



Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 07:24 am GMT

PDB ID : 7A4P
EMDB ID : EMD-11640
Title : Structure of small high-light grown *Chlorella ohadii* photosystem I
Authors : Caspy, I.; Nelson, N.; Nechushtai, R.; Shkolnisky, Y.; Neumann, E.
Deposited on : 2020-08-20
Resolution : 4.20 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.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

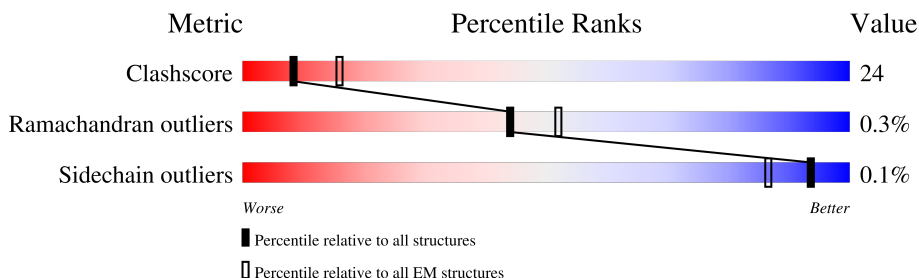
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	741	<div> <div>55%</div> <div>68%</div> <div>31%</div> <div>.</div> </div>
2	B	731	<div> <div>73%</div> <div>69%</div> <div>31%</div> <div>.</div> </div>
3	C	80	<div> <div>39%</div> <div>75%</div> <div>24%</div> <div>.</div> </div>
4	D	143	<div> <div>83%</div> <div>71%</div> <div>29%</div> <div>.</div> </div>
5	E	64	<div> <div>59%</div> <div>80%</div> <div>17%</div> <div>.</div> </div>
6	F	165	<div> <div>71%</div> <div>71%</div> <div>28%</div> <div>.</div> </div>
7	G	99	<div> <div>100%</div> <div>59%</div> <div>40%</div> <div>.</div> </div>
8	J	41	<div> <div>59%</div> <div>71%</div> <div>27%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
9	K	86	
10	M	31	
11	I	35	
12	L	157	
13	1	192	
13	a	192	
14	3	241	
15	4	207	
16	5	227	
17	6	231	
18	7	221	
19	8	219	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL0	A	1011	X	-	-	-
22	CLA	1	601	X	-	-	-
22	CLA	1	602	X	-	-	-
22	CLA	1	603	X	-	-	-
22	CLA	1	604	X	-	-	-
22	CLA	1	605	X	-	-	-
22	CLA	1	606	X	-	-	-
22	CLA	1	607	X	-	-	-
22	CLA	1	608	X	-	-	-
22	CLA	1	610	X	-	-	-
22	CLA	1	611	X	-	-	-
22	CLA	1	612	X	-	-	-
22	CLA	1	615	X	-	-	-
22	CLA	3	601	X	-	-	-
22	CLA	3	602	X	-	-	-
22	CLA	3	603	X	-	-	-
22	CLA	3	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	3	605	X	-	-	-
22	CLA	3	606	X	-	-	-
22	CLA	3	607	X	-	-	-
22	CLA	3	610	X	-	-	-
22	CLA	3	612	X	-	-	-
22	CLA	3	613	X	-	-	-
22	CLA	3	616	X	-	-	-
22	CLA	3	618	X	-	-	-
22	CLA	4	601	X	-	-	-
22	CLA	4	602	X	-	-	-
22	CLA	4	603	X	-	-	-
22	CLA	4	604	X	-	-	-
22	CLA	4	605	X	-	-	-
22	CLA	4	606	X	-	-	-
22	CLA	4	607	X	-	-	-
22	CLA	4	608	X	-	-	-
22	CLA	4	610	X	-	-	-
22	CLA	4	611	X	-	-	-
22	CLA	4	612	X	-	-	-
22	CLA	4	615	X	-	-	-
22	CLA	4	616	X	-	-	-
22	CLA	4	617	X	-	-	-
22	CLA	5	601	X	-	-	-
22	CLA	5	602	X	-	-	-
22	CLA	5	603	X	-	-	-
22	CLA	5	604	X	-	-	-
22	CLA	5	605	X	-	-	-
22	CLA	5	606	X	-	-	-
22	CLA	5	607	X	-	-	-
22	CLA	5	608	X	-	-	-
22	CLA	5	609	X	-	-	-
22	CLA	5	612	X	-	-	-
22	CLA	5	614	X	-	-	-
22	CLA	5	616	X	-	-	-
22	CLA	5	617	X	-	-	-
22	CLA	5	618	X	-	-	-
22	CLA	6	601	X	-	X	-
22	CLA	6	602	X	-	-	-
22	CLA	6	603	X	-	-	-
22	CLA	6	604	X	-	X	-
22	CLA	6	605	X	-	-	-
22	CLA	6	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	6	607	X	-	-	-
22	CLA	6	608	X	-	-	-
22	CLA	6	609	X	-	X	-
22	CLA	6	612	X	-	-	-
22	CLA	6	615	X	-	-	-
22	CLA	6	617	X	-	-	-
22	CLA	6	618	X	-	-	-
22	CLA	7	601	X	-	-	-
22	CLA	7	602	X	-	-	-
22	CLA	7	603	X	-	-	-
22	CLA	7	604	X	-	-	-
22	CLA	7	605	X	-	-	-
22	CLA	7	606	X	-	-	-
22	CLA	7	607	X	-	-	-
22	CLA	7	608	X	-	-	-
22	CLA	7	609	X	-	-	-
22	CLA	7	610	X	-	-	-
22	CLA	7	611	X	-	-	-
22	CLA	7	612	X	-	-	-
22	CLA	7	615	X	-	-	-
22	CLA	7	617	X	-	-	-
22	CLA	8	602	X	-	-	-
22	CLA	8	603	X	-	-	-
22	CLA	8	605	X	-	-	-
22	CLA	8	606	X	-	-	-
22	CLA	8	607	X	-	-	-
22	CLA	8	608	X	-	-	-
22	CLA	8	609	X	-	-	-
22	CLA	8	610	X	-	-	-
22	CLA	8	611	X	-	-	-
22	CLA	8	612	X	-	-	-
22	CLA	8	615	X	-	-	-
22	CLA	8	618	X	-	-	-
22	CLA	8	620	X	-	-	-
22	CLA	A	1012	X	-	-	-
22	CLA	A	1013	X	-	-	-
22	CLA	A	1101	X	-	-	-
22	CLA	A	1102	X	-	-	-
22	CLA	A	1103	X	-	-	-
22	CLA	A	1104	X	-	-	-
22	CLA	A	1105	X	-	-	-
22	CLA	A	1106	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	1107	X	-	-	-
22	CLA	A	1108	X	-	-	-
22	CLA	A	1109	X	-	-	-
22	CLA	A	1110	X	-	-	-
22	CLA	A	1111	X	-	-	-
22	CLA	A	1112	X	-	-	-
22	CLA	A	1113	X	-	-	-
22	CLA	A	1114	X	-	-	-
22	CLA	A	1115	X	-	-	-
22	CLA	A	1116	X	-	-	-
22	CLA	A	1117	X	-	-	-
22	CLA	A	1118	X	-	-	-
22	CLA	A	1119	X	-	-	-
22	CLA	A	1120	X	-	-	-
22	CLA	A	1121	X	-	-	-
22	CLA	A	1122	X	-	-	-
22	CLA	A	1123	X	-	-	-
22	CLA	A	1124	X	-	-	-
22	CLA	A	1125	X	-	-	-
22	CLA	A	1126	X	-	-	-
22	CLA	A	1127	X	-	-	-
22	CLA	A	1128	X	-	-	-
22	CLA	A	1129	X	-	-	-
22	CLA	A	1130	X	-	-	-
22	CLA	A	1131	X	-	-	-
22	CLA	A	1132	X	-	-	-
22	CLA	A	1133	X	-	-	-
22	CLA	A	1134	X	-	-	-
22	CLA	A	1135	X	-	-	-
22	CLA	A	1136	X	-	-	-
22	CLA	A	1137	X	-	-	-
22	CLA	A	1138	X	-	-	-
22	CLA	A	1139	X	-	-	-
22	CLA	A	1140	X	-	-	-
22	CLA	A	1141	X	-	-	-
22	CLA	B	1021	X	-	-	-
22	CLA	B	1022	X	-	-	-
22	CLA	B	1023	X	-	-	-
22	CLA	B	1201	X	-	-	-
22	CLA	B	1202	X	-	-	-
22	CLA	B	1203	X	-	-	-
22	CLA	B	1204	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	1205	X	-	-	-
22	CLA	B	1206	X	-	-	-
22	CLA	B	1207	X	-	-	-
22	CLA	B	1208	X	-	-	-
22	CLA	B	1209	X	-	-	-
22	CLA	B	1210	X	-	-	-
22	CLA	B	1211	X	-	-	-
22	CLA	B	1212	X	-	-	-
22	CLA	B	1213	X	-	-	-
22	CLA	B	1214	X	-	-	-
22	CLA	B	1215	X	-	-	-
22	CLA	B	1216	X	-	-	-
22	CLA	B	1217	X	-	-	-
22	CLA	B	1218	X	-	-	-
22	CLA	B	1219	X	-	-	-
22	CLA	B	1220	X	-	-	-
22	CLA	B	1221	X	-	-	-
22	CLA	B	1222	X	-	-	-
22	CLA	B	1223	X	-	-	-
22	CLA	B	1224	X	-	-	-
22	CLA	B	1225	X	-	-	-
22	CLA	B	1226	X	-	-	-
22	CLA	B	1227	X	-	-	-
22	CLA	B	1228	X	-	-	-
22	CLA	B	1229	X	-	-	-
22	CLA	B	1230	X	-	-	-
22	CLA	B	1231	X	-	-	-
22	CLA	B	1232	X	-	-	-
22	CLA	B	1234	X	-	-	-
22	CLA	B	1235	X	-	-	-
22	CLA	B	1236	X	-	-	-
22	CLA	B	1237	X	-	-	-
22	CLA	B	1238	X	-	-	-
22	CLA	B	1239	X	-	-	-
22	CLA	B	1240	X	-	-	-
22	CLA	F	1301	X	-	-	-
22	CLA	F	1302	X	-	-	-
22	CLA	G	1601	X	-	-	-
22	CLA	G	1602	X	-	-	-
22	CLA	G	1603	X	-	-	-
22	CLA	J	1901	X	-	-	-
22	CLA	K	1401	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	K	1402	X	-	-	-
22	CLA	K	1403	X	-	X	-
22	CLA	K	1404	X	-	-	-
22	CLA	L	1501	X	-	-	-
22	CLA	L	1502	X	-	-	-
22	CLA	L	1503	X	-	-	-
22	CLA	a	601	X	-	-	-
22	CLA	a	602	X	-	-	-
22	CLA	a	603	X	-	-	-
22	CLA	a	604	X	-	-	-
22	CLA	a	605	X	-	-	-
22	CLA	a	607	X	-	-	-
22	CLA	a	608	X	-	-	-
22	CLA	a	611	X	-	-	-
22	CLA	a	612	X	-	-	-
22	CLA	a	615	X	-	-	-
34	ERG	G	5002	X	-	-	-
35	RRX	J	4002	X	-	-	-
38	LUT	1	503	X	-	-	-
38	LUT	5	505	X	-	-	-
38	LUT	6	501	X	-	-	-
38	LUT	6	502	X	-	-	-
38	LUT	7	501	X	-	-	-
38	LUT	a	502	X	-	-	-
39	CHL	1	609	X	-	-	-
39	CHL	1	613	X	-	-	-
39	CHL	3	608	X	-	-	-
39	CHL	3	611	X	-	-	-
39	CHL	4	609	X	-	-	-
39	CHL	4	613	X	-	-	-
39	CHL	4	618	X	-	-	-
39	CHL	5	610	X	-	-	-
39	CHL	5	611	X	-	-	-
39	CHL	5	613	X	-	-	-
39	CHL	6	610	X	-	-	-
39	CHL	6	611	X	-	X	-
39	CHL	6	613	X	-	-	-
39	CHL	6	619	X	-	-	-
39	CHL	7	613	X	-	-	-
39	CHL	8	601	X	-	-	-
39	CHL	8	604	X	-	-	-
39	CHL	8	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
39	CHL	a	606	X	-	-	-
39	CHL	a	609	X	-	-	-
39	CHL	a	610	X	-	-	-
39	CHL	a	613	X	-	-	-
41	QTB	3	506	X	-	-	-
46	XAT	7	502	X	-	-	-
48	C7Z	7	504	X	-	-	-

2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 48636 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 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	4	LYS	THR	conflict	UNP W8SUA3
B	5	LEU	LYS	conflict	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	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 PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	140	Total	C	N	O	S	0	0
			1041	682	167	188	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 13 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1	192	Total	C	N	O	S	0	0
			1405	900	237	261	7		
13	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 14 is a protein called Glutathione reductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	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
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 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	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	conflict	UNP A0A2P6TQ14

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	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 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	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 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	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 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	8	219	Total	C	N	O	S	0	0
			1669	1073	285	305	6		

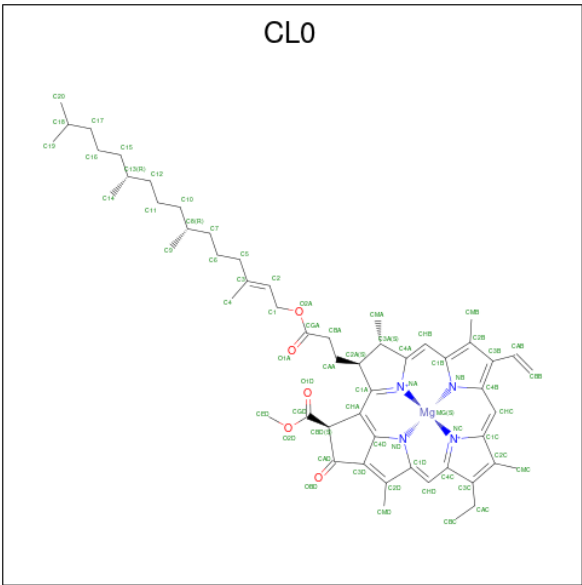
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 20 is a protein called Photosystem I reaction center subunit VI-chloroplastic-like.

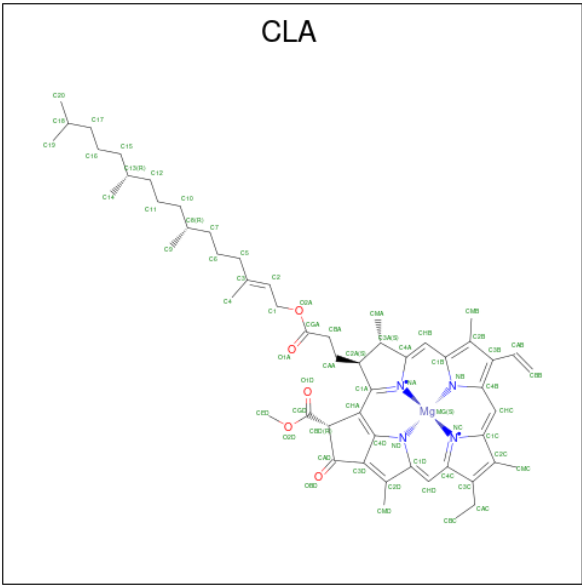
Mol	Chain	Residues	Atoms	AltConf	Trace
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- Molecule 21 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C₅₅H₇₂MgN₄O₅).



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

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	F	1	Total	C	Mg	N	O	0
			105	85	2	8	10	
22	F	1	Total	C	Mg	N	O	0
			105	85	2	8	10	

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Mol	Chain	Residues	Atoms					AltConf
22	G	1	Total 141	C 111	Mg 3	N 12	O 15	0
22	G	1	Total 141	C 111	Mg 3	N 12	O 15	0
22	G	1	Total 141	C 111	Mg 3	N 12	O 15	0
22	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	K	1	Total 204	C 164	Mg 4	N 16	O 20	0
22	K	1	Total 204	C 164	Mg 4	N 16	O 20	0
22	K	1	Total 204	C 164	Mg 4	N 16	O 20	0
22	K	1	Total 204	C 164	Mg 4	N 16	O 20	0
22	L	1	Total 155	C 125	Mg 3	N 12	O 15	0
22	L	1	Total 155	C 125	Mg 3	N 12	O 15	0
22	L	1	Total 155	C 125	Mg 3	N 12	O 15	0
22	1	1	Total 693	C 573	Mg 12	N 48	O 60	0
22	1	1	Total 693	C 573	Mg 12	N 48	O 60	0
22	1	1	Total 693	C 573	Mg 12	N 48	O 60	0
22	1	1	Total 693	C 573	Mg 12	N 48	O 60	0
22	1	1	Total 693	C 573	Mg 12	N 48	O 60	0
22	1	1	Total 693	C 573	Mg 12	N 48	O 60	0
22	1	1	Total 693	C 573	Mg 12	N 48	O 60	0
22	1	1	Total 693	C 573	Mg 12	N 48	O 60	0
22	1	1	Total 693	C 573	Mg 12	N 48	O 60	0
22	1	1	Total 693	C 573	Mg 12	N 48	O 60	0

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Mol	Chain	Residues	Atoms					AltConf
22	1	1	Total	C	Mg	N	O	0
			693	573	12	48	60	
22	1	1	Total	C	Mg	N	O	0
			693	573	12	48	60	
22	a	1	Total	C	Mg	N	O	0
			571	471	10	40	50	
22	a	1	Total	C	Mg	N	O	0
			571	471	10	40	50	
22	a	1	Total	C	Mg	N	O	0
			571	471	10	40	50	
22	a	1	Total	C	Mg	N	O	0
			571	471	10	40	50	
22	a	1	Total	C	Mg	N	O	0
			571	471	10	40	50	
22	a	1	Total	C	Mg	N	O	0
			571	471	10	40	50	
22	a	1	Total	C	Mg	N	O	0
			571	471	10	40	50	
22	a	1	Total	C	Mg	N	O	0
			571	471	10	40	50	
22	a	1	Total	C	Mg	N	O	0
			571	471	10	40	50	
22	3	1	Total	C	Mg	N	O	0
			719	599	12	48	60	
22	3	1	Total	C	Mg	N	O	0
			719	599	12	48	60	
22	3	1	Total	C	Mg	N	O	0
			719	599	12	48	60	
22	3	1	Total	C	Mg	N	O	0
			719	599	12	48	60	
22	3	1	Total	C	Mg	N	O	0
			719	599	12	48	60	
22	3	1	Total	C	Mg	N	O	0
			719	599	12	48	60	
22	3	1	Total	C	Mg	N	O	0
			719	599	12	48	60	
22	3	1	Total	C	Mg	N	O	0
			719	599	12	48	60	

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Mol	Chain	Residues	Atoms					AltConf
22	3	1	Total	C	Mg	N	O	0
			719	599	12	48	60	
22	3	1	Total	C	Mg	N	O	0
			719	599	12	48	60	
22	3	1	Total	C	Mg	N	O	0
			719	599	12	48	60	
22	4	1	Total	C	Mg	N	O	0
			768	628	14	56	70	
22	4	1	Total	C	Mg	N	O	0
			768	628	14	56	70	
22	4	1	Total	C	Mg	N	O	0
			768	628	14	56	70	
22	4	1	Total	C	Mg	N	O	0
			768	628	14	56	70	
22	4	1	Total	C	Mg	N	O	0
			768	628	14	56	70	
22	4	1	Total	C	Mg	N	O	0
			768	628	14	56	70	
22	4	1	Total	C	Mg	N	O	0
			768	628	14	56	70	
22	4	1	Total	C	Mg	N	O	0
			768	628	14	56	70	
22	4	1	Total	C	Mg	N	O	0
			768	628	14	56	70	
22	4	1	Total	C	Mg	N	O	0
			768	628	14	56	70	
22	4	1	Total	C	Mg	N	O	0
			768	628	14	56	70	
22	4	1	Total	C	Mg	N	O	0
			768	628	14	56	70	
22	5	1	Total	C	Mg	N	O	0
			739	599	14	56	70	
22	5	1	Total	C	Mg	N	O	0
			739	599	14	56	70	
22	5	1	Total	C	Mg	N	O	0
			739	599	14	56	70	
22	5	1	Total	C	Mg	N	O	0
			739	599	14	56	70	

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Mol	Chain	Residues	Atoms					AltConf
22	5	1	Total	C	Mg	N	O	0
			739	599	14	56	70	
22	5	1	Total	C	Mg	N	O	0
			739	599	14	56	70	
22	5	1	Total	C	Mg	N	O	0
			739	599	14	56	70	
22	5	1	Total	C	Mg	N	O	0
			739	599	14	56	70	
22	5	1	Total	C	Mg	N	O	0
			739	599	14	56	70	
22	5	1	Total	C	Mg	N	O	0
			739	599	14	56	70	
22	5	1	Total	C	Mg	N	O	0
			739	599	14	56	70	
22	5	1	Total	C	Mg	N	O	0
			739	599	14	56	70	
22	5	1	Total	C	Mg	N	O	0
			739	599	14	56	70	
22	6	1	Total	C	Mg	N	O	0
			711	581	13	52	65	
22	6	1	Total	C	Mg	N	O	0
			711	581	13	52	65	
22	6	1	Total	C	Mg	N	O	0
			711	581	13	52	65	
22	6	1	Total	C	Mg	N	O	0
			711	581	13	52	65	
22	6	1	Total	C	Mg	N	O	0
			711	581	13	52	65	
22	6	1	Total	C	Mg	N	O	0
			711	581	13	52	65	
22	6	1	Total	C	Mg	N	O	0
			711	581	13	52	65	
22	6	1	Total	C	Mg	N	O	0
			711	581	13	52	65	
22	6	1	Total	C	Mg	N	O	0
			711	581	13	52	65	
22	6	1	Total	C	Mg	N	O	0
			711	581	13	52	65	

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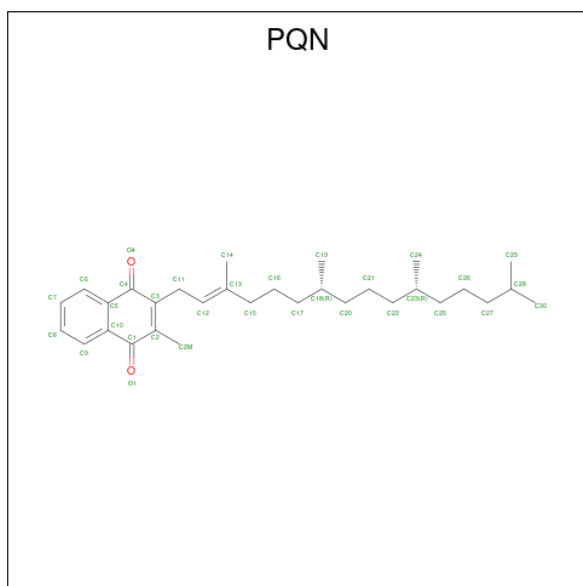
Mol	Chain	Residues	Atoms					AltConf
22	6	1	Total	C	Mg	N	O	0
			711	581	13	52	65	
22	6	1	Total	C	Mg	N	O	0
			711	581	13	52	65	
22	7	1	Total	C	Mg	N	O	0
			778	641	14	56	67	
22	7	1	Total	C	Mg	N	O	0
			778	641	14	56	67	
22	7	1	Total	C	Mg	N	O	0
			778	641	14	56	67	
22	7	1	Total	C	Mg	N	O	0
			778	641	14	56	67	
22	7	1	Total	C	Mg	N	O	0
			778	641	14	56	67	
22	7	1	Total	C	Mg	N	O	0
			778	641	14	56	67	
22	7	1	Total	C	Mg	N	O	0
			778	641	14	56	67	
22	7	1	Total	C	Mg	N	O	0
			778	641	14	56	67	
22	7	1	Total	C	Mg	N	O	0
			778	641	14	56	67	
22	7	1	Total	C	Mg	N	O	0
			778	641	14	56	67	
22	7	1	Total	C	Mg	N	O	0
			778	641	14	56	67	
22	7	1	Total	C	Mg	N	O	0
			778	641	14	56	67	
22	8	1	Total	C	Mg	N	O	0
			699	569	13	52	65	
22	8	1	Total	C	Mg	N	O	0
			699	569	13	52	65	
22	8	1	Total	C	Mg	N	O	0
			699	569	13	52	65	
22	8	1	Total	C	Mg	N	O	0
			699	569	13	52	65	
22	8	1	Total	C	Mg	N	O	0
			699	569	13	52	65	

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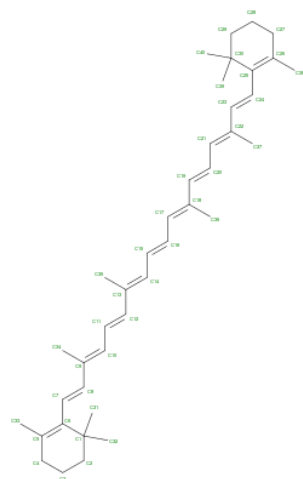
Mol	Chain	Residues	Atoms					AltConf
22	8	1	Total	C	Mg	N	O	0
			699	569	13	52	65	
22	8	1	Total	C	Mg	N	O	0
			699	569	13	52	65	
22	8	1	Total	C	Mg	N	O	0
			699	569	13	52	65	
22	8	1	Total	C	Mg	N	O	0
			699	569	13	52	65	
22	8	1	Total	C	Mg	N	O	0
			699	569	13	52	65	
22	8	1	Total	C	Mg	N	O	0
			699	569	13	52	65	
22	8	1	Total	C	Mg	N	O	0
			699	569	13	52	65	

- Molecule 23 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



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

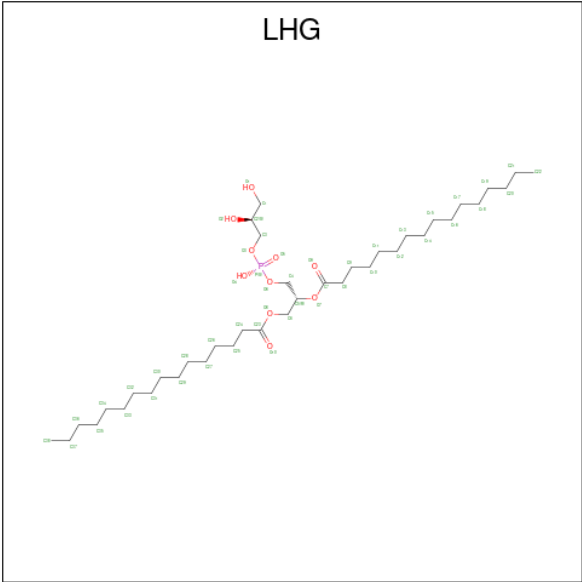
- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).

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Mol	Chain	Residues	Atoms		AltConf
24	J	1	Total 40	C 40	0
24	K	1	Total 80	C 80	0
24	K	1	Total 80	C 80	0
24	I	1	Total 40	C 40	0
24	L	1	Total 120	C 120	0
24	L	1	Total 120	C 120	0
24	L	1	Total 120	C 120	0
24	3	1	Total 120	C 120	0
24	3	1	Total 120	C 120	0
24	3	1	Total 120	C 120	0
24	4	1	Total 40	C 40	0
24	5	1	Total 80	C 80	0
24	5	1	Total 80	C 80	0
24	6	1	Total 80	C 80	0
24	6	1	Total 80	C 80	0
24	7	1	Total 40	C 40	0
24	8	1	Total 40	C 40	0

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



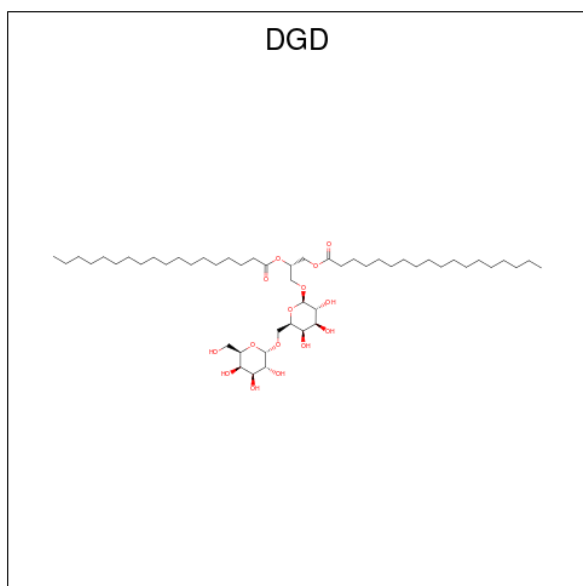
Mol	Chain	Residues	Atoms				AltConf
25	A	1	Total	C	O	P	0
			120	87	30	3	
25	A	1	Total	C	O	P	0
			120	87	30	3	
25	A	1	Total	C	O	P	0
			120	87	30	3	
25	B	1	Total	C	O	P	0
			95	73	20	2	
25	B	1	Total	C	O	P	0
			95	73	20	2	
25	F	1	Total	C	O	P	0
			79	57	20	2	
25	F	1	Total	C	O	P	0
			79	57	20	2	
25	1	1	Total	C	O	P	0
			77	55	20	2	
25	1	1	Total	C	O	P	0
			77	55	20	2	
25	a	1	Total	C	O	P	0
			35	24	10	1	
25	3	1	Total	C	O	P	0
			49	38	10	1	
25	4	1	Total	C	O	P	0
			81	59	20	2	
25	4	1	Total	C	O	P	0
			81	59	20	2	
25	5	1	Total	C	O	P	0
			49	38	10	1	

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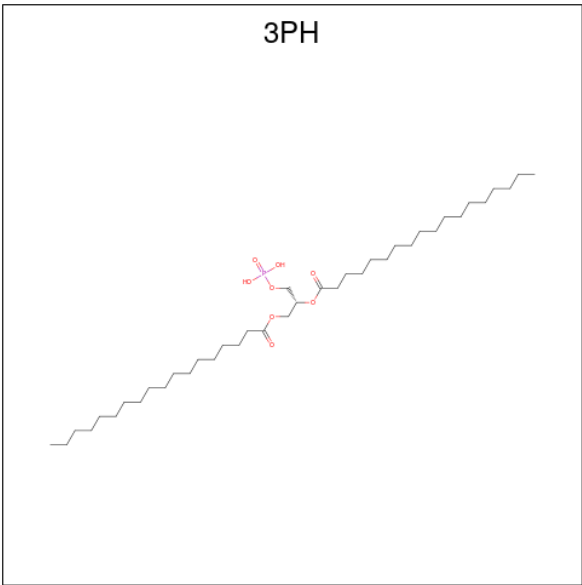
Mol	Chain	Residues	Atoms				AltConf
25	6	1	Total	C	O	P	0
			86	64	20	2	
25	6	1	Total	C	O	P	0
			86	64	20	2	
25	7	1	Total	C	O	P	0
			128	95	30	3	
25	7	1	Total	C	O	P	0
			128	95	30	3	
25	7	1	Total	C	O	P	0
			128	95	30	3	
25	8	1	Total	C	O	P	0
			37	26	10	1	

- Molecule 26 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



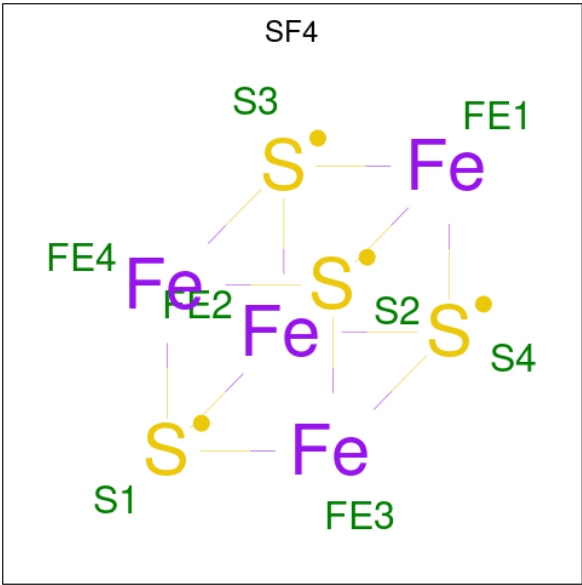
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			51	36	15	
26	B	1	Total	C	O	0
			66	51	15	
26	8	1	Total	C	O	0
			66	51	15	

- Molecule 27 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: $C_{39}H_{77}O_8P$).



