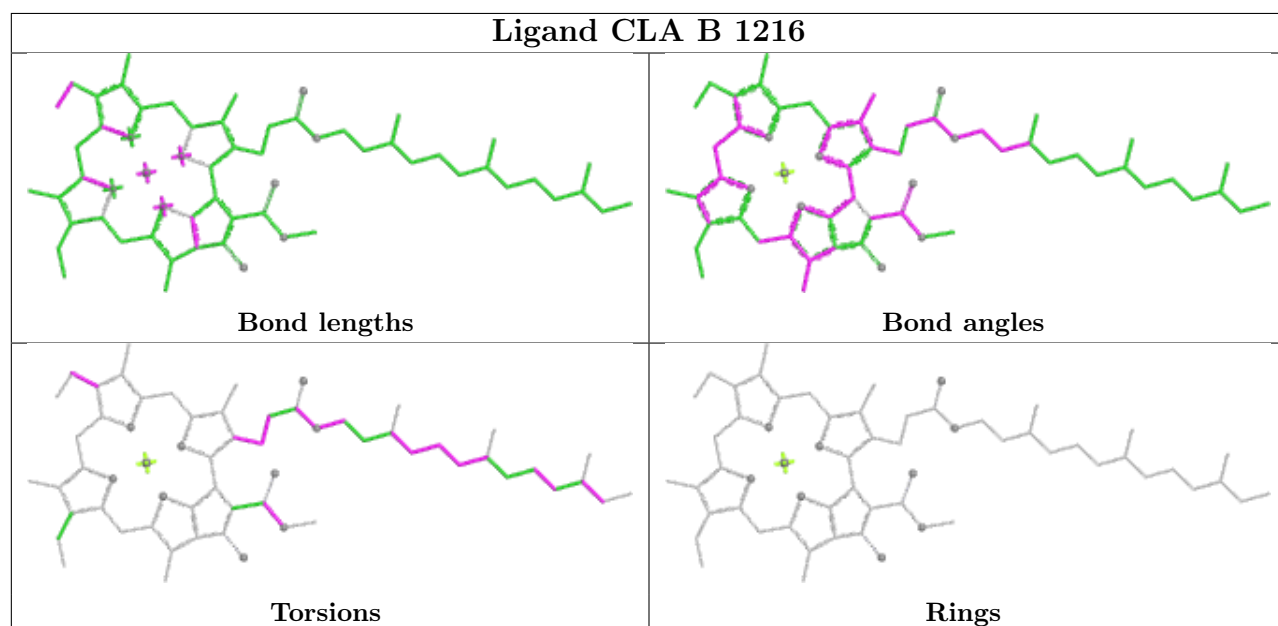
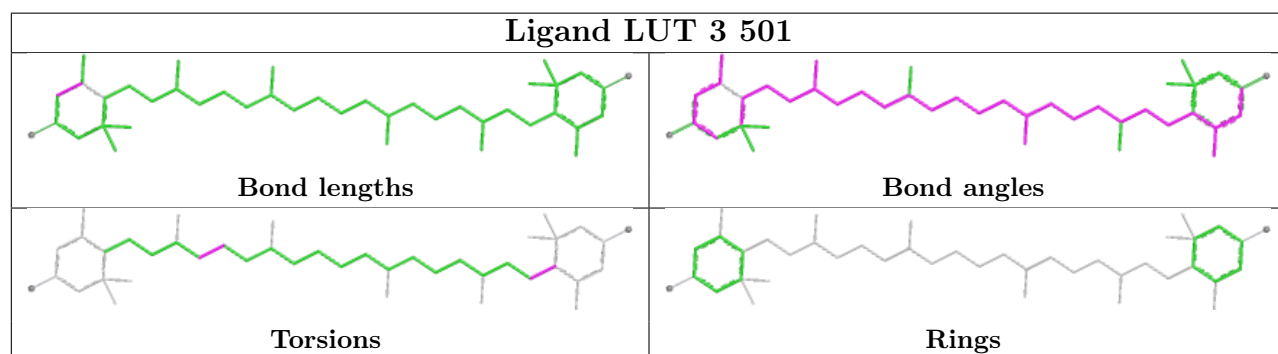
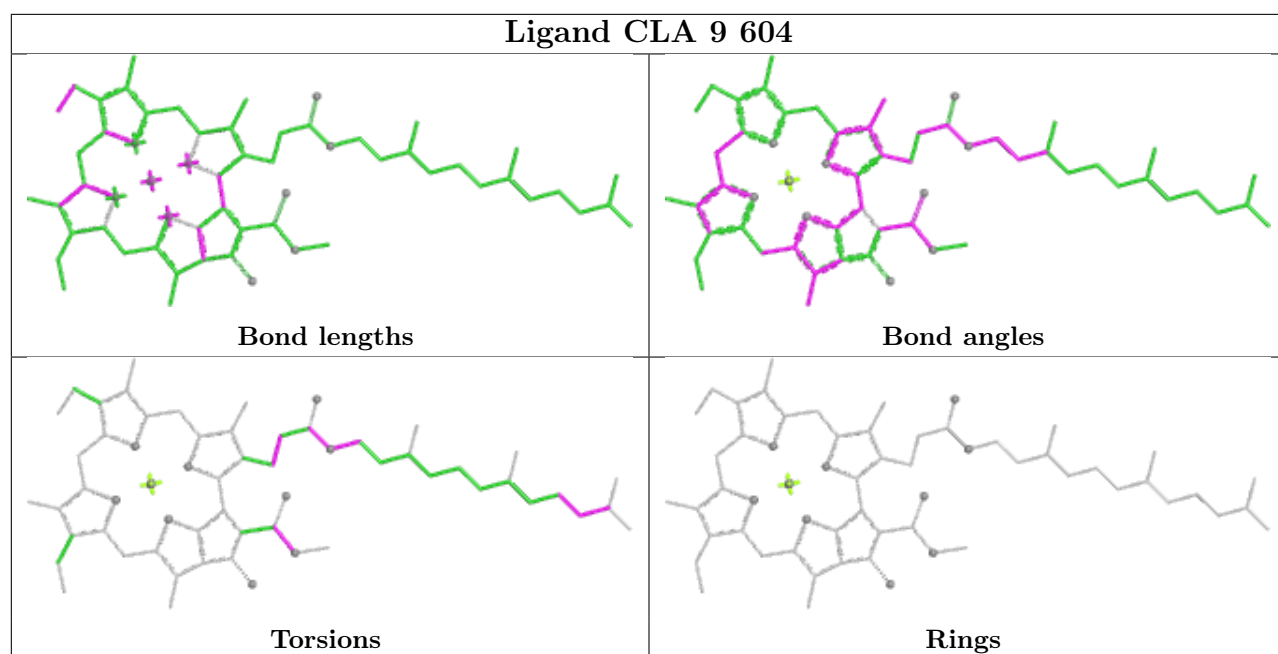
Ligand CHL 8 613

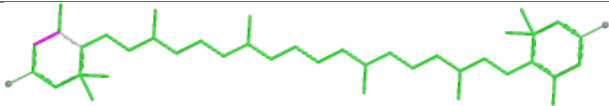
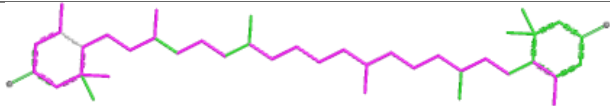
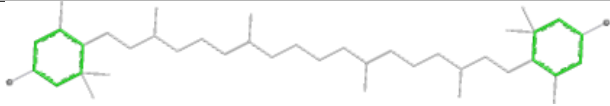


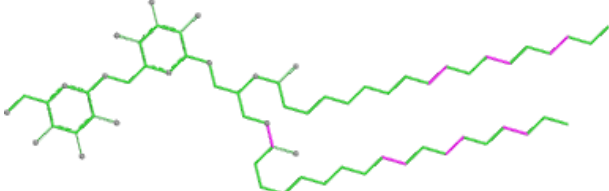
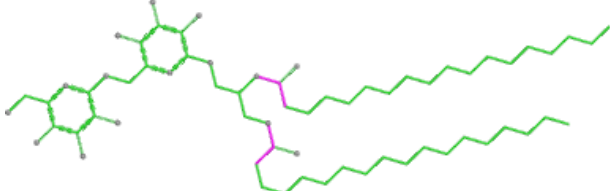
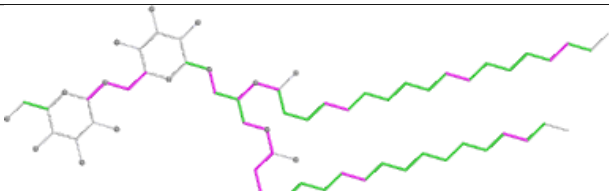
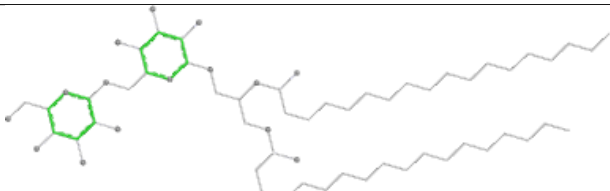
Ligand CLA B 1207

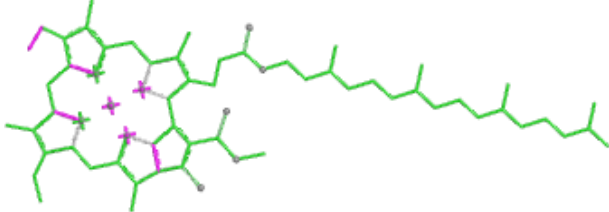
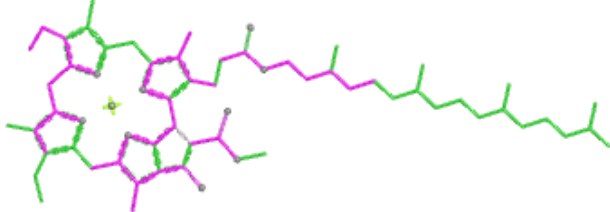
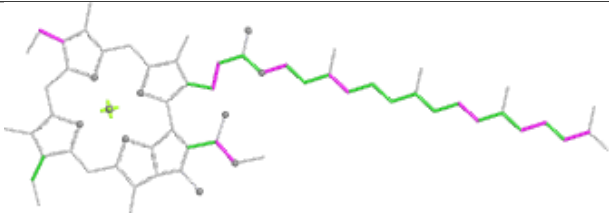
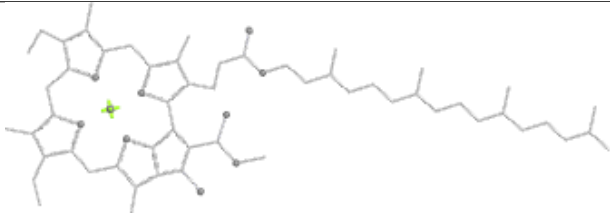


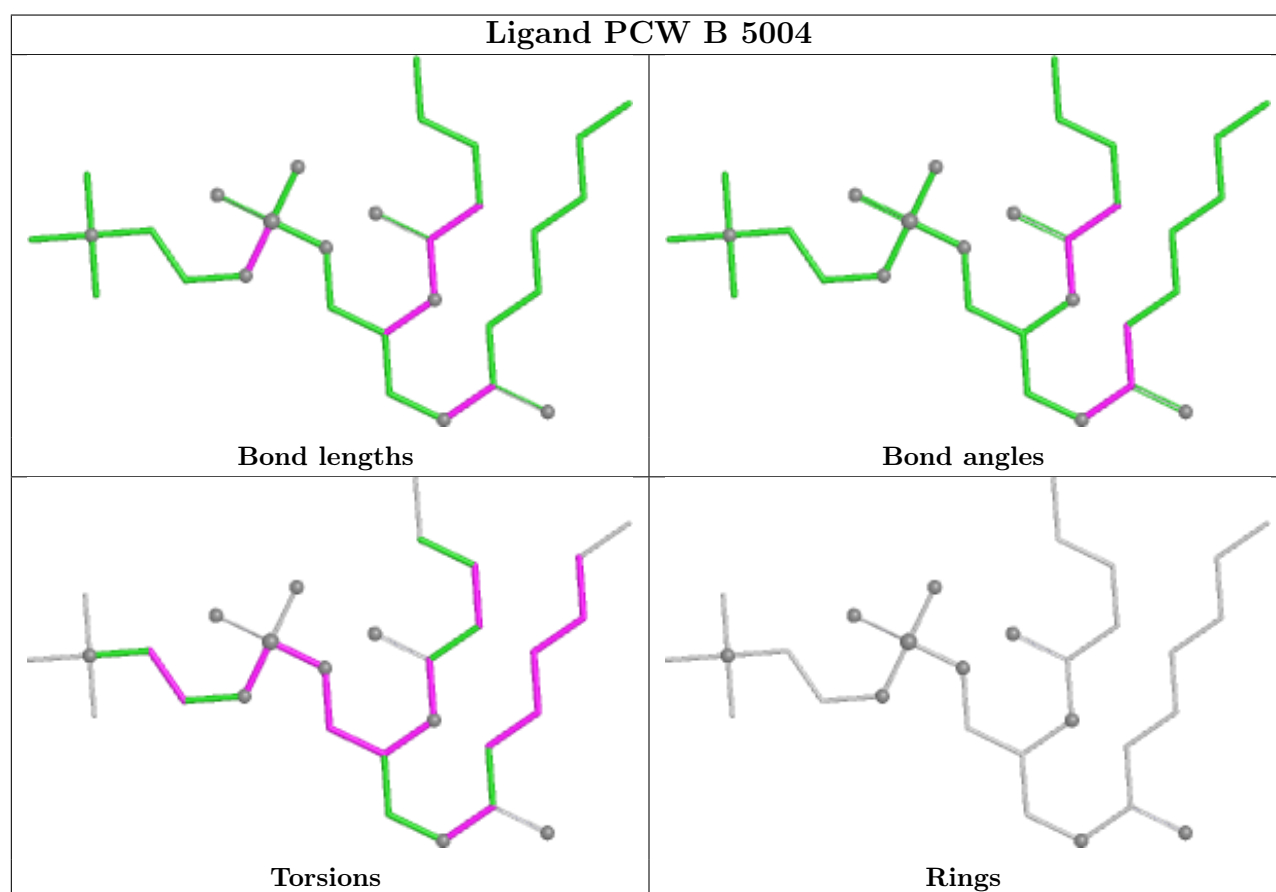
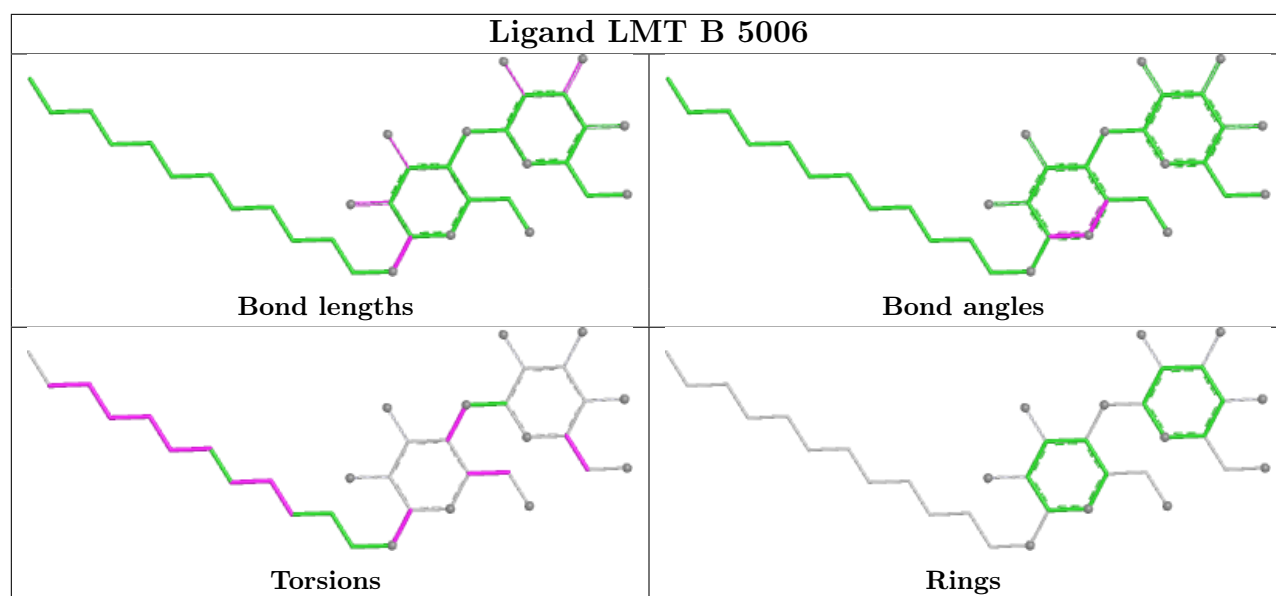




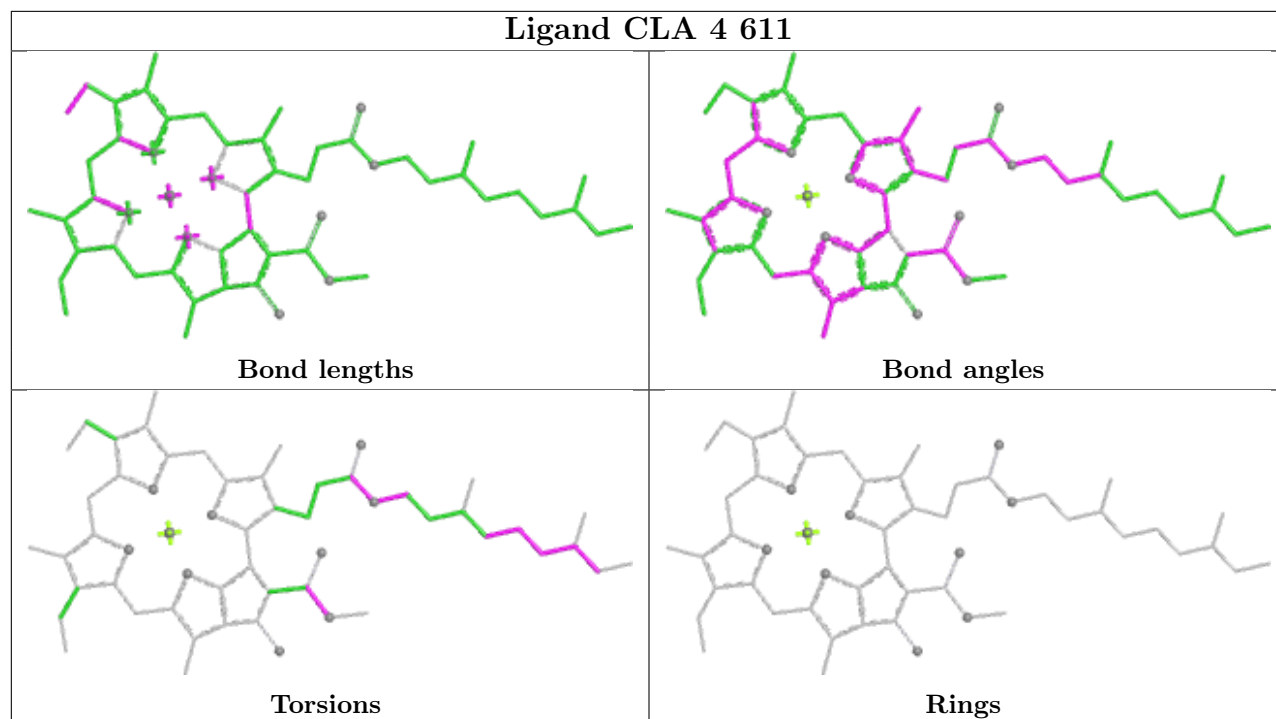
Ligand LUT 8 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGD 8 802	
	
Bond lengths	Bond angles
	
Torsions	Rings

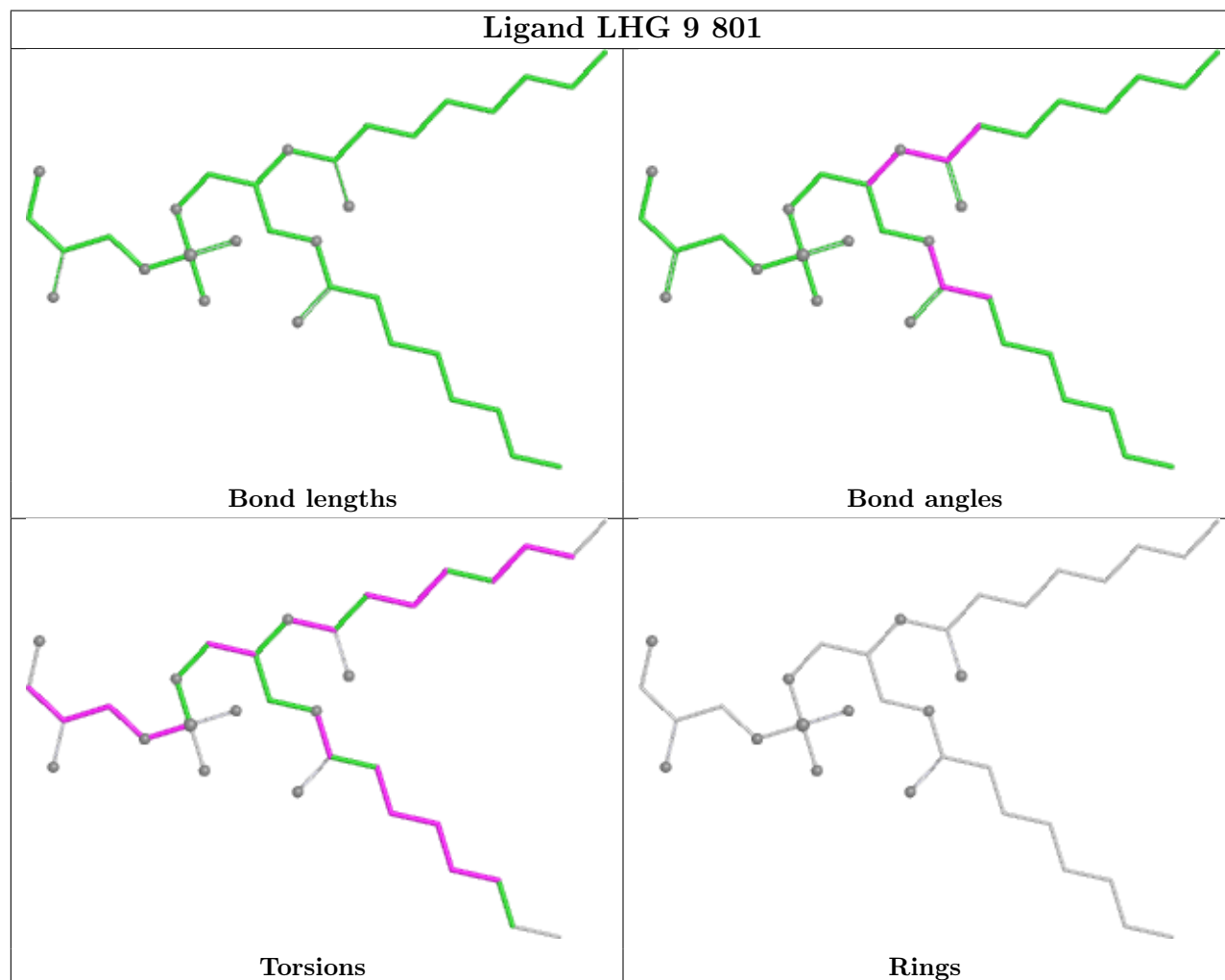
Ligand CLA B 1022	
	
Bond lengths	Bond angles
	
Torsions	Rings



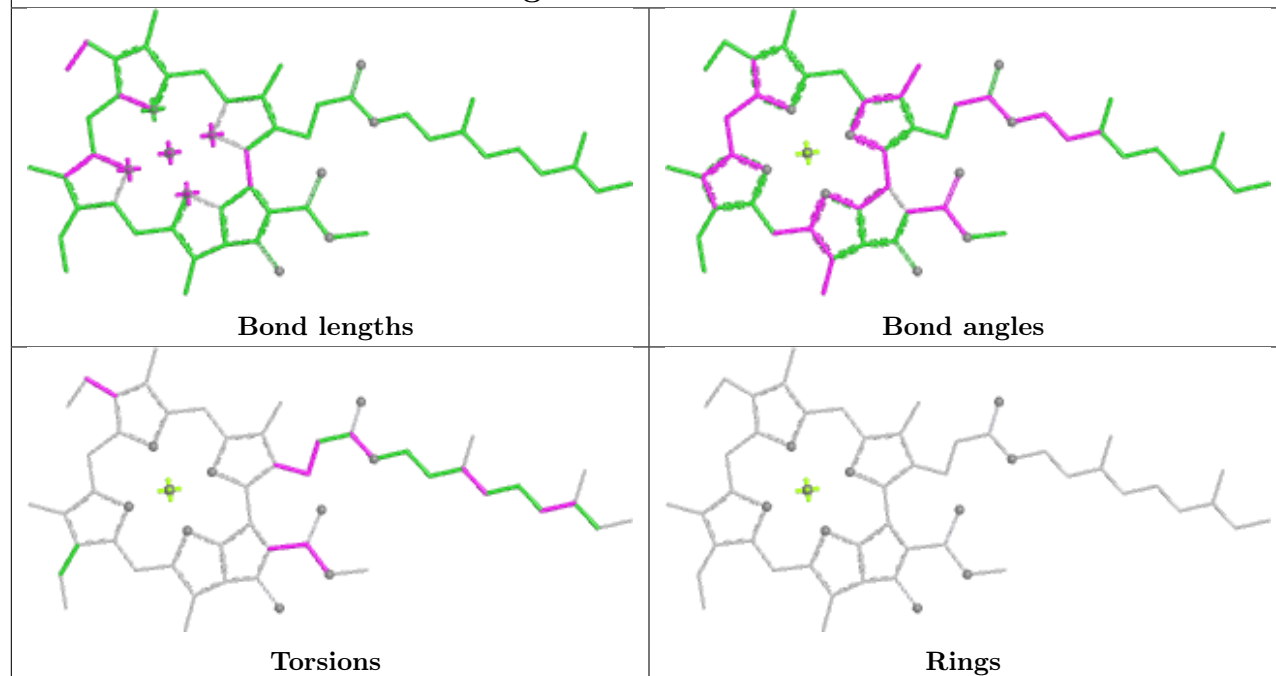
Ligand CLA 4 611



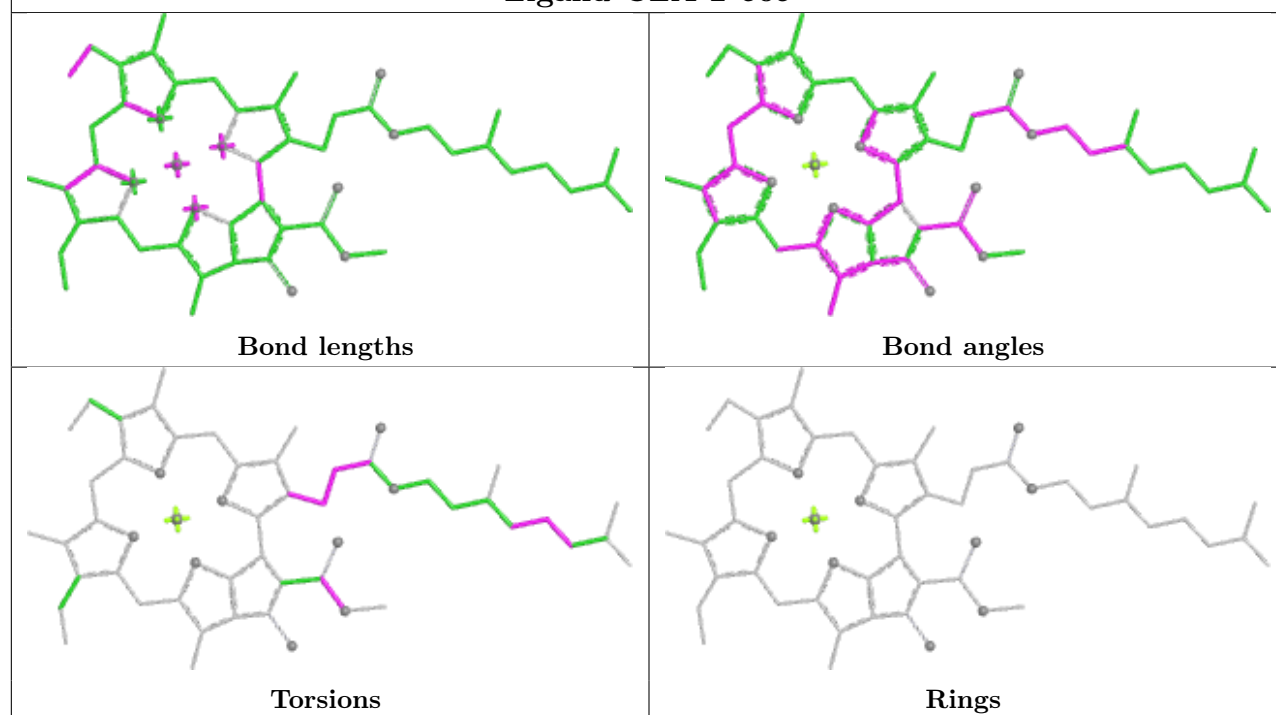
Ligand LHG 9 801

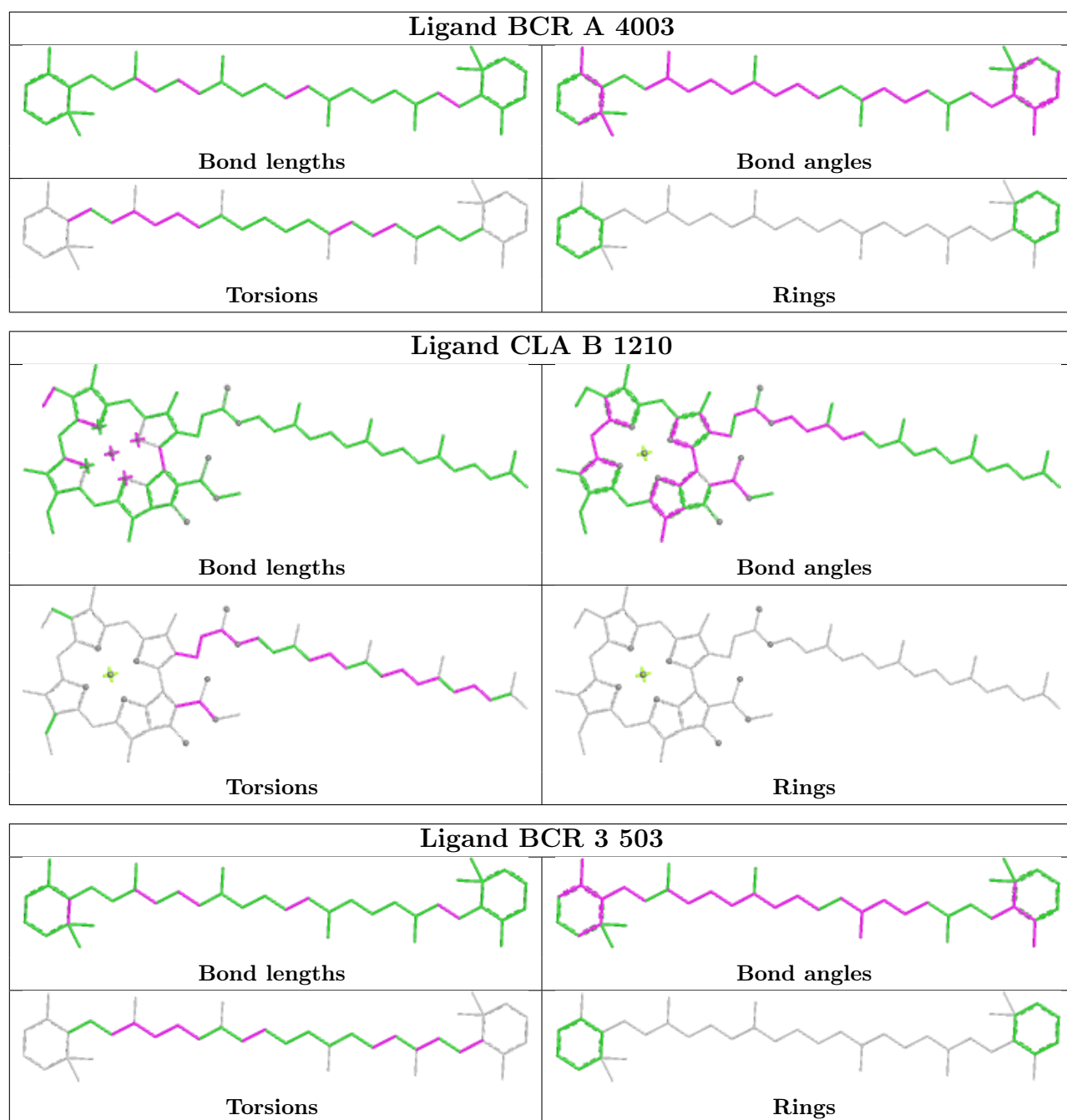


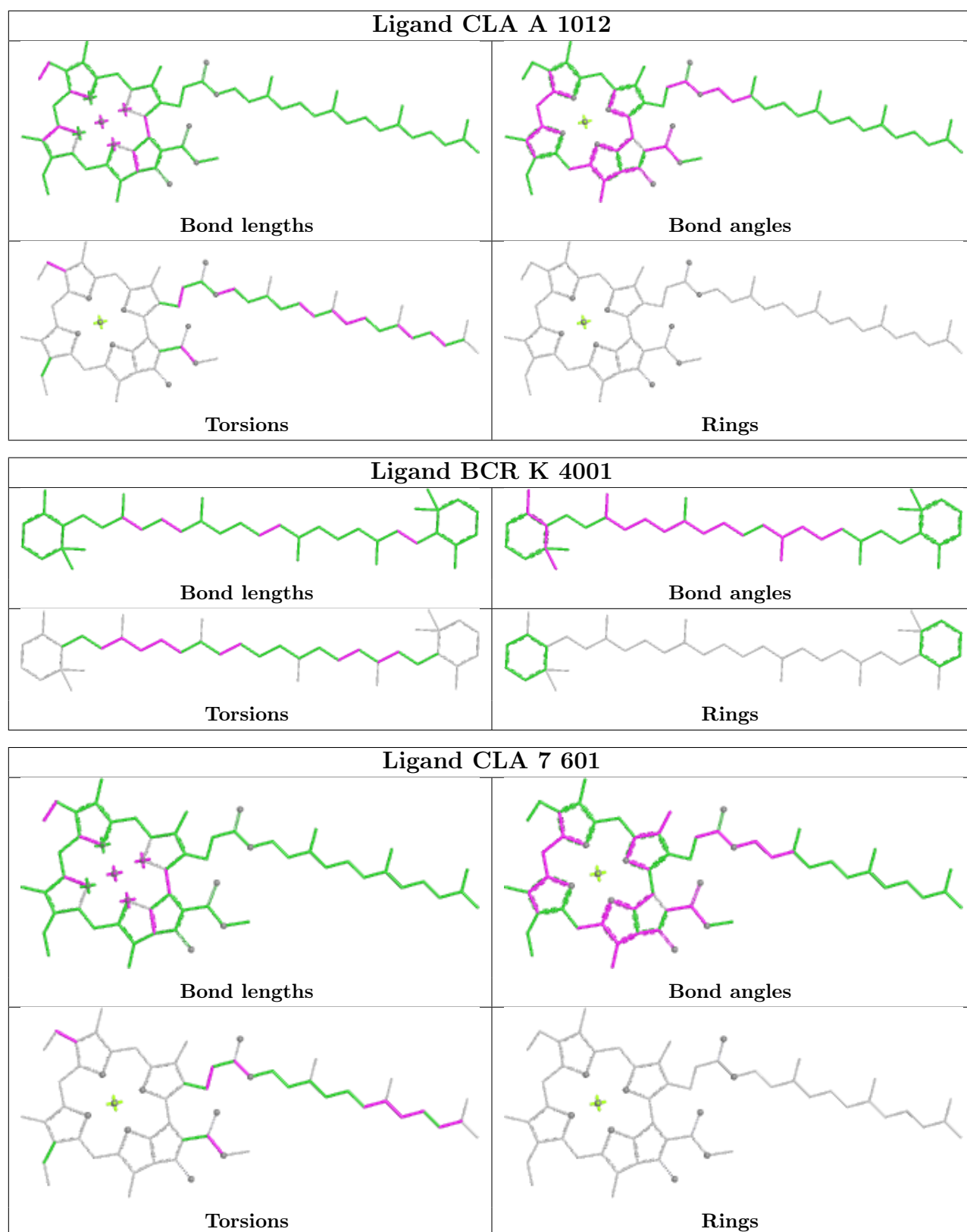
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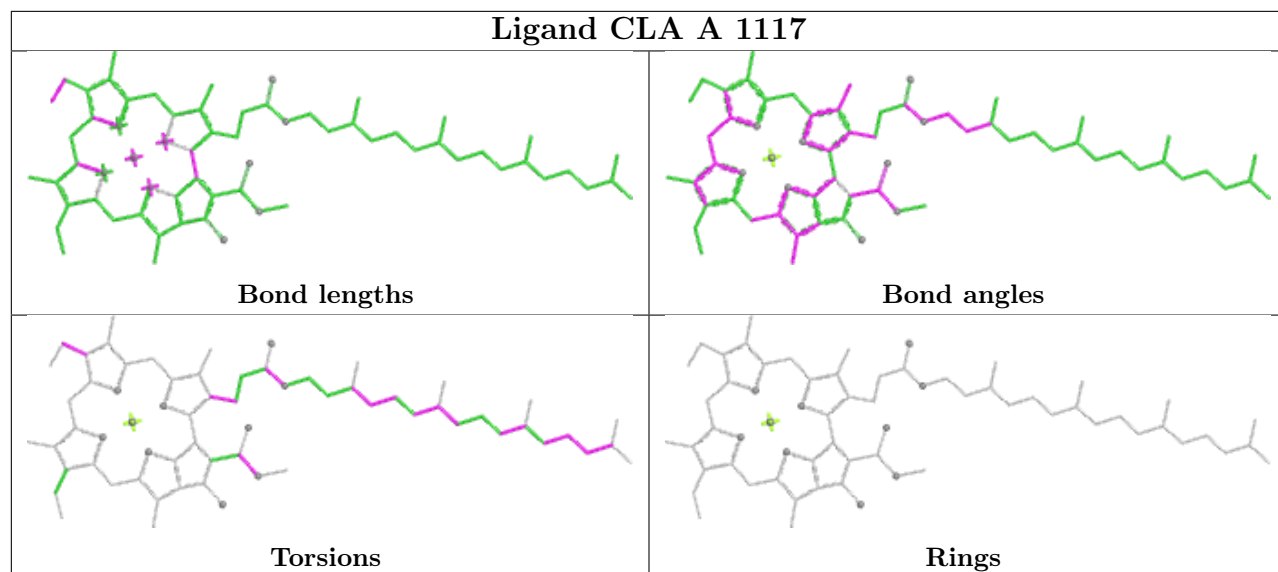
Ligand CLA 2 609



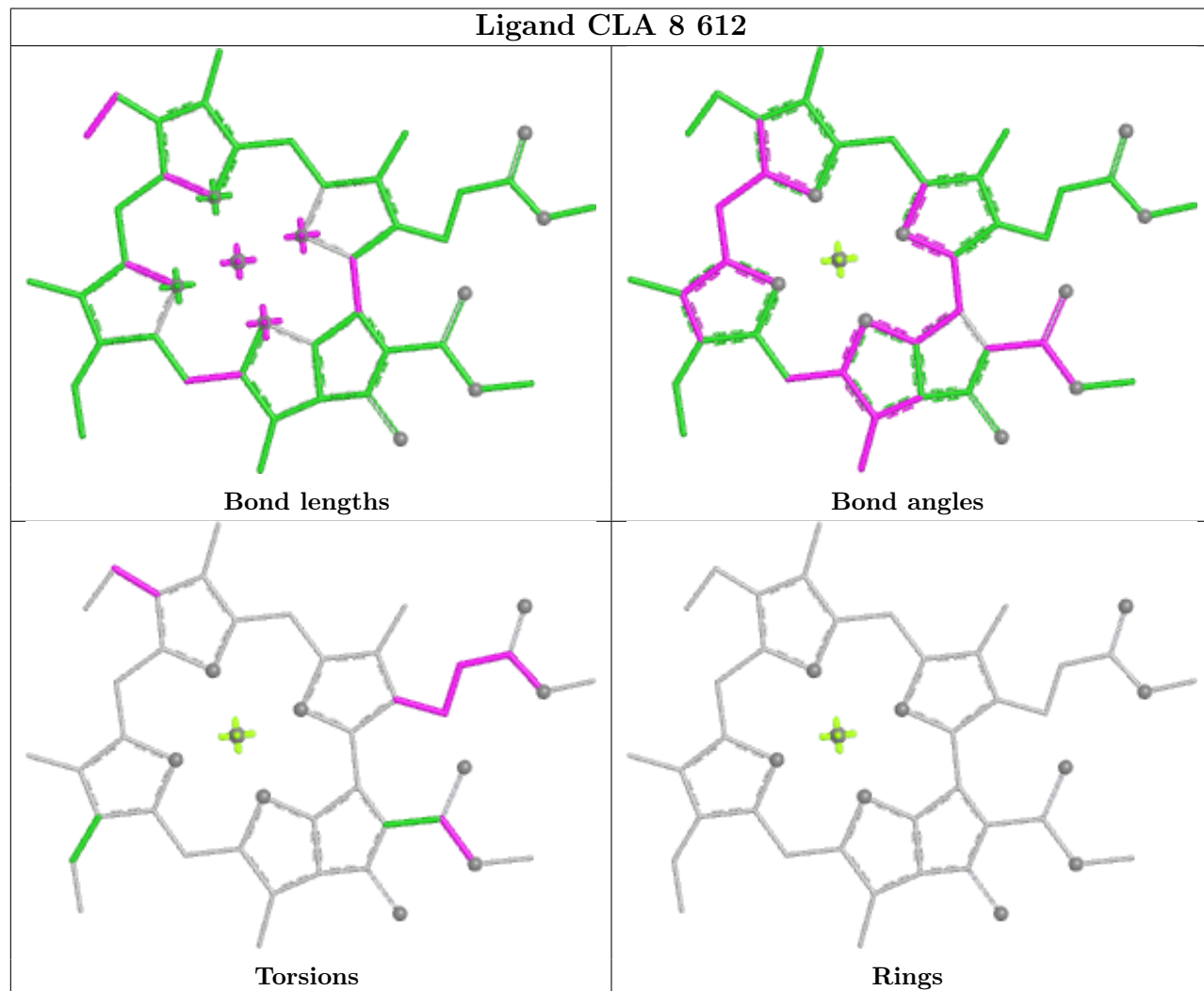


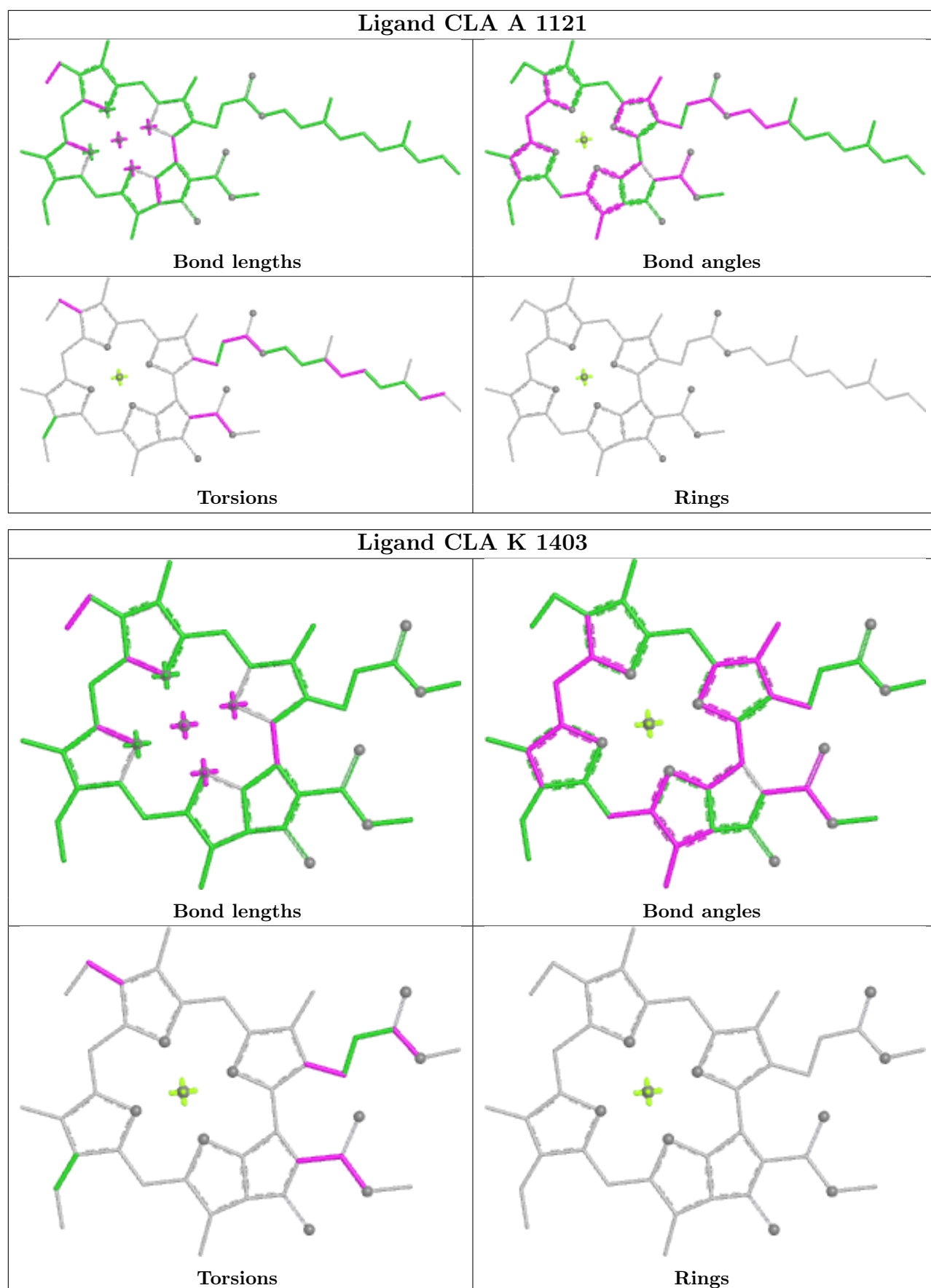


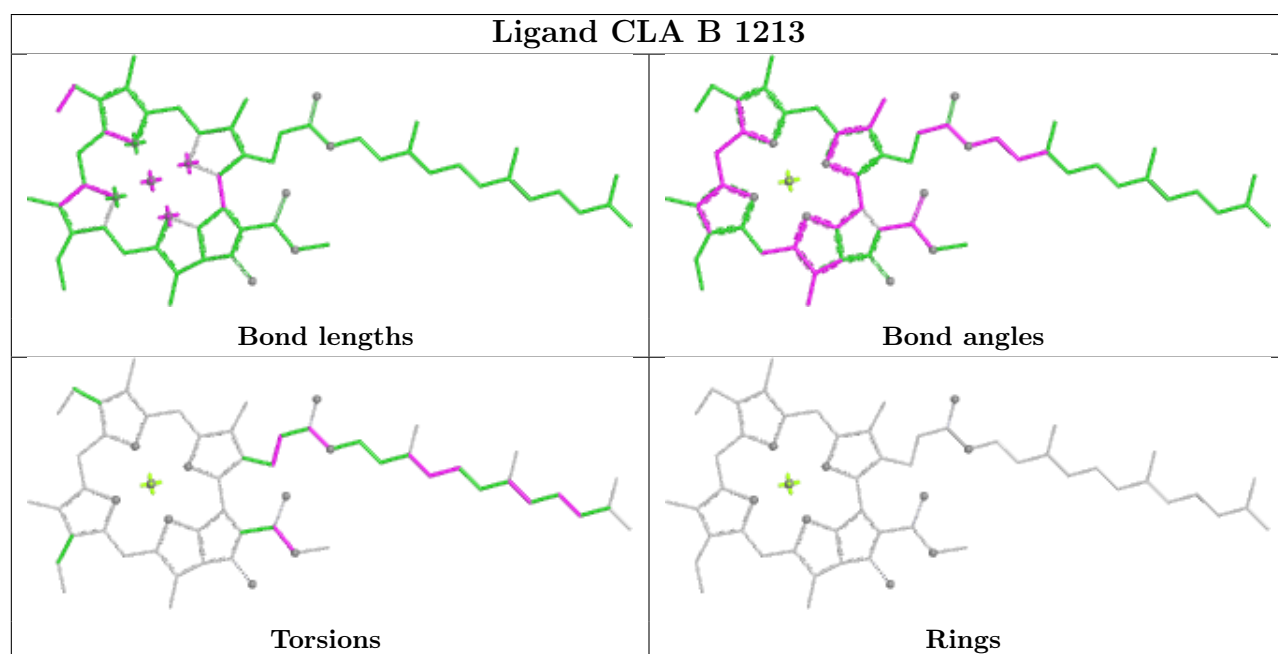
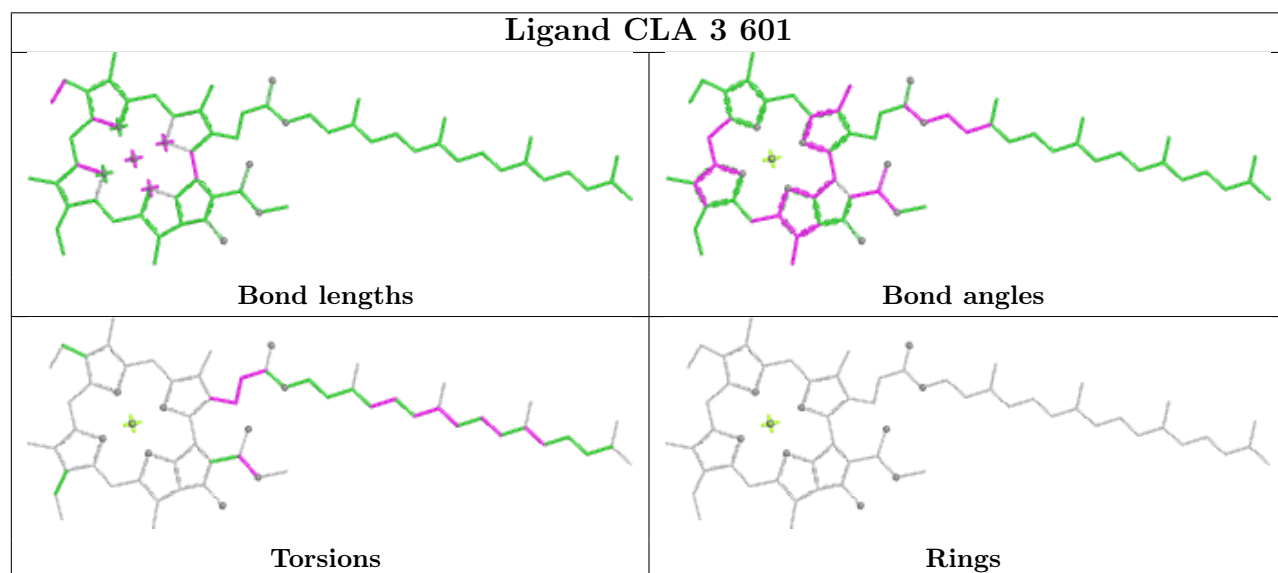
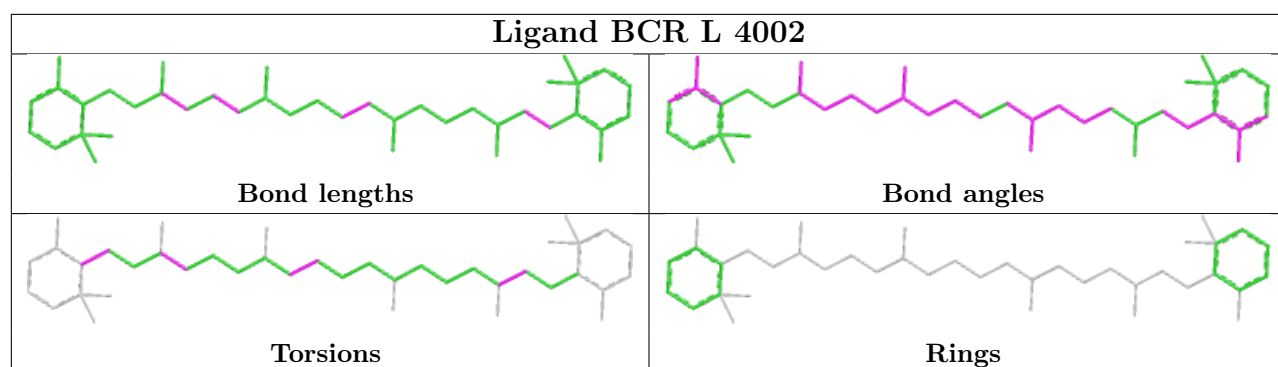
Ligand CLA A 1117

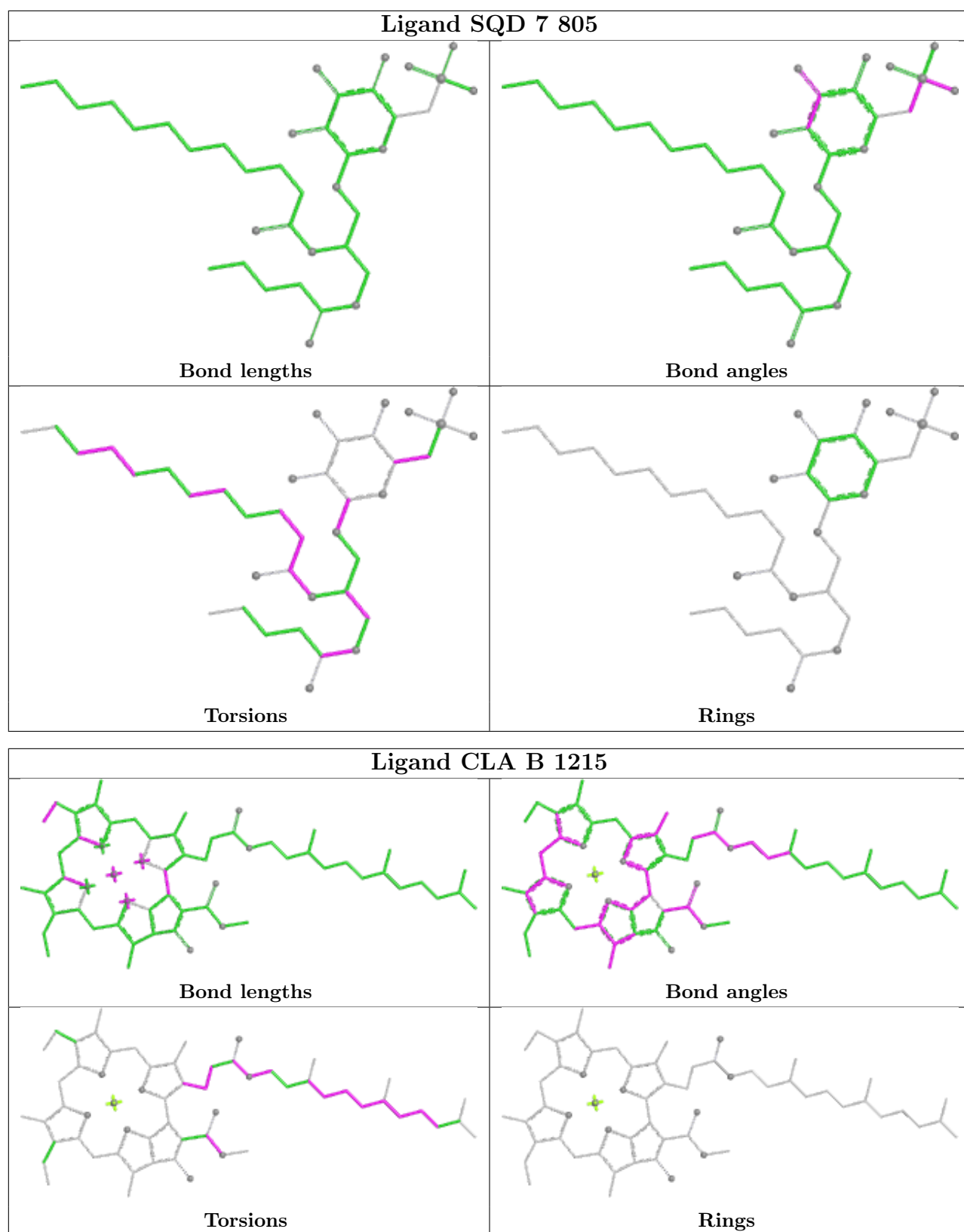


Ligand CLA 8 612

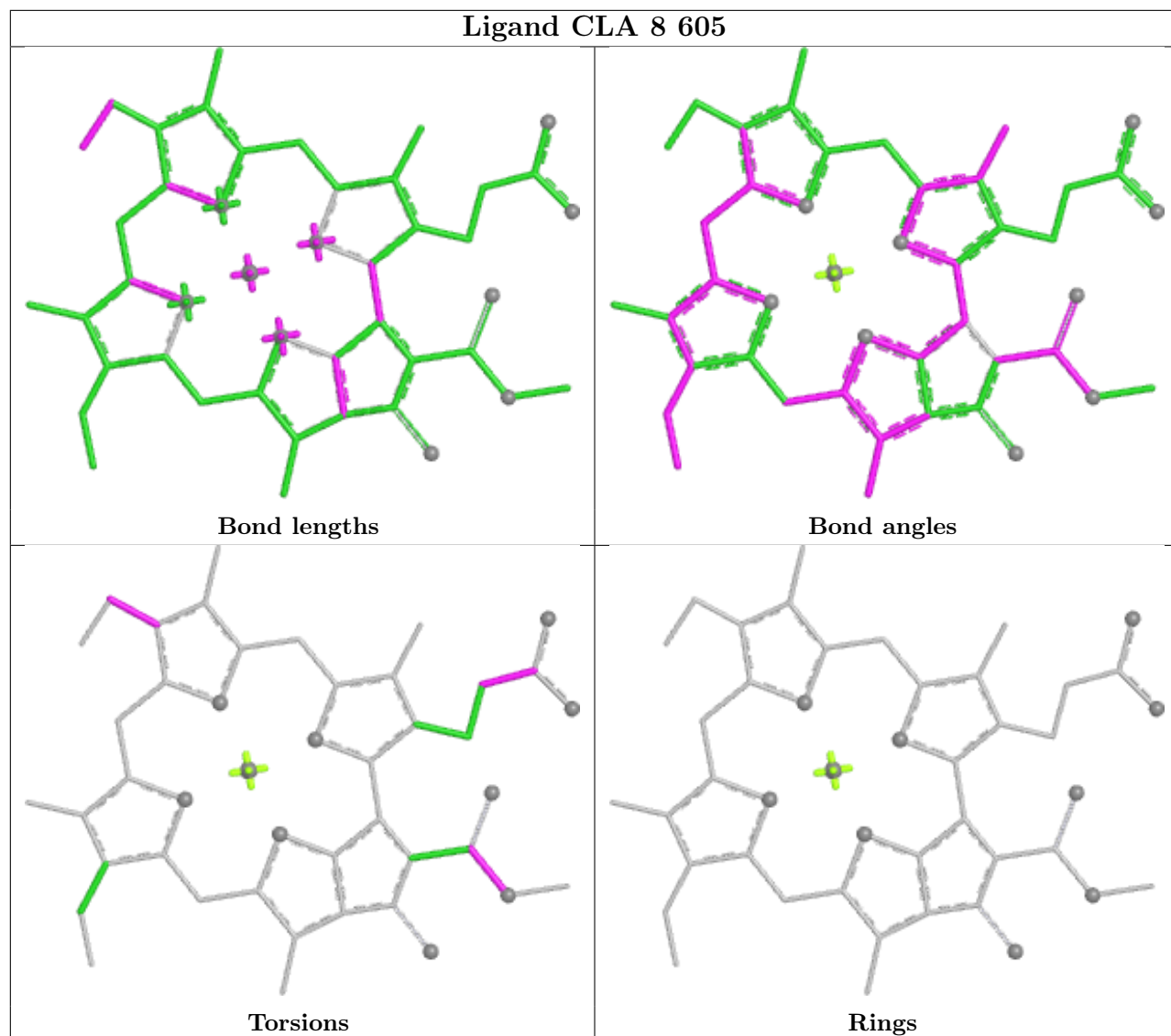




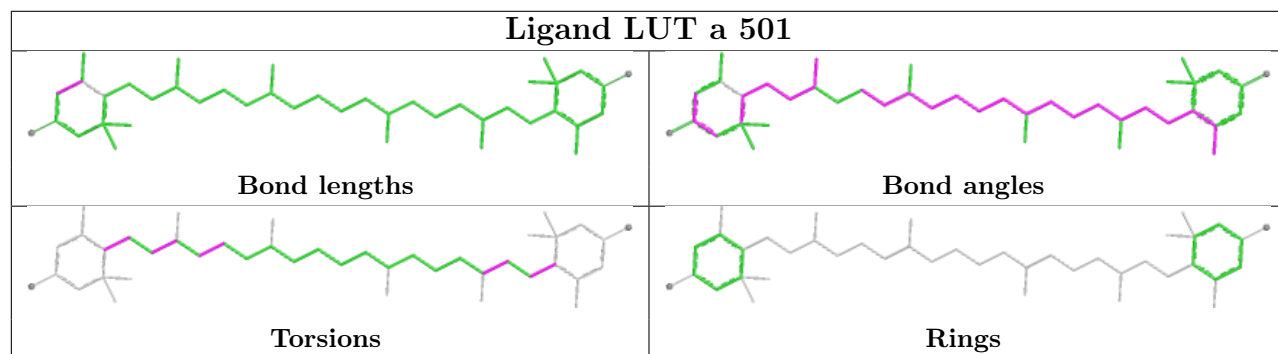




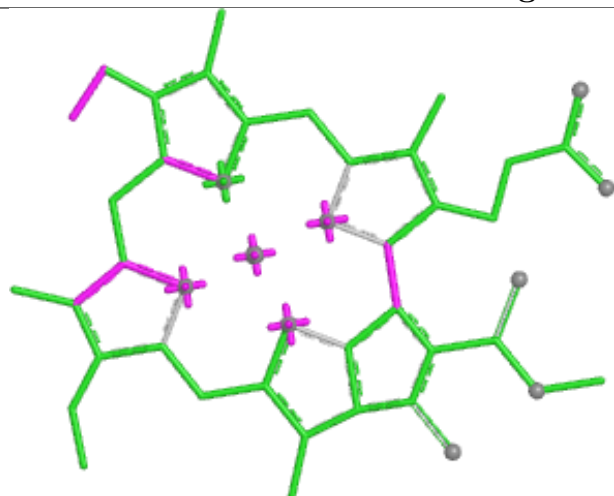
Ligand CLA 8 605



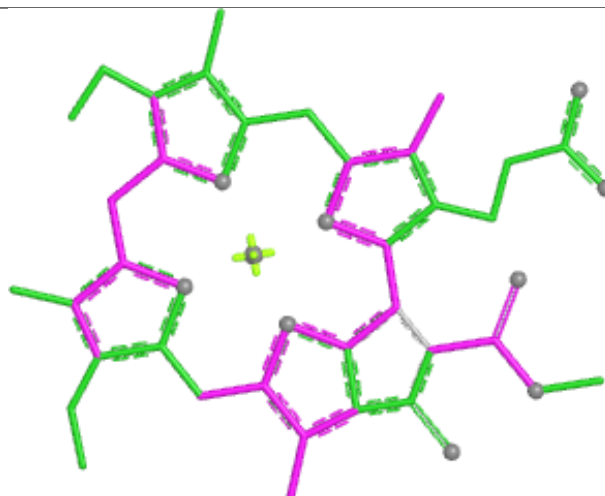
Ligand LUT a 501



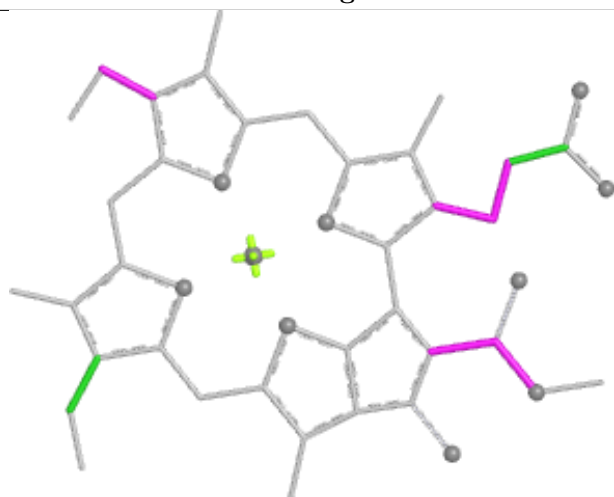
Ligand CLA 5 608



Bond lengths



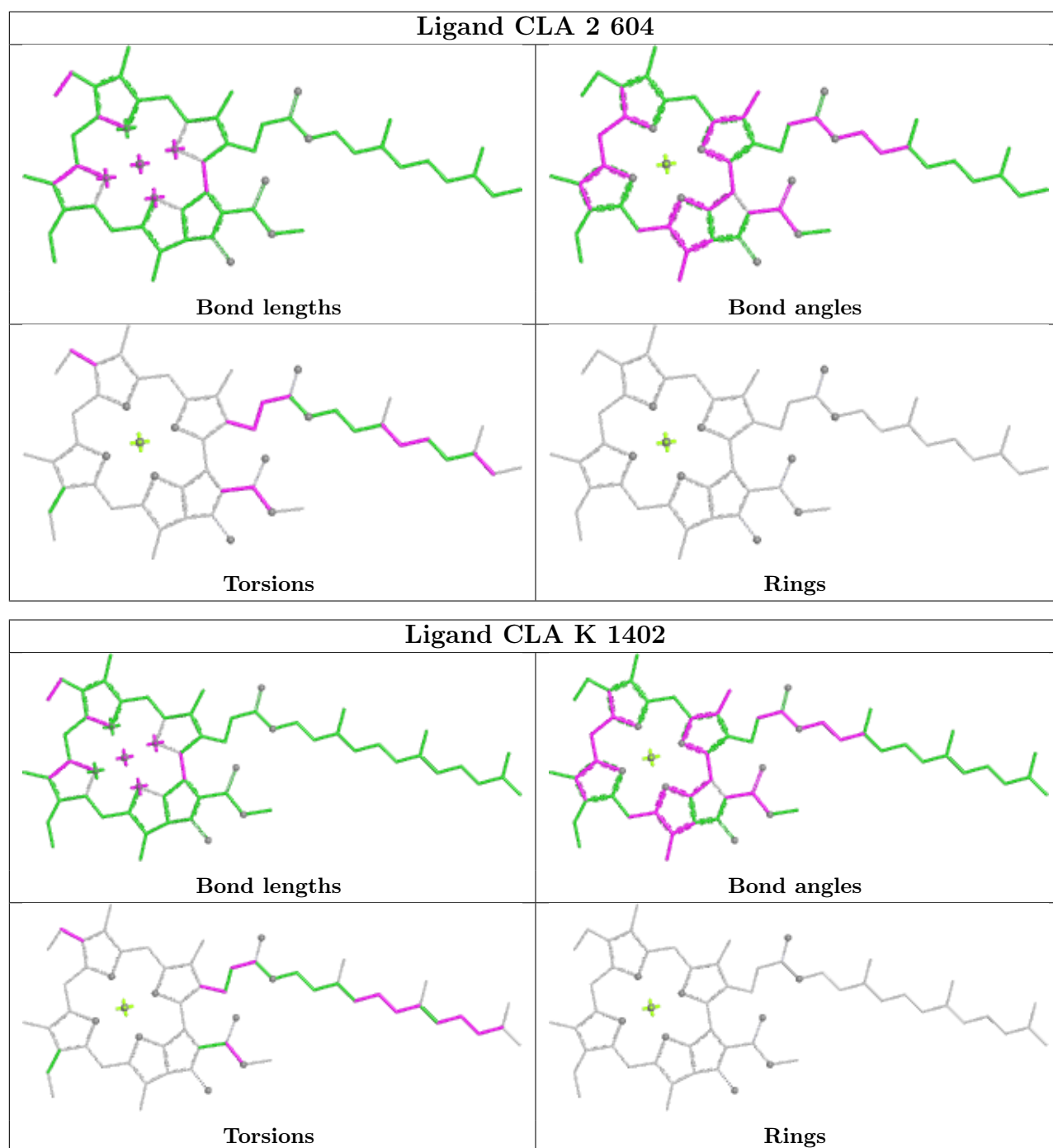
Bond angles

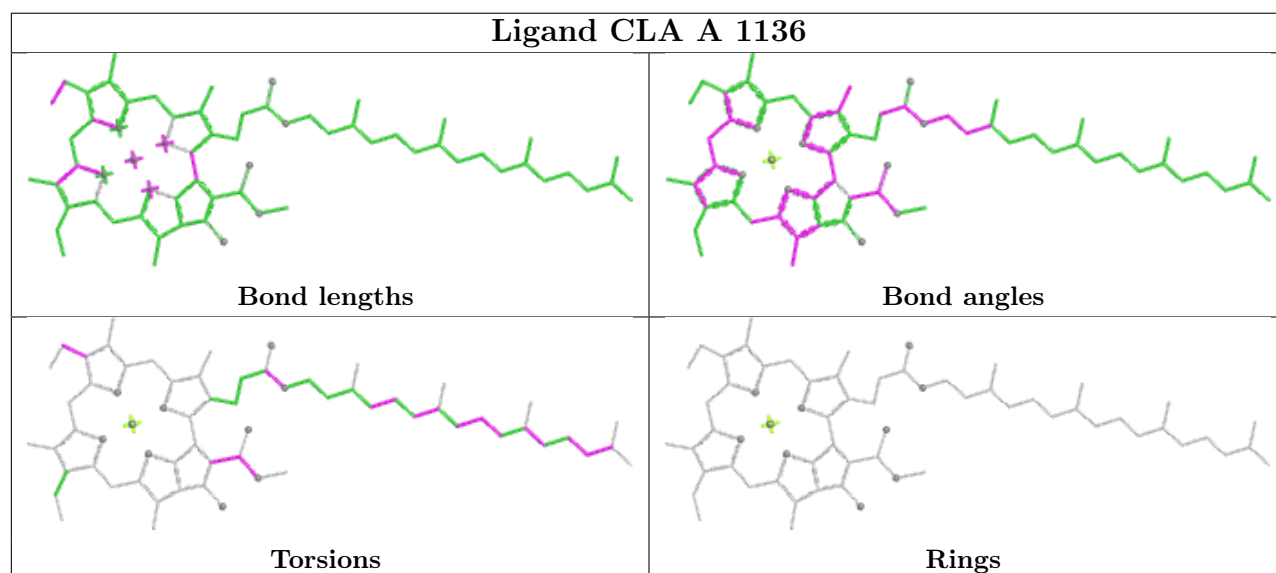
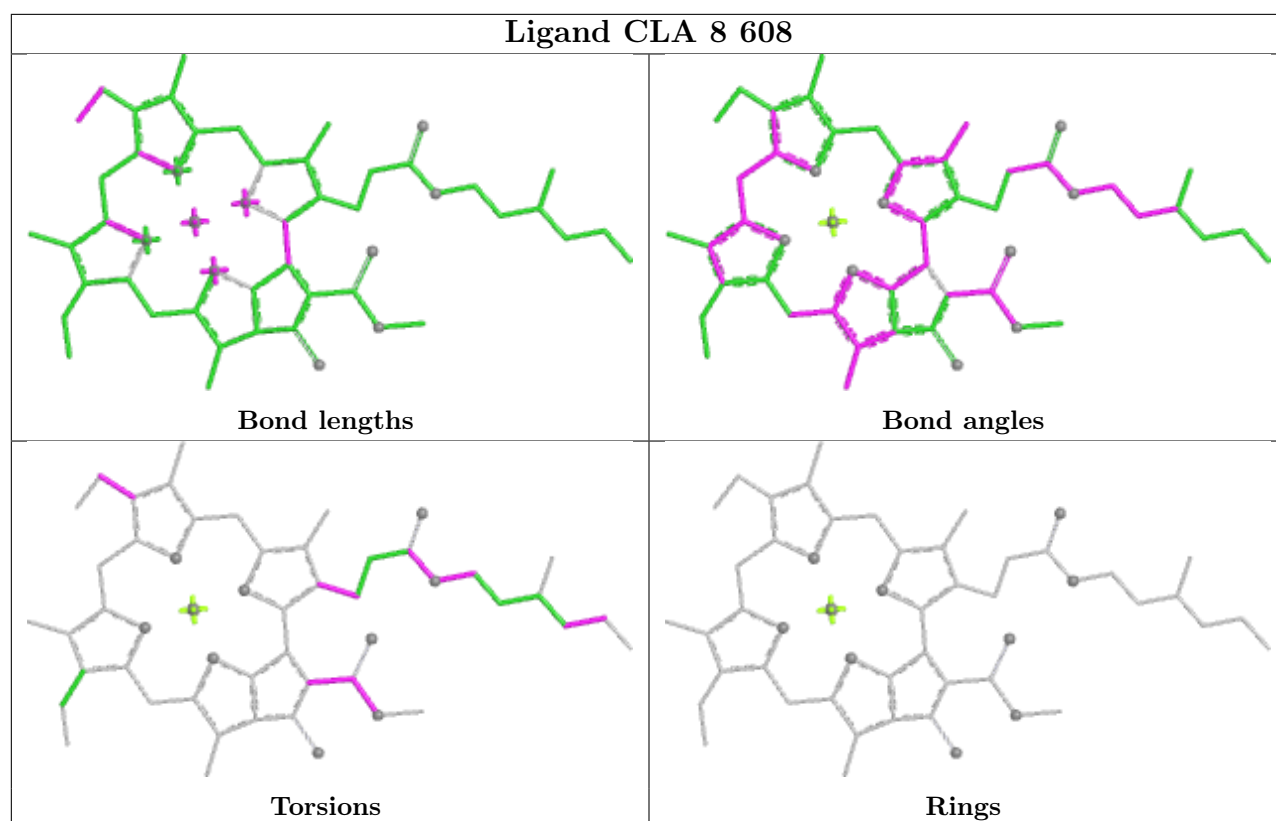


Torsions

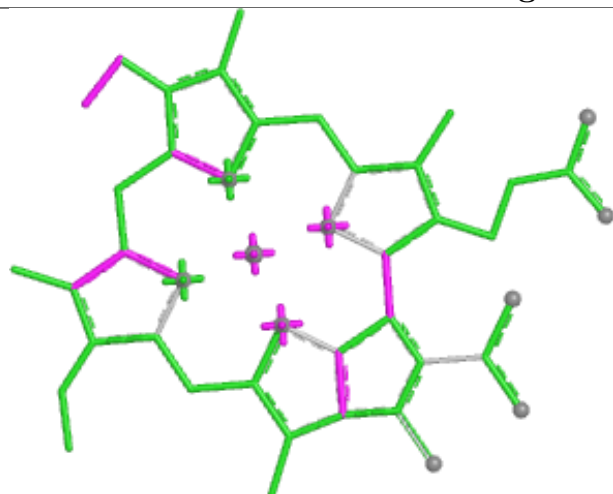


Rings

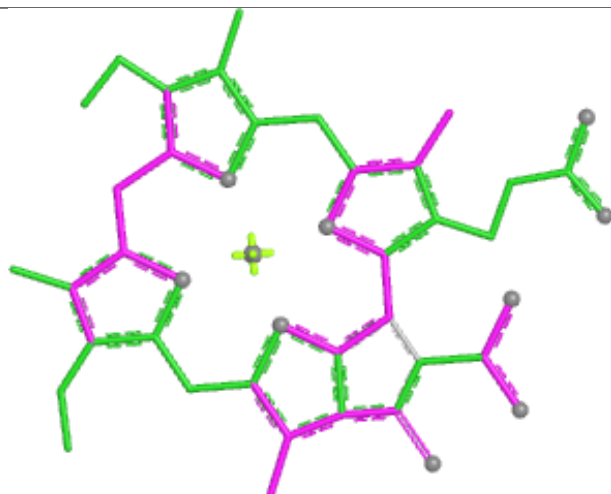




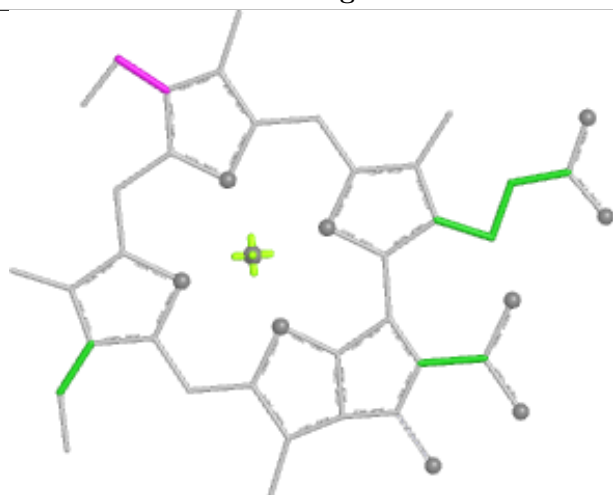
Ligand CLA 7 605



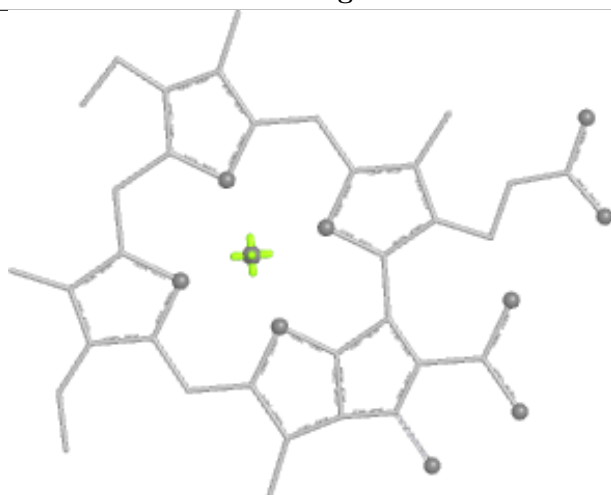
Bond lengths



Bond angles

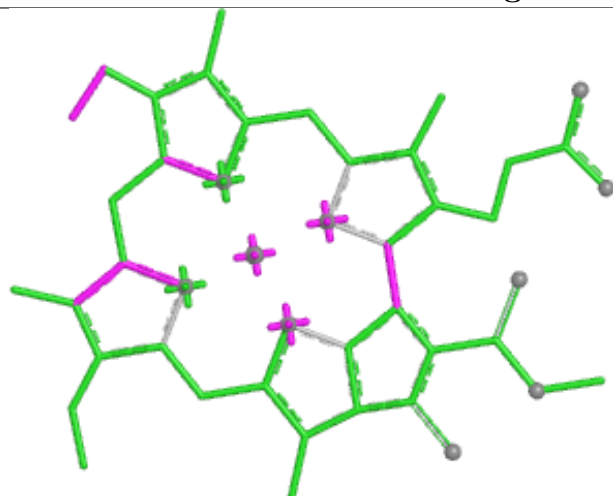


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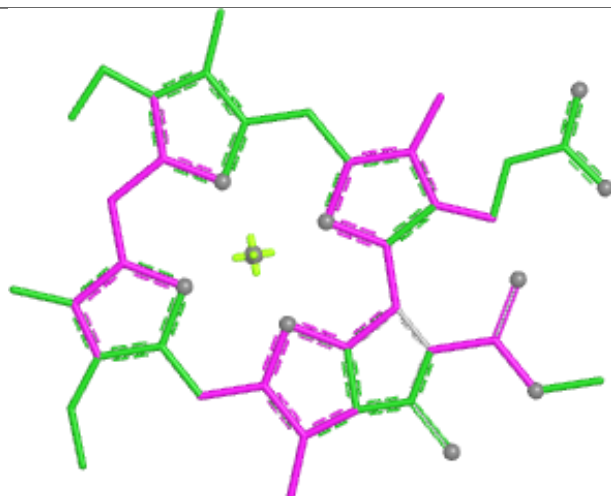


Rings

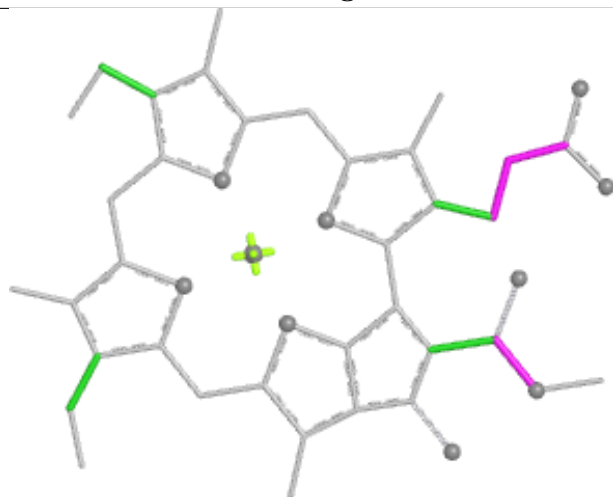
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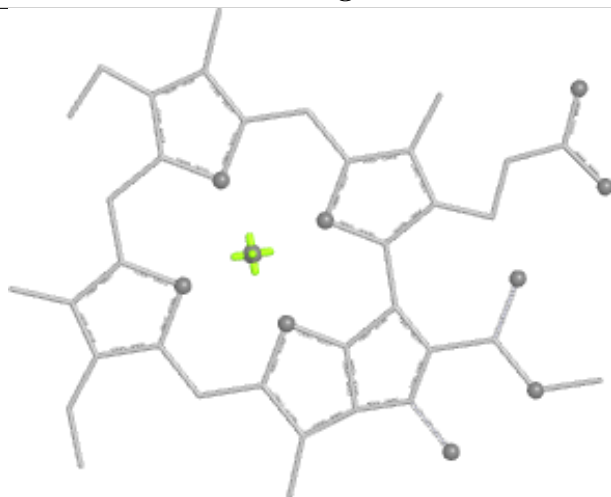
Bond lengths



Bond angles

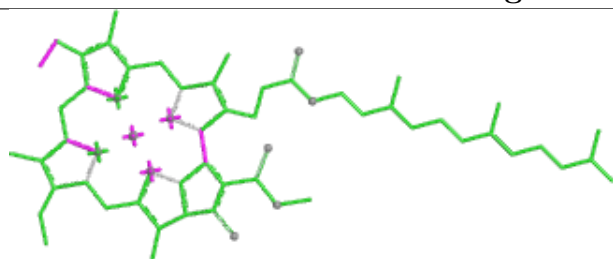


Torsions

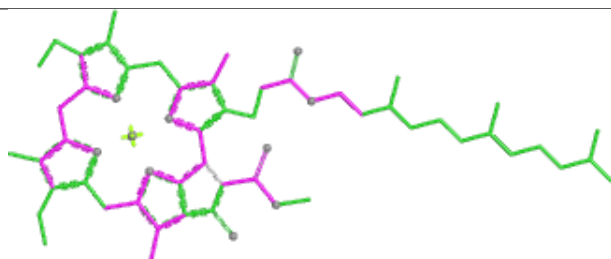


Rings

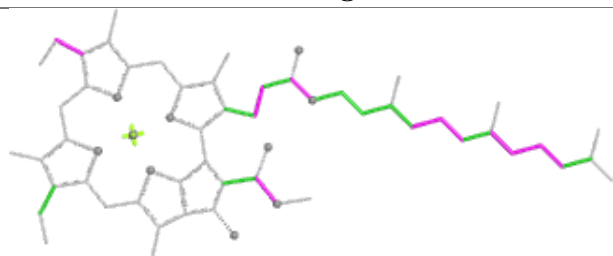
Ligand CLA A 1110



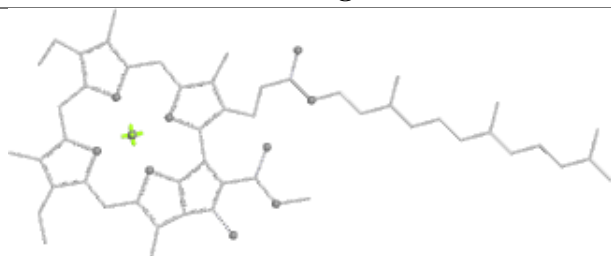
Bond lengths



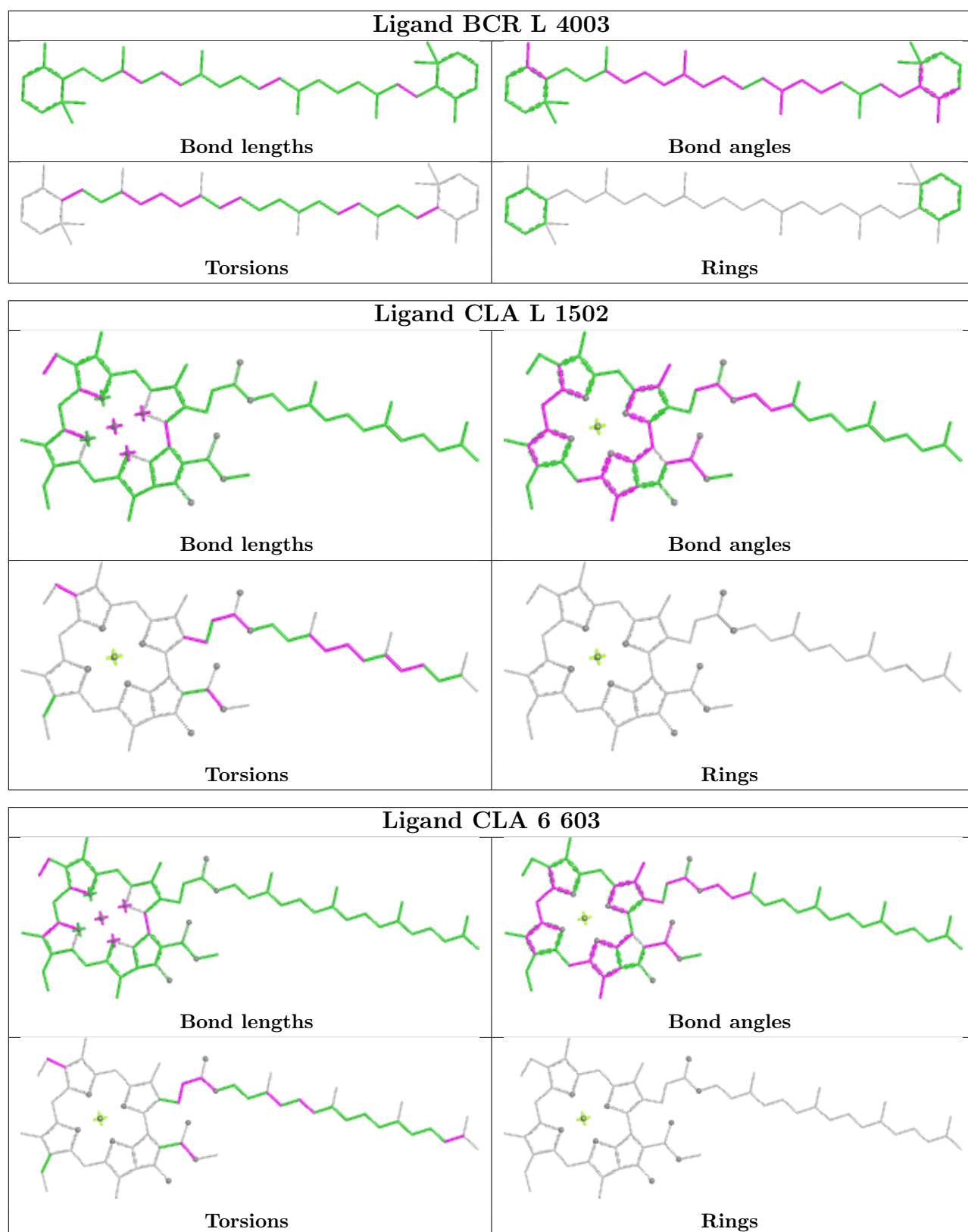
Bond angles



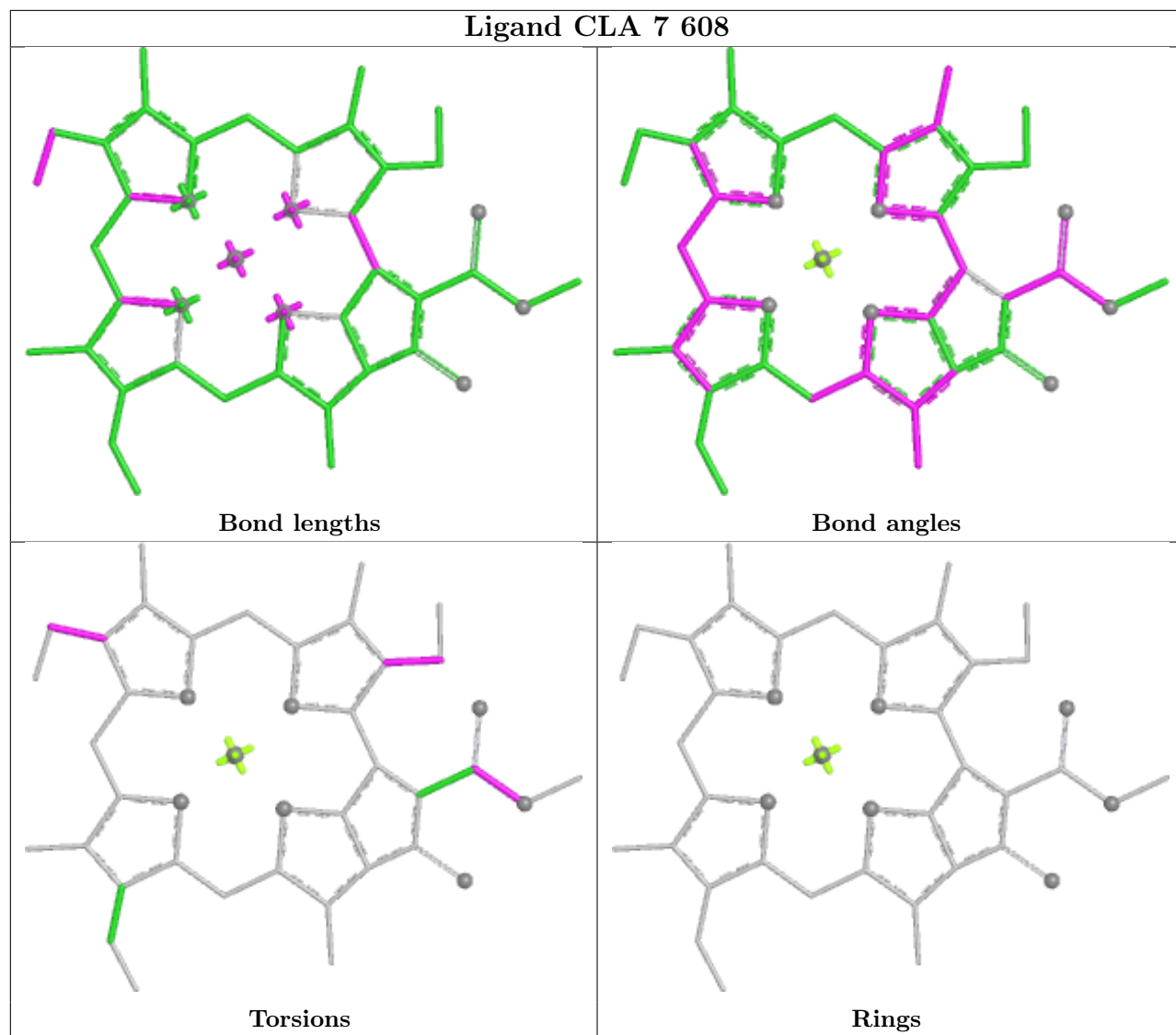
Torsions



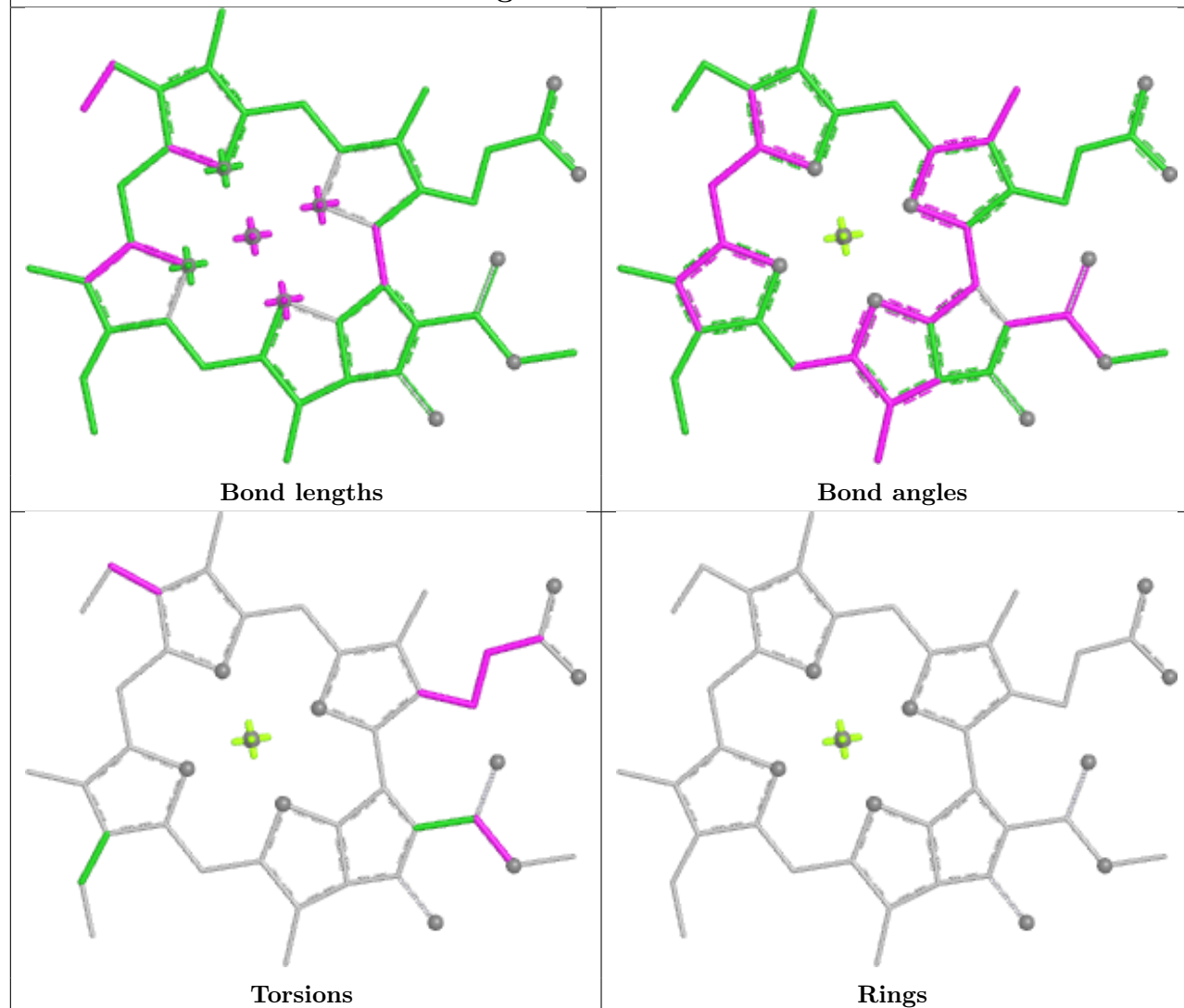
Rings



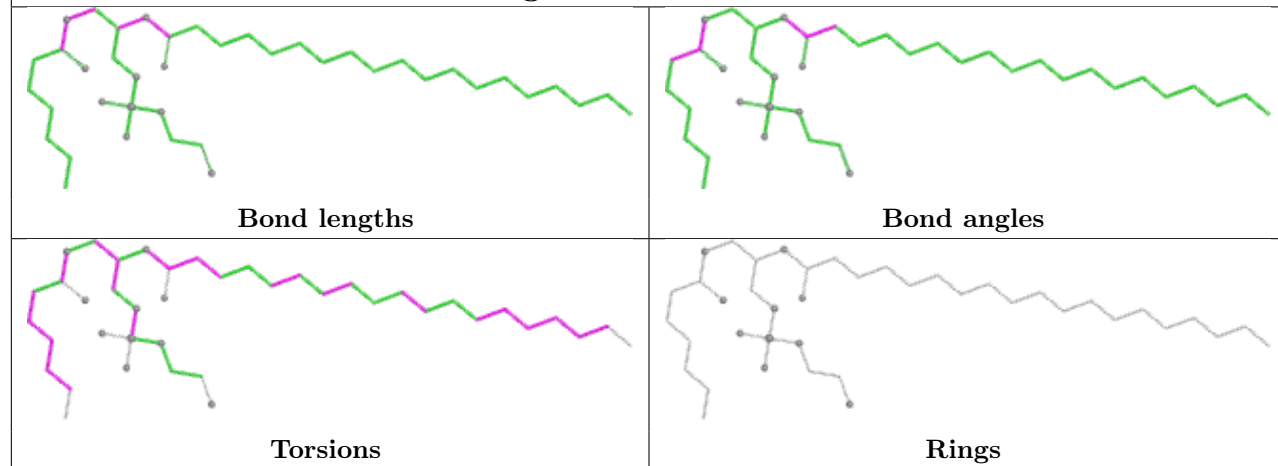
Ligand CLA 7 608

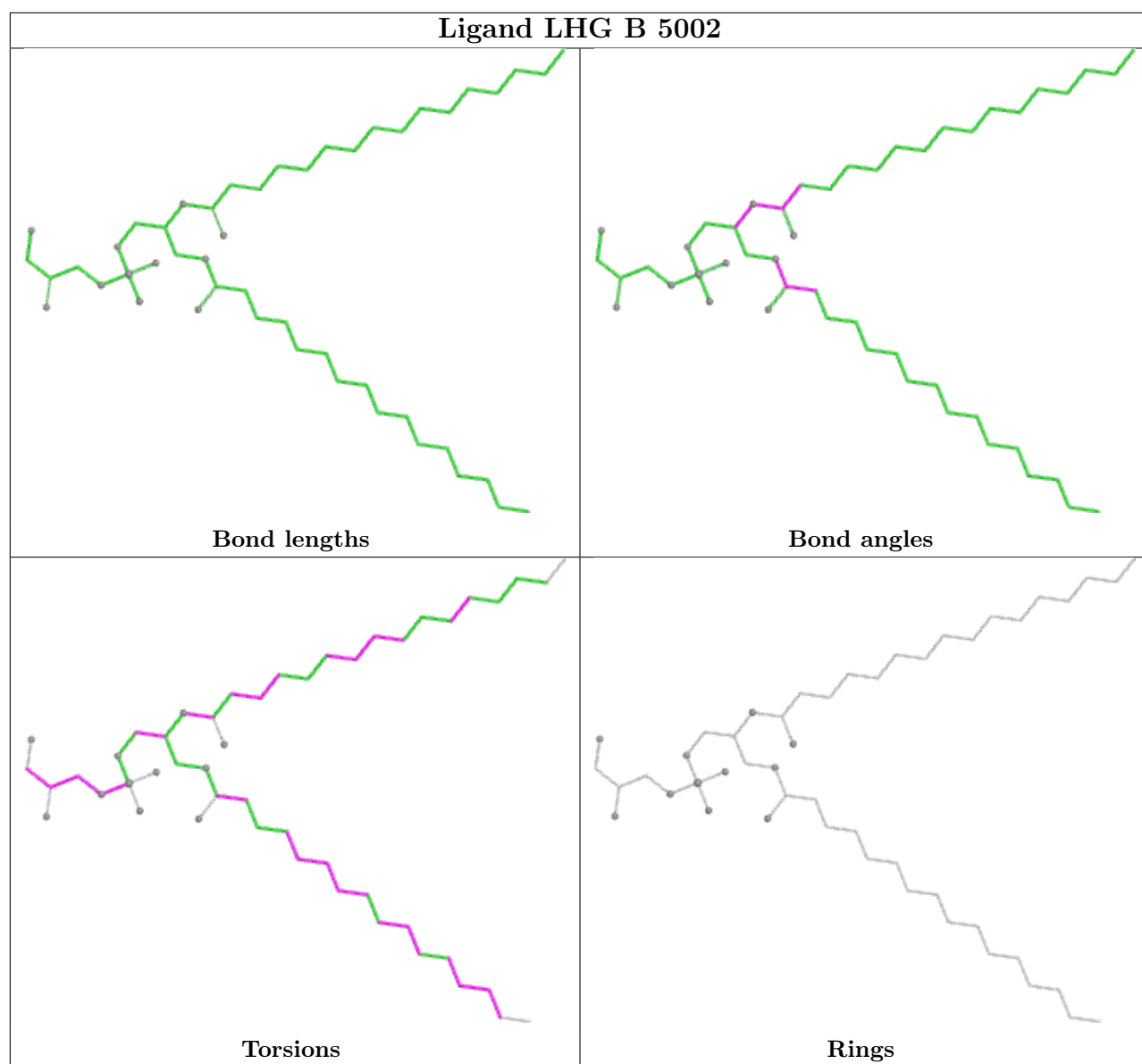


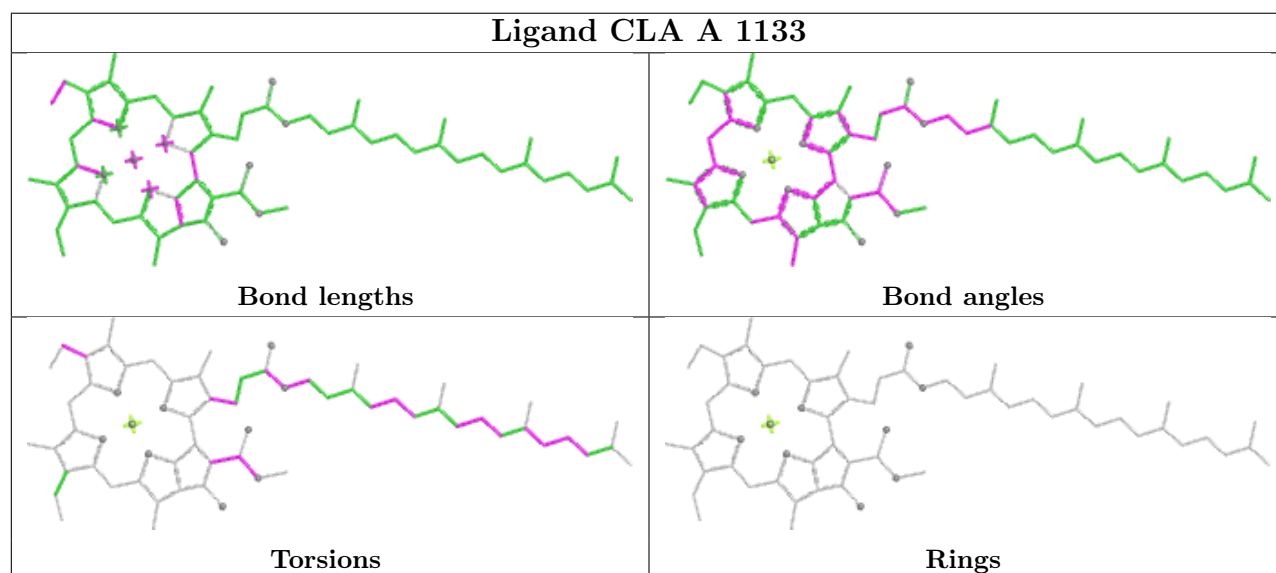
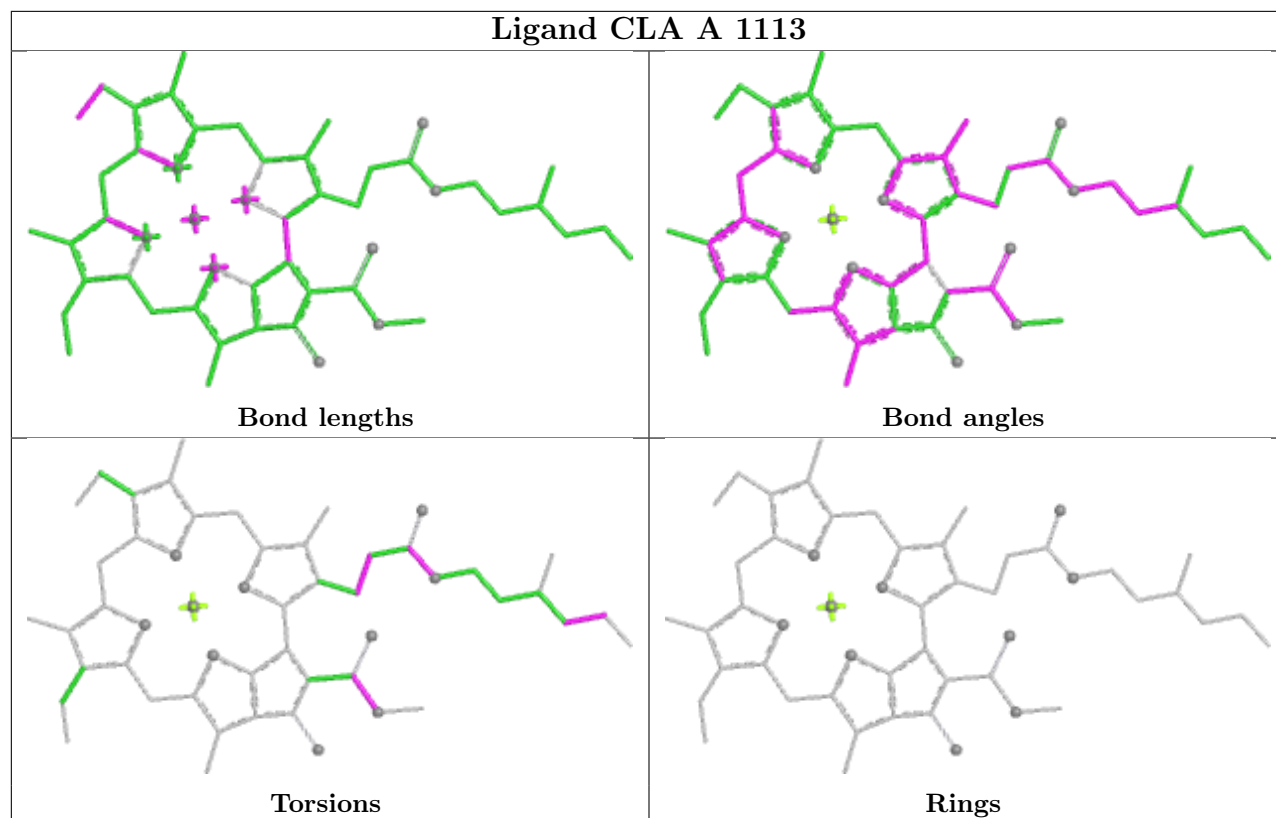
Ligand CLA 4 617

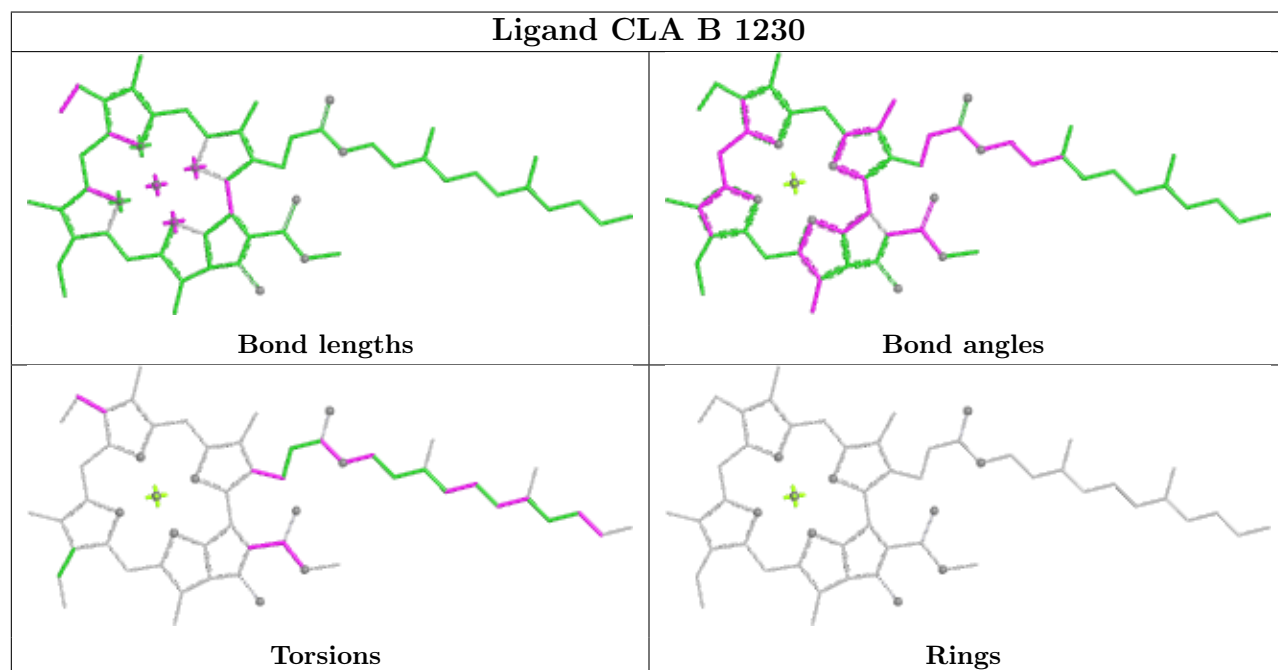
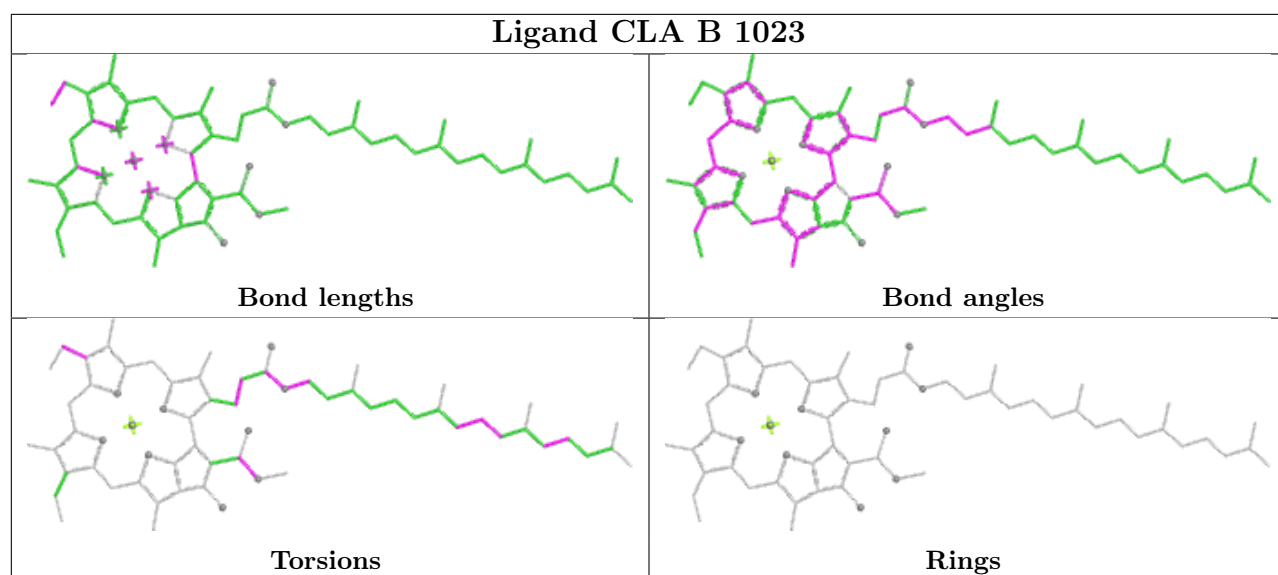


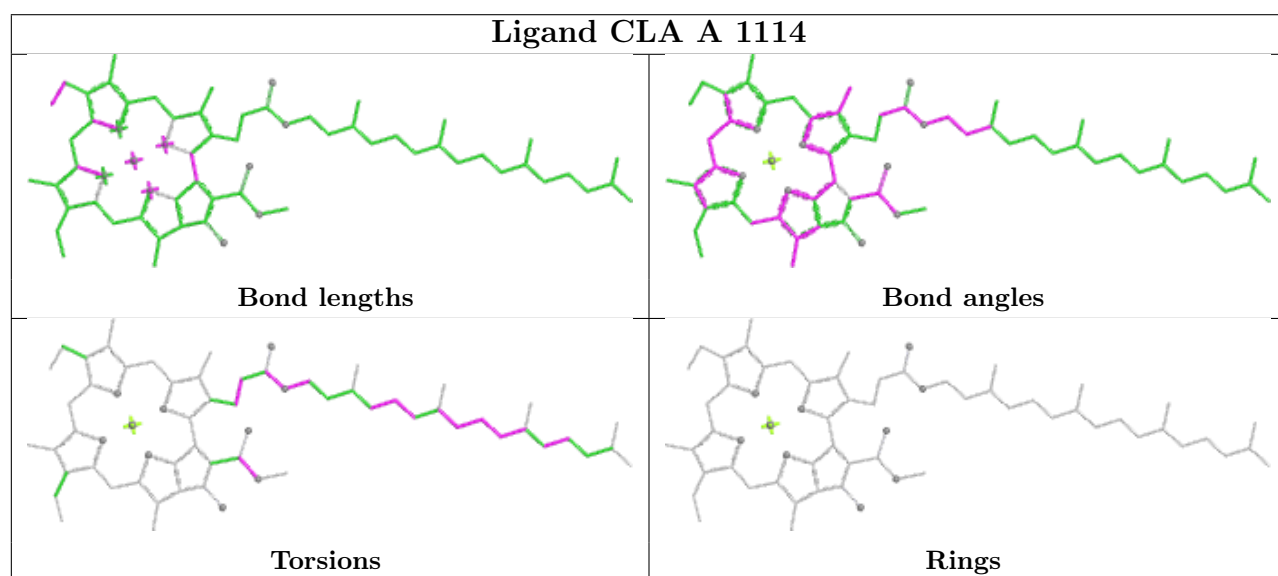
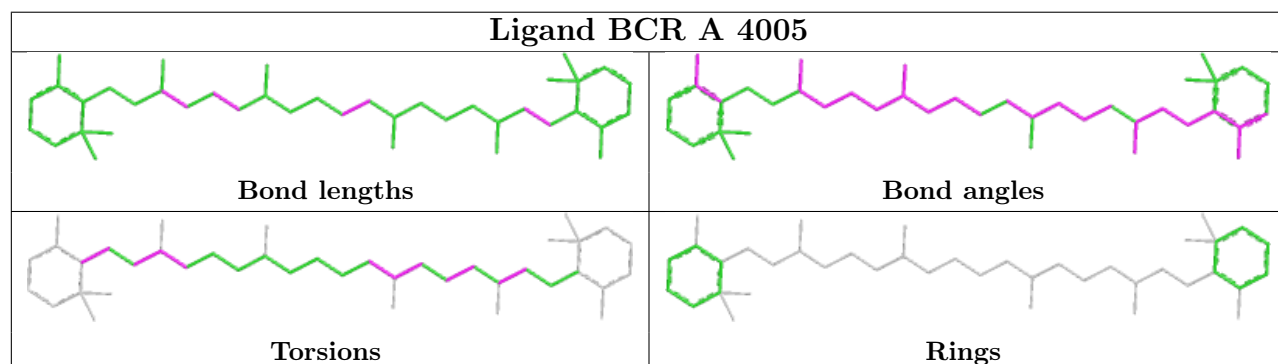
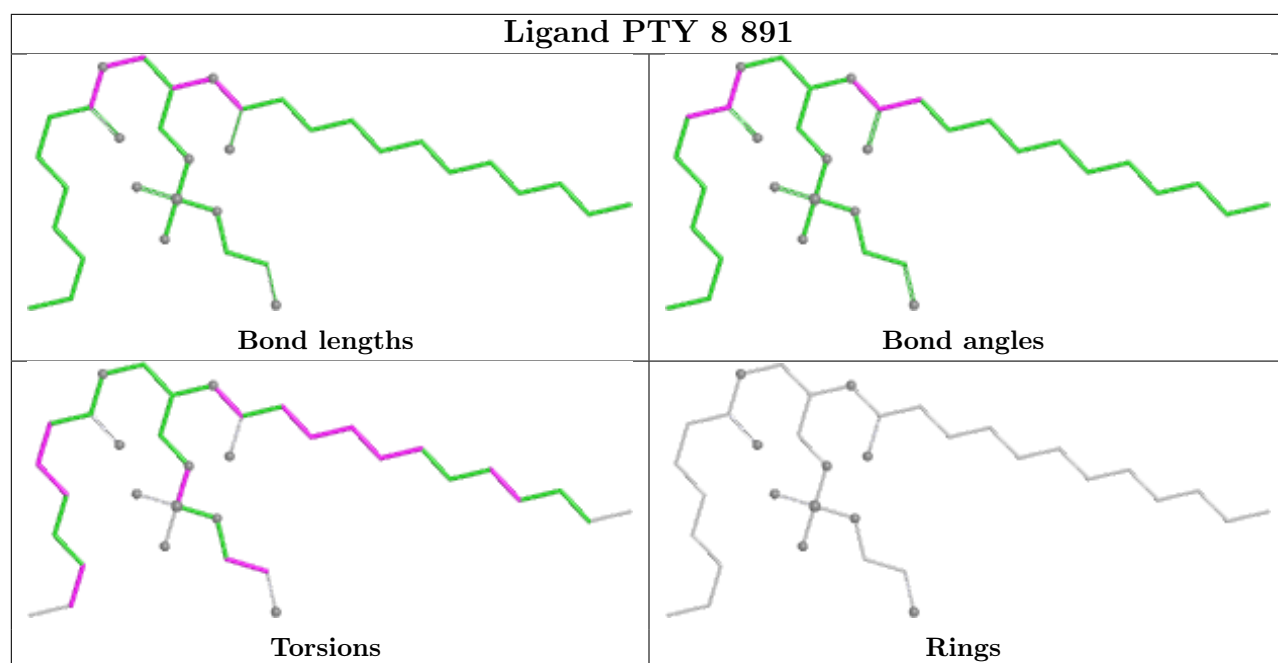
Ligand PTY B 5005

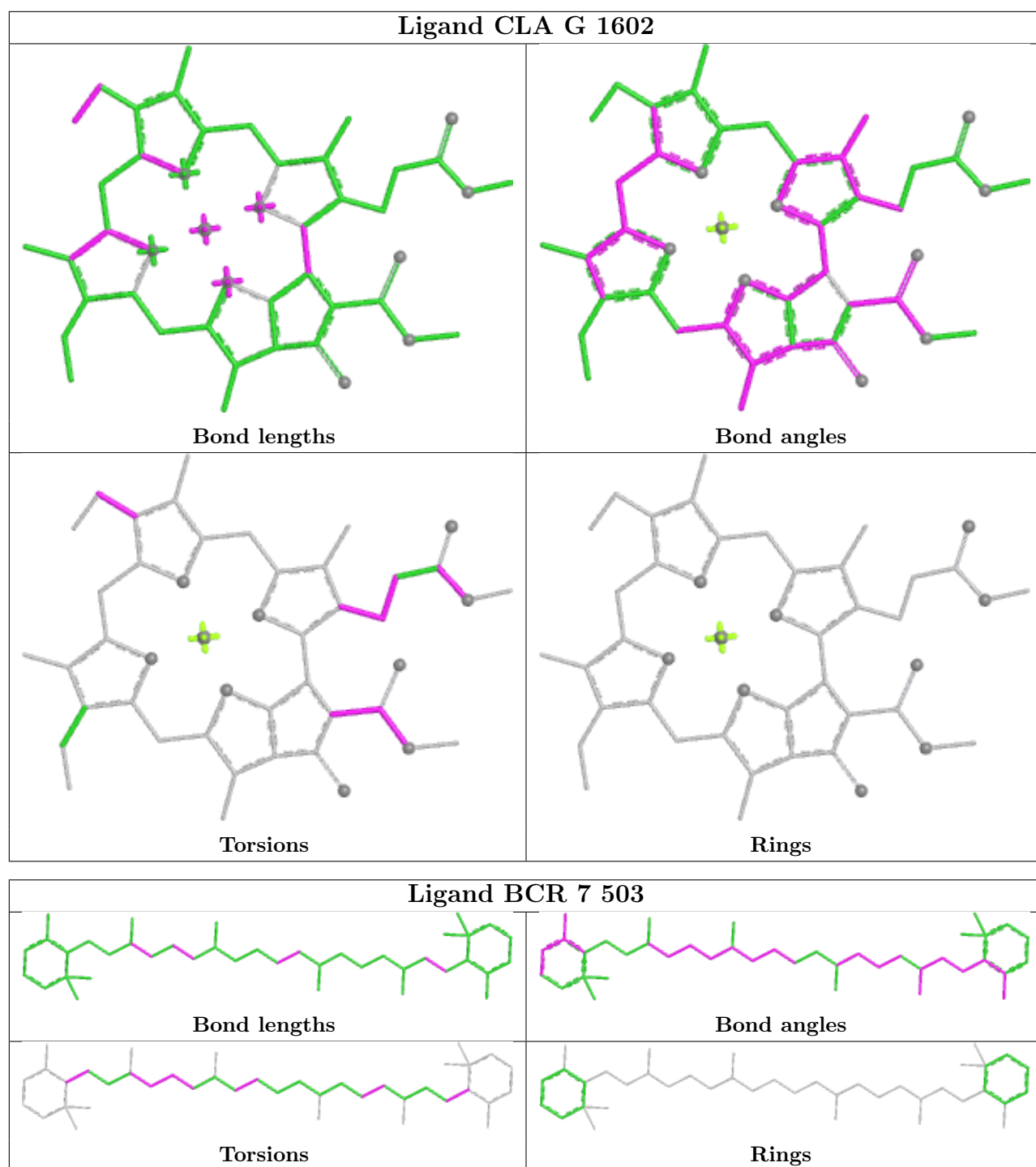




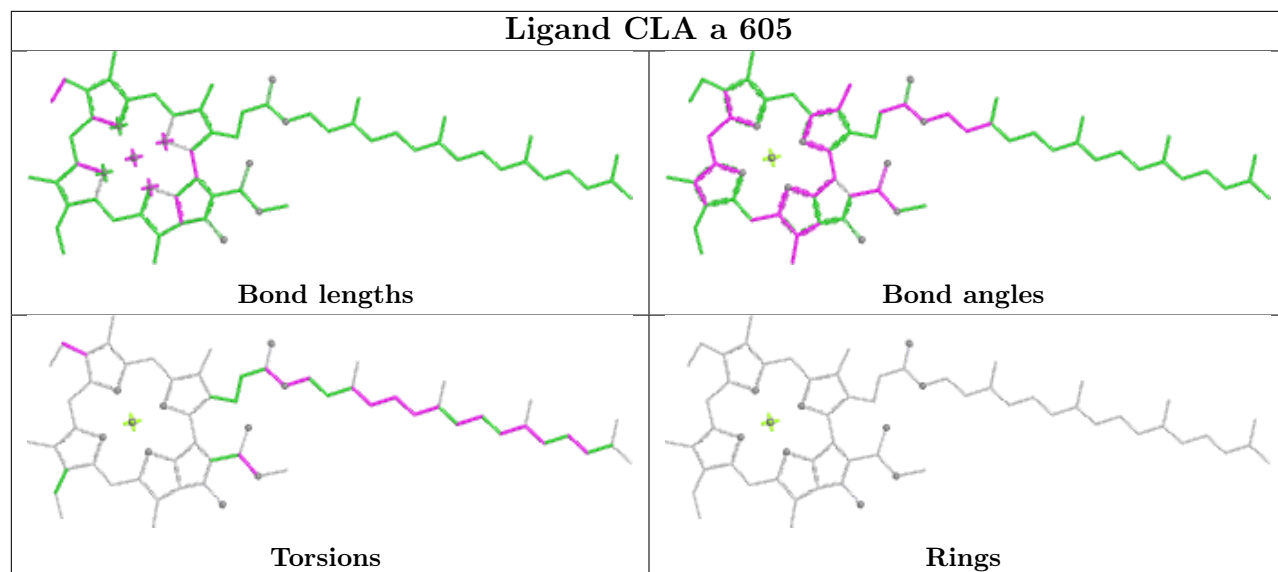




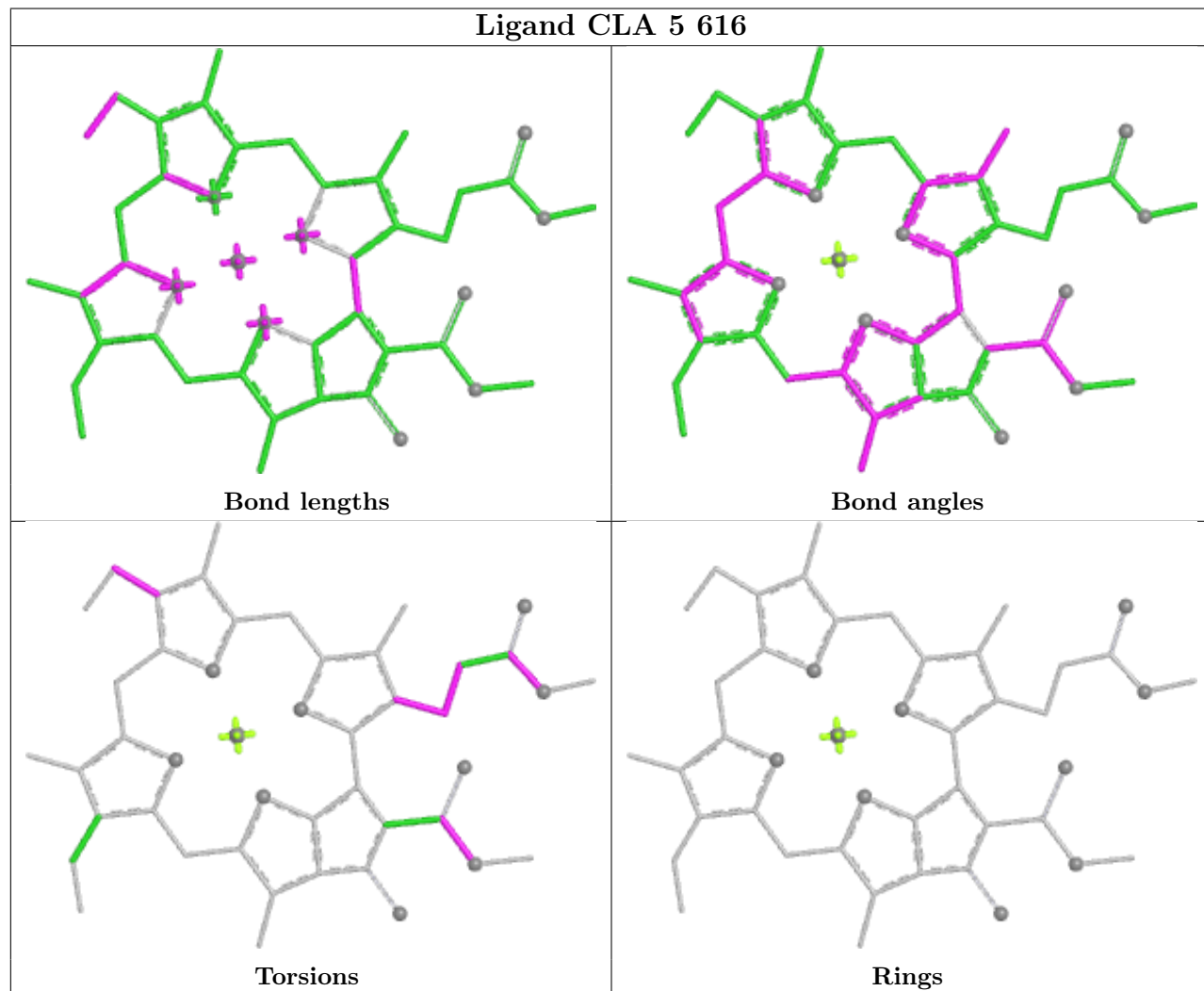


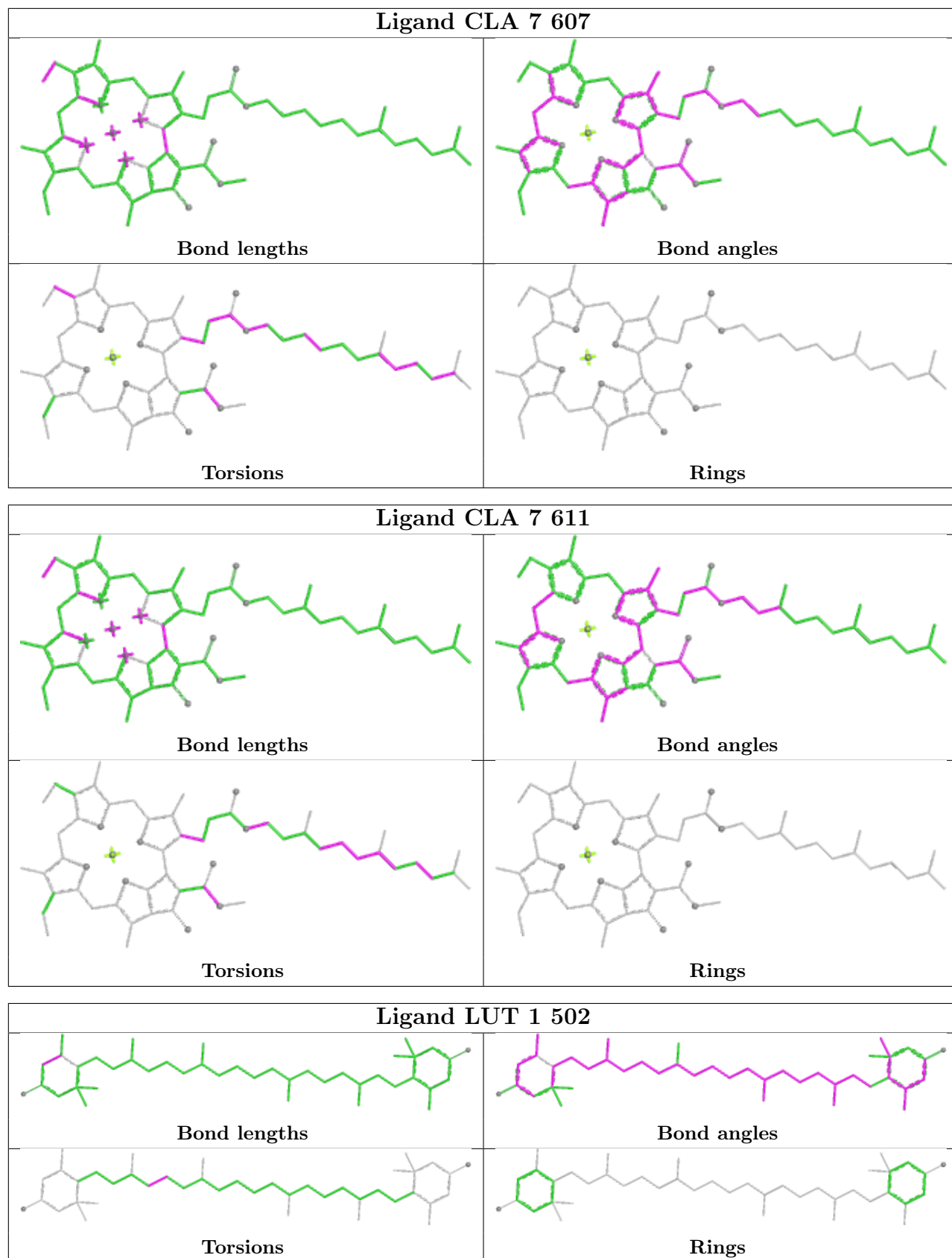


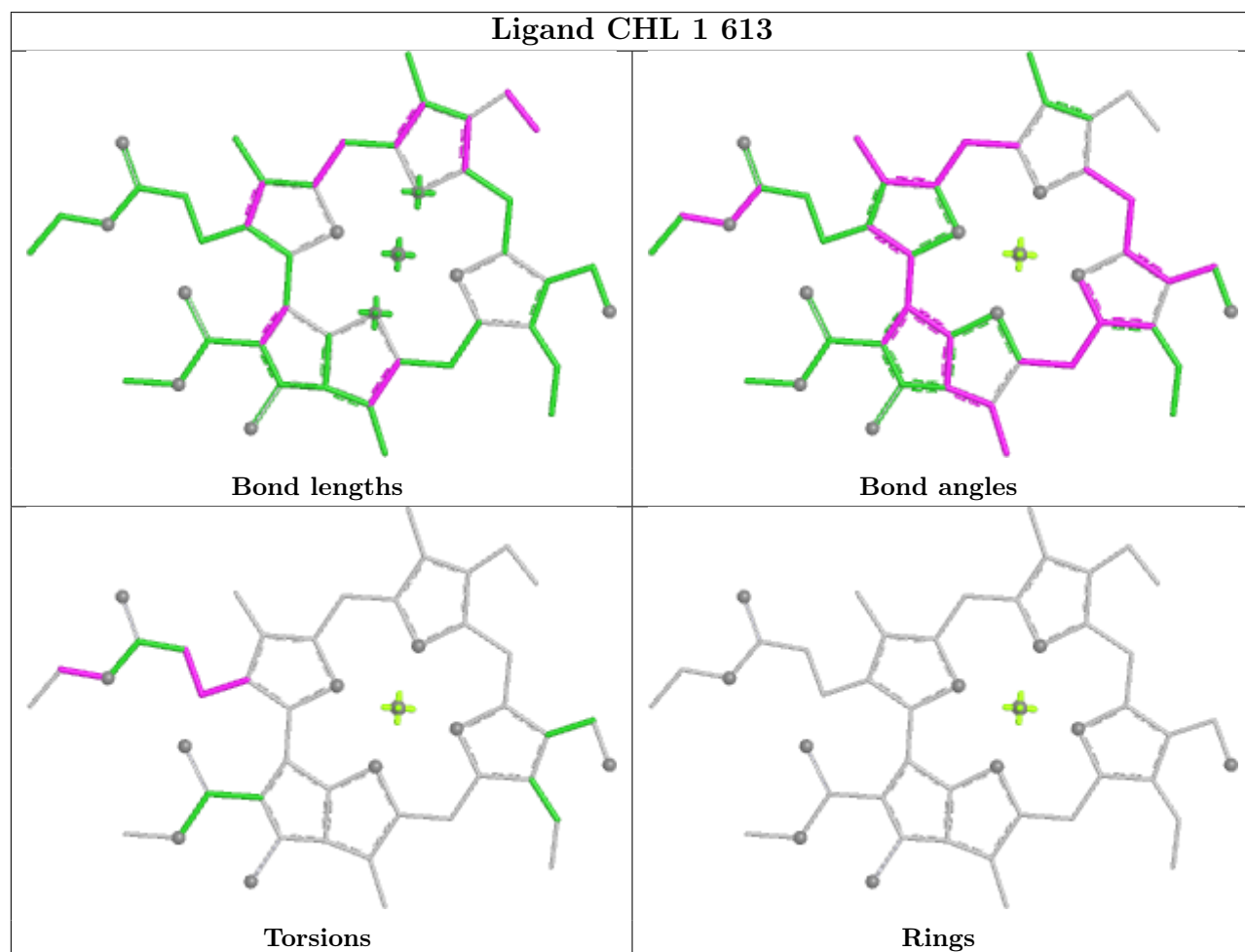
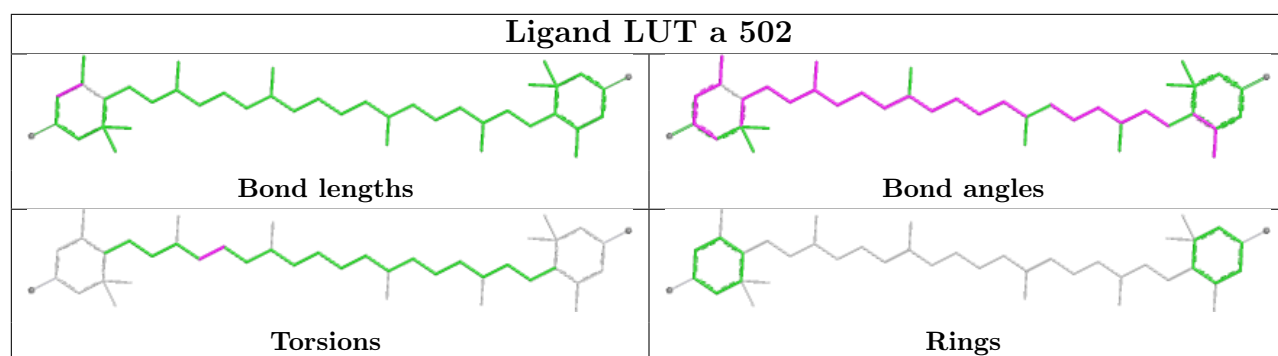
Ligand CLA a 605