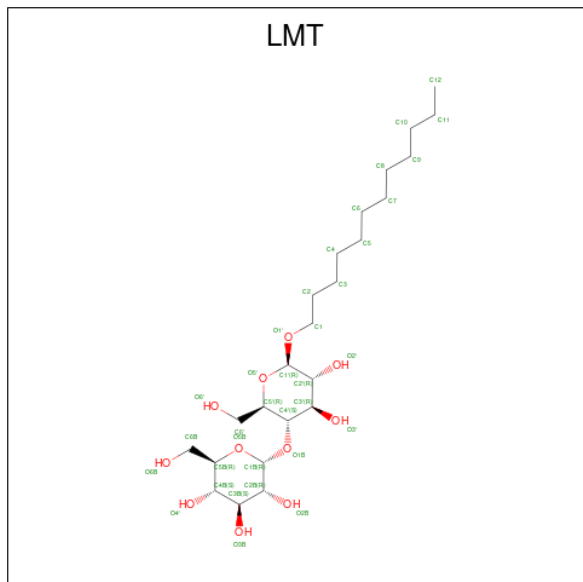
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
27	A	1	33	24	8	1	0

- Molecule 28 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



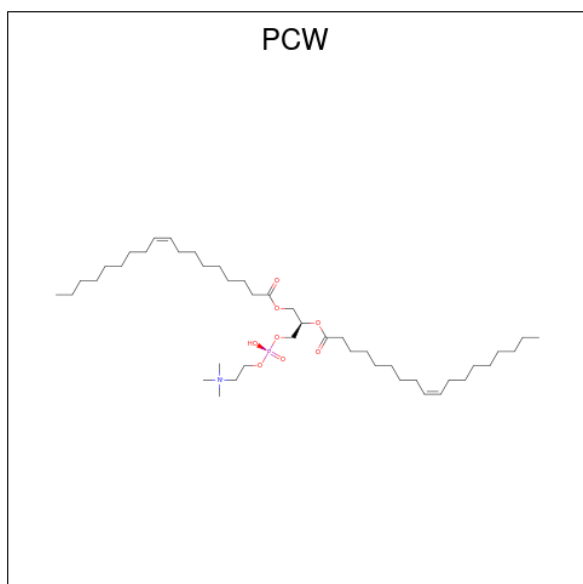
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
28	A	1	8	4	4	0
28	C	1	16	8	8	0
28	C	1	16	8	8	0

- Molecule 29 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



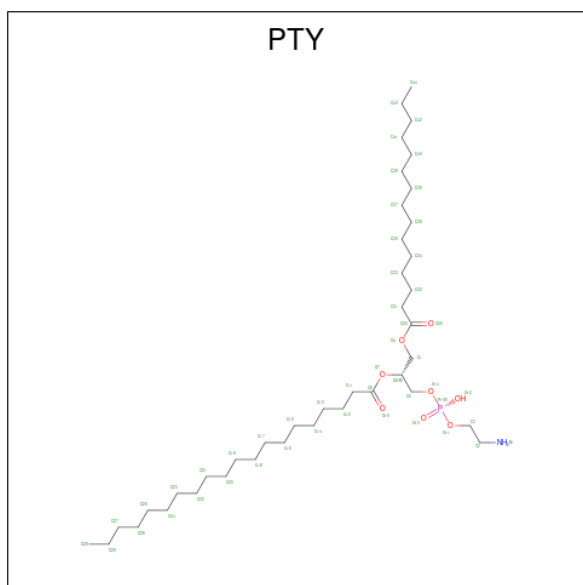
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			35	24	11	
29	B	1	Total	C	O	0
			35	24	11	
29	1	1	Total	C	O	0
			35	24	11	

- Molecule 30 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).



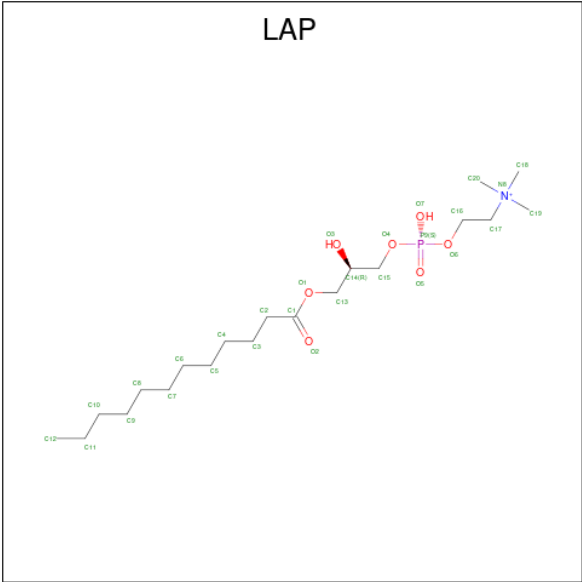
Mol	Chain	Residues	Atoms					AltConf
30	B	1	Total	C	N	O	P	0
			30	20	1	8	1	
30	6	1	Total	C	N	O	P	0
			36	26	1	8	1	

- Molecule 31 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



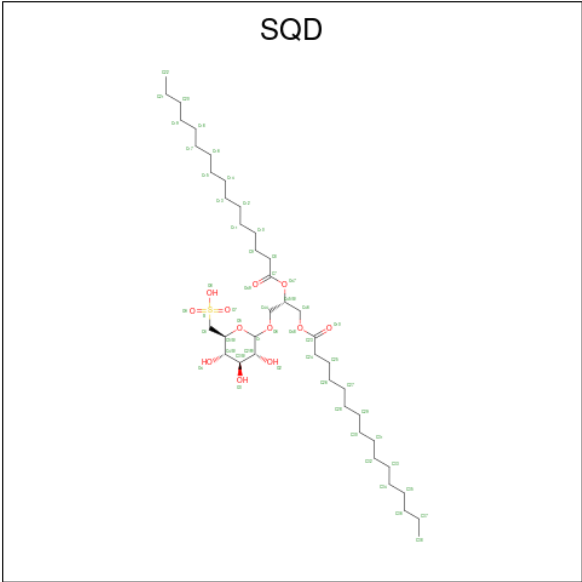
Mol	Chain	Residues	Atoms					AltConf
31	B	1	Total	C	N	O	P	0
			41	31	1	8	1	
31	3	1	Total	C	N	O	P	0
			38	28	1	8	1	
31	5	1	Total	C	N	O	P	0
			38	28	1	8	1	
31	7	1	Total	C	N	O	P	0
			33	23	1	8	1	
31	8	1	Total	C	N	O	P	0
			35	25	1	8	1	

- Molecule 32 is [2-((1-OXODODECANOXY-(2-HYDROXY-3-PROPANYL))-PHOSPHONATE-OXY)-ETHYL]-TRIMETHYLAMMONIUM (three-letter code: LAP) (formula: $C_{20}H_{43}NO_7P$).



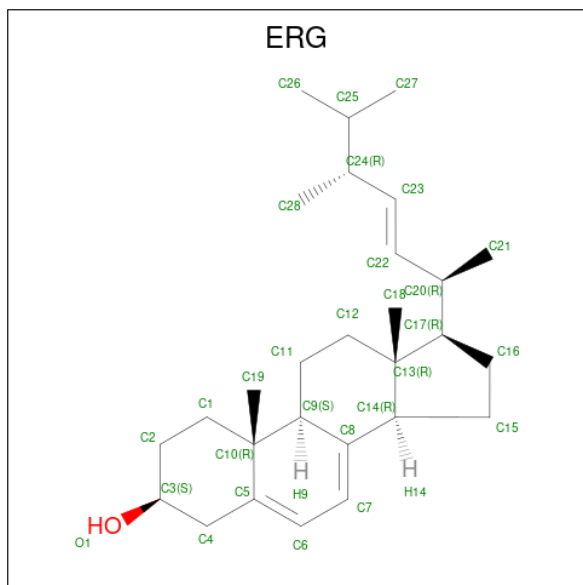
Mol	Chain	Residues	Atoms					AltConf
32	B	1	Total	C	N	O	P	0
			29	20	1	7	1	
32	F	1	Total	C	N	O	P	0
			29	20	1	7	1	
32	K	1	Total	C	N	O	P	0
			29	20	1	7	1	

- Molecule 33 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



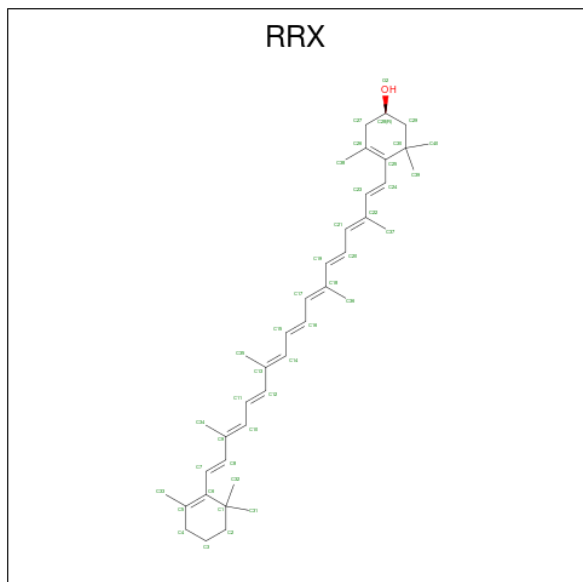
Mol	Chain	Residues	Atoms				AltConf
33	G	1	Total	C	O	S	0
			46	33	12	1	
33	7	1	Total	C	O	S	0
			39	26	12	1	

- Molecule 34 is ERGOSTEROL (three-letter code: ERG) (formula: $C_{28}H_{44}O$).



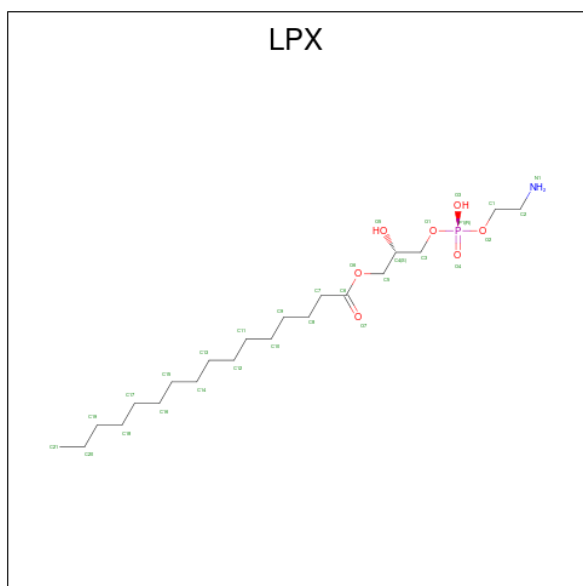
Mol	Chain	Residues	Atoms				AltConf
34	G	1	Total	C	O		0
			29	28	1		

- Molecule 35 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: $C_{40}H_{56}O$).



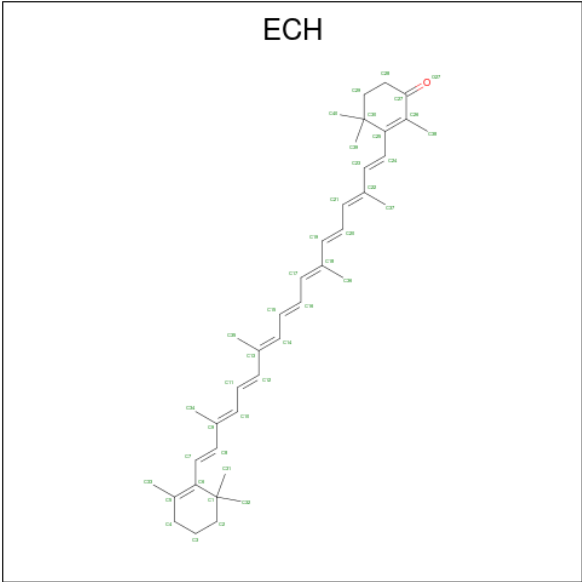
Mol	Chain	Residues	Atoms			AltConf
35	J	1	Total	C	O	0
			41	40	1	

- Molecule 36 is (2S)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (three-letter code: LPX) (formula: C₂₁H₄₄NO₇P).



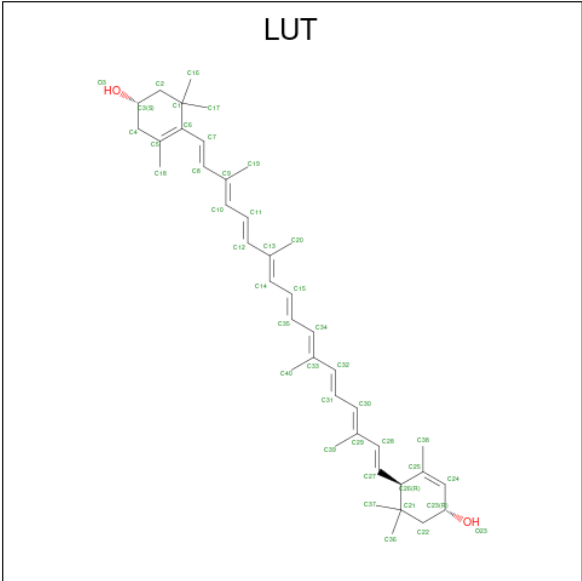
Mol	Chain	Residues	Atoms					AltConf
36	J	1	Total	C	N	O	P	0
			17	8	1	7	1	
36	a	1	Total	C	N	O	P	0
			30	21	1	7	1	

- Molecule 37 is beta,beta-caroten-4-one (three-letter code: ECH) (formula: C₄₀H₅₄O).



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

- Molecule 38 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



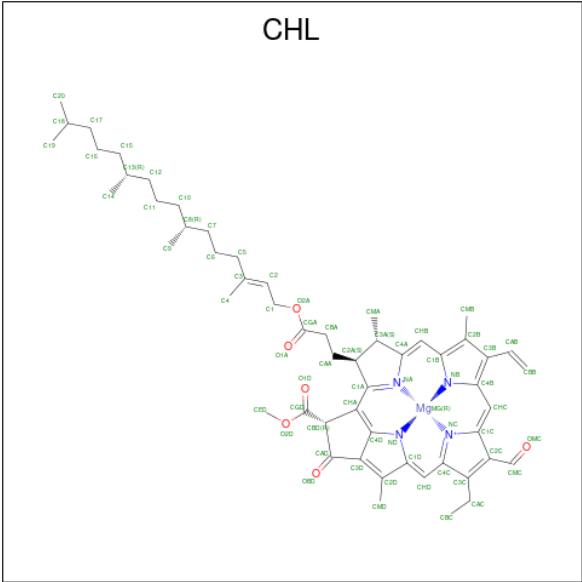
Mol	Chain	Residues	Atoms			AltConf
38	1	1	Total	C	O	0
			126	120	6	
38	1	1	Total	C	O	0
			126	120	6	

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Mol	Chain	Residues	Atoms			AltConf
38	1	1	Total	C	O	0
			126	120	6	
38	a	1	Total	C	O	0
			126	120	6	
38	a	1	Total	C	O	0
			126	120	6	
38	a	1	Total	C	O	0
			126	120	6	
38	3	1	Total	C	O	0
			84	80	4	
38	3	1	Total	C	O	0
			84	80	4	
38	4	1	Total	C	O	0
			84	80	4	
38	4	1	Total	C	O	0
			84	80	4	
38	5	1	Total	C	O	0
			126	120	6	
38	5	1	Total	C	O	0
			126	120	6	
38	5	1	Total	C	O	0
			126	120	6	
38	6	1	Total	C	O	0
			84	80	4	
38	6	1	Total	C	O	0
			84	80	4	
38	7	1	Total	C	O	0
			42	40	2	
38	8	1	Total	C	O	0
			84	80	4	
38	8	1	Total	C	O	0
			84	80	4	

- Molecule 39 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



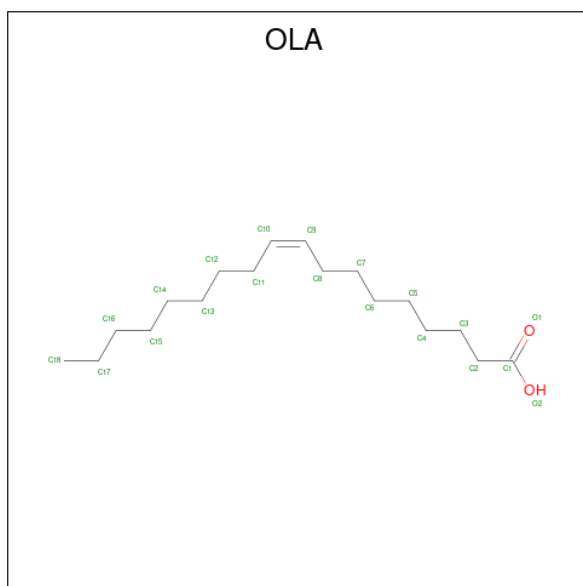
Mol	Chain	Residues	Atoms					AltConf
39	1	1	Total	C	Mg	N	O	0
			114	92	2	8	12	
39	1	1	Total	C	Mg	N	O	0
			114	92	2	8	12	
39	a	1	Total	C	Mg	N	O	0
			203	159	4	16	24	
39	a	1	Total	C	Mg	N	O	0
			203	159	4	16	24	
39	a	1	Total	C	Mg	N	O	0
			203	159	4	16	24	
39	a	1	Total	C	Mg	N	O	0
			203	159	4	16	24	
39	3	1	Total	C	Mg	N	O	0
			98	78	2	8	10	
39	3	1	Total	C	Mg	N	O	0
			98	78	2	8	10	
39	4	1	Total	C	Mg	N	O	0
			174	141	3	12	18	
39	4	1	Total	C	Mg	N	O	0
			174	141	3	12	18	
39	4	1	Total	C	Mg	N	O	0
			174	141	3	12	18	
39	5	1	Total	C	Mg	N	O	0
			173	140	3	12	18	
39	5	1	Total	C	Mg	N	O	0
			173	140	3	12	18	
39	5	1	Total	C	Mg	N	O	0
			173	140	3	12	18	

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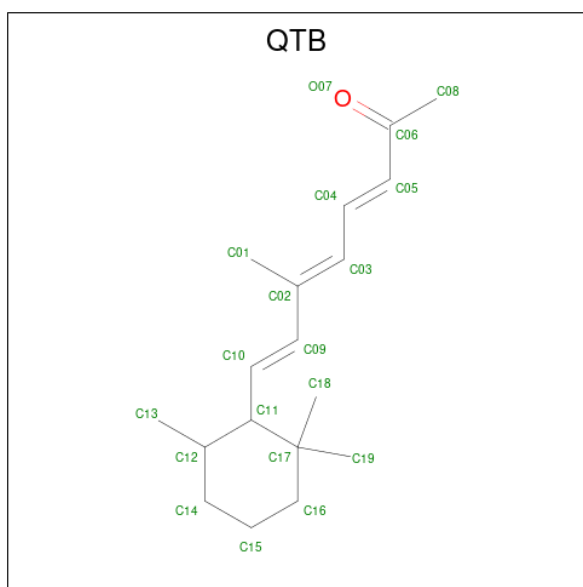
Mol	Chain	Residues	Atoms					AltConf
39	6	1	Total	C	Mg	N	O	0
			224	180	4	16	24	
39	6	1	Total	C	Mg	N	O	0
			224	180	4	16	24	
39	6	1	Total	C	Mg	N	O	0
			224	180	4	16	24	
39	6	1	Total	C	Mg	N	O	0
			224	180	4	16	24	
39	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	8	1	Total	C	Mg	N	O	0
			174	141	3	12	18	
39	8	1	Total	C	Mg	N	O	0
			174	141	3	12	18	
39	8	1	Total	C	Mg	N	O	0
			174	141	3	12	18	

- Molecule 40 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



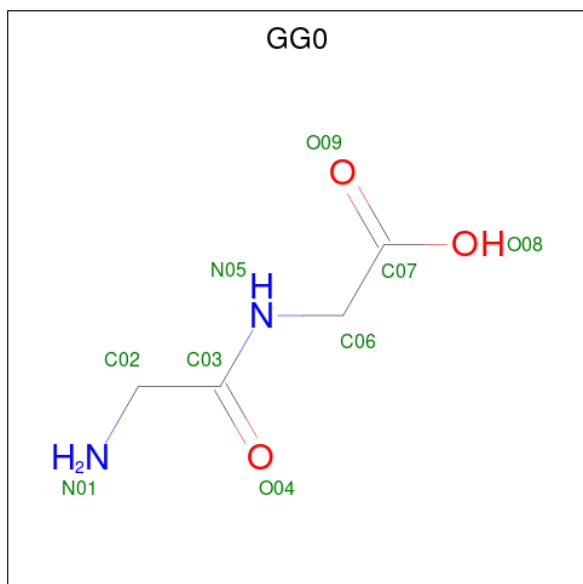
Mol	Chain	Residues	Atoms			AltConf
40	1	1	Total	C	O	0
			20	18	2	
40	8	1	Total	C	O	0
			20	18	2	

- Molecule 41 is (3 {E},5 {E},7 {E})-6-methyl-8-[(6 {R})-2,2,6-trimethylcyclohexyl]octa-3,5,7-trien-2-one (three-letter code: QTB) (formula: $C_{18}H_{28}O$).



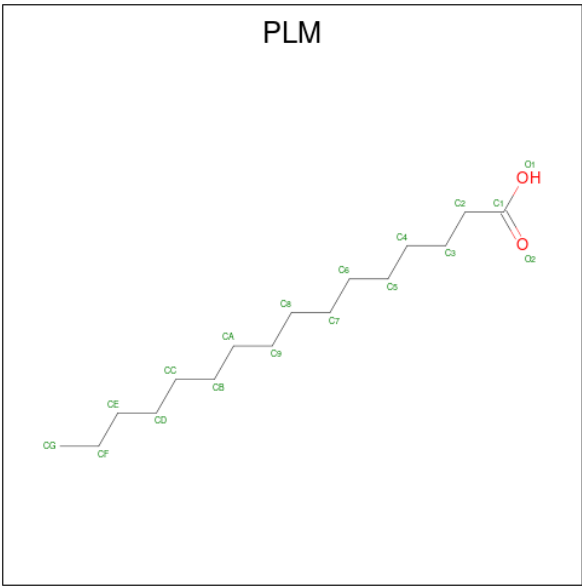
Mol	Chain	Residues	Atoms			AltConf
41	a	1	Total	C	O	0
			19	18	1	
41	3	1	Total	C	O	0
			19	18	1	

- Molecule 42 is 2-(2-azanylethanoylamino)ethanoic acid (three-letter code: GG0) (formula: $C_4H_8N_2O_3$).



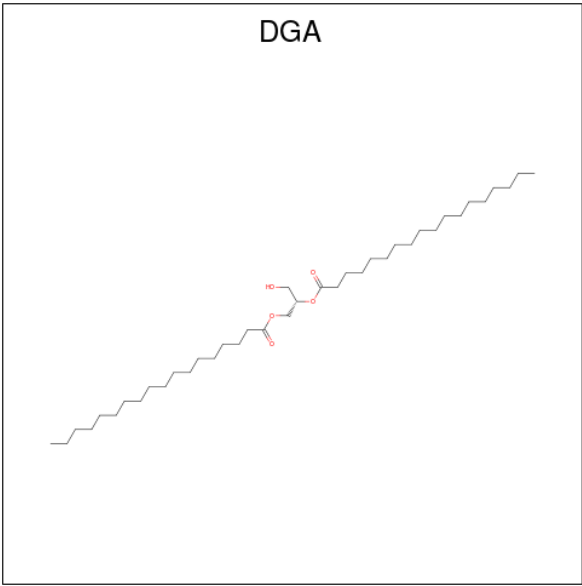
Mol	Chain	Residues	Atoms				AltConf
42	a	1	Total	C	N	O	0
			9	4	2	3	

- Molecule 43 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms			AltConf
43	4	1	Total	C	O	0
			17	16	1	
43	6	1	Total	C	O	0
			18	16	2	

- Molecule 44 is DIACYL GLYCEROL (three-letter code: DGA) (formula: C₃₉H₇₆O₅).



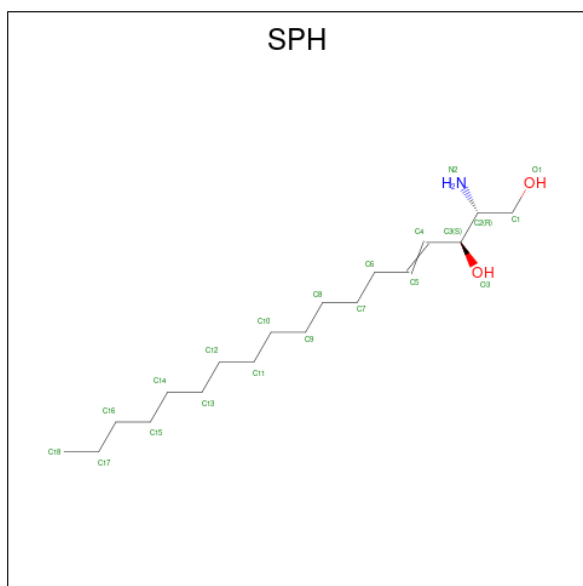
Mol	Chain	Residues	Atoms			AltConf
44	5	1	Total	C	O	0
			23	18	5	

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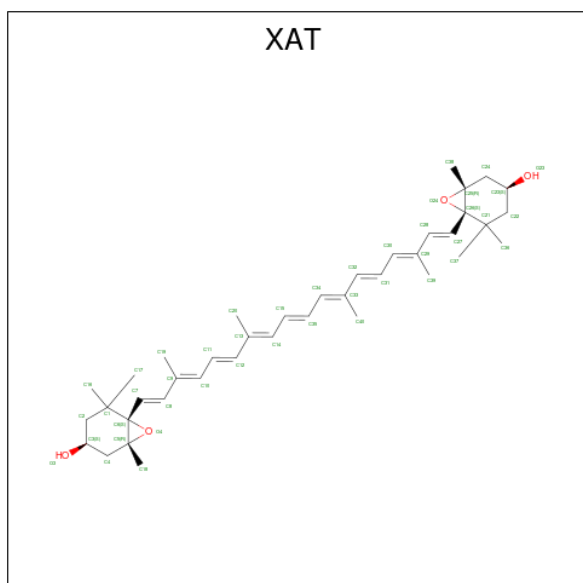
Mol	Chain	Residues	Atoms			AltConf
44	8	1	Total	C	O	0
			30	25	5	

- Molecule 45 is SPHINGOSINE (three-letter code: SPH) (formula: $C_{18}H_{37}NO_2$).



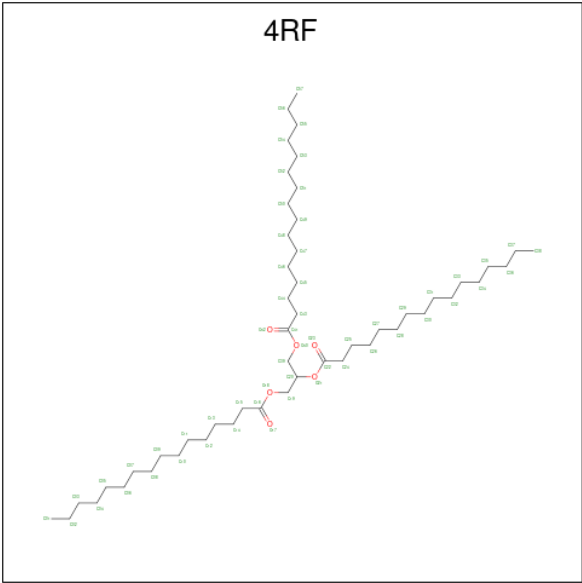
Mol	Chain	Residues	Atoms				AltConf
45	6	1	Total	C	N	O	0
			21	18	1	2	

- Molecule 46 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 (three-letter code: XAT) (formula: $C_{40}H_{56}O_4$).



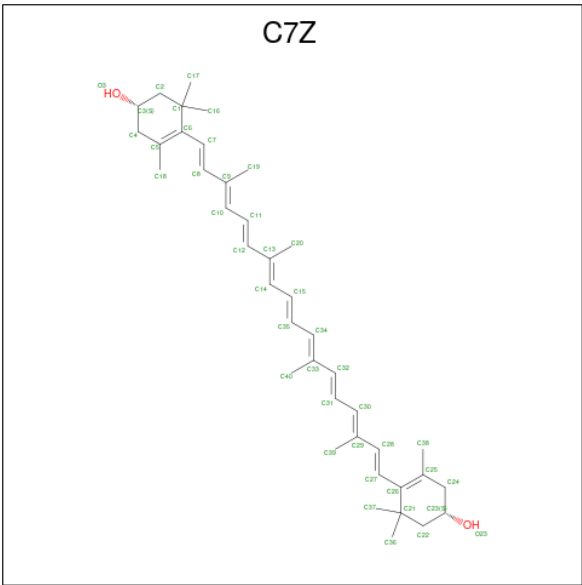
Mol	Chain	Residues	Atoms			AltConf
46	7	1	Total	C	O	0
			44	40	4	

- Molecule 47 is Tripalmitoylglycerol (three-letter code: 4RF) (formula: C₅₁H₉₈O₆).



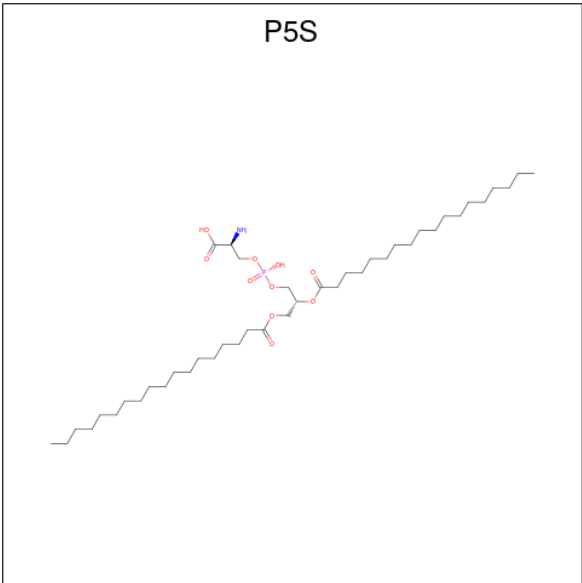
Mol	Chain	Residues	Atoms			AltConf
47	7	1	Total	C	O	0
			32	26	6	
47	8	1	Total	C	O	0
			96	84	12	
47	8	1	Total	C	O	0
			96	84	12	

- Molecule 48 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (three-letter code: C7Z) (formula: C₄₀H₅₆O₂).



Mol	Chain	Residues	Atoms			AltConf
48	7	1	Total	C	O	0
			42	40	2	

- Molecule 49 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (three-letter code: P5S) (formula: C₄₂H₈₂NO₁₀P).