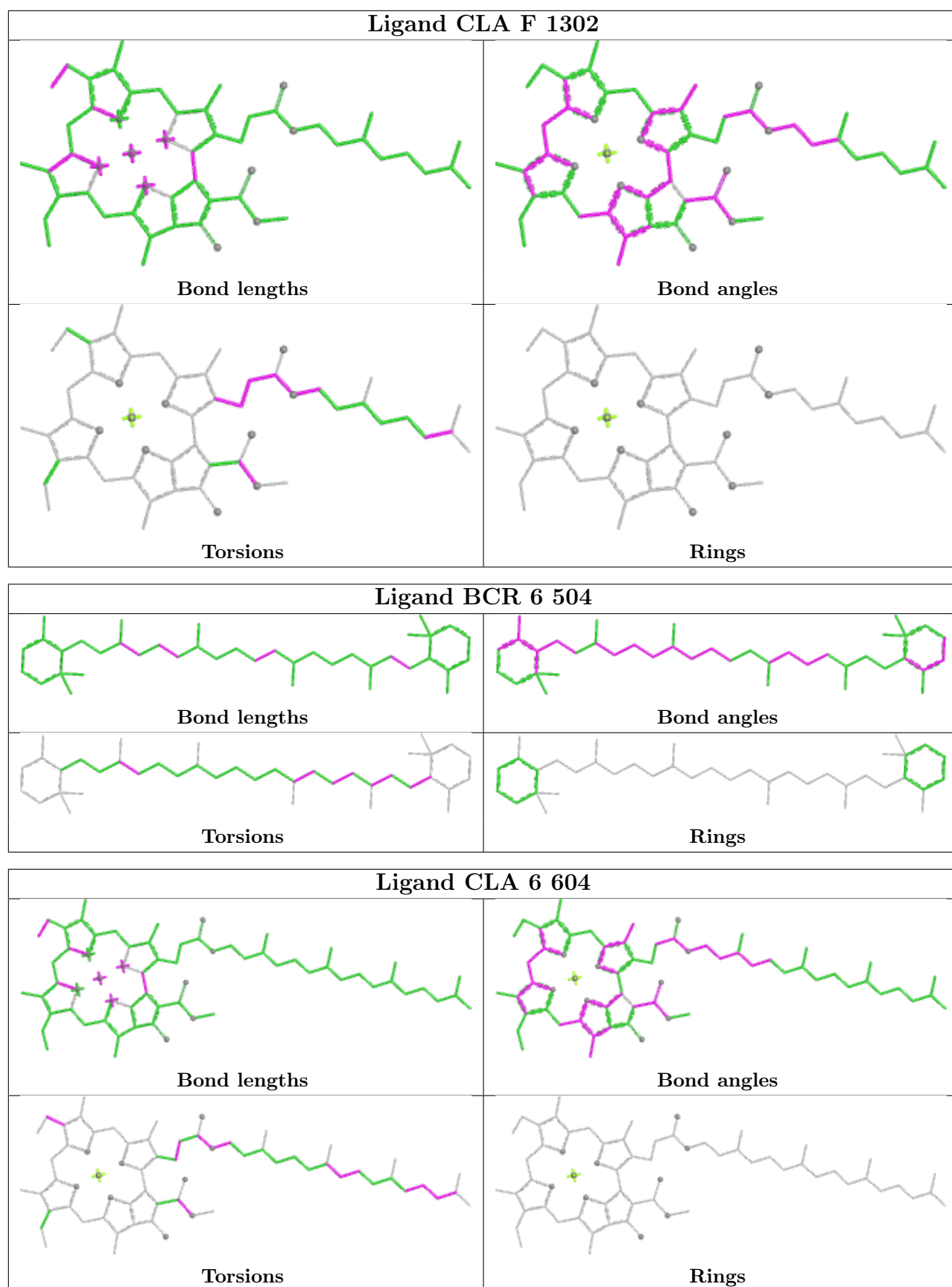


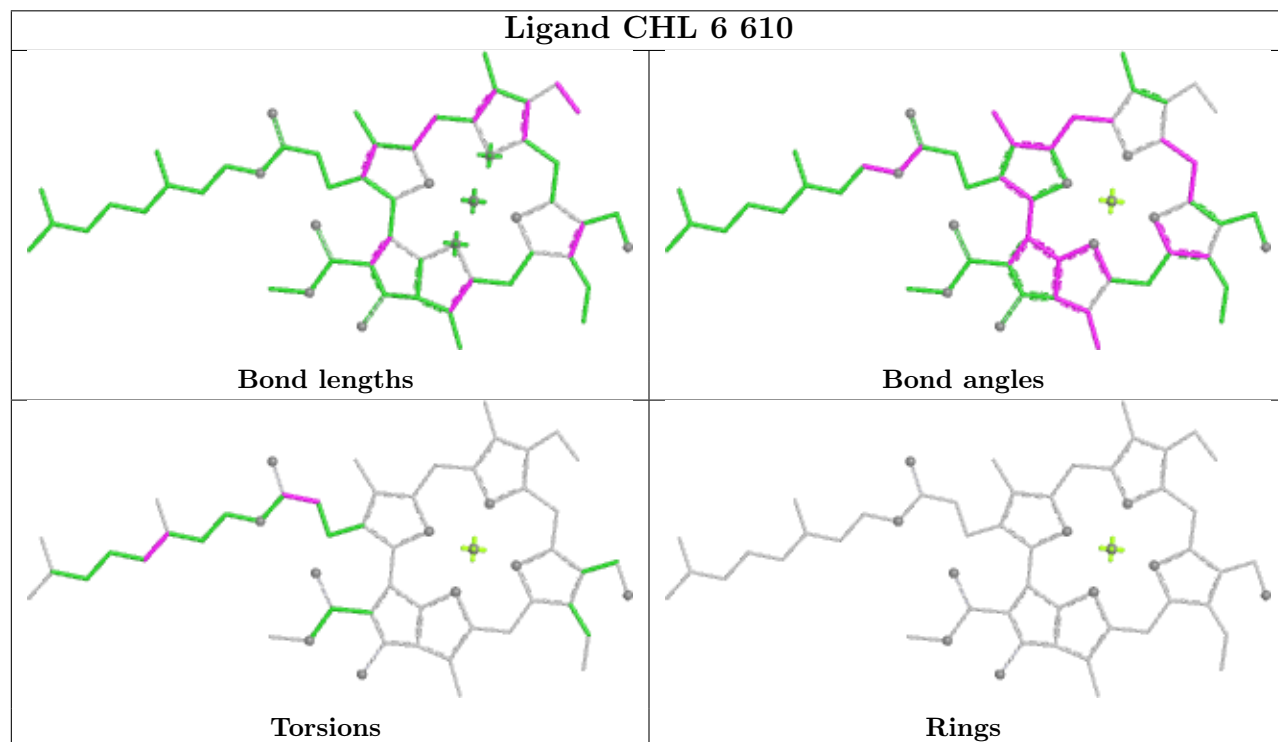
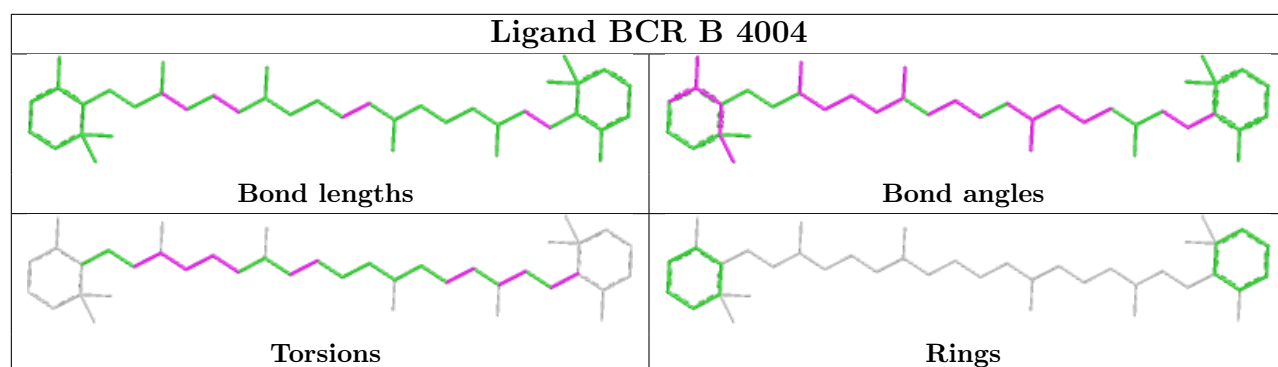
Ligand CLA 5 616



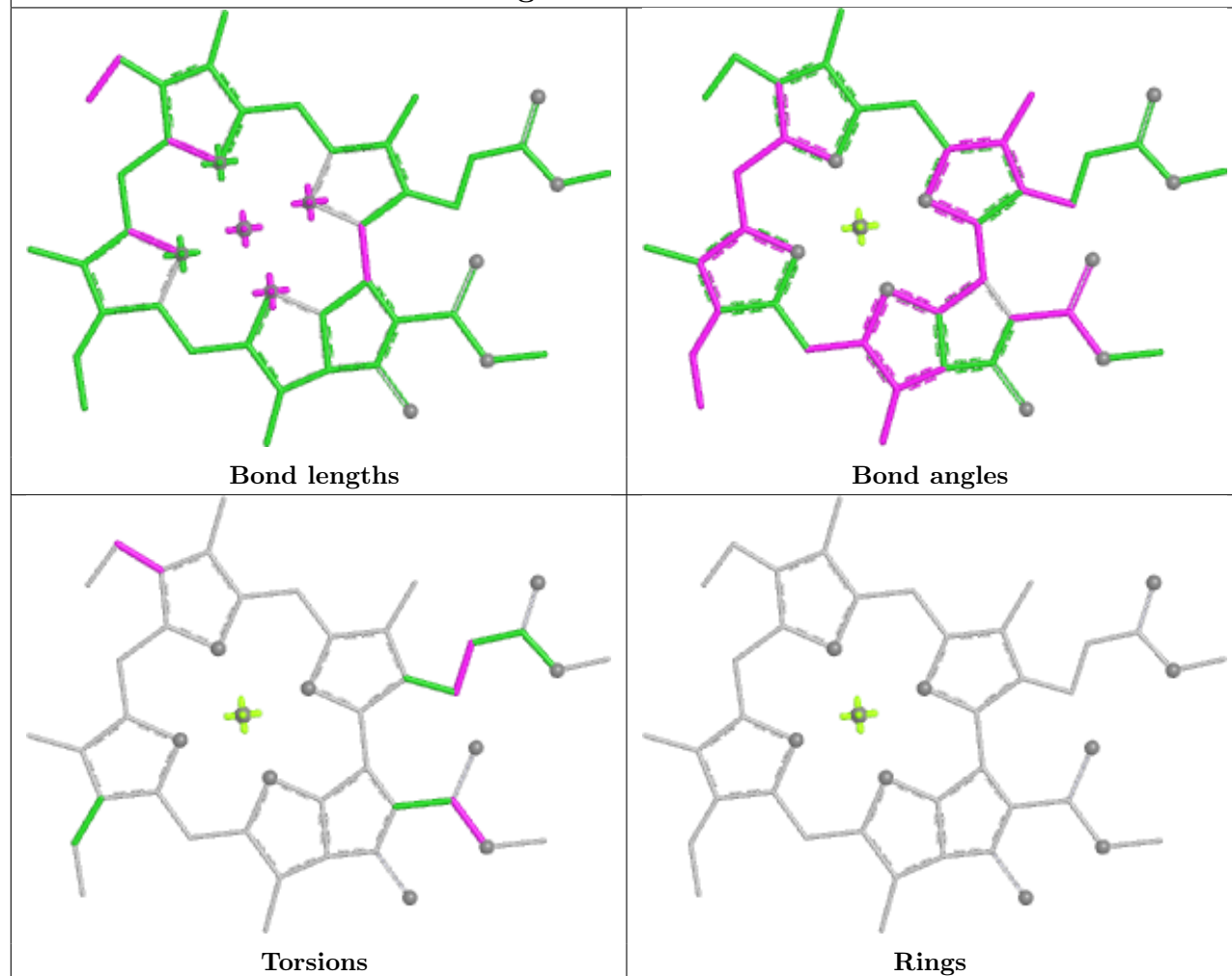




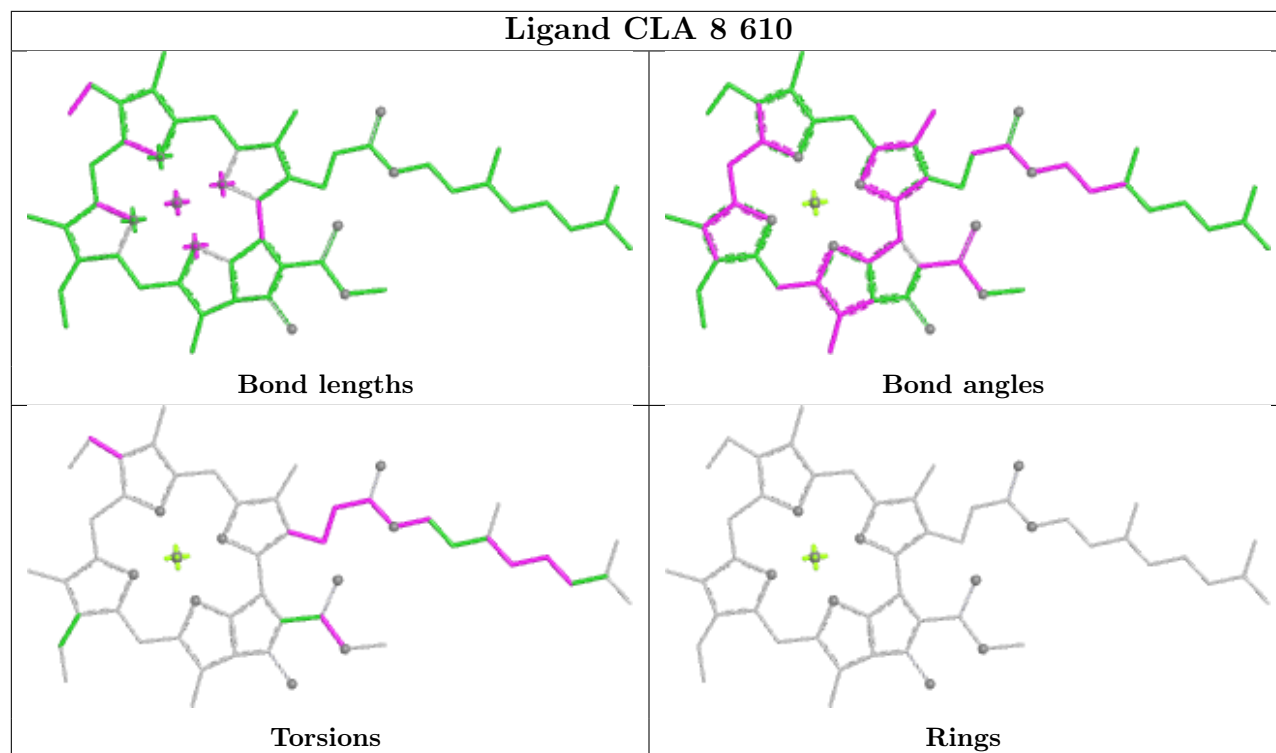




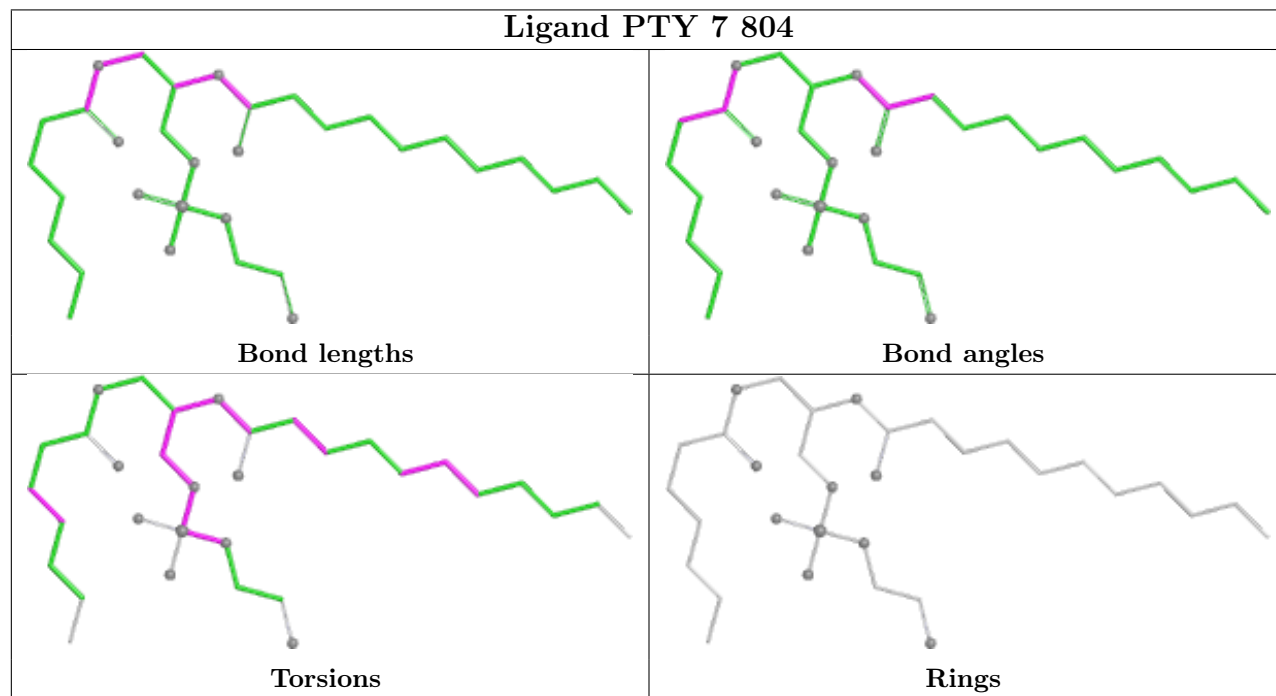
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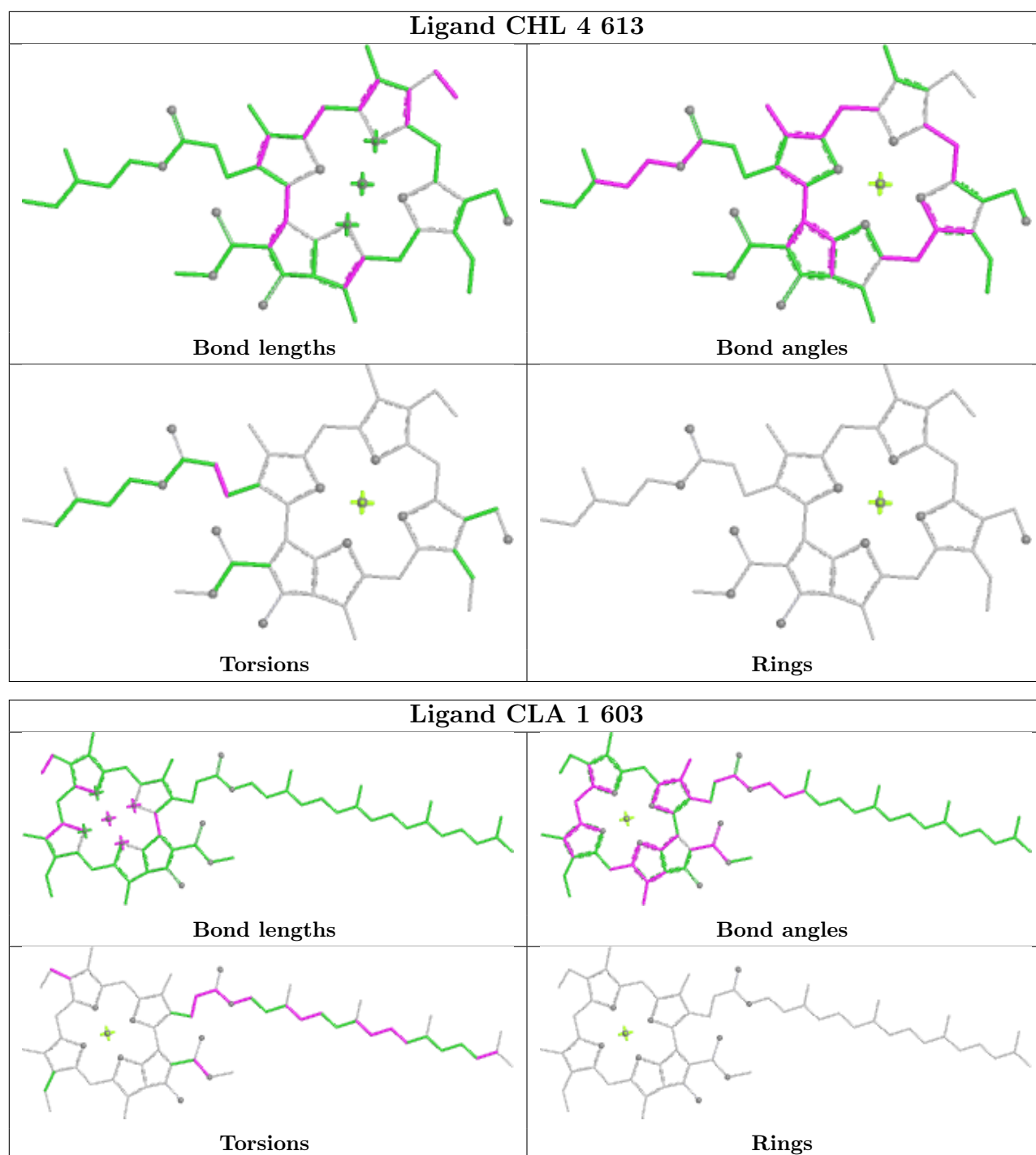


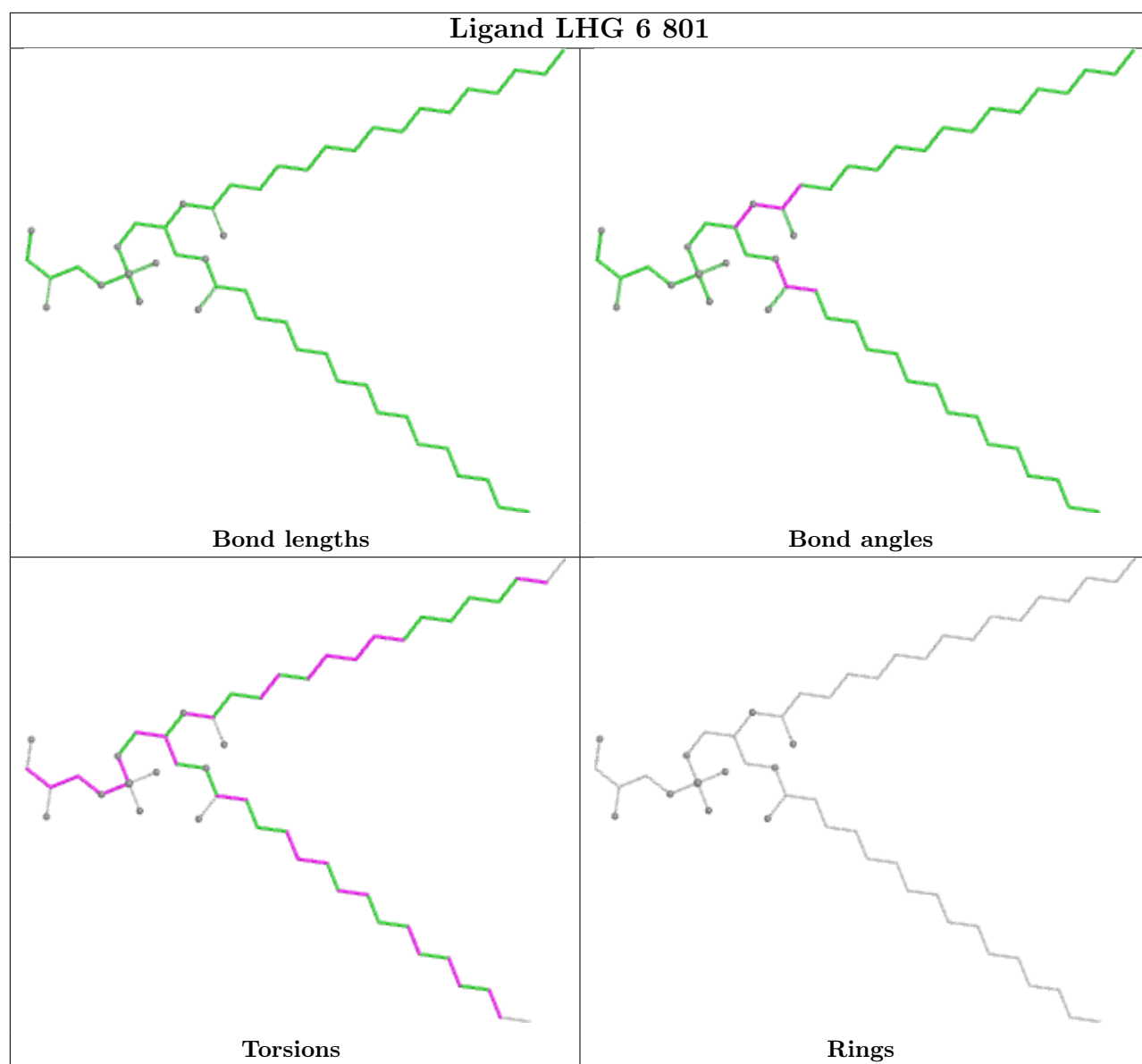
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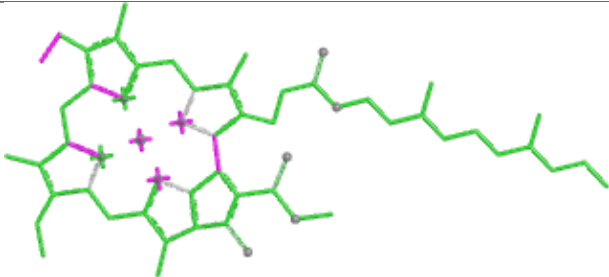
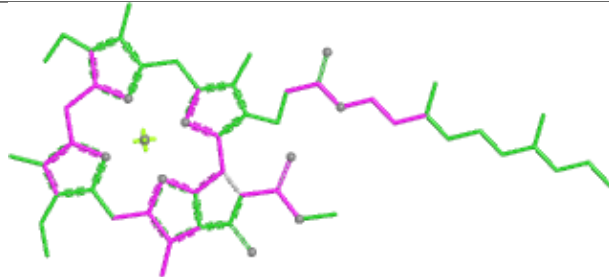
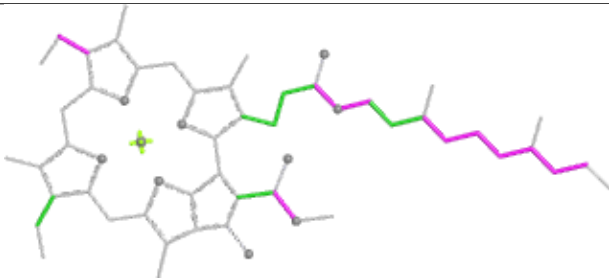
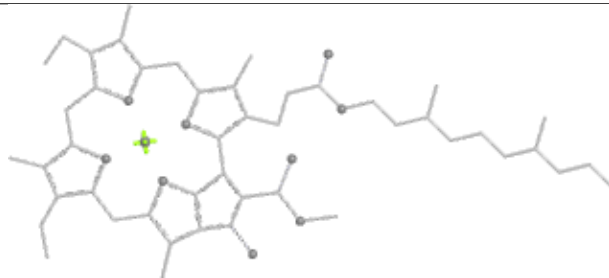
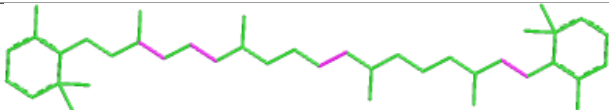
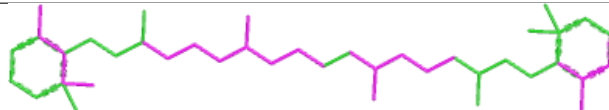
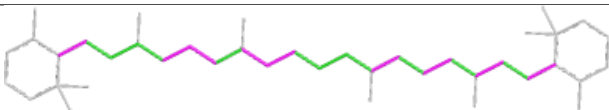
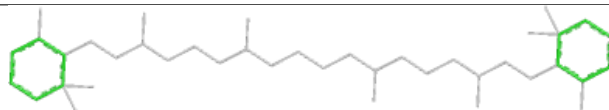
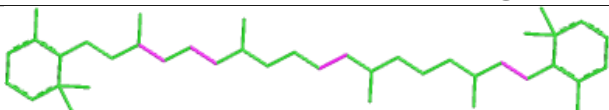
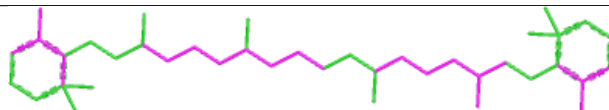
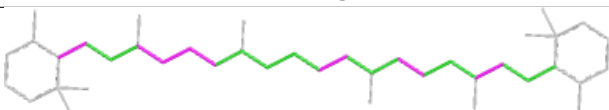
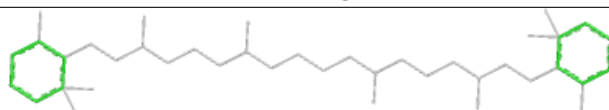


Ligand PTY 7 804

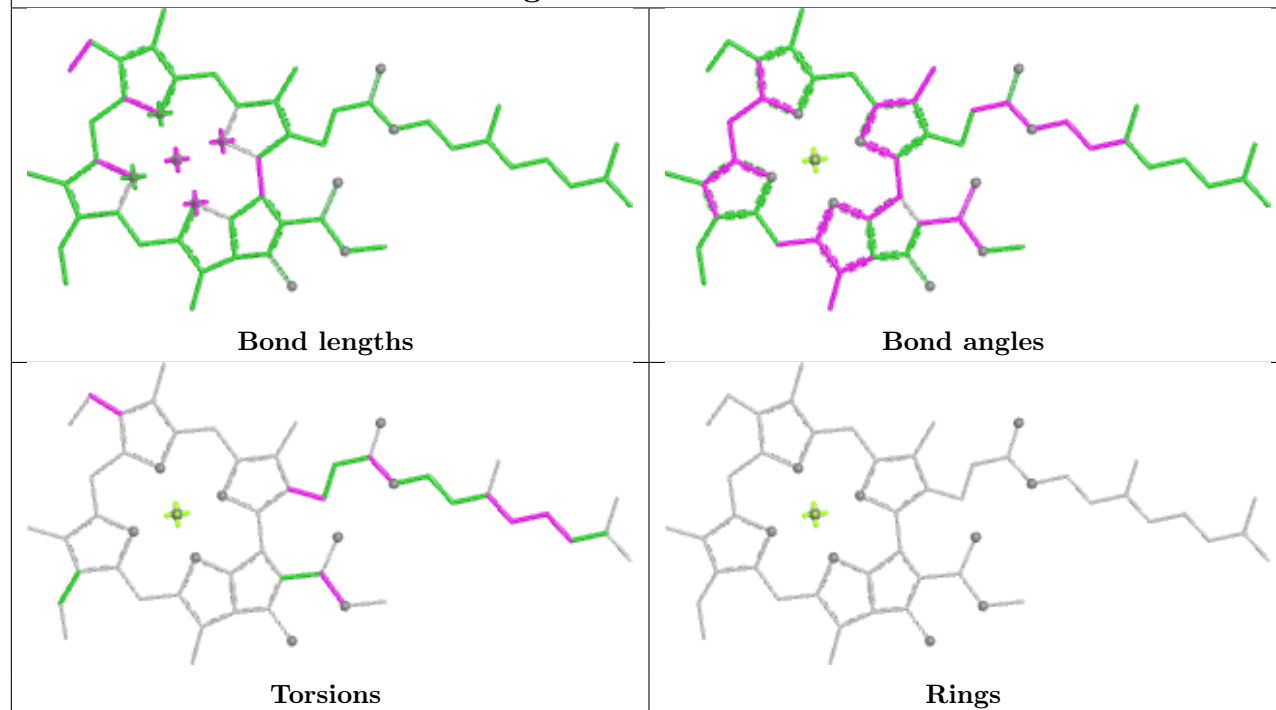




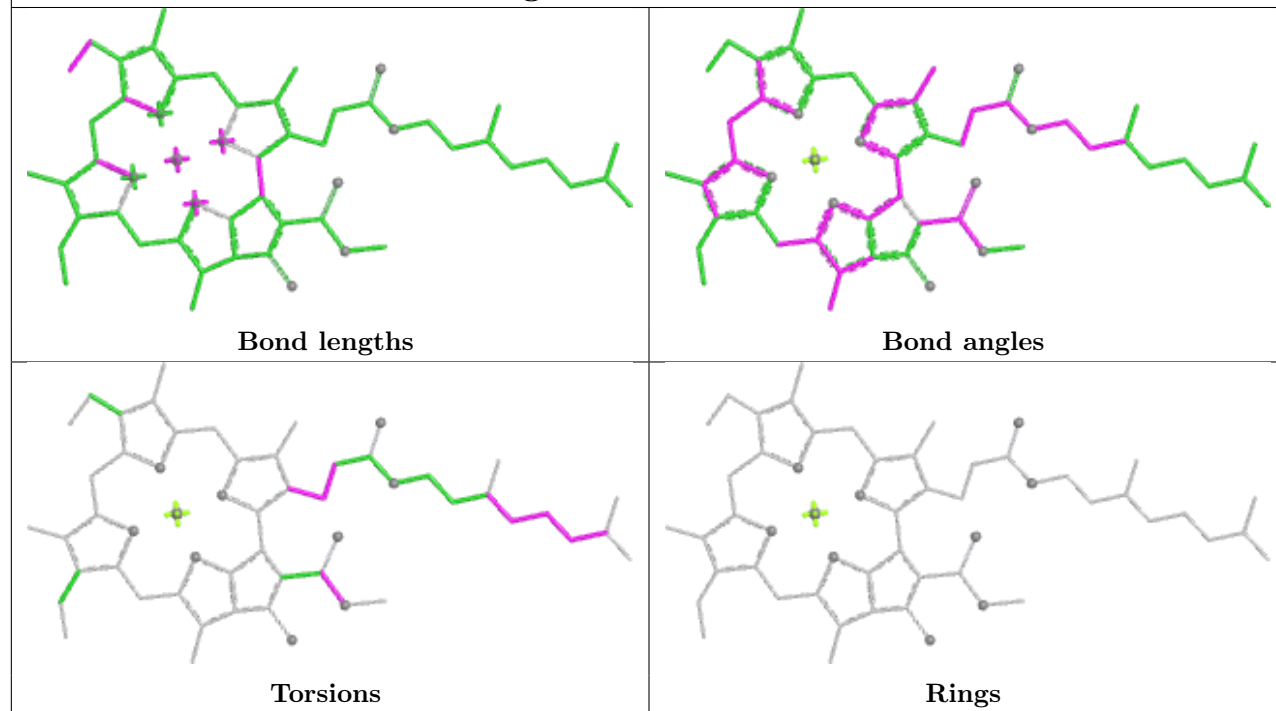


Ligand CLA 8 606	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR F 4001	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR H 4001	
	
Bond lengths	Bond angles
	
Torsions	Rings

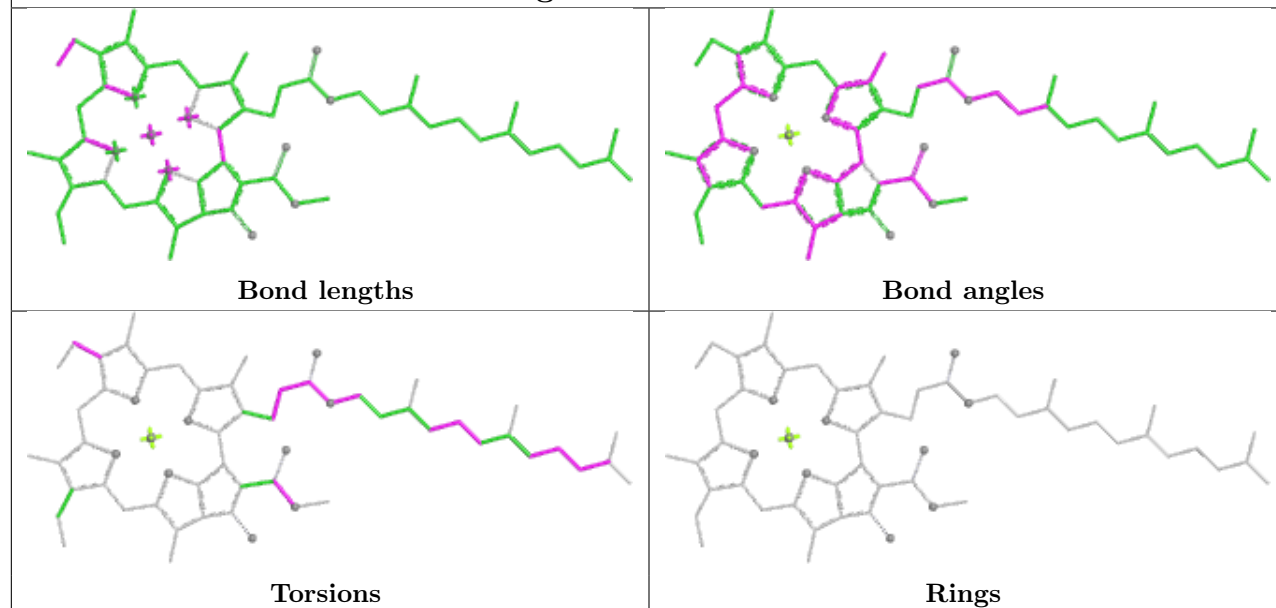
Ligand CLA B 1218



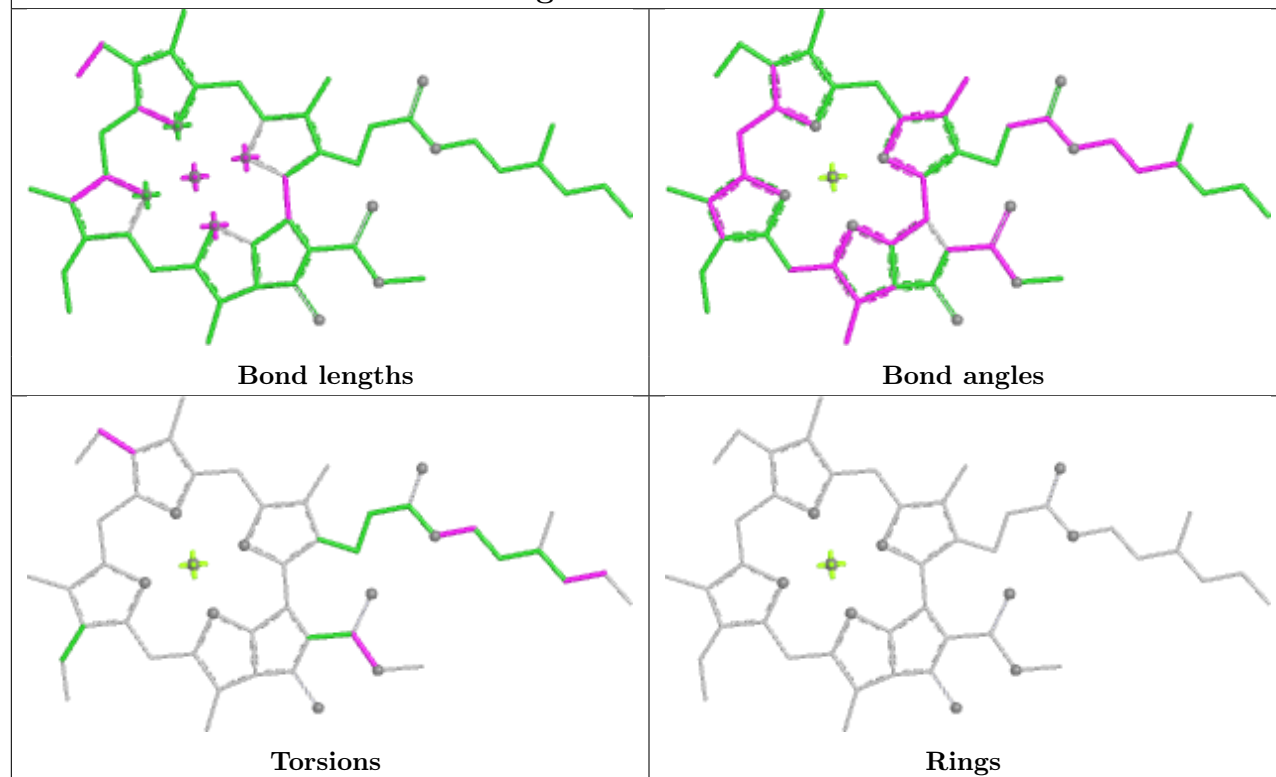
Ligand CLA A 1107

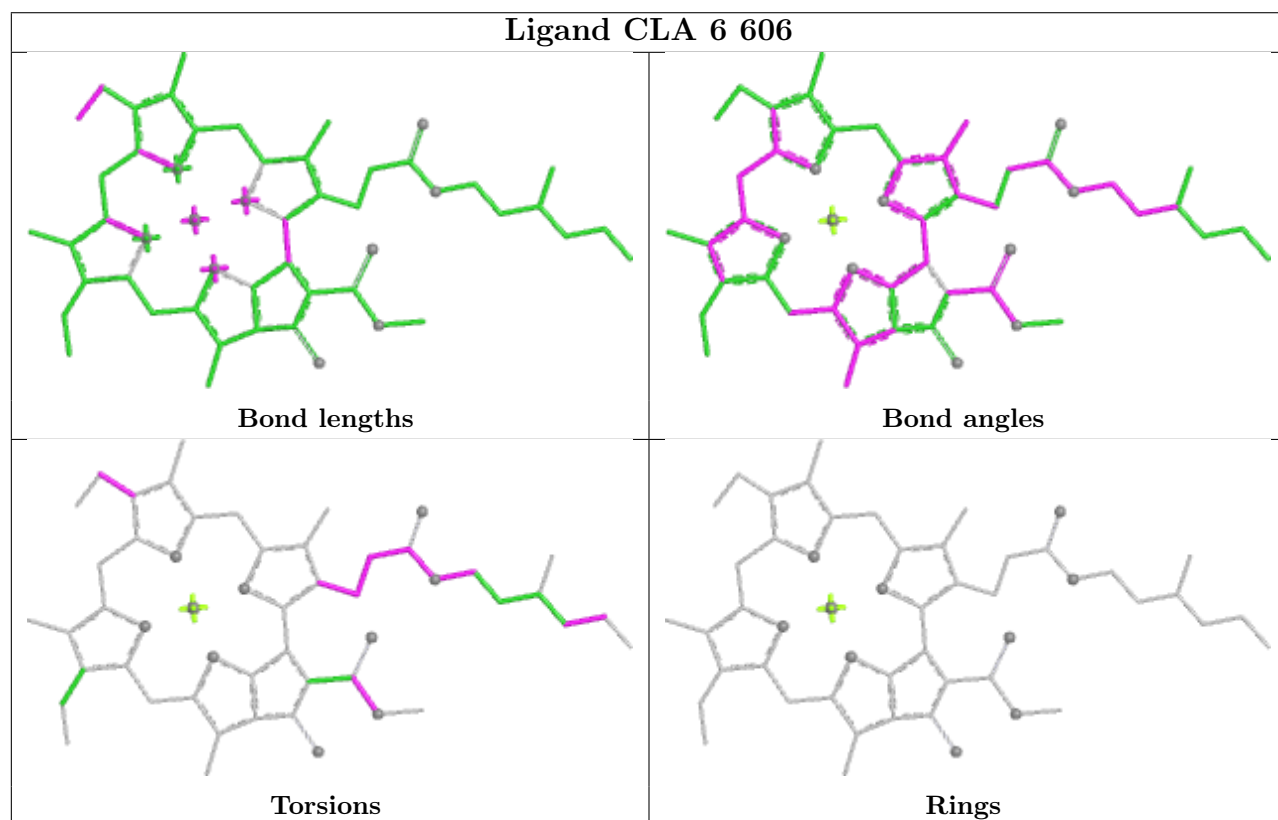
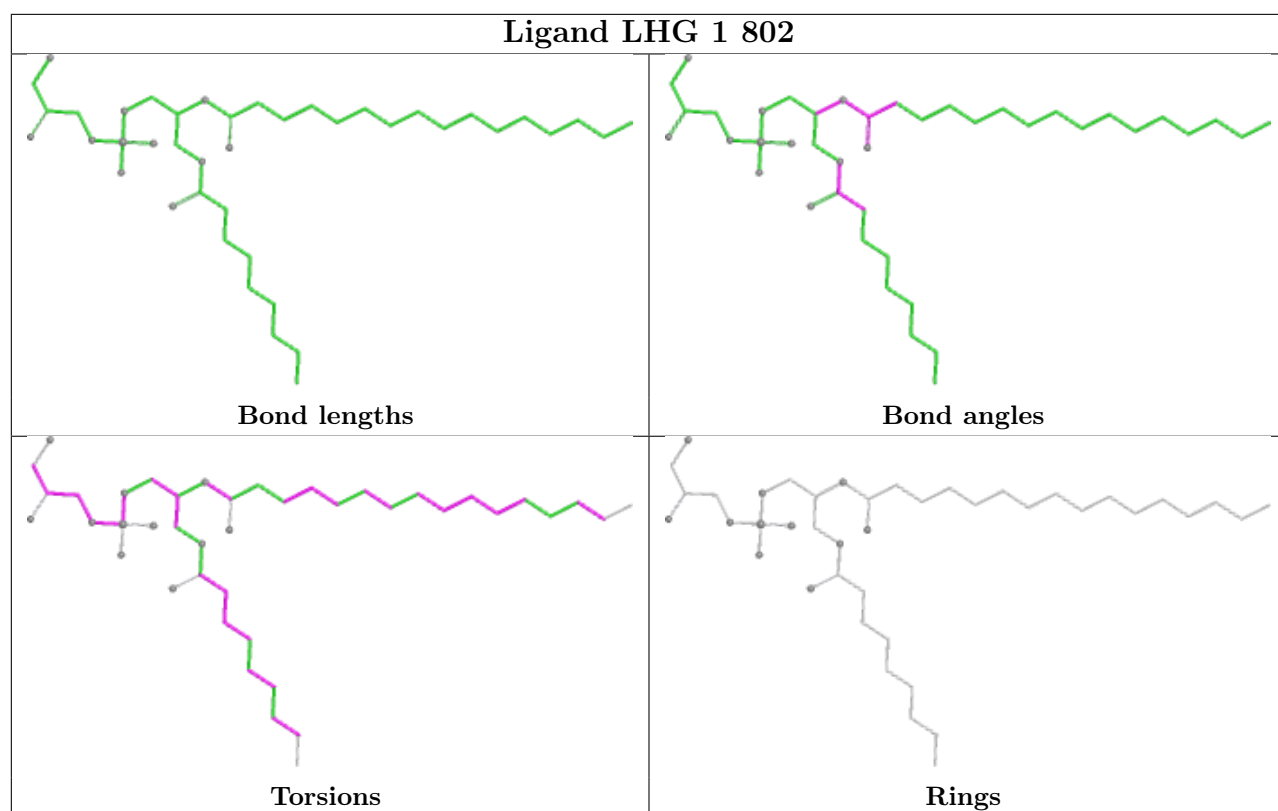


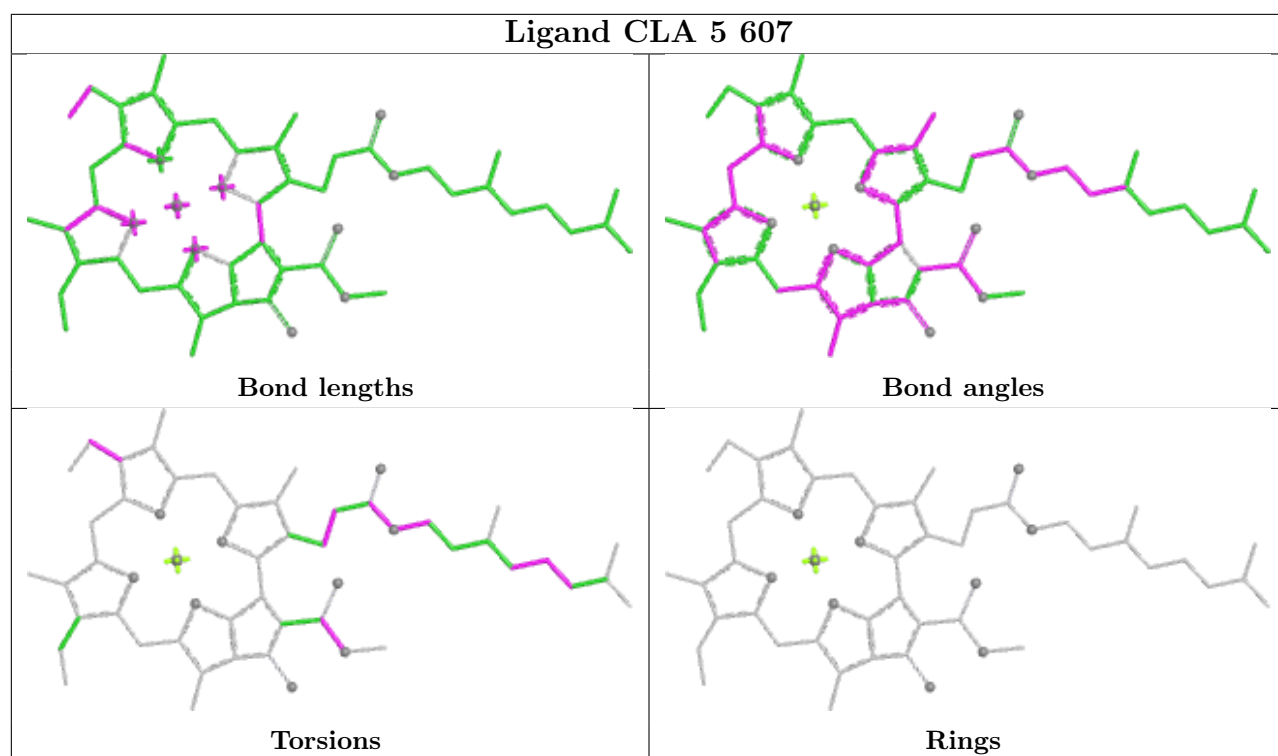
Ligand CLA 8 618



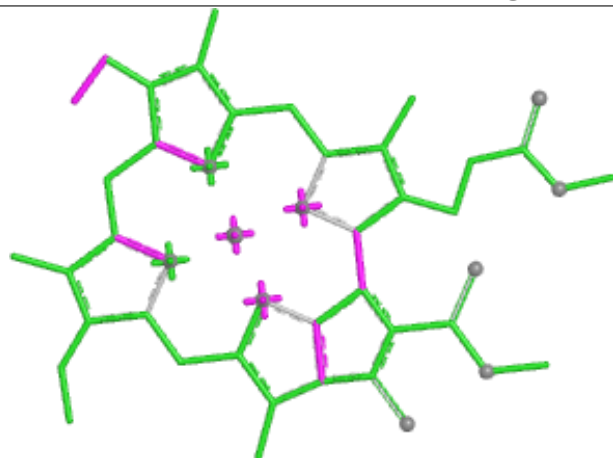
Ligand CLA 6 602



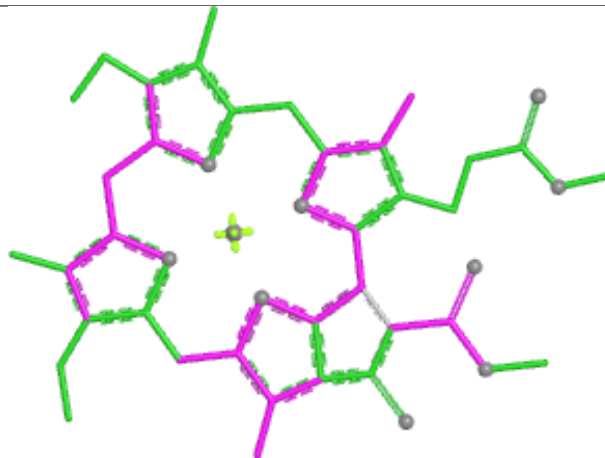




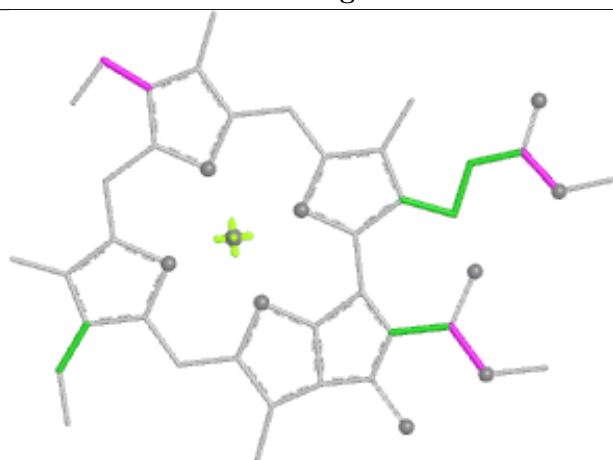
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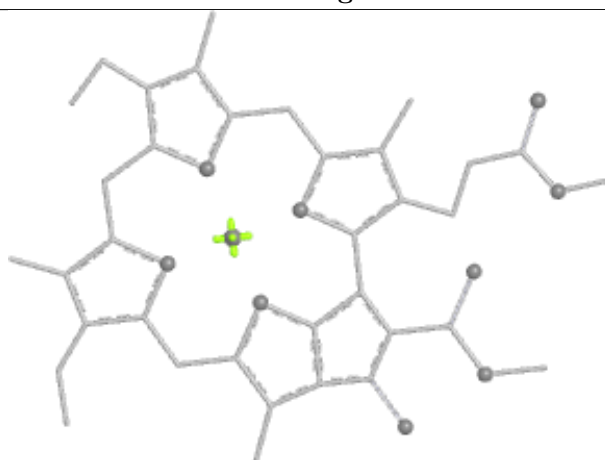
Bond lengths



Bond angles

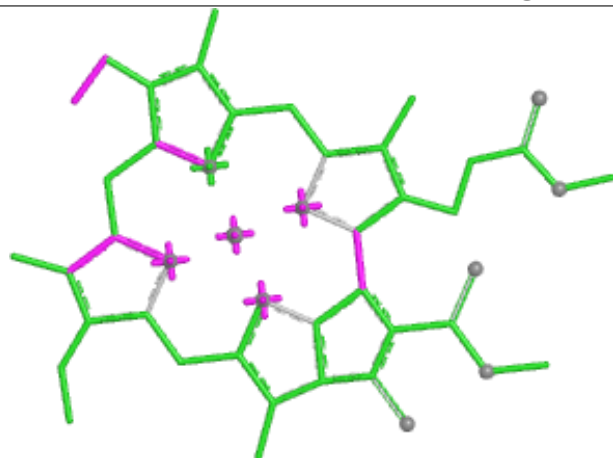


Torsions

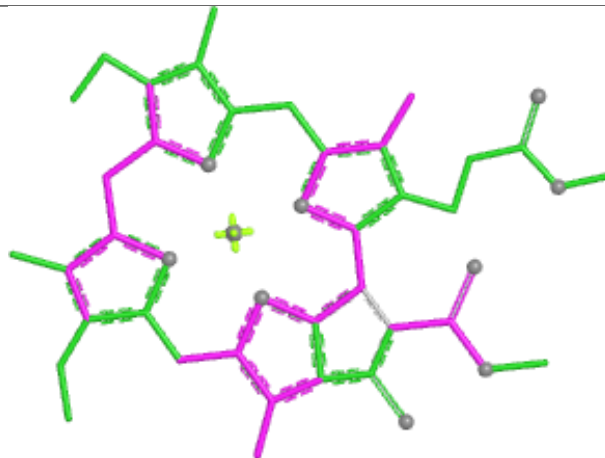


Rings

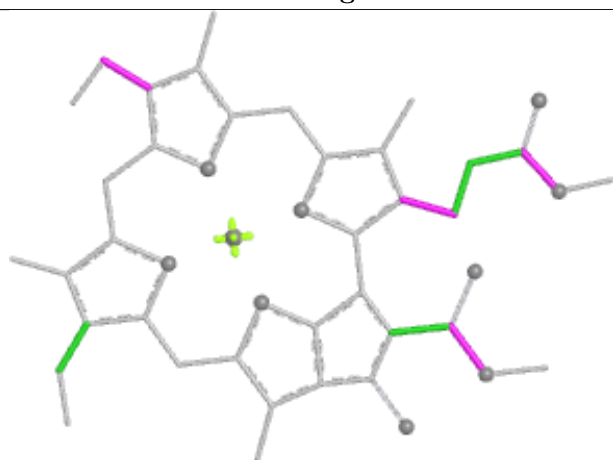
Ligand CLA 1 615



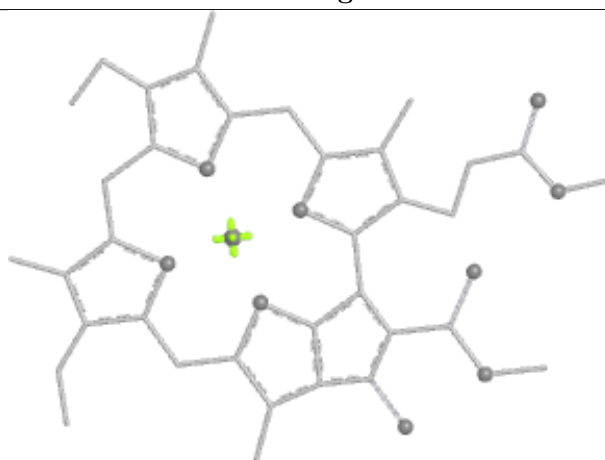
Bond lengths



Bond angles

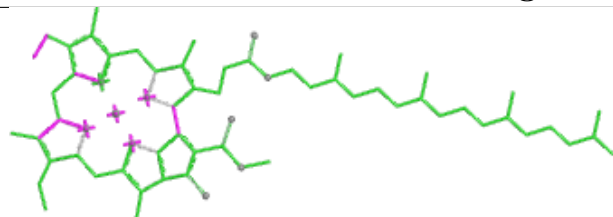


Torsions

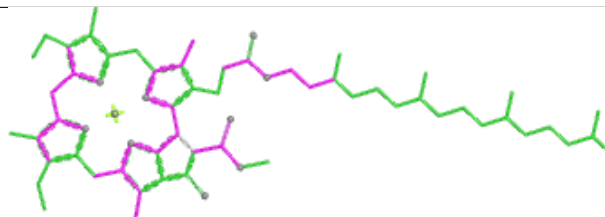


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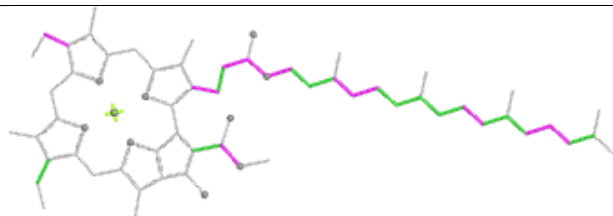
Ligand CLA 3 607



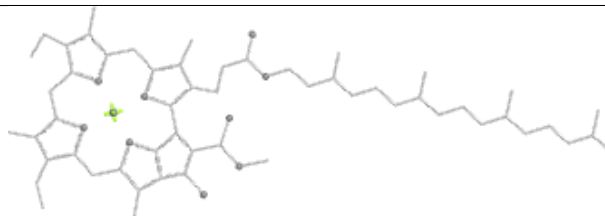
Bond lengths



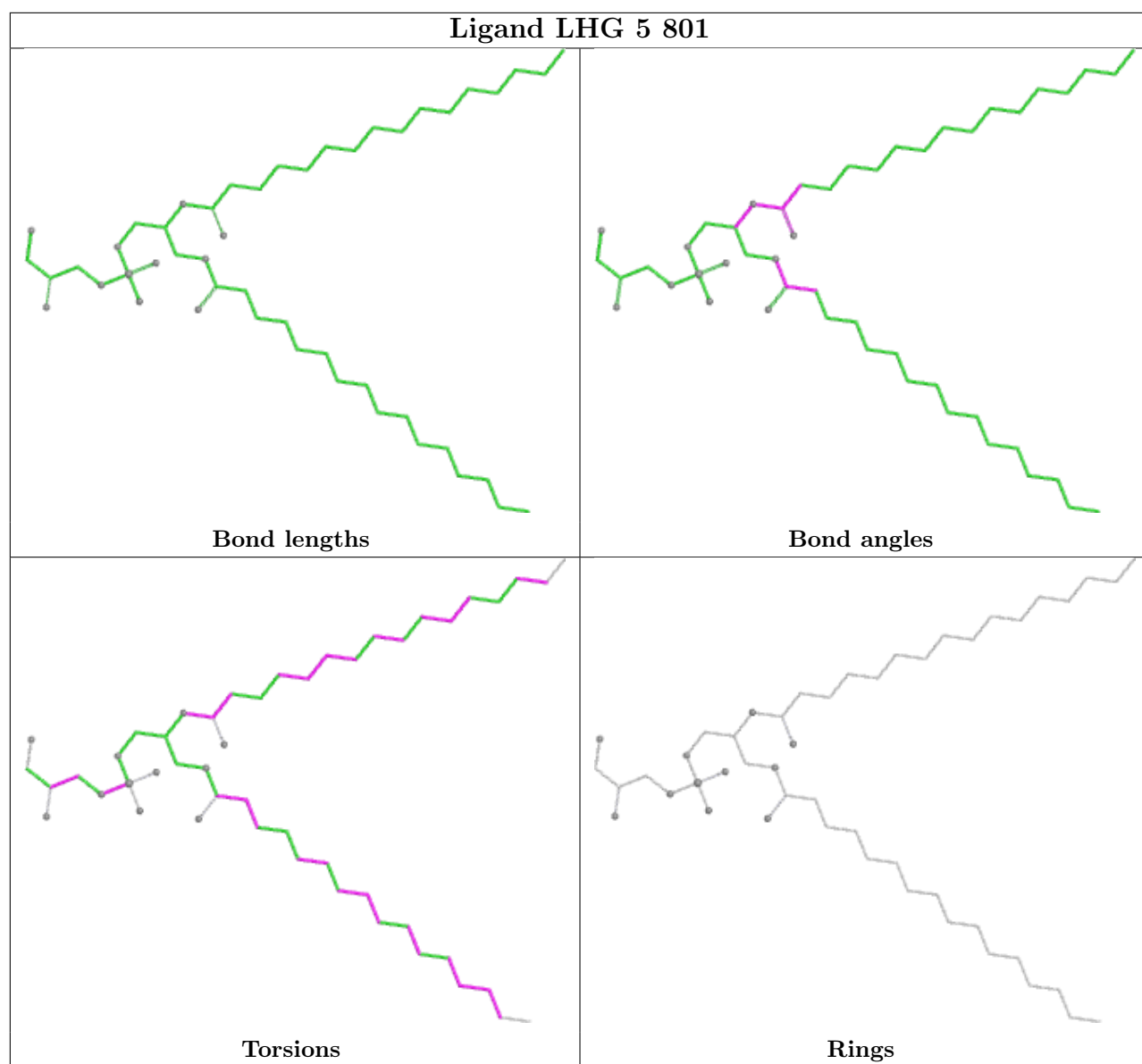
Bond angles



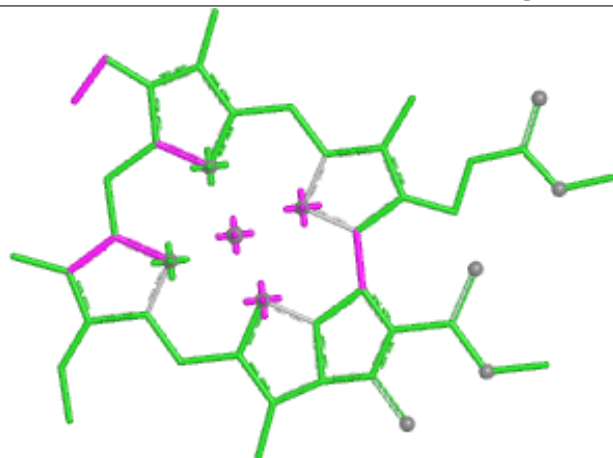
Torsions



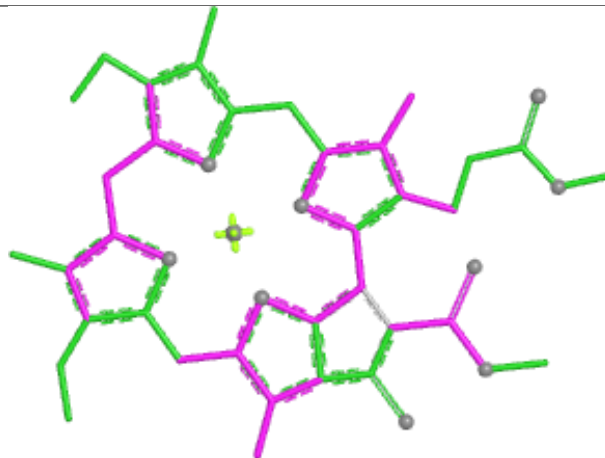
Rings



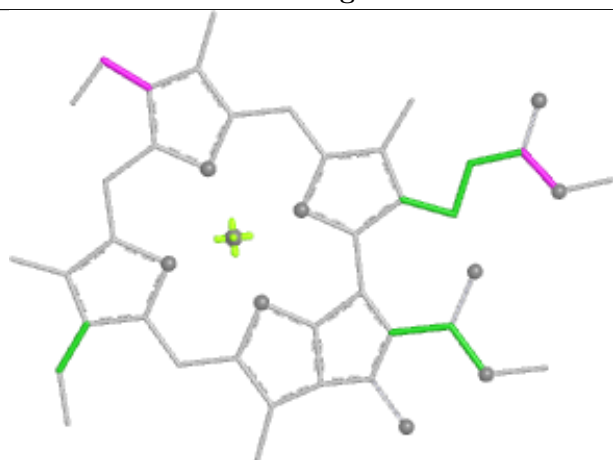
Ligand CLA 8 607



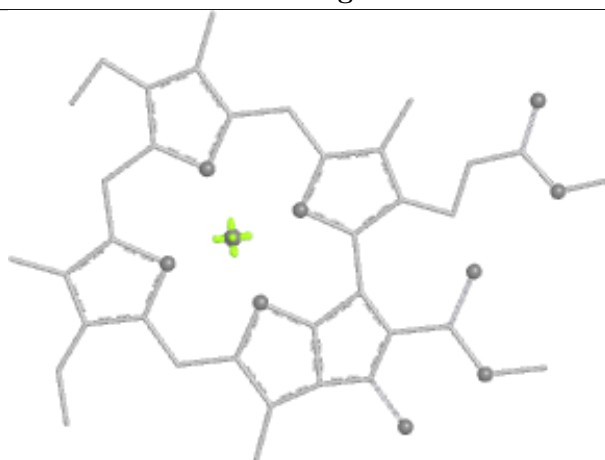
Bond lengths



Bond angles

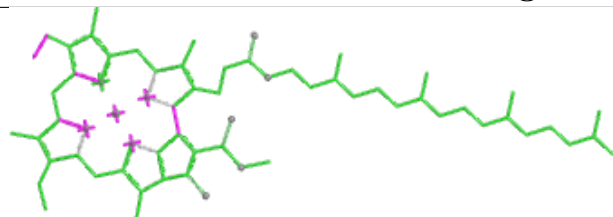


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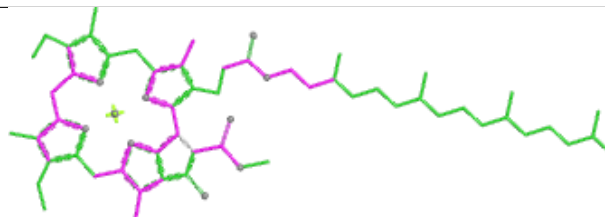


Rings

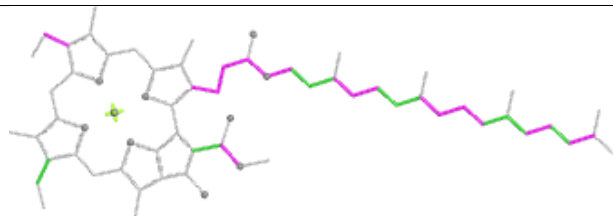
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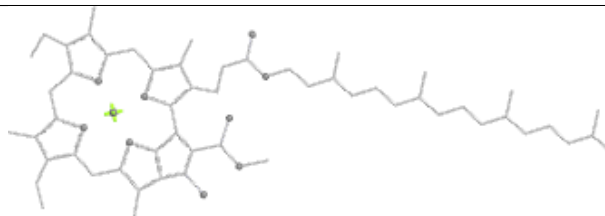
Bond lengths