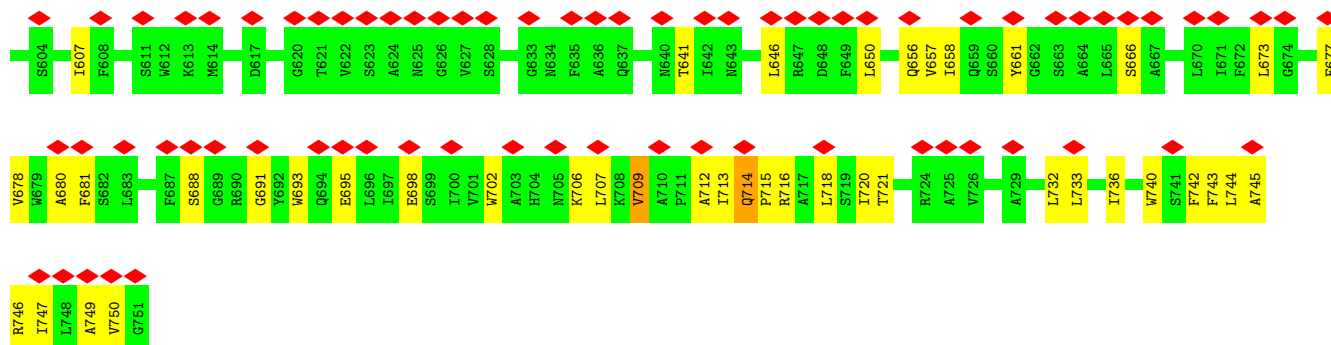
Mol	Chain	Residues	Atoms					AltConf
49	8	1	Total	C	N	O	P	0
			37	25	1	10	1	

3 Residue-property plots

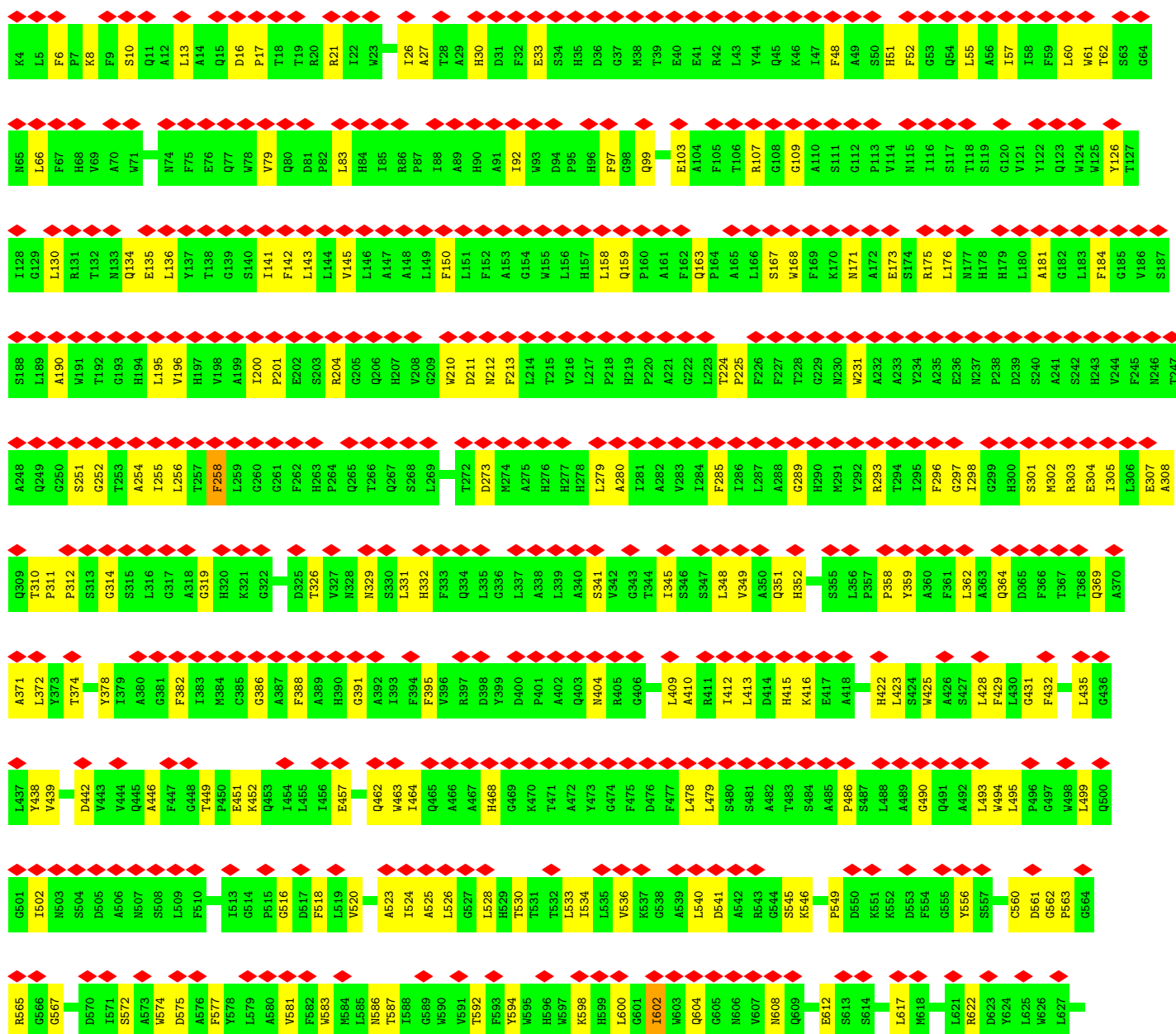
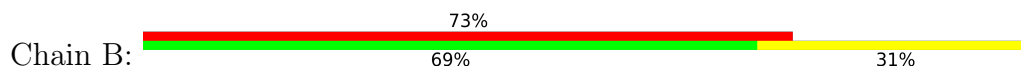
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

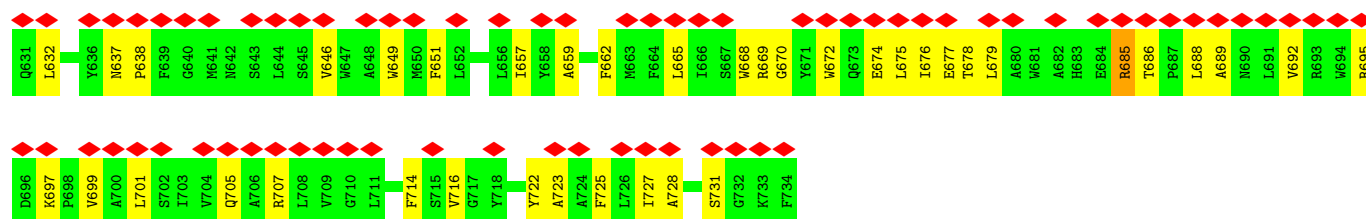
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



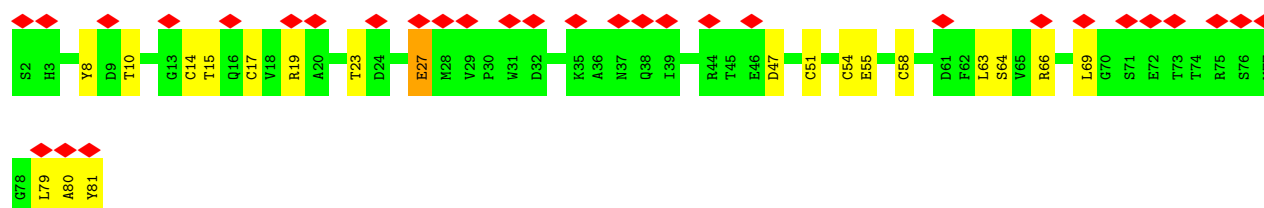
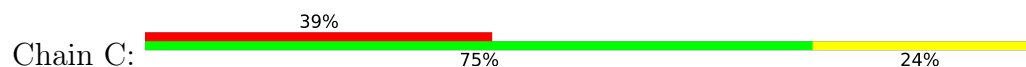


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

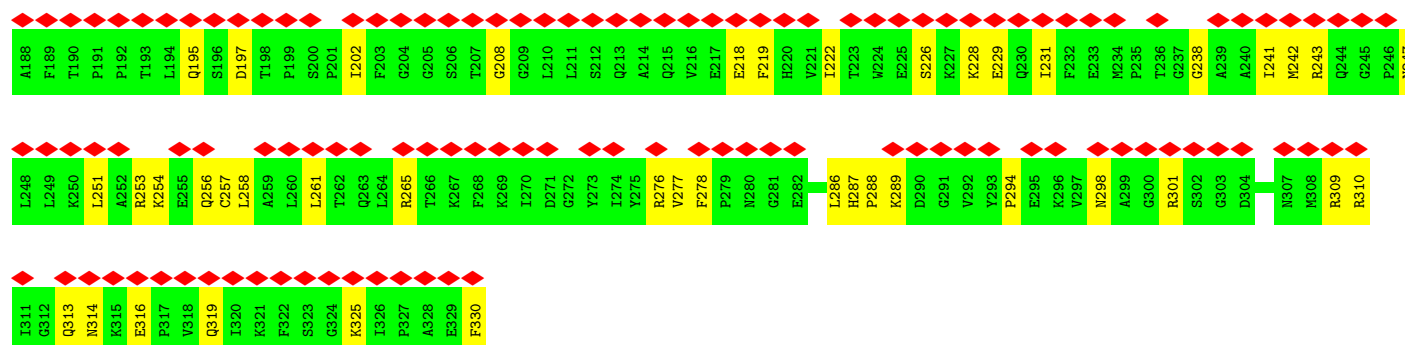
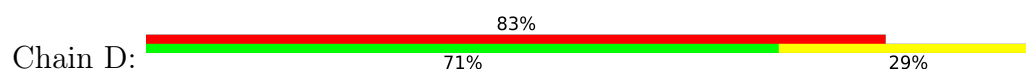




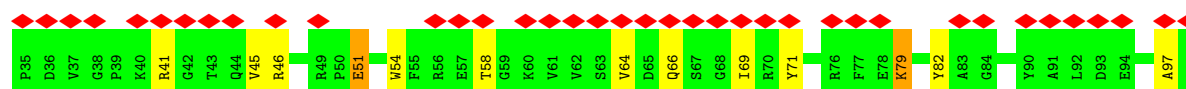
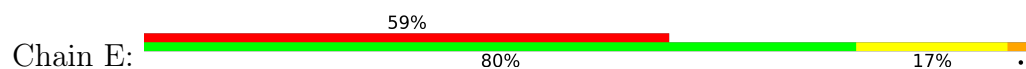
• Molecule 3: Photosystem I iron-sulfur center



• Molecule 4: Photosystem I reaction center subunit chloroplastic

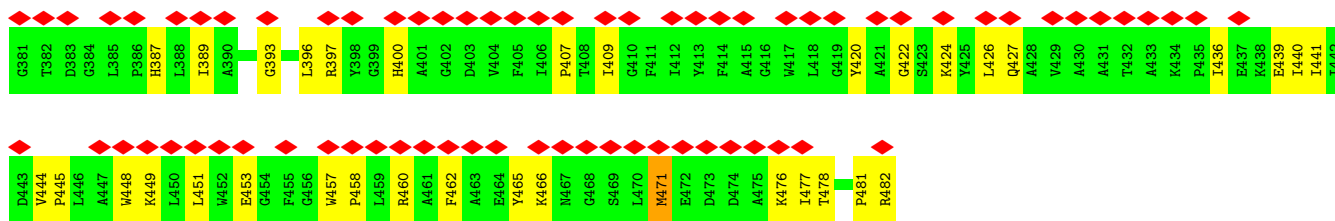


• Molecule 5: Photosystem I reaction center subunit IV

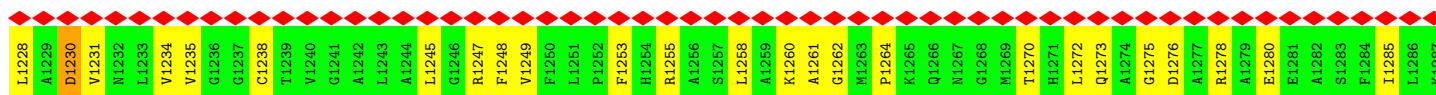


• Molecule 6: PSI-F

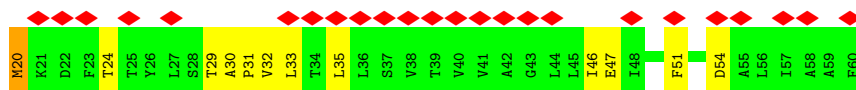




• Molecule 7: Photosystem I reaction center subunit chloroplastic



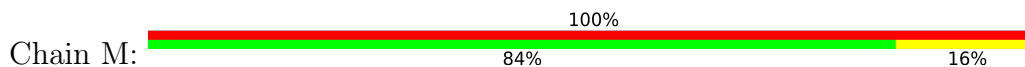
• Molecule 8: Photosystem I reaction center subunit IX



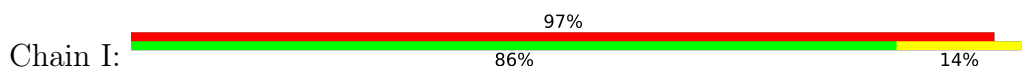
• Molecule 9: PSI-K

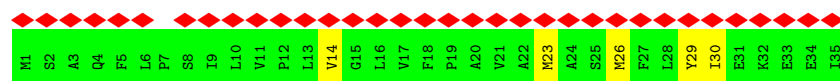


• Molecule 10: Photosystem I reaction center subunit XII

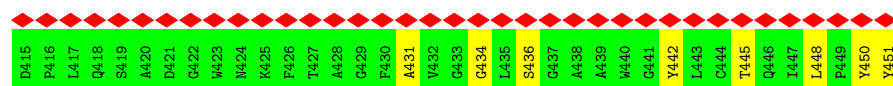
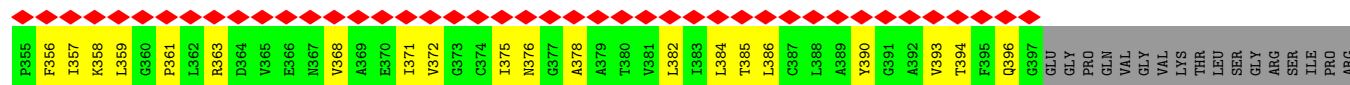
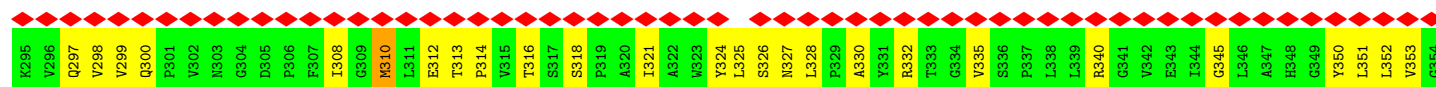
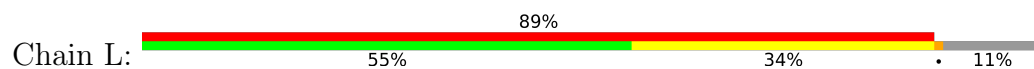


• Molecule 11: Photosystem I reaction center subunit VIII

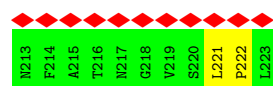
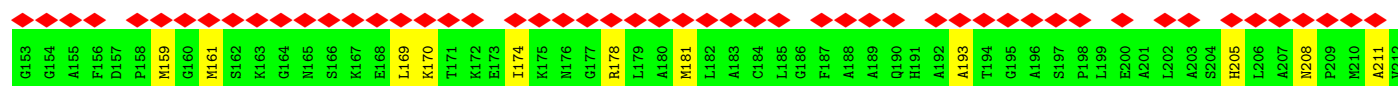
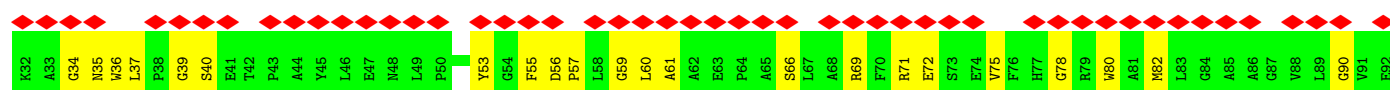
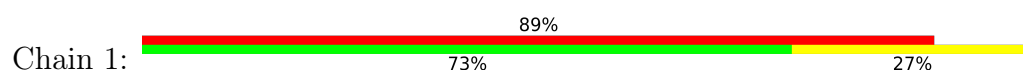




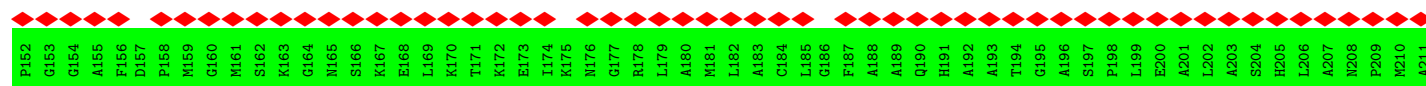
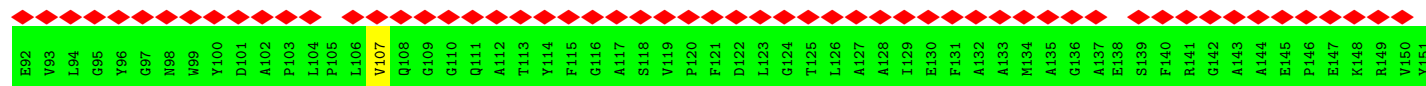
• Molecule 12: PSI subunit V

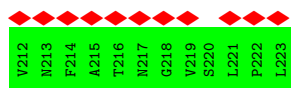


• Molecule 13: Chlorophyll a-b binding protein, chloroplastic

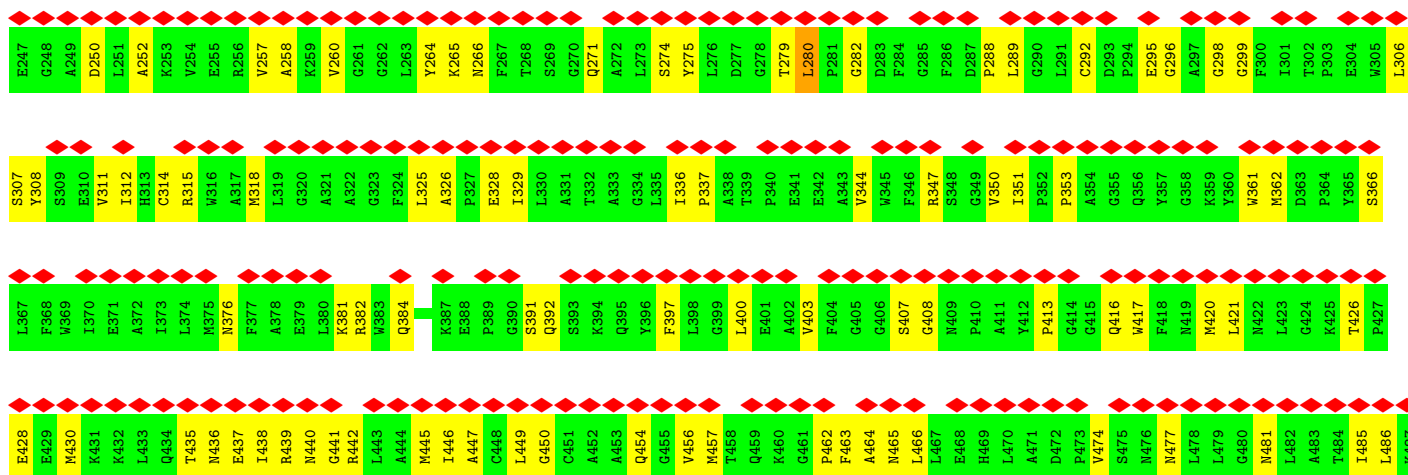
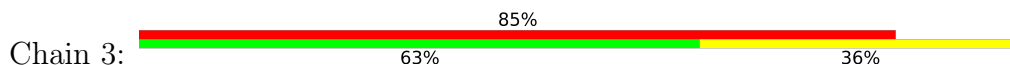


• Molecule 13: Chlorophyll a-b binding protein, chloroplastic

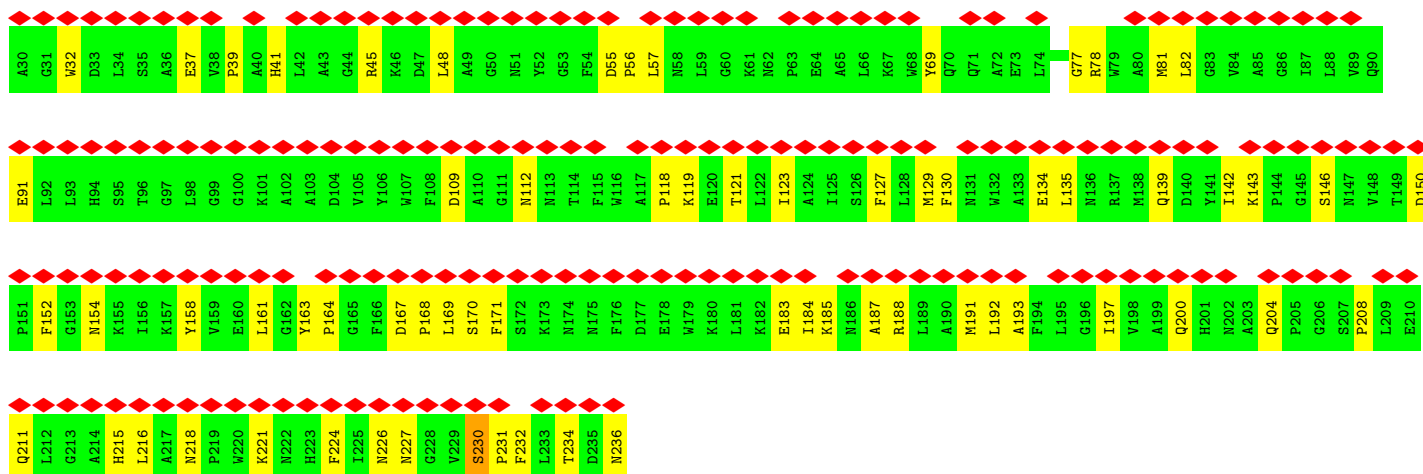
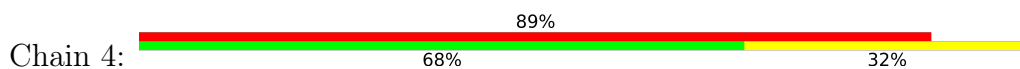




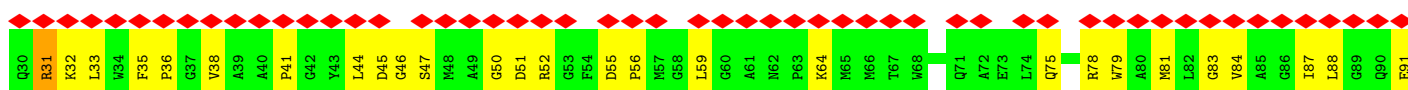
• Molecule 14: Glutathione reductase

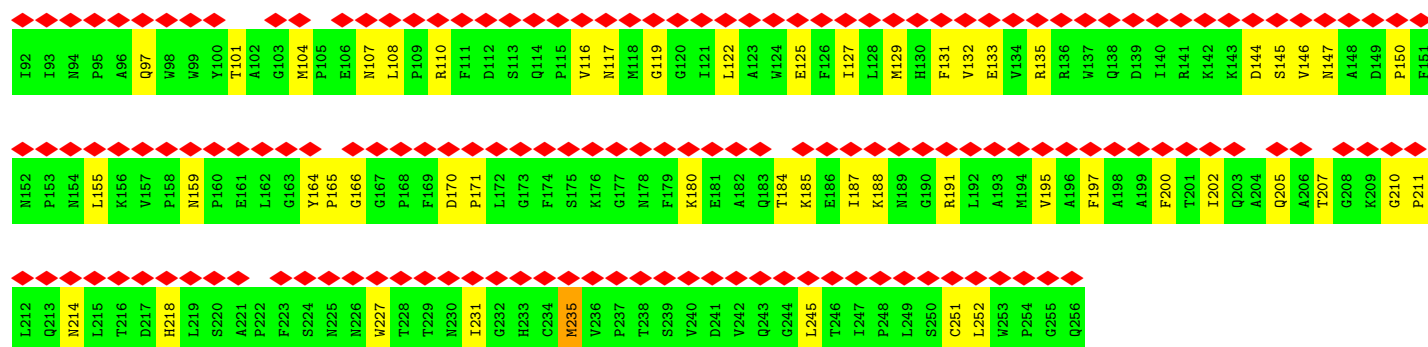


• Molecule 15: Chlorophyll a-b binding protein, chloroplastic



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

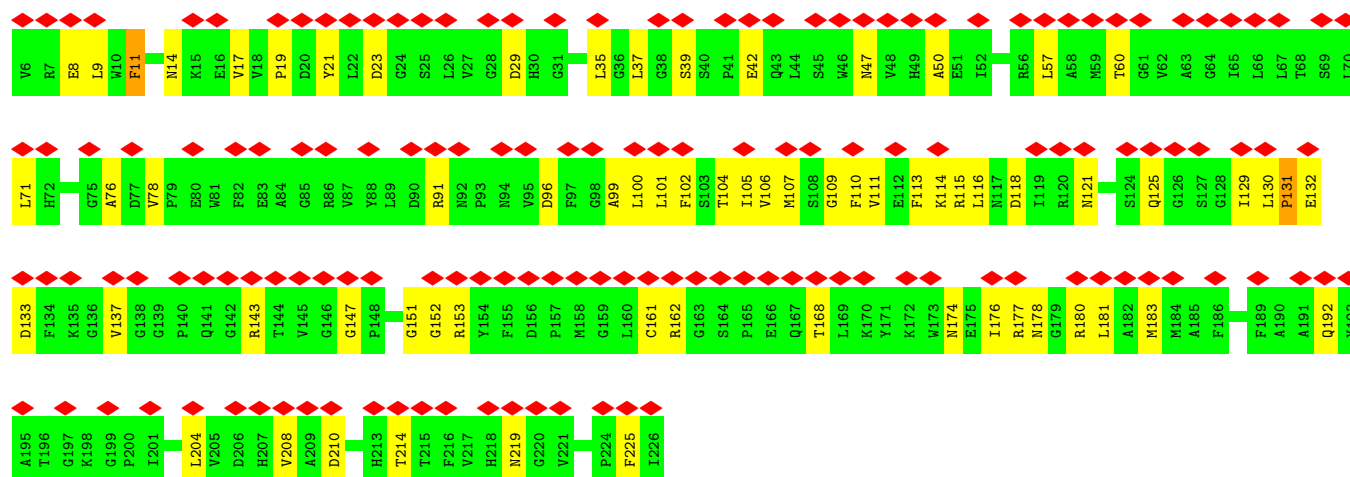




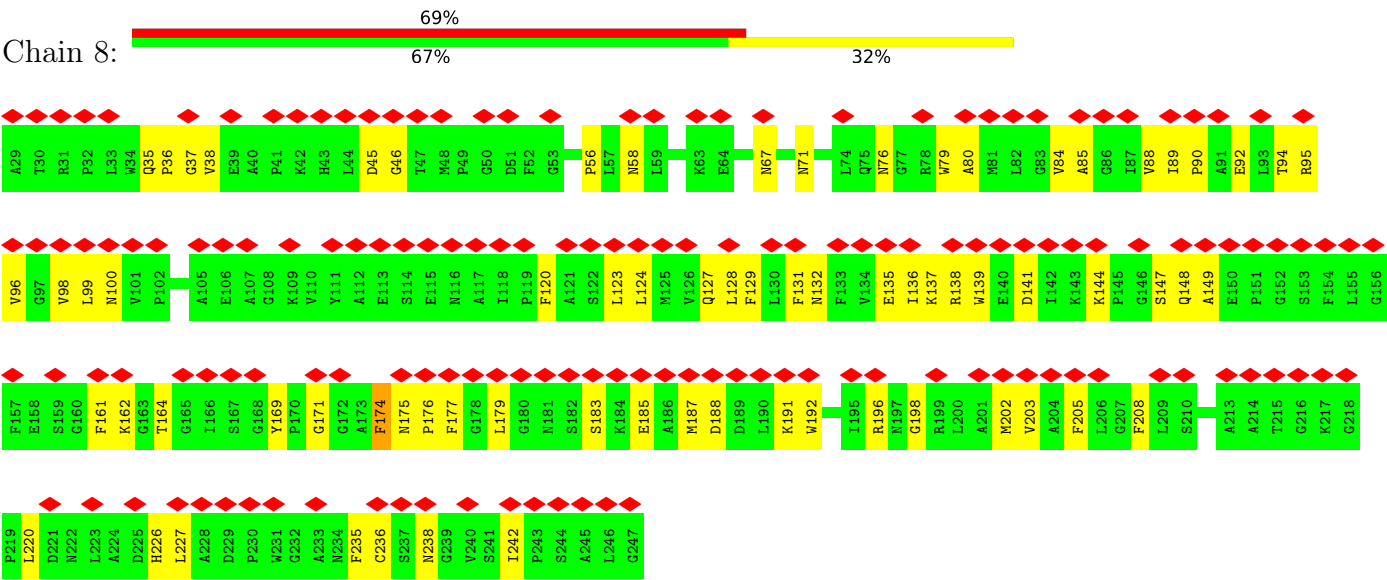
• Molecule 17: Chlorophyll a-b binding protein, chloroplastic



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	25248	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	0.034	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.01	Depositor
Map size (\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 (\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: LMT, BCR, QTB, DGA, GG0, LUT, 4RF, SF4, ERG, PTY, SPH, SQD, XAT, CL0, PLM, CHL, OLA, LPX, DGD, LAP, P5S, LHG, 3PH, RRX, PQN, ECH, C7Z, CLA, PCW

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	0.41	0/6022	0.54	4/8215 (0.0%)
2	B	0.42	3/6006 (0.0%)	0.51	1/8205 (0.0%)
3	C	0.48	0/611	0.67	2/828 (0.2%)
4	D	0.44	0/1150	0.57	0/1551
5	E	1.09	4/520 (0.8%)	0.76	1/705 (0.1%)
6	F	0.39	1/1309 (0.1%)	0.76	2/1771 (0.1%)
7	G	0.35	0/743	0.55	0/1007
8	J	0.43	0/322	0.72	1/439 (0.2%)
9	K	0.31	0/622	0.51	0/844
10	M	0.36	0/244	0.46	0/330
11	I	0.36	0/276	0.51	0/373
12	L	0.36	0/1068	0.66	2/1462 (0.1%)
13	1	0.36	0/1443	0.57	1/1960 (0.1%)
13	a	0.38	0/1443	0.59	0/1960
14	3	0.37	0/1896	0.53	0/2573
15	4	0.35	0/1681	0.52	0/2285
16	5	0.34	0/1825	0.55	1/2483 (0.0%)
17	6	0.38	0/1845	0.58	1/2515 (0.0%)
18	7	0.42	0/1748	0.54	2/2372 (0.1%)
19	8	0.42	0/1717	0.53	1/2330 (0.0%)
All	All	0.42	8/32491 (0.0%)	0.56	19/44208 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	E	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	79	LYS	CE-NZ	17.65	1.93	1.49
5	E	51	GLU	CB-CG	-9.11	1.34	1.52
5	E	79	LYS	CB-CG	-8.41	1.29	1.52
2	B	258	PHE	CE1-CZ	-5.74	1.26	1.37
6	F	471	MET	CB-CG	-5.46	1.33	1.51
5	E	79	LYS	CD-CE	5.35	1.64	1.51
2	B	685	ARG	CB-CG	-5.09	1.38	1.52
2	B	258	PHE	CG-CD2	-5.04	1.31	1.38

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	471	MET	CB-CG-SD	-18.05	58.27	112.40
13	1	221	LEU	CB-CG-CD1	-10.38	93.35	111.00
6	F	471	MET	CG-SD-CE	-9.62	84.81	100.20
1	A	374	MET	CG-SD-CE	-9.00	85.80	100.20
17	6	200	MET	CA-CB-CG	-8.72	98.47	113.30
12	L	310	MET	CB-CG-SD	-8.65	86.44	112.40
1	A	714	GLN	CB-CA-C	-8.02	94.36	110.40
1	A	714	GLN	CA-CB-CG	6.35	127.36	113.40
16	5	235	MET	CA-CB-CG	6.26	123.94	113.30
5	E	51	GLU	CG-CD-OE2	-6.12	106.06	118.30
12	L	310	MET	CG-SD-CE	5.88	109.61	100.20
18	7	11	PHE	CB-CG-CD2	-5.73	116.79	120.80
3	C	27	GLU	CG-CD-OE1	-5.54	107.21	118.30
2	B	602	ILE	CG1-CB-CG2	-5.42	99.47	111.40
8	J	20	MET	CG-SD-CE	-5.35	91.64	100.20
19	8	174	PHE	CB-CG-CD2	-5.28	117.10	120.80
1	A	709	VAL	C-N-CA	-5.13	108.88	121.70
18	7	11	PHE	CB-CG-CD1	5.10	124.37	120.80
3	C	27	GLU	OE1-CD-OE2	5.05	129.35	123.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	51	GLU	Sidechain

5.2 Too-close contacts ⓘ

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	240	0
2	B	5796	0	5576	242	0
3	C	601	0	576	23	0
4	D	1124	0	1129	44	0
5	E	509	0	507	11	0
6	F	1277	0	1296	58	0
7	G	727	0	724	55	0
8	J	316	0	332	18	0
9	K	613	0	639	48	0
10	M	239	0	255	9	0
11	I	270	0	287	19	0
12	L	1041	0	1047	51	0
13	1	1405	0	1370	52	0
13	a	1405	0	1370	0	0
14	3	1844	0	1805	91	0
15	4	1631	0	1575	61	0
16	5	1769	0	1719	98	0
17	6	1787	0	1762	187	0
18	7	1698	0	1640	80	0
19	8	1669	0	1619	70	0
21	A	65	0	72	3	0
22	1	693	0	678	75	0
22	3	719	0	726	66	0
22	4	768	0	686	52	0
22	5	739	0	638	64	0
22	6	711	0	649	117	0
22	7	778	0	720	69	0
22	8	699	0	617	65	0
22	A	2621	0	2695	265	0
22	B	2583	0	2678	288	0
22	F	105	0	87	13	0
22	G	141	0	105	11	0
22	J	42	0	31	1	0
22	K	204	0	167	41	0
22	L	155	0	130	23	0
22	a	571	0	540	0	0
23	A	33	0	46	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	B	33	0	46	8	0
24	3	120	0	159	14	0
24	4	40	0	53	3	0
24	5	80	0	104	10	0
24	6	80	0	105	16	0
24	7	40	0	52	9	0
24	8	40	0	53	5	0
24	A	200	0	264	22	0
24	B	280	0	369	35	0
24	F	40	0	53	5	0
24	G	40	0	53	3	0
24	I	40	0	52	8	0
24	J	40	0	53	3	0
24	K	80	0	106	7	0
24	L	120	0	159	23	0
25	1	77	0	97	5	0
25	3	49	0	74	5	0
25	4	81	0	108	20	0
25	5	49	0	74	9	0
25	6	86	0	118	19	0
25	7	128	0	175	12	0
25	8	37	0	44	5	0
25	A	120	0	159	16	0
25	B	95	0	139	9	0
25	F	79	0	101	8	0
25	a	35	0	40	0	0
26	8	66	0	96	13	0
26	A	51	0	60	3	0
26	B	66	0	96	10	0
27	A	33	0	39	1	0
28	A	8	0	0	0	0
28	C	16	0	0	2	0
29	1	35	0	45	8	0
29	A	35	0	46	4	0
29	B	35	0	44	2	0
30	6	36	0	44	3	0
30	B	30	0	34	6	0
31	3	38	0	49	5	0
31	5	38	0	49	2	0
31	7	33	0	39	3	0
31	8	35	0	43	6	0
31	B	41	0	55	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	B	29	0	42	3	0
32	F	29	0	42	6	0
32	K	29	0	42	3	0
33	7	39	0	41	1	0
33	G	46	0	55	4	0
34	G	29	0	38	16	0
35	J	41	0	56	10	0
36	J	17	0	14	3	0
36	a	30	0	43	0	0
37	M	41	0	54	6	0
38	1	126	0	165	16	0
38	3	84	0	110	10	0
38	4	84	0	110	9	0
38	5	126	0	165	20	0
38	6	84	0	110	29	0
38	7	42	0	55	4	0
38	8	84	0	110	17	0
38	a	126	0	165	0	0
39	1	114	0	102	16	0
39	3	98	0	73	11	0
39	4	174	0	154	18	0
39	5	173	0	153	22	0
39	6	224	0	188	56	0
39	7	66	0	70	6	0
39	8	174	0	153	20	0
39	a	203	0	148	0	0
40	1	20	0	33	2	0
40	8	20	0	33	4	0
41	3	19	0	0	0	0
41	a	19	0	0	0	0
42	a	9	0	0	0	0
43	4	17	0	31	0	0
43	6	18	0	31	1	0
44	5	23	0	28	3	0
44	8	30	0	42	5	0
45	6	21	0	37	7	0
46	7	44	0	56	5	0
47	7	32	0	39	6	0
47	8	96	0	142	16	0
48	7	42	0	0	4	0
49	8	37	0	40	0	0
All	All	48636	0	48687	2217	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 24.

All (2217) 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)
34:G:5002:ERG:O1	34:G:5002:ERG:C3	1.70	1.40
5:E:79:LYS:NZ	5:E:79:LYS:CE	1.93	1.29
22:B:1201:CLA:H72	11:I:29:TYR:CE2	1.77	1.17
17:6:135:ARG:NE	39:6:611:CHL:OMC	1.78	1.14
7:G:1317:SER:HA	34:G:5002:ERG:H7	1.13	1.11
22:B:1204:CLA:H12	11:I:14:VAL:HG21	1.35	1.09
22:B:1204:CLA:H61	24:I:4001:BCR:HC31	1.37	1.06
30:B:5004:PCW:H322	24:F:4001:BCR:H351	1.41	1.01
17:6:131:TRP:HE1	39:6:611:CHL:CBB	1.73	1.00
2:B:412:ILE:HD13	24:B:4004:BCR:H402	1.41	1.00
16:5:32:LYS:HZ2	22:5:609:CLA:H2A	1.24	0.99
29:1:804:LMT:H82	22:1:605:CLA:HMD3	1.45	0.99
1:A:442:ASN:HD22	2:B:675:LEU:HD11	1.26	0.99
11:I:30:ILE:HD13	24:L:4001:BCR:C33	1.95	0.97
22:B:1228:CLA:H2	24:F:4001:BCR:H353	1.48	0.96
7:G:1317:SER:HA	34:G:5002:ERG:C7	1.96	0.94
18:7:11:PHE:CE2	18:7:14:ASN:HB2	2.01	0.94
17:6:152:PHE:CZ	22:6:617:CLA:HBA2	2.02	0.93
1:A:369:HIS:HA	1:A:372:TYR:CE2	2.03	0.93
17:6:40:LEU:CD1	22:6:609:CLA:HED2	1.99	0.92
17:6:131:TRP:HE1	39:6:611:CHL:HBB2	1.34	0.91
34:G:5002:ERG:H122	13:1:123:LEU:HD23	1.53	0.91
22:8:610:CLA:H12	47:8:808:4RF:H29	1.53	0.91
7:G:1253:PHE:CZ	29:1:804:LMT:H2'	2.06	0.90
7:G:1317:SER:CA	34:G:5002:ERG:H7	2.01	0.90
22:B:1208:CLA:HAA1	7:G:1278:ARG:NH2	1.88	0.89
17:6:169:PHE:HD1	39:6:611:CHL:H11	1.36	0.89
2:B:134:GLN:HE22	10:M:3:ILE:HG22	1.37	0.89
1:A:396:TRP:CD1	22:A:1126:CLA:HAB	2.08	0.88
13:1:35:ASN:O	13:1:37:LEU:N	2.07	0.88
1:A:389:SER:HB3	22:A:1126:CLA:HMA1	1.55	0.88
16:5:64:LYS:HE2	44:5:803:DGA:HG2	1.57	0.87
1:A:190:TRP:CZ2	22:A:1108:CLA:HMA1	2.09	0.87
12:L:357:ILE:HG13	12:L:372:VAL:HG11	1.55	0.87
25:4:801:LHG:HC92	24:6:503:BCR:HC22	1.54	0.87
1:A:673:LEU:HB3	22:A:1012:CLA:H2	1.56	0.87
22:B:1218:CLA:HMD2	24:B:4001:BCR:HC7	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:7:11:PHE:HE2	18:7:14:ASN:HB2	1.39	0.86
22:A:1131:CLA:HBB1	22:A:1132:CLA:H2	1.55	0.86
17:6:58:TYR:CD1	22:6:609:CLA:HBC2	2.10	0.86
17:6:164:TYR:O	22:6:601:CLA:HED2	1.74	0.86
18:7:113:PHE:HD2	22:8:609:CLA:HAA2	1.40	0.86
22:B:1220:CLA:HAB	22:B:1227:CLA:HMD2	1.58	0.86
11:I:30:ILE:HD13	24:L:4001:BCR:H332	1.55	0.86
1:A:577:GLY:HA2	2:B:563:PRO:HD3	1.57	0.85
14:3:314:CYS:HB2	14:3:441:GLY:HA3	1.57	0.85
22:B:1240:CLA:H11	25:B:5001:LHG:H242	1.57	0.85
38:4:501:LUT:H32	22:4:601:CLA:HAB	1.57	0.85
1:A:578:PRO:HD3	2:B:562:GLY:HA2	1.57	0.85
22:A:1130:CLA:H102	22:L:1502:CLA:H92	1.57	0.85
17:6:40:LEU:HD12	22:6:609:CLA:HED2	1.58	0.84
25:4:801:LHG:H222	22:6:618:CLA:HMC3	1.57	0.83
1:A:442:ASN:ND2	2:B:675:LEU:HD11	1.93	0.83
2:B:258:PHE:CE2	2:B:494:TRP:HE3	1.96	0.83
3:C:55:GLU:OE2	3:C:66:ARG:NH1	2.10	0.83
22:B:1227:CLA:H12	25:B:5001:LHG:H252	1.59	0.83
2:B:657:ILE:HG12	22:B:1239:CLA:HMB3	1.60	0.83
17:6:128:VAL:CG1	24:6:503:BCR:H17C	2.08	0.83
22:B:1220:CLA:HBA1	24:B:4004:BCR:H16C	1.60	0.83
22:B:1205:CLA:HAB	22:B:1206:CLA:HBA1	1.61	0.83
17:6:165:PRO:HD2	22:6:601:CLA:CAD	2.09	0.83
1:A:45:THR:HG22	1:A:714:GLN:HG2	1.59	0.82
22:4:607:CLA:H11	22:4:607:CLA:H3A	1.59	0.82
22:A:1012:CLA:H41	2:B:439:VAL:HG13	1.60	0.82
2:B:258:PHE:HE2	2:B:494:TRP:HE3	1.25	0.82
31:7:804:PTY:H351	26:8:802:DGD:HAV2	1.62	0.82
1:A:363:LEU:HD11	22:A:1117:CLA:H72	1.62	0.82
1:A:707:LEU:HD13	24:F:4001:BCR:H321	1.61	0.82
6:F:336:LYS:O	6:F:340:LYS:HG2	1.80	0.82
29:1:804:LMT:H22	22:1:612:CLA:O1A	1.78	0.82
2:B:196:VAL:HG21	22:B:1212:CLA:HBC3	1.59	0.81
22:B:1218:CLA:HED1	7:G:1258:LEU:HA	1.61	0.81
1:A:657:VAL:HG22	1:A:745:ALA:HB3	1.61	0.81
2:B:57:ILE:HD11	37:M:4001:ECH:H39A	1.60	0.81
22:B:1237:CLA:H151	24:L:4002:BCR:H17C	1.63	0.81
22:B:1204:CLA:H102	24:I:4001:BCR:HC21	1.63	0.81
11:I:26:MET:HG3	24:L:4001:BCR:H312	1.63	0.81
16:5:64:LYS:NZ	44:5:803:DGA:OA1	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:PRO:HG3	1:A:149:ARG:HH12	1.46	0.80
8:J:29:THR:HG22	8:J:31:PRO:HD2	1.62	0.80
2:B:301:SER:OG	7:G:1262:GLY:O	1.99	0.80
17:6:165:PRO:HD2	22:6:601:CLA:OBD	1.82	0.80
17:6:75:PHE:CB	22:6:604:CLA:HMA1	2.11	0.79
22:B:1238:CLA:O1A	24:L:4001:BCR:H351	1.82	0.79
22:B:1207:CLA:HBA2	12:L:361:PRO:HG3	1.65	0.79
16:5:129:MET:HG3	22:5:612:CLA:HMC3	1.65	0.79
22:B:1234:CLA:HBA2	22:B:1235:CLA:HAA2	1.65	0.78
9:K:58:PRO:HD3	22:K:1403:CLA:CHB	2.13	0.78
15:4:234:THR:HG23	24:6:504:BCR:H332	1.66	0.78
15:4:234:THR:CG2	24:6:504:BCR:H332	2.13	0.78
14:3:376:ASN:ND2	22:7:609:CLA:O1A	2.16	0.78
17:6:39:TRP:CZ3	17:6:40:LEU:HB2	2.18	0.78
17:6:136:ARG:HG3	39:6:611:CHL:C2D	2.13	0.78
13:1:178:ARG:HB3	22:1:604:CLA:HBC3	1.64	0.78
39:1:609:CHL:HED1	19:8:136:ILE:HG22	1.65	0.78
22:5:617:CLA:HED2	22:5:617:CLA:HAA2	1.65	0.78
1:A:369:HIS:CD2	22:A:1124:CLA:HED2	2.19	0.78
29:B:5006:LMT:O4'	7:G:1260:LYS:HG2	1.84	0.77
16:5:75:GLN:NE2	39:5:611:CHL:O1D	2.15	0.77
12:L:356:PHE:HB2	12:L:372:VAL:HG13	1.65	0.77
17:6:128:VAL:HG11	24:6:503:BCR:H17C	1.65	0.77
25:4:802:LHG:H102	22:6:618:CLA:HBA1	1.66	0.77
24:6:503:BCR:H16C	39:6:613:CHL:H43	1.66	0.77
17:6:184:GLU:HB2	22:6:601:CLA:HMB3	1.66	0.77
17:6:136:ARG:HG3	39:6:611:CHL:C1D	2.15	0.76
1:A:561:ARG:NH2	4:D:208:GLY:HA2	2.01	0.76
22:A:1130:CLA:H11	22:L:1502:CLA:H102	1.67	0.76
1:A:11:LYS:HD2	1:A:12:LYS:HG2	1.68	0.76
2:B:525:ALA:HA	22:B:1236:CLA:HED1	1.65	0.76
14:3:439:ARG:NH1	22:3:607:CLA:O1D	2.18	0.76
3:C:27:GLU:OE2	4:D:294:PRO:HA	1.86	0.76
8:J:31:PRO:HB2	35:J:4002:RRX:H1	1.67	0.76
18:7:107:MET:HE3	39:7:613:CHL:H2A	1.68	0.76
7:G:1323:ARG:NH1	22:G:1603:CLA:OBD	2.19	0.75
17:6:164:TYR:HB3	22:6:601:CLA:HED3	1.68	0.75
4:D:243:ARG:H	4:D:247:ASN:HD21	1.32	0.75
7:G:1249:VAL:HG13	13:1:139:SER:OG	1.86	0.75
17:6:184:GLU:HB2	22:6:601:CLA:C2B	2.17	0.75
2:B:173:GLU:OE2	7:G:1264:PRO:HB3	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:1228:LEU:N	7:G:1317:SER:HG	1.84	0.75
1:A:442:ASN:HD22	2:B:675:LEU:CD1	2.00	0.75
12:L:324:TYR:OH	22:L:1502:CLA:O1A	2.04	0.75
38:5:505:LUT:H173	22:7:608:CLA:HAB	1.66	0.74
22:B:1236:CLA:HHC	22:B:1236:CLA:HBB1	1.70	0.74
22:A:1101:CLA:HBB1	22:A:1101:CLA:HHC	1.70	0.74
17:6:87:MET:SD	22:6:601:CLA:HAB	2.27	0.74
26:8:802:DGD:HBN2	22:8:609:CLA:H141	1.68	0.74
22:A:1114:CLA:H93	22:3:610:CLA:HMC2	1.69	0.74
9:K:58:PRO:CD	22:K:1403:CLA:CHB	2.65	0.74
1:A:121:ILE:HD13	35:J:4002:RRX:H18	1.70	0.74
22:A:1113:CLA:HBD	14:3:485:ILE:HD11	1.68	0.74
2:B:541:ASP:OD1	2:B:545:SER:OG	2.05	0.74
22:B:1216:CLA:HMB2	22:B:1221:CLA:HMA3	1.70	0.73
32:F:5003:LAP:H132	22:1:615:CLA:HMA1	1.71	0.73
15:4:109:ASP:OD1	15:4:112:ASN:ND2	2.21	0.73
15:4:78:ARG:HA	15:4:81:MET:HE2	1.69	0.73
12:L:357:ILE:HA	12:L:372:VAL:HG21	1.71	0.73
16:5:32:LYS:NZ	22:5:609:CLA:H2A	2.02	0.73
16:5:117:ASN:HD22	17:6:222:GLY:HA2	1.52	0.73
22:1:603:CLA:HBB1	22:1:603:CLA:H91	1.70	0.73
9:K:107:ILE:HG12	22:K:1402:CLA:CBB	2.18	0.72
17:6:75:PHE:HB3	22:6:604:CLA:HMA1	1.70	0.72
14:3:329:ILE:HG21	24:3:504:BCR:H272	1.71	0.72
22:3:618:CLA:HHC	22:3:618:CLA:HBB1	1.71	0.72
6:F:444:VAL:HG11	36:J:5001:LPX:H7A	1.70	0.72
22:1:603:CLA:HMA1	22:1:608:CLA:HBC3	1.71	0.72
16:5:145:SER:OG	17:6:42:GLY:O	2.05	0.72
22:G:1603:CLA:HMC2	22:1:610:CLA:HBA2	1.71	0.72
17:6:183:LYS:HD3	22:6:602:CLA:HBD	1.71	0.72
22:B:1201:CLA:H43	22:B:1201:CLA:H121	1.71	0.72
22:B:1208:CLA:H2	22:B:1209:CLA:HMD2	1.71	0.72
19:8:187:MET:HG3	19:8:191:LYS:HE3	1.72	0.72
22:7:610:CLA:H91	25:7:803:LHG:H311	1.72	0.72
1:A:46:THR:HG23	1:A:714:GLN:O	1.89	0.72
2:B:298:ILE:HD13	7:G:1297:VAL:HG12	1.71	0.72
2:B:575:ASP:OD1	2:B:707:ARG:NH1	2.23	0.72
16:5:117:ASN:HD21	17:6:227:SER:HB2	1.55	0.72
22:B:1206:CLA:HBB1	22:B:1206:CLA:HMB1	1.71	0.71
22:A:1102:CLA:HBB1	22:A:1102:CLA:HMB1	1.70	0.71
22:A:1109:CLA:HBA1	22:A:1109:CLA:CHA	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:5:56:PRO:HD2	38:5:502:LUT:H23	1.72	0.71
17:6:194:ALA:HB1	38:6:501:LUT:H7	1.71	0.71
1:A:575:CYS:SG	2:B:563:PRO:HB3	2.30	0.71
22:A:1103:CLA:H11	22:A:1104:CLA:HBB1	1.71	0.71
39:4:609:CHL:HH2	39:4:609:CHL:HBC3	1.71	0.71
17:6:186:LYS:NZ	22:6:607:CLA:O1D	2.22	0.71
22:A:1107:CLA:H43	24:J:4001:BCR:H10C	1.73	0.71
22:A:1107:CLA:HMB1	22:A:1107:CLA:HBB1	1.73	0.71
22:A:1138:CLA:HBB2	6:F:422:GLY:HA3	1.73	0.71
39:6:613:CHL:HMB1	39:6:613:CHL:HBB1	1.72	0.71
7:G:1255:ARG:NH2	7:G:1293:GLY:O	2.24	0.71
2:B:371:ALA:HB1	22:B:1224:CLA:HMA1	1.72	0.70
22:B:1218:CLA:CE2	7:G:1258:LEU:HD23	2.21	0.70
24:A:4005:BCR:H24C	22:B:1230:CLA:HMC2	1.70	0.70
2:B:258:PHE:HE2	2:B:494:TRP:CE3	2.07	0.70
38:8:501:LUT:H373	39:8:601:CHL:H51	1.73	0.70
22:A:1109:CLA:H201	35:J:4002:RRX:H43	1.72	0.70
22:6:609:CLA:HMB1	22:6:609:CLA:HBB1	1.73	0.70
22:3:603:CLA:H172	25:3:801:LHG:H322	1.72	0.70
22:3:616:CLA:HHC	22:3:616:CLA:HBB1	1.73	0.70
22:5:607:CLA:HBB1	22:5:607:CLA:HHC	1.72	0.70
17:6:131:TRP:NE1	39:6:611:CHL:CBB	2.52	0.70
22:7:601:CLA:HMB1	22:7:601:CLA:HBB1	1.73	0.70
1:A:178:TRP:CZ2	31:3:802:PTY:H342	2.27	0.70
4:D:222:ILE:HD11	4:D:261:LEU:HD13	1.73	0.70
19:8:94:THR:HG23	19:8:100:ASN:HA	1.74	0.70
22:A:1013:CLA:HBA2	2:B:428:LEU:HD23	1.74	0.70
22:B:1217:CLA:HBB1	22:B:1217:CLA:HHC	1.73	0.70
5:E:46:ARG:HH22	6:F:476:LYS:HE3	1.57	0.70
1:A:356:ASN:ND2	22:A:1103:CLA:OBD	2.20	0.70
22:5:604:CLA:HMB1	22:5:604:CLA:HBB1	1.73	0.69
22:A:1012:CLA:H43	2:B:439:VAL:HG22	1.74	0.69
14:3:381:LYS:HD2	39:3:611:CHL:HBB1	1.73	0.69
16:5:97:GLN:HE22	16:5:107:ASN:HD22	1.38	0.69
2:B:378:TYR:CD2	22:B:1224:CLA:HAB	2.28	0.69
2:B:168:TRP:CZ2	22:B:1208:CLA:HMA1	2.27	0.69
2:B:688:LEU:HB3	24:L:4002:BCR:HC31	1.73	0.69
17:6:265:PRO:HD2	22:6:615:CLA:HED2	1.74	0.69
22:B:1213:CLA:H92	24:G:4001:BCR:HC21	1.74	0.69
9:K:69:ILE:HG23	9:K:70:LYS:HE3	1.74	0.69
14:3:289:LEU:HD12	38:3:502:LUT:H222	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:3:504:BCR:C10	39:3:611:CHL:HBA1	2.23	0.69
25:4:801:LHG:C9	24:6:503:BCR:HC22	2.22	0.69
16:5:78:ARG:NH1	39:5:611:CHL:OBD	2.25	0.69
1:A:265:PHE:HD2	32:K:5001:LAP:H71	1.58	0.69
12:L:442:TYR:O	12:L:445:THR:OG1	2.10	0.69
17:6:193:LEU:HD11	25:6:801:LHG:H302	1.72	0.69
22:1:602:CLA:HBB1	22:1:602:CLA:HHC	1.74	0.69
16:5:150:PRO:HD3	22:5:618:CLA:HMC2	1.74	0.69
18:7:11:PHE:CD2	18:7:14:ASN:HB2	2.27	0.69
22:7:617:CLA:HHC	22:7:617:CLA:HBB1	1.74	0.69
19:8:137:LYS:HE3	22:8:611:CLA:HMC3	1.75	0.69
16:5:146:VAL:HG13	17:6:42:GLY:HA3	1.76	0.68
25:6:801:LHG:H121	25:6:801:LHG:H312	1.76	0.68
2:B:598:LYS:O	2:B:602:ILE:HG12	1.94	0.68
38:5:502:LUT:H31	22:5:604:CLA:H161	1.75	0.68
24:7:503:BCR:HC31	25:8:801:LHG:HC81	1.75	0.68
22:B:1209:CLA:HBB2	22:B:1217:CLA:H102	1.74	0.68
3:C:58:CYS:HB3	3:C:63:LEU:HD22	1.74	0.68
6:F:369:ARG:NH1	8:J:54:ASP:OD2	2.23	0.68
31:8:810:PTY:HN11	31:8:810:PTY:HC51	1.57	0.68
2:B:258:PHE:CE2	2:B:494:TRP:CE3	2.81	0.68
22:B:1207:CLA:H112	12:L:378:ALA:HB2	1.75	0.68
24:3:504:BCR:H10C	39:3:611:CHL:HBA1	1.74	0.68
19:8:128:LEU:HD13	22:8:618:CLA:HAB	1.74	0.68
12:L:326:SER:O	12:L:332:ARG:NH1	2.27	0.68
17:6:75:PHE:C	22:6:604:CLA:HMA1	2.14	0.68
17:6:164:TYR:HB3	22:6:601:CLA:O1D	1.94	0.68
17:6:186:LYS:NZ	25:6:801:LHG:O5	2.26	0.68
22:4:604:CLA:H71	22:4:605:CLA:HMA1	1.74	0.68
17:6:186:LYS:HG3	22:6:607:CLA:O1D	1.94	0.68
1:A:439:SER:OG	2:B:678:THR:HG22	1.94	0.67
22:1:607:CLA:H51	22:1:607:CLA:H92	1.76	0.67
15:4:192:LEU:HD11	25:4:801:LHG:H282	1.75	0.67
25:A:5002:LHG:H161	22:A:1101:CLA:HMB2	1.76	0.67
22:B:1201:CLA:HBA2	10:M:30:TYR:HD1	1.58	0.67
17:6:135:ARG:HB3	39:6:611:CHL:CMC	2.23	0.67
17:6:184:GLU:HB2	22:6:601:CLA:CMB	2.24	0.67
39:7:613:CHL:HHC	39:7:613:CHL:HBB1	1.76	0.67
1:A:293:ASP:HB3	22:A:1116:CLA:HMA1	1.75	0.67
13:1:222:PRO:HG2	22:1:615:CLA:HBB1	1.76	0.67
22:B:1221:CLA:HBB1	22:B:1221:CLA:HMB1	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:6:229:ALA:HB2	17:6:239:PRO:HD3	1.77	0.67
1:A:318:ILE:HG13	22:A:1118:CLA:HED1	1.77	0.67
22:A:1106:CLA:HBB2	22:A:1126:CLA:H171	1.75	0.67
22:B:1208:CLA:HBB1	22:B:1208:CLA:HMB1	1.75	0.67
1:A:245:LEU:HD11	22:A:1114:CLA:HAC2	1.76	0.67
35:J:4002:RRX:H46	35:J:4002:RRX:H51	1.76	0.67
15:4:45:ARG:HG3	15:4:48:LEU:HD13	1.77	0.67
22:5:618:CLA:HBB1	22:5:618:CLA:HHC	1.77	0.67
2:B:258:PHE:CE2	2:B:494:TRP:HB3	2.30	0.67
22:B:1204:CLA:C1	11:I:14:VAL:HG21	2.21	0.67
14:3:481:ASN:HD21	22:3:603:CLA:HED2	1.58	0.67
12:L:335:VAL:HB	12:L:340:ARG:HD2	1.75	0.67
16:5:227:TRP:NE1	22:5:608:CLA:O1D	2.26	0.67
46:7:502:XAT:C33	22:7:605:CLA:HAB	2.25	0.67
19:8:124:LEU:HD21	40:8:809:OLA:H141	1.77	0.67
22:A:1116:CLA:H111	22:A:1134:CLA:HBA1	1.75	0.66
16:5:32:LYS:HZ2	22:5:609:CLA:C2A	2.02	0.66
19:8:120:PHE:CZ	47:8:808:4RF:H41	2.30	0.66
47:8:808:4RF:H42	47:8:808:4RF:H69	1.76	0.66
39:5:613:CHL:HBB1	39:5:613:CHL:HMB1	1.75	0.66
17:6:125:GLU:OE1	39:6:613:CHL:CHB	2.43	0.66
17:6:150:PRO:HD3	22:6:617:CLA:HMC2	1.78	0.66
25:5:801:LHG:H121	25:5:801:LHG:H241	1.75	0.66
22:B:1219:CLA:HBB1	22:B:1219:CLA:HMB1	1.77	0.66
14:3:417:TRP:O	14:3:420:MET:HG3	1.94	0.66
39:6:619:CHL:HBB1	39:6:619:CHL:HMB1	1.78	0.66
24:7:503:BCR:H333	22:8:607:CLA:HAB	1.78	0.66
22:8:620:CLA:HBB1	22:8:620:CLA:HMB1	1.76	0.66
18:7:99:ALA:N	19:8:236:CYS:SG	2.69	0.66
1:A:369:HIS:HA	1:A:372:TYR:HE2	1.57	0.66
38:5:501:LUT:H371	22:5:601:CLA:H92	1.78	0.66
1:A:587:SER:OG	1:A:590:ASP:OD2	2.12	0.66
22:A:1136:CLA:H102	22:A:1136:CLA:HBB1	1.78	0.66
2:B:175:ARG:HB2	22:B:1210:CLA:HBC2	1.78	0.66
2:B:310:THR:HG22	2:B:319:GLY:HA3	1.77	0.66
2:B:572:SER:OG	2:B:575:ASP:OD2	2.13	0.66
22:A:1104:CLA:H92	25:A:5002:LHG:H352	1.78	0.66
22:A:1120:CLA:HMD2	24:K:4001:BCR:H23C	1.77	0.66
22:F:1301:CLA:HBB1	22:F:1301:CLA:HHC	1.76	0.66
8:J:20:MET:CE	18:7:37:LEU:HA	2.26	0.66
7:G:1316:THR:HG21	34:G:5002:ERG:H181	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:2001:PQN:H162	24:B:4006:BCR:H382	1.77	0.65
16:5:131:PHE:HB2	22:6:609:CLA:H42	1.78	0.65
9:K:102:ILE:HG22	22:K:1402:CLA:HBC1	1.77	0.65
2:B:143:LEU:HD21	24:B:4003:BCR:H23C	1.77	0.65
22:B:1231:CLA:HBC1	25:1:802:LHG:H211	1.78	0.65
44:8:803:DGA:HB81	44:8:803:DGA:HA32	1.78	0.65
22:A:1012:CLA:H201	22:A:1106:CLA:H122	1.78	0.65
9:K:64:THR:CG2	22:K:1403:CLA:HMA2	2.26	0.65
24:3:504:BCR:H363	22:3:601:CLA:H121	1.78	0.65
18:7:125:GLN:NE2	19:8:36:PRO:O	2.27	0.65
1:A:712:ALA:N	6:F:439:GLU:OE2	2.29	0.65
13:1:181:MET:HE3	22:1:604:CLA:HMC3	1.78	0.65
18:7:100:LEU:HG	22:7:610:CLA:HBC1	1.78	0.65
18:7:210:ASP:O	18:7:214:THR:OG1	2.15	0.65
1:A:370:HIS:ND1	22:A:1116:CLA:OBD	2.28	0.65
4:D:309:ARG:NH2	4:D:330:PHE:O	2.30	0.65
14:3:435:THR:HA	14:3:438:ILE:HG22	1.79	0.65
1:A:217:GLN:HA	1:A:221:SER:HB3	1.79	0.64
39:4:609:CHL:H161	22:4:608:CLA:H2	1.78	0.64
39:5:610:CHL:HBB1	39:5:610:CHL:HHC	1.78	0.64
39:6:610:CHL:HMB1	39:6:610:CHL:HBB1	1.78	0.64
34:G:5002:ERG:O1	34:G:5002:ERG:C2	2.41	0.64
11:I:23:MET:HG2	24:L:4001:BCR:H10C	1.80	0.64
22:A:1102:CLA:HMA2	22:A:1109:CLA:HMD2	1.77	0.64
22:L:1503:CLA:HMB1	22:L:1503:CLA:HBB1	1.80	0.64
22:A:1123:CLA:HMB1	22:A:1123:CLA:HBB1	1.80	0.64
35:J:4002:RRX:H17	35:J:4002:RRX:H21	1.80	0.64
9:K:56:LEU:HD23	22:K:1403:CLA:HHD	1.80	0.64
17:6:80:ARG:HH11	17:6:163:GLY:HA3	1.61	0.64
7:G:1234:VAL:HG21	7:G:1314:LEU:HD21	1.79	0.64
47:8:808:4RF:H50	40:8:809:OLA:H152	1.79	0.64
22:A:1125:CLA:HBB1	22:A:1125:CLA:HHC	1.78	0.64
12:L:352:LEU:O	12:L:376:ASN:ND2	2.31	0.64
17:6:164:TYR:HA	22:6:601:CLA:O1D	1.96	0.64
18:7:111:VAL:CG1	24:7:503:BCR:H16C	2.28	0.64
39:1:613:CHL:HMB1	39:1:613:CHL:HBB1	1.79	0.64
1:A:369:HIS:NE2	22:A:1124:CLA:OBD	2.30	0.64
2:B:464:ILE:HD12	22:B:1234:CLA:O1A	1.97	0.64
2:B:646:VAL:HG21	22:B:1205:CLA:HAC1	1.79	0.64
38:1:501:LUT:H27	22:1:611:CLA:H42	1.80	0.64
16:5:135:ARG:NH1	22:6:609:CLA:OBD	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:336:LYS:HG3	6:F:340:LYS:HE3	1.79	0.64
13:1:134:MET:HG3	22:1:612:CLA:HMC3	1.80	0.64
22:1:601:CLA:HBB1	22:1:601:CLA:HMB1	1.78	0.64
17:6:39:TRP:CE3	17:6:40:LEU:HB2	2.33	0.64
18:7:116:LEU:HD13	22:7:612:CLA:HMA2	1.80	0.64
1:A:72:LYS:HD3	22:A:1109:CLA:OBD	1.99	0.63
2:B:351:GLN:HE21	22:B:1223:CLA:HMD2	1.63	0.63
2:B:518:PHE:HA	22:B:1235:CLA:HED1	1.79	0.63
22:4:616:CLA:HBD	22:4:616:CLA:H2	1.79	0.63
19:8:227:LEU:HD21	22:8:608:CLA:HMC3	1.80	0.63
14:3:420:MET:O	16:5:38:VAL:HG23	1.98	0.63
39:1:609:CHL:HMB1	31:8:810:PTY:C37	2.28	0.63
15:4:150:ASP:OD1	15:4:154:ASN:N	2.31	0.63
15:4:169:LEU:HB2	15:4:171:PHE:CE1	2.34	0.63
2:B:60:LEU:CD1	37:M:4001:ECH:H37A	2.28	0.63
16:5:32:LYS:NZ	22:5:609:CLA:C2A	2.61	0.63
16:5:59:LEU:HD13	22:5:604:CLA:H42	1.79	0.63
18:7:29:ASP:HA	22:7:604:CLA:O1D	1.98	0.63
39:4:618:CHL:HBB1	39:4:618:CHL:HHC	1.81	0.63
17:6:190:LEU:HG	38:6:501:LUT:H191	1.81	0.63
22:A:1102:CLA:HBA2	22:A:1109:CLA:H61	1.80	0.63
22:B:1230:CLA:HMA1	31:B:5005:PTY:H161	1.81	0.63
16:5:47:SER:O	16:5:180:LYS:NZ	2.31	0.63
22:A:1137:CLA:H43	24:A:4004:BCR:H19C	1.80	0.63
2:B:33:GLU:OE1	2:B:332:HIS:NE2	2.21	0.63
22:8:606:CLA:HMA2	39:8:613:CHL:HBC3	1.79	0.63
47:8:808:4RF:H77	47:8:808:4RF:H12	1.81	0.63
38:5:505:LUT:H371	38:5:505:LUT:H28	1.81	0.63
22:A:1111:CLA:HMB1	22:A:1111:CLA:HBB1	1.81	0.62
2:B:99:GLN:O	2:B:103:GLU:HG3	1.99	0.62
22:B:1201:CLA:H72	11:I:29:TYR:CD2	2.33	0.62
8:J:31:PRO:O	8:J:35:LEU:HD23	1.99	0.62
29:1:804:LMT:H61	22:1:612:CLA:H61	1.80	0.62
19:8:198:GLY:O	19:8:202:MET:HG3	1.99	0.62
6:F:462:PHE:CD2	44:8:803:DGA:HB72	2.34	0.62
13:1:140:PHE:HB3	22:1:611:CLA:HMC3	1.81	0.62
22:4:610:CLA:HBA1	22:4:612:CLA:HBC3	1.81	0.62
22:A:1013:CLA:H101	24:A:4005:BCR:H23C	1.81	0.62
38:4:502:LUT:H28	22:4:604:CLA:H52	1.80	0.62
17:6:80:ARG:NH1	17:6:163:GLY:HA3	2.14	0.62
22:6:604:CLA:HBC2	22:6:609:CLA:HBB2	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:358:LYS:HG2	22:L:1503:CLA:HMA1	1.80	0.62