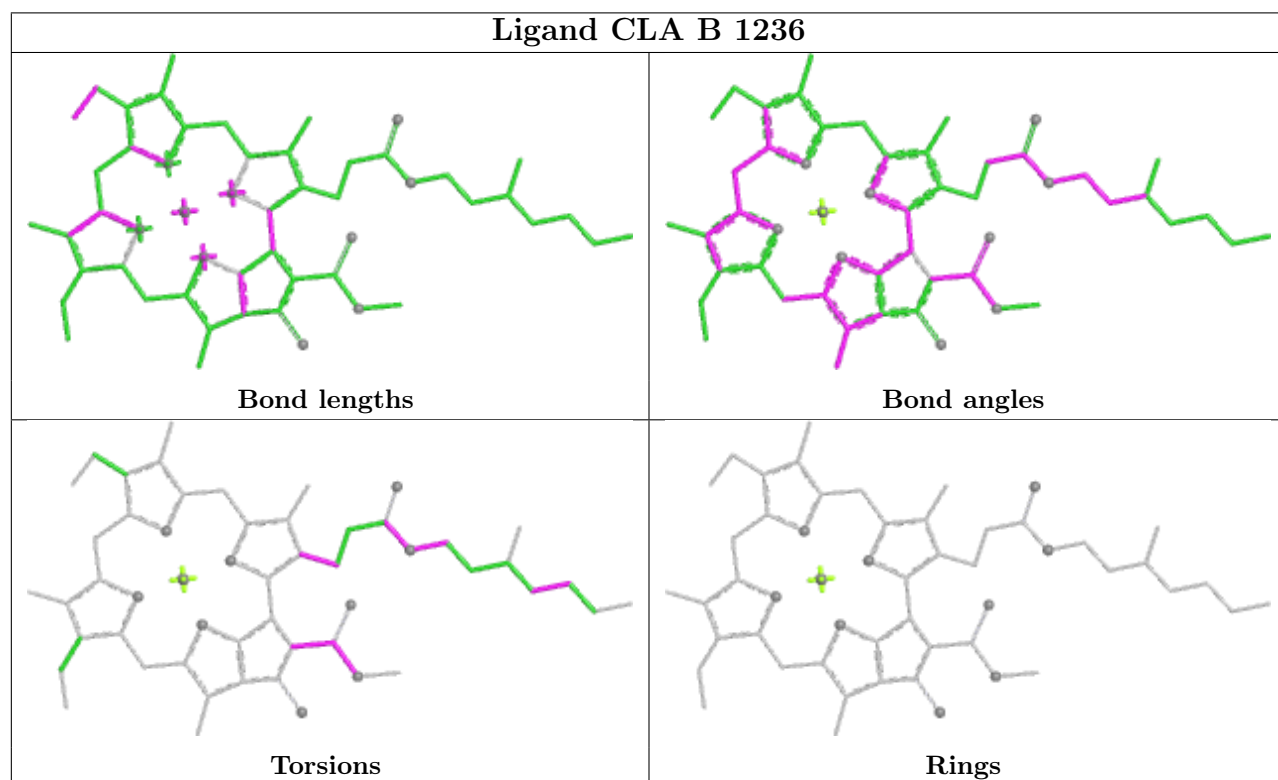
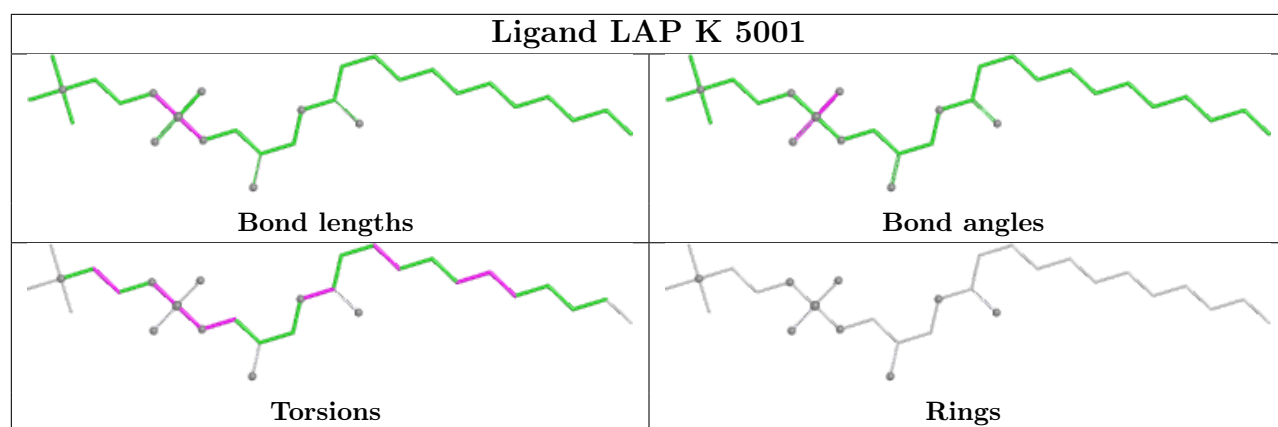
Bond angles



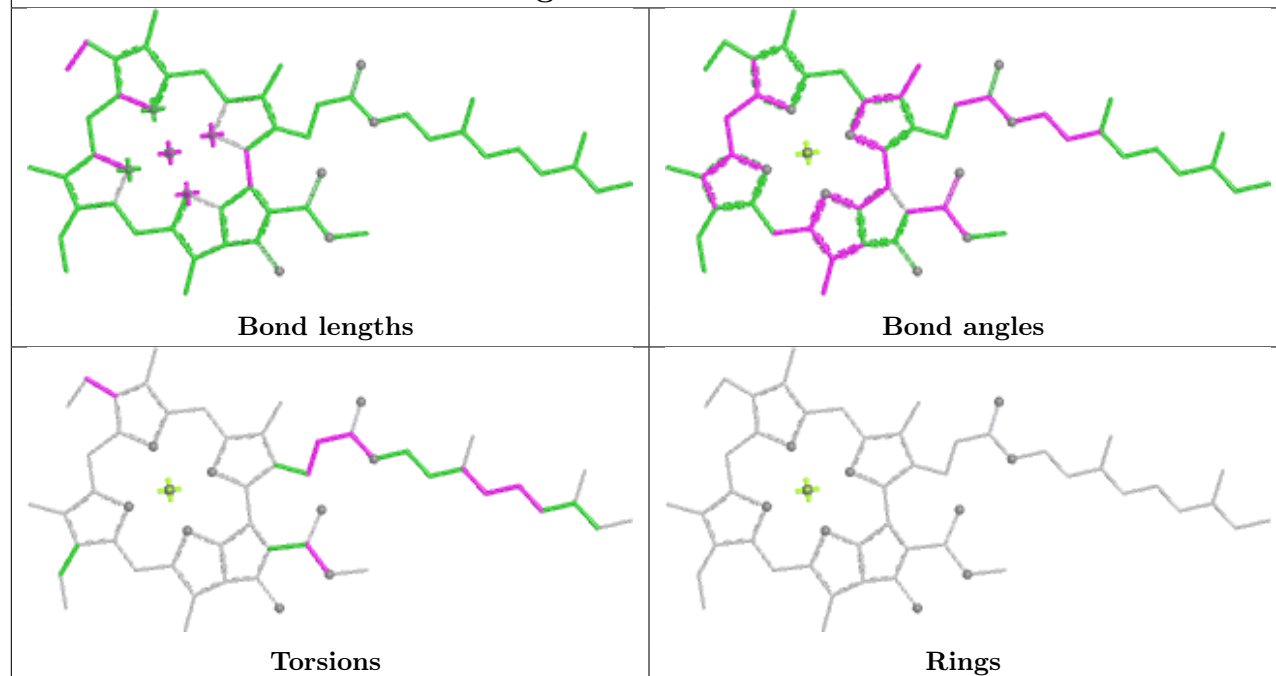
Torsions



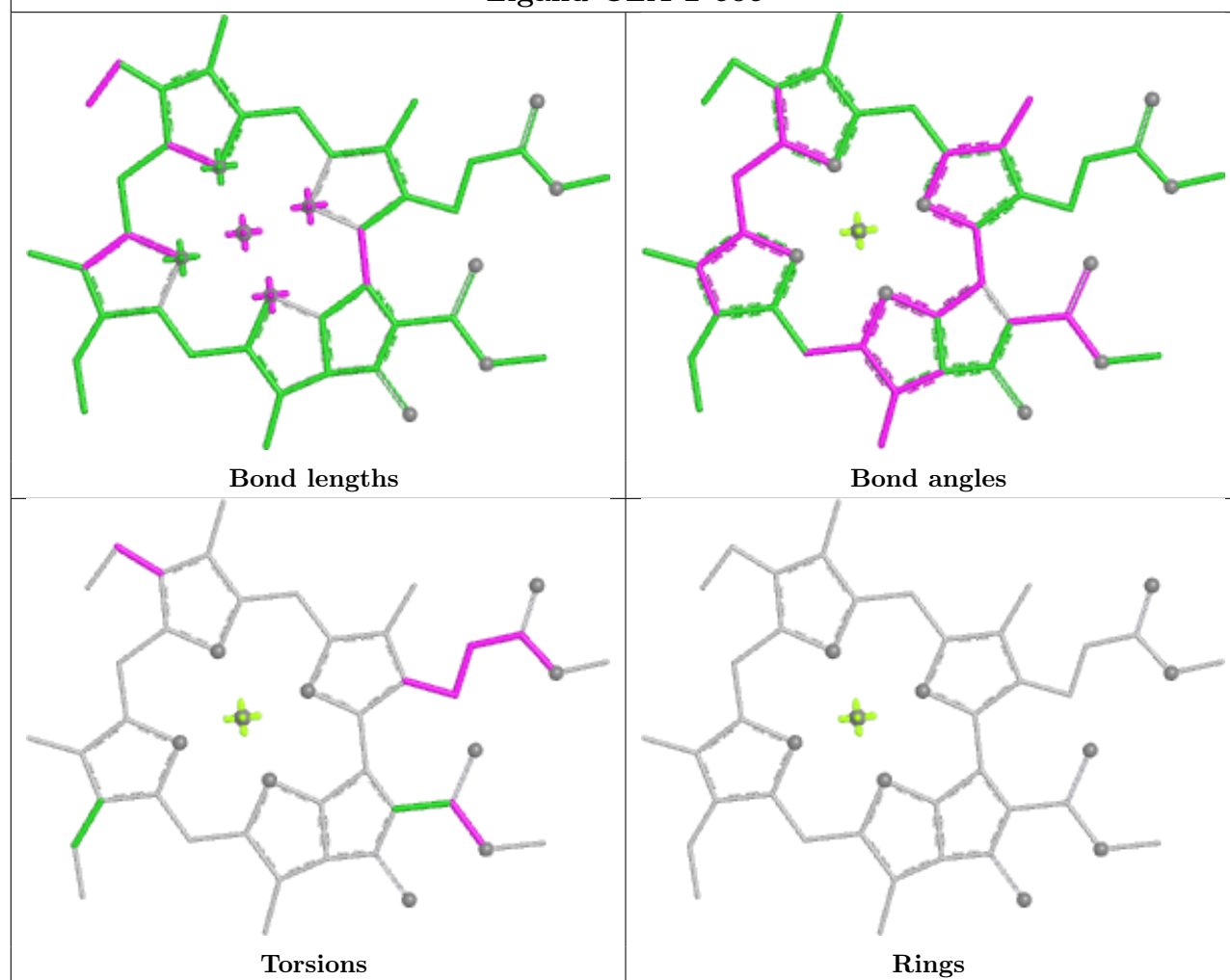
Rings



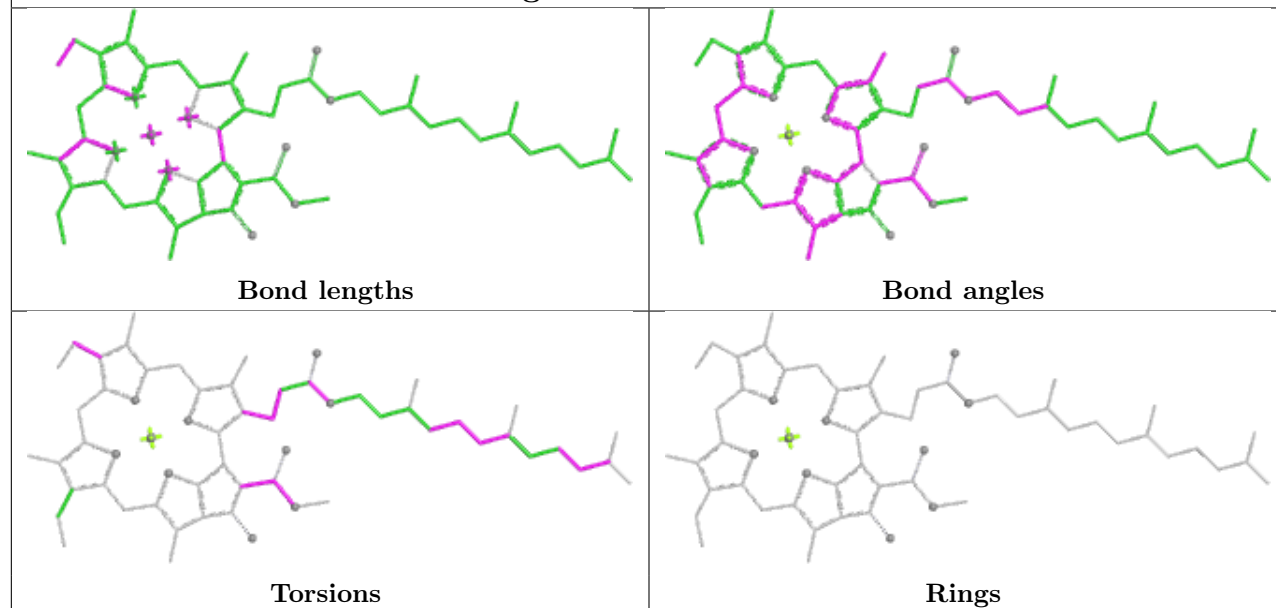
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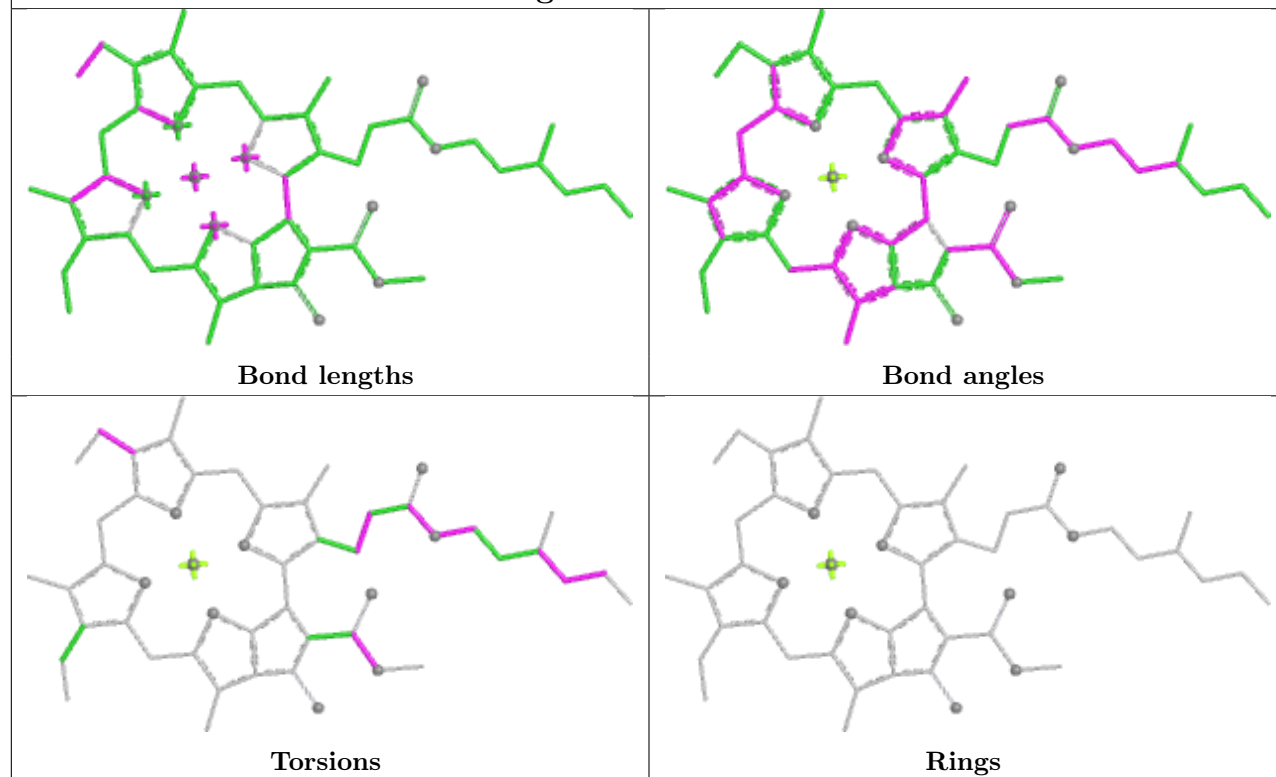
Ligand CLA 2 606



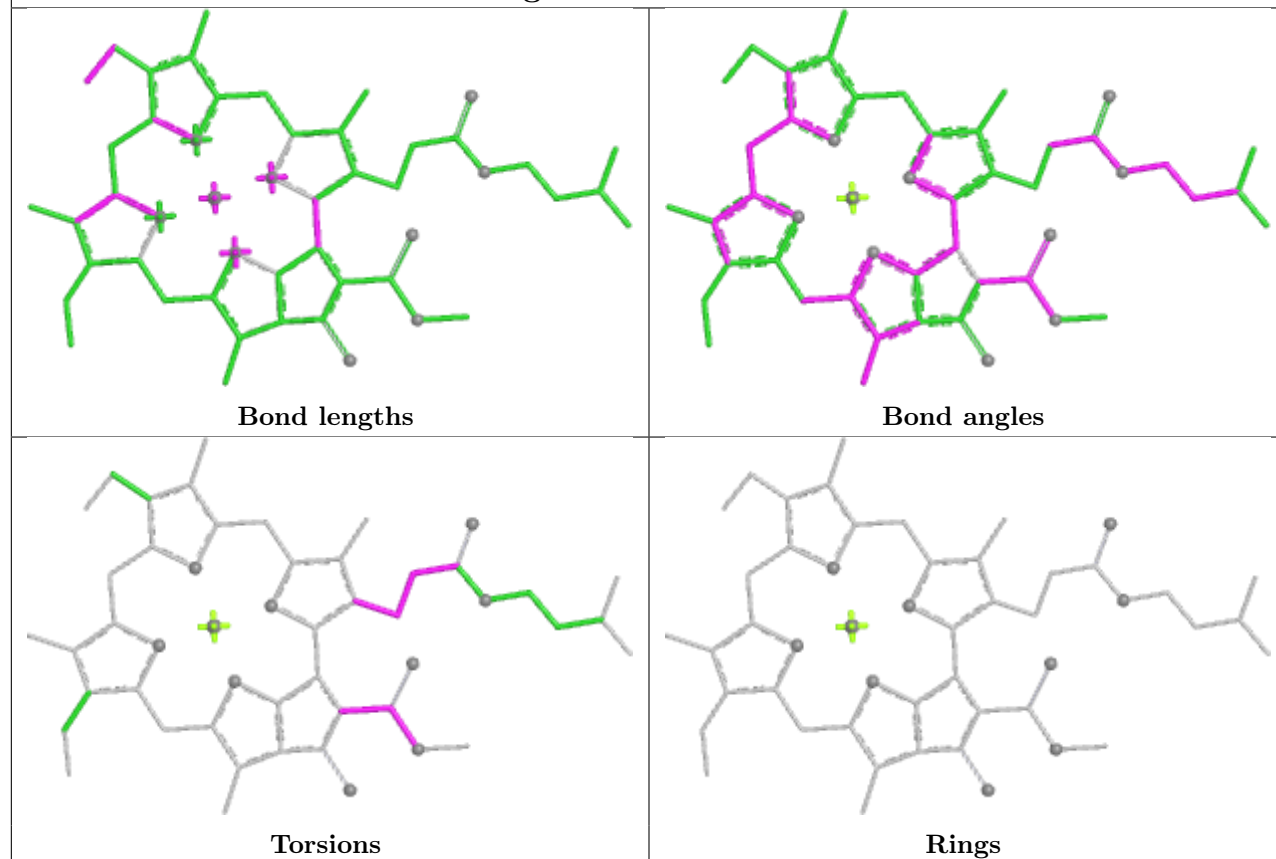
Ligand CLA A 1134



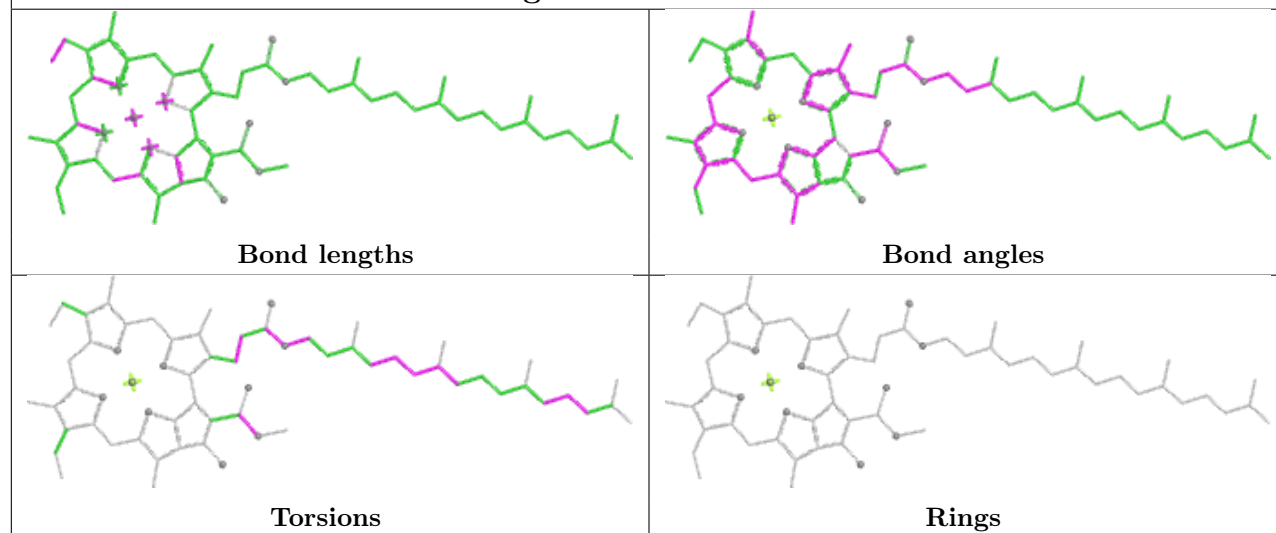
Ligand CLA 8 602

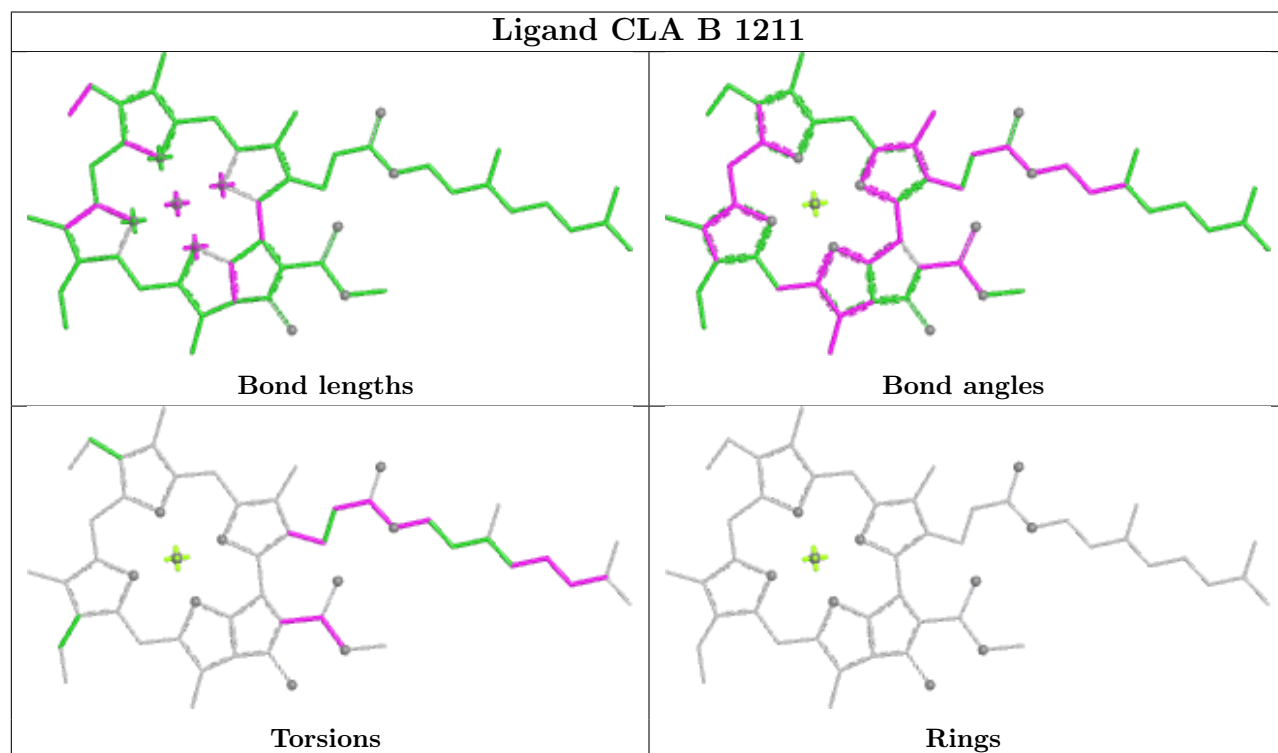
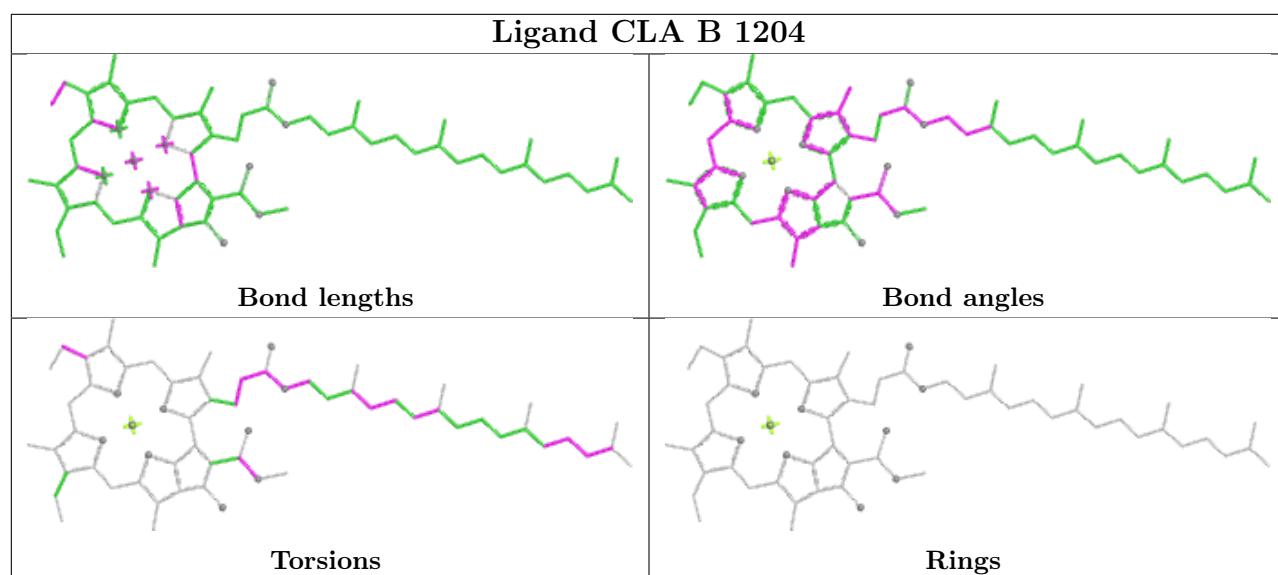


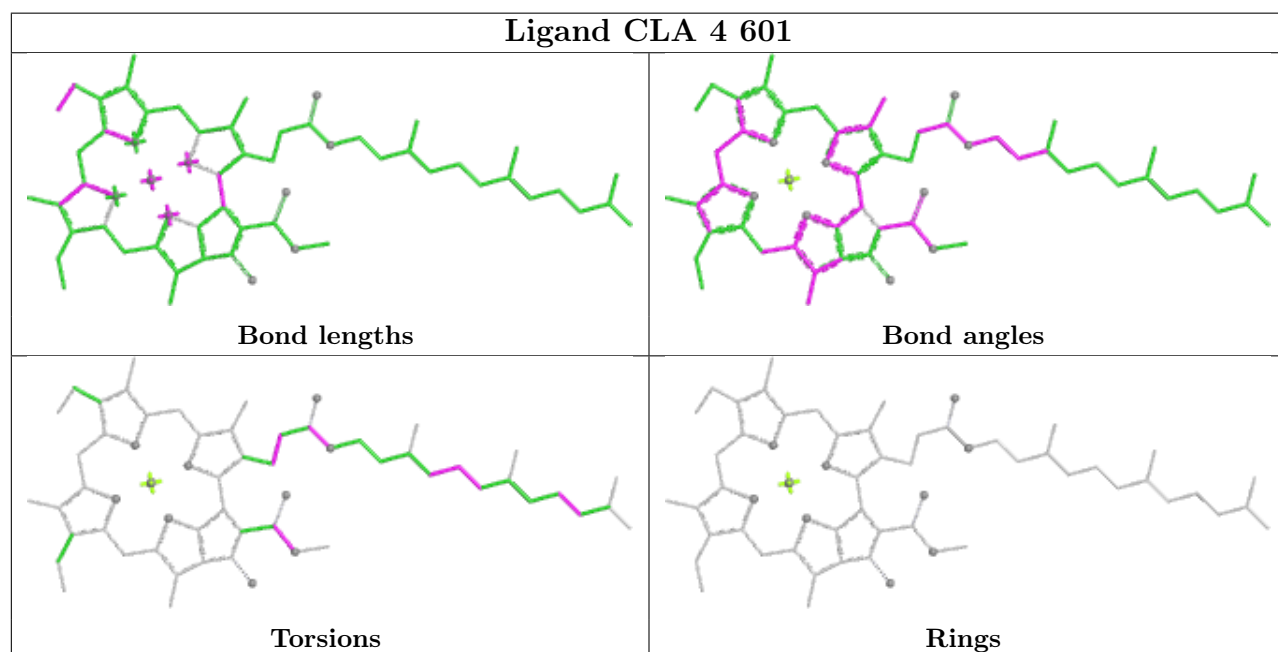
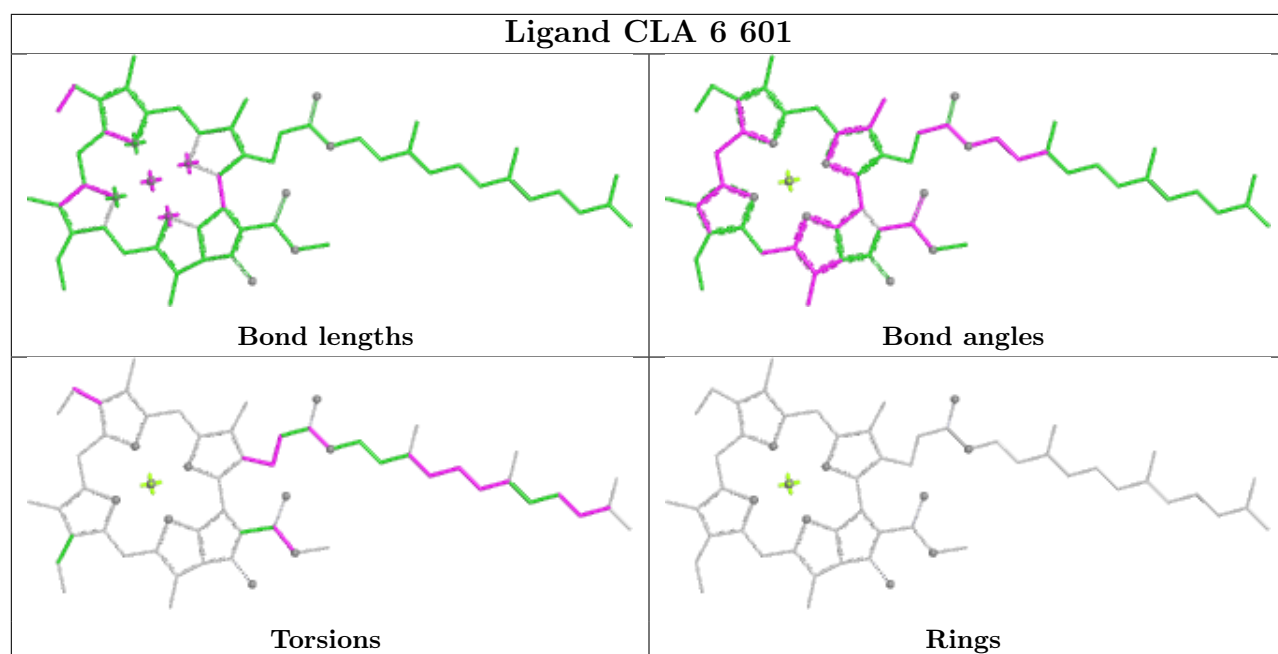
Ligand CLA B 1227

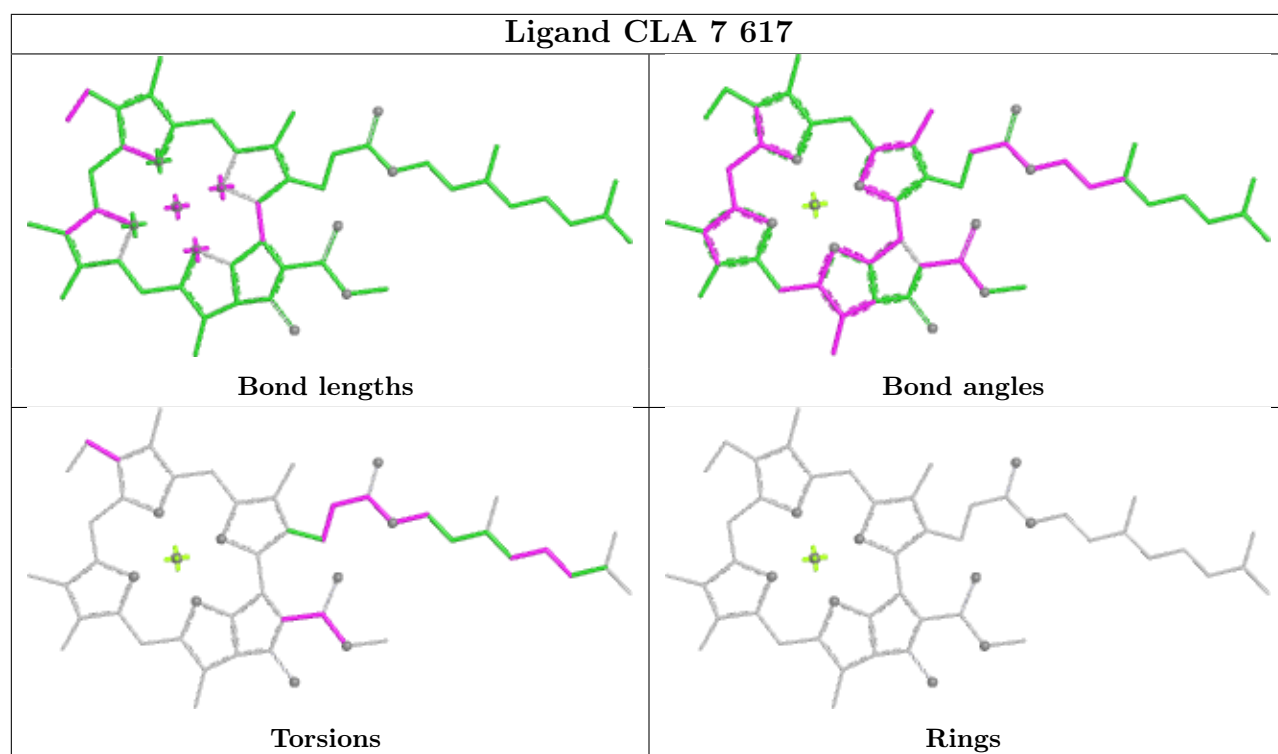


Ligand CLA B 1226

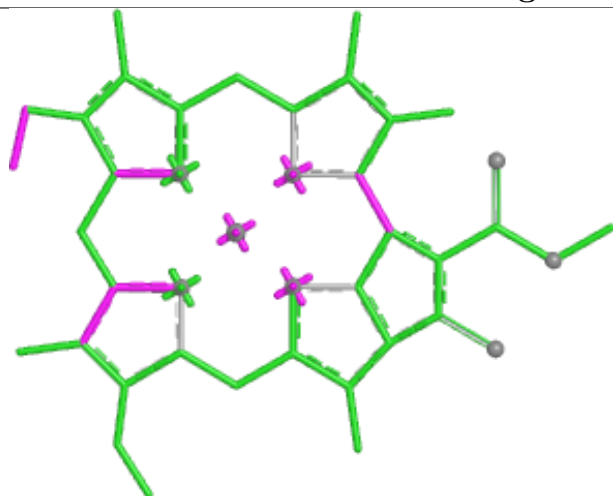




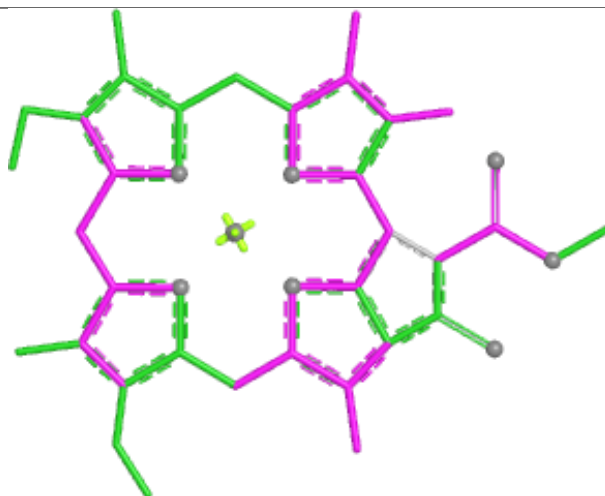




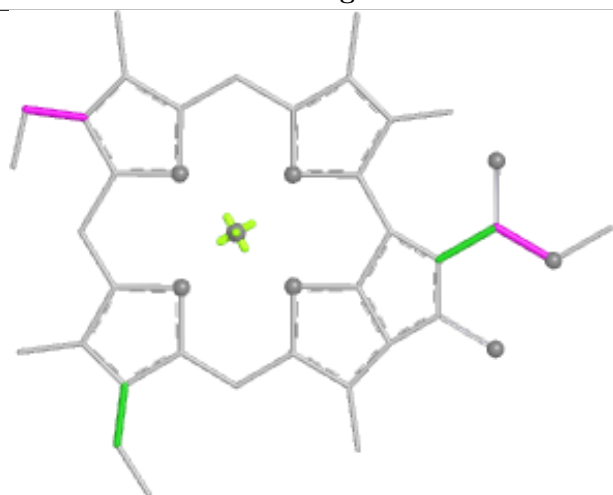
Ligand CLA 2 613



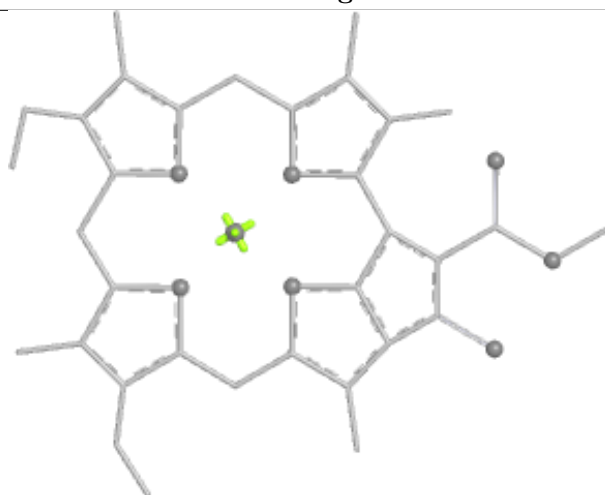
Bond lengths



Bond angles

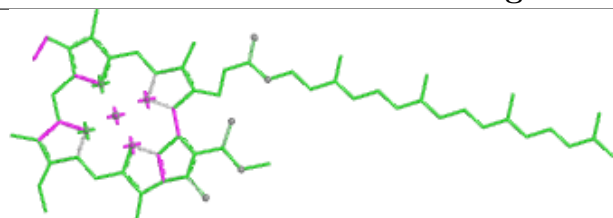


Torsions

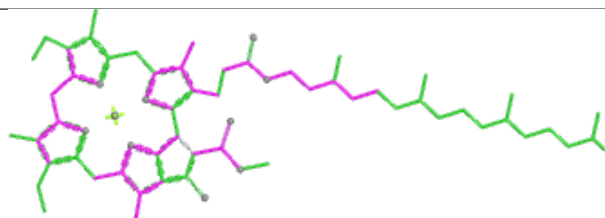


Rings

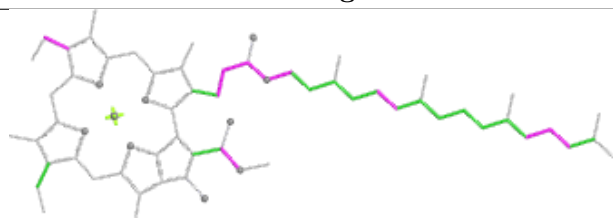
Ligand CLA B 1238



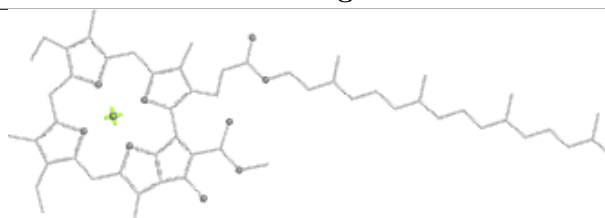
Bond lengths



Bond angles

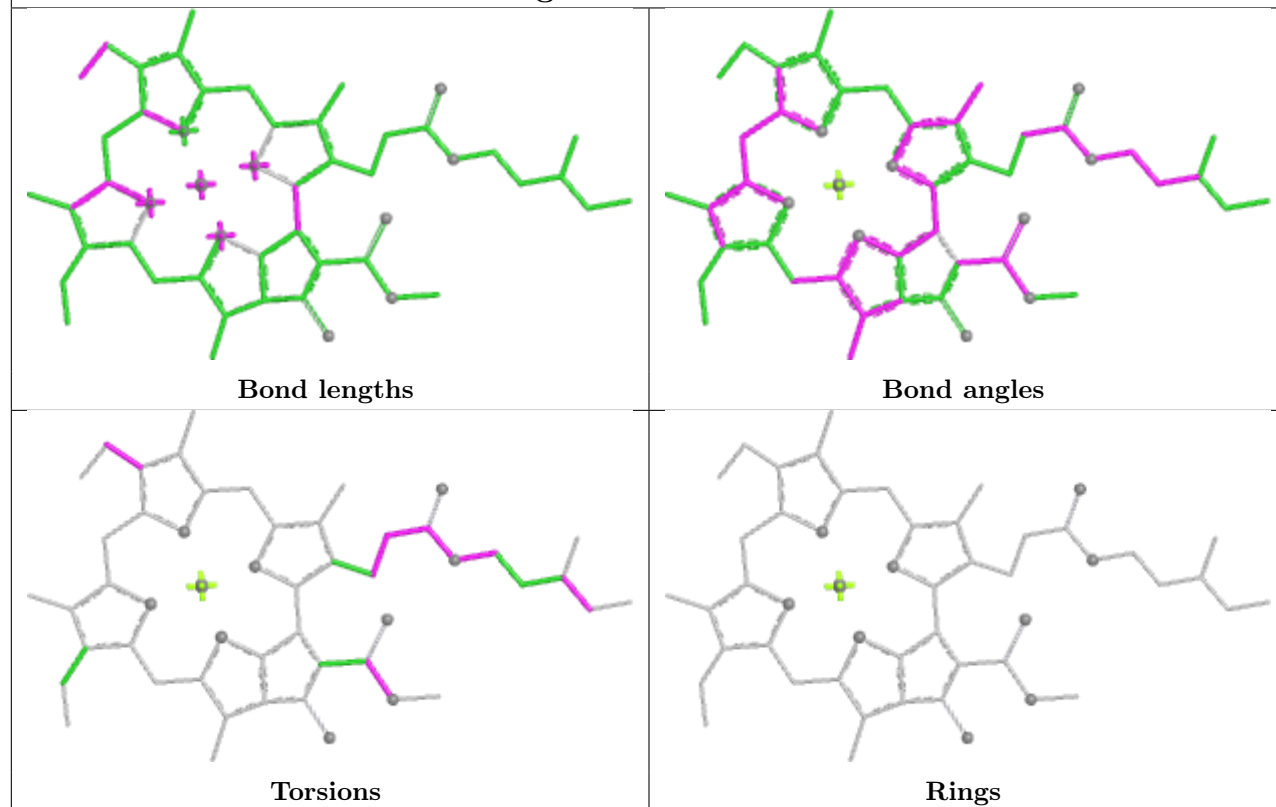


Torsions

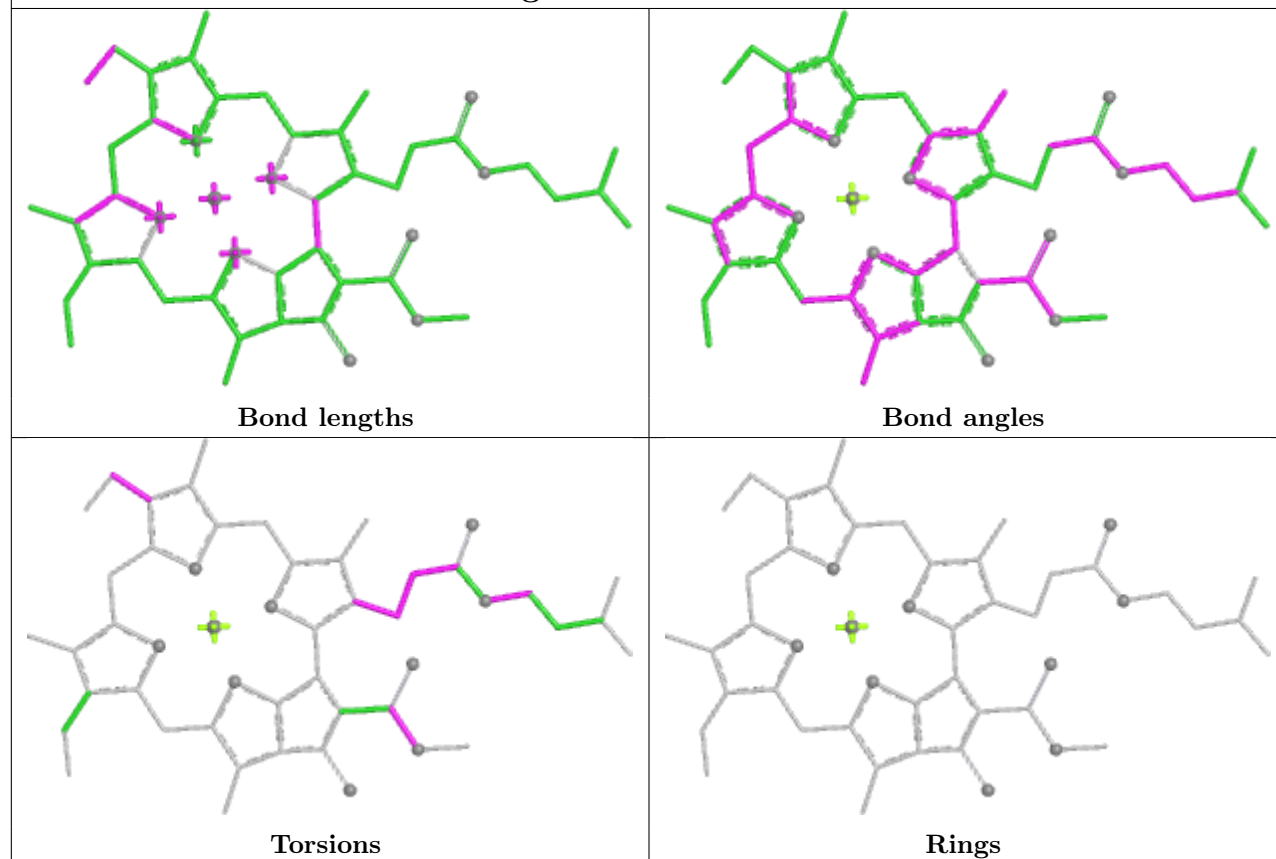


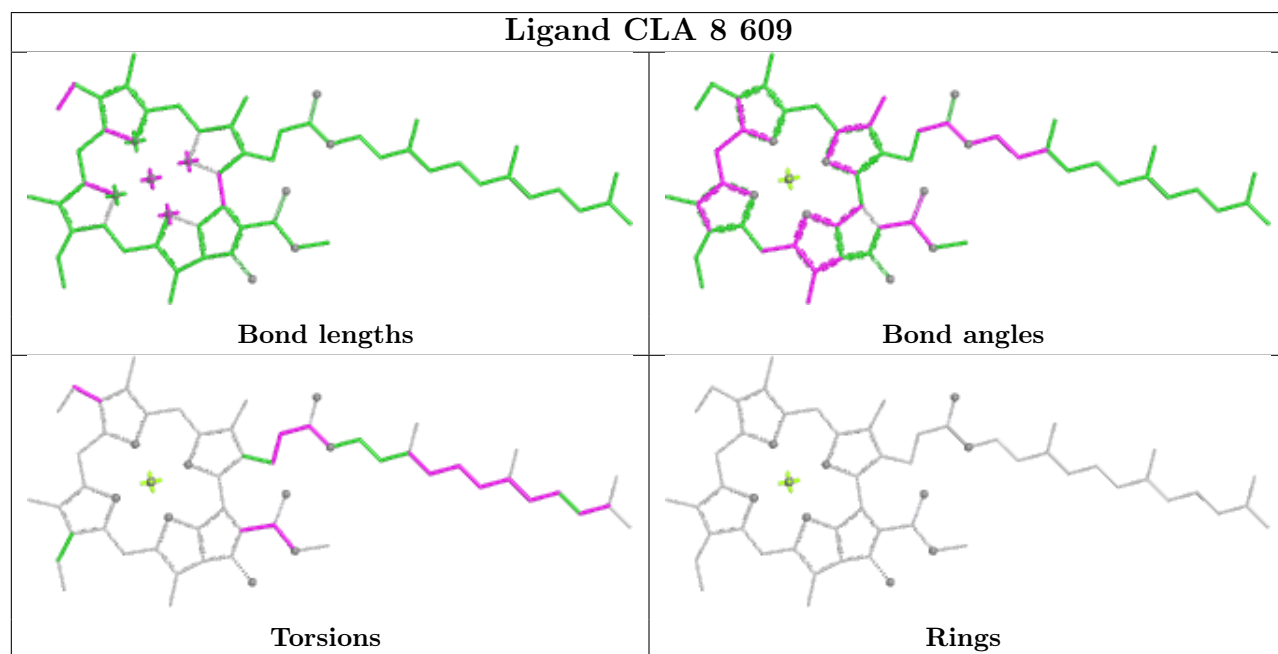
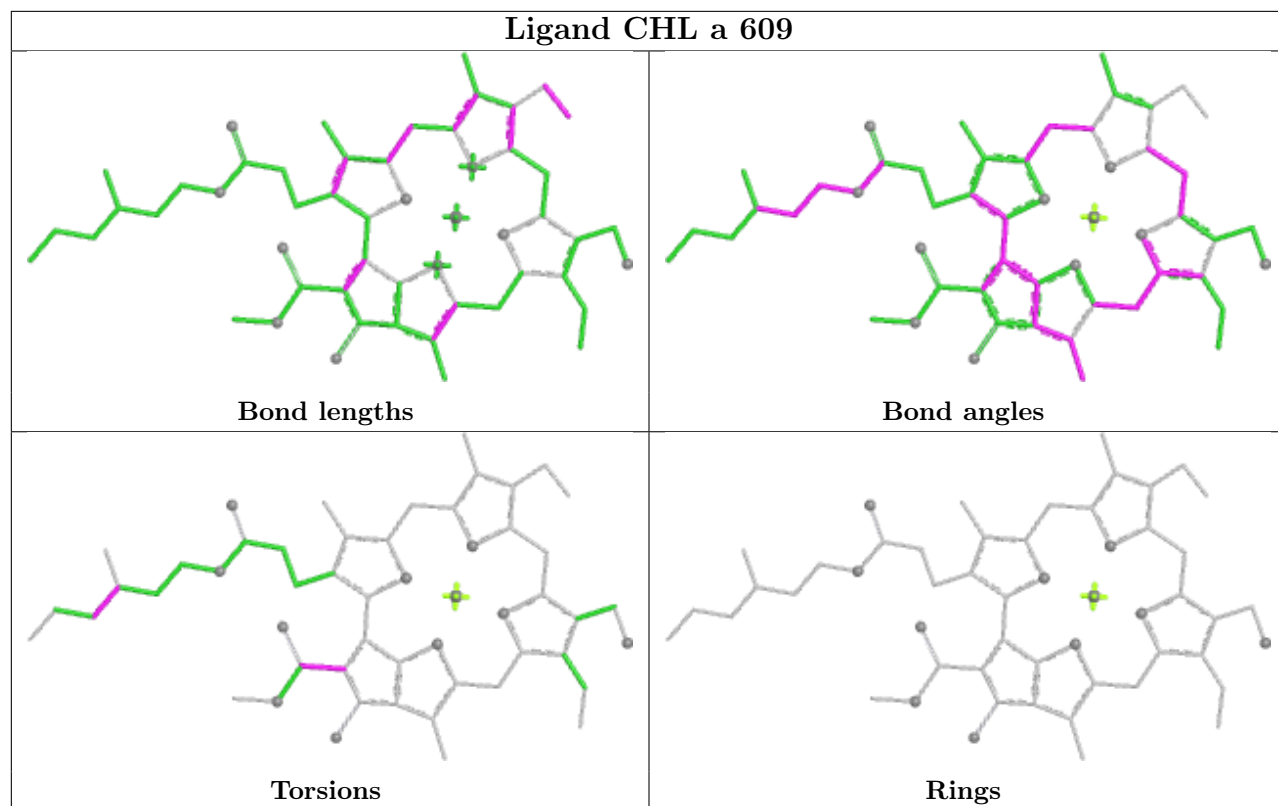
Rings

Ligand CLA 5 609

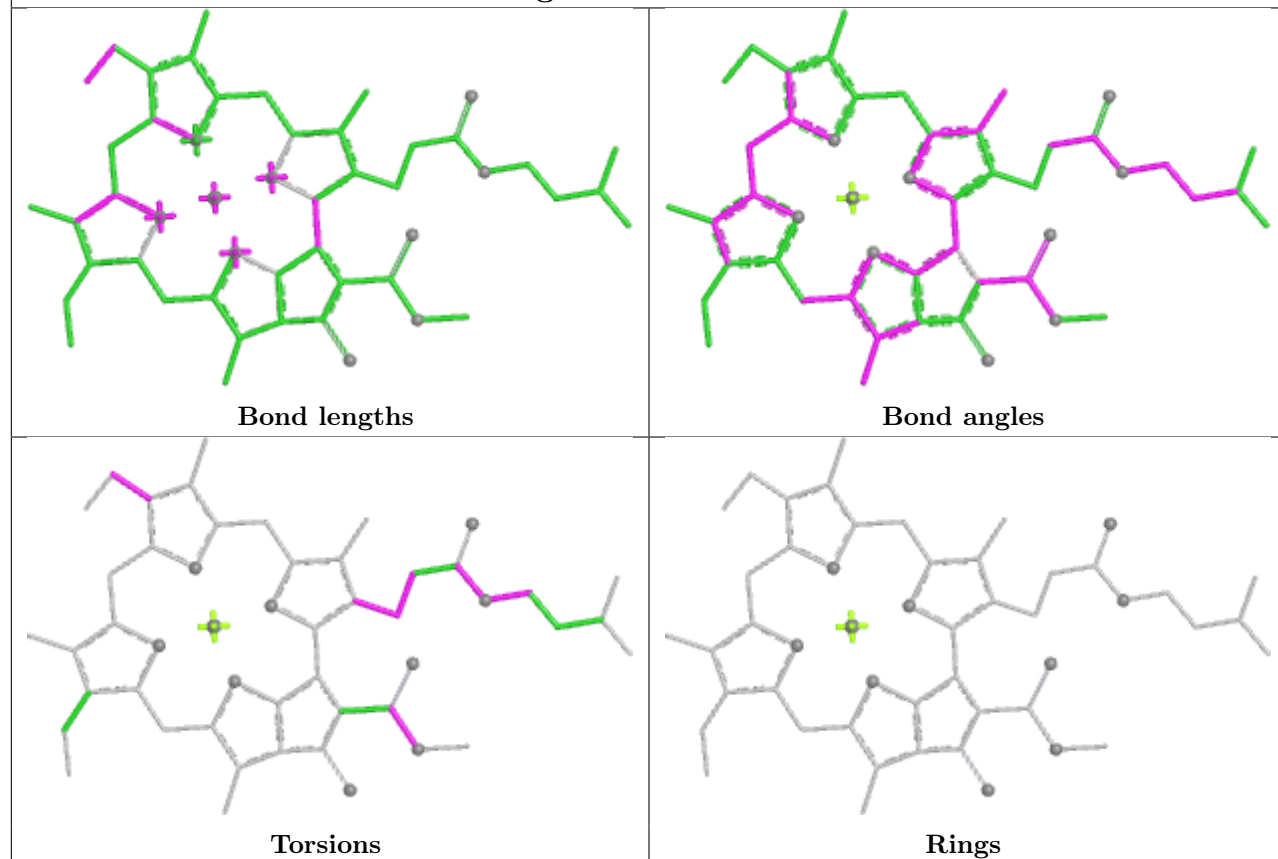


Ligand CLA G 1601

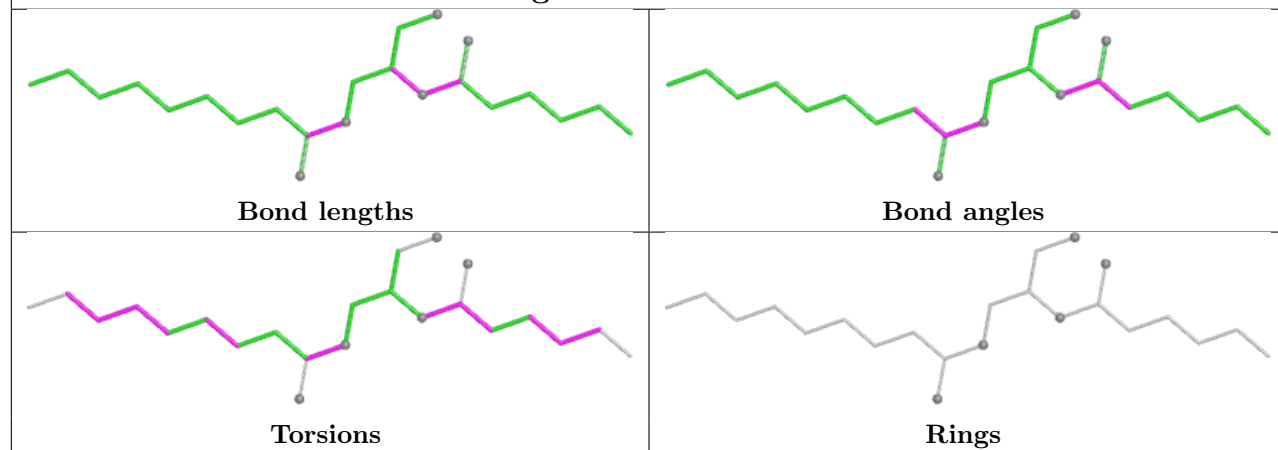


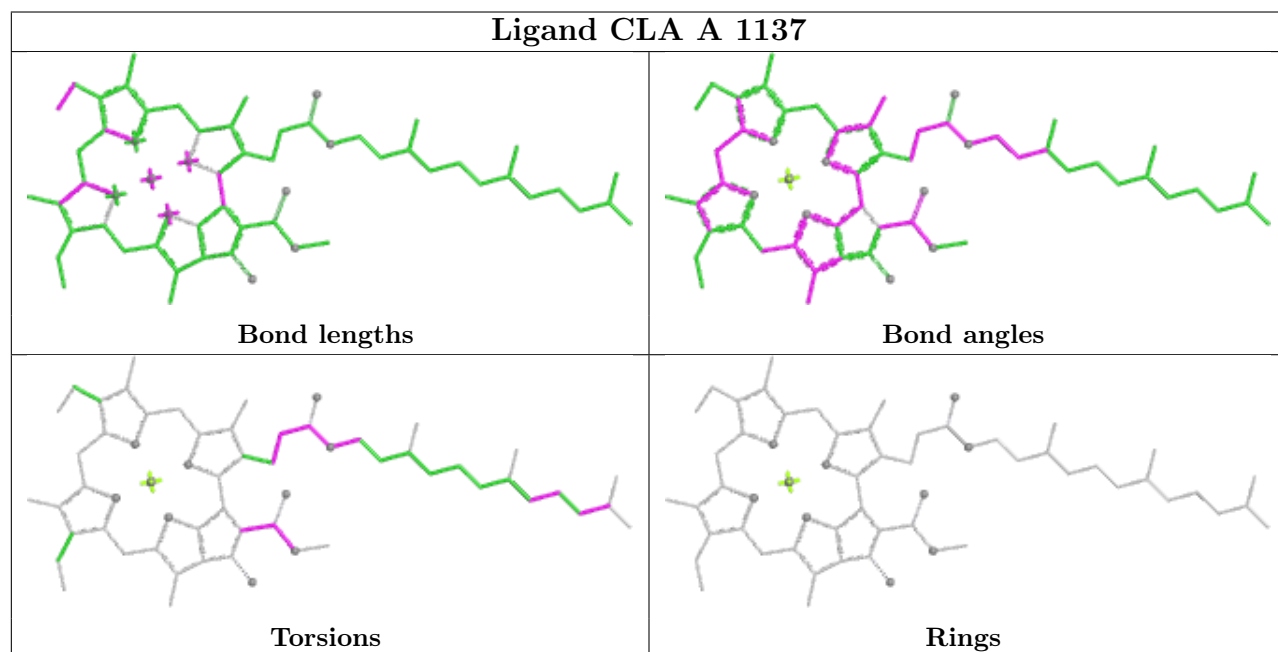
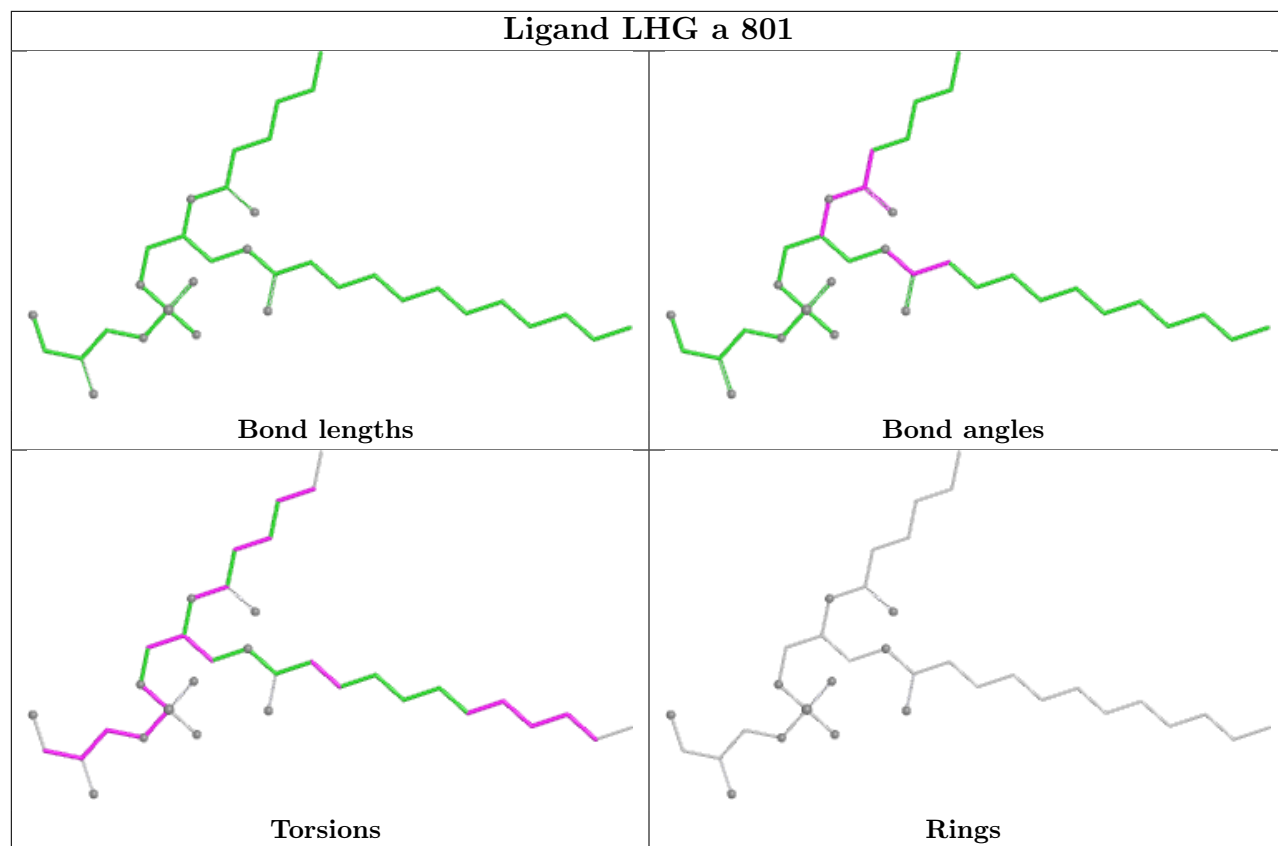