19:8:135:GLU:OE1	19:8:138:ARG:NH2	2.21	0.62
22:A:1108:CLA:HHC	22:A:1108:CLA:HBB1	1.81	0.62
18:7:101:LEU:HD21	25:7:803:LHG:H192	1.81	0.62
9:K:58:PRO:HD2	22:K:1403:CLA:C1B	2.29	0.62
7:G:1247:ARG:NH1	7:G:1290:ASP:OD1	2.32	0.62
12:L:393:VAL:O	12:L:396:GLN:NE2	2.33	0.62
16:5:159:ASN:HB3	16:5:165:PRO:HA	1.82	0.62
18:7:118:ASP:HB2	22:7:611:CLA:HAC2	1.82	0.62
1:A:45:THR:HG22	1:A:714:GLN:CG	2.30	0.62
22:A:1112:CLA:HBA2	22:A:1114:CLA:HMB3	1.80	0.62
5:E:45:VAL:HG12	5:E:97:ALA:HA	1.81	0.62
13:1:61:ALA:HB2	22:1:604:CLA:HBA1	1.82	0.62
17:6:182:VAL:CG1	22:6:607:CLA:HED2	2.29	0.62
18:7:11:PHE:CD2	18:7:14:ASN:CB	2.83	0.62
4:D:218:GLU:HG2	4:D:277:VAL:O	1.99	0.62
39:3:608:CHL:HHC	39:3:608:CHL:HBB1	1.81	0.62
22:6:604:CLA:HMB1	22:6:604:CLA:HBB1	1.81	0.62
39:4:609:CHL:HHC	39:4:609:CHL:HBB1	1.80	0.62
17:6:125:GLU:OE2	39:6:613:CHL:HMB3	1.99	0.62
1:A:95:GLY:O	1:A:99:SER:OG	2.17	0.61
2:B:451:GLU:OE2	6:F:369:ARG:NE	2.33	0.61
22:B:1201:CLA:HMB1	22:B:1201:CLA:HBB1	1.82	0.61
9:K:51:ALA:HB2	22:K:1403:CLA:HBC2	1.82	0.61
18:7:19:PRO:O	18:7:21:TYR:N	2.32	0.61
5:E:54:TRP:CD1	5:E:79:LYS:NZ	2.68	0.61
17:6:164:TYR:CA	22:6:601:CLA:O1D	2.48	0.61
22:8:605:CLA:HHC	22:8:605:CLA:HBB1	1.81	0.61
22:3:602:CLA:HBB1	22:3:602:CLA:HMB1	1.82	0.61
15:4:39:PRO:HG3	15:4:55:ASP:HB3	1.81	0.61
17:6:164:TYR:CB	22:6:601:CLA:O1D	2.48	0.61
1:A:178:TRP:HB2	22:A:1109:CLA:HMC3	1.81	0.61
1:A:279:GLN:HG2	1:A:503:LEU:HD12	1.82	0.61
22:A:1138:CLA:H2	22:B:1229:CLA:H42	1.81	0.61
6:F:393:GLY:O	6:F:397:ARG:HG2	2.00	0.61
6:F:420:TYR:HE2	6:F:460:ARG:HE	1.49	0.61
22:A:1118:CLA:H51	14:3:288:PRO:HG3	1.82	0.61
22:A:1130:CLA:C3	22:L:1502:CLA:H8	2.30	0.61
12:L:363:ARG:HA	12:L:368:VAL:HG21	1.82	0.61
14:3:318:MET:HE3	22:3:601:CLA:HMC3	1.82	0.61
19:8:238:ASN:ND2	22:8:603:CLA:OBD	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:688:LEU:HD12	24:L:4002:BCR:HC41	1.82	0.61
22:B:1229:CLA:HMC3	31:B:5005:PTY:H202	1.80	0.61
22:7:609:CLA:H2	25:7:801:LHG:H282	1.81	0.61
1:A:220:VAL:HG13	1:A:240:PRO:HB3	1.83	0.61
1:A:299:LEU:HD22	22:A:1113:CLA:HMC1	1.82	0.61
1:A:577:GLY:CA	2:B:563:PRO:HD3	2.29	0.61
4:D:202:ILE:HG13	4:D:243:ARG:HE	1.66	0.61
9:K:48:PRO:HA	22:K:1403:CLA:HMC3	1.82	0.61
13:1:82:MET:SD	22:1:601:CLA:HAB	2.40	0.61
17:6:121:LEU:HD21	39:6:613:CHL:C1D	2.31	0.61
2:B:62:THR:HG23	2:B:143:LEU:HD13	1.83	0.61
22:B:1202:CLA:H11	22:B:1203:CLA:HBB1	1.83	0.61
22:B:1204:CLA:O1A	11:I:14:VAL:HB	2.01	0.61
4:D:243:ARG:N	4:D:247:ASN:HD21	1.98	0.61
9:K:51:ALA:HB2	22:K:1403:CLA:C2C	2.31	0.61
22:4:606:CLA:HBA2	22:4:616:CLA:HMB3	1.83	0.61
38:6:501:LUT:H373	39:6:611:CHL:H42	1.82	0.61
2:B:646:VAL:HA	22:B:1206:CLA:CBC	2.31	0.60
1:A:438:ILE:HG13	1:A:556:TYR:HE1	1.67	0.60
22:A:1140:CLA:H61	8:J:33:LEU:HD21	1.81	0.60
22:B:1221:CLA:HMA2	22:B:1221:CLA:H2	1.84	0.60
22:B:1231:CLA:HHC	22:B:1231:CLA:HBB1	1.81	0.60
24:3:504:BCR:H14C	39:3:611:CHL:H72	1.82	0.60
16:5:117:ASN:ND2	17:6:222:GLY:HA2	2.17	0.60
22:A:1130:CLA:HBB1	22:A:1136:CLA:H192	1.81	0.60
12:L:330:ALA:HB2	22:L:1502:CLA:HMD1	1.83	0.60
18:7:111:VAL:HG11	24:7:503:BCR:H16C	1.84	0.60
22:A:1012:CLA:C4	2:B:439:VAL:HG13	2.32	0.60
22:B:1240:CLA:HHB	25:B:5001:LHG:HC81	1.82	0.60
14:3:382:ARG:HG3	39:3:611:CHL:CHD	2.31	0.60
16:5:170:ASP:OD1	38:5:501:LUT:O23	2.19	0.60
24:5:503:BCR:H16C	39:5:611:CHL:HMB3	1.82	0.60
19:8:96:VAL:HG21	22:8:620:CLA:HMB3	1.82	0.60
22:A:1102:CLA:HMC1	25:A:5002:LHG:H171	1.82	0.60
2:B:258:PHE:HD1	22:B:1214:CLA:HMB2	1.67	0.60
2:B:659:ALA:HB3	22:B:1023:CLA:HBB2	1.82	0.60
12:L:445:THR:HG22	12:L:451:TYR:CE1	2.36	0.60
18:7:125:GLN:HB3	22:7:611:CLA:HMC1	1.83	0.60
1:A:510:TRP:CZ2	22:A:1125:CLA:HMC3	2.36	0.60
2:B:478:LEU:HD22	2:B:486:PRO:HG3	1.82	0.60
2:B:659:ALA:O	22:B:1023:CLA:HAB	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:1212:CLA:H203	24:B:4002:BCR:H311	1.83	0.60
14:3:325:LEU:HD23	22:3:607:CLA:H202	1.84	0.60
14:3:403:VAL:HG12	14:3:416:GLN:HB3	1.84	0.60
16:5:52:ARG:HE	22:5:609:CLA:HED2	1.65	0.60
17:6:142:LYS:HG3	17:6:145:SER:HB3	1.84	0.60
22:B:1227:CLA:HBB2	22:B:1236:CLA:HMC2	1.84	0.60
7:G:1312:TYR:OH	34:G:5002:ERG:H272	2.02	0.60
9:K:64:THR:HG21	22:K:1403:CLA:HMA2	1.82	0.60
25:4:801:LHG:H111	25:4:801:LHG:H271	1.83	0.60
22:A:1120:CLA:H12	22:K:1403:CLA:HMB2	1.82	0.59
6:F:444:VAL:HG22	8:J:33:LEU:HD11	1.83	0.59
9:K:56:LEU:HD23	22:K:1403:CLA:CHD	2.32	0.59
34:G:5002:ERG:O1	34:G:5002:ERG:C4	2.42	0.59
16:5:166:GLY:N	22:5:601:CLA:OBD	2.30	0.59
22:5:603:CLA:H2	22:5:608:CLA:HMD1	1.84	0.59
17:6:181:LYS:HG3	22:6:601:CLA:CMA	2.31	0.59
17:6:182:VAL:HG12	22:6:607:CLA:HED2	1.84	0.59
22:7:604:CLA:O1A	22:7:604:CLA:H3A	2.02	0.59
1:A:384:TYR:HB3	1:A:747:ILE:HD11	1.83	0.59
22:B:1232:CLA:HAA2	22:G:1603:CLA:HMA1	1.84	0.59
14:3:260:VAL:O	25:3:801:LHG:HC11	2.02	0.59
17:6:164:TYR:C	22:6:601:CLA:HED2	2.22	0.59
22:A:1128:CLA:HBB1	22:A:1128:CLA:HMB1	1.83	0.59
2:B:676:ILE:HG23	22:B:1238:CLA:HMC3	1.85	0.59
18:7:42:GLU:HG2	47:7:807:4RF:H41	1.84	0.59
12:L:328:LEU:HD21	22:L:1501:CLA:HAB	1.84	0.59
14:3:457:MET:HG2	22:3:603:CLA:HMD1	1.84	0.59
22:7:617:CLA:HAA1	26:8:802:DGD:HA81	1.83	0.59
1:A:554:VAL:HG21	24:A:4004:BCR:HC31	1.85	0.59
25:A:5003:LHG:H101	14:3:456:VAL:HG23	1.85	0.59
12:L:371:ILE:O	12:L:375:ILE:HG12	2.03	0.59
39:1:609:CHL:HHC	39:1:609:CHL:HBB1	1.83	0.59
1:A:39:LEU:O	1:A:48:TRP:NE1	2.26	0.59
1:A:396:TRP:HB3	22:A:1126:CLA:HMC3	1.84	0.59
2:B:352:HIS:ND1	22:B:1214:CLA:OBD	2.34	0.59
4:D:218:GLU:OE2	4:D:219:PHE:O	2.21	0.59
15:4:39:PRO:O	15:4:41:HIS:N	2.34	0.59
16:5:146:VAL:CG1	17:6:42:GLY:HA3	2.33	0.59
38:6:501:LUT:H23	22:6:601:CLA:H11	1.84	0.59
22:7:601:CLA:H92	22:7:602:CLA:HMA1	1.84	0.59
1:A:15:ILE:HG21	22:A:1108:CLA:HAA2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:2001:PQN:H201	22:A:1101:CLA:H42	1.84	0.59
2:B:296:PHE:C	7:G:1285:ILE:HD13	2.23	0.59
39:5:611:CHL:HBB1	39:5:611:CHL:HHC	1.84	0.59
2:B:171:ASN:ND2	7:G:1276:ASP:OD2	2.28	0.59
12:L:300:GLN:O	12:L:312:GLU:N	2.35	0.59
38:8:502:LUT:H32	39:8:604:CHL:CBB	2.33	0.59
2:B:167:SER:OG	7:G:1276:ASP:N	2.36	0.59
13:1:141:ARG:NH2	22:1:612:CLA:O1D	2.34	0.59
22:B:1232:CLA:HMD2	22:G:1603:CLA:CBB	2.32	0.58
9:K:83:ASN:HB3	22:K:1404:CLA:CAD	2.32	0.58
38:3:501:LUT:H28	22:3:601:CLA:H43	1.84	0.58
22:A:1116:CLA:HHC	22:A:1116:CLA:HBB1	1.84	0.58
22:B:1201:CLA:HAA1	10:M:30:TYR:HA	1.85	0.58
4:D:298:ASN:HB2	4:D:301:ARG:CZ	2.33	0.58
16:5:101:THR:OG1	16:5:104:MET:SD	2.61	0.58
19:8:164:THR:OG1	19:8:169:TYR:O	2.20	0.58
22:1:606:CLA:HMA2	39:1:613:CHL:HBC3	1.85	0.58
16:5:145:SER:O	17:6:42:GLY:HA2	2.03	0.58
17:6:41:PRO:CD	22:6:609:CLA:C3D	2.80	0.58
17:6:216:HIS:ND1	17:6:223:THR:OG1	2.34	0.58
2:B:27:ALA:HB2	26:B:5003:DGD:HA51	1.84	0.58
2:B:181:ALA:HB2	2:B:289:GLY:HA3	1.85	0.58
22:B:1228:CLA:C4A	22:B:1228:CLA:HBA2	2.29	0.58
25:F:5001:LHG:H302	25:F:5001:LHG:H251	1.84	0.58
13:1:130:GLU:HA	39:1:613:CHL:HMA3	1.85	0.58
2:B:429:PHE:CE1	22:B:1235:CLA:HAB	2.38	0.58
13:1:39:GLY:HA3	19:8:147:SER:HB3	1.85	0.58
15:4:163:TYR:HB3	22:4:601:CLA:O1D	2.04	0.58
15:4:167:ASP:HB3	15:4:170:SER:HA	1.86	0.58
16:5:44:LEU:HD22	16:5:51:ASP:OD2	2.04	0.58
11:I:26:MET:HG3	24:L:4001:BCR:C31	2.32	0.58
13:1:169:LEU:HB3	22:1:601:CLA:HMA1	1.85	0.58
17:6:87:MET:HG2	38:6:501:LUT:C15	2.34	0.58
25:B:5001:LHG:H332	32:B:5007:LAP:H71	1.84	0.58
15:4:224:PHE:HA	15:4:227:ASN:HD21	1.68	0.58
17:6:193:LEU:HD13	22:6:603:CLA:H91	1.86	0.58
22:6:615:CLA:HMC3	39:6:619:CHL:HBC3	1.84	0.58
22:B:1202:CLA:H93	22:B:1210:CLA:H2	1.86	0.58
22:B:1237:CLA:H203	22:L:1502:CLA:CBB	2.34	0.58
22:F:1302:CLA:HBD	47:7:807:4RF:H5	1.85	0.58
29:1:804:LMT:H82	22:1:605:CLA:CMD	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:6:155:PHE:HE2	22:6:617:CLA:HAA1	1.69	0.58
2:B:285:PHE:HE1	22:B:1216:CLA:HAB	1.68	0.58
17:6:181:LYS:HG3	22:6:601:CLA:HMA3	1.86	0.58
2:B:546:LYS:NZ	6:F:478:THR:OG1	2.36	0.58
15:4:184:ILE:O	15:4:188:ARG:HG3	2.04	0.58
25:4:801:LHG:HC81	24:6:503:BCR:HC31	1.86	0.58
16:5:51:ASP:OD2	22:5:604:CLA:HED2	2.04	0.58
22:A:1130:CLA:H42	22:L:1502:CLA:H102	1.84	0.57
22:B:1201:CLA:H93	11:I:26:MET:HE3	1.86	0.57
22:B:1211:CLA:H3A	24:B:4003:BCR:H383	1.86	0.57
22:B:1232:CLA:HAA2	22:G:1603:CLA:CMA	2.34	0.57
22:F:1302:CLA:HBB1	22:F:1302:CLA:HMB1	1.86	0.57
13:1:37:LEU:HD21	39:1:609:CHL:HMA3	1.85	0.57
22:1:608:CLA:H11	39:1:609:CHL:H42	1.86	0.57
17:6:155:PHE:CE2	22:6:617:CLA:HAA1	2.38	0.57
22:6:604:CLA:O1A	22:6:604:CLA:H3A	2.03	0.57
22:A:1012:CLA:HMB3	22:B:1021:CLA:H18	1.86	0.57
22:A:1107:CLA:HBA2	22:A:1107:CLA:CHA	2.34	0.57
2:B:659:ALA:C	22:B:1023:CLA:HAB	2.24	0.57
7:G:1313:ILE:HD12	34:G:5002:ERG:H213	1.86	0.57
22:K:1402:CLA:HHC	22:K:1402:CLA:HBB1	1.86	0.57
19:8:149:ALA:HB2	19:8:162:LYS:HA	1.85	0.57
1:A:16:VAL:HB	1:A:187:LYS:HD2	1.86	0.57
22:A:1012:CLA:HBC2	2:B:586:ASN:HB2	1.87	0.57
25:B:5002:LHG:H112	25:B:5002:LHG:H272	1.86	0.57
39:4:613:CHL:HHC	39:4:613:CHL:HBB1	1.86	0.57
17:6:186:LYS:HB3	22:6:607:CLA:CMD	2.34	0.57
22:A:1122:CLA:H11	22:A:1133:CLA:H202	1.86	0.57
22:B:1201:CLA:HAB	22:B:1203:CLA:CAD	2.34	0.57
3:C:23:THR:HG22	3:C:47:ASP:HB3	1.86	0.57
38:1:503:LUT:H28	38:1:503:LUT:H361	1.87	0.57
16:5:52:ARG:HB2	22:5:604:CLA:HMD1	1.87	0.57
18:7:8:GLU:OE2	25:7:801:LHG:O2	2.21	0.57
12:L:298:VAL:HG23	12:L:299:VAL:HG23	1.86	0.57
12:L:327:ASN:HB3	22:L:1501:CLA:HAC1	1.86	0.57
17:6:165:PRO:CD	22:6:601:CLA:OBD	2.53	0.57
22:A:1104:CLA:HAB	22:A:1127:CLA:HBB1	1.85	0.57
22:A:1107:CLA:C4	24:J:4001:BCR:H10C	2.34	0.57
1:A:465:LEU:HG	22:B:1206:CLA:HMC3	1.86	0.57
4:D:316:GLU:HB3	4:D:319:GLN:HG3	1.87	0.57
13:1:178:ARG:HA	13:1:181:MET:HE2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:ILE:HA	22:B:1201:CLA:HMD3	1.87	0.57
14:3:275:TYR:HE2	14:3:292:CYS:HB3	1.70	0.57
14:3:366:SER:HB3	22:7:608:CLA:HED1	1.87	0.57
22:5:617:CLA:HED3	45:6:806:SPH:H141	1.86	0.57
17:6:62:PRO:HG3	45:6:806:SPH:H122	1.87	0.57
38:7:501:LUT:H30	22:7:601:CLA:H71	1.86	0.57
22:A:1137:CLA:HBB1	22:A:1137:CLA:HHC	1.87	0.57
2:B:359:TYR:CE2	22:B:1225:CLA:HED2	2.40	0.57
5:E:46:ARG:NH2	6:F:476:LYS:HE3	2.20	0.57
18:7:219:ASN:ND2	22:7:603:CLA:OBD	2.36	0.57
19:8:76:ASN:HD22	39:8:604:CHL:HBB2	1.69	0.57
1:A:402:ILE:HG23	24:A:4004:BCR:H343	1.87	0.56
2:B:457:GLU:OE1	2:B:462:GLN:NE2	2.35	0.56
22:B:1210:CLA:HBB1	22:B:1210:CLA:HMB1	1.87	0.56
18:7:101:LEU:O	18:7:105:ILE:HG12	2.05	0.56
24:7:503:BCR:H372	39:7:613:CHL:H152	1.88	0.56
1:A:43:PRO:HB3	1:A:48:TRP:CE3	2.40	0.56
1:A:374:MET:SD	22:A:1116:CLA:HBD	2.44	0.56
22:A:1131:CLA:H18	24:L:4001:BCR:H343	1.86	0.56
22:B:1235:CLA:HBC2	31:B:5005:PTY:H251	1.88	0.56
4:D:325:LYS:HE3	4:D:330:PHE:CE1	2.40	0.56
6:F:449:LYS:O	6:F:453:GLU:HG3	2.04	0.56
22:F:1301:CLA:C2	32:F:5003:LAP:H21	2.34	0.56
9:K:51:ALA:CB	22:K:1403:CLA:C2C	2.83	0.56
14:3:436:ASN:O	14:3:440:ASN:ND2	2.31	0.56
25:4:801:LHG:H111	25:4:801:LHG:H292	1.87	0.56
17:6:122:LEU:O	17:6:126:LEU:HG	2.05	0.56
1:A:646:LEU:HD12	1:A:650:LEU:HD23	1.86	0.56
22:A:1012:CLA:H172	22:A:1126:CLA:H143	1.86	0.56
2:B:130:LEU:HD13	2:B:136:LEU:HD23	1.85	0.56
2:B:499:LEU:HA	2:B:502:ILE:HG22	1.88	0.56
22:B:1201:CLA:H203	22:B:1201:CLA:H141	1.87	0.56
9:K:64:THR:CG2	22:K:1403:CLA:CMA	2.83	0.56
22:3:612:CLA:HMC1	22:3:613:CLA:HBB1	1.86	0.56
17:6:58:TYR:CD1	22:6:609:CLA:CBC	2.86	0.56
17:6:89:GLY:HA2	38:6:502:LUT:H182	1.87	0.56
17:6:193:LEU:HD13	22:6:603:CLA:C9	2.36	0.56
39:6:610:CHL:CBB	39:6:613:CHL:HBB2	2.35	0.56
22:B:1201:CLA:HBA2	10:M:30:TYR:CD1	2.41	0.56
9:K:58:PRO:HD2	22:K:1403:CLA:CHB	2.35	0.56
13:1:60:LEU:HD12	22:1:604:CLA:H2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:4:618:CHL:HBD	39:4:618:CHL:HBA1	1.87	0.56
17:6:128:VAL:HG13	24:6:503:BCR:C14	2.35	0.56
39:6:611:CHL:CBB	22:6:617:CLA:HMC3	2.36	0.56
22:B:1220:CLA:HMA1	22:B:1240:CLA:CGD	2.36	0.56
4:D:287:HIS:HB3	4:D:288:PRO:HD3	1.86	0.56
12:L:386:LEU:HD22	24:L:4001:BCR:H17C	1.85	0.56
16:5:52:ARG:HG2	22:5:609:CLA:OBD	2.06	0.56
1:A:390:LEU:HD11	22:A:1127:CLA:HED3	1.86	0.56
13:1:107:VAL:HG12	13:1:108:GLN:HG3	1.87	0.56
22:3:606:CLA:H201	25:5:801:LHG:H372	1.87	0.56
1:A:175:PHE:HE1	31:3:802:PTY:H162	1.71	0.56
2:B:701:LEU:HD11	22:B:1239:CLA:HMD3	1.87	0.56
12:L:436:SER:HB3	24:L:4003:BCR:H312	1.87	0.56
15:4:57:LEU:HD23	38:4:502:LUT:H222	1.86	0.56
22:7:611:CLA:HMB1	22:7:611:CLA:HBB1	1.88	0.56
19:8:183:SER:O	19:8:185:GLU:N	2.38	0.56
1:A:178:TRP:HZ2	31:3:802:PTY:H342	1.70	0.56
2:B:51:HIS:O	2:B:55:LEU:HD12	2.06	0.56
6:F:441:ILE:HD13	8:J:29:THR:HG23	1.87	0.56
7:G:1248:PHE:HB3	38:1:503:LUT:H373	1.87	0.56
22:7:605:CLA:HBC2	22:7:605:CLA:HHD	1.87	0.56
19:8:235:PHE:HE1	22:8:608:CLA:O1D	1.88	0.56
38:8:501:LUT:H32	39:8:601:CHL:CBB	2.36	0.56
1:A:359:LEU:HD21	22:A:1123:CLA:HMB2	1.88	0.56
2:B:646:VAL:HA	22:B:1206:CLA:HBC1	1.87	0.56
22:B:1232:CLA:CAA	22:G:1603:CLA:HMA1	2.36	0.56
9:K:51:ALA:HB2	22:K:1403:CLA:CBC	2.36	0.56
39:5:611:CHL:CBB	22:5:618:CLA:HMC3	2.35	0.56
22:6:604:CLA:H43	22:6:604:CLA:HMB2	1.86	0.56
1:A:359:LEU:HG	22:A:1123:CLA:HHB	1.87	0.56
2:B:608:ASN:O	2:B:612:GLU:HG2	2.06	0.56
22:B:1207:CLA:HBB1	22:B:1207:CLA:HHC	1.87	0.56
17:6:77:GLU:HG2	17:6:140:ILE:HG13	1.88	0.56
17:6:205:THR:HG22	17:6:207:LYS:HG2	1.87	0.56
18:7:11:PHE:CE2	18:7:14:ASN:CB	2.84	0.56
1:A:67:GLU:O	1:A:71:ARG:HG3	2.05	0.55
1:A:341:LEU:HD13	1:A:344:ILE:HD11	1.88	0.55
2:B:258:PHE:HE2	2:B:494:TRP:HB3	1.70	0.55
22:B:1222:CLA:H52	22:B:1231:CLA:HBB2	1.88	0.55
15:4:164:PRO:HD3	22:4:611:CLA:HMD2	1.88	0.55
17:6:164:TYR:O	22:6:601:CLA:CED	2.52	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:6:169:PHE:CD1	39:6:611:CHL:H11	2.28	0.55
2:B:258:PHE:CD1	22:B:1214:CLA:HMB2	2.42	0.55
2:B:395:PHE:CE1	2:B:413:LEU:HD21	2.41	0.55
2:B:395:PHE:CZ	2:B:413:LEU:HD21	2.41	0.55
24:5:503:BCR:HC41	25:6:801:LHG:HC81	1.87	0.55
19:8:196:ARG:NH1	25:8:801:LHG:O4	2.38	0.55
22:A:1111:CLA:H201	22:3:605:CLA:H62	1.88	0.55
22:B:1022:CLA:OBD	22:B:1021:CLA:HMB3	2.07	0.55
6:F:445:PRO:HD2	36:J:5001:LPX:O3	2.05	0.55
38:3:502:LUT:H162	22:3:606:CLA:HMB3	1.89	0.55
22:7:609:CLA:HBB2	22:7:604:CLA:HBC2	1.89	0.55
19:8:131:PHE:CG	22:8:612:CLA:HMC3	2.41	0.55
22:A:1119:CLA:H152	24:A:4003:BCR:H21C	1.88	0.55
2:B:10:SER:OG	2:B:13:LEU:HB2	2.06	0.55
6:F:393:GLY:H	6:F:396:LEU:HD12	1.71	0.55
13:1:37:LEU:O	13:1:40:SER:OG	2.15	0.55
22:3:616:CLA:HBC3	16:5:227:TRP:CZ3	2.41	0.55
17:6:124:PHE:CZ	39:6:613:CHL:HED3	2.41	0.55
2:B:293:ARG:HH21	2:B:297:GLY:HA2	1.70	0.55
5:E:64:VAL:O	5:E:66:GLN:NE2	2.39	0.55
11:I:30:ILE:HD13	24:L:4001:BCR:H333	1.86	0.55
19:8:139:TRP:HZ3	22:8:618:CLA:HAC2	1.70	0.55
2:B:211:ASP:OD1	2:B:212:ASN:N	2.40	0.55
2:B:362:LEU:HG	2:B:369:GLN:OE1	2.06	0.55
2:B:577:PHE:CZ	26:B:5003:DGD:HB81	2.41	0.55
14:3:449:LEU:HD23	22:3:603:CLA:HMC1	1.89	0.55
17:6:189:ARG:CB	25:6:801:LHG:H241	2.36	0.55
47:8:807:4RF:H10	22:8:610:CLA:HMB2	1.87	0.55
1:A:327:GLU:OE1	1:A:339:LYS:HA	2.07	0.55
22:A:1117:CLA:HBB1	22:A:1117:CLA:HMB1	1.89	0.55
22:3:607:CLA:HMB1	22:3:607:CLA:HBB1	1.88	0.55
22:A:1140:CLA:HHC	22:A:1140:CLA:HBB1	1.89	0.55
22:3:616:CLA:H43	16:5:231:ILE:HG12	1.88	0.55
16:5:81:MET:SD	22:5:601:CLA:HAB	2.47	0.55
22:8:610:CLA:CAD	47:8:808:4RF:H66	2.36	0.55
2:B:416:LYS:HB2	2:B:540:LEU:HD23	1.89	0.55
38:1:501:LUT:H162	22:1:608:CLA:HBC1	1.87	0.55
22:A:1138:CLA:HED2	2:B:425:TRP:HB2	1.89	0.55
2:B:175:ARG:HE	22:B:1221:CLA:HMD1	1.72	0.55
22:A:1120:CLA:C3D	24:K:4001:BCR:H271	2.38	0.54
22:B:1236:CLA:HHD	22:B:1236:CLA:HBC2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:B:5007:LAP:O5	32:B:5007:LAP:H14	2.06	0.54
14:3:391:SER:OG	14:3:392:GLN:N	2.39	0.54
16:5:210:GLY:O	16:5:214:ASN:ND2	2.39	0.54
1:A:102:GLU:HG3	1:A:156:GLU:HG3	1.88	0.54
1:A:733:LEU:HD22	22:A:1139:CLA:HMA1	1.88	0.54
22:A:1118:CLA:HMA1	9:K:94:LEU:HB3	1.89	0.54
22:A:1125:CLA:H143	22:A:1133:CLA:H13	1.89	0.54
22:B:1022:CLA:CAD	22:B:1021:CLA:HMB3	2.38	0.54
22:B:1219:CLA:HMB3	22:B:1240:CLA:C1D	2.37	0.54
25:F:5002:LHG:H102	22:8:610:CLA:H93	1.89	0.54
8:J:20:MET:HE3	18:7:37:LEU:HA	1.89	0.54
22:4:615:CLA:HAA2	22:4:615:CLA:H2	1.89	0.54
1:A:691:GLY:O	1:A:695:GLU:HG2	2.08	0.54
2:B:134:GLN:NE2	10:M:3:ILE:HG22	2.15	0.54
2:B:685:ARG:O	2:B:685:ARG:HG3	2.07	0.54
22:B:1209:CLA:HAA1	7:G:1278:ARG:HD3	1.89	0.54
3:C:54:CYS:HB3	28:C:3002:SF4:S4	2.47	0.54
34:G:5002:ERG:C3	34:G:5002:ERG:HO1	2.14	0.54
19:8:76:ASN:HD22	39:8:604:CHL:CBB	2.20	0.54
1:A:175:PHE:CE1	31:3:802:PTY:H162	2.43	0.54
2:B:167:SER:OG	7:G:1275:GLY:C	2.46	0.54
2:B:672:TRP:CH2	23:B:2002:PQN:H2M3	2.42	0.54
22:B:1234:CLA:HHD	22:B:1234:CLA:HBC2	1.89	0.54
6:F:424:LYS:NZ	6:F:427:GLN:OE1	2.32	0.54
9:K:64:THR:HG21	22:K:1403:CLA:CMA	2.37	0.54
16:5:164:TYR:HB3	22:5:601:CLA:O1D	2.07	0.54
1:A:656:GLN:HG2	1:A:749:ALA:HB3	1.90	0.54
21:A:1011:CL0:CGD	21:A:1011:CL0:H8	2.38	0.54
2:B:423:LEU:HD13	2:B:533:LEU:HA	1.89	0.54
22:B:1023:CLA:H121	24:I:4001:BCR:H281	1.90	0.54
14:3:311:VAL:O	14:3:315:ARG:HG3	2.08	0.54
22:A:1109:CLA:H101	22:A:1101:CLA:HBB2	1.88	0.54
12:L:353:VAL:HA	12:L:376:ASN:OD1	2.08	0.54
22:1:605:CLA:HBC1	22:1:612:CLA:HAC1	1.89	0.54
17:6:170:ALA:HB1	22:6:601:CLA:HBA2	1.90	0.54
2:B:670:GLY:O	2:B:674:GLU:HG3	2.07	0.54
22:B:1228:CLA:CBA	6:F:471:MET:HE2	2.37	0.54
24:A:4001:BCR:H362	24:A:4002:BCR:H21C	1.89	0.54
7:G:1231:VAL:O	7:G:1235:VAL:HG12	2.08	0.54
14:3:271:GLN:O	14:3:274:SER:OG	2.25	0.54
25:4:801:LHG:HC81	24:6:503:BCR:C3	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:6:801:LHG:H372	25:6:801:LHG:H191	1.90	0.54
18:7:176:ILE:O	18:7:180:ARG:HG3	2.08	0.54
1:A:316:TRP:CD1	9:K:91:VAL:HG21	2.43	0.53
2:B:204:ARG:NH2	2:B:254:ALA:O	2.36	0.53
22:B:1209:CLA:HBD	7:G:1278:ARG:HD3	1.90	0.53
24:B:4004:BCR:H313	22:1:605:CLA:HED1	1.89	0.53
22:B:1204:CLA:H61	24:I:4001:BCR:C3	2.26	0.53
22:1:610:CLA:HMB1	22:1:610:CLA:HBB1	1.90	0.53
14:3:421:LEU:HD22	16:5:35:PHE:CD2	2.44	0.53
17:6:41:PRO:O	22:6:609:CLA:HED1	2.08	0.53
17:6:150:PRO:HD2	22:6:617:CLA:CHC	2.38	0.53
38:7:501:LUT:H361	38:7:501:LUT:H28	1.90	0.53
1:A:714:GLN:HG3	1:A:716:ARG:NH2	2.23	0.53
22:A:1102:CLA:HAB	22:A:1104:CLA:CAD	2.39	0.53
23:A:2001:PQN:H291	25:A:5002:LHG:H141	1.88	0.53
2:B:326:THR:OG1	2:B:404:ASN:OD1	2.25	0.53
22:B:1201:CLA:HBA1	22:B:1201:CLA:CHA	2.37	0.53
9:K:56:LEU:HB3	22:K:1403:CLA:CHD	2.38	0.53
38:1:501:LUT:H30	22:1:601:CLA:H52	1.89	0.53
22:7:610:CLA:HBB1	25:7:803:LHG:H312	1.89	0.53
1:A:452:SER:HB3	1:A:538:ILE:HD13	1.90	0.53
22:A:1130:CLA:C2	22:L:1502:CLA:H72	2.38	0.53
22:B:1201:CLA:H93	11:I:26:MET:CE	2.38	0.53
4:D:195:GLN:NE2	4:D:197:ASP:O	2.40	0.53
16:5:125:GLU:HA	39:5:613:CHL:HMA3	1.90	0.53
16:5:188:LYS:NZ	25:5:801:LHG:O5	2.40	0.53
18:7:114:LYS:HB3	22:7:611:CLA:HMC3	1.90	0.53
18:7:115:ARG:NH1	22:7:612:CLA:O1D	2.37	0.53
17:6:41:PRO:HG2	22:6:609:CLA:OBD	2.08	0.53
1:A:661:TYR:OH	2:B:442:ASP:OD1	2.19	0.53
22:A:1104:CLA:H43	25:A:5002:LHG:H262	1.90	0.53
2:B:176:LEU:HD12	2:B:302:MET:CE	2.39	0.53
22:B:1219:CLA:HBB2	24:B:4004:BCR:H343	1.90	0.53
22:F:1302:CLA:HBC3	22:F:1302:CLA:HHD	1.90	0.53
13:1:71:ARG:HH12	13:1:151:TYR:HE2	1.55	0.53
24:3:503:BCR:C16	39:3:611:CHL:HMB3	2.38	0.53
17:6:82:HIS:HD2	38:6:502:LUT:H15	1.74	0.53
22:7:604:CLA:H102	22:7:605:CLA:HMB3	1.91	0.53
1:A:357:LEU:HD23	22:A:1103:CLA:HED1	1.91	0.53
22:A:1111:CLA:HAA2	22:A:1123:CLA:H52	1.91	0.53
22:B:1239:CLA:H11	23:B:2002:PQN:H302	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:226:SER:OG	4:D:228:LYS:O	2.27	0.53
18:7:91:ARG:HH22	22:7:606:CLA:HED1	1.74	0.53
1:A:421:ASN:ND2	1:A:421:ASN:O	2.42	0.53
13:1:169:LEU:HB3	22:1:601:CLA:CMA	2.38	0.53
16:5:50:GLY:O	16:5:191:ARG:NH1	2.39	0.53
17:6:261:HIS:O	17:6:262:SER:OG	2.22	0.53
22:6:612:CLA:HHD	22:6:612:CLA:HBC3	1.89	0.53
31:7:804:PTY:O10	31:7:804:PTY:HC12	2.09	0.53
22:B:1223:CLA:HBB1	22:B:1231:CLA:HMA2	1.91	0.53
22:B:1232:CLA:HMB1	24:B:4005:BCR:HC32	1.90	0.53
15:4:193:ALA:O	15:4:197:ILE:HG12	2.08	0.53
17:6:233:PRO:HD2	39:6:619:CHL:O1D	2.07	0.53
22:A:1103:CLA:H141	24:A:4002:BCR:H353	1.90	0.53
22:A:1131:CLA:H143	23:B:2002:PQN:H191	1.91	0.53
7:G:1299:VAL:HG21	22:G:1602:CLA:HMA1	1.90	0.53
1:A:485:GLN:NE2	1:A:528:LEU:O	2.41	0.53
22:A:1105:CLA:HMA1	22:A:1106:CLA:HMB3	1.90	0.53
2:B:493:LEU:HD22	22:B:1213:CLA:HED2	1.91	0.53
22:B:1202:CLA:H11	22:B:1203:CLA:CBB	2.39	0.53
22:B:1204:CLA:H2	24:I:4001:BCR:HC31	1.90	0.53
12:L:390:TYR:O	12:L:394:THR:HG22	2.09	0.53
16:5:55:ASP:HB2	22:5:604:CLA:HBA2	1.89	0.53
16:5:133:GLU:HG3	22:5:612:CLA:C4B	2.38	0.53
16:5:165:PRO:HD3	39:5:611:CHL:HMD2	1.90	0.53
16:5:185:LYS:HG3	22:5:607:CLA:HED2	1.90	0.53
17:6:189:ARG:HB2	25:6:801:LHG:H241	1.90	0.53
18:7:161:CYS:SG	22:7:601:CLA:HAA2	2.48	0.53
38:8:501:LUT:H32	39:8:601:CHL:HBB1	1.90	0.53
2:B:30:HIS:HD2	22:B:1202:CLA:HBB2	1.74	0.52
2:B:478:LEU:HD13	22:B:1231:CLA:HMD3	1.91	0.52
12:L:353:VAL:HA	12:L:376:ASN:CG	2.30	0.52
14:3:350:VAL:HG13	14:3:351:ILE:HG13	1.91	0.52
15:4:91:GLU:HG3	15:4:208:PRO:HD2	1.91	0.52
25:7:803:LHG:P	25:7:803:LHG:HC12	2.50	0.52
1:A:45:THR:HB	1:A:716:ARG:HG3	1.91	0.52
2:B:190:ALA:HA	22:B:1212:CLA:HAB	1.91	0.52
2:B:659:ALA:CB	22:B:1023:CLA:HBB2	2.40	0.52
22:B:1022:CLA:H151	22:B:1207:CLA:HBC3	1.90	0.52
39:5:610:CHL:HBB2	22:5:612:CLA:HBC3	1.91	0.52
22:5:612:CLA:H121	22:5:617:CLA:HAB	1.92	0.52
17:6:85:TRP:CE2	39:6:611:CHL:HED3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:549:PRO:HB3	6:F:481:PRO:HG2	1.91	0.52
7:G:1238:CYS:HB3	7:G:1310:ALA:HB2	1.92	0.52
12:L:313:THR:H	12:L:316:THR:HG1	1.58	0.52
15:4:191:MET:HE3	22:4:604:CLA:HMC3	1.92	0.52
22:4:617:CLA:HHC	22:4:617:CLA:HBB1	1.91	0.52
16:5:35:PHE:HB3	16:5:38:VAL:HB	1.90	0.52
45:6:806:SPH:H161	38:6:502:LUT:H361	1.90	0.52
22:B:1224:CLA:CGA	22:B:1224:CLA:H3A	2.35	0.52
17:6:152:PHE:CE1	22:6:617:CLA:HBA2	2.42	0.52
2:B:438:TYR:CD2	22:B:1021:CLA:H203	2.45	0.52
8:J:30:ALA:N	8:J:31:PRO:HD2	2.24	0.52
11:I:14:VAL:HG13	24:I:4001:BCR:H333	1.92	0.52
14:3:258:ALA:HB2	14:3:265:LYS:HD2	1.90	0.52
14:3:382:ARG:NH2	22:3:612:CLA:O1D	2.41	0.52
15:4:82:LEU:HG	22:4:601:CLA:HMC1	1.90	0.52
25:4:802:LHG:H141	25:4:802:LHG:HC92	1.91	0.52
22:5:605:CLA:HMD2	22:5:612:CLA:C1D	2.40	0.52
17:6:133:GLU:OE1	17:6:136:ARG:NH2	2.42	0.52
19:8:138:ARG:NH1	22:8:612:CLA:O1D	2.40	0.52
22:A:1128:CLA:H41	25:A:5002:LHG:H111	1.91	0.52
22:A:1132:CLA:HMA2	12:L:359:LEU:HD22	1.91	0.52
22:A:1138:CLA:CBB	6:F:422:GLY:HA3	2.37	0.52
22:B:1023:CLA:CGA	22:B:1023:CLA:H3A	2.40	0.52
4:D:218:GLU:HG3	4:D:278:PHE:CD1	2.44	0.52
14:3:438:ILE:O	14:3:442:ARG:HG3	2.10	0.52
17:6:254:ILE:HD12	39:6:610:CHL:OBD	2.09	0.52
24:7:503:BCR:C19	39:7:613:CHL:HBA2	2.39	0.52
48:7:504:C7Z:C10	19:8:242:ILE:HD13	2.40	0.52
22:A:1119:CLA:HMB3	22:A:1123:CLA:HED2	1.92	0.52
22:B:1209:CLA:H171	22:B:1217:CLA:H11	1.92	0.52
14:3:257:VAL:O	14:3:260:VAL:HG22	2.09	0.52
16:5:84:VAL:HG11	38:5:501:LUT:H12	1.91	0.52
16:5:97:GLN:NE2	16:5:107:ASN:HB3	2.24	0.52
17:6:104:PHE:HA	17:6:208:ASN:HD21	1.74	0.52
22:6:604:CLA:H3A	22:6:604:CLA:CGA	2.39	0.52
39:6:610:CHL:HBB2	39:6:613:CHL:HBB2	1.90	0.52
1:A:514:VAL:HG13	1:A:524:MET:HB3	1.91	0.52
22:A:1012:CLA:HMA2	2:B:617:LEU:HD13	1.92	0.52
22:A:1125:CLA:HMB3	22:A:1133:CLA:H2	1.91	0.52
22:1:602:CLA:HMD3	22:1:607:CLA:H43	1.91	0.52
22:1:604:CLA:H202	22:8:618:CLA:H91	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:6:501:LUT:H161	38:6:501:LUT:H8	1.91	0.52
19:8:84:VAL:O	19:8:88:VAL:HG22	2.09	0.52
19:8:175:ASN:HB2	39:8:601:CHL:HBD	1.92	0.52
1:A:329:HIS:HB2	1:A:338:HIS:HD2	1.75	0.52
22:A:1114:CLA:H192	25:A:5003:LHG:H271	1.92	0.52
2:B:561:ASP:OD1	3:C:66:ARG:NH1	2.38	0.52
4:D:229:GLU:HA	4:D:242:MET:O	2.09	0.52
13:1:75:VAL:HG22	13:1:174:ILE:HD11	1.90	0.52
16:5:75:GLN:HE22	39:5:611:CHL:CGD	2.16	0.52
17:6:124:PHE:CE2	39:6:613:CHL:HED3	2.44	0.52
25:6:801:LHG:O9	25:6:801:LHG:H261	2.10	0.52
2:B:16:ASP:HB3	2:B:21:ARG:HB2	1.91	0.52
22:B:1225:CLA:H171	24:B:4002:BCR:H352	1.92	0.52
38:5:505:LUT:H173	22:7:608:CLA:CAB	2.37	0.52
22:5:617:CLA:HBC3	22:5:617:CLA:HMC1	1.92	0.52
17:6:135:ARG:HD3	39:6:611:CHL:HBB1	1.91	0.52
1:A:197:MET:HE2	22:A:1111:CLA:HBC2	1.93	0.51
22:B:1209:CLA:HHC	22:B:1209:CLA:HBB1	1.93	0.51
22:B:1230:CLA:H12	31:B:5005:PTY:H111	1.91	0.51
7:G:1228:LEU:HD22	7:G:1318:SER:HA	1.92	0.51
9:K:83:ASN:HB3	22:K:1404:CLA:OBD	2.11	0.51
14:3:306:LEU:HB3	22:3:604:CLA:HMA1	1.92	0.51
14:3:407:SER:OG	14:3:408:GLY:N	2.36	0.51
15:4:39:PRO:O	15:4:41:HIS:ND1	2.43	0.51
2:B:577:PHE:O	2:B:581:VAL:HG23	2.10	0.51
9:K:56:LEU:HB3	22:K:1403:CLA:C1D	2.40	0.51
15:4:216:LEU:HD21	22:4:608:CLA:HMC3	1.92	0.51
16:5:202:ILE:HG22	22:5:603:CLA:HMD3	1.92	0.51
17:6:40:LEU:CG	22:6:609:CLA:HED2	2.40	0.51
17:6:186:LYS:HD2	25:6:801:LHG:O10	2.11	0.51
19:8:92:GLU:HG2	19:8:220:LEU:HD21	1.92	0.51
2:B:705:GLN:HG3	26:B:5003:DGD:HA31	1.93	0.51
9:K:51:ALA:HB2	22:K:1403:CLA:C3C	2.40	0.51
13:1:170:LYS:O	13:1:174:ILE:HG12	2.10	0.51
24:6:503:BCR:H21C	39:6:613:CHL:HBA1	1.92	0.51
22:A:1131:CLA:H18	24:L:4001:BCR:C34	2.41	0.51
9:K:96:LEU:CD2	22:K:1403:CLA:HBB1	2.40	0.51
12:L:297:GLN:O	12:L:297:GLN:HG2	2.11	0.51
18:7:107:MET:CG	22:8:608:CLA:H12	2.41	0.51
1:A:721:THR:HG22	25:A:5002:LHG:HC62	1.93	0.51
22:A:1012:CLA:C4	2:B:439:VAL:HG22	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:3:474:VAL:O	14:3:477:ASN:ND2	2.43	0.51
15:4:81:MET:HE3	22:4:601:CLA:HMC3	1.93	0.51
16:5:144:ASP:HA	16:5:147:ASN:HD21	1.74	0.51
26:8:802:DGD:HAS2	22:8:607:CLA:HBB2	1.92	0.51
1:A:128:ASN:HB3	1:A:136:GLN:HB3	1.93	0.51
1:A:440:HIS:O	1:A:444:VAL:HG23	2.10	0.51
1:A:460:ASP:OD1	1:A:641:THR:HB	2.10	0.51
1:A:481:PRO:HB3	22:A:1136:CLA:O2D	2.11	0.51
21:A:1011:CL0:H13	22:A:1012:CLA:CAD	2.41	0.51
22:A:1012:CLA:HAB	2:B:583:TRP:CH2	2.45	0.51
22:A:1107:CLA:H61	26:A:5005:DGD:HB72	1.93	0.51
22:A:1118:CLA:HMB2	9:K:94:LEU:HD22	1.92	0.51
6:F:346:LEU:O	6:F:348:ASN:N	2.38	0.51
22:1:603:CLA:HBB1	22:1:603:CLA:H111	1.93	0.51
14:3:337:PRO:HG3	22:3:616:CLA:OBD	2.11	0.51
11:I:30:ILE:CD1	24:L:4001:BCR:H332	2.36	0.51
17:6:122:LEU:HD12	39:6:610:CHL:HAC2	1.93	0.51
22:7:601:CLA:H3A	22:7:601:CLA:CGA	2.41	0.51
1:A:136:GLN:HG3	6:F:355:PRO:HB3	1.92	0.51
25:A:5003:LHG:H162	22:3:610:CLA:HAC2	1.92	0.51
22:B:1225:CLA:H8	24:B:4002:BCR:H21C	1.92	0.51
22:3:605:CLA:OBD	22:3:612:CLA:HBA2	2.11	0.51
24:7:503:BCR:H391	22:7:606:CLA:H12	1.93	0.51
21:A:1011:CL0:H13	22:A:1012:CLA:OBD	2.10	0.51
2:B:279:LEU:HG	22:B:1213:CLA:HAB	1.93	0.51
22:F:1301:CLA:HBD	32:F:5003:LAP:H151	1.91	0.51
39:4:609:CHL:H51	17:6:127:PHE:CD1	2.46	0.51
17:6:121:LEU:HD21	39:6:613:CHL:C2D	2.40	0.51
4:D:298:ASN:HB3	4:D:301:ARG:HG3	1.93	0.51
22:3:601:CLA:C2B	22:3:601:CLA:H42	2.41	0.51
16:5:83:GLY:O	16:5:87:ILE:HG12	2.11	0.51
17:6:39:TRP:CD1	17:6:59:GLY:O	2.64	0.51
17:6:54:LEU:HD12	22:6:604:CLA:CED	2.41	0.51
17:6:62:PRO:HB2	45:6:806:SPH:H101	1.93	0.51
17:6:99:VAL:HG23	17:6:100:LYS:HG3	1.93	0.51
46:7:502:XAT:H183	22:7:606:CLA:C3B	2.42	0.51
1:A:16:VAL:HG12	14:3:296:GLY:HA3	1.93	0.50
1:A:533:PHE:HA	22:A:1136:CLA:HED1	1.93	0.50
22:B:1207:CLA:H71	12:L:375:ILE:HD13	1.93	0.50
7:G:1270:THR:OG1	7:G:1273:GLN:HG3	2.12	0.50
16:5:110:ARG:NH2	16:5:116:VAL:HB	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:6:62:PRO:HD2	38:6:502:LUT:H23	1.93	0.50
1:A:153:ILE:HG21	1:A:159:LEU:HD12	1.93	0.50
22:B:1237:CLA:H203	22:L:1502:CLA:CAB	2.42	0.50
16:5:45:ASP:OD1	16:5:46:GLY:N	2.43	0.50
24:5:504:BCR:H362	39:5:610:CHL:C1C	2.42	0.50
38:6:502:LUT:H24	22:6:604:CLA:O2A	2.11	0.50
22:7:604:CLA:H191	25:7:802:LHG:H131	1.93	0.50
1:A:208:LEU:HD22	24:A:4001:BCR:H361	1.94	0.50
1:A:366:ILE:HG21	22:A:1117:CLA:H191	1.93	0.50
1:A:376:PRO:HG3	22:A:1117:CLA:HBA1	1.92	0.50
22:A:1118:CLA:H92	25:3:801:LHG:H291	1.93	0.50
2:B:331:LEU:HD21	22:B:1202:CLA:H192	1.92	0.50
2:B:692:VAL:HG11	22:B:1237:CLA:HAB	1.93	0.50
12:L:382:LEU:O	12:L:385:THR:HG22	2.11	0.50
13:1:130:GLU:OE1	22:1:610:CLA:HMC1	2.11	0.50
15:4:77:GLY:HA3	15:4:187:ALA:HB1	1.92	0.50
15:4:236:ASN:N	25:6:802:LHG:HC2	2.27	0.50
1:A:746:ARG:O	1:A:750:VAL:HG22	2.12	0.50
22:B:1222:CLA:HMB3	24:B:4005:BCR:C17	2.41	0.50
15:4:158:TYR:OH	15:4:161:LEU:HA	2.12	0.50
1:A:190:TRP:CE2	22:A:1108:CLA:HMA1	2.46	0.50
1:A:650:LEU:HD21	22:B:1021:CLA:CBB	2.42	0.50
1:A:736:ILE:HG21	22:A:1126:CLA:HMC2	1.92	0.50
2:B:686:THR:HG23	2:B:689:ALA:HB3	1.93	0.50
17:6:149:ASP:OD1	17:6:151:ILE:N	2.45	0.50
48:7:504:C7Z:C14	22:8:615:CLA:HAC1	2.41	0.50
1:A:375:PRO:HG3	1:A:381:ALA:HB2	1.94	0.50
1:A:666:SER:OG	2:B:446:ALA:O	2.26	0.50
13:1:69:ARG:NH1	22:1:605:CLA:O1A	2.45	0.50
22:4:604:CLA:HED2	22:4:604:CLA:H2A	1.92	0.50
39:4:609:CHL:HAC1	25:4:801:LHG:HC41	1.93	0.50
17:6:105:TRP:O	17:6:108:SER:OG	2.27	0.50
18:7:60:THR:HG22	22:7:606:CLA:HAB	1.93	0.50
22:8:611:CLA:HBB1	22:8:611:CLA:HMB1	1.93	0.50
1:A:351:ALA:HB1	24:A:4003:BCR:H391	1.93	0.50
1:A:392:THR:HG23	1:A:607:ILE:HG21	1.92	0.50
22:A:1110:CLA:H92	14:3:289:LEU:HD11	1.94	0.50
6:F:466:LYS:HB2	44:8:803:DGA:HB32	1.93	0.50
13:1:208:ASN:OD1	13:1:211:ALA:HB3	2.12	0.50
17:6:186:LYS:CB	22:6:607:CLA:CMD	2.90	0.50
18:7:9:LEU:HD22	18:7:17:VAL:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:8:226:HIS:CG	22:8:603:CLA:HAA2	2.47	0.50
1:A:432:ARG:HG3	4:D:238:GLY:HA3	1.93	0.50
1:A:453:PHE:HD2	22:B:1023:CLA:H41	1.76	0.50
22:B:1218:CLA:HED2	7:G:1258:LEU:HD23	1.93	0.50
6:F:457:TRP:CD1	6:F:458:PRO:HD3	2.46	0.50
12:L:445:THR:HG22	12:L:451:TYR:HE1	1.77	0.50
16:5:205:GLN:NE2	16:5:251:CYS:O	2.45	0.50
24:5:503:BCR:H271	22:5:606:CLA:C1B	2.42	0.50
1:A:34:HIS:NE2	22:A:1109:CLA:HBA2	2.26	0.50
22:A:1013:CLA:H3A	22:A:1013:CLA:CGA	2.41	0.50
25:F:5001:LHG:H182	39:8:604:CHL:H102	1.94	0.50
22:1:605:CLA:HBB1	22:1:605:CLA:HMB1	1.94	0.50
22:1:607:CLA:C4C	25:1:801:LHG:HC62	2.42	0.50
15:4:224:PHE:CE1	22:4:608:CLA:HED2	2.47	0.50
17:6:139:ASP:CG	39:6:611:CHL:HBC1	2.32	0.50
18:7:114:LYS:HE3	22:7:611:CLA:HMC3	1.94	0.50
18:7:129:ILE:HG13	18:7:130:LEU:N	2.27	0.50
18:7:133:ASP:HB3	18:7:152:GLY:HA3	1.93	0.50
1:A:172:ALA:HB2	22:3:605:CLA:H203	1.94	0.49
1:A:680:ALA:HB3	22:A:1013:CLA:HBB2	1.93	0.49
22:A:1114:CLA:H203	25:A:5003:LHG:H251	1.93	0.49
2:B:520:VAL:HG11	2:B:594:TYR:CG	2.47	0.49
22:B:1205:CLA:O1A	22:B:1224:CLA:HBD	2.12	0.49
7:G:1245:LEU:HD11	13:1:135:ALA:HB3	1.94	0.49
15:4:130:PHE:CD2	22:4:612:CLA:HMC3	2.47	0.49
17:6:41:PRO:HD2	22:6:609:CLA:O2D	2.12	0.49
18:7:76:ALA:HB2	33:7:805:SQD:H172	1.93	0.49
19:8:132:ASN:O	19:8:136:ILE:HG12	2.12	0.49
15:4:152:PHE:CE2	22:4:617:CLA:HMA3	2.48	0.49
1:A:370:HIS:O	1:A:374:MET:HG2	2.13	0.49
22:B:1021:CLA:HHC	22:B:1021:CLA:HBB1	1.94	0.49
9:K:98:ALA:O	9:K:102:ILE:HG12	2.13	0.49
22:5:616:CLA:HBB2	39:6:619:CHL:H171	1.94	0.49
17:6:132:VAL:HG12	39:6:611:CHL:C2B	2.42	0.49
18:7:96:ASP:OD1	19:8:236:CYS:SG	2.70	0.49
19:8:132:ASN:N	22:8:612:CLA:HAB	2.27	0.49
19:8:176:PRO:HD2	38:8:501:LUT:H23	1.93	0.49
1:A:539:HIS:HB3	22:A:1135:CLA:HAB	1.93	0.49
1:A:578:PRO:HD3	2:B:562:GLY:CA	2.37	0.49
3:C:10:THR:OG1	3:C:64:SER:OG	2.25	0.49
6:F:379:LEU:HD11	6:F:400:HIS:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:3:336:ILE:HG22	22:3:616:CLA:CHD	2.41	0.49
31:8:810:PTY:O4	31:8:810:PTY:H112	2.12	0.49
1:A:105:LEU:HD11	1:A:154:THR:HA	1.93	0.49
22:A:1130:CLA:C10	22:L:1502:CLA:H92	2.37	0.49
18:7:204:LEU:O	18:7:208:VAL:HG23	2.12	0.49
22:8:609:CLA:H51	25:8:801:LHG:H121	1.93	0.49
22:8:605:CLA:HMD2	22:8:612:CLA:C1D	2.41	0.49
22:B:1235:CLA:HMA1	22:B:1236:CLA:HED3	1.95	0.49
22:B:1240:CLA:HBB2	22:1:604:CLA:H52	1.93	0.49
22:B:1240:CLA:HMC2	13:1:66:SER:OG	2.13	0.49
12:L:298:VAL:HB	12:L:314:PRO:HG3	1.94	0.49
17:6:169:PHE:HD1	39:6:611:CHL:C1	2.16	0.49
24:6:504:BCR:H352	25:6:802:LHG:H112	1.95	0.49
1:A:14:LYS:HE2	14:3:295:GLU:OE2	2.13	0.49
2:B:55:LEU:HD21	22:B:1210:CLA:O1A	2.12	0.49
2:B:677:GLU:HG3	3:C:81:TYR:CD2	2.48	0.49
7:G:1316:THR:HG21	34:G:5002:ERG:C18	2.42	0.49
14:3:430:MET:HE1	22:3:601:CLA:HED3	1.94	0.49
22:4:610:CLA:HBB1	22:8:620:CLA:H18	1.95	0.49
16:5:131:PHE:CB	22:6:609:CLA:H42	2.42	0.49
17:6:89:GLY:HA2	38:6:502:LUT:C18	2.42	0.49
17:6:258:CYS:SG	17:6:261:HIS:HB2	2.52	0.49
39:6:611:CHL:HBB1	39:6:611:CHL:HHC	1.94	0.49
19:8:129:PHE:CE1	22:8:618:CLA:HMA1	2.47	0.49
1:A:531:ALA:O	1:A:535:VAL:HG22	2.13	0.49
1:A:577:GLY:HA3	3:C:51:CYS:O	2.12	0.49
22:A:1110:CLA:HED2	22:A:1111:CLA:HAC1	1.93	0.49
22:A:1121:CLA:HED1	9:K:66:GLN:HG2	1.95	0.49
22:B:1216:CLA:HBB1	22:B:1221:CLA:H61	1.93	0.49
22:B:1226:CLA:HMB1	22:B:1226:CLA:HBB1	1.95	0.49
14:3:250:ASP:O	14:3:252:ALA:N	2.43	0.49
15:4:232:PHE:HE2	22:4:615:CLA:HMA3	1.78	0.49
1:A:303:VAL:HG21	22:A:1115:CLA:HBB2	1.95	0.49
1:A:423:TYR:CE2	4:D:241:ILE:HD11	2.48	0.49
22:A:1124:CLA:H3A	22:A:1124:CLA:HBA2	1.50	0.49
2:B:130:LEU:HD23	22:B:1211:CLA:HED3	1.95	0.49
6:F:359:LEU:O	6:F:363:ILE:HG13	2.13	0.49
25:F:5001:LHG:HC91	19:8:56:PRO:HG3	1.95	0.49
17:6:125:GLU:OE2	39:6:613:CHL:C2B	2.61	0.49
17:6:183:LYS:NZ	22:6:602:CLA:OBD	2.46	0.49
18:7:174:ASN:O	18:7:178:ASN:ND2	2.34	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:702:TRP:CD1	6:F:477:ILE:HG21	2.48	0.49
22:A:1112:CLA:HBB1	22:A:1112:CLA:HMB1	1.93	0.49
2:B:668:TRP:HA	23:B:2002:PQN:H8	1.94	0.49
22:B:1201:CLA:HMC3	22:B:1203:CLA:HED2	1.94	0.49
25:4:802:LHG:H102	22:6:618:CLA:CBA	2.42	0.49
19:8:235:PHE:CE1	22:8:608:CLA:O1D	2.66	0.49
1:A:150:ALA:HB2	1:A:378:PRO:HD2	1.94	0.48
22:A:1106:CLA:H62	24:J:4001:BCR:H343	1.95	0.48
22:A:1131:CLA:HMD3	22:A:1136:CLA:H13	1.95	0.48
26:A:5005:DGD:HA21	26:A:5005:DGD:HG11	1.70	0.48
25:A:5003:LHG:C10	14:3:456:VAL:HG23	2.42	0.48
22:B:1218:CLA:HBB2	29:B:5006:LMT:H112	1.95	0.48
35:J:4002:RRX:H17	35:J:4002:RRX:C23	2.43	0.48
38:5:505:LUT:H181	39:5:610:CHL:H43	1.95	0.48
22:A:1013:CLA:H12	2:B:432:PHE:N	2.29	0.48
2:B:561:ASP:OD2	2:B:565:ARG:NH2	2.43	0.48
22:B:1212:CLA:HED2	22:B:1212:CLA:H2A	1.94	0.48
15:4:200:GLN:HB3	15:4:211:GLN:OE1	2.13	0.48
18:7:192:GLN:HE22	38:7:501:LUT:H42	1.76	0.48
22:7:604:CLA:H3A	22:7:604:CLA:CGA	2.42	0.48
1:A:43:PRO:HG3	6:F:440:ILE:HD13	1.95	0.48
22:A:1117:CLA:H203	22:A:1125:CLA:HBA2	1.95	0.48
25:A:5003:LHG:O3	25:A:5003:LHG:O1	2.14	0.48
2:B:83:LEU:HD21	2:B:364:GLN:HB3	1.95	0.48
2:B:429:PHE:CD1	22:B:1235:CLA:HAB	2.47	0.48
4:D:261:LEU:HG	4:D:265:ARG:HH12	1.79	0.48
22:G:1603:CLA:HHC	22:G:1603:CLA:HBB1	1.95	0.48
38:1:503:LUT:H173	22:1:606:CLA:H101	1.95	0.48
16:5:117:ASN:ND2	17:6:227:SER:HB2	2.23	0.48
39:8:604:CHL:HHC	39:8:604:CHL:HBB1	1.95	0.48
17:6:194:ALA:HA	38:6:501:LUT:H181	1.95	0.48
2:B:231:TRP:HH2	24:G:4001:BCR:HC32	1.78	0.48
13:1:72:GLU:OE2	13:1:149:ARG:HB3	2.13	0.48
38:3:501:LUT:C30	22:3:601:CLA:H101	2.44	0.48
18:7:42:GLU:CG	47:7:807:4RF:H41	2.44	0.48
24:8:503:BCR:H271	22:8:606:CLA:C1B	2.44	0.48
1:A:13:VAL:HG13	1:A:193:ASN:ND2	2.27	0.48
1:A:428:ASP:O	1:A:432:ARG:HB2	2.13	0.48
22:A:1120:CLA:O1A	9:K:58:PRO:HG3	2.14	0.48
24:A:4003:BCR:H351	24:A:4003:BCR:H15C	1.58	0.48
2:B:200:ILE:HB	2:B:201:PRO:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:304:GLU:HG3	7:G:1261:ALA:HA	1.93	0.48
6:F:444:VAL:HG22	8:J:33:LEU:CD1	2.43	0.48