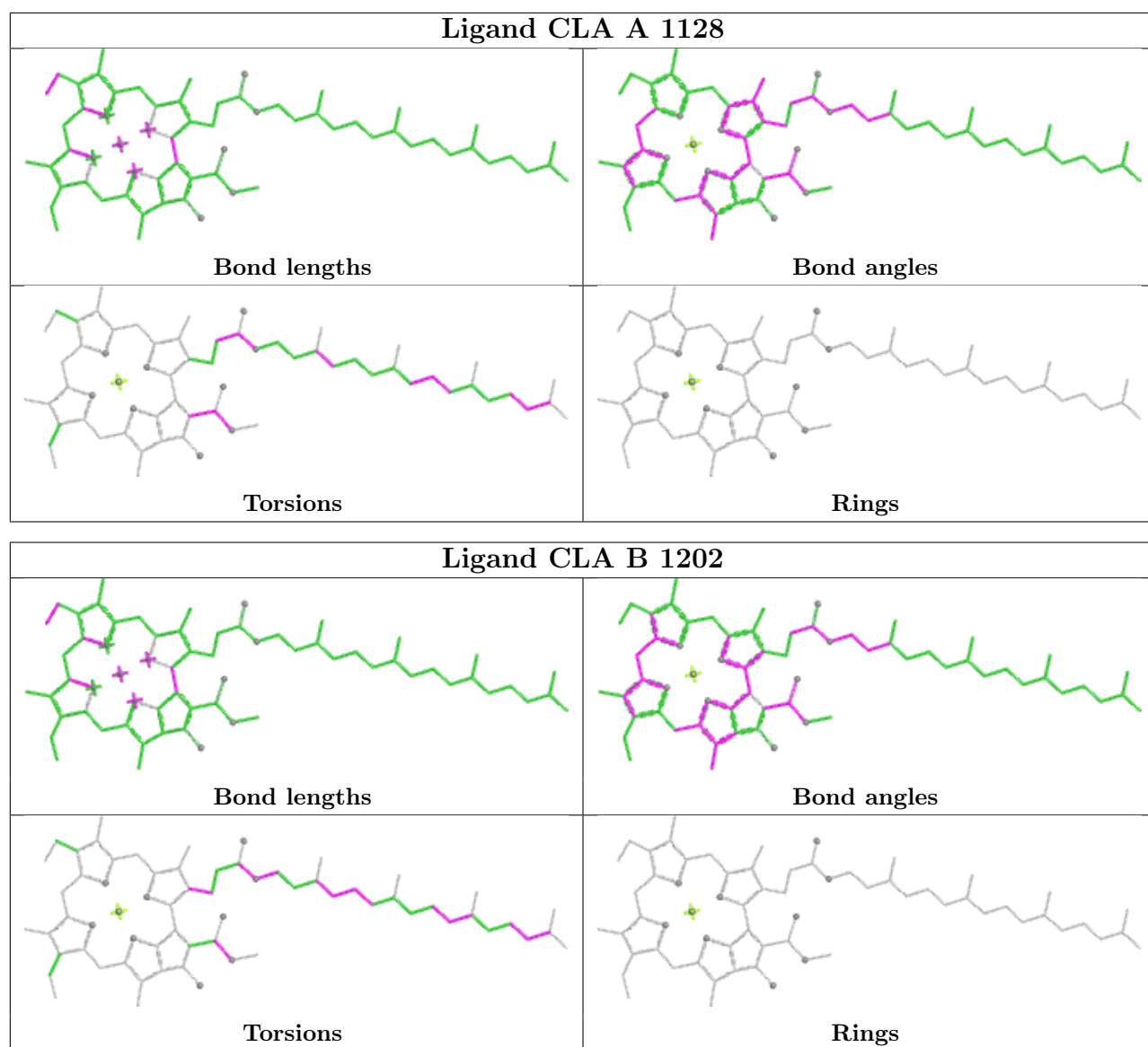
Ligand CLA 2 621



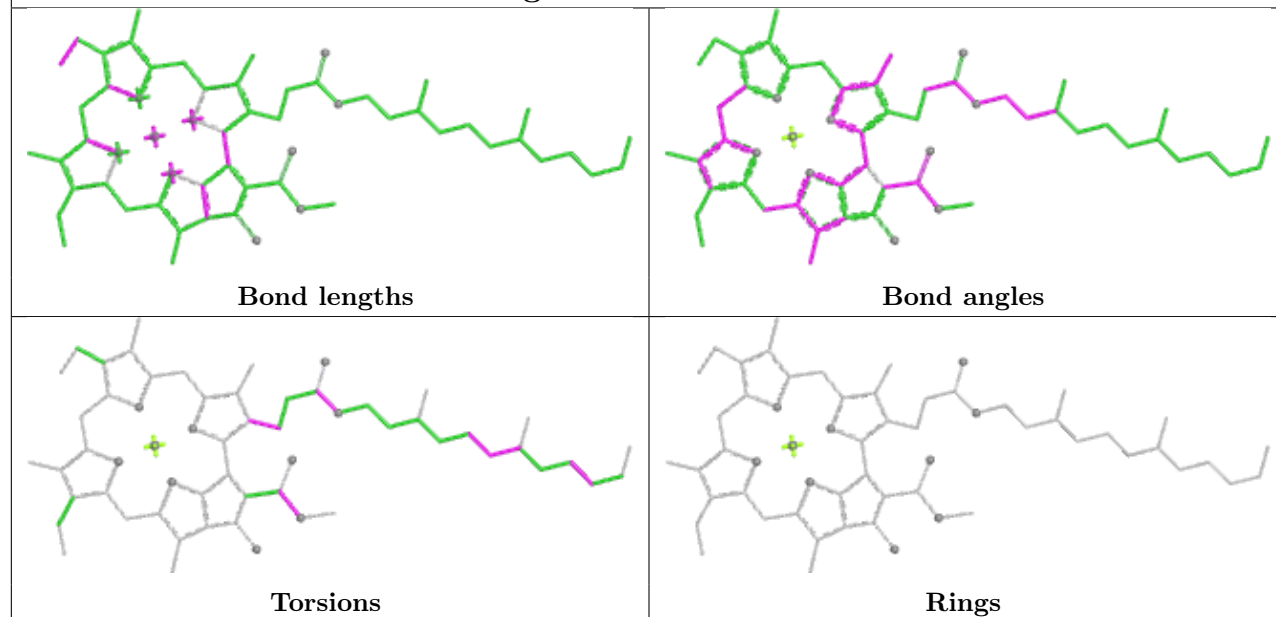
Ligand DGA 5 803



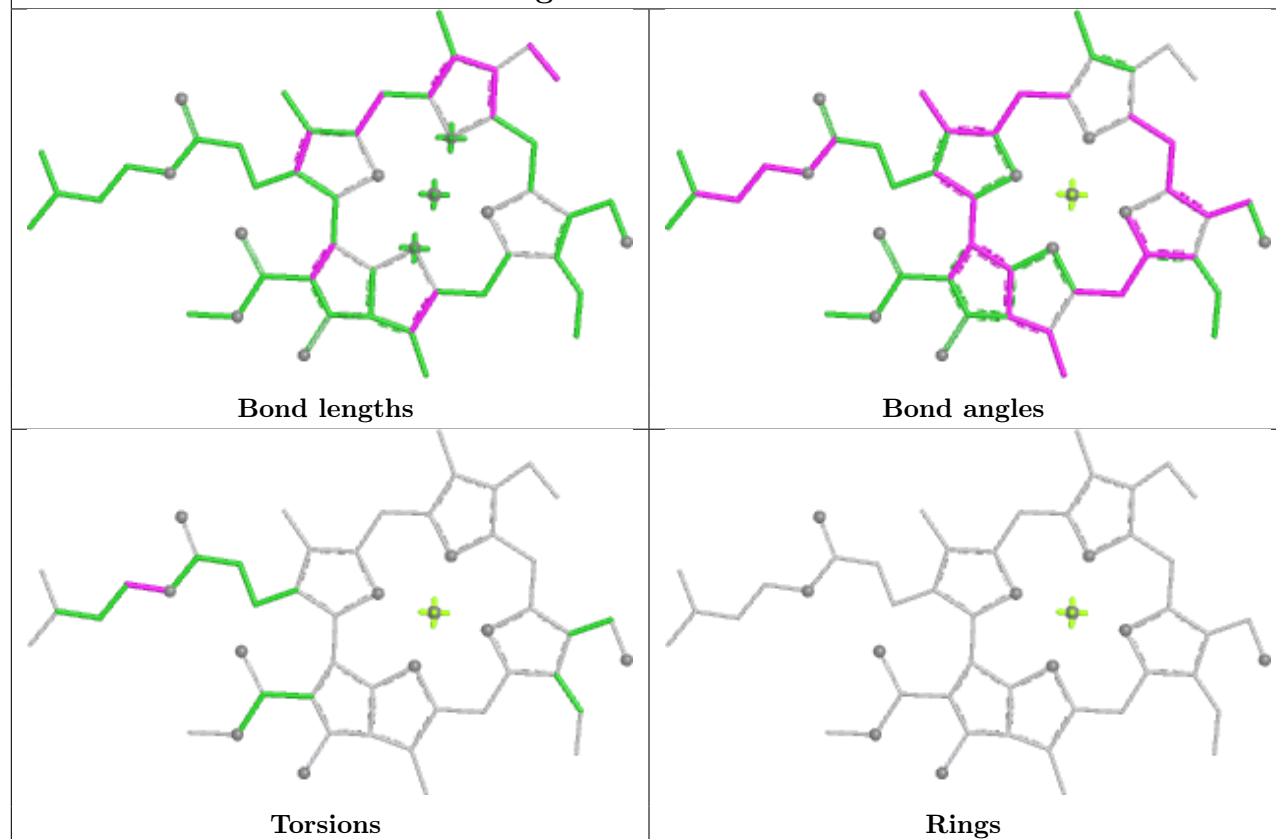


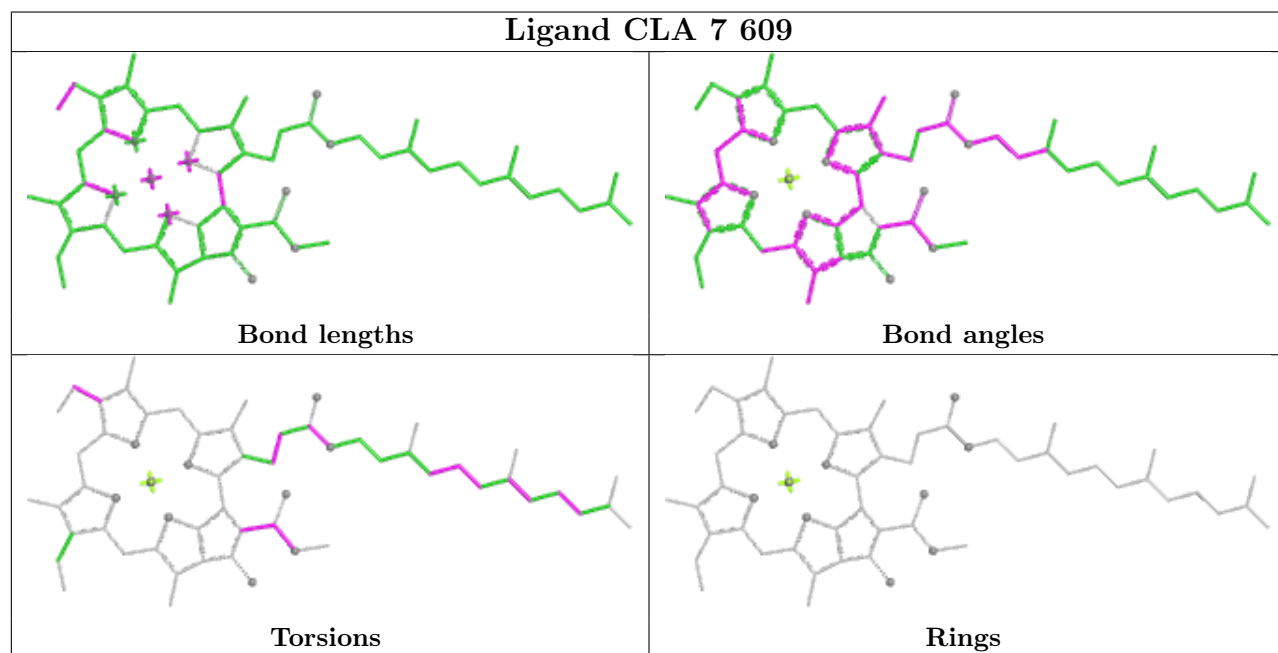
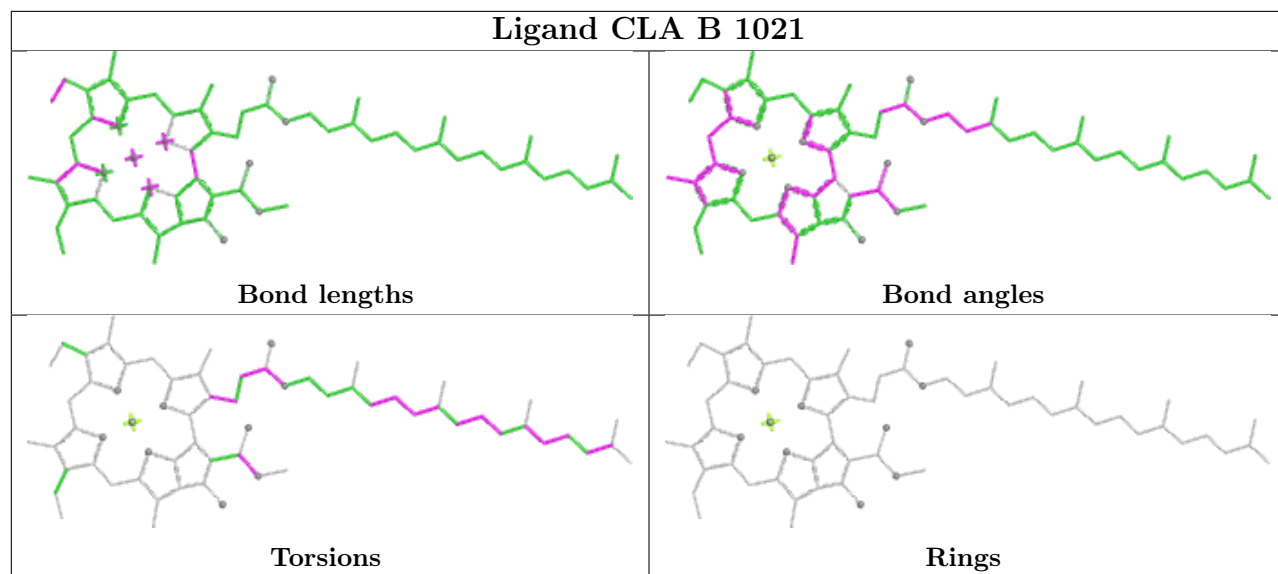


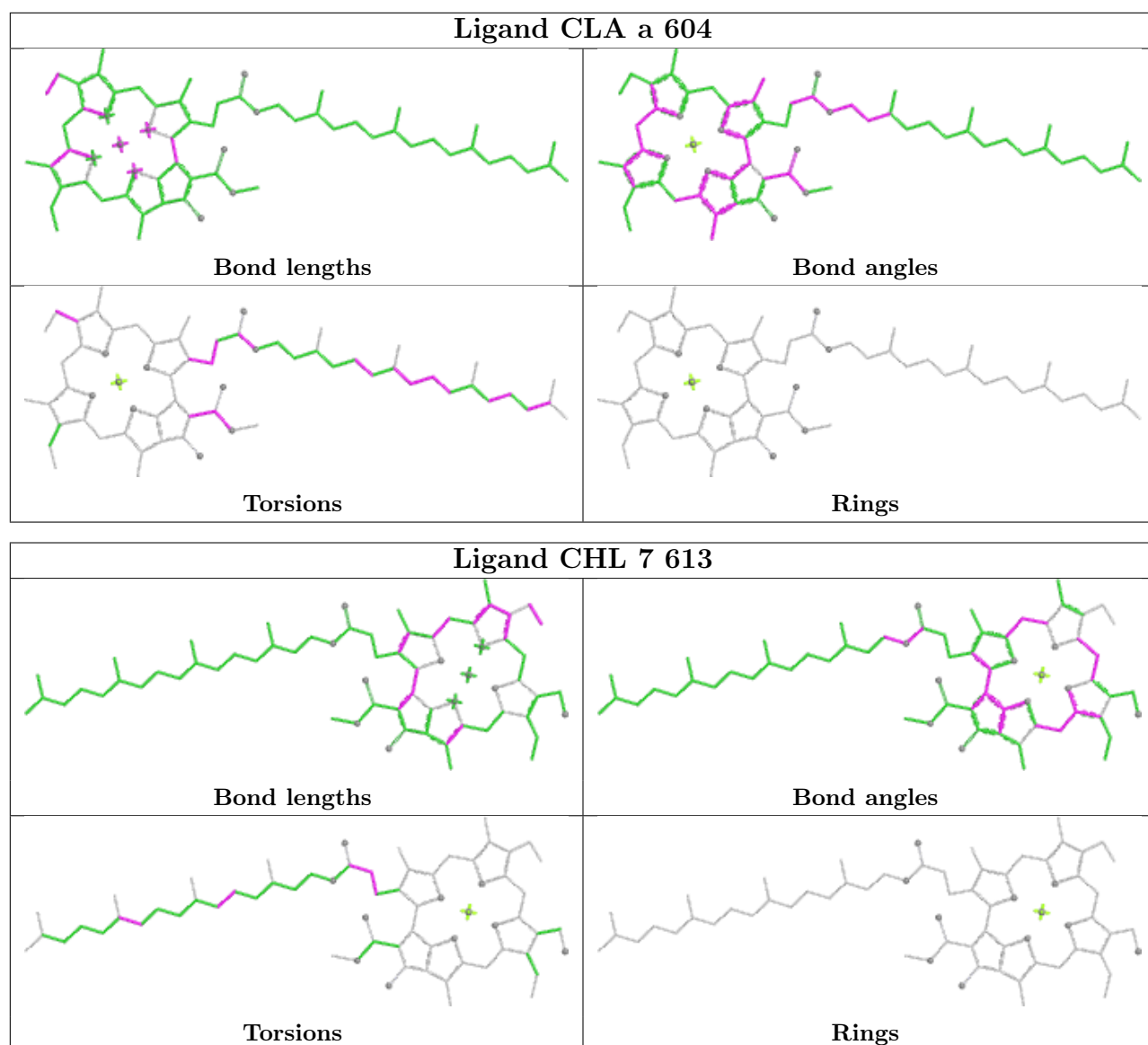
Ligand CLA B 1219



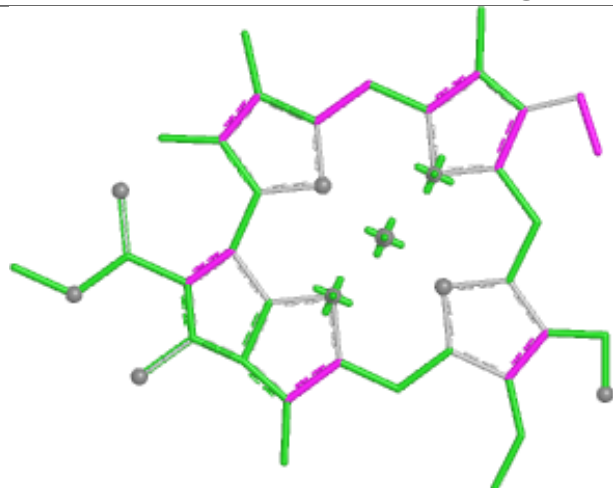
Ligand CHL 6 611



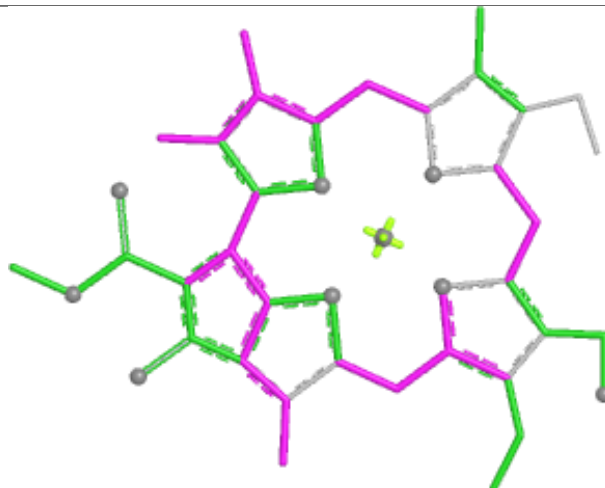




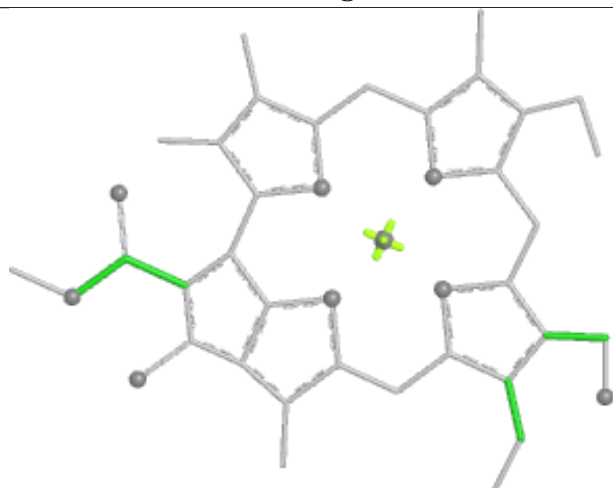
Ligand CHL 9 613



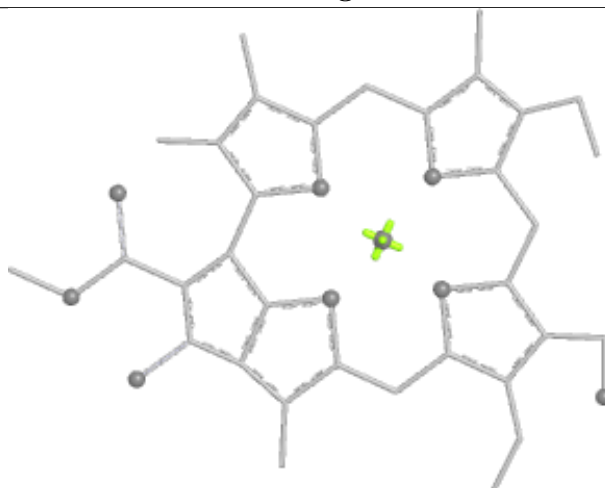
Bond lengths



Bond angles

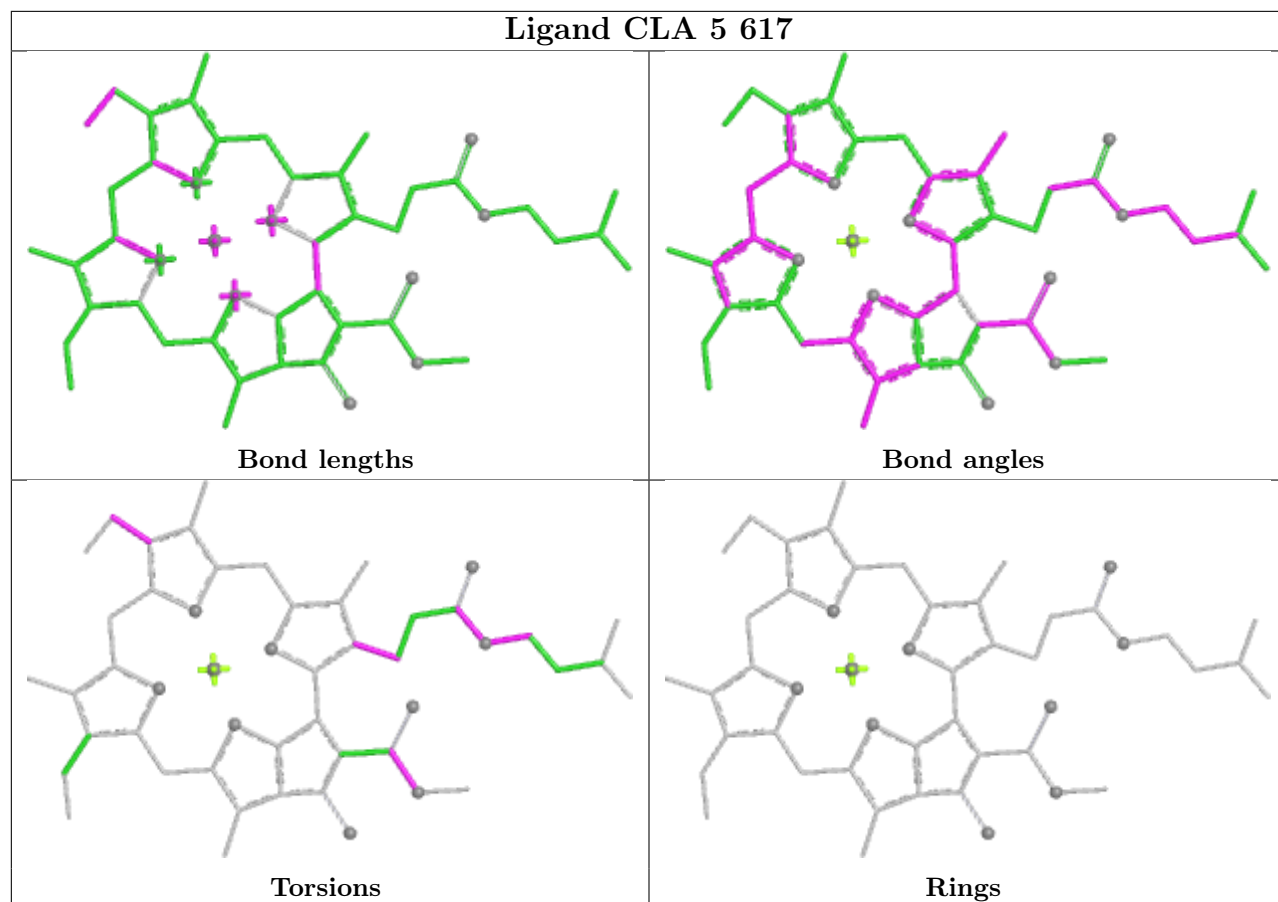


Torsions

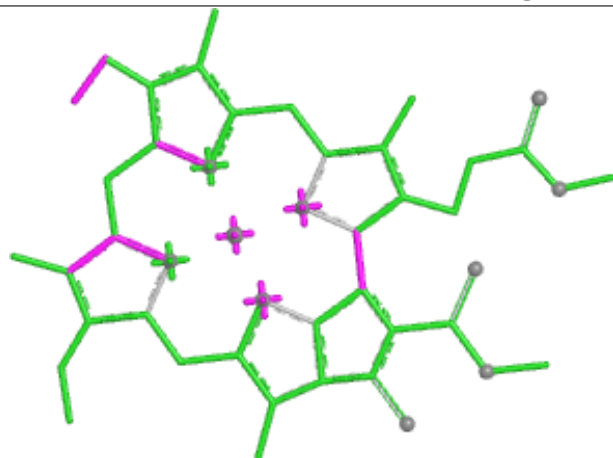


Rings

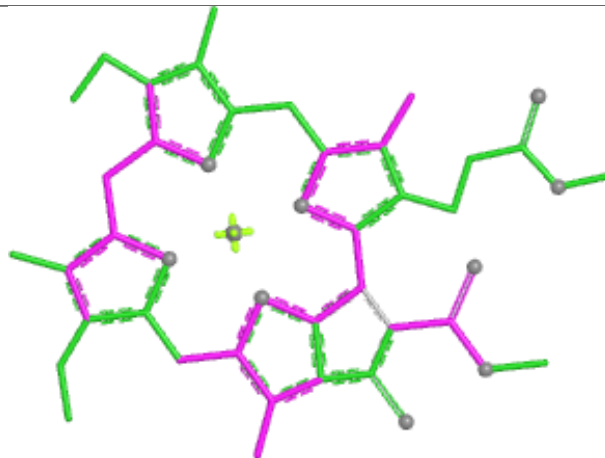
Ligand CLA 5 617



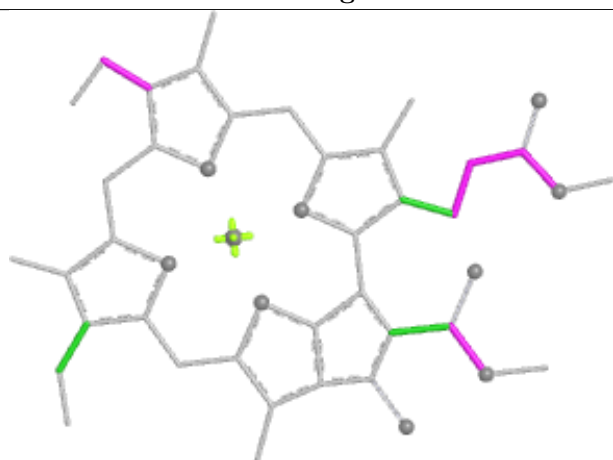
Ligand CLA 9 609



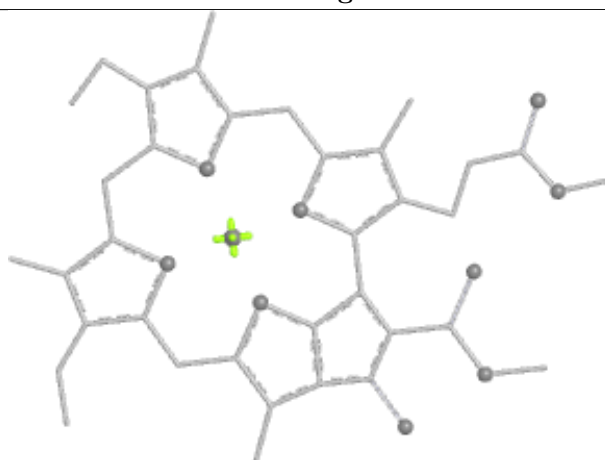
Bond lengths



Bond angles

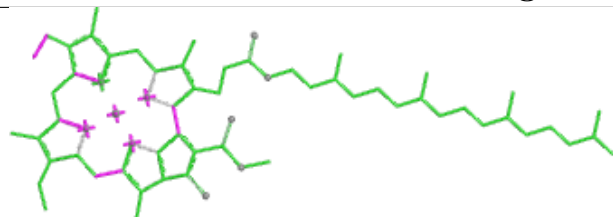


Torsions

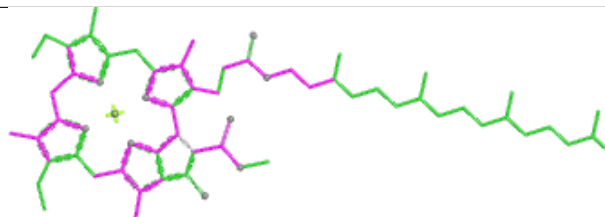


Rings

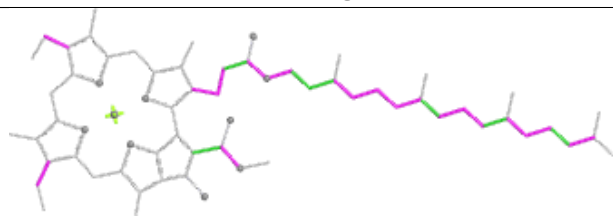
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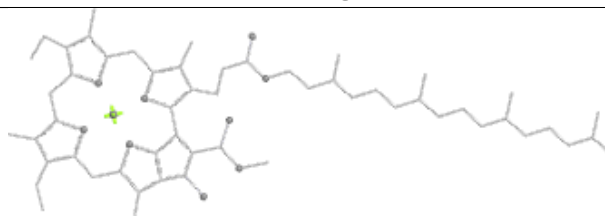
Bond lengths



Bond angles

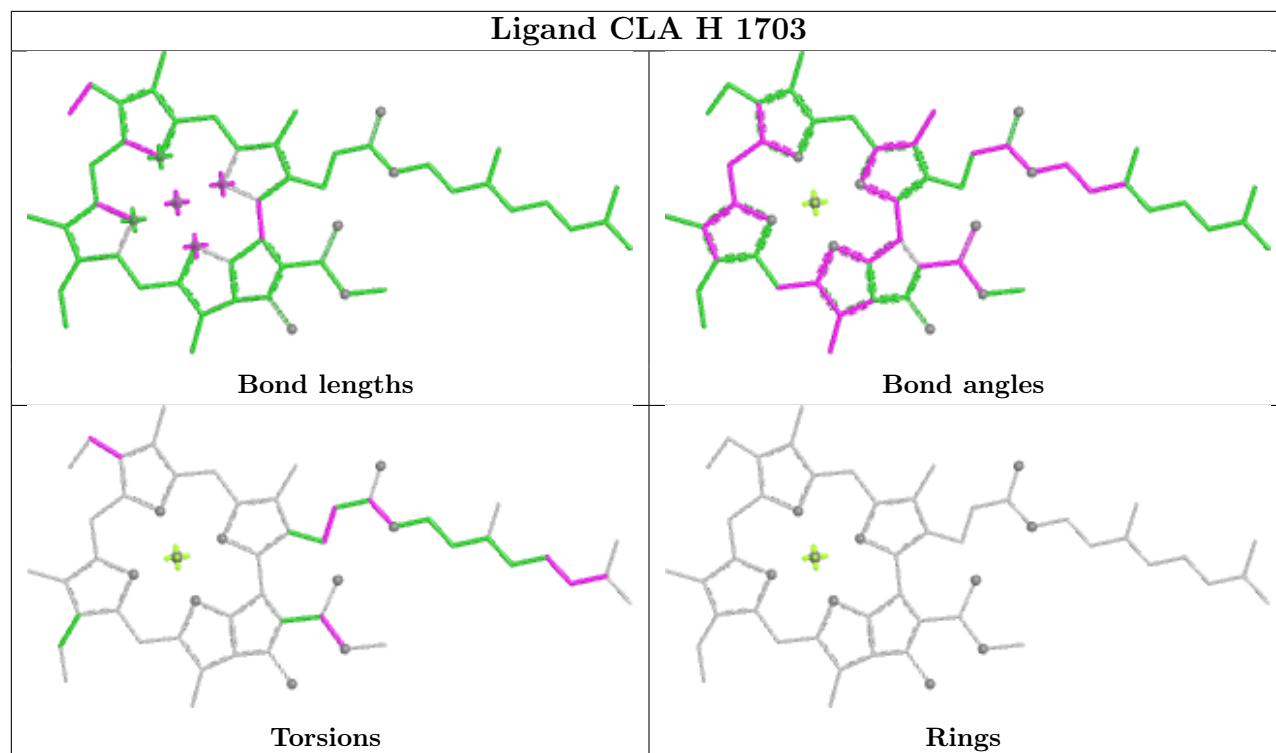


Torsions

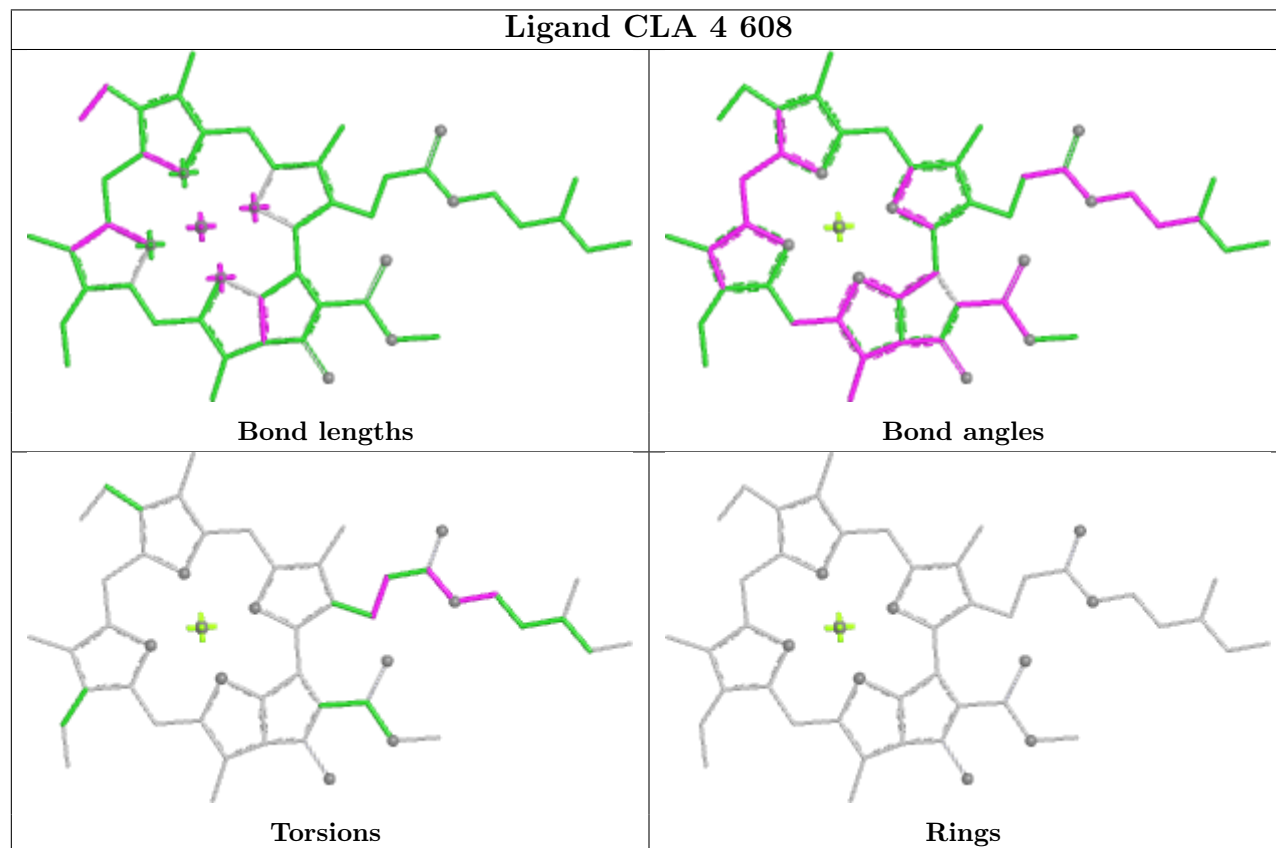


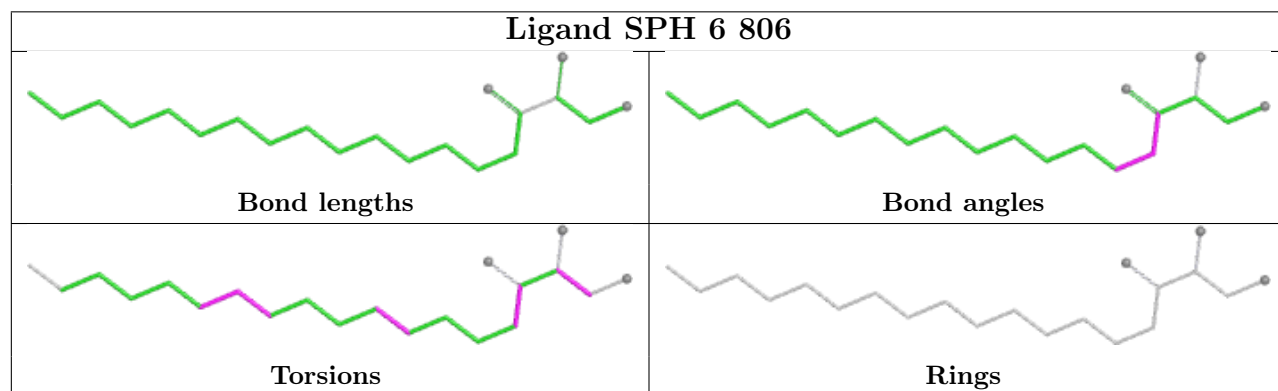
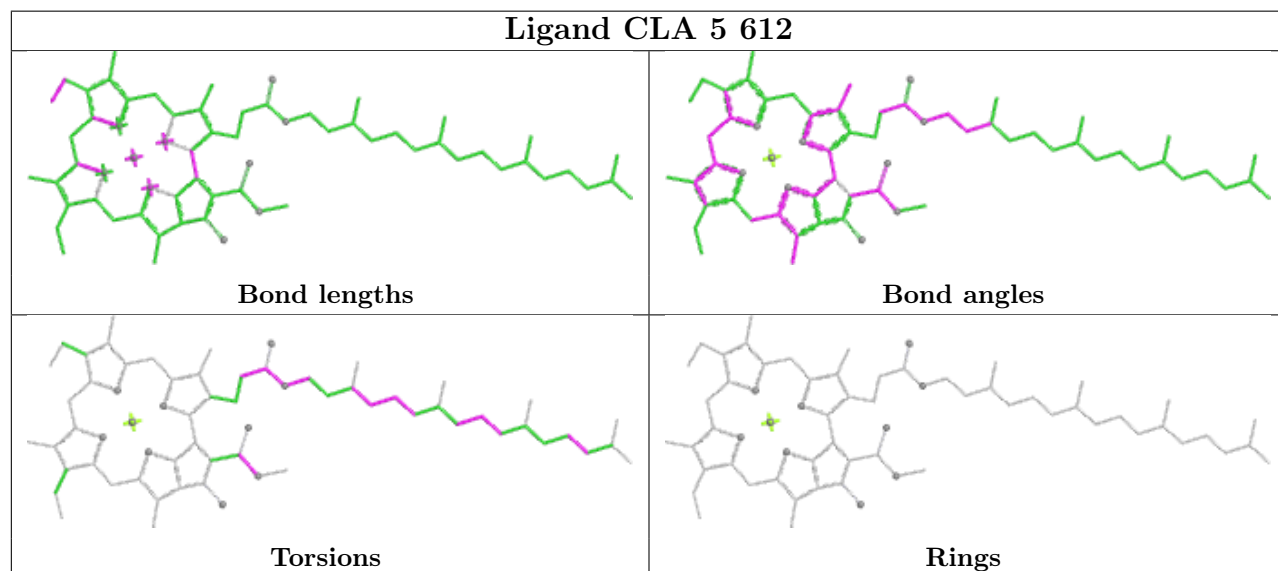
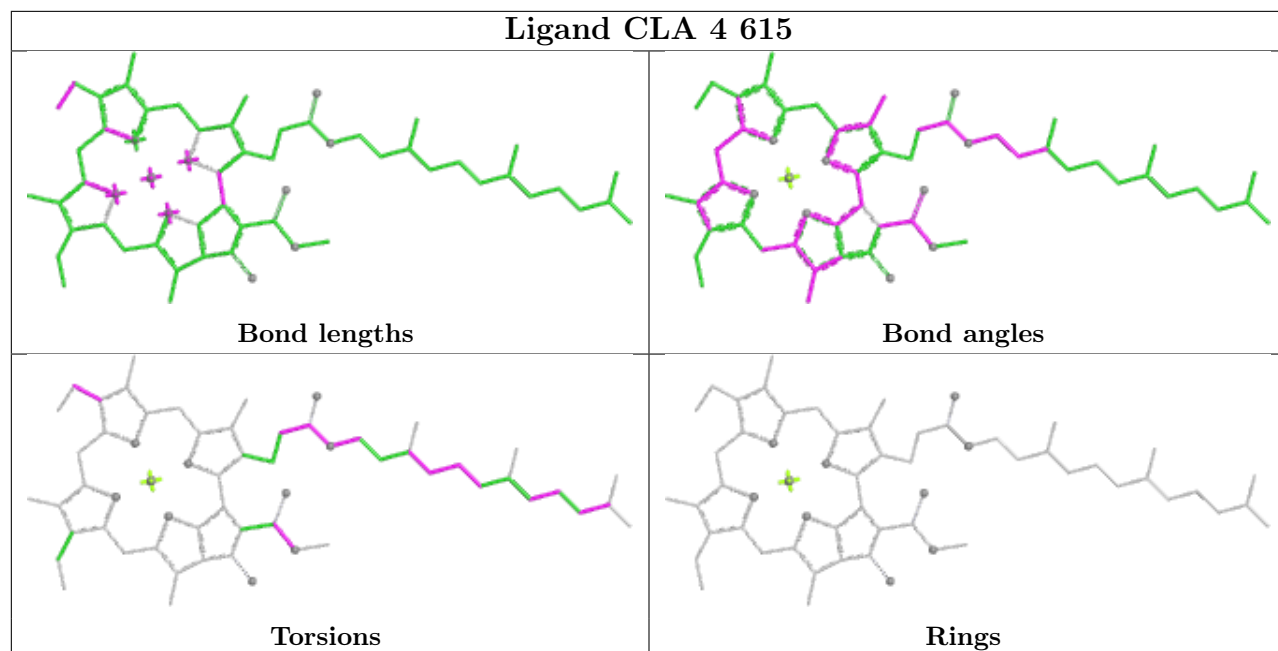
Rings

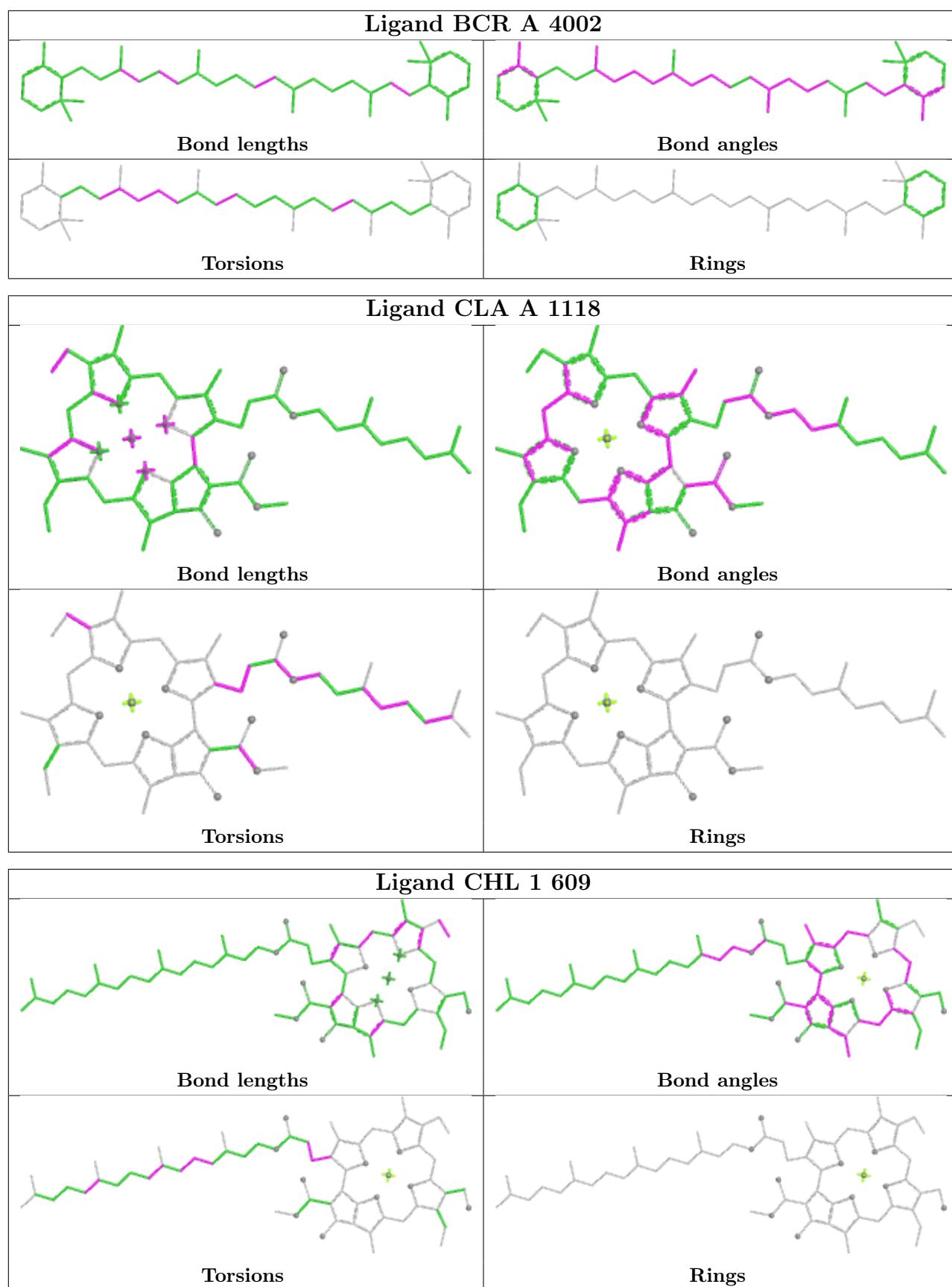
Ligand CLA H 1703

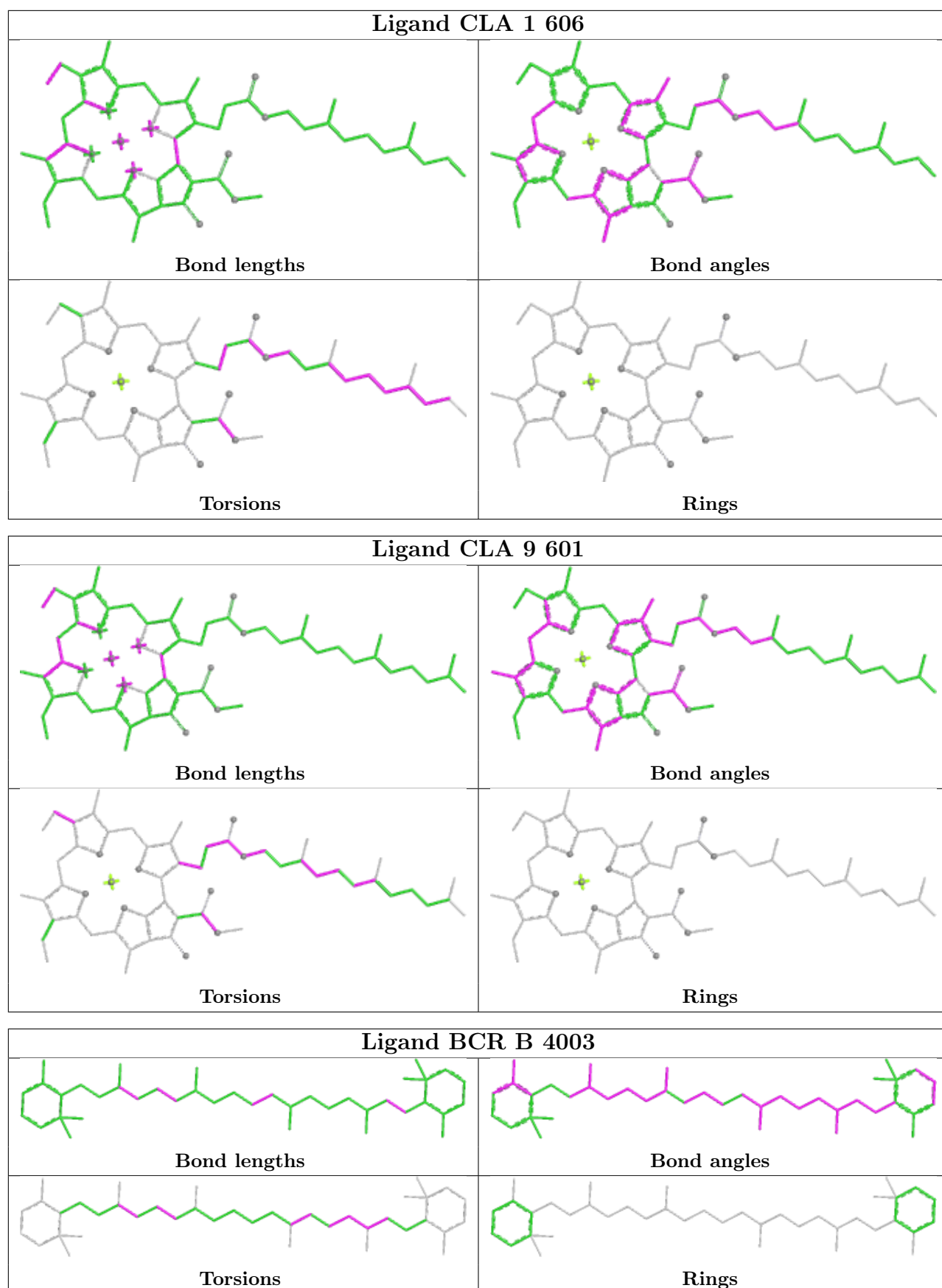


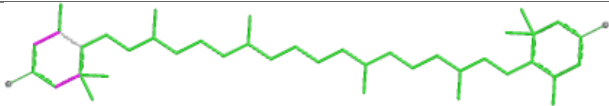
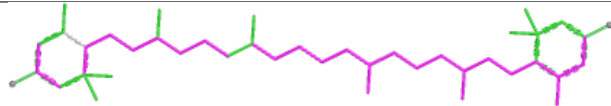
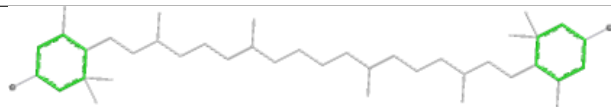
Ligand CLA 4 608

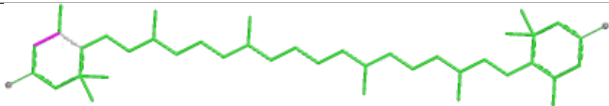
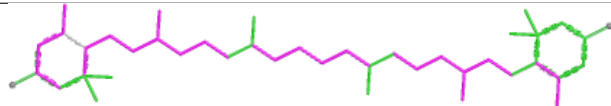
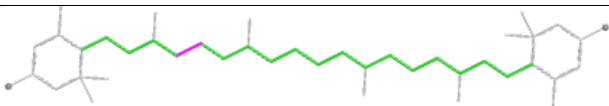
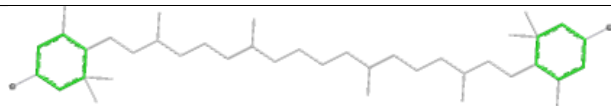


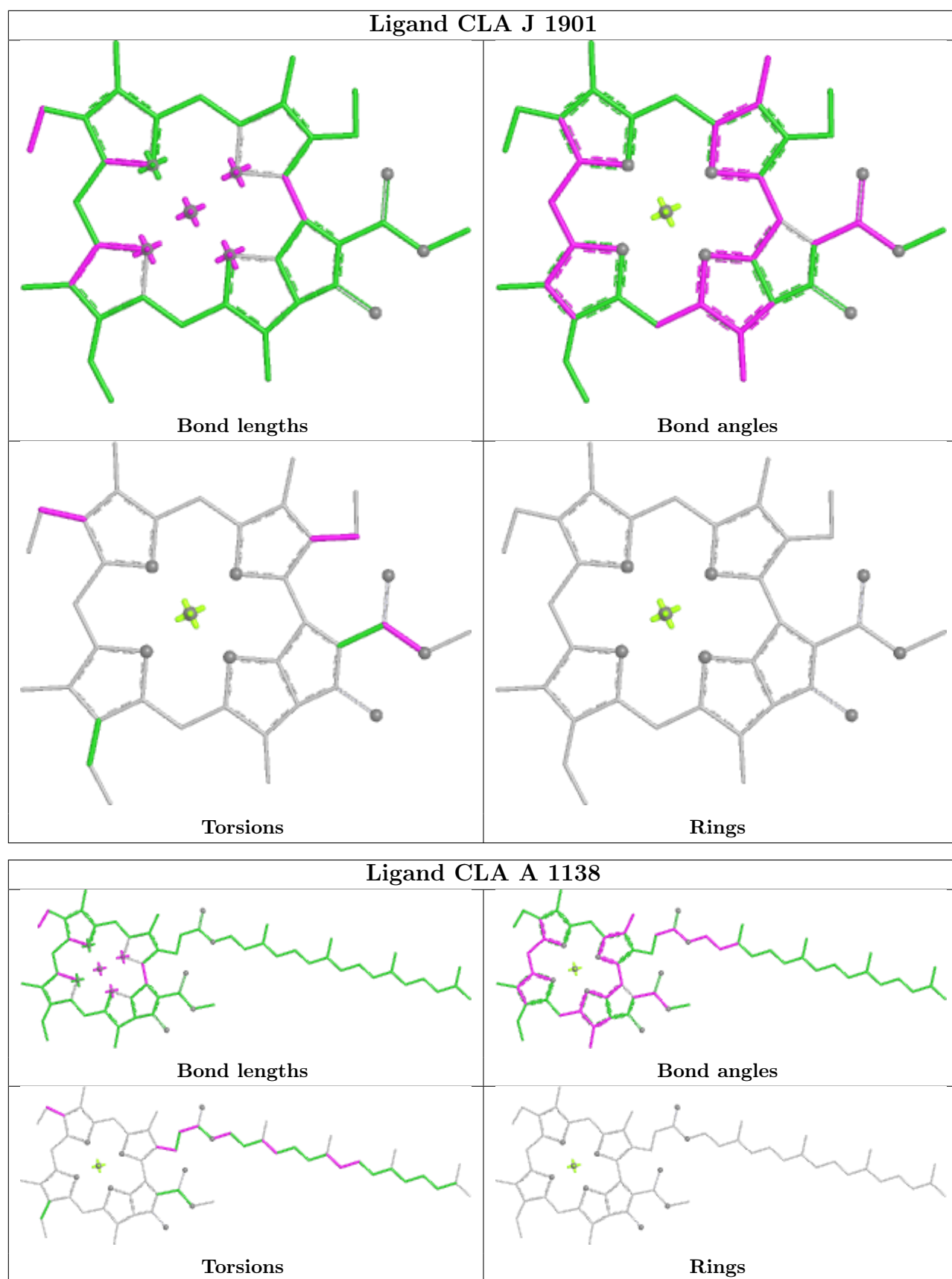


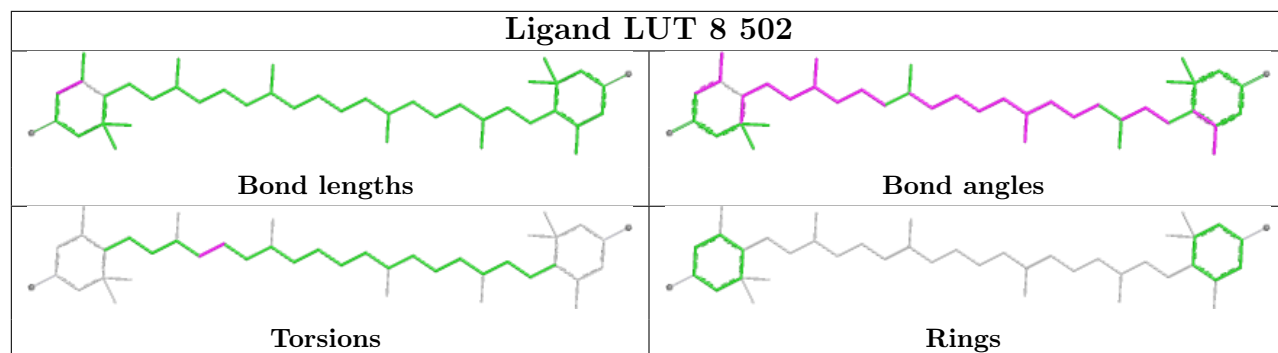
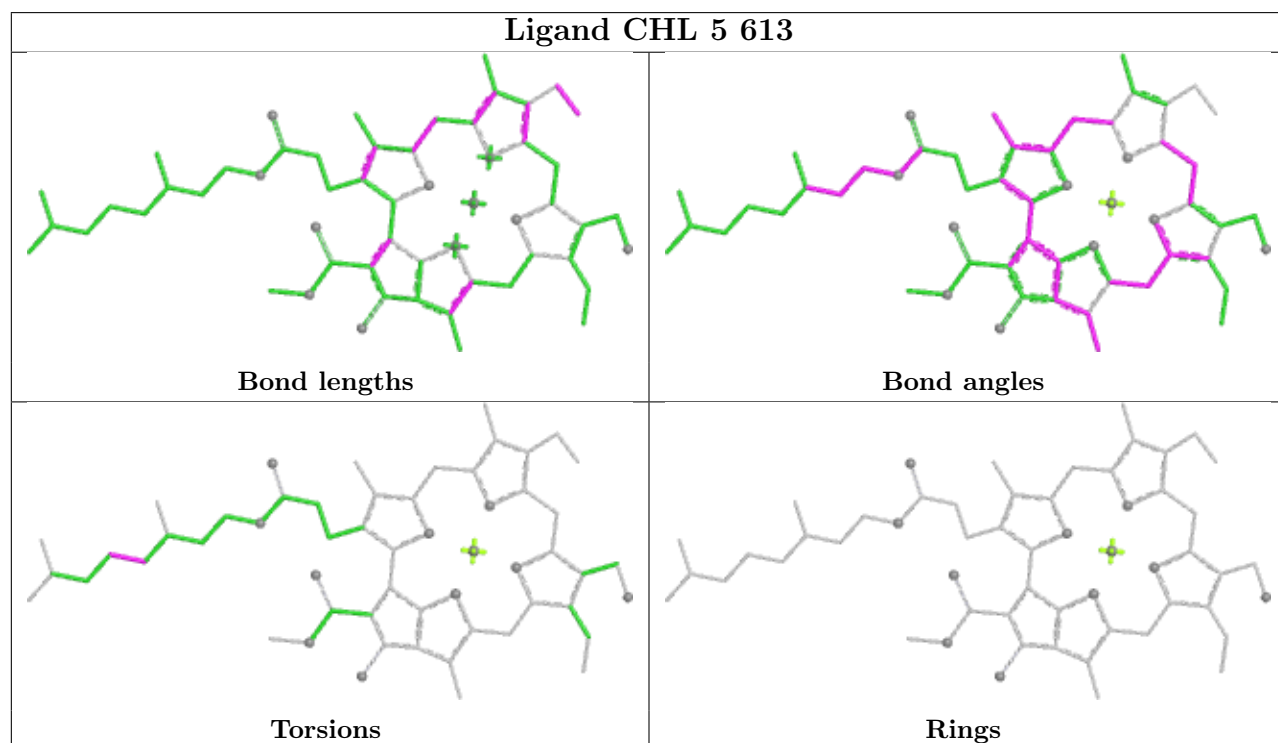
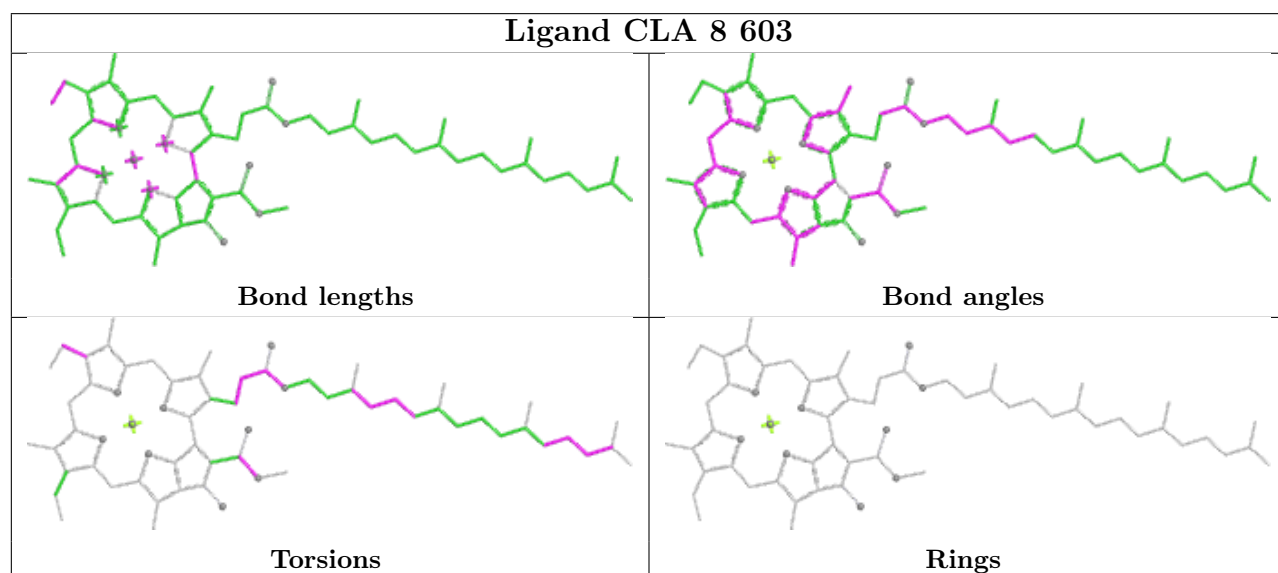


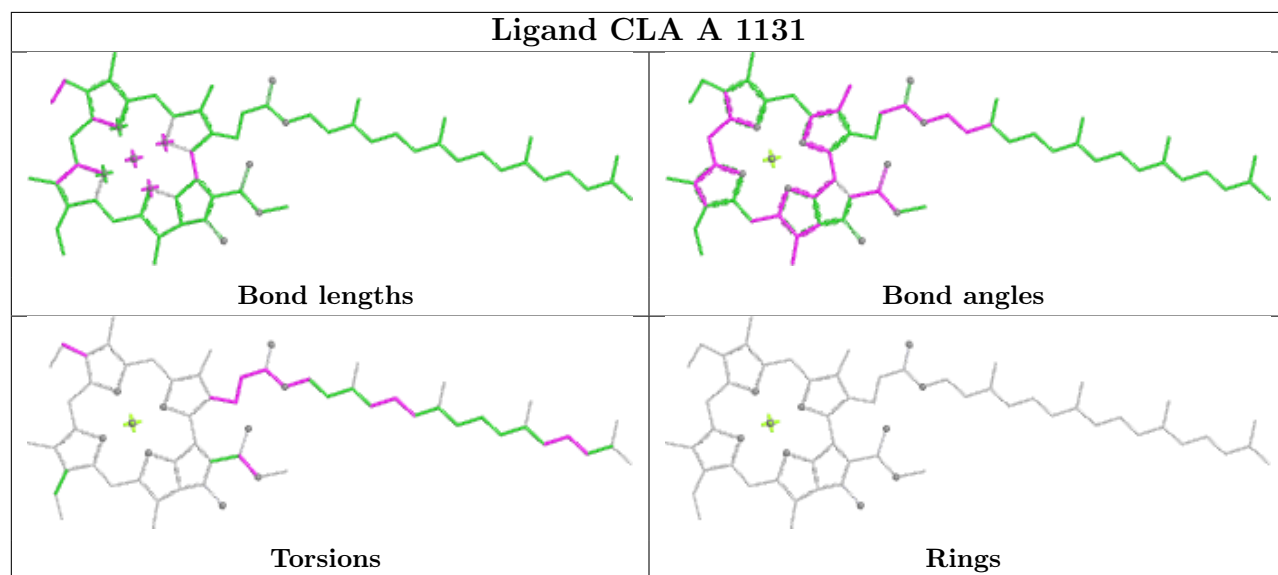
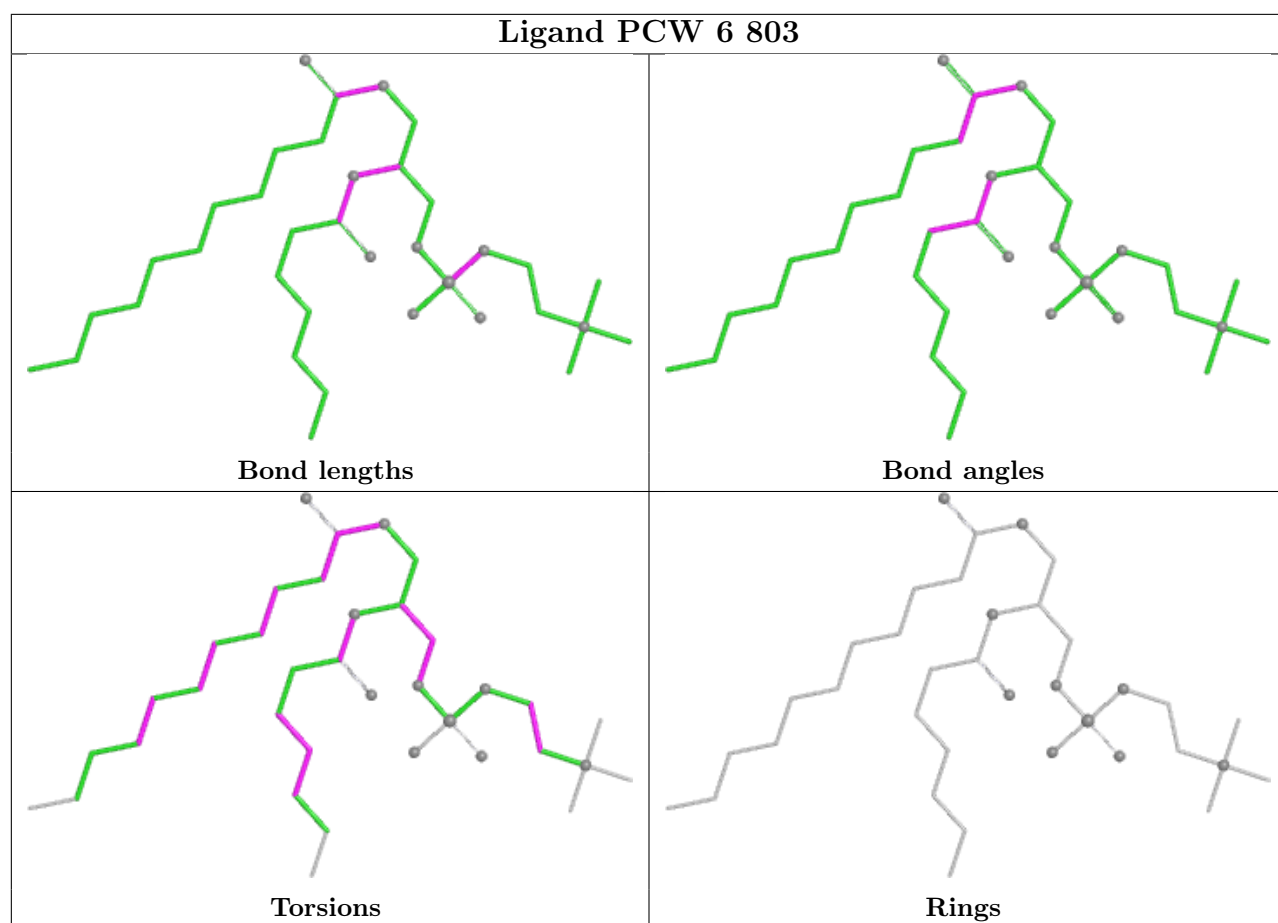


Ligand LUT 5 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

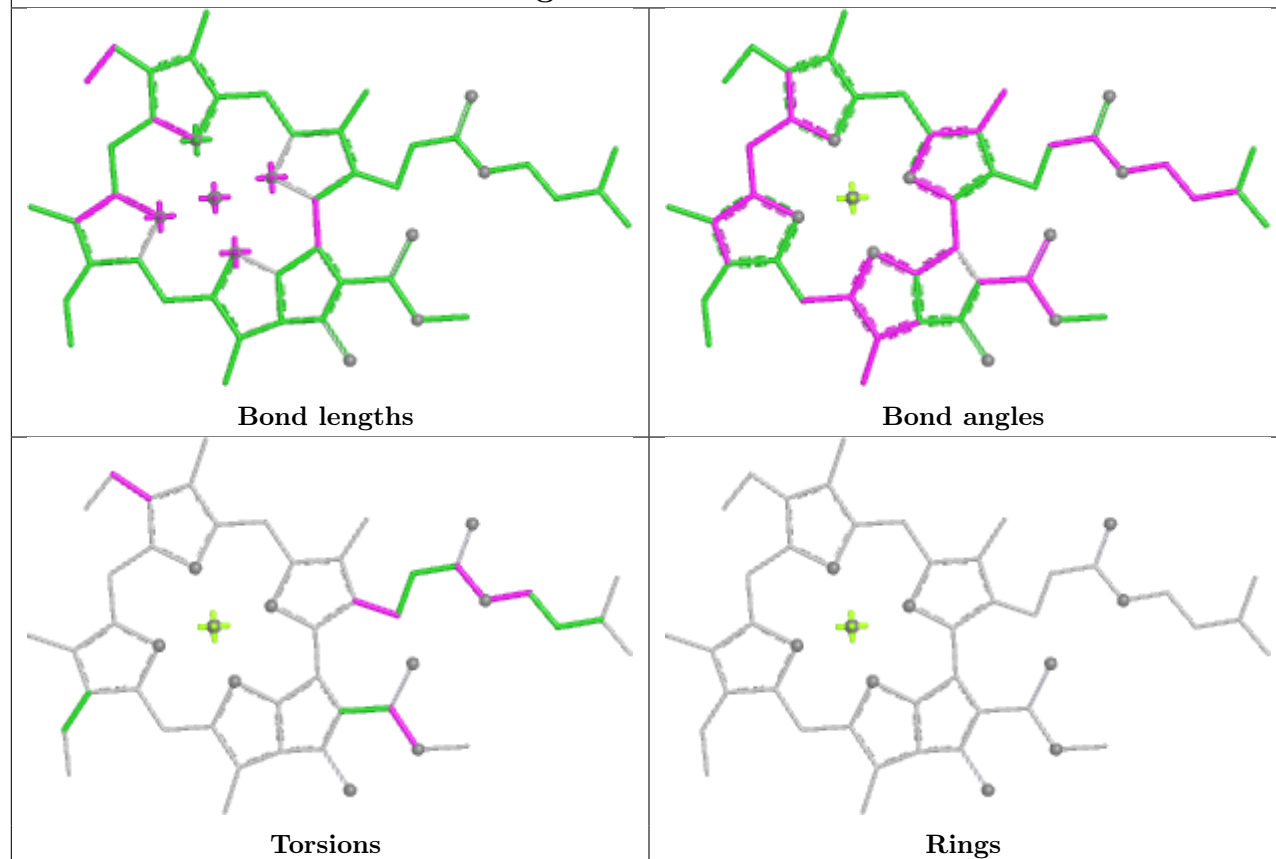
Ligand LUT 3 502	
	
Bond lengths	Bond angles
	
Torsions	Rings



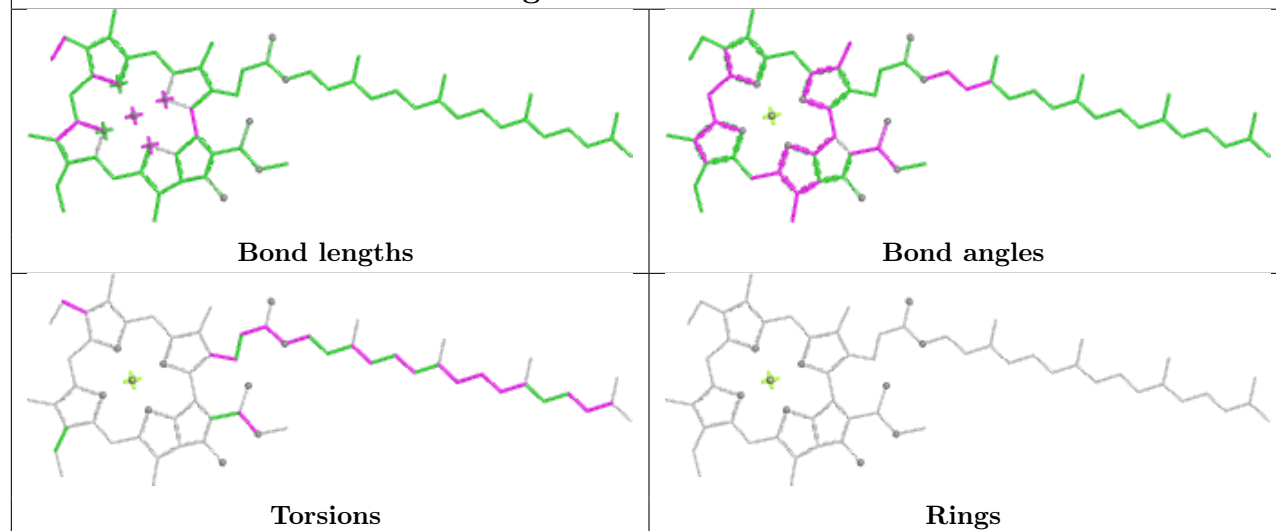
Ligand LUT 8 502**Ligand CHL 5 613****Ligand CLA 8 603**

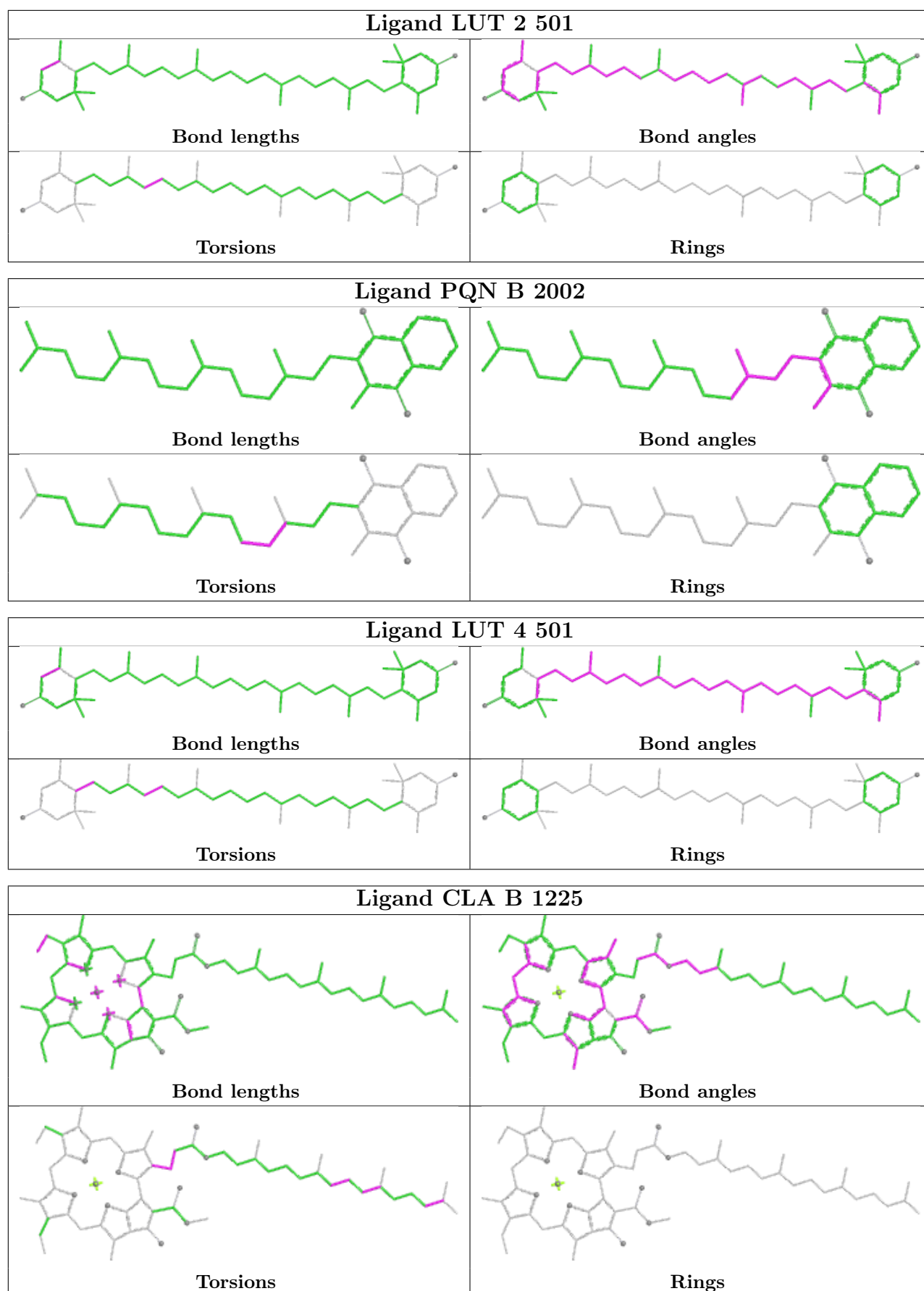


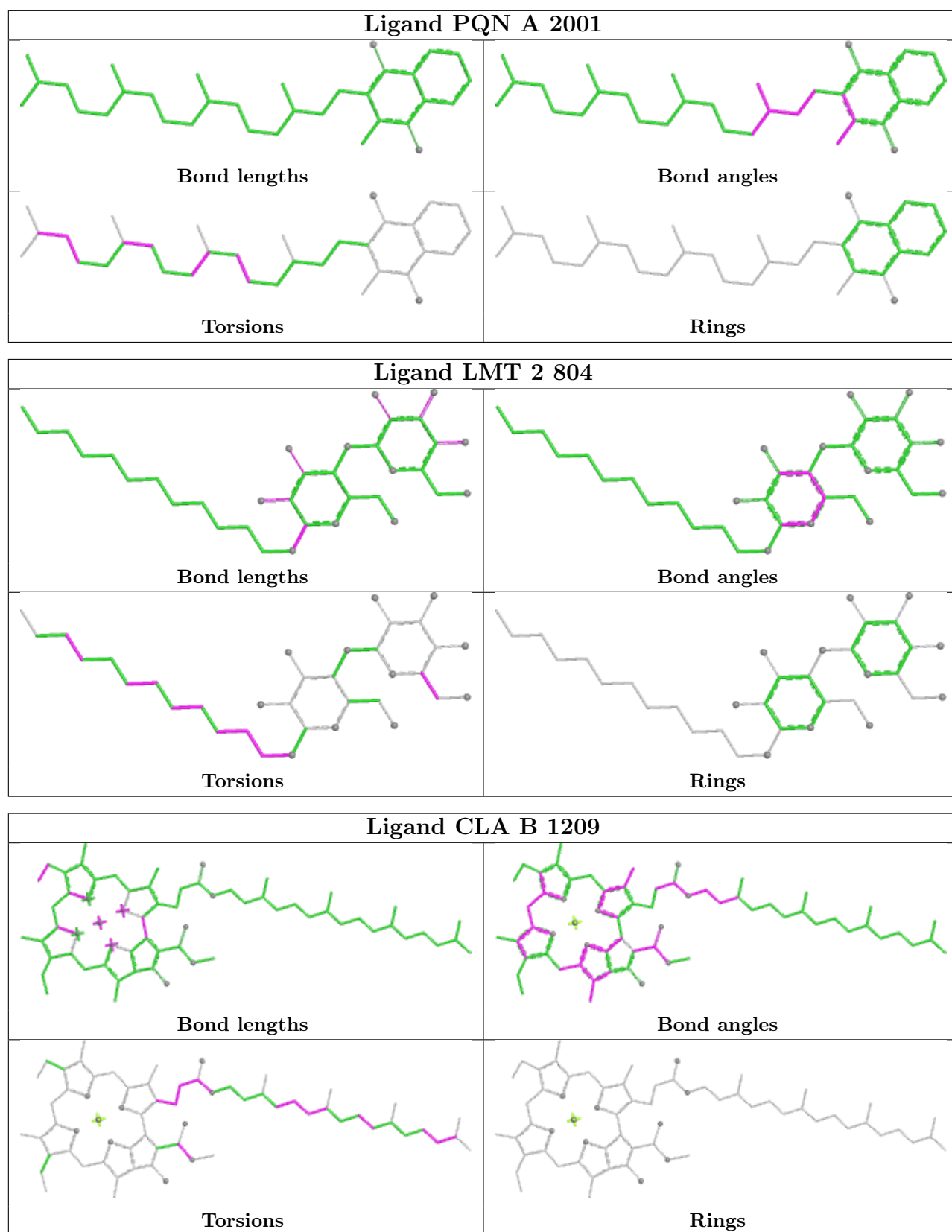
Ligand CLA 4 616

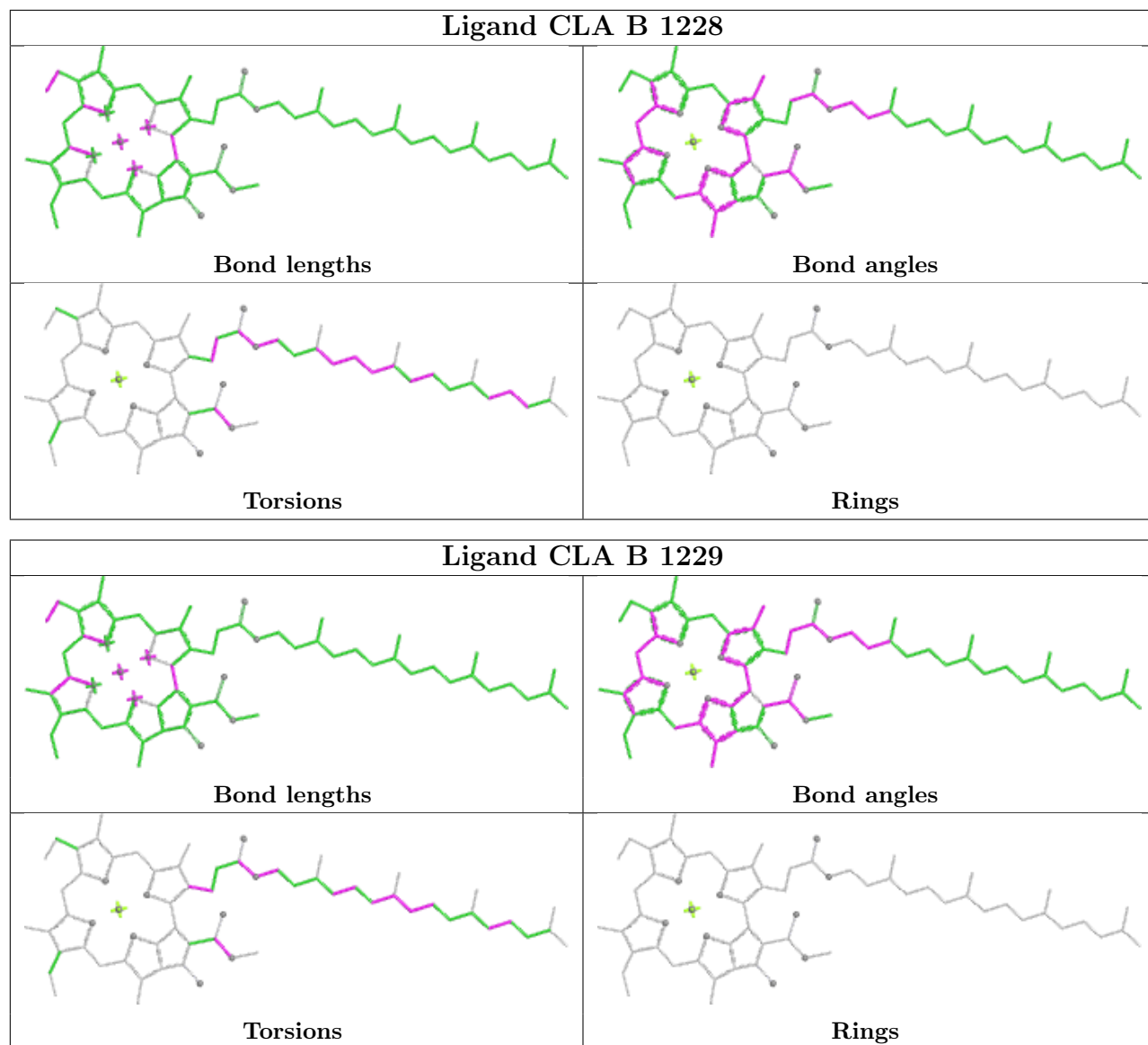


Ligand CLA A 1126

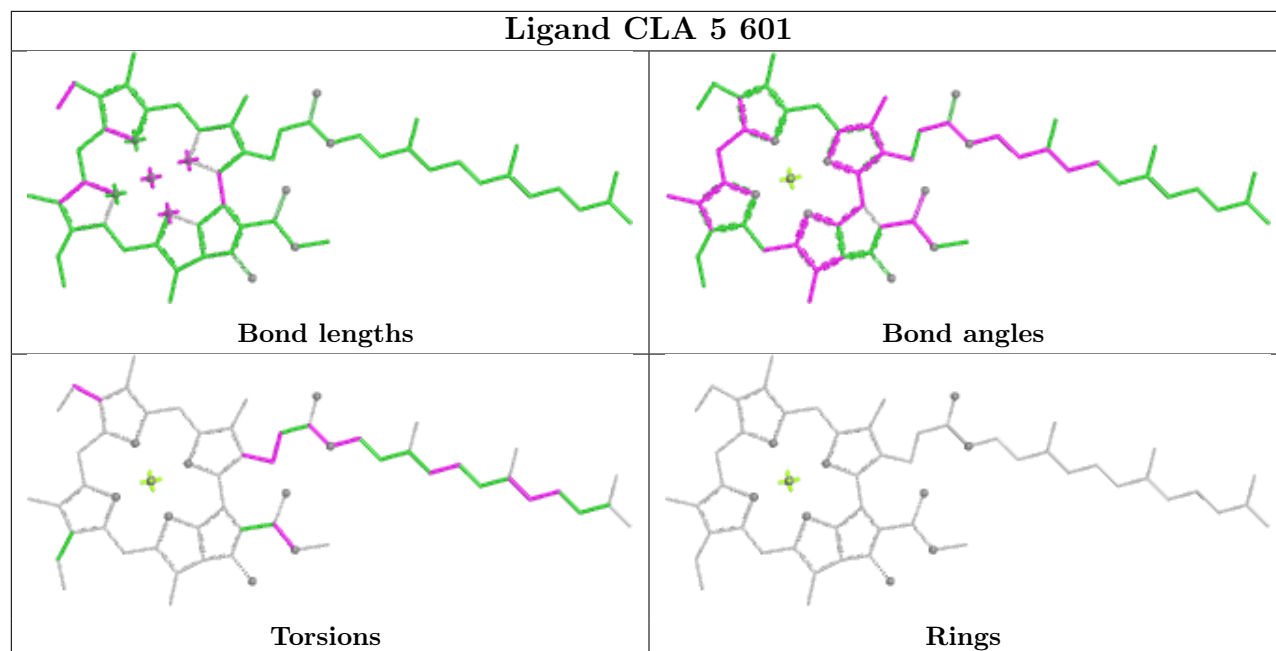




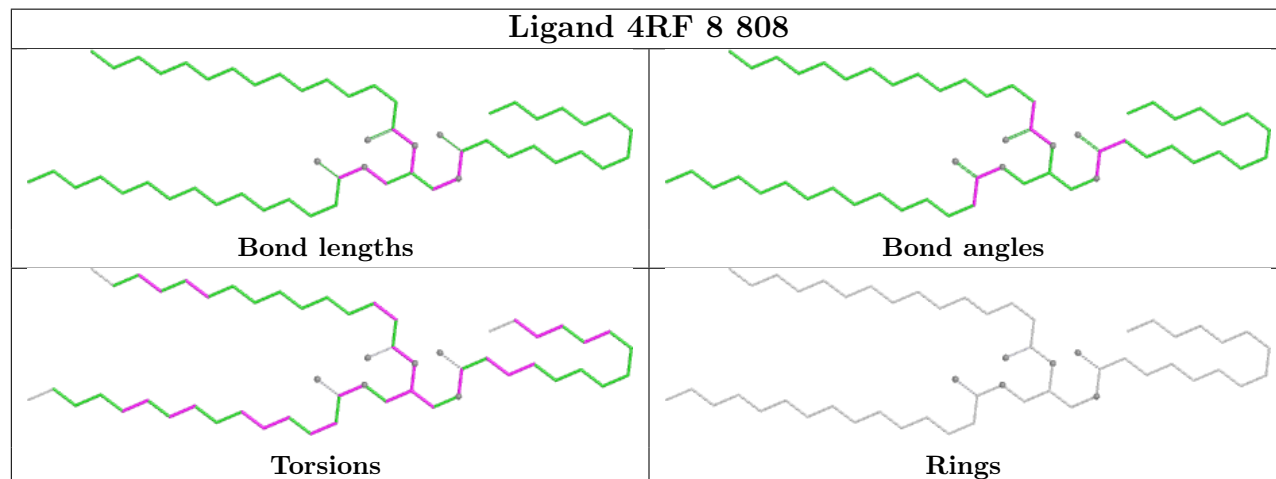




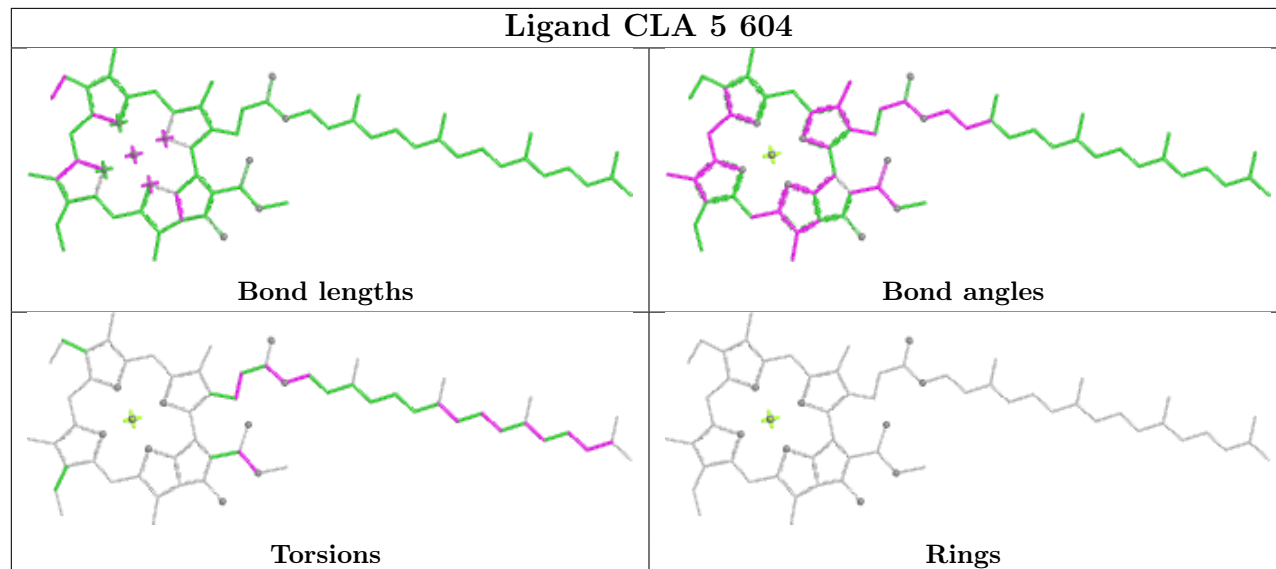
Ligand CLA 5 601

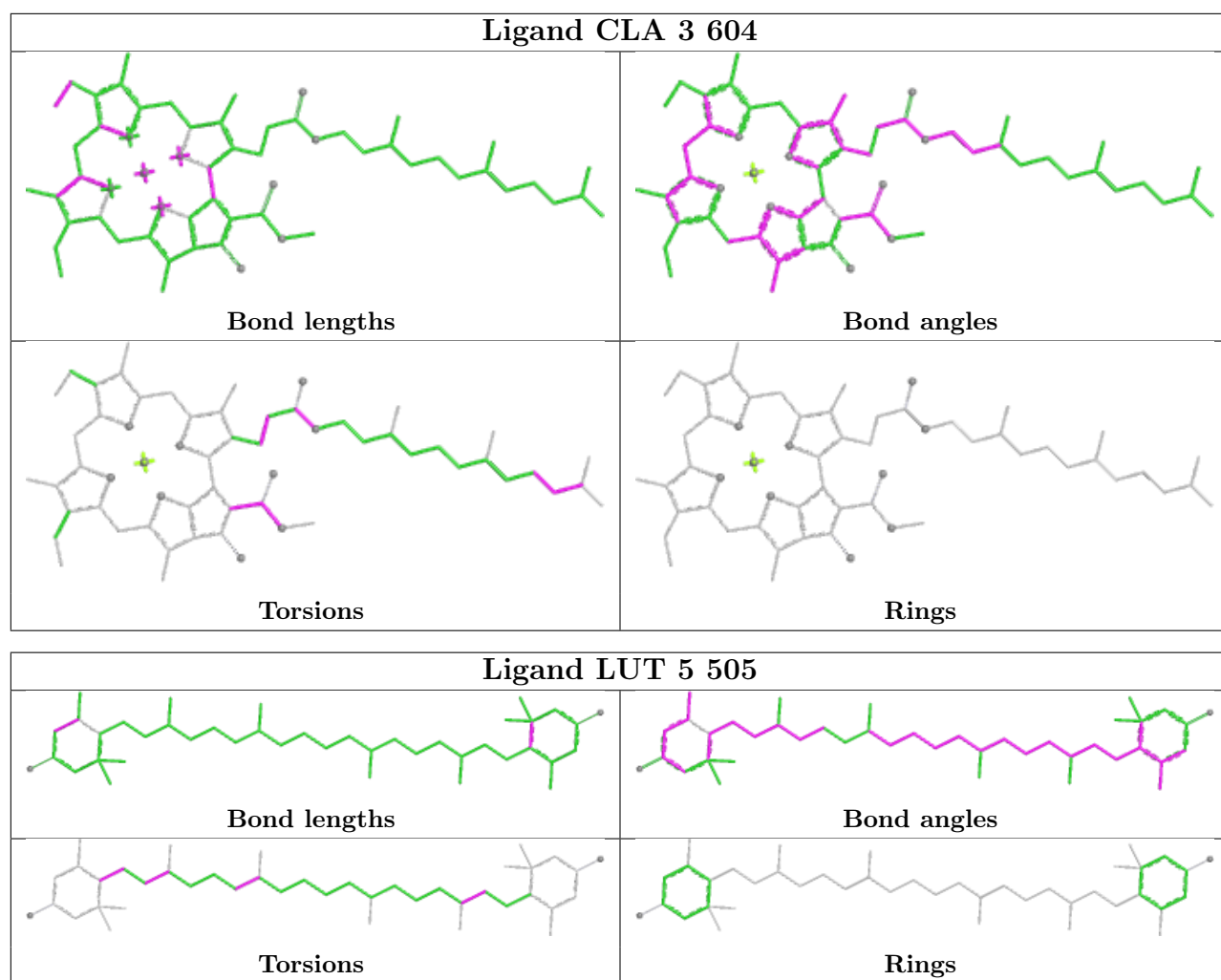


Ligand 4RF 8 808

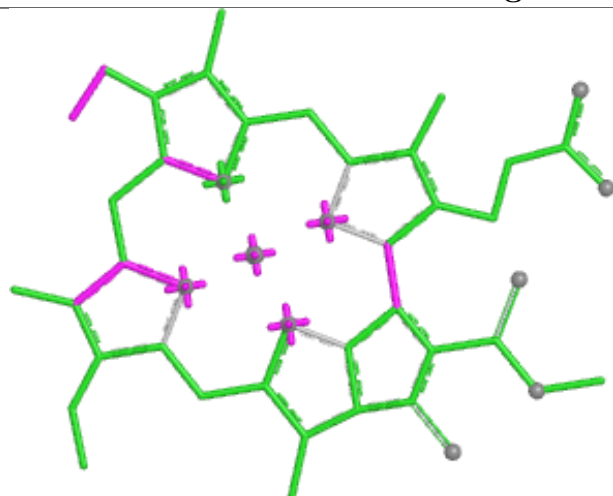


Ligand CLA 5 604

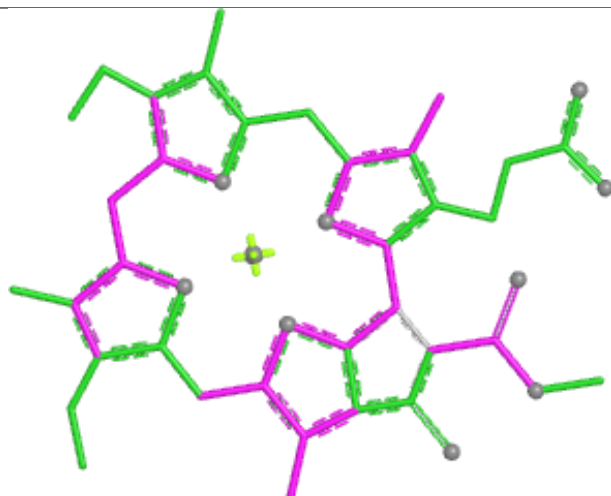




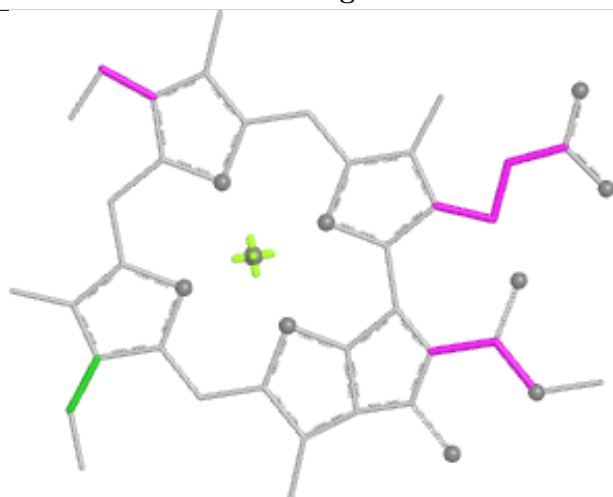
Ligand CLA A 1141



Bond lengths



Bond angles

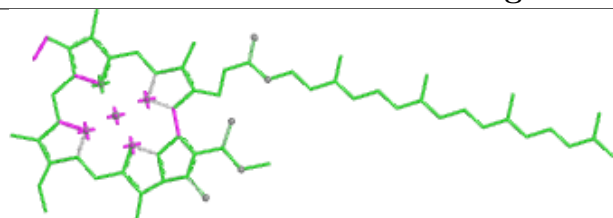


Torsions

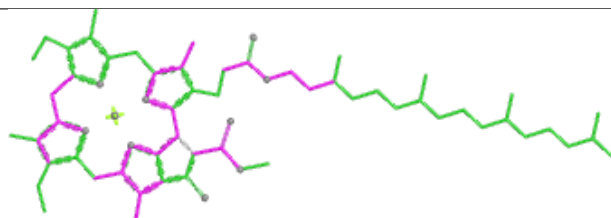


Rings

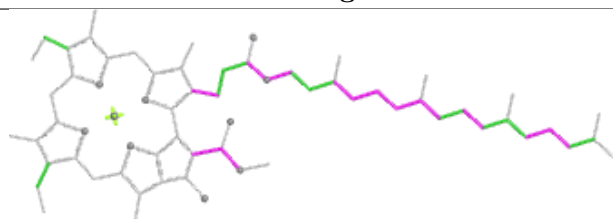
Ligand CLA A 1123



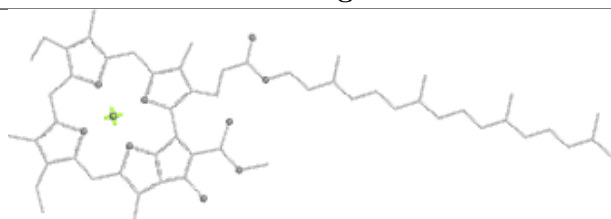
Bond lengths



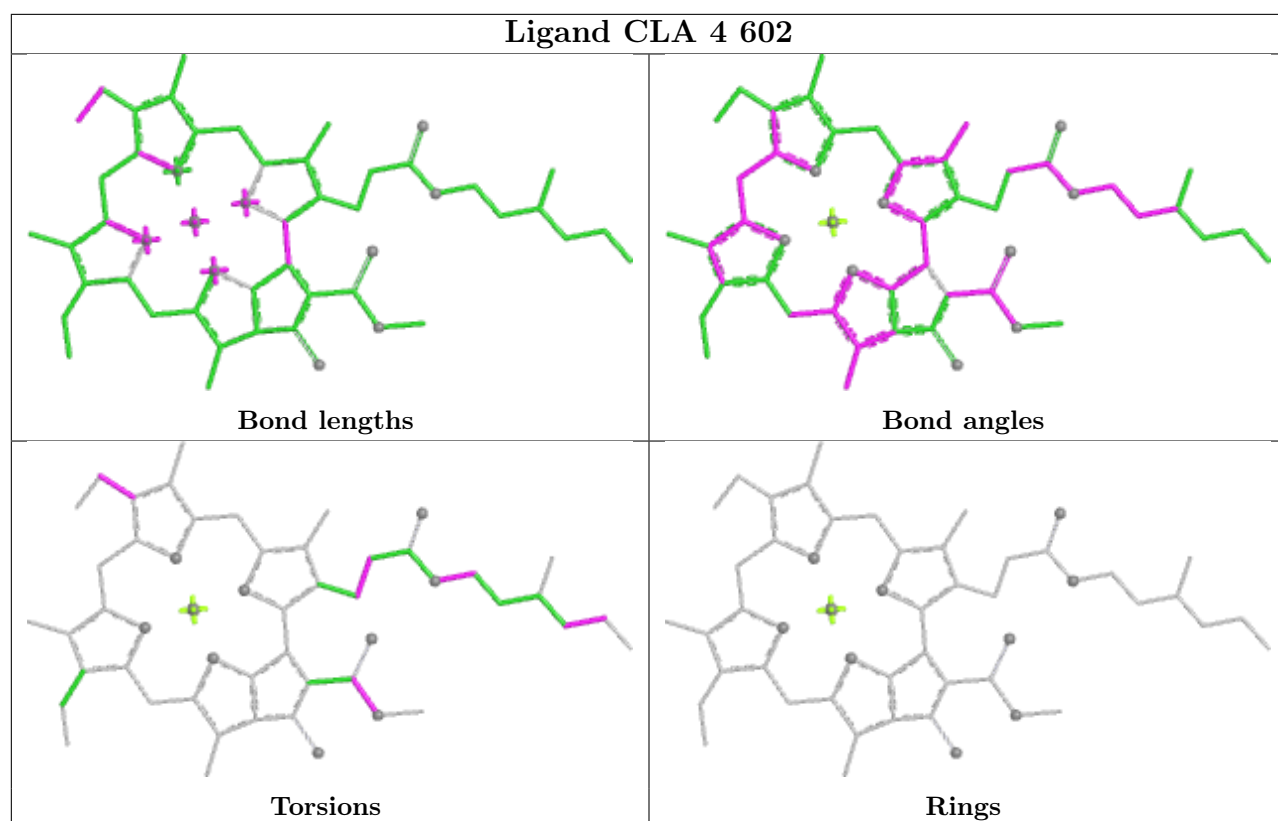
Bond angles



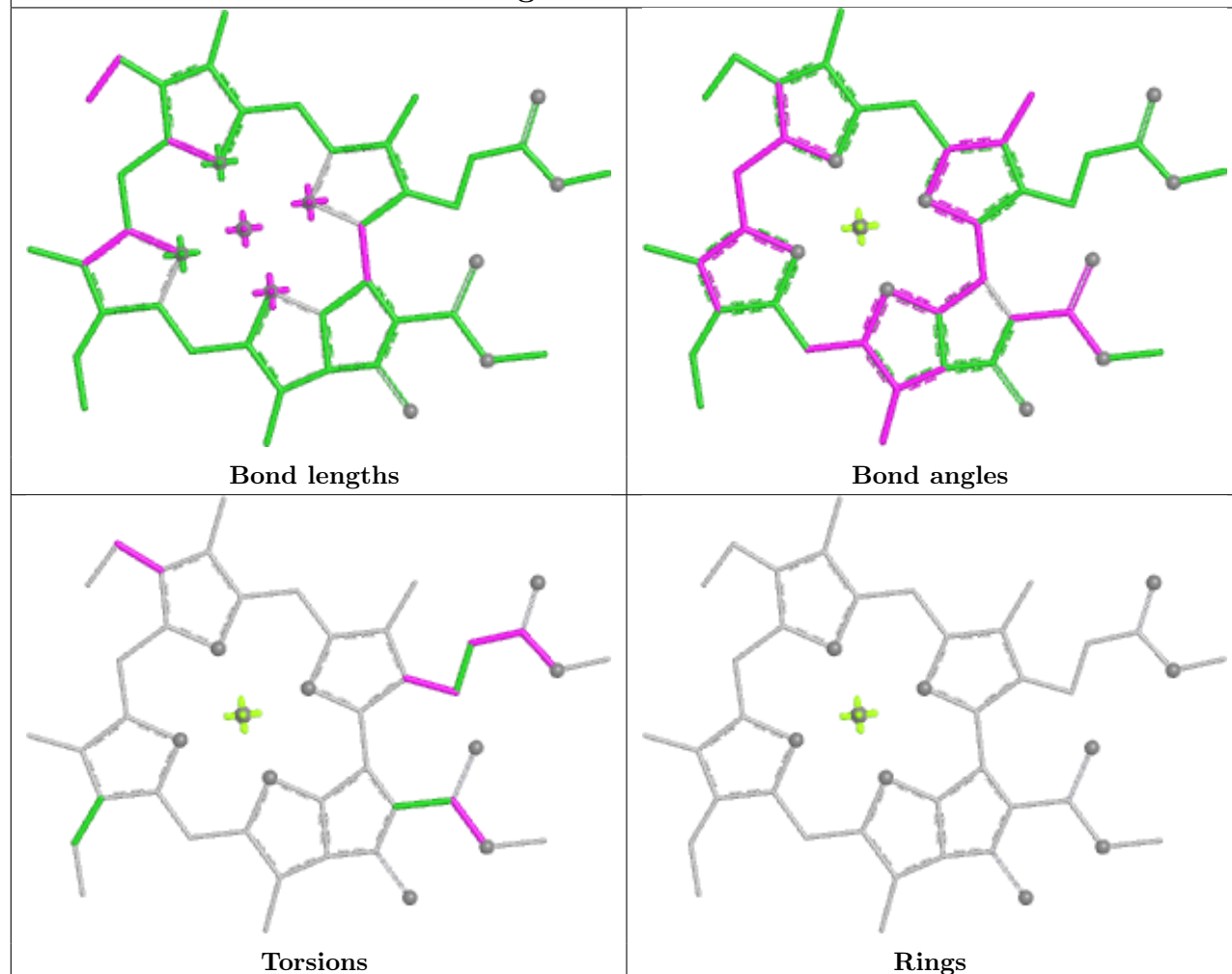
Torsions



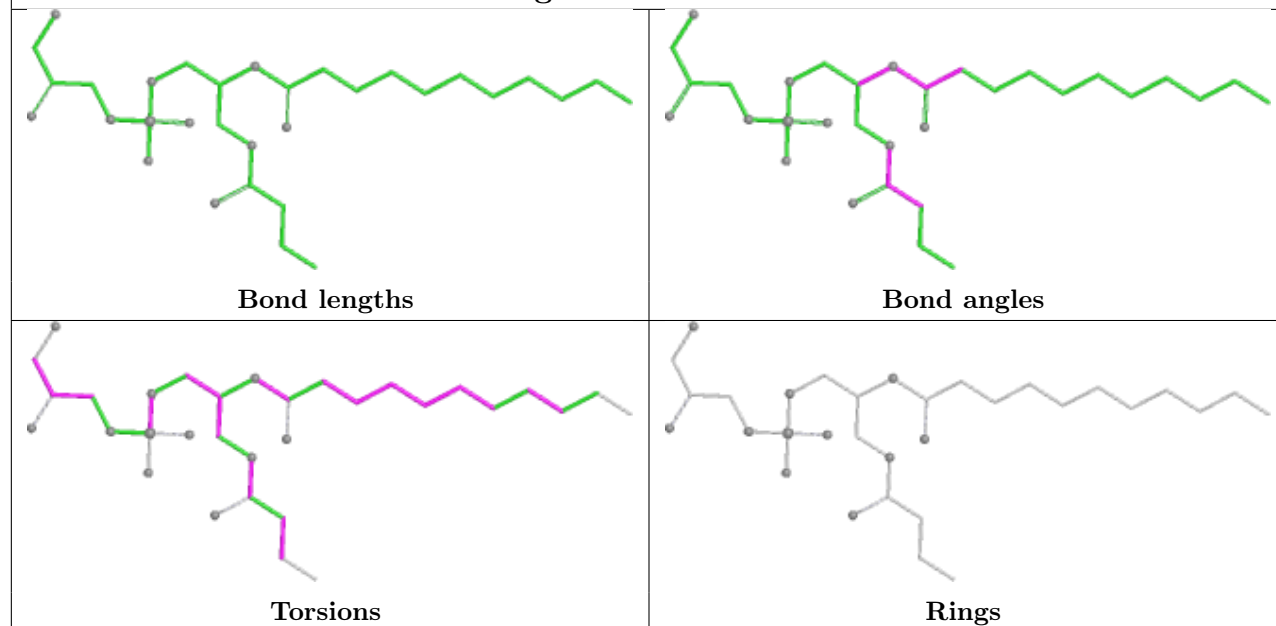
Rings

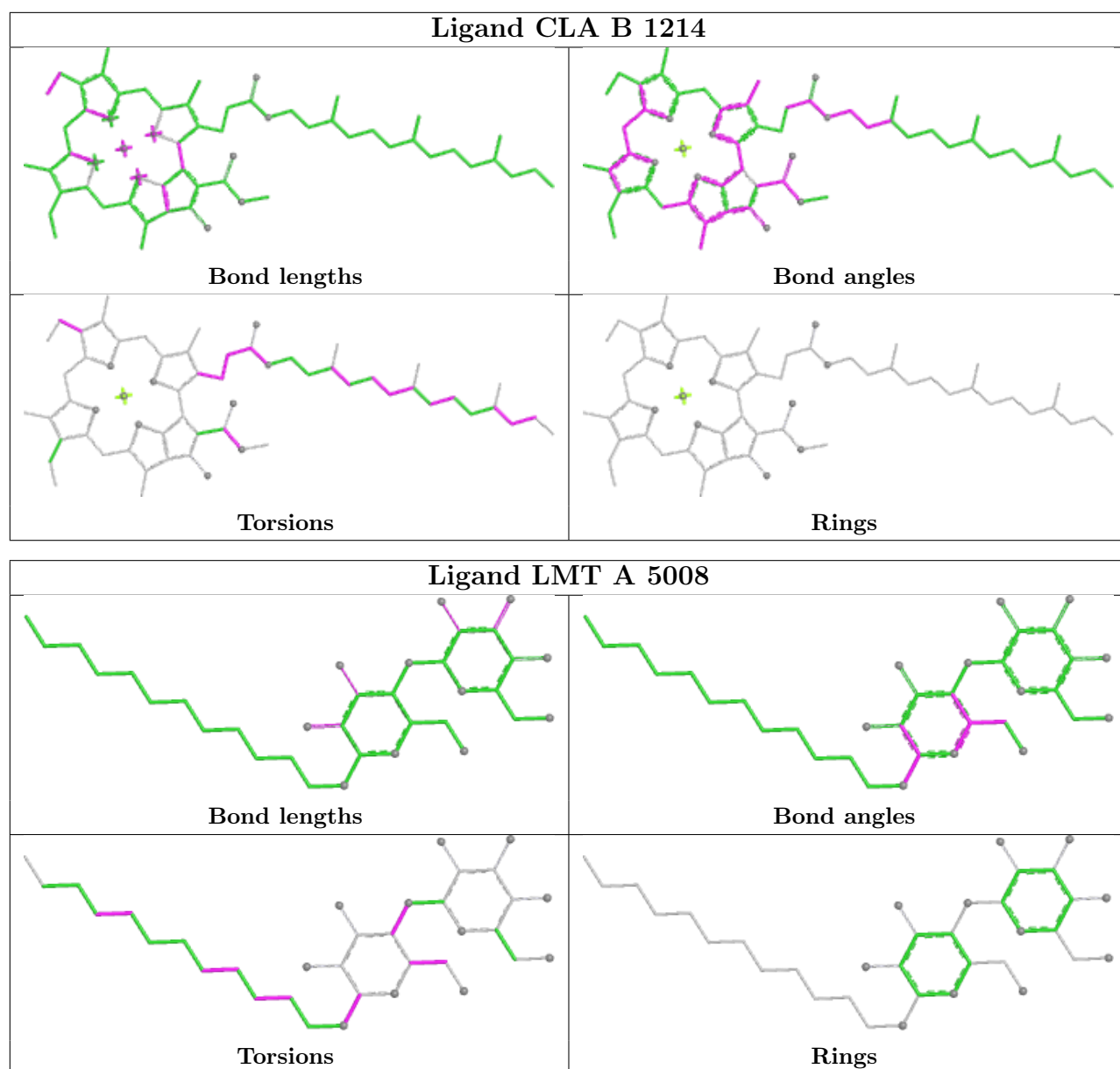


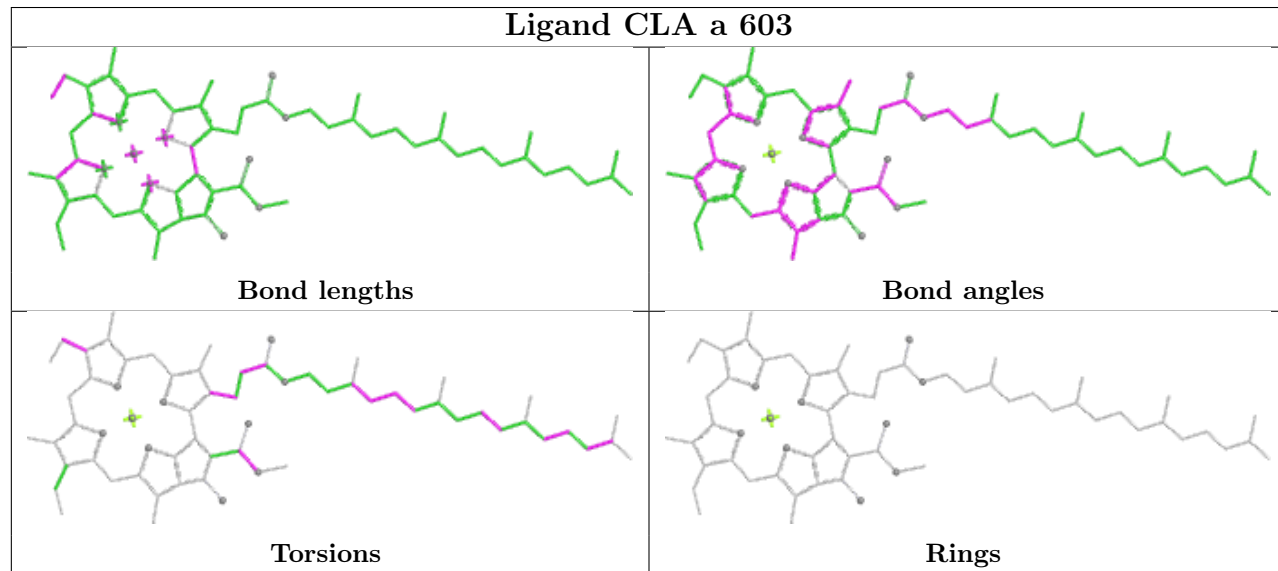
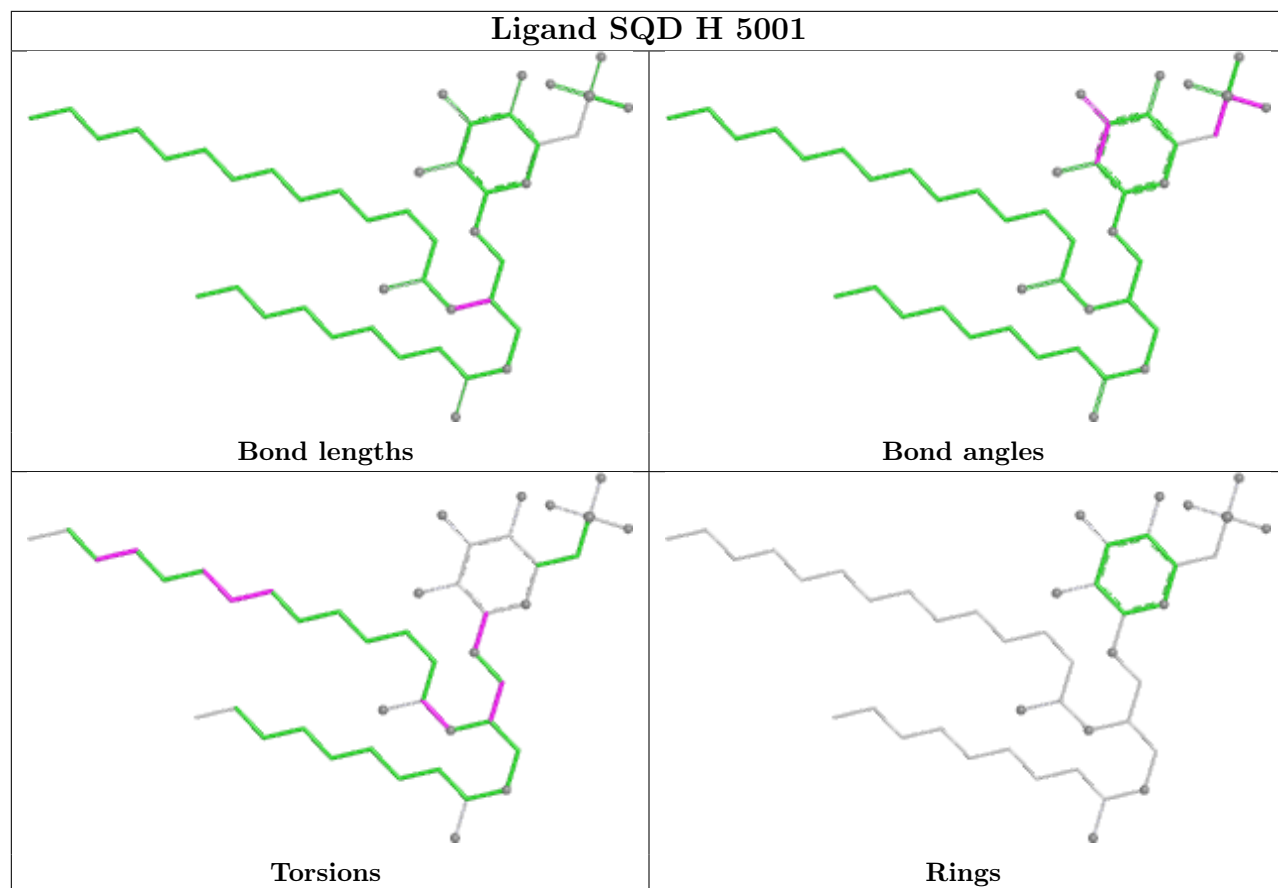
Ligand CLA 6 618

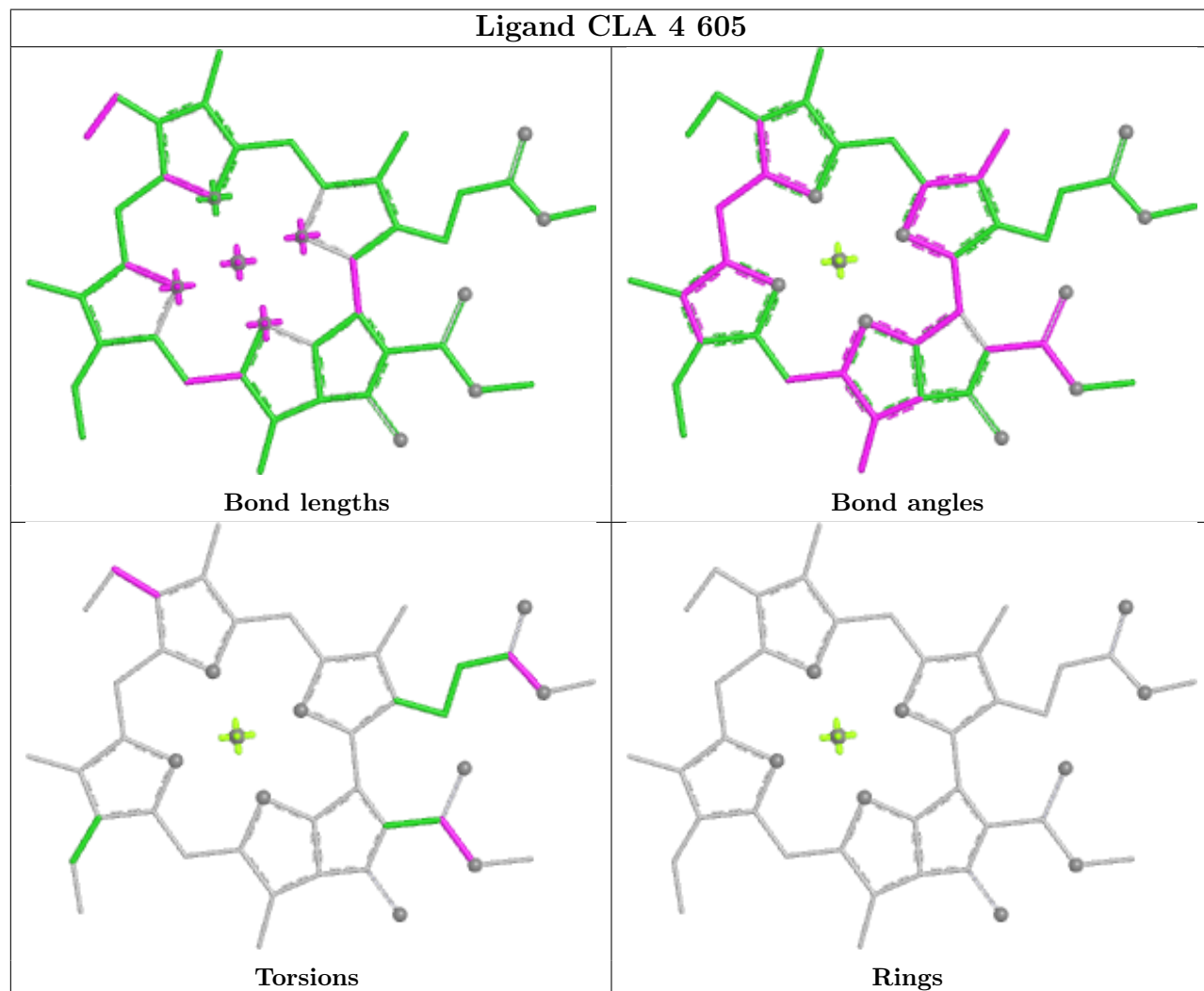
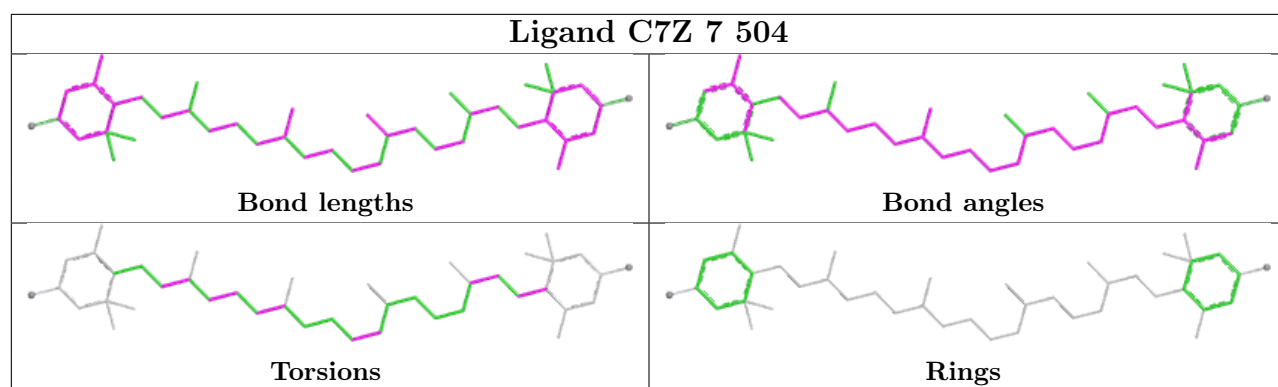


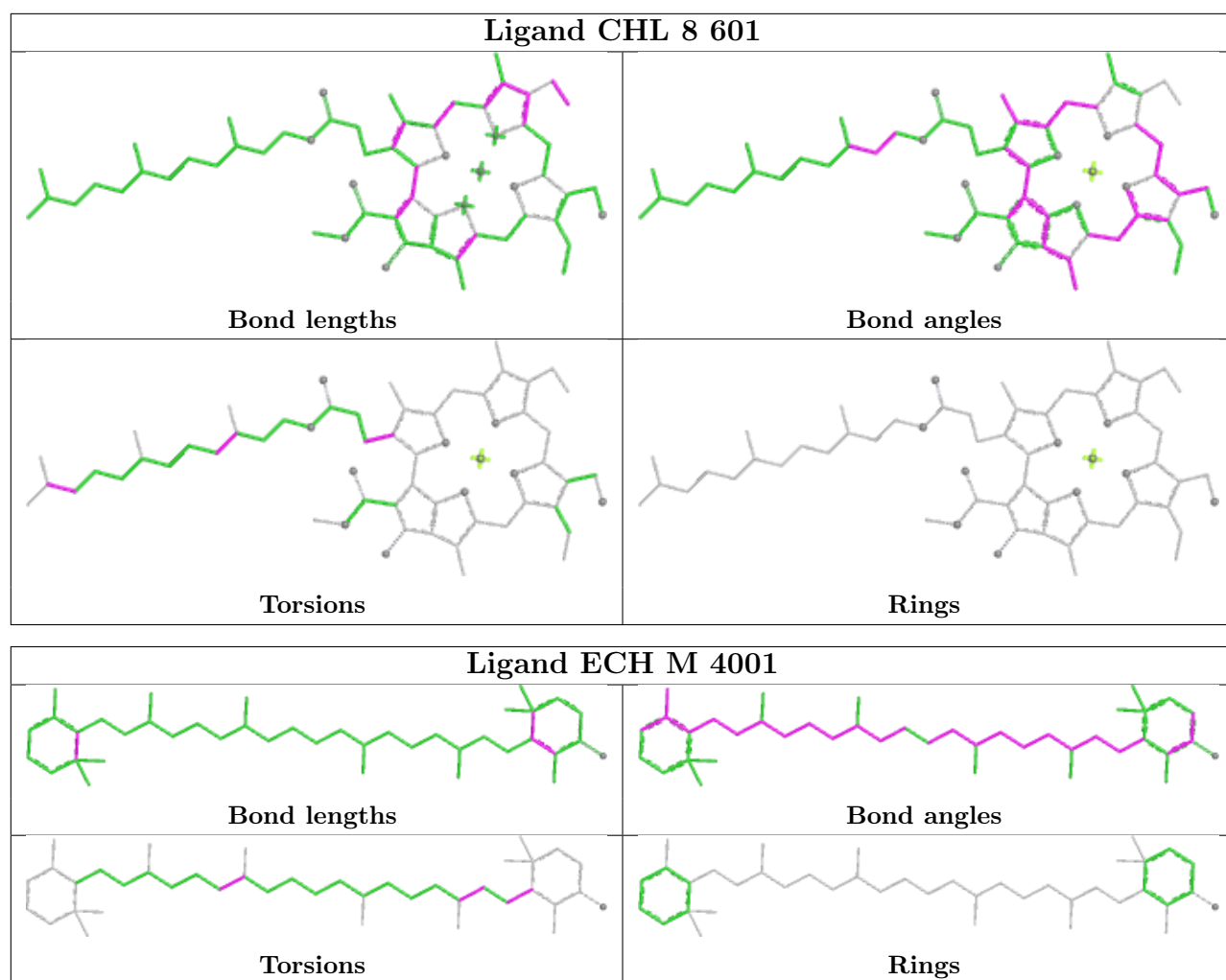
Ligand LHG 4 802

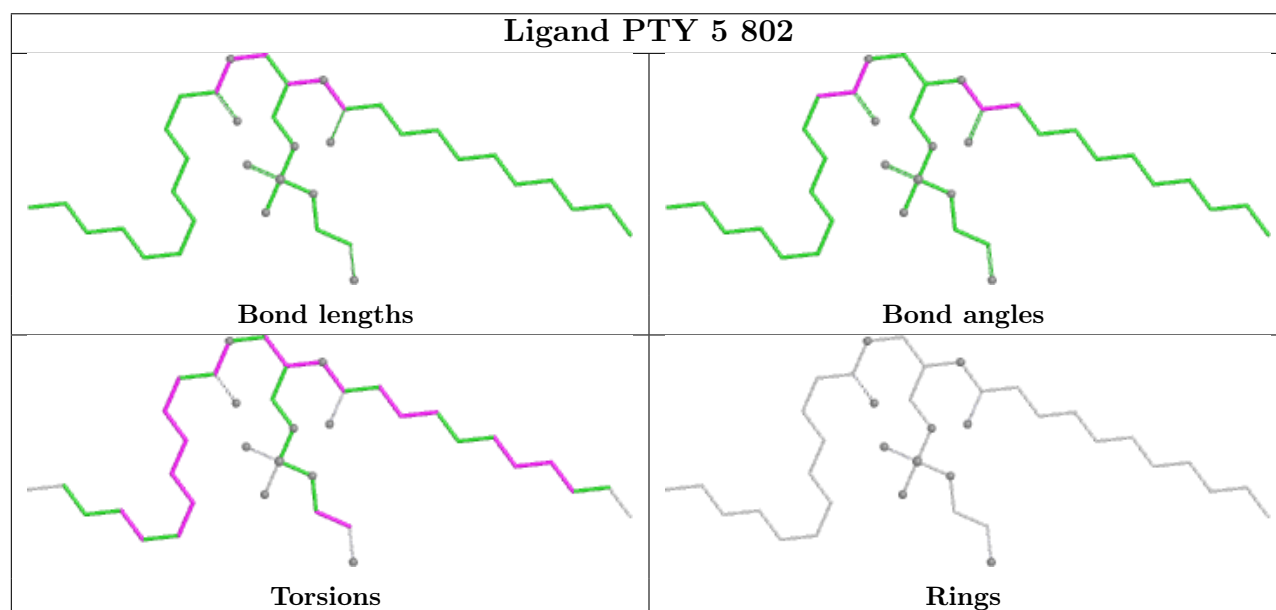
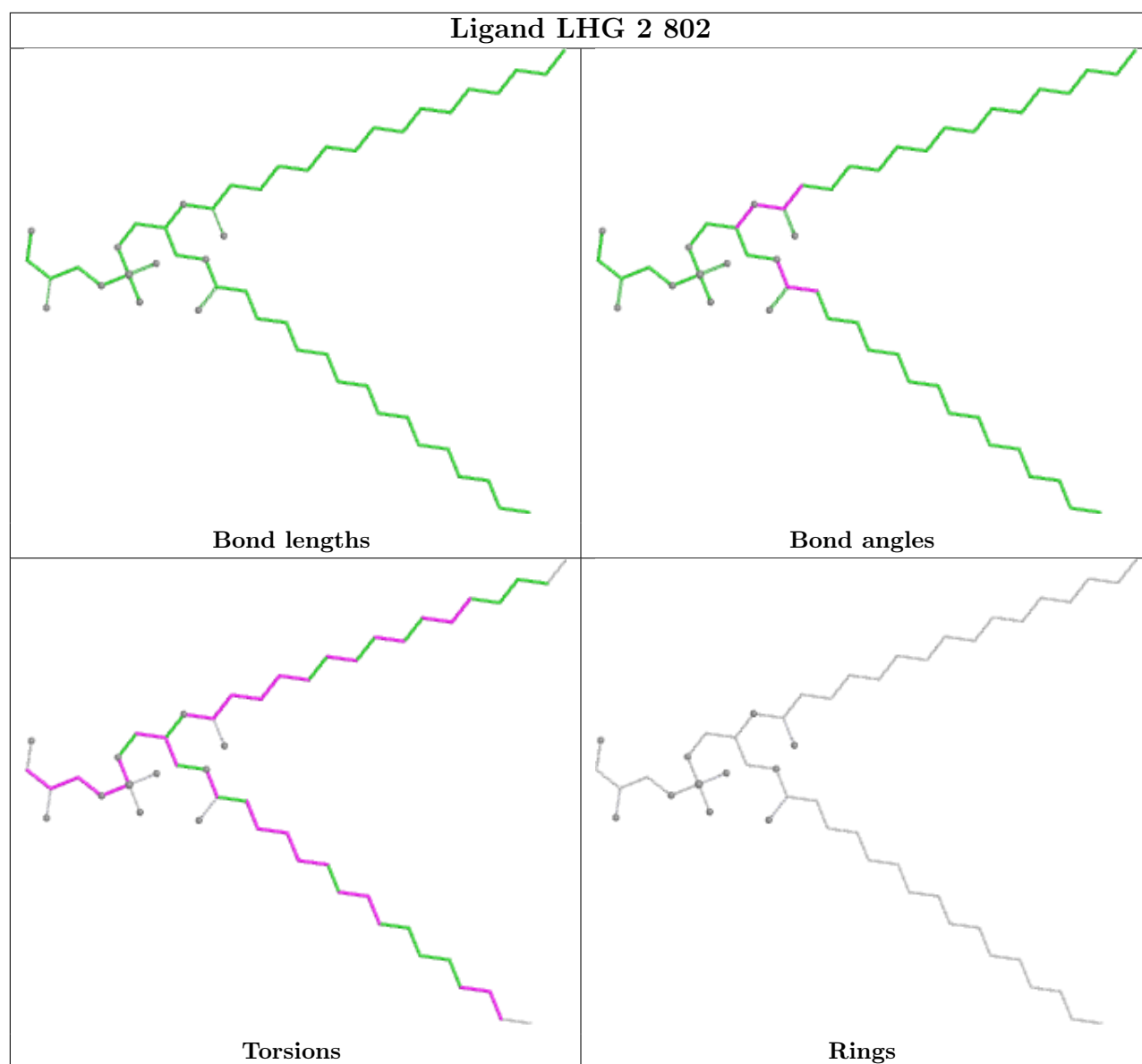