6:F:453:GLU:OE2	19:8:58:ASN:ND2	2.46	0.48
13:1:78:GLY:O	13:1:82:MET:HG3	2.13	0.48
39:6:610:CHL:H91	22:6:615:CLA:H202	1.95	0.48
38:8:502:LUT:H32	39:8:604:CHL:HBB1	1.96	0.48
22:8:618:CLA:HBC2	31:8:810:PTY:O10	2.13	0.48
1:A:255:PRO:O	1:A:258:SER:OG	2.23	0.48
2:B:130:LEU:HD22	2:B:135:GLU:HB3	1.96	0.48
2:B:382:PHE:HB3	22:B:1203:CLA:H112	1.95	0.48
2:B:677:GLU:HG3	3:C:81:TYR:HD2	1.79	0.48
22:B:1215:CLA:HHC	22:B:1215:CLA:HBB1	1.95	0.48
32:K:5001:LAP:H62	32:K:5001:LAP:H31	1.74	0.48
17:6:61:ASP:OD1	17:6:64:GLY:N	2.45	0.48
22:6:617:CLA:HHC	22:6:617:CLA:HBB1	1.94	0.48
18:7:161:CYS:HB3	18:7:168:THR:HG23	1.95	0.48
1:A:454:GLY:C	22:A:1132:CLA:HAB	2.34	0.48
1:A:598:TRP:CH2	22:B:1022:CLA:HAB	2.49	0.48
22:A:1103:CLA:HBB1	22:A:1103:CLA:HHC	1.96	0.48
31:B:5005:PTY:H151	6:F:407:PRO:HB3	1.95	0.48
22:F:1301:CLA:HAA1	32:F:5003:LAP:H151	1.96	0.48
12:L:318:SER:HB3	12:L:321:ILE:HD13	1.94	0.48
14:3:315:ARG:HA	14:3:318:MET:HE2	1.94	0.48
14:3:337:PRO:HG2	22:3:616:CLA:O1D	2.13	0.48
39:4:618:CHL:H8	19:8:177:PHE:HE2	1.79	0.48
16:5:32:LYS:HD3	16:5:33:LEU:O	2.13	0.48
38:5:505:LUT:H362	22:5:617:CLA:HBC2	1.96	0.48
17:6:254:ILE:O	17:6:256:ALA:N	2.46	0.48
18:7:102:PHE:CD2	19:8:235:PHE:HZ	2.32	0.48
19:8:127:GLN:OE1	22:8:610:CLA:HMC1	2.13	0.48
22:A:1105:CLA:HBA1	22:A:1107:CLA:H2	1.95	0.48
22:A:1118:CLA:HBA2	22:A:1118:CLA:H3A	1.37	0.48
2:B:722:TYR:HB2	22:B:1021:CLA:HED3	1.96	0.48
22:3:616:CLA:H102	22:3:616:CLA:H62	1.53	0.48
25:4:802:LHG:O9	25:4:802:LHG:HC61	2.12	0.48
39:6:610:CHL:CAB	39:6:613:CHL:HBB2	2.43	0.48
26:8:802:DGD:HG11	26:8:802:DGD:HA91	1.95	0.48
38:8:502:LUT:H34	39:8:604:CHL:HBB2	1.96	0.48
1:A:153:ILE:HG21	1:A:159:LEU:CD1	2.44	0.48
22:A:1127:CLA:HBB1	22:A:1127:CLA:HHC	1.96	0.48
2:B:431:GLY:HA2	2:B:526:LEU:HD22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:1022:CLA:H101	22:B:1023:CLA:H141	1.95	0.48
22:B:1204:CLA:HBB1	22:B:1204:CLA:H111	1.95	0.48
4:D:310:ARG:HB2	4:D:313:GLN:HG3	1.95	0.48
22:F:1302:CLA:H62	47:7:807:4RF:H4	1.95	0.48
22:K:1401:CLA:HBB1	24:K:4002:BCR:C11	2.44	0.48
39:1:609:CHL:HBA2	22:8:618:CLA:O1D	2.14	0.48
15:4:119:LYS:HD2	22:4:610:CLA:HBC3	1.96	0.48
17:6:68:ASN:OD1	17:6:69:GLU:N	2.46	0.48
1:A:720:ILE:HD11	2:B:567:GLY:HA3	1.96	0.47
22:A:1013:CLA:HBB1	22:A:1013:CLA:HMB1	1.95	0.47
22:A:1109:CLA:C10	22:A:1101:CLA:HBB2	2.44	0.47
22:A:1129:CLA:HBB2	22:A:1137:CLA:HMC2	1.96	0.47
2:B:256:LEU:HD21	22:B:1212:CLA:HBC1	1.95	0.47
2:B:662:PHE:HE1	2:B:714:PHE:CE2	2.32	0.47
22:B:1234:CLA:HBA2	22:B:1235:CLA:CAA	2.41	0.47
22:B:1228:CLA:H111	6:F:462:PHE:HD1	1.79	0.47
8:J:24:THR:HB	36:J:5001:LPX:H4	1.95	0.47
16:5:197:PHE:CD2	38:5:502:LUT:H12	2.48	0.47
17:6:183:LYS:HA	22:6:607:CLA:OBD	2.13	0.47
19:8:208:PHE:HE1	38:8:501:LUT:H41	1.78	0.47
1:A:508:PRO:HG2	1:A:523:MET:HB3	1.96	0.47
1:A:677:PHE:HB2	22:A:1012:CLA:O1A	2.14	0.47
22:A:1126:CLA:H3A	22:A:1126:CLA:HBA2	1.45	0.47
2:B:27:ALA:HA	22:B:1226:CLA:H43	1.96	0.47
2:B:435:LEU:O	2:B:439:VAL:HG23	2.13	0.47
2:B:632:LEU:HD22	2:B:725:PHE:HA	1.95	0.47
3:C:8:TYR:HD1	4:D:309:ARG:O	1.97	0.47
22:3:612:CLA:HBB1	22:3:612:CLA:HMB1	1.95	0.47
38:6:501:LUT:H373	39:6:611:CHL:H12	1.95	0.47
18:7:101:LEU:O	18:7:104:THR:HG22	2.14	0.47
1:A:714:GLN:HG3	1:A:716:ARG:CZ	2.43	0.47
22:B:1206:CLA:H41	22:B:1206:CLA:H61	1.58	0.47
22:B:1212:CLA:HBA2	22:B:1212:CLA:H3A	1.54	0.47
13:1:90:GLY:HA2	13:1:93:VAL:HG12	1.96	0.47
14:3:450:GLY:O	14:3:454:GLN:HG3	2.15	0.47
14:3:454:GLN:HB3	14:3:465:ASN:ND2	2.30	0.47
17:6:186:LYS:HE3	25:6:801:LHG:HC62	1.94	0.47
38:6:502:LUT:H193	39:6:610:CHL:CBB	2.44	0.47
18:7:110:PHE:HE2	22:7:611:CLA:CBB	2.27	0.47
1:A:197:MET:HB2	22:A:1111:CLA:CBC	2.44	0.47
22:A:1133:CLA:H41	22:A:1133:CLA:H61	1.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:329:ASN:HD22	2:B:329:ASN:N	2.10	0.47
2:B:479:LEU:HD22	2:B:495:LEU:HD21	1.95	0.47
22:B:1209:CLA:H162	22:B:1209:CLA:H141	1.64	0.47
22:B:1223:CLA:H2	24:B:4005:BCR:H14C	1.96	0.47
6:F:448:TRP:HZ3	22:F:1302:CLA:C4A	2.28	0.47
13:1:205:HIS:CG	22:1:603:CLA:HAA2	2.50	0.47
25:1:802:LHG:H121	25:1:802:LHG:HC92	1.55	0.47
14:3:328:GLU:OE2	14:3:464:ALA:N	2.47	0.47
22:4:610:CLA:H111	22:4:610:CLA:H142	1.74	0.47
16:5:188:LYS:NZ	25:5:801:LHG:HC41	2.28	0.47
17:6:104:PHE:HB3	17:6:107:THR:OG1	2.14	0.47
38:6:501:LUT:H30	22:6:601:CLA:H72	1.97	0.47
22:7:603:CLA:H143	22:7:603:CLA:H161	1.74	0.47
22:7:605:CLA:H3A	22:7:605:CLA:HBA1	1.61	0.47
1:A:115:ALA:HB3	1:A:140:ILE:HG21	1.96	0.47
1:A:413:MET:SD	1:A:431:LEU:HD11	2.55	0.47
1:A:457:ILE:HD12	22:B:1023:CLA:C9	2.45	0.47
22:B:1222:CLA:H41	22:B:1234:CLA:H92	1.96	0.47
30:B:5004:PCW:H322	24:F:4001:BCR:C35	2.28	0.47
7:G:1272:LEU:HD22	7:G:1280:GLU:HA	1.96	0.47
7:G:1316:THR:CG2	34:G:5002:ERG:H181	2.43	0.47
22:4:610:CLA:CBB	22:8:620:CLA:H18	2.44	0.47
17:6:61:ASP:OD2	22:6:604:CLA:HBA2	2.15	0.47
1:A:197:MET:HB2	22:A:1111:CLA:HBC3	1.95	0.47
1:A:718:LEU:HD11	22:A:1139:CLA:HMD3	1.96	0.47
23:A:2001:PQN:H261	23:A:2001:PQN:H222	1.74	0.47
2:B:530:THR:O	2:B:534:ILE:HG13	2.14	0.47
22:B:1021:CLA:H8	22:B:1021:CLA:H51	1.60	0.47
24:B:4004:BCR:HC22	22:1:612:CLA:H41	1.95	0.47
8:J:32:VAL:HA	35:J:4002:RRX:H49	1.97	0.47
22:4:605:CLA:HMD2	22:4:612:CLA:C1D	2.45	0.47
30:6:803:PCW:H141	30:6:803:PCW:H321	1.95	0.47
18:7:21:TYR:CZ	18:7:39:SER:HA	2.50	0.47
19:8:161:PHE:CG	22:8:611:CLA:HMC2	2.49	0.47
22:A:1132:CLA:HBC3	22:B:1023:CLA:H143	1.96	0.47
2:B:662:PHE:HE1	2:B:714:PHE:HE2	1.63	0.47
2:B:676:ILE:HG23	22:B:1238:CLA:CMC	2.44	0.47
22:B:1208:CLA:H91	22:B:1208:CLA:H112	1.69	0.47
22:B:1212:CLA:H8	24:B:4001:BCR:H24C	1.97	0.47
4:D:254:LYS:HG2	4:D:258:LEU:HD13	1.95	0.47
22:1:605:CLA:H62	22:1:605:CLA:H41	1.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:3:282:GLY:HA3	14:3:438:ILE:HD13	1.97	0.47
38:6:501:LUT:H35	38:6:501:LUT:H401	1.75	0.47
22:6:603:CLA:H62	22:6:603:CLA:CHC	2.44	0.47
22:6:609:CLA:H3A	22:6:609:CLA:HBA2	1.46	0.47
22:7:603:CLA:H121	25:7:801:LHG:H341	1.96	0.47
25:7:803:LHG:HC12	25:7:803:LHG:O6	2.14	0.47
22:8:618:CLA:H52	22:8:618:CLA:H11	1.57	0.47
22:B:1203:CLA:H43	26:B:5003:DGD:HB51	1.96	0.47
14:3:421:LEU:HD13	16:5:35:PHE:CZ	2.50	0.47
22:4:608:CLA:O1A	17:6:124:PHE:HA	2.15	0.47
18:7:71:LEU:HB2	18:7:78:VAL:HG21	1.97	0.47
18:7:181:LEU:HD21	22:7:602:CLA:HBC3	1.97	0.47
19:8:144:LYS:HE3	19:8:147:SER:HA	1.97	0.47
1:A:356:ASN:O	1:A:360:PHE:HB2	2.15	0.47
32:B:5007:LAP:H162	32:B:5007:LAP:H193	1.68	0.47
4:D:231:ILE:HG12	4:D:241:ILE:HG12	1.97	0.47
32:F:5003:LAP:H62	32:F:5003:LAP:H31	1.63	0.47
22:1:611:CLA:HBA1	40:1:803:OLA:H162	1.97	0.47
14:3:307:SER:O	14:3:311:VAL:HG23	2.15	0.47
1:A:219:HIS:CE1	22:A:1113:CLA:HED2	2.49	0.47
1:A:658:ILE:HD12	2:B:622:ARG:HG3	1.96	0.47
2:B:231:TRP:CH2	24:G:4001:BCR:HC32	2.50	0.47
2:B:536:VAL:HG13	24:B:4004:BCR:H282	1.97	0.47
22:B:1211:CLA:HMB1	22:B:1211:CLA:HBB1	1.97	0.47
22:B:1220:CLA:H143	22:B:1220:CLA:H111	1.71	0.47
4:D:309:ARG:HB2	4:D:313:GLN:HB2	1.96	0.47
38:1:503:LUT:H15	38:1:503:LUT:H201	1.77	0.47
14:3:279:THR:O	14:3:280:LEU:HB2	2.14	0.47
15:4:143:LYS:HD3	15:4:146:SER:HB3	1.97	0.47
17:6:199:THR:O	17:6:203:GLN:HG2	2.14	0.47
38:8:501:LUT:H24	39:8:601:CHL:HBA1	1.97	0.47
1:A:678:VAL:HG11	1:A:733:LEU:HD23	1.97	0.46
22:A:1105:CLA:H8	26:A:5005:DGD:HB52	1.98	0.46
22:A:1136:CLA:H41	22:A:1136:CLA:H61	1.54	0.46
2:B:386:GLY:HA3	22:B:1226:CLA:C2C	2.45	0.46
2:B:388:PHE:HZ	22:B:1222:CLA:HAB	1.81	0.46
2:B:412:ILE:HA	2:B:415:HIS:CE1	2.50	0.46
2:B:688:LEU:CB	24:L:4002:BCR:HC31	2.44	0.46
24:B:4001:BCR:H321	7:G:1301:ALA:HB1	1.97	0.46
22:F:1302:CLA:C3D	47:7:807:4RF:H35	2.45	0.46
14:3:326:ALA:HB2	24:3:504:BCR:H383	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:3:362:MET:SD	22:7:608:CLA:HMA2	2.55	0.46
22:5:601:CLA:HMB2	22:5:602:CLA:HBA2	1.97	0.46
17:6:106:TYR:CE1	17:6:243:ILE:HD13	2.50	0.46
17:6:150:PRO:HD3	22:6:617:CLA:CMC	2.45	0.46
22:7:611:CLA:H61	22:7:611:CLA:H41	1.44	0.46
1:A:365:ILE:O	1:A:369:HIS:HD2	1.98	0.46
1:A:688:SER:HB3	1:A:693:TRP:HE1	1.81	0.46
22:A:1102:CLA:HBA1	22:A:1102:CLA:H3A	1.46	0.46
22:A:1105:CLA:H11	22:A:1105:CLA:H51	1.65	0.46
22:A:1120:CLA:HMB2	22:A:1121:CLA:H2	1.97	0.46
2:B:298:ILE:CD1	7:G:1297:VAL:HG12	2.42	0.46
2:B:358:PRO:HG3	22:B:1215:CLA:HBA1	1.97	0.46
9:K:56:LEU:O	22:K:1403:CLA:C4D	2.63	0.46
22:4:601:CLA:H92	22:4:602:CLA:HMA1	1.95	0.46
38:5:505:LUT:H381	38:5:505:LUT:H27	1.58	0.46
17:6:75:PHE:CB	22:6:604:CLA:CMA	2.89	0.46
17:6:184:GLU:CB	22:6:601:CLA:HMB3	2.43	0.46
22:6:604:CLA:H192	22:6:604:CLA:H161	1.74	0.46
22:8:606:CLA:H52	22:8:606:CLA:H11	1.73	0.46
1:A:365:ILE:O	1:A:369:HIS:CD2	2.67	0.46
22:A:1133:CLA:H121	22:A:1133:CLA:H161	1.40	0.46
2:B:312:PRO:C	2:B:314:GLY:H	2.18	0.46
22:B:1223:CLA:HMA3	24:B:4005:BCR:HC21	1.96	0.46
22:B:1226:CLA:H193	22:B:1226:CLA:H161	1.73	0.46
3:C:80:ALA:HB2	4:D:253:ARG:HD3	1.97	0.46
22:1:604:CLA:HBA2	22:1:604:CLA:H3A	1.50	0.46
39:6:619:CHL:H121	39:6:619:CHL:H161	1.72	0.46
18:7:113:PHE:CE1	22:7:612:CLA:CMB	2.99	0.46
1:A:198:LEU:HD12	1:A:322:LEU:HD11	1.96	0.46
1:A:740:TRP:CG	24:A:4005:BCR:HC42	2.51	0.46
22:B:1201:CLA:H72	11:I:29:TYR:CZ	2.42	0.46
22:B:1209:CLA:O1D	22:B:1210:CLA:HMC1	2.15	0.46
9:K:64:THR:HG22	22:K:1403:CLA:HMA2	1.95	0.46
13:1:55:PHE:HB3	22:1:604:CLA:CAD	2.46	0.46
13:1:193:ALA:HB2	22:1:615:CLA:HED3	1.98	0.46
14:3:306:LEU:HB3	22:3:604:CLA:CMA	2.45	0.46
14:3:315:ARG:NE	14:3:437:GLU:OE2	2.45	0.46
22:5:603:CLA:H62	22:5:603:CLA:H41	1.69	0.46
17:6:54:LEU:HD12	22:6:604:CLA:HED2	1.98	0.46
17:6:198:PHE:HE1	38:6:501:LUT:C6	2.29	0.46
26:8:802:DGD:HBH2	26:8:802:DGD:HB92	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:8:802:DGD:HE1	26:8:802:DGD:HD5	1.52	0.46
2:B:341:SER:HB3	22:B:1221:CLA:H2	1.98	0.46
14:3:275:TYR:CE2	14:3:292:CYS:HB3	2.48	0.46
22:4:601:CLA:O1A	22:4:601:CLA:H3A	2.15	0.46
22:6:603:CLA:H72	25:6:801:LHG:H172	1.97	0.46
30:6:803:PCW:H321	30:6:803:PCW:H122	1.97	0.46
18:7:131:PRO:HB3	22:7:617:CLA:HMB3	1.97	0.46
46:7:502:XAT:C34	22:7:605:CLA:HAB	2.45	0.46
44:8:803:DGA:HB91	22:8:605:CLA:HED3	1.96	0.46
39:8:604:CHL:H3A	39:8:604:CHL:HBA2	1.45	0.46
1:A:323:LYS:O	1:A:327:GLU:HG2	2.15	0.46
1:A:328:ALA:CB	22:A:1121:CLA:HED1	2.46	0.46
2:B:60:LEU:HD12	37:M:4001:ECH:H37A	1.96	0.46
2:B:374:THR:HG23	2:B:592:THR:HG21	1.97	0.46
2:B:464:ILE:HD11	22:B:1234:CLA:H43	1.98	0.46
22:B:1021:CLA:HBA2	22:B:1021:CLA:H3A	1.50	0.46
4:D:251:LEU:HD12	4:D:257:CYS:SG	2.55	0.46
5:E:54:TRP:HD1	5:E:79:LYS:NZ	2.12	0.46
12:L:351:LEU:HD11	22:L:1503:CLA:HBC3	1.97	0.46
15:4:56:PRO:O	22:7:617:CLA:H11	2.16	0.46
16:5:35:PHE:HE1	22:5:609:CLA:CBB	2.29	0.46
22:A:1103:CLA:H51	22:A:1111:CLA:H12	1.98	0.46
22:A:1135:CLA:H102	22:A:1135:CLA:H62	1.56	0.46
2:B:649:TRP:CE3	24:B:4007:BCR:HC31	2.50	0.46
3:C:15:THR:O	3:C:19:ARG:HG3	2.15	0.46
14:3:264:TYR:C	14:3:266:ASN:H	2.18	0.46
22:3:601:CLA:H192	22:3:601:CLA:H162	1.75	0.46
22:3:616:CLA:H2	22:5:616:CLA:O2D	2.16	0.46
38:4:502:LUT:H32	22:4:604:CLA:CAB	2.46	0.46
22:4:607:CLA:H3A	22:4:607:CLA:H43	1.98	0.46
22:5:605:CLA:OBD	22:5:612:CLA:HBA2	2.15	0.46
17:6:105:TRP:HZ2	17:6:199:THR:HA	1.81	0.46
18:7:113:PHE:CD2	22:8:609:CLA:HAA2	2.32	0.46
2:B:168:TRP:CE2	22:B:1208:CLA:HMA1	2.51	0.46
2:B:280:ALA:HA	22:B:1213:CLA:HMC3	1.96	0.46
4:D:218:GLU:OE2	4:D:277:VAL:N	2.49	0.46
39:4:609:CHL:HBA2	25:4:801:LHG:H161	1.97	0.46
19:8:98:VAL:HG12	19:8:99:LEU:HG	1.98	0.46
1:A:116:GLN:NE2	22:A:1107:CLA:OBD	2.45	0.46
29:A:5008:LMT:H12	18:7:225:PHE:HB3	1.97	0.46
2:B:273:ASP:HB3	22:B:1214:CLA:HMA1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:311:PRO:HB2	25:B:5001:LHG:O4	2.16	0.46
2:B:685:ARG:HD3	2:B:685:ARG:HA	1.60	0.46
7:G:1234:VAL:HG21	7:G:1314:LEU:CD2	2.46	0.46
14:3:454:GLN:HB3	14:3:465:ASN:HD22	1.81	0.46
22:3:607:CLA:C1B	25:3:801:LHG:HC2	2.46	0.46
15:4:230:SER:HB3	15:4:231:PRO:HD2	1.97	0.46
22:6:604:CLA:H2	22:6:604:CLA:H61	1.63	0.46
18:7:110:PHE:O	18:7:114:LYS:HG2	2.15	0.46
18:7:111:VAL:HG13	24:7:503:BCR:H16C	1.98	0.46
22:8:610:CLA:H93	22:8:610:CLA:H61	1.66	0.46
1:A:205:LEU:HD11	22:A:1111:CLA:H42	1.97	0.46
1:A:334:THR:HG1	25:A:5001:LHG:H02	1.62	0.46
1:A:374:MET:O	1:A:374:MET:HG3	2.16	0.46
1:A:698:GLU:OE2	5:E:82:TYR:OH	2.29	0.46
22:A:1109:CLA:H61	22:A:1109:CLA:H92	1.75	0.46
22:A:1119:CLA:HMB2	22:A:1123:CLA:HMA3	1.98	0.46
22:A:1134:CLA:H62	22:A:1134:CLA:H92	1.71	0.46
22:A:1140:CLA:HMD1	6:F:426:LEU:HD11	1.98	0.46
2:B:55:LEU:HD22	2:B:150:PHE:HE2	1.81	0.46
2:B:159:GLN:O	2:B:163:GLN:N	2.49	0.46
2:B:404:ASN:O	2:B:410:ALA:HB2	2.16	0.46
22:B:1224:CLA:O1D	22:B:1225:CLA:HMA1	2.15	0.46
3:C:17:CYS:HB3	28:C:3003:SF4:S4	2.55	0.46
7:G:1260:LYS:O	7:G:1260:LYS:HD3	2.15	0.46
38:1:502:LUT:H24	22:1:604:CLA:O1A	2.17	0.46
22:1:611:CLA:HBB1	40:1:803:OLA:H111	1.98	0.46
14:3:481:ASN:ND2	22:3:603:CLA:HED2	2.28	0.46
14:3:486:LEU:HD23	14:3:486:LEU:HA	1.77	0.46
18:7:9:LEU:C	18:7:11:PHE:H	2.19	0.46
26:8:802:DGD:HA62	26:8:802:DGD:HA32	1.58	0.46
26:8:802:DGD:O1A	25:8:801:LHG:O1	2.31	0.46
1:A:154:THR:CG2	1:A:228:LEU:HD11	2.46	0.45
1:A:222:LEU:HG	1:A:254:TYR:CE2	2.50	0.45
1:A:363:LEU:HD22	22:A:1127:CLA:H193	1.97	0.45
1:A:657:VAL:HG21	1:A:742:PHE:HA	1.97	0.45
22:A:1126:CLA:H102	22:A:1126:CLA:H62	1.31	0.45
2:B:669:ARG:HB2	23:B:2002:PQN:H7	1.97	0.45
22:B:1228:CLA:H141	22:B:1228:CLA:H162	1.78	0.45
22:K:1402:CLA:H51	22:K:1402:CLA:H11	1.71	0.45
38:3:502:LUT:H161	22:3:613:CLA:HAB	1.99	0.45
22:3:606:CLA:H11	22:3:616:CLA:HMB2	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:4:127:PHE:CD1	22:4:610:CLA:HED3	2.51	0.45
17:6:145:SER:OG	17:6:146:MET:N	2.46	0.45
31:8:810:PTY:H172	31:8:810:PTY:H142	1.63	0.45
22:A:1103:CLA:H3A	22:A:1103:CLA:HBA1	1.57	0.45
22:A:1125:CLA:H2	22:A:1125:CLA:H61	1.84	0.45
22:A:1101:CLA:HHC	22:A:1101:CLA:CBB	2.44	0.45
2:B:468:HIS:HA	2:B:479:LEU:HD12	1.98	0.45
2:B:516:GLY:O	2:B:520:VAL:HG23	2.16	0.45
22:B:1205:CLA:H143	22:B:1205:CLA:H161	1.73	0.45
13:1:161:MET:HG3	13:1:169:LEU:HD11	1.98	0.45
14:3:329:ILE:HD13	24:3:504:BCR:H282	1.98	0.45
16:5:41:PRO:HD2	16:5:44:LEU:HB2	1.97	0.45
16:5:79:TRP:HD1	22:5:612:CLA:HMD3	1.82	0.45
22:5:603:CLA:H2	22:5:608:CLA:CMD	2.47	0.45
17:6:186:LYS:HB3	22:6:607:CLA:HMD3	1.98	0.45
17:6:193:LEU:CD1	25:6:801:LHG:H302	2.45	0.45
38:6:502:LUT:C35	22:6:605:CLA:HAB	2.45	0.45
22:6:602:CLA:H11	22:6:602:CLA:H51	1.61	0.45
47:8:808:4RF:H46	40:8:809:OLA:H132	1.99	0.45
1:A:21:PRO:HG2	1:A:185:ALA:HB3	1.99	0.45
1:A:377:TYR:HB2	1:A:380:LEU:HD13	1.99	0.45
1:A:709:VAL:HG13	6:F:426:LEU:HD12	1.98	0.45
1:A:715:PRO:HB3	22:A:1140:CLA:C1C	2.46	0.45
22:A:1103:CLA:H121	24:A:4002:BCR:H343	1.97	0.45
2:B:649:TRP:CZ3	24:B:4007:BCR:HC31	2.51	0.45
22:B:1229:CLA:H152	22:B:1229:CLA:H112	1.71	0.45
7:G:1288:THR:OG1	22:G:1602:CLA:O1A	2.28	0.45
9:K:55:GLY:O	22:K:1403:CLA:HED2	2.16	0.45
38:1:501:LUT:H15	38:1:501:LUT:H201	1.86	0.45
22:1:601:CLA:H92	22:1:601:CLA:H61	1.78	0.45
22:1:604:CLA:H121	22:1:604:CLA:H162	1.74	0.45
14:3:442:ARG:HA	14:3:445:MET:HG3	1.97	0.45
25:4:801:LHG:C8	24:6:503:BCR:HC22	2.46	0.45
18:7:35:LEU:HD12	46:7:502:XAT:H221	1.98	0.45
18:7:107:MET:HG2	22:8:608:CLA:H12	1.99	0.45
18:7:137:VAL:HG13	18:7:151:GLY:H	1.81	0.45
19:8:205:PHE:CE1	38:8:502:LUT:H10	2.52	0.45
1:A:157:LEU:HD11	29:A:5008:LMT:H11	1.97	0.45
1:A:299:LEU:HD22	22:A:1113:CLA:HAC1	1.97	0.45
22:A:1121:CLA:H111	24:K:4001:BCR:H381	1.99	0.45
22:A:1122:CLA:HBB1	22:A:1129:CLA:HBC2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:231:TRP:CZ2	7:G:1311:PHE:HD2	2.34	0.45
2:B:308:ALA:HB3	22:B:1219:CLA:O1D	2.16	0.45
2:B:679:LEU:HD13	22:B:1237:CLA:HMD3	1.99	0.45
22:B:1201:CLA:H203	22:B:1201:CLA:H162	1.67	0.45
22:B:1226:CLA:H41	22:B:1226:CLA:H62	1.50	0.45
3:C:23:THR:HG22	3:C:23:THR:O	2.16	0.45
33:G:5001:SQD:H171	33:G:5001:SQD:H321	1.98	0.45
38:4:501:LUT:H35	38:4:501:LUT:H401	1.83	0.45
17:6:125:GLU:OE1	39:6:613:CHL:C1B	2.64	0.45
22:7:601:CLA:H3A	22:7:601:CLA:O1A	2.17	0.45
19:8:203:VAL:HG21	25:8:801:LHG:H261	1.98	0.45
22:A:1103:CLA:H151	24:A:4001:BCR:H323	1.98	0.45
22:A:1116:CLA:H61	22:A:1134:CLA:HMA2	1.99	0.45
22:A:1121:CLA:CED	9:K:66:GLN:HG2	2.47	0.45
2:B:422:HIS:CD2	22:B:1227:CLA:HMB1	2.51	0.45
25:B:5001:LHG:H131	25:B:5001:LHG:H161	1.81	0.45
22:1:602:CLA:HMD2	22:1:607:CLA:C1D	2.47	0.45
25:5:801:LHG:H311	25:5:801:LHG:H281	1.42	0.45
17:6:265:PRO:HB2	39:6:619:CHL:HAB	1.98	0.45
1:A:120:PRO:HA	1:A:125:GLU:HG3	1.98	0.45
22:A:1104:CLA:H2	22:A:1104:CLA:HED2	1.99	0.45
22:A:1106:CLA:HBA2	22:A:1106:CLA:H3A	1.35	0.45
30:B:5004:PCW:H62	30:B:5004:PCW:H42	1.68	0.45
22:B:1204:CLA:HMB2	24:I:4001:BCR:H322	1.99	0.45
9:K:113:SER:O	9:K:113:SER:OG	2.31	0.45
12:L:448:LEU:HD22	12:L:450:TYR:CE1	2.51	0.45
13:1:56:ASP:OD2	13:1:59:GLY:HA2	2.16	0.45
14:3:344:VAL:HG21	14:3:347:ARG:HH21	1.81	0.45
16:5:155:LEU:HD13	22:5:618:CLA:CBD	2.47	0.45
38:6:501:LUT:H362	22:6:601:CLA:H42	1.98	0.45
31:7:804:PTY:H142	31:7:804:PTY:H112	1.64	0.45
22:7:617:CLA:HHC	22:7:617:CLA:CBB	2.46	0.45
1:A:69:ILE:O	1:A:73:VAL:HG23	2.16	0.45
2:B:577:PHE:CE2	26:B:5003:DGD:HB81	2.52	0.45
22:B:1208:CLA:C2	22:B:1209:CLA:HMD2	2.43	0.45
3:C:47:ASP:OD2	4:D:254:LYS:NZ	2.37	0.45
6:F:319:VAL:HG22	6:F:379:LEU:HD22	1.99	0.45
7:G:1313:ILE:CD1	34:G:5002:ERG:H213	2.46	0.45
12:L:350:TYR:OH	22:L:1503:CLA:OBD	2.34	0.45
24:L:4001:BCR:H281	22:L:1502:CLA:CHD	2.47	0.45
14:3:308:TYR:O	14:3:312:ILE:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:3:606:CLA:H2	22:3:613:CLA:CAD	2.46	0.45
22:4:603:CLA:H2	22:4:608:CLA:HMD1	1.98	0.45