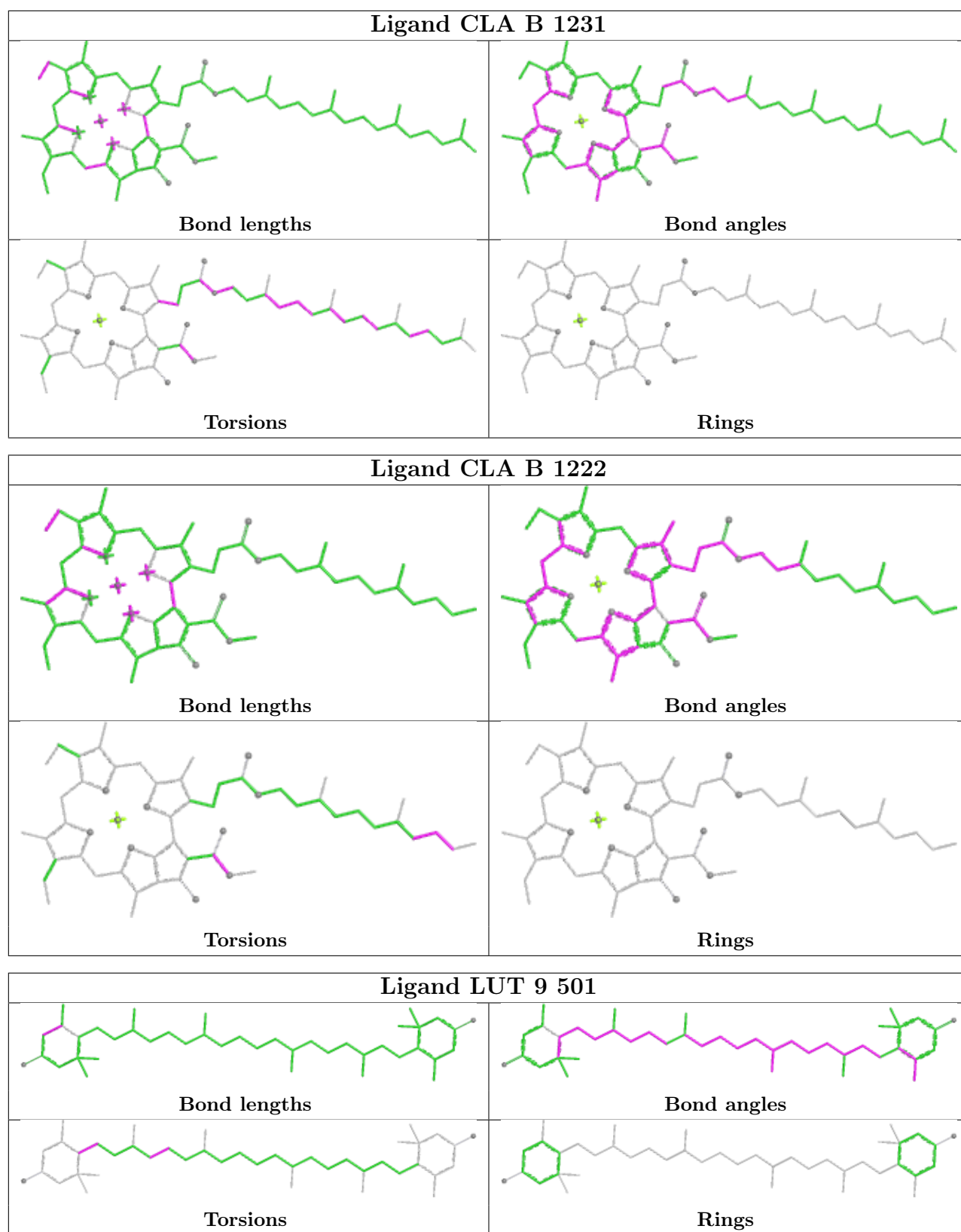




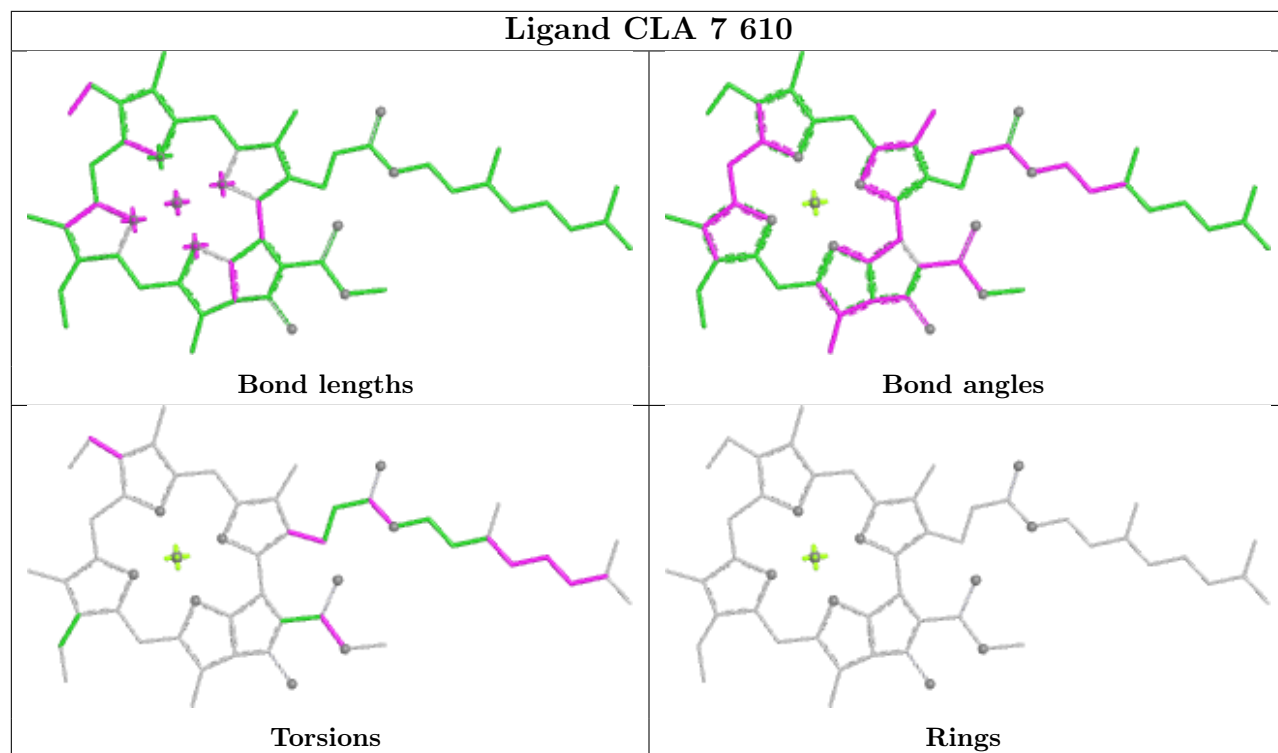




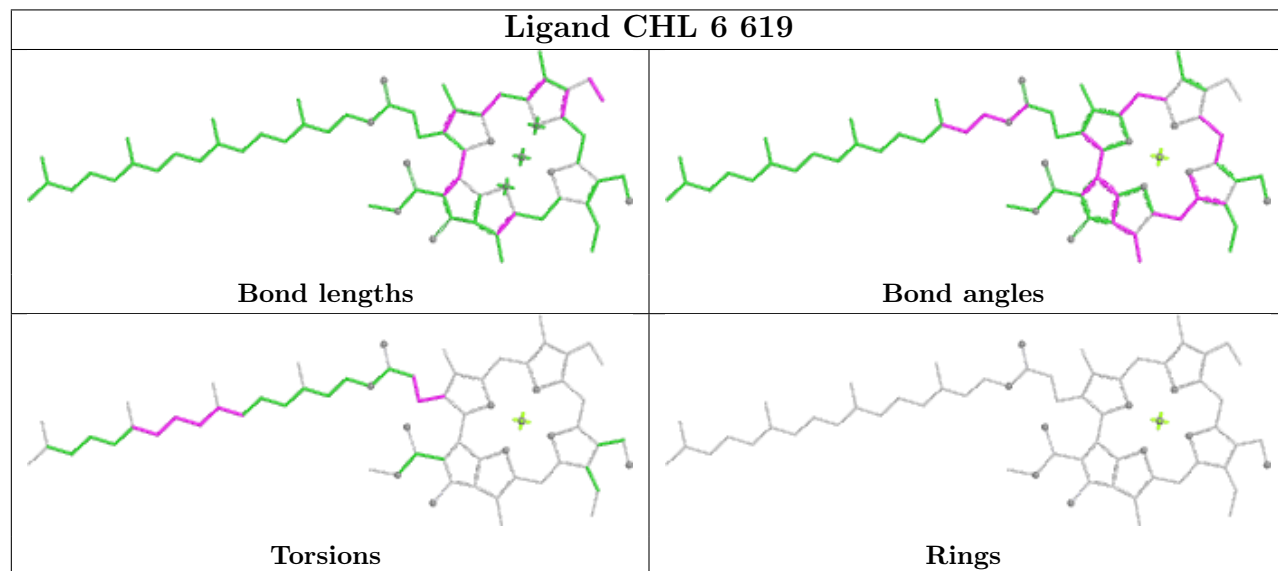




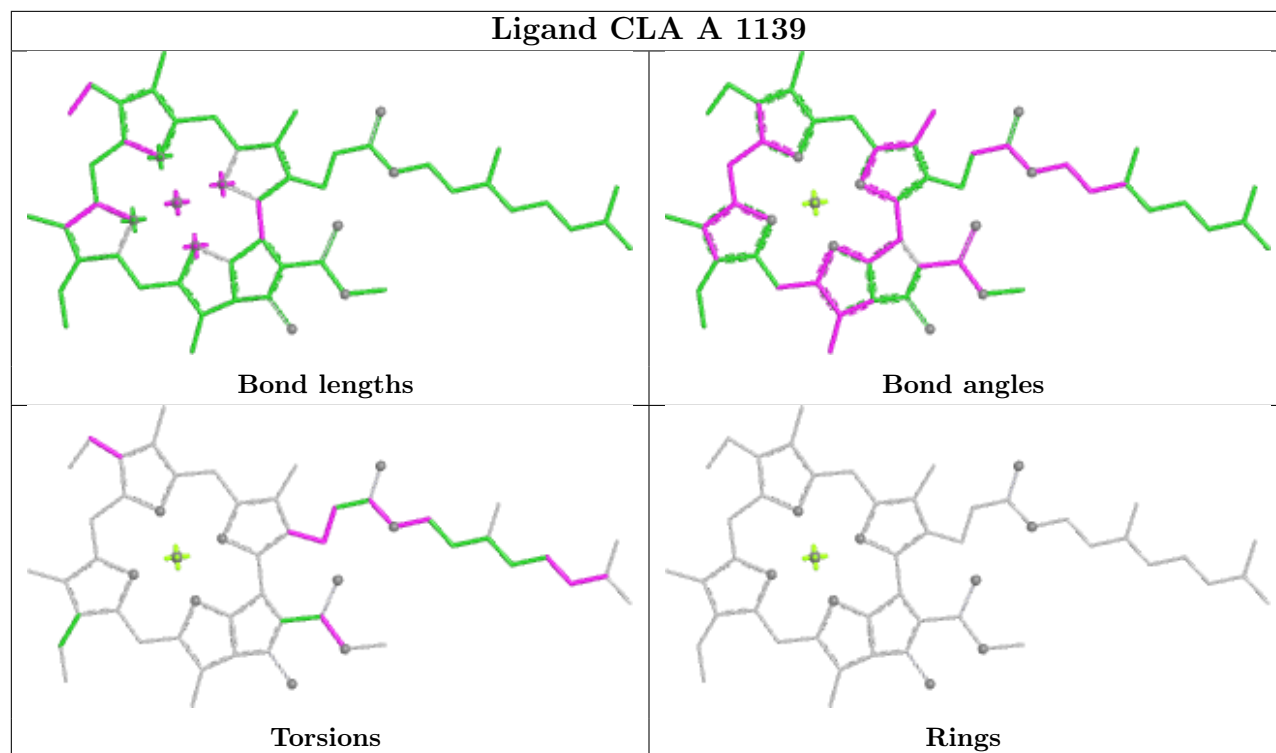
Ligand CLA 7 610



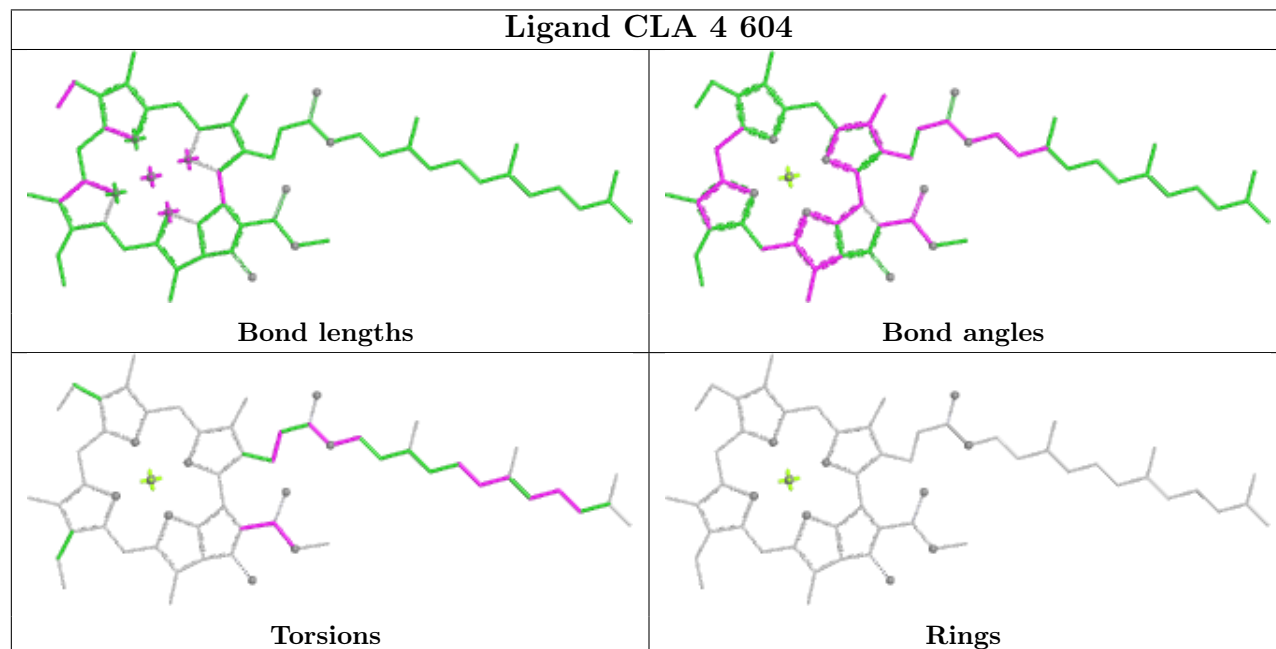
Ligand CHL 6 619



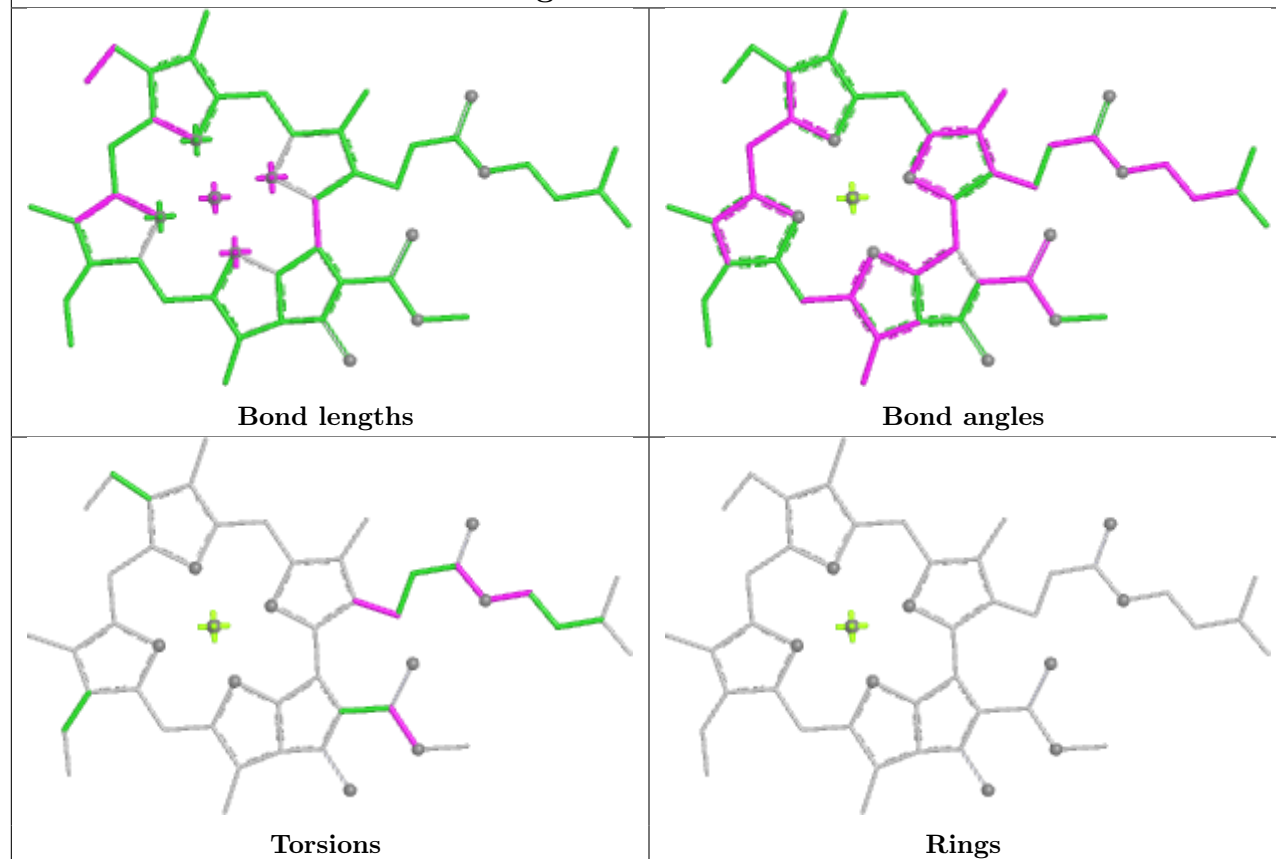
Ligand CLA A 1139



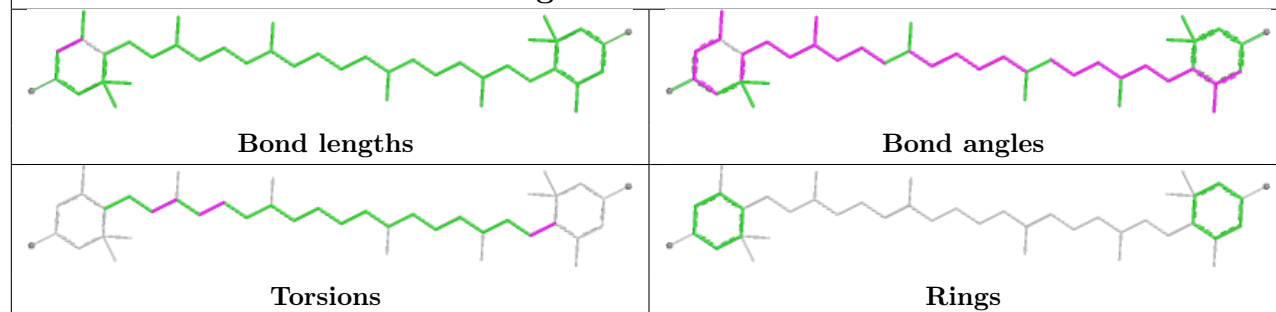
Ligand CLA 4 604

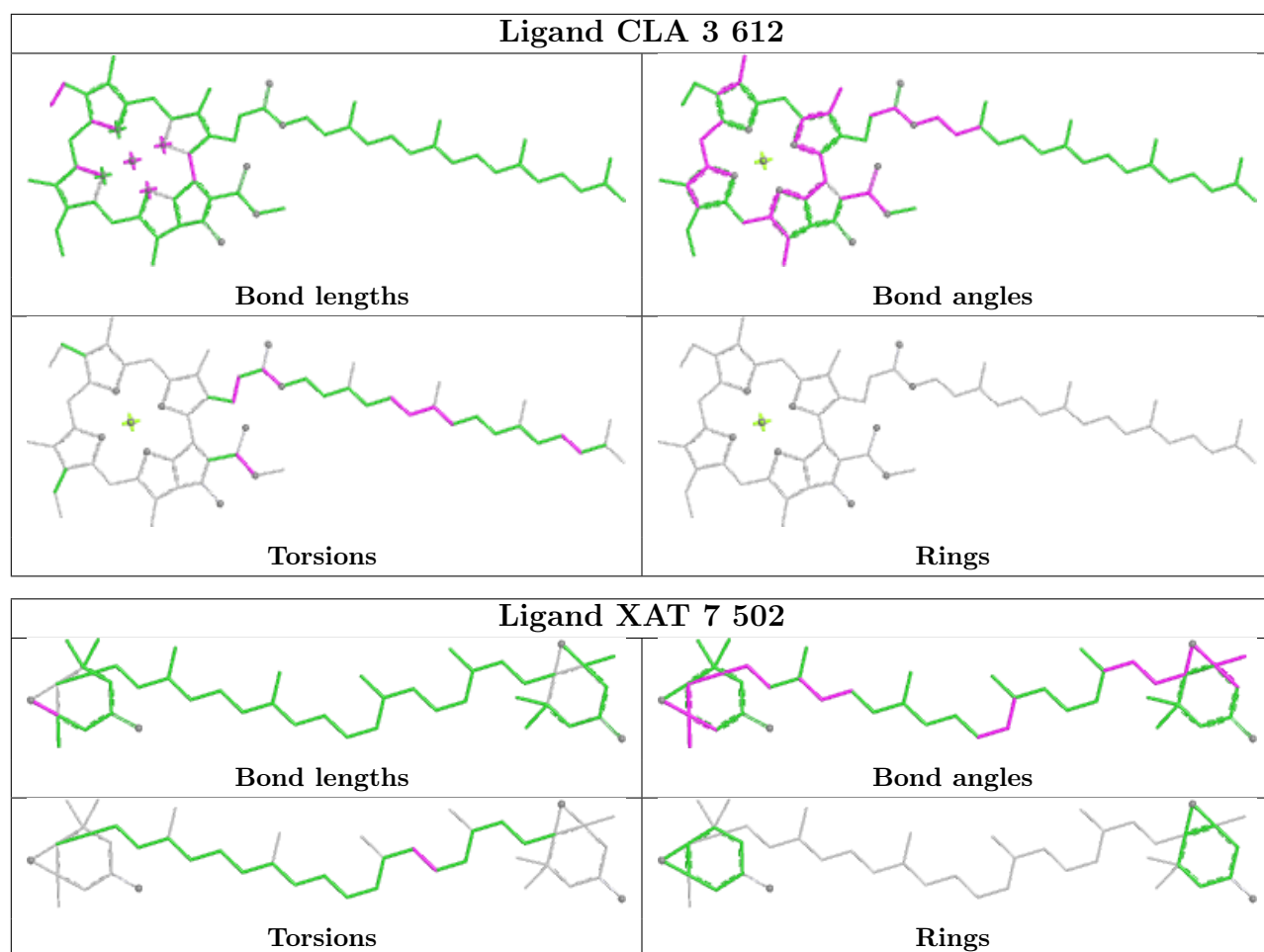


Ligand CLA 4 606

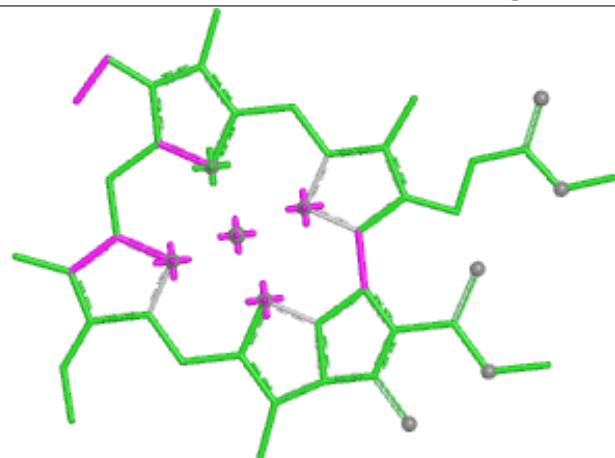


Ligand LUT 1 501

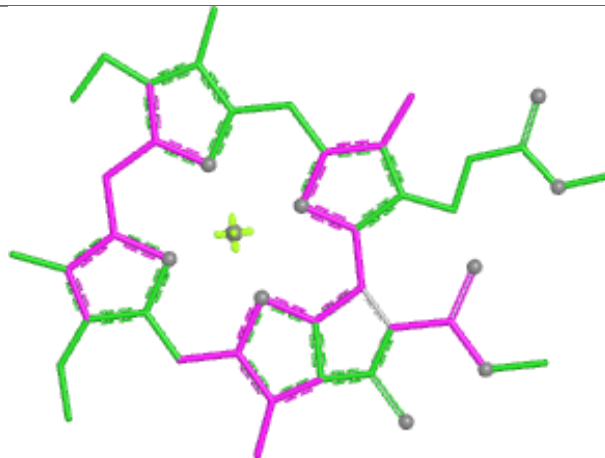




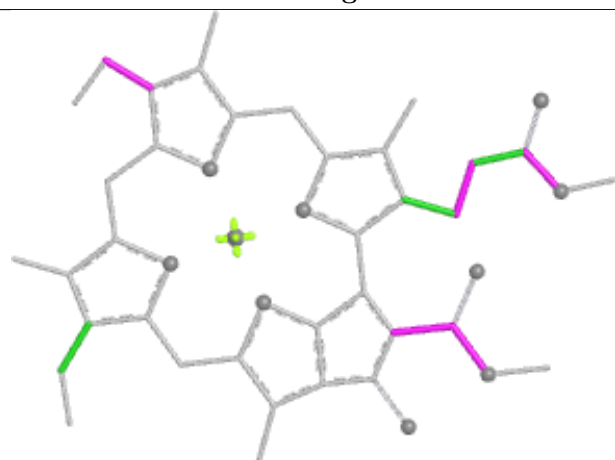
Ligand CLA H 1702



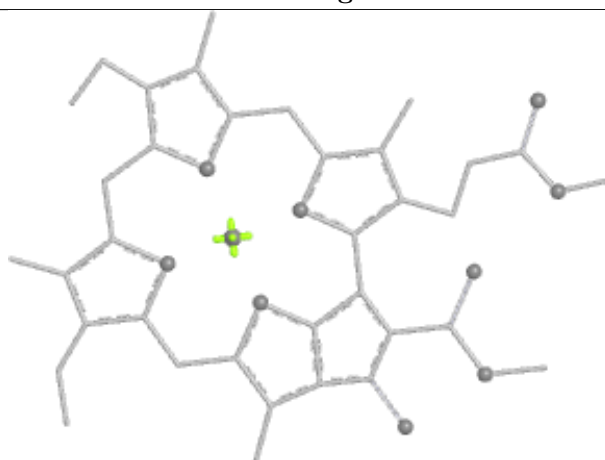
Bond lengths



Bond angles

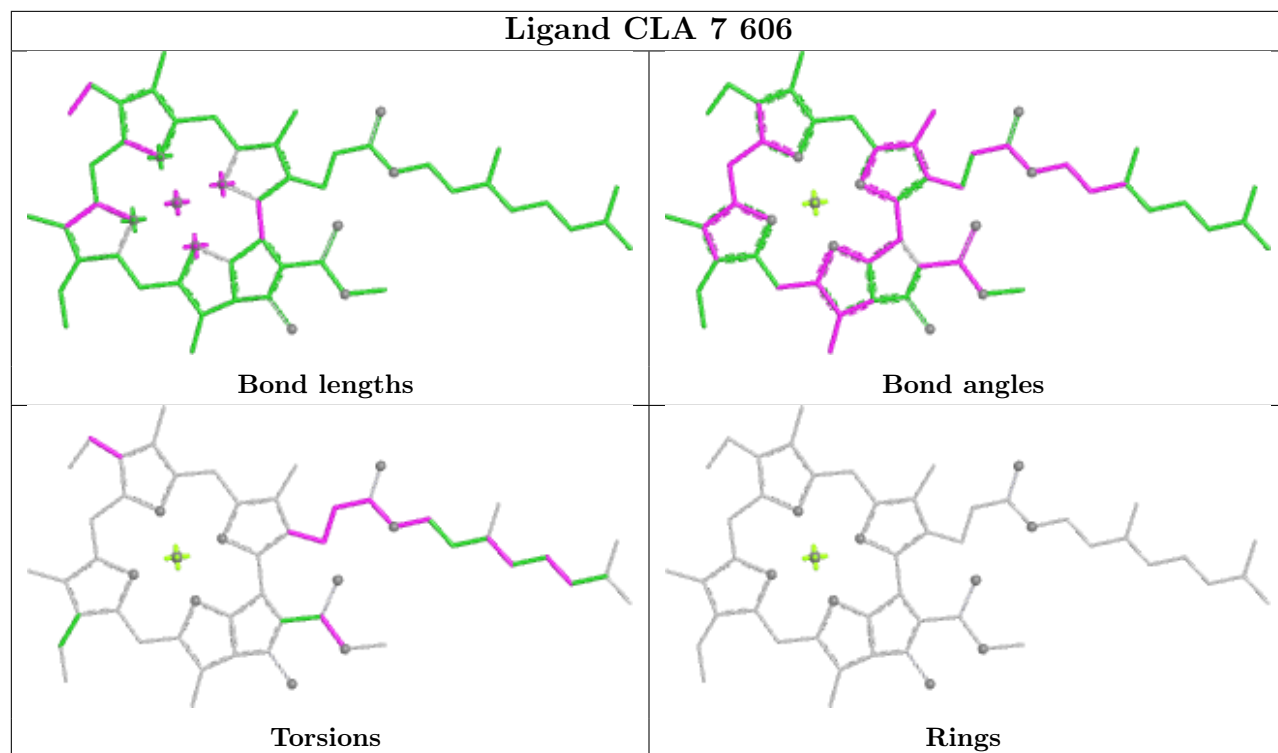


Torsions

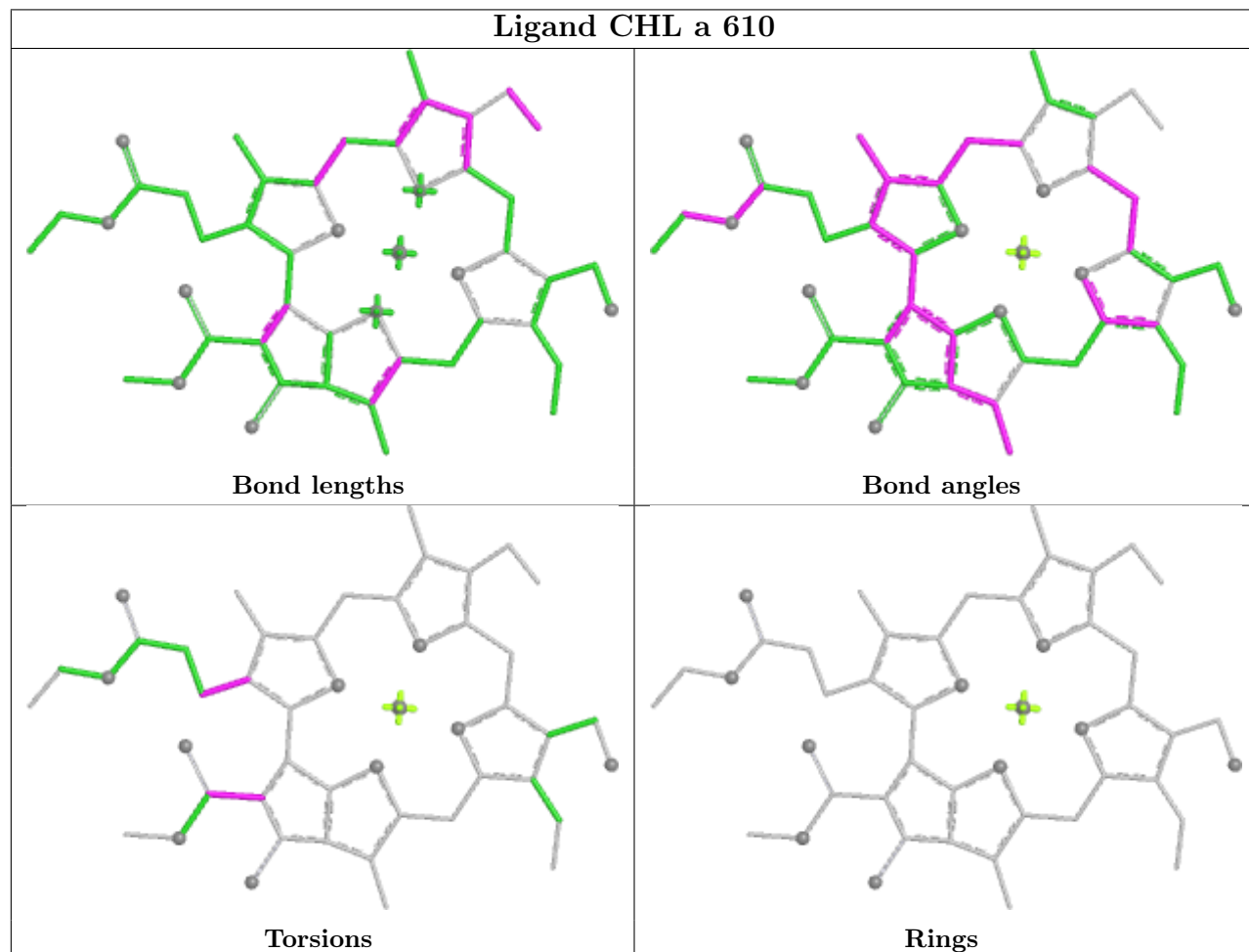


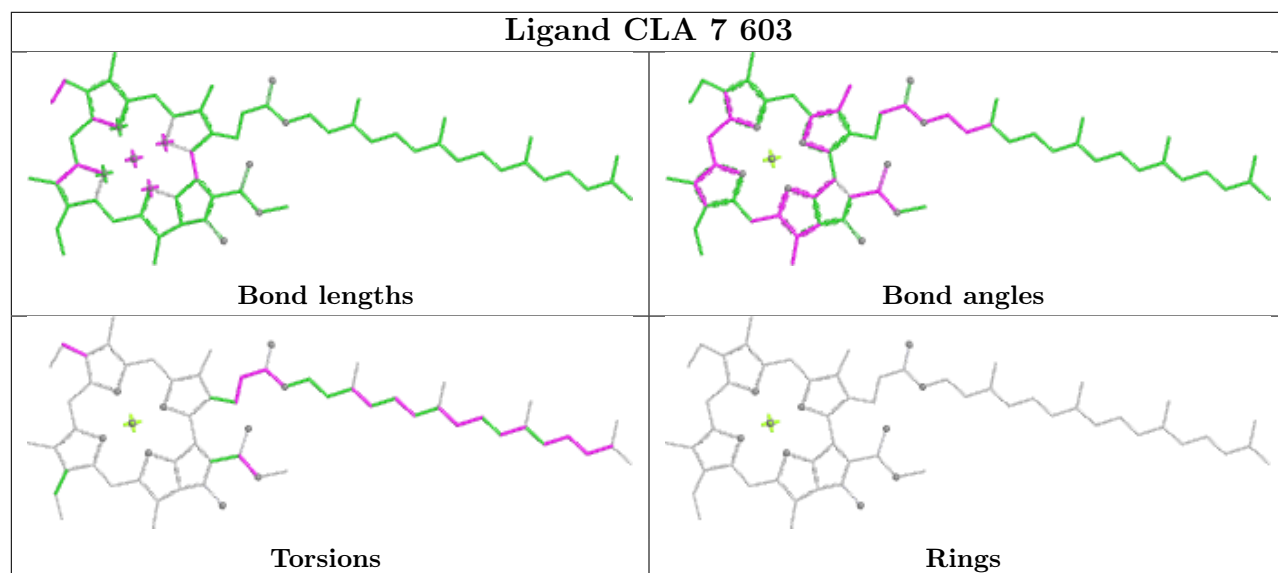
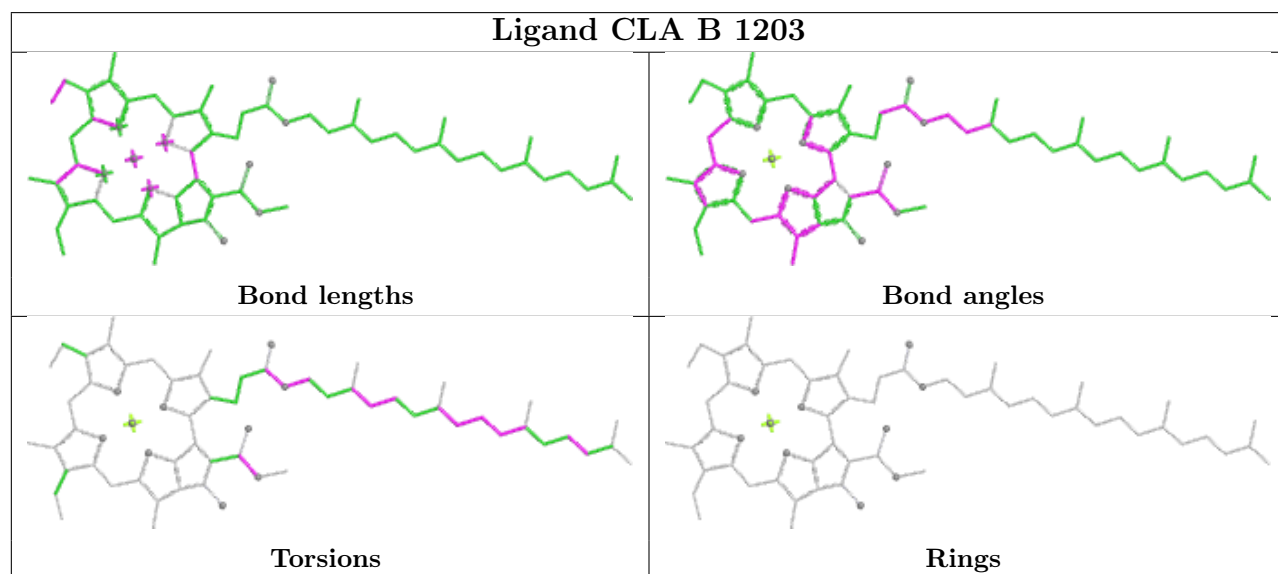
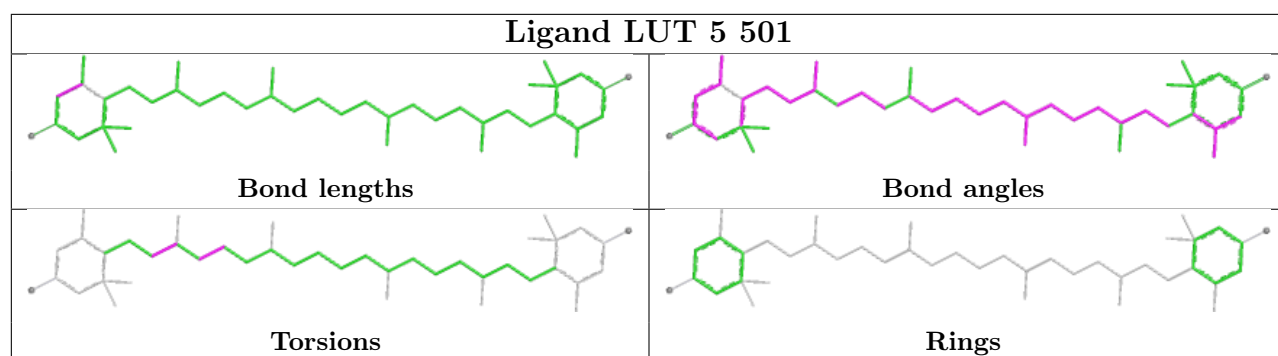
Rings

Ligand CLA 7 606

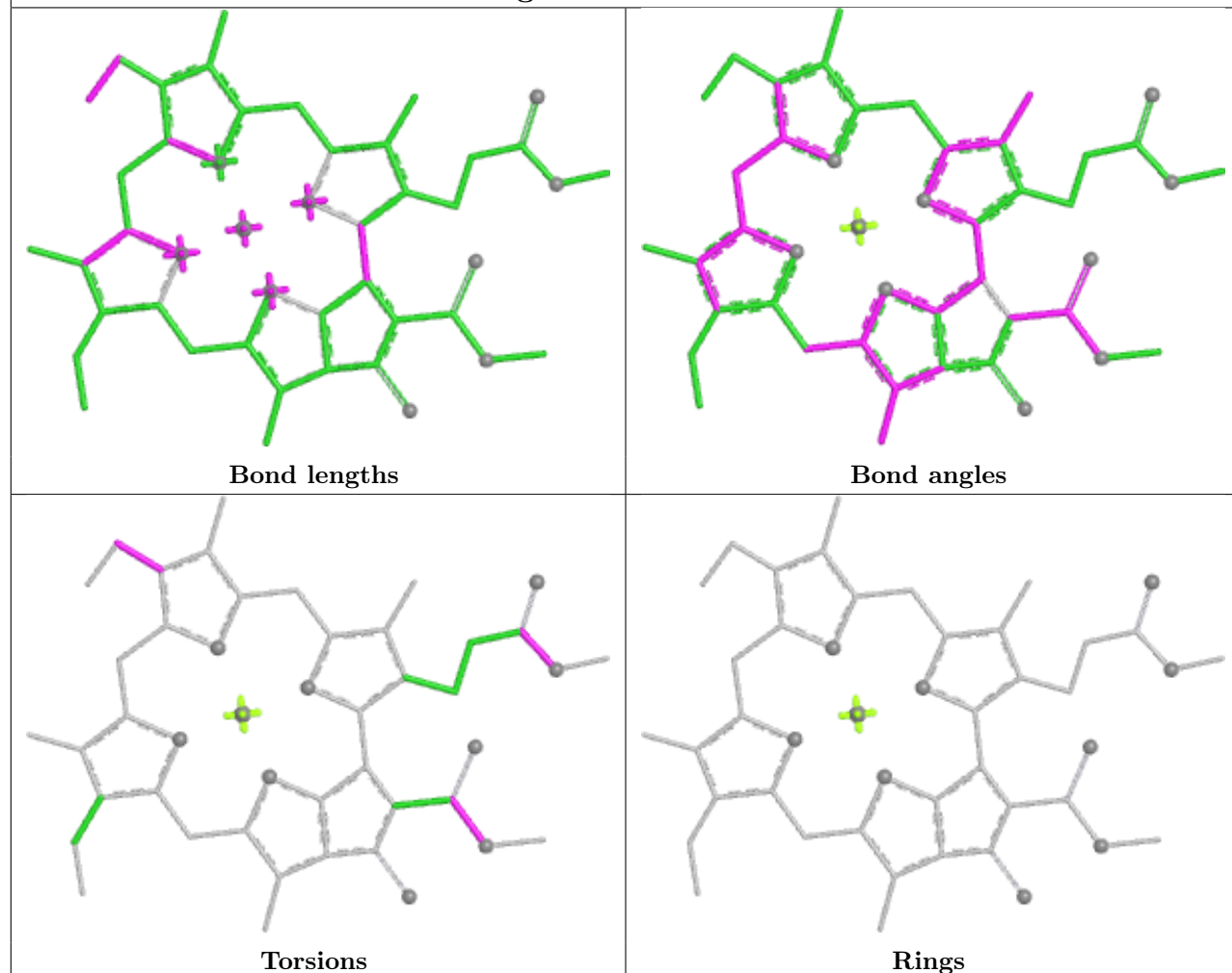


Ligand CHL a 610

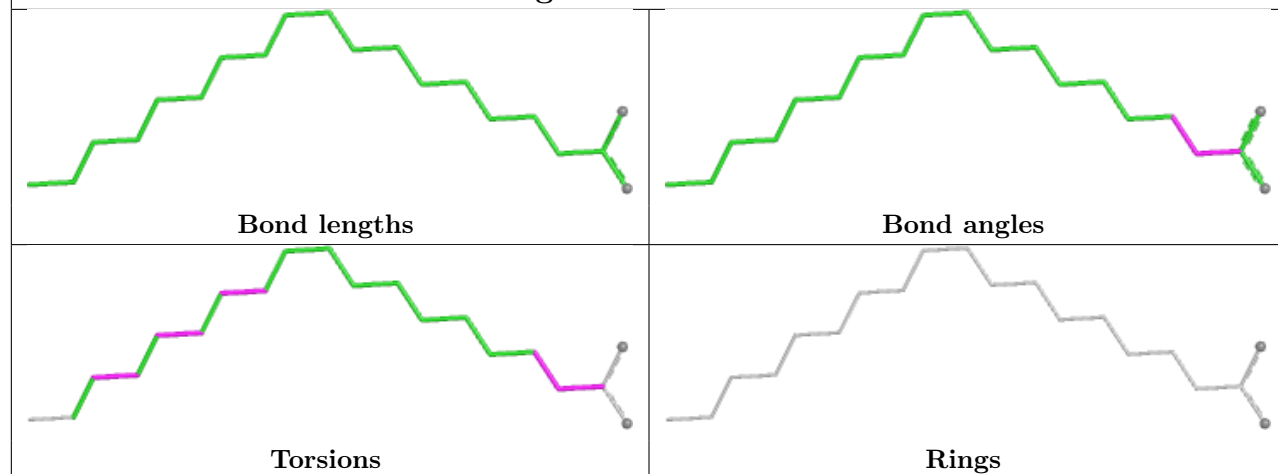


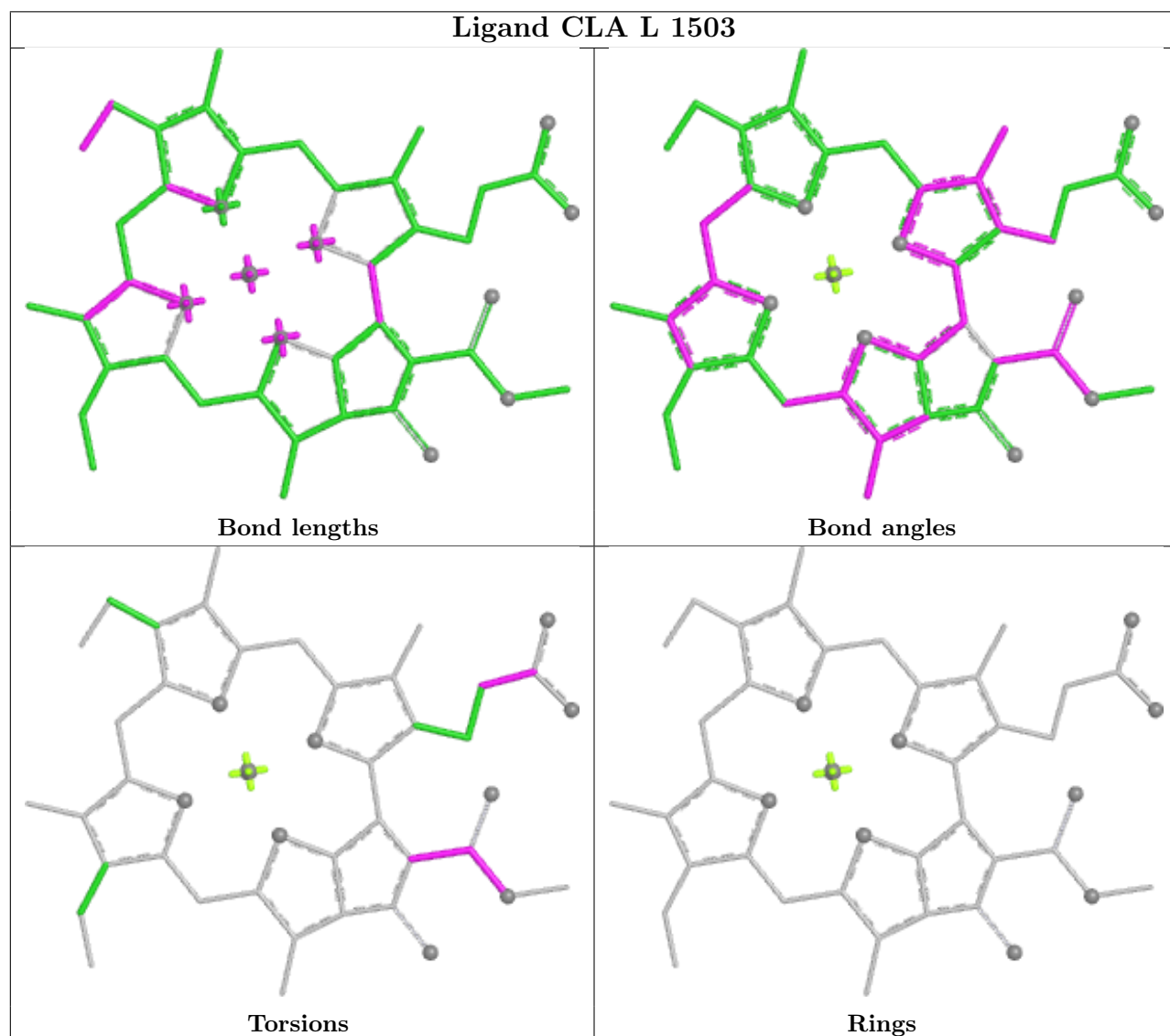
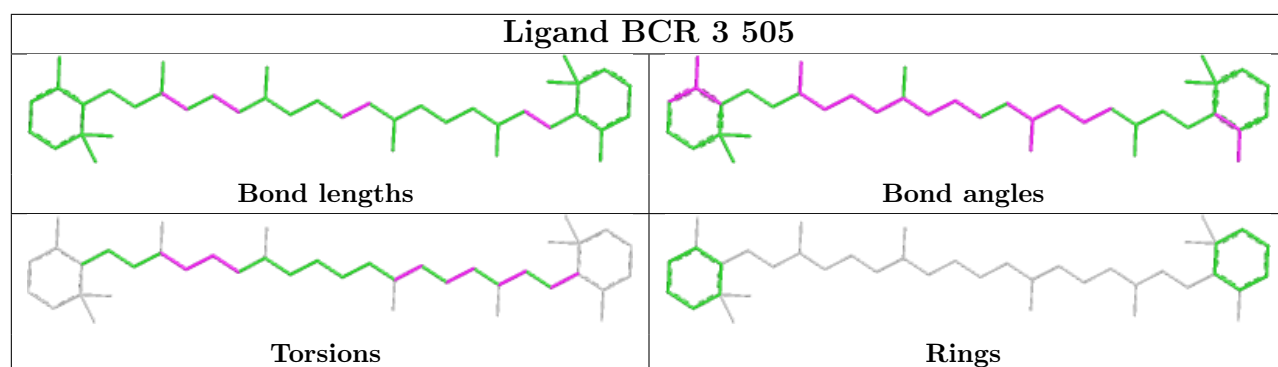


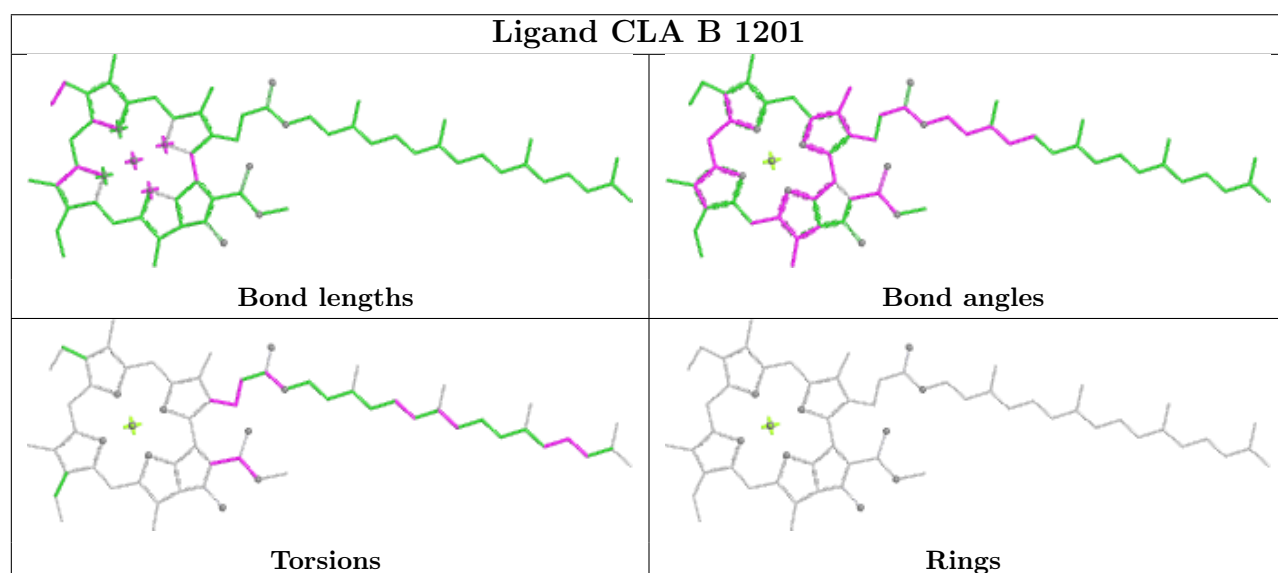
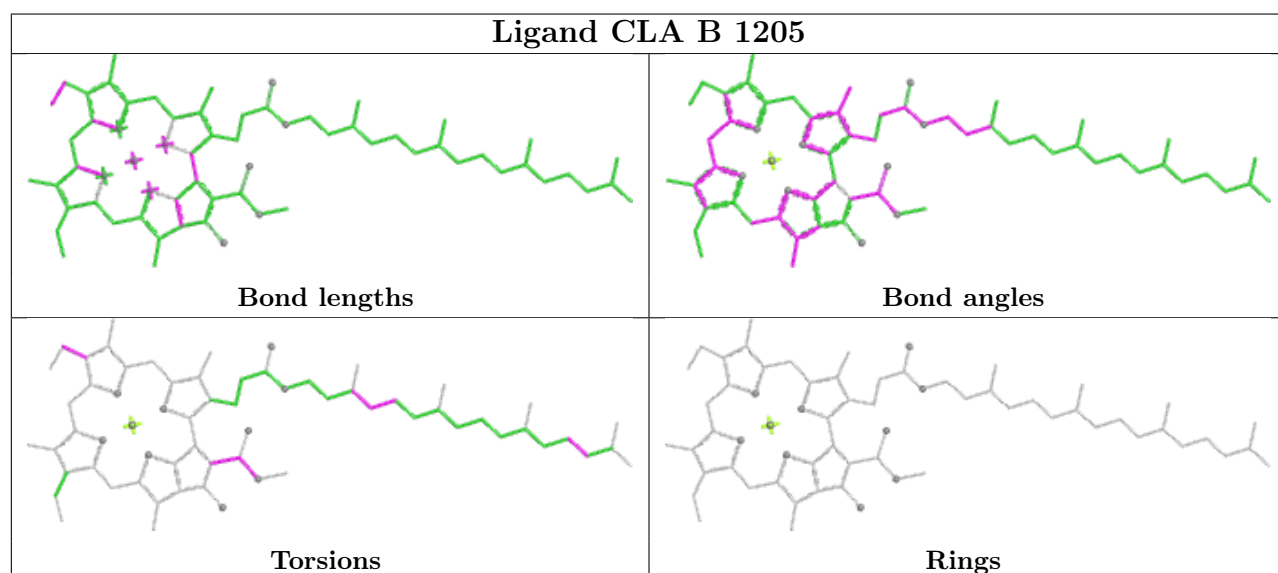
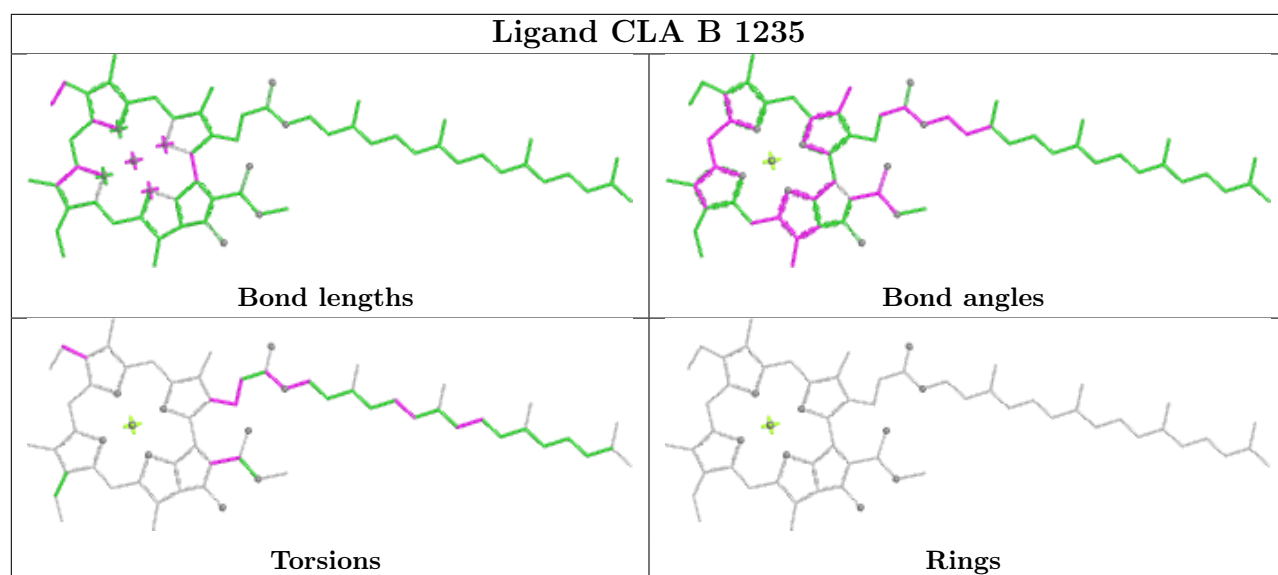
Ligand CLA 2 607

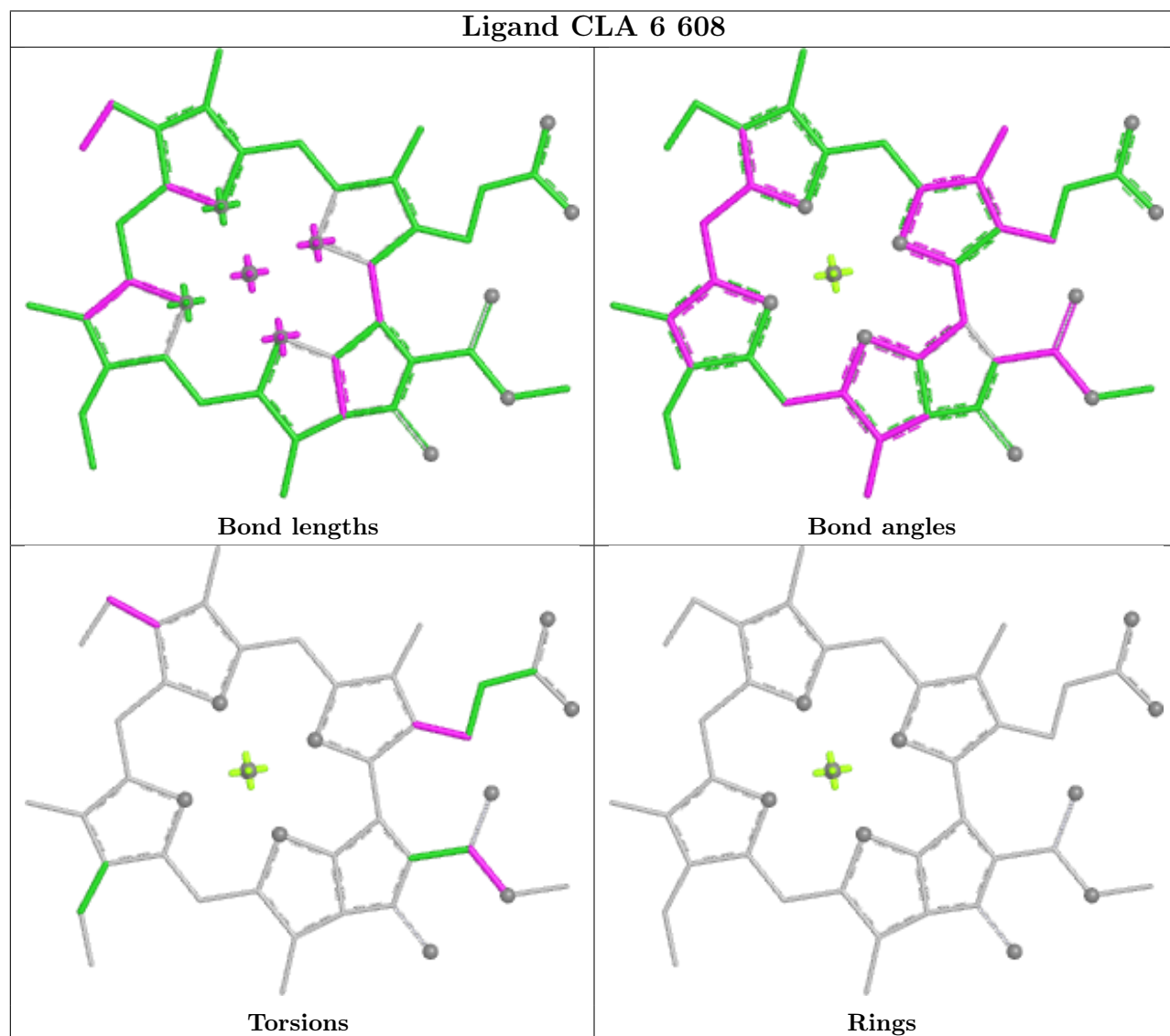
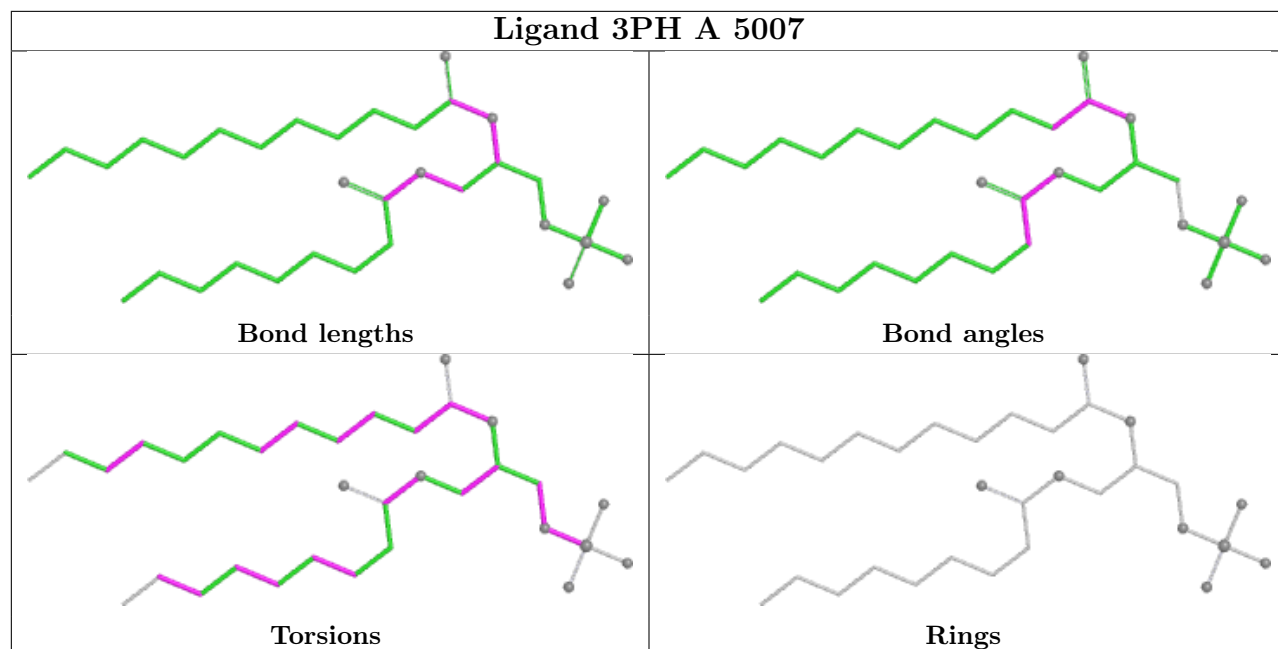


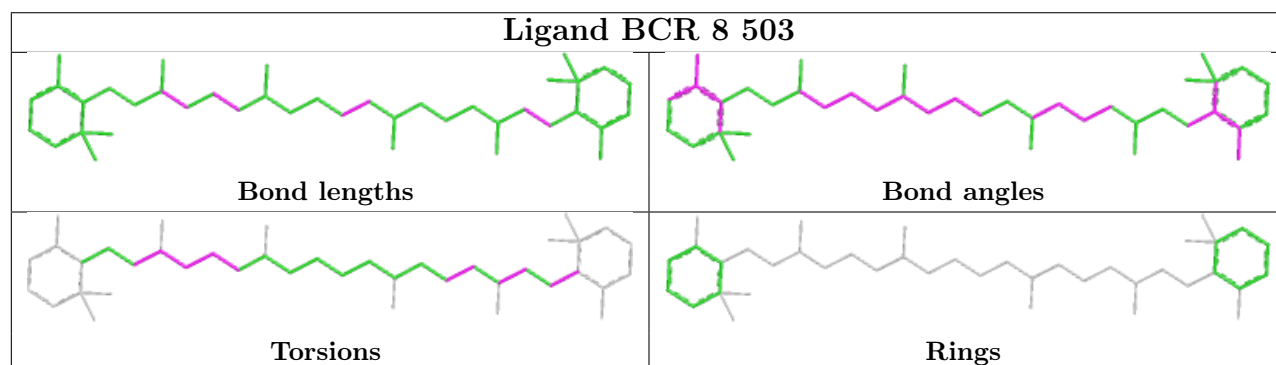
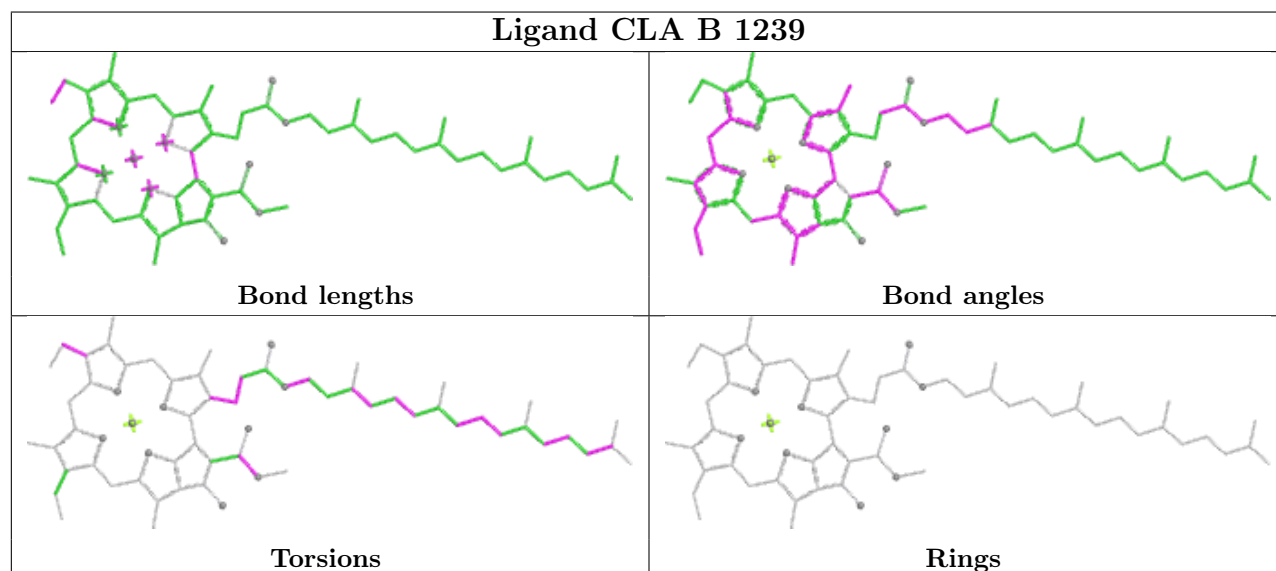
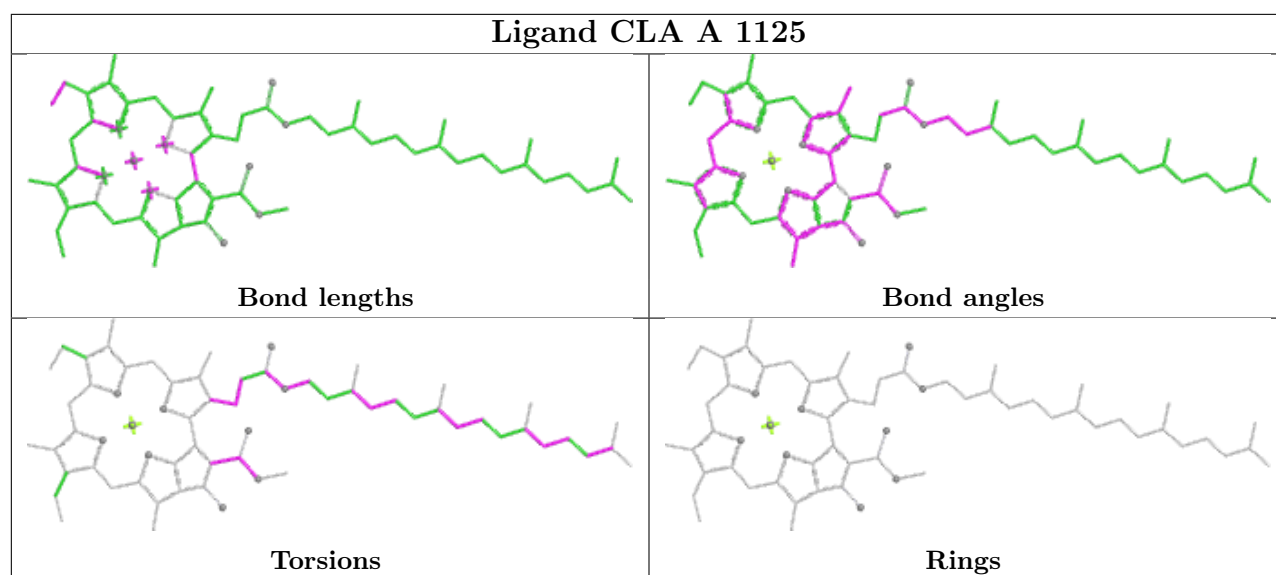
Ligand OLA 1 803

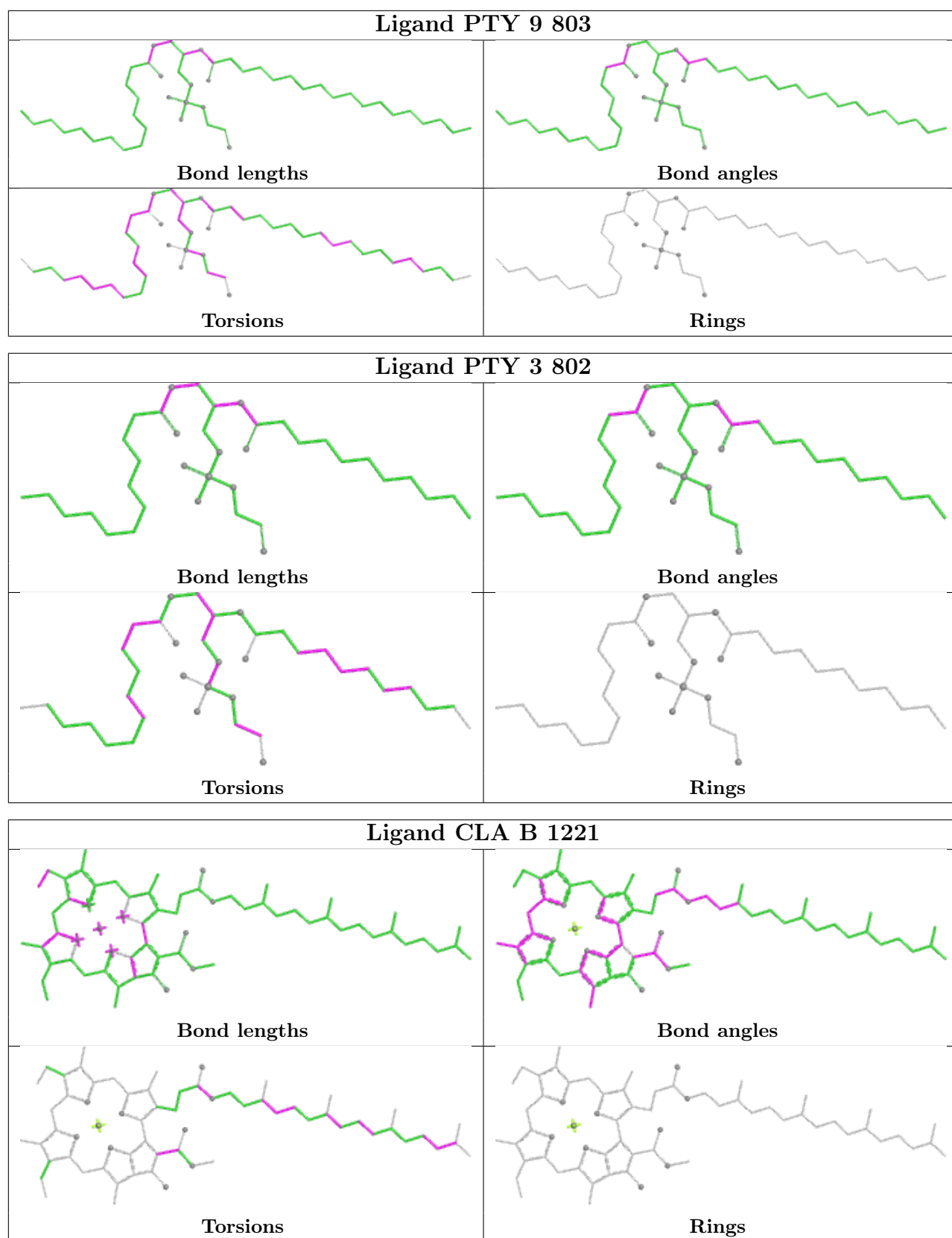


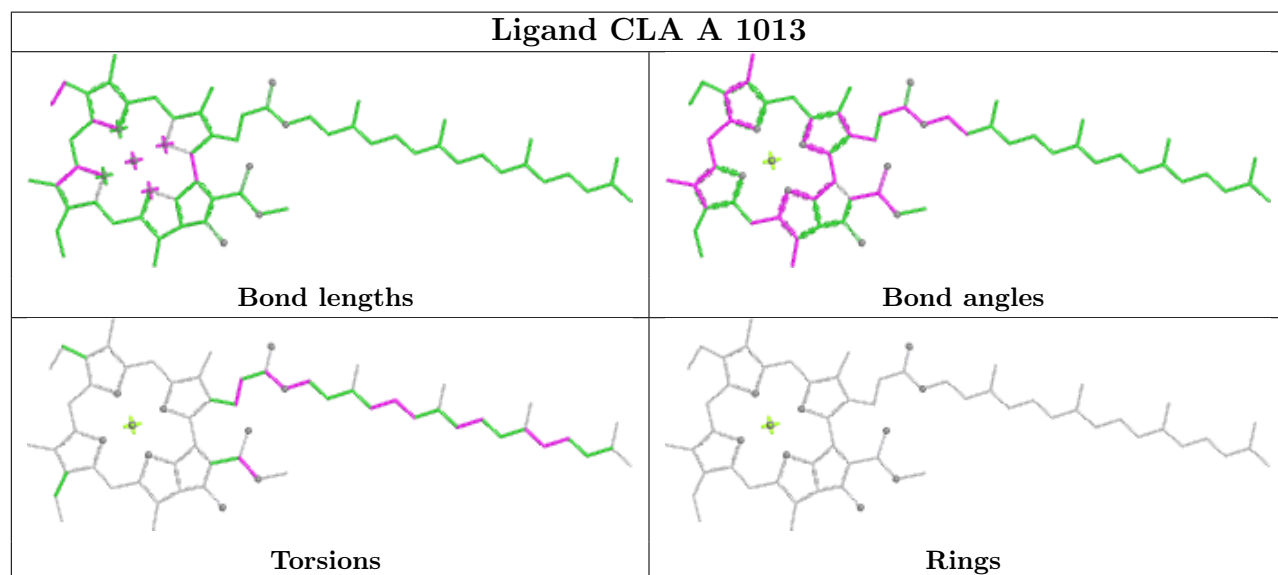
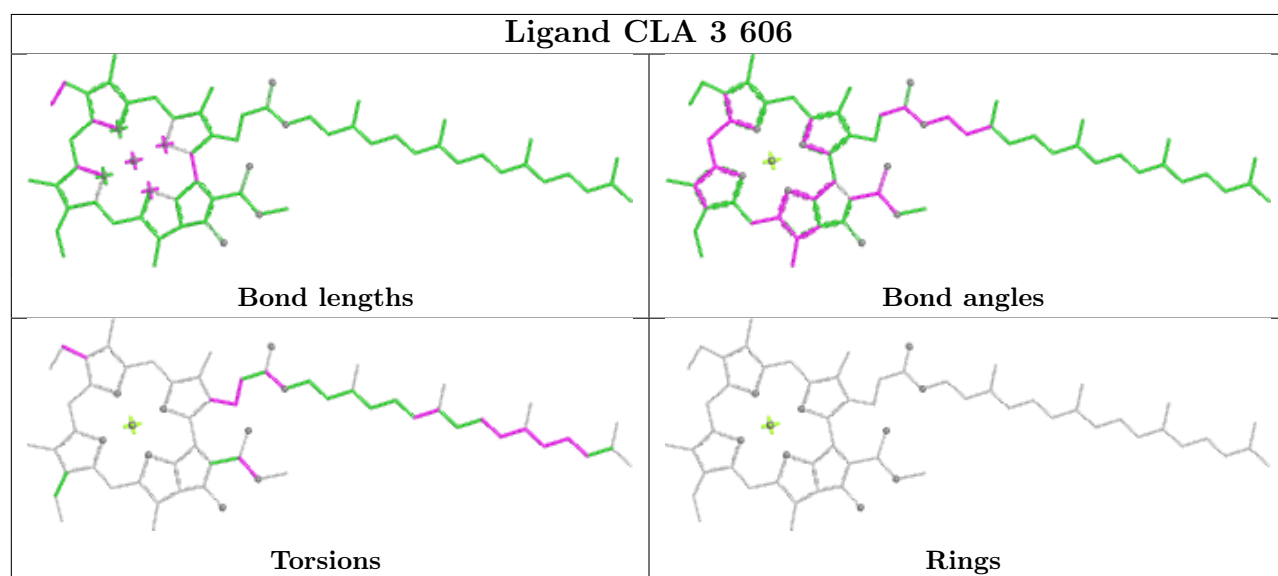
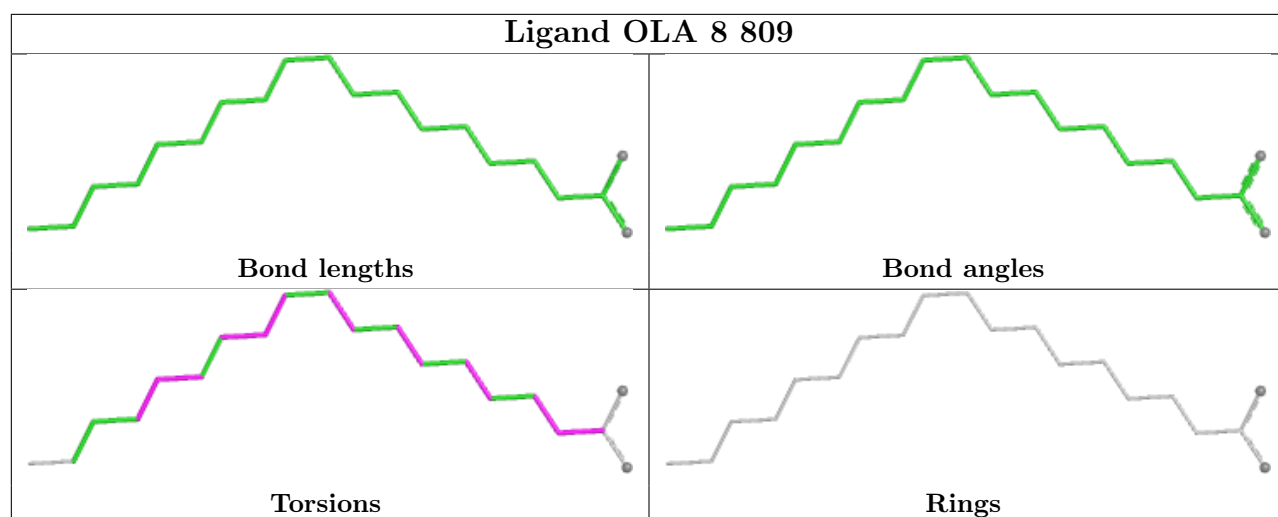


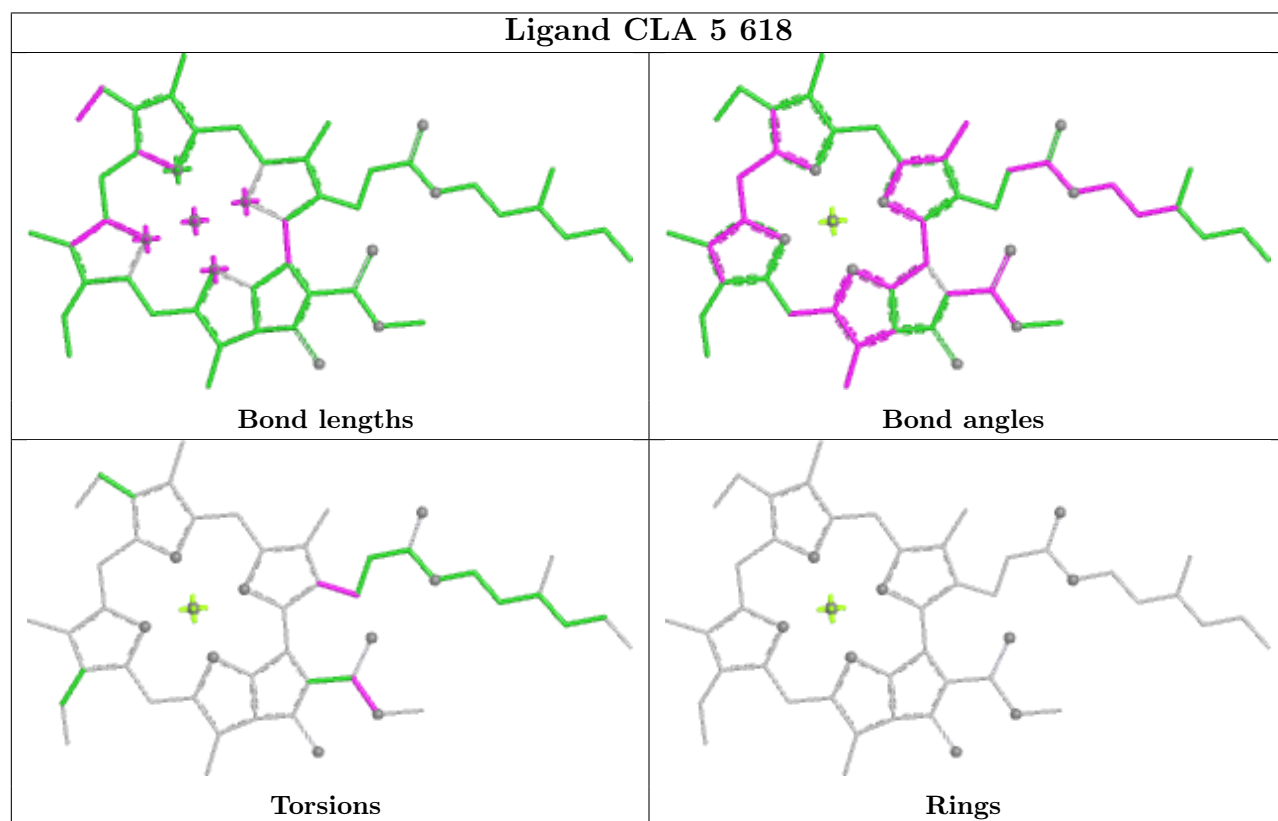
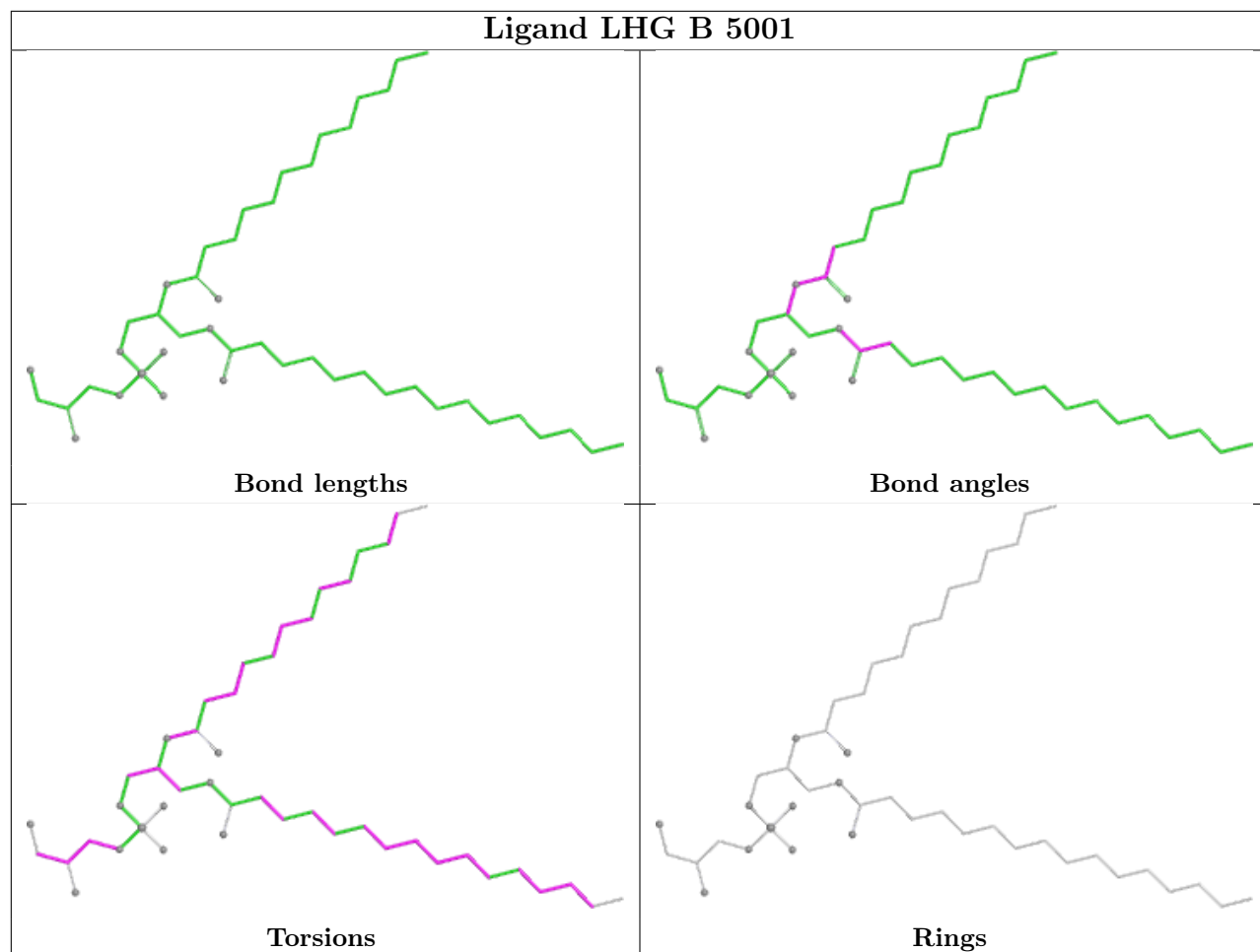


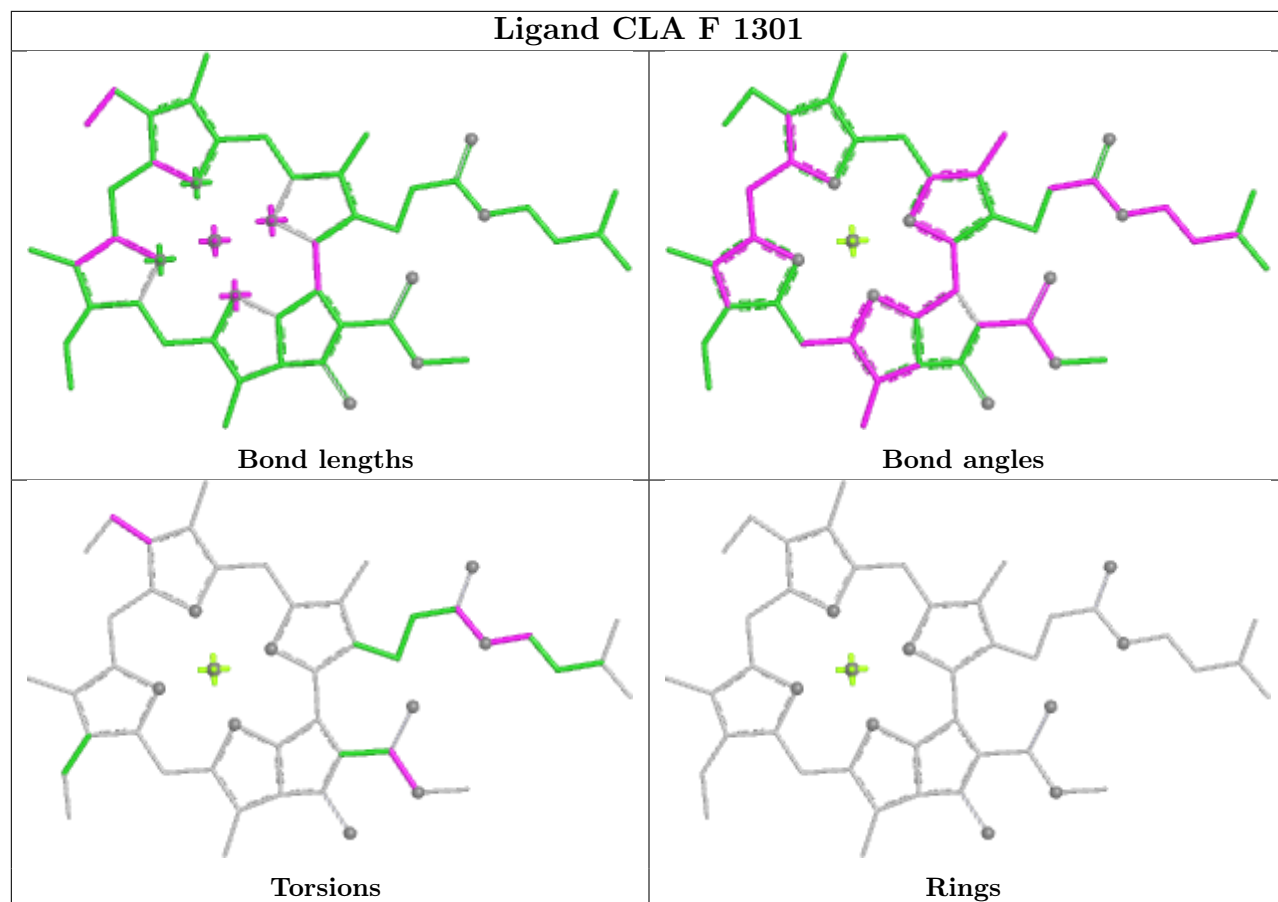


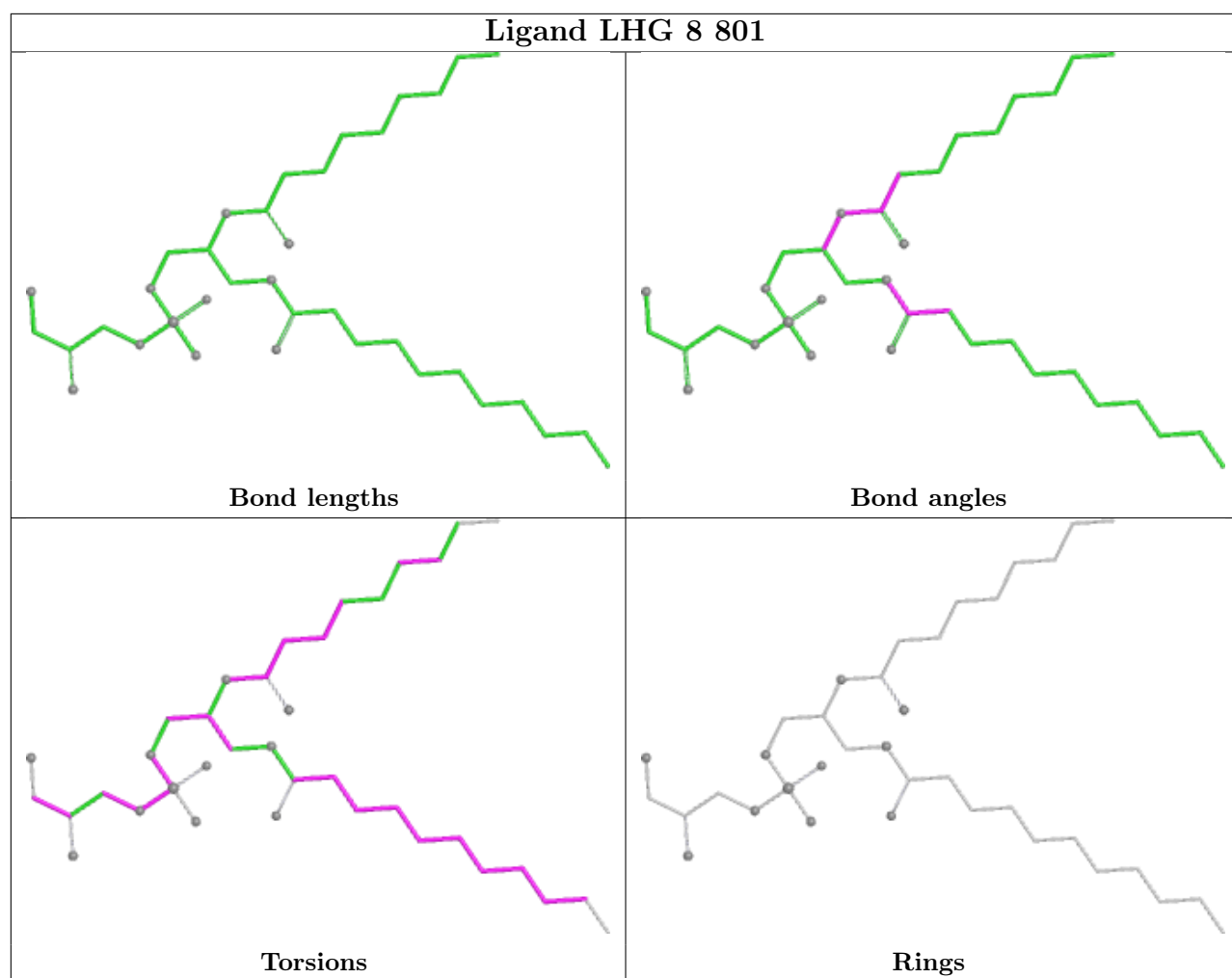




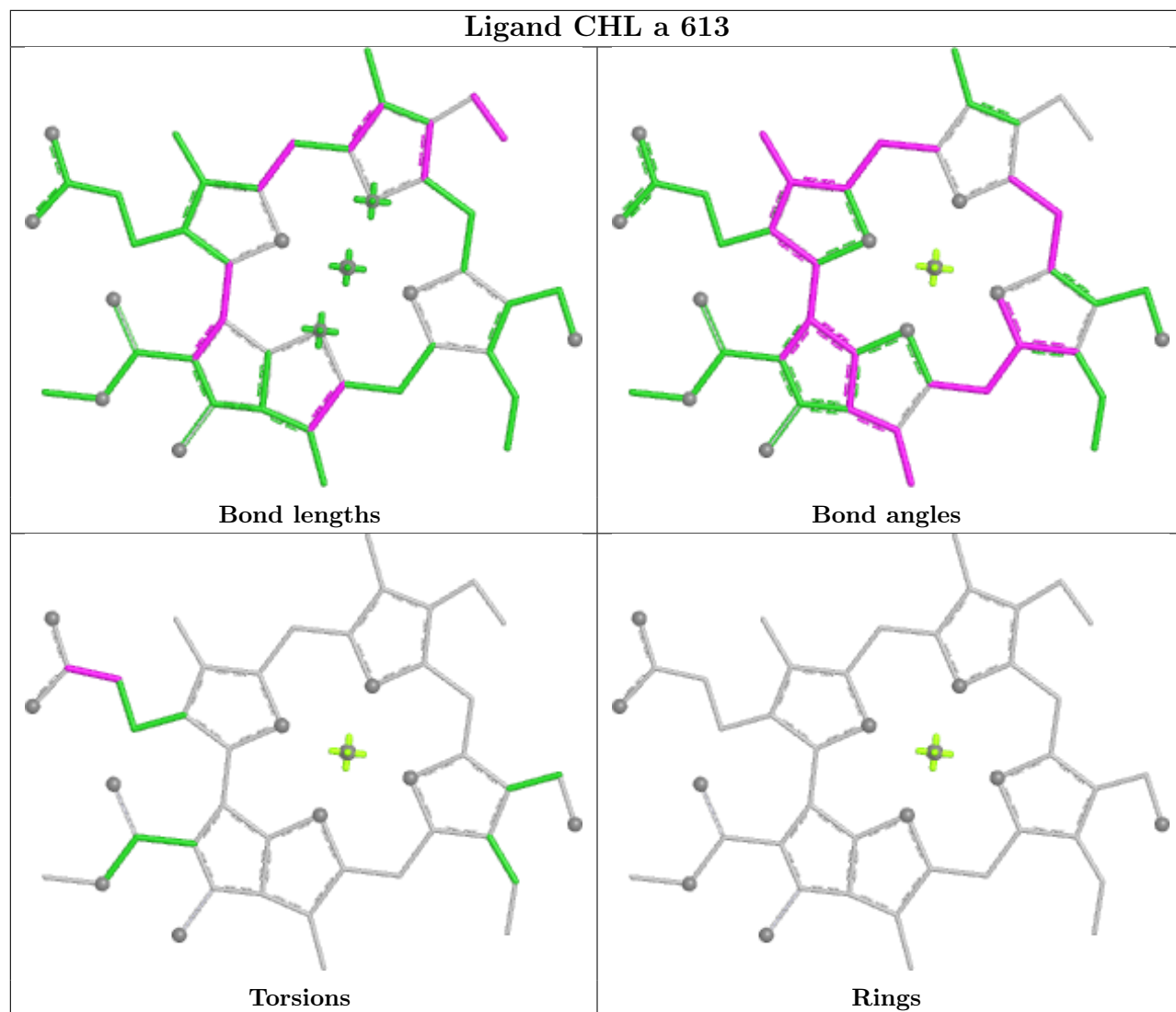




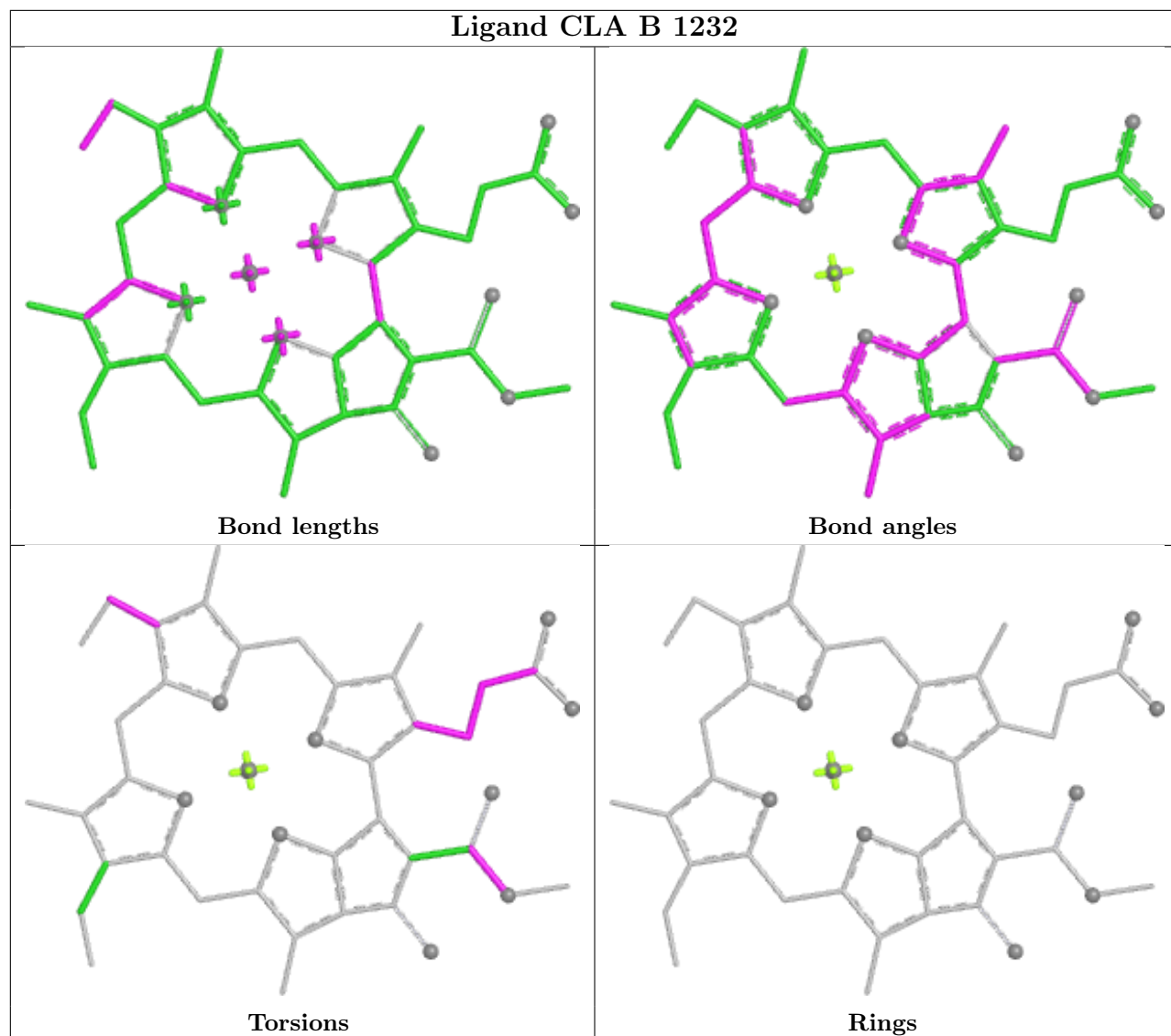




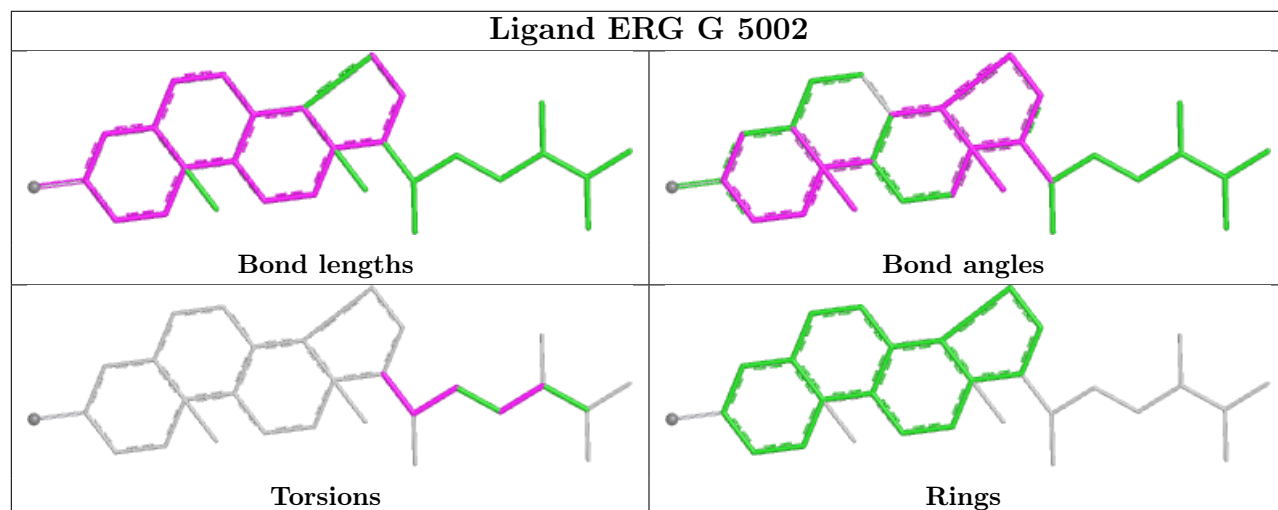
Ligand CHL a 613

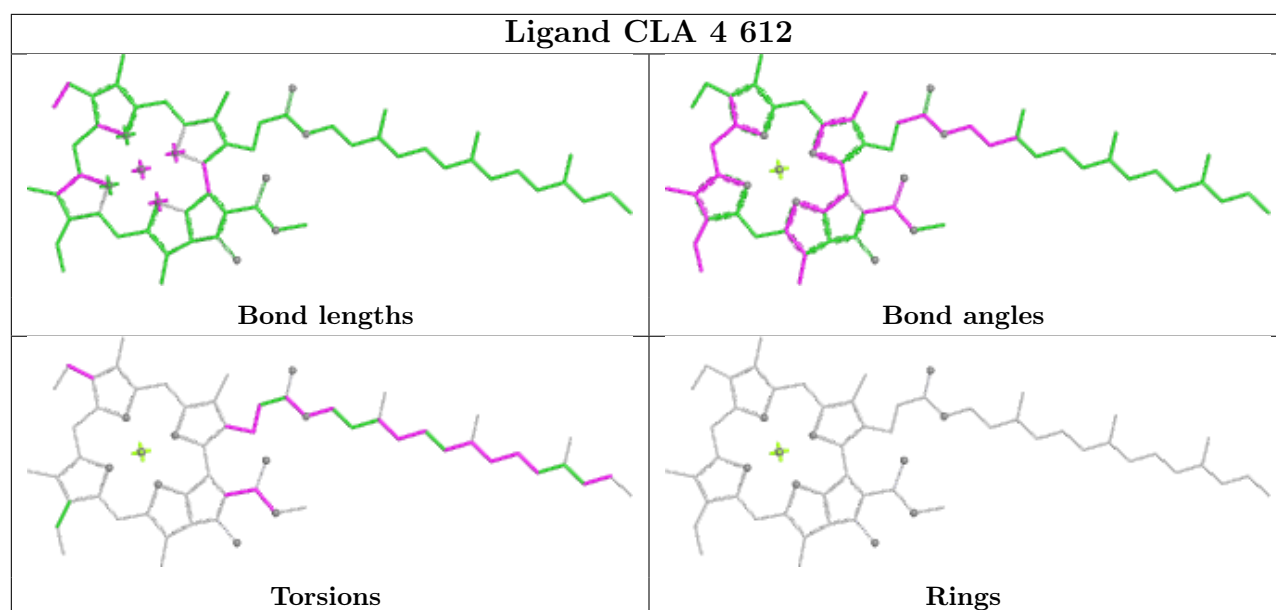


Ligand CLA B 1232



Ligand ERG G 5002





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.

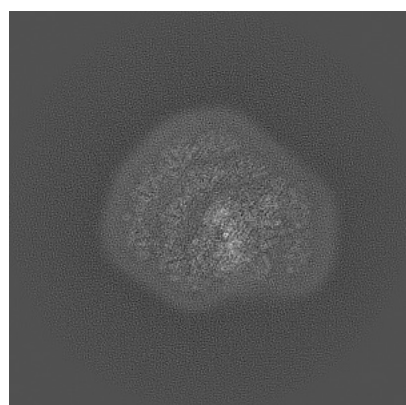
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11589. These allow visual inspection of the internal detail of the map and identification of artifacts.

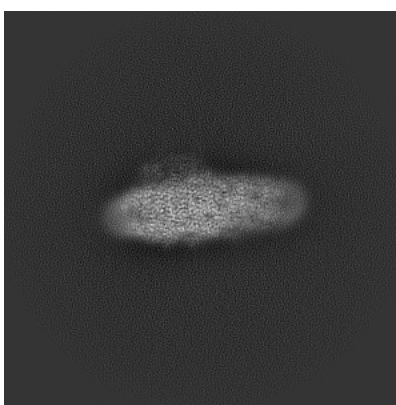
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

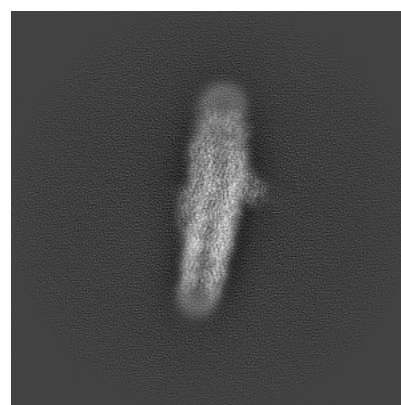
6.1.1 Primary map



X



Y

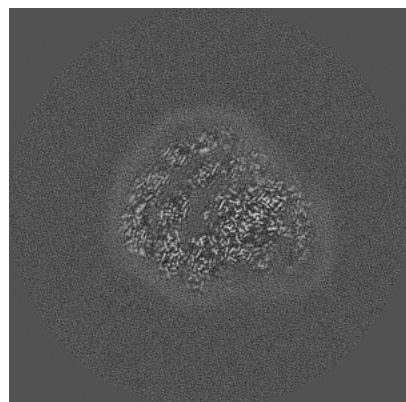


Z

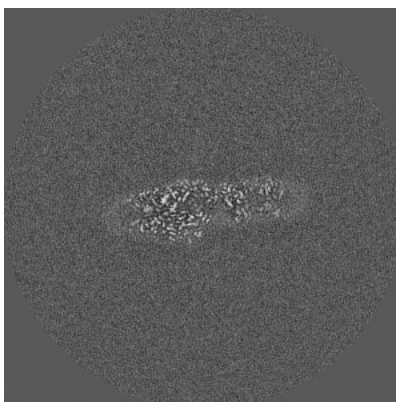
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

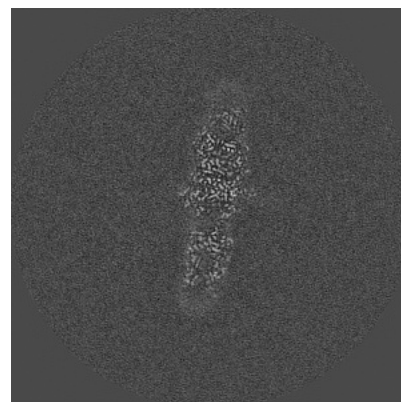
6.2.1 Primary map



X Index: 256



Y Index: 256

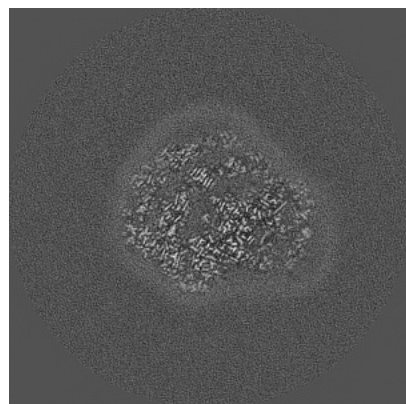


Z Index: 256

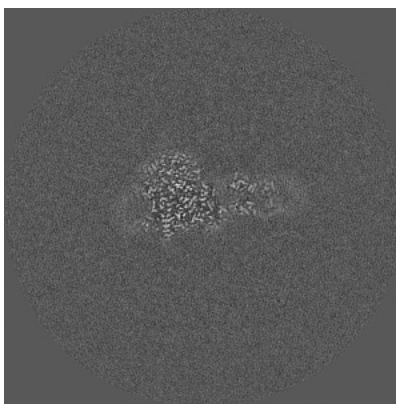
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

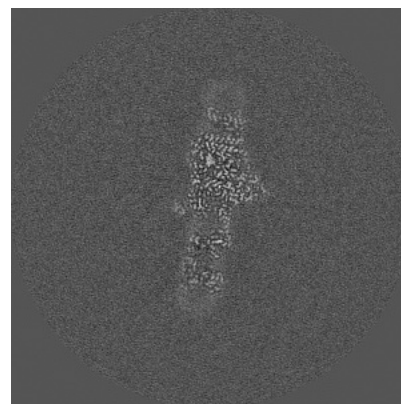
6.3.1 Primary map



X Index: 261



Y Index: 285

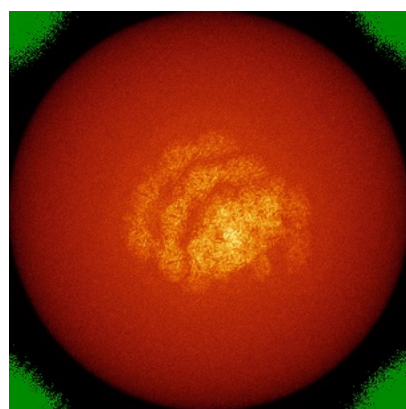


Z Index: 238

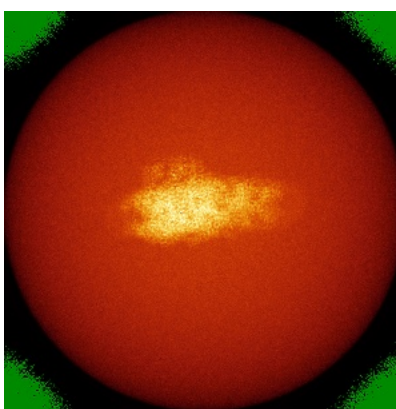
The images above show the largest variance slices of the map in three orthogonal directions.

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

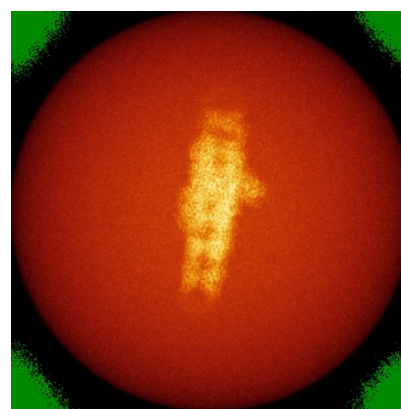
6.4.1 Primary map



X



Y

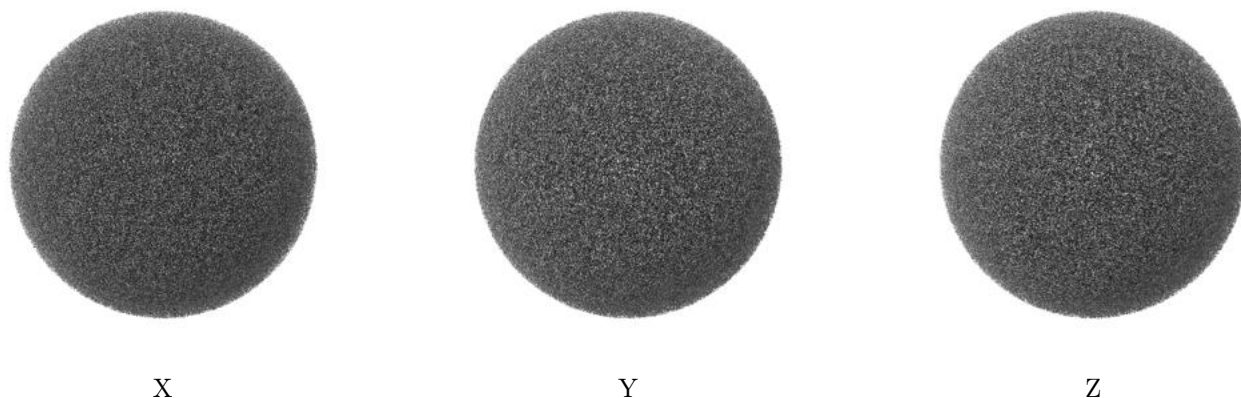


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

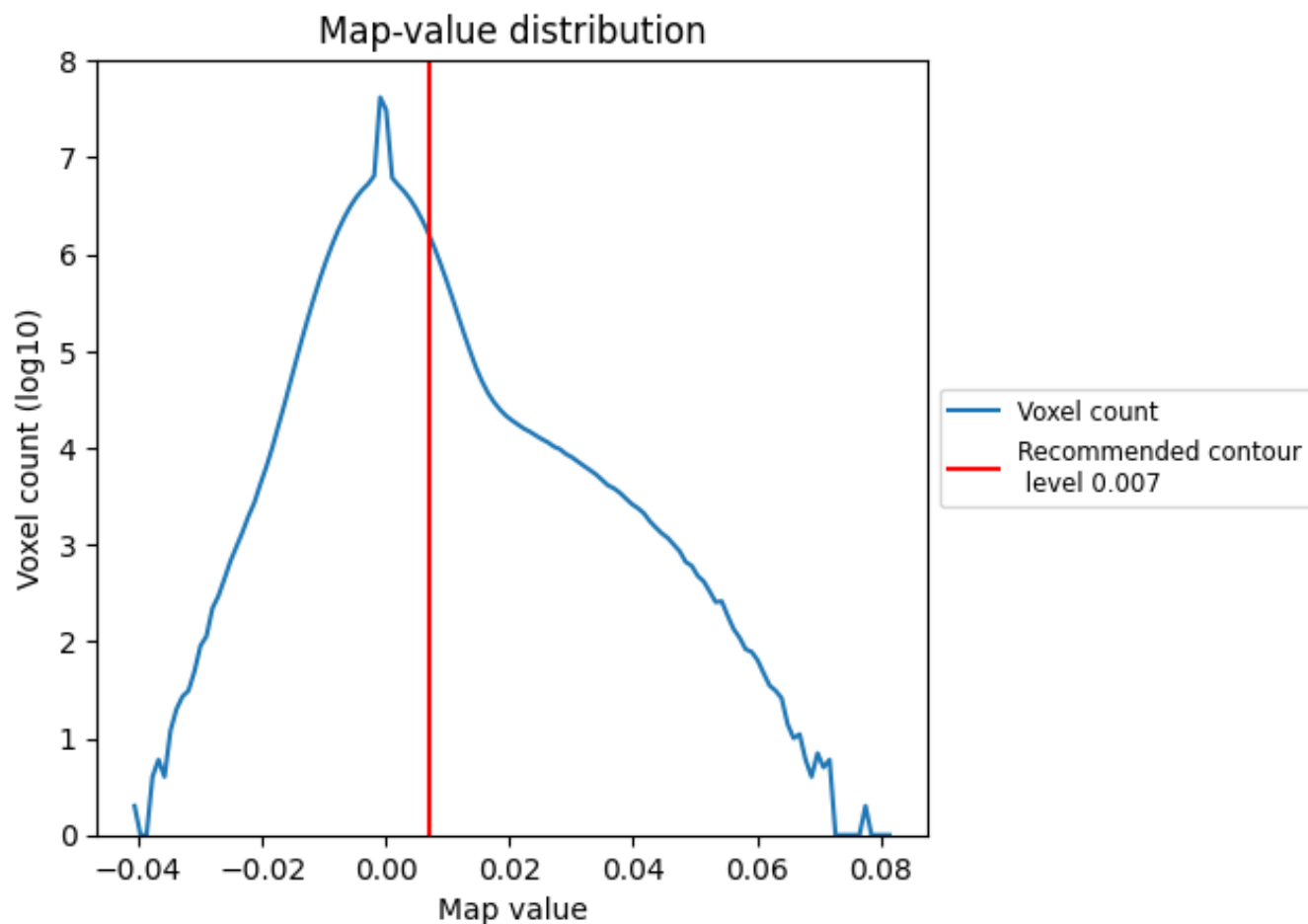
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

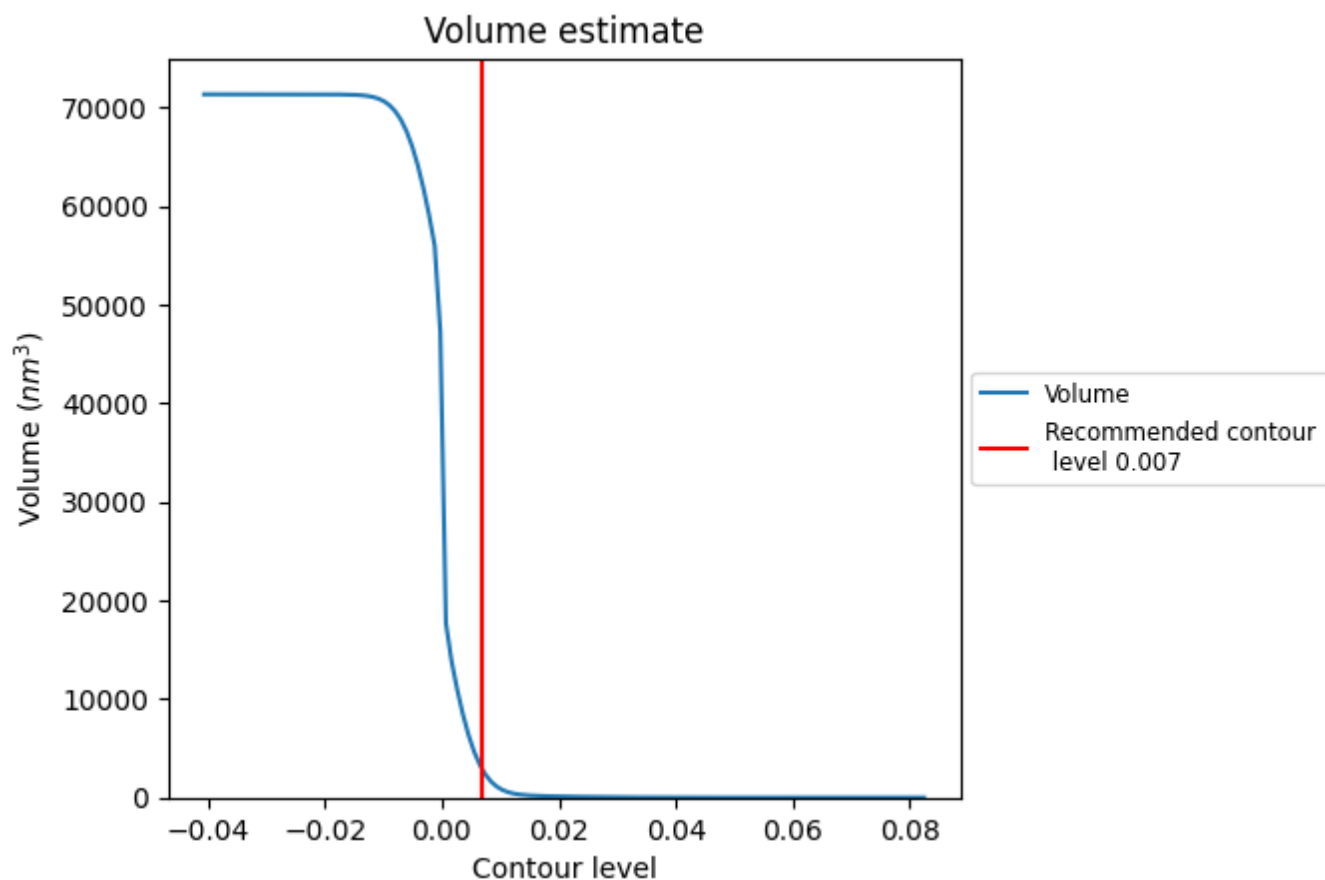
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

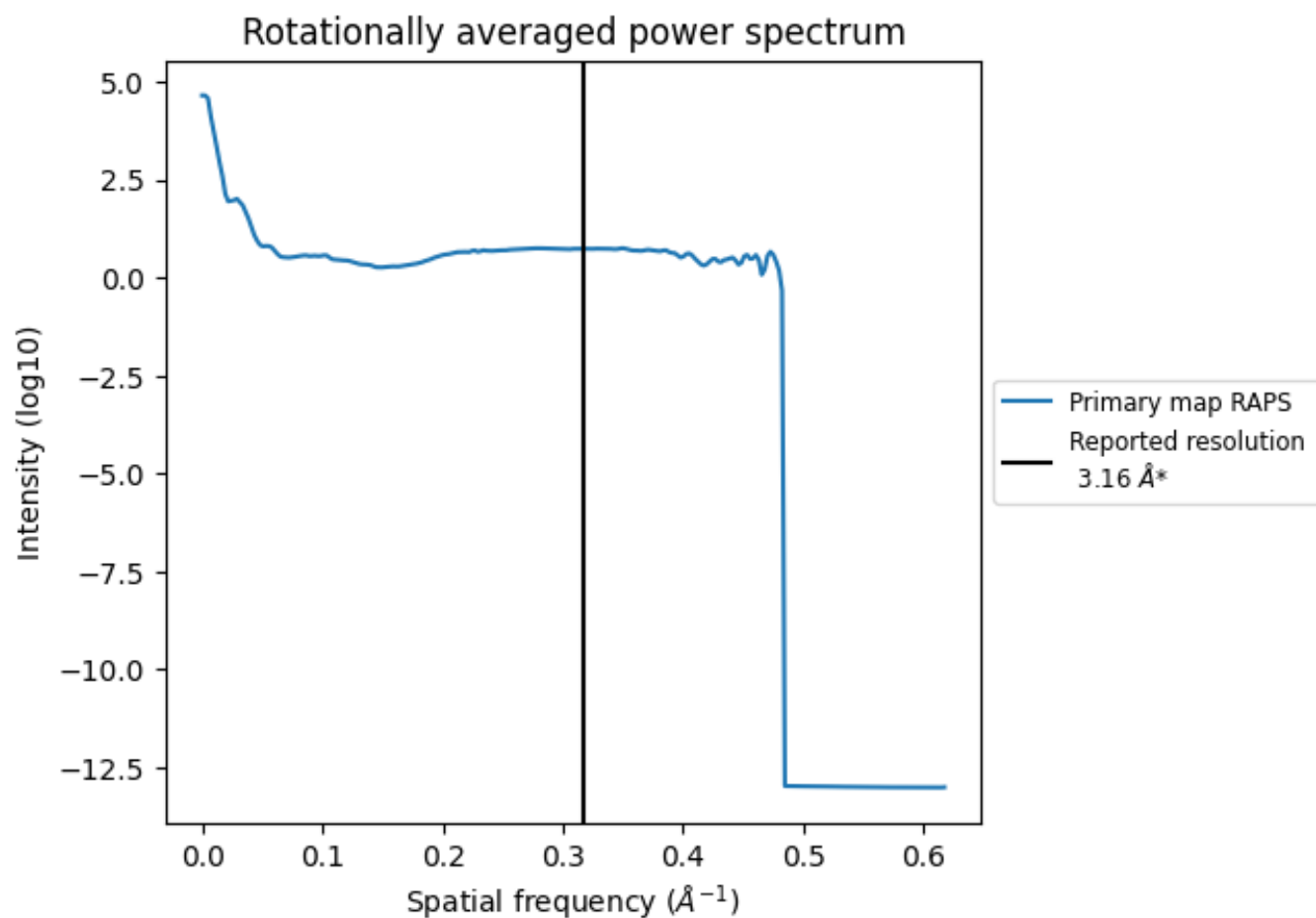
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2795 nm³; this corresponds to an approximate mass of 2525 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

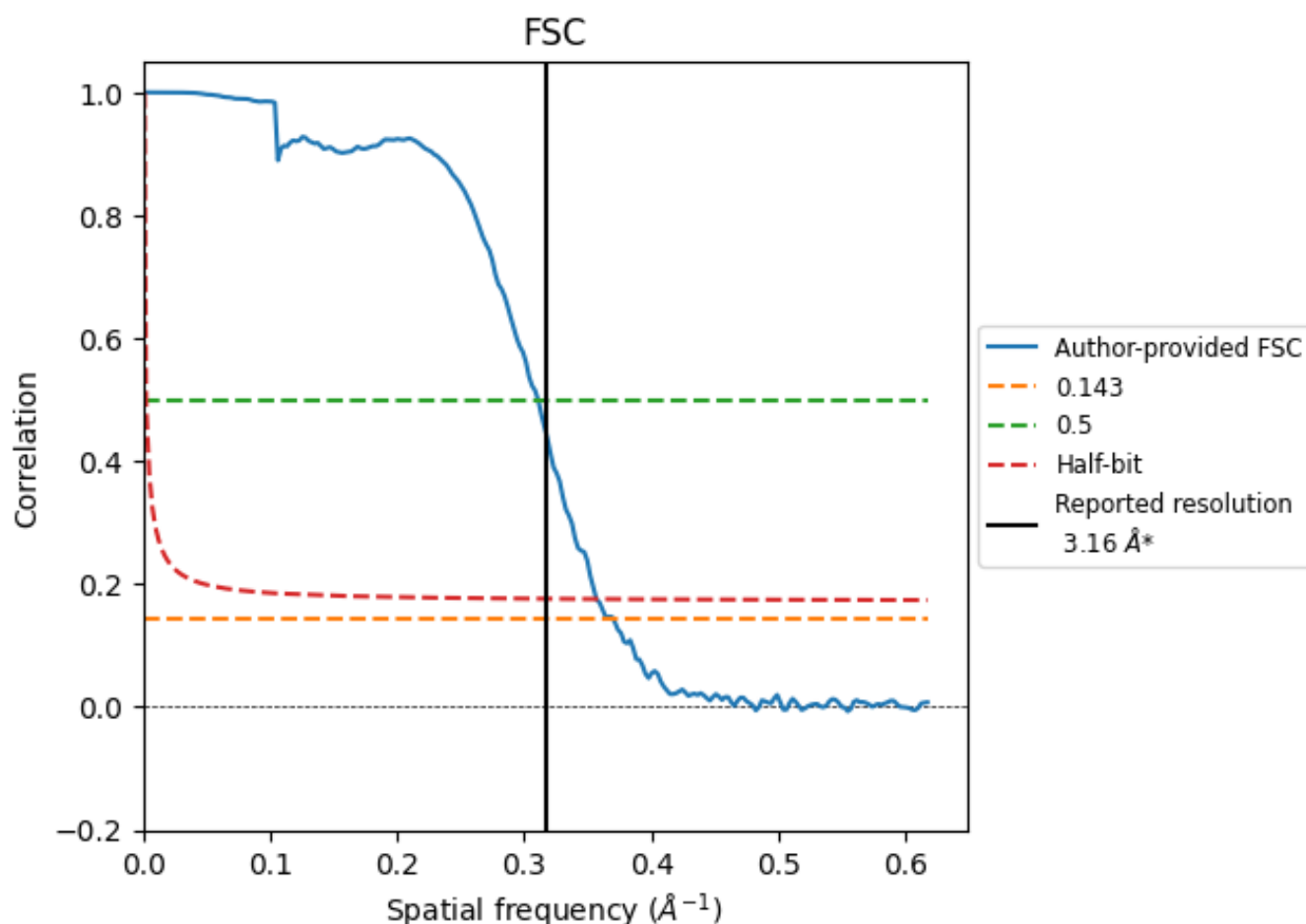


*Reported resolution corresponds to spatial frequency of 0.316 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.316 Å⁻¹

8.2 Resolution estimates [i](#)

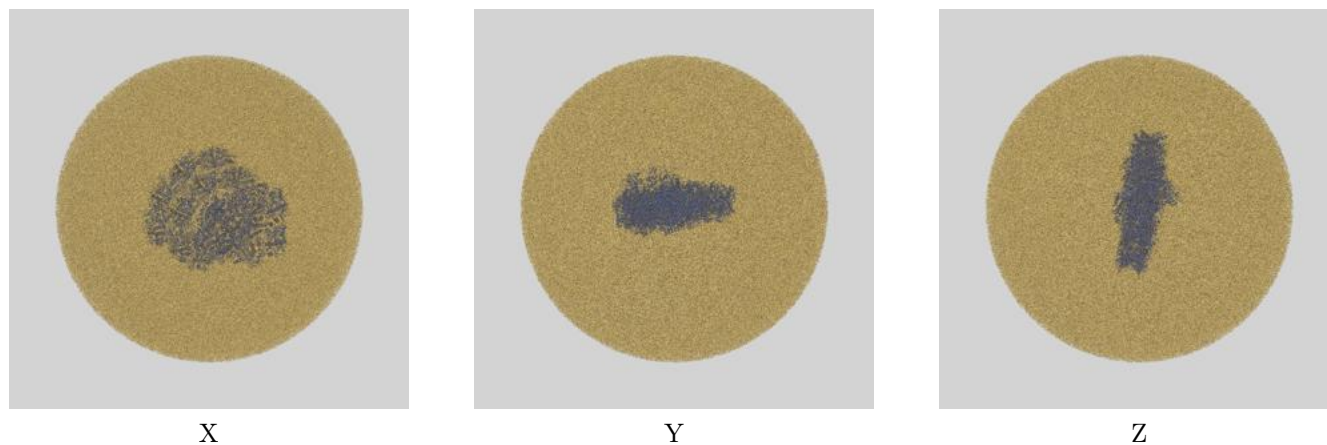
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.16	-	-
Author-provided FSC curve	2.70	3.22	2.80
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 2.70 differs from the reported value 3.16 by more than 10 %

9 Map-model fit [i](#)

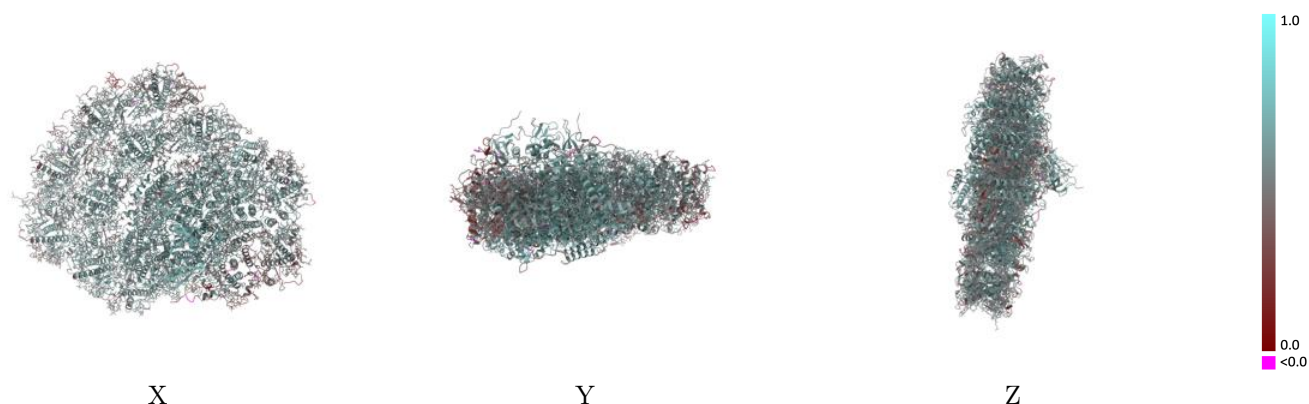
This section contains information regarding the fit between EMDB map EMD-11589 and PDB model 6ZZY. Per-residue inclusion information can be found in section [3](#) on page [52](#).

9.1 Map-model overlay [i](#)



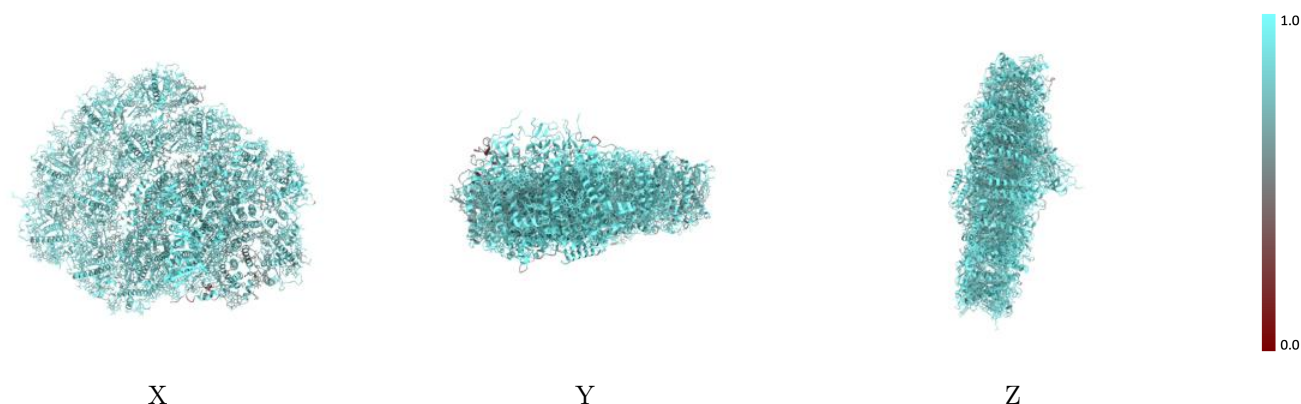
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



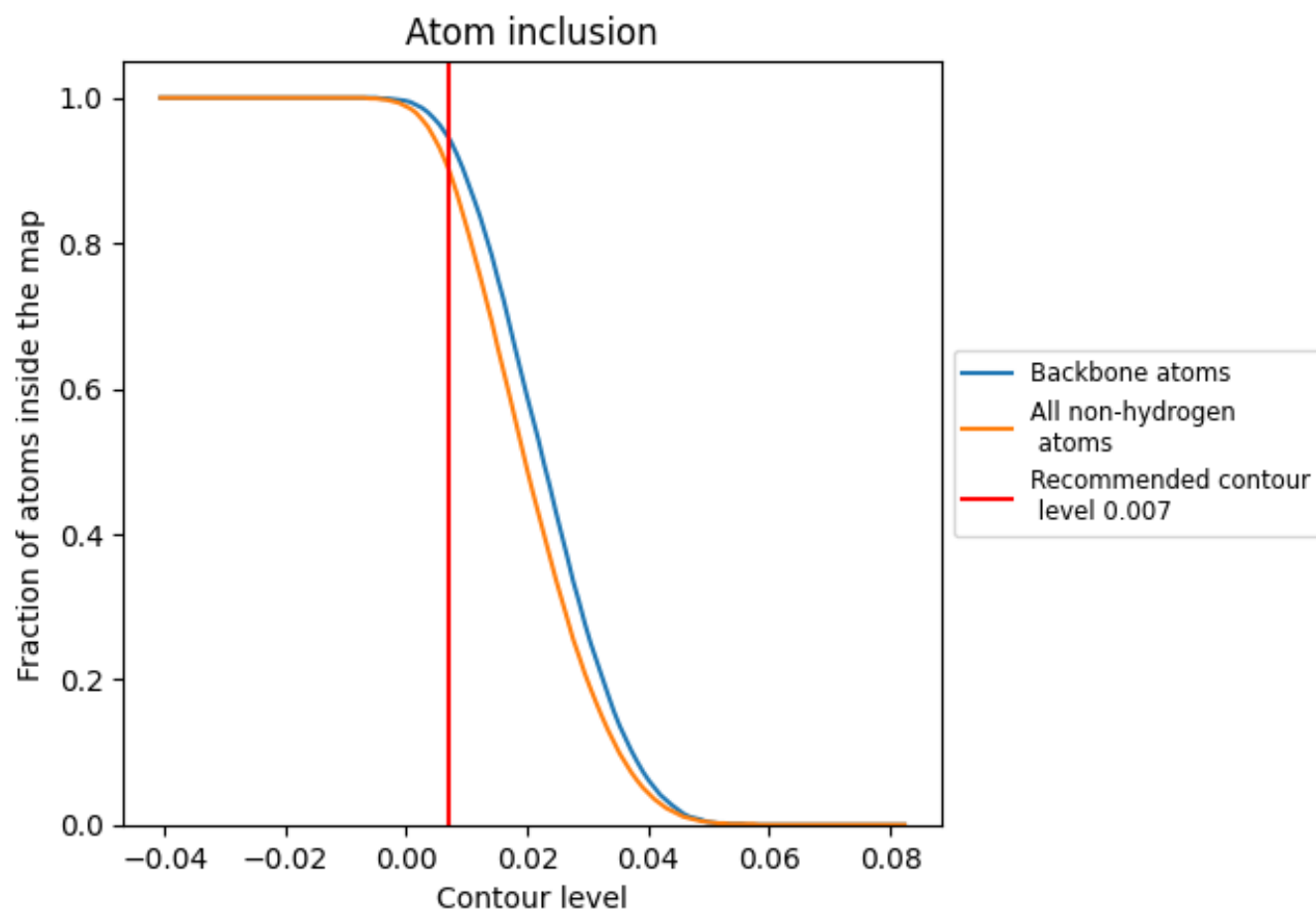
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.007).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 90% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9020	0.5610
1	0.8850	0.5400
2	0.8000	0.4480
3	0.9190	0.5830
4	0.8810	0.5090
5	0.8870	0.5350
6	0.8780	0.5150
7	0.9170	0.5720
8	0.9150	0.5740
9	0.8750	0.5300
A	0.9510	0.6240
B	0.9500	0.6240
C	0.9780	0.6340
D	0.9150	0.5590
E	0.9110	0.5560
F	0.9200	0.5790
G	0.8790	0.5390
H	0.6450	0.3690
I	0.8740	0.5420
J	0.9400	0.5980
K	0.8670	0.5190
L	0.8300	0.4810
M	0.9240	0.5900
a	0.8340	0.4620

1.0

0.0

<0.0