16:5:131:PHE:HB2	22:6:609:CLA:H11	1.98	0.45
16:5:218:HIS:CG	22:5:603:CLA:HAA2	2.52	0.45
18:7:50:ALA:CA	22:7:612:CLA:HED2	2.46	0.45
18:7:109:GLY:HA2	22:7:612:CLA:CAB	2.47	0.45
1:A:85:PHE:CZ	1:A:169:MET:HG2	2.52	0.45
1:A:377:TYR:CE2	22:A:1127:CLA:HED2	2.52	0.45
2:B:210:TRP:HA	2:B:213:PHE:CD1	2.52	0.45
33:G:5001:SQD:O49	33:G:5001:SQD:H441	2.11	0.45
9:K:89:ASN:N	9:K:92:ASP:OD2	2.41	0.45
22:3:603:CLA:H41	22:3:603:CLA:H62	1.57	0.45
1:A:303:VAL:HG21	22:A:1115:CLA:CBB	2.47	0.45
1:A:448:LEU:HD11	22:A:1136:CLA:HMB1	1.99	0.45
1:A:709:VAL:HG11	22:A:1138:CLA:HMB3	1.99	0.45
9:K:52:GLY:HA3	9:K:96:LEU:CD1	2.47	0.45
10:M:30:TYR:CE2	11:I:29:TYR:OH	2.65	0.45
15:4:184:ILE:HD12	15:4:184:ILE:HA	1.88	0.45
24:5:504:BCR:H21C	39:5:610:CHL:CGA	2.47	0.45
22:5:612:CLA:H62	22:5:612:CLA:H2	1.64	0.45
17:6:46:PRO:HB2	17:6:47:ALA:H	1.64	0.45
17:6:128:VAL:HG11	24:6:503:BCR:C17	2.39	0.45
22:6:604:CLA:H102	22:6:605:CLA:HMB3	1.99	0.45
22:8:609:CLA:H3A	22:8:609:CLA:HBA1	1.63	0.45
22:8:602:CLA:HHC	22:8:602:CLA:HBB1	1.99	0.45
1:A:316:TRP:HH2	14:3:289:LEU:HD23	1.81	0.45
1:A:396:TRP:HE1	1:A:607:ILE:HD13	1.82	0.45
22:A:1109:CLA:H18	22:A:1109:CLA:H152	1.49	0.45
22:A:1131:CLA:HBB2	12:L:359:LEU:HD13	1.99	0.45
2:B:665:LEU:HD23	2:B:665:LEU:HA	1.81	0.45
22:B:1228:CLA:CGA	6:F:471:MET:HE2	2.47	0.45
25:F:5002:LHG:H271	25:F:5002:LHG:H242	1.51	0.45
12:L:356:PHE:HD2	12:L:376:ASN:HD21	1.65	0.45
24:L:4002:BCR:H333	22:L:1502:CLA:NB	2.32	0.45
14:3:306:LEU:HD12	22:3:604:CLA:H12	1.99	0.45
14:3:384:GLN:HG2	18:7:11:PHE:CE2	2.52	0.45
22:5:609:CLA:HBD	25:5:801:LHG:HC62	1.98	0.45
17:6:135:ARG:NE	22:6:617:CLA:HMC1	2.31	0.45
22:6:603:CLA:H152	22:6:603:CLA:H111	1.67	0.45
18:7:23:ASP:OD1	18:7:23:ASP:N	2.50	0.45
18:7:102:PHE:CG	19:8:235:PHE:HZ	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ILE:HD13	22:A:1108:CLA:HAA2	1.99	0.44
1:A:45:THR:HG22	1:A:714:GLN:HB2	1.99	0.44
1:A:105:LEU:CD1	1:A:154:THR:HA	2.47	0.44
6:F:397:ARG:NH2	32:F:5003:LAP:H182	2.31	0.44
15:4:171:PHE:HB2	22:4:601:CLA:CGA	2.47	0.44
16:5:132:VAL:HG11	24:5:503:BCR:H16C	1.98	0.44
17:6:41:PRO:HD3	22:6:609:CLA:C3D	2.47	0.44
17:6:62:PRO:CB	45:6:806:SPH:H101	2.48	0.44
17:6:125:GLU:OE1	39:6:613:CHL:C4A	2.66	0.44
17:6:136:ARG:CG	39:6:611:CHL:HMD3	2.47	0.44
22:6:602:CLA:OBD	22:6:607:CLA:H2	2.17	0.44
18:7:102:PHE:O	18:7:106:VAL:HG23	2.18	0.44
18:7:177:ARG:NE	25:7:801:LHG:O5	2.50	0.44
1:A:453:PHE:CE1	22:B:1022:CLA:HMA1	2.52	0.44
22:A:1114:CLA:H121	22:A:1114:CLA:CBB	2.47	0.44
22:B:1023:CLA:H41	22:B:1023:CLA:H62	1.67	0.44
3:C:55:GLU:HG2	3:C:63:LEU:HD13	1.98	0.44
4:D:253:ARG:HB2	4:D:256:GLN:HG3	1.99	0.44
4:D:309:ARG:NH1	4:D:314:ASN:OD1	2.50	0.44
11:I:30:ILE:HG21	24:L:4001:BCR:C33	2.47	0.44
22:3:603:CLA:H112	22:3:603:CLA:H72	1.67	0.44
15:4:200:GLN:NE2	15:4:211:GLN:OE1	2.47	0.44
25:4:801:LHG:H321	25:4:801:LHG:H142	1.99	0.44
16:5:195:VAL:HG21	25:5:801:LHG:H131	1.98	0.44
17:6:207:LYS:HE3	17:6:207:LYS:HB3	1.73	0.44
24:6:504:BCR:H351	24:6:504:BCR:H15C	1.53	0.44
1:A:400:PHE:CZ	1:A:732:LEU:HD23	2.53	0.44
1:A:457:ILE:HD12	22:B:1023:CLA:H92	2.00	0.44
1:A:736:ILE:HD13	22:A:1126:CLA:HMC2	1.99	0.44
22:A:1108:CLA:H13	24:A:4002:BCR:H372	1.99	0.44
22:A:1134:CLA:H111	22:A:1134:CLA:H91	1.65	0.44
22:A:1135:CLA:HBA2	22:A:1136:CLA:HAA1	1.99	0.44
2:B:195:LEU:O	2:B:200:ILE:HG12	2.18	0.44
2:B:303:ARG:O	2:B:307:GLU:HG2	2.17	0.44
22:B:1213:CLA:HMD3	22:B:1214:CLA:H142	2.00	0.44
22:B:1239:CLA:H141	22:B:1239:CLA:H162	1.78	0.44
3:C:27:GLU:OE2	4:D:294:PRO:O	2.35	0.44
9:K:96:LEU:HD22	22:K:1403:CLA:HBB1	1.99	0.44
39:1:609:CHL:H92	39:1:609:CHL:H62	1.73	0.44
15:4:118:PRO:HG2	15:4:121:THR:HG22	1.99	0.44
15:4:218:ASN:HD22	15:4:221:LYS:HB3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:5:127:ILE:HG23	16:5:127:ILE:HD12	1.72	0.44
39:6:610:CHL:HAB	39:6:613:CHL:HBB2	1.98	0.44
1:A:552:LYS:NZ	2:B:674:GLU:OE1	2.51	0.44
22:A:1125:CLA:HAC2	22:A:1125:CLA:HMC1	1.82	0.44
2:B:224:THR:OG1	2:B:225:PRO:HD3	2.17	0.44
2:B:637:ASN:HB2	2:B:638:PRO:HD2	2.00	0.44
22:B:1218:CLA:CMD	24:B:4001:BCR:HC7	2.36	0.44
4:D:287:HIS:O	4:D:289:LYS:N	2.50	0.44
14:3:312:ILE:HG21	14:3:382:ARG:HH12	1.82	0.44
24:4:503:BCR:H271	22:4:606:CLA:NB	2.33	0.44
24:5:503:BCR:H343	22:5:618:CLA:HAB	1.98	0.44
17:6:247:ILE:HD11	17:6:254:ILE:HB	1.98	0.44
38:6:502:LUT:H35	38:6:502:LUT:H401	1.79	0.44
39:6:613:CHL:HMB1	39:6:613:CHL:CBB	2.46	0.44
18:7:131:PRO:HB2	18:7:132:GLU:H	1.61	0.44
19:8:137:LYS:HD2	19:8:148:GLN:HE21	1.81	0.44
1:A:286:THR:HG22	1:A:379:TYR:CE2	2.52	0.44
1:A:297:HIS:HB2	22:A:1116:CLA:C1B	2.48	0.44
22:A:1128:CLA:H41	22:A:1128:CLA:H61	1.56	0.44
22:A:1131:CLA:H71	22:B:1238:CLA:H71	1.98	0.44
29:A:5008:LMT:H5'	29:A:5008:LMT:H1B	1.64	0.44
22:B:1221:CLA:HMA2	22:B:1221:CLA:C2	2.45	0.44
24:B:4007:BCR:H351	24:B:4007:BCR:H15C	1.76	0.44
5:E:69:ILE:HG22	5:E:71:TYR:H	1.82	0.44
22:1:605:CLA:H51	22:1:605:CLA:H11	1.86	0.44
22:1:605:CLA:H61	22:1:605:CLA:H92	1.79	0.44
39:4:609:CHL:HHD	39:4:609:CHL:CBC	2.44	0.44
39:5:613:CHL:H62	39:5:613:CHL:H41	1.60	0.44
22:5:617:CLA:HED1	25:6:801:LHG:H321	1.98	0.44
39:6:613:CHL:HBA1	39:6:613:CHL:H3A	1.75	0.44
18:7:21:TYR:CE2	18:7:39:SER:HA	2.53	0.44
22:7:603:CLA:H2	22:7:608:CLA:HMD1	2.00	0.44
19:8:171:GLY:O	19:8:174:PHE:HB2	2.17	0.44
1:A:423:TYR:CZ	4:D:241:ILE:HD11	2.52	0.44
2:B:438:TYR:CE2	22:B:1021:CLA:H162	2.53	0.44
2:B:463:TRP:CD1	22:F:1301:CLA:HMA2	2.53	0.44
2:B:490:GLY:O	2:B:495:LEU:HB2	2.17	0.44
22:B:1201:CLA:H101	22:B:1201:CLA:C3	2.47	0.44
22:B:1228:CLA:H192	22:B:1228:CLA:H161	1.80	0.44
3:C:54:CYS:SG	3:C:55:GLU:N	2.90	0.44
4:D:261:LEU:HD23	4:D:287:HIS:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:336:LYS:O	6:F:340:LYS:HE2	2.18	0.44
22:G:1602:CLA:HED2	22:G:1602:CLA:H2A	1.99	0.44
22:1:602:CLA:HMA2	22:1:602:CLA:O1A	2.17	0.44
22:4:603:CLA:H61	22:4:603:CLA:H101	1.56	0.44
22:4:610:CLA:H62	22:4:610:CLA:H2	1.71	0.44
17:6:41:PRO:HG3	22:6:609:CLA:HMD3	1.99	0.44
1:A:355:ILE:O	1:A:359:LEU:HD23	2.17	0.44
22:A:1122:CLA:H91	22:A:1122:CLA:H111	1.67	0.44
22:A:1138:CLA:HBA2	22:A:1138:CLA:H3A	1.56	0.44
6:F:379:LEU:O	6:F:387:HIS:N	2.48	0.44
13:1:181:MET:HE2	13:1:181:MET:HB2	1.71	0.44
16:5:97:GLN:HE22	16:5:107:ASN:ND2	2.12	0.44
17:6:80:ARG:HD3	17:6:164:TYR:CZ	2.52	0.44
19:8:89:ILE:HB	19:8:90:PRO:HD3	2.00	0.44
22:8:603:CLA:C4A	22:8:603:CLA:HBA2	2.47	0.44
1:A:264:PHE:HZ	24:K:4001:BCR:H343	1.83	0.44
1:A:441:LEU:HD13	22:A:1137:CLA:CAB	2.47	0.44
22:B:1221:CLA:H3A	22:B:1221:CLA:HBA1	1.84	0.44
22:B:1226:CLA:H92	22:B:1226:CLA:H61	1.77	0.44
22:B:1234:CLA:H93	22:B:1235:CLA:O1A	2.18	0.44
22:B:1229:CLA:HBB1	22:B:1229:CLA:HHC	1.98	0.44
14:3:318:MET:SD	22:3:601:CLA:HAB	2.58	0.44
14:3:328:GLU:CD	14:3:463:PHE:HB3	2.38	0.44
24:3:503:BCR:C2	22:7:609:CLA:HMD2	2.48	0.44
24:3:504:BCR:HC7	39:3:611:CHL:HMB2	1.99	0.44
15:4:168:PRO:HD2	38:4:501:LUT:H23	2.00	0.44
16:5:35:PHE:CG	16:5:36:PRO:HD2	2.53	0.44
16:5:122:LEU:HD13	39:5:610:CHL:HBC3	1.99	0.44
17:6:41:PRO:HG3	22:6:609:CLA:CMD	2.47	0.44
31:8:810:PTY:H112	31:8:810:PTY:C1	2.47	0.44
1:A:357:LEU:CD2	22:A:1103:CLA:HED1	2.48	0.44
22:A:1013:CLA:H151	22:A:1013:CLA:H112	1.64	0.44
22:A:1135:CLA:H141	22:A:1135:CLA:H162	1.76	0.44
22:B:1209:CLA:C3D	22:B:1210:CLA:HMC3	2.48	0.44
22:B:1235:CLA:H143	22:B:1235:CLA:H111	1.84	0.44
22:B:1237:CLA:H152	22:B:1237:CLA:H112	1.69	0.44
25:F:5001:LHG:HC61	22:8:609:CLA:HMA1	1.99	0.44
22:4:607:CLA:H62	22:4:607:CLA:H41	1.76	0.44
25:4:801:LHG:H342	25:4:801:LHG:H372	1.34	0.44
22:5:604:CLA:H2A	22:5:604:CLA:O2D	2.18	0.44
22:5:604:CLA:H3A	22:5:604:CLA:CGA	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:5:611:CHL:HBB2	22:5:618:CLA:HMC3	1.99	0.44
22:7:609:CLA:H142	22:7:609:CLA:H111	1.78	0.44
47:8:807:4RF:C10	22:8:615:CLA:HBA2	2.47	0.44
22:A:1106:CLA:H193	22:A:1106:CLA:H162	1.81	0.43
22:A:1123:CLA:H193	22:A:1123:CLA:H161	1.75	0.43
22:B:1230:CLA:HMB2	22:B:1229:CLA:CAB	2.48	0.43
12:L:351:LEU:HD21	22:L:1502:CLA:HMB3	2.00	0.43
13:1:82:MET:HB2	22:1:601:CLA:HMC3	2.00	0.43
22:1:603:CLA:H62	22:1:603:CLA:H41	1.45	0.43
22:1:610:CLA:CAB	39:1:613:CHL:HBB2	2.48	0.43
14:3:413:PRO:HD2	22:3:601:CLA:OBD	2.18	0.43
15:4:134:GLU:HG3	22:4:612:CLA:NB	2.34	0.43
24:5:504:BCR:H402	39:5:610:CHL:H3A	2.00	0.43
24:7:503:BCR:H313	22:8:609:CLA:C2D	2.48	0.43
19:8:79:TRP:CD1	22:8:612:CLA:HMD3	2.52	0.43
1:A:425:ASN:O	1:A:429:ARG:HG2	2.18	0.43
1:A:681:PHE:HZ	22:A:1139:CLA:HBC2	1.83	0.43
1:A:744:LEU:HA	1:A:744:LEU:HD23	1.76	0.43
22:A:1114:CLA:HMD2	14:3:353:PRO:HG3	2.00	0.43
22:A:1119:CLA:OBD	22:A:1121:CLA:HHD	2.18	0.43
2:B:695:ARG:HG3	12:L:393:VAL:CG1	2.48	0.43
22:B:1203:CLA:H41	26:B:5003:DGD:HB72	2.00	0.43
22:B:1208:CLA:HBD	22:B:1208:CLA:HBA1	2.01	0.43
22:B:1213:CLA:H61	22:B:1213:CLA:H102	1.43	0.43
25:F:5001:LHG:H112	25:F:5001:LHG:H311	1.99	0.43
9:K:69:ILE:HG13	22:K:1403:CLA:O1A	2.17	0.43
22:3:601:CLA:H3A	22:3:601:CLA:HBA2	1.43	0.43
15:4:226:ASN:ND2	24:6:504:BCR:HC21	2.33	0.43
15:4:236:ASN:HB2	25:6:802:LHG:C1	2.48	0.43
25:4:801:LHG:H142	25:4:801:LHG:H301	2.01	0.43
16:5:125:GLU:OE1	39:5:610:CHL:HMC	2.18	0.43
22:5:618:CLA:H3A	22:5:618:CLA:HBA2	1.80	0.43
18:7:11:PHE:HD2	18:7:14:ASN:CB	2.30	0.43
19:8:35:GLN:HB3	19:8:38:VAL:HB	2.00	0.43
19:8:235:PHE:CD1	22:8:603:CLA:H11	2.54	0.43
1:A:442:ASN:ND2	2:B:675:LEU:CD1	2.70	0.43
2:B:51:HIS:HE1	22:B:1202:CLA:H171	1.82	0.43
2:B:51:HIS:ND1	22:B:1210:CLA:OBD	2.49	0.43
2:B:701:LEU:HD22	2:B:705:GLN:NE2	2.33	0.43
22:B:1021:CLA:H142	22:B:1021:CLA:H111	1.67	0.43
22:B:1201:CLA:HBC1	26:B:5003:DGD:HAT1	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:1212:CLA:NB	24:B:4001:BCR:H271	2.33	0.43
7:G:1253:PHE:CE1	29:1:804:LMT:H4'	2.53	0.43
12:L:345:GLY:O	12:L:434:GLY:HA2	2.18	0.43
12:L:357:ILE:HG13	12:L:372:VAL:CG1	2.37	0.43
14:3:361:TRP:CE3	14:3:362:MET:HG3	2.53	0.43
14:3:466:LEU:HD22	38:3:501:LUT:H163	2.01	0.43
39:4:609:CHL:H61	39:4:609:CHL:H41	1.47	0.43
16:5:97:GLN:HE22	16:5:107:ASN:HB3	1.83	0.43
17:6:148:GLN:OE1	17:6:156:LYS:HE2	2.18	0.43
18:7:143:ARG:HH22	18:7:147:GLY:HA2	1.83	0.43
1:A:175:PHE:CE2	22:3:605:CLA:H161	2.53	0.43
24:A:4001:BCR:H282	32:K:5001:LAP:H111	1.99	0.43
22:B:1216:CLA:H111	22:B:1216:CLA:H152	1.30	0.43
26:B:5003:DGD:HA81	26:B:5003:DGD:HAE2	1.77	0.43
6:F:482:ARG:HA	6:F:482:ARG:HD3	1.89	0.43
9:K:58:PRO:HD2	22:K:1403:CLA:C2B	2.48	0.43
12:L:324:TYR:CD2	12:L:325:LEU:HD22	2.54	0.43
13:1:119:VAL:HG21	39:1:613:CHL:CMD	2.48	0.43
22:3:616:CLA:H61	22:3:616:CLA:H41	1.65	0.43
22:5:612:CLA:H112	22:5:612:CLA:H72	1.68	0.43
17:6:100:LYS:HE2	17:6:103:VAL:HG21	2.00	0.43
17:6:186:LYS:CE	25:6:801:LHG:O5	2.66	0.43
17:6:236:ALA:HB2	43:6:804:PLM:H51	2.01	0.43
19:8:123:LEU:HD21	39:8:613:CHL:CHD	2.48	0.43
22:8:612:CLA:H3A	22:8:612:CLA:HBA2	1.23	0.43
1:A:87:TRP:O	1:A:91:MET:HG2	2.18	0.43
1:A:587:SER:O	1:A:591:HIS:ND1	2.38	0.43
2:B:409:LEU:O	2:B:413:LEU:HD23	2.19	0.43
2:B:540:LEU:HD11	24:B:4004:BCR:H291	2.00	0.43
2:B:723:ALA:O	2:B:727:ILE:HG12	2.19	0.43
22:B:1215:CLA:H62	22:B:1215:CLA:H41	1.48	0.43
22:B:1231:CLA:H61	24:B:4005:BCR:H313	2.01	0.43
5:E:41:ARG:HE	5:E:41:ARG:HB2	1.56	0.43
6:F:457:TRP:CG	6:F:458:PRO:HD3	2.54	0.43
9:K:71:LEU:HD13	22:K:1403:CLA:HMA3	2.01	0.43
22:K:1401:CLA:HED2	22:K:1401:CLA:H2A	1.99	0.43
37:M:4001:ECH:H15	37:M:4001:ECH:H35	1.78	0.43
39:4:609:CHL:HAC1	25:4:801:LHG:C4	2.49	0.43
17:6:150:PRO:HG2	22:6:617:CLA:HBB1	2.01	0.43
45:6:806:SPH:H131	45:6:806:SPH:H162	1.36	0.43
38:6:502:LUT:H15	38:6:502:LUT:H201	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:6:601:CLA:H61	22:6:601:CLA:H92	1.68	0.43
1:A:706:LYS:NZ	6:F:471:MET:SD	2.92	0.43
22:A:1115:CLA:H3A	22:A:1115:CLA:HBA2	1.76	0.43
22:A:1135:CLA:HED2	22:A:1135:CLA:H2A	2.00	0.43
2:B:107:ARG:O	2:B:109:GLY:N	2.45	0.43
22:B:1225:CLA:H52	24:B:4002:BCR:H23C	2.00	0.43
22:B:1237:CLA:C20	22:L:1502:CLA:CBB	2.96	0.43
4:D:325:LYS:HE3	4:D:330:PHE:HE1	1.82	0.43
10:M:20:ILE:O	10:M:24:ARG:HG2	2.18	0.43
12:L:308:ILE:O	12:L:310:MET:N	2.43	0.43
12:L:356:PHE:CD1	12:L:375:ILE:HG21	2.53	0.43
22:1:607:CLA:CHD	25:1:801:LHG:HC62	2.49	0.43
22:3:602:CLA:H3A	22:3:602:CLA:HBA1	1.81	0.43
22:3:607:CLA:H141	22:3:607:CLA:H161	1.67	0.43
39:4:618:CHL:H62	39:4:618:CHL:H41	1.86	0.43
22:6:609:CLA:HMB1	22:6:609:CLA:CBB	2.45	0.43
1:A:410:ALA:HB1	1:A:588:ALA:HB1	1.99	0.43
1:A:596:LEU:HD21	22:A:1128:CLA:HBC1	2.00	0.43
22:B:1214:CLA:O1D	22:B:1215:CLA:HMA1	2.19	0.43
30:B:5004:PCW:O2P	6:F:471:MET:CE	2.67	0.43
4:D:218:GLU:OE2	4:D:276:ARG:CG	2.66	0.43
22:K:1401:CLA:HBA2	22:K:1401:CLA:H3A	1.73	0.43
38:1:503:LUT:H11	38:1:503:LUT:H191	1.83	0.43
22:1:605:CLA:HMD2	22:1:612:CLA:C1D	2.49	0.43
22:4:615:CLA:H92	22:4:615:CLA:H62	1.83	0.43
17:6:41:PRO:HG2	22:6:609:CLA:CAD	2.48	0.43
22:7:606:CLA:HBB1	22:7:606:CLA:HMB1	2.01	0.43
1:A:483:PHE:O	1:A:487:VAL:HG23	2.18	0.43
1:A:715:PRO:HG3	22:A:1140:CLA:HBC2	2.00	0.43
22:A:1115:CLA:H42	22:K:1402:CLA:O1D	2.19	0.43
2:B:305:ILE:HD13	22:B:1219:CLA:HMD3	2.01	0.43
6:F:466:LYS:CB	44:8:803:DGA:HB32	2.49	0.43
35:J:4002:RRX:H51	35:J:4002:RRX:C8	2.48	0.43
13:1:72:GLU:OE2	13:1:149:ARG:HD2	2.18	0.43
22:1:602:CLA:HAC2	22:1:603:CLA:H191	2.01	0.43
15:4:142:ILE:HG13	15:4:143:LYS:N	2.34	0.43
39:4:618:CHL:HBA1	39:4:618:CHL:CHA	2.48	0.43
16:5:97:GLN:HG2	22:5:606:CLA:HED3	2.01	0.43
16:5:144:ASP:HA	16:5:147:ASN:ND2	2.34	0.43
16:5:184:THR:HA	16:5:187:ILE:HG22	2.00	0.43
17:6:150:PRO:CD	22:6:617:CLA:HMC2	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:6:265:PRO:CB	39:6:619:CHL:HAB	2.49	0.43
47:8:807:4RF:H2	22:8:615:CLA:HBA2	2.01	0.43
39:8:601:CHL:C4	22:8:602:CLA:HBA1	2.48	0.43
47:8:808:4RF:H10	47:8:808:4RF:H72	2.00	0.43
1:A:20:ASN:N	1:A:21:PRO:HD3	2.34	0.43
1:A:65:ASP:O	1:A:69:ILE:HG13	2.18	0.43
1:A:113:PRO:HB3	1:A:145:PHE:CD2	2.54	0.43
1:A:296:HIS:ND1	22:A:1116:CLA:HMB1	2.33	0.43
2:B:79:VAL:HG13	2:B:126:TYR:HE1	1.83	0.43
2:B:145:VAL:HG11	25:B:5002:LHG:H192	2.01	0.43
2:B:255:ILE:HG13	2:B:256:LEU:HG	2.01	0.43
2:B:574:TRP:CD1	22:B:1226:CLA:HMD1	2.54	0.43
2:B:672:TRP:CZ2	23:B:2002:PQN:H2M3	2.53	0.43
9:K:59:THR:HB	9:K:92:ASP:OD1	2.18	0.43
13:1:71:ARG:O	13:1:75:VAL:HG23	2.19	0.43
14:3:315:ARG:HD2	39:3:611:CHL:OBD	2.19	0.43
22:3:603:CLA:H112	22:3:603:CLA:H151	1.84	0.43
16:5:207:THR:C	16:5:235:MET:HG3	2.40	0.43
1:A:407:ALA:HB2	1:A:592:VAL:HG11	2.00	0.43
2:B:348:LEU:HD23	22:B:1215:CLA:H62	2.01	0.43
2:B:349:VAL:HG21	22:B:1225:CLA:HHD	1.99	0.43
2:B:388:PHE:CZ	22:B:1222:CLA:HAB	2.53	0.43
22:B:1023:CLA:C12	24:I:4001:BCR:H281	2.48	0.43
22:B:1218:CLA:HMD2	24:B:4001:BCR:H342	2.01	0.43
22:B:1239:CLA:H3A	22:B:1239:CLA:HBA2	1.61	0.43
5:E:45:VAL:O	5:E:58:THR:HA	2.19	0.43
22:4:604:CLA:H62	22:4:604:CLA:H41	1.79	0.43
16:5:200:PHE:HE1	38:5:501:LUT:H41	1.84	0.43
22:5:612:CLA:H71	39:6:619:CHL:H43	2.00	0.43
17:6:186:LYS:HB2	22:6:607:CLA:HMD1	2.00	0.43
25:7:801:LHG:H241	25:7:801:LHG:H271	1.44	0.43
1:A:702:TRP:CD1	6:F:477:ILE:CG2	3.02	0.42
22:A:1106:CLA:CBB	22:A:1126:CLA:H171	2.45	0.42
2:B:520:VAL:HG11	2:B:594:TYR:HB2	2.01	0.42
22:B:1216:CLA:H41	22:B:1216:CLA:H61	1.64	0.42
9:K:69:ILE:HG13	22:K:1403:CLA:CGA	2.49	0.42
38:1:502:LUT:H15	38:1:502:LUT:H201	1.89	0.42
22:1:607:CLA:H111	22:1:607:CLA:H72	1.53	0.42
22:1:607:CLA:H61	22:1:607:CLA:H41	1.89	0.42
38:3:501:LUT:H35	38:3:501:LUT:H401	1.89	0.42
39:4:618:CHL:H8	19:8:177:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:5:150:PRO:HB3	22:6:609:CLA:HMD1	2.01	0.42
46:7:502:XAT:H31	46:7:502:XAT:H391	1.77	0.42
1:A:18:ASP:CG	1:A:71:ARG:HH22	2.22	0.42
1:A:130:ASP:OD1	1:A:136:GLN:NE2	2.51	0.42
22:A:1131:CLA:H72	22:A:1131:CLA:H111	1.61	0.42
22:A:1140:CLA:H62	22:A:1140:CLA:H41	1.67	0.42
2:B:561:ASP:CG	2:B:565:ARG:HH22	2.21	0.42
22:B:1218:CLA:H41	22:B:1218:CLA:H62	1.48	0.42
22:B:1207:CLA:H43	12:L:371:ILE:CG2	2.48	0.42
13:1:145:GLU:OE1	13:1:145:GLU:N	2.47	0.42
14:3:397:PHE:HD2	14:3:400:LEU:HB2	1.85	0.42
38:5:502:LUT:H15	38:5:502:LUT:H201	1.89	0.42
22:6:615:CLA:H161	22:6:615:CLA:H122	1.82	0.42
22:7:612:CLA:HBC2	39:7:613:CHL:H192	2.00	0.42
39:7:613:CHL:H152	39:7:613:CHL:H111	1.71	0.42
22:8:608:CLA:O2D	22:8:608:CLA:H2A	2.19	0.42
1:A:75:SER:OG	1:A:181:TYR:HB2	2.19	0.42
1:A:578:PRO:HB3	2:B:560:CYS:SG	2.60	0.42
1:A:743:PHE:O	1:A:747:ILE:HG22	2.19	0.42
22:A:1131:CLA:HMD2	22:A:1136:CLA:H161	2.00	0.42
2:B:142:PHE:CE2	22:B:1211:CLA:H52	2.54	0.42
22:B:1234:CLA:H2	22:B:1234:CLA:H62	1.71	0.42
22:B:1236:CLA:HBC3	25:B:5001:LHG:H371	2.01	0.42
3:C:14:CYS:O	3:C:15:THR:OG1	2.28	0.42
7:G:1245:LEU:HD11	13:1:135:ALA:CB	2.49	0.42
9:K:47:LEU:HD23	9:K:47:LEU:HA	1.90	0.42
22:1:604:CLA:H203	22:1:604:CLA:H161	1.86	0.42
38:5:501:LUT:H11	38:5:501:LUT:H191	1.90	0.42
38:6:501:LUT:H191	38:6:501:LUT:H11	1.79	0.42
19:8:120:PHE:CG	47:8:808:4RF:H9	2.54	0.42
22:A:1108:CLA:HHC	22:A:1108:CLA:CBB	2.50	0.42
22:A:1109:CLA:H161	22:A:1109:CLA:H143	1.69	0.42
22:A:1134:CLA:HBA2	22:A:1134:CLA:H3A	1.65	0.42
2:B:600:LEU:O	2:B:604:GLN:HG3	2.20	0.42
22:B:1231:CLA:H2	22:B:1232:CLA:HMB2	2.00	0.42
9:K:96:LEU:CD2	22:K:1403:CLA:CBB	2.98	0.42
12:L:324:TYR:HD2	12:L:325:LEU:HD22	1.83	0.42
15:4:135:LEU:HD23	15:4:135:LEU:HA	1.89	0.42
24:4:503:BCR:H271	22:4:606:CLA:C4B	2.48	0.42
22:4:604:CLA:H112	22:4:604:CLA:H91	1.82	0.42
17:6:112:VAL:HG23	22:6:606:CLA:HED1	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:8:610:CLA:HBA2	47:8:808:4RF:H71	2.00	0.42
39:8:613:CHL:HHC	39:8:613:CHL:HBB1	2.00	0.42
1:A:26:PHE:HE1	27:A:5007:3PH:H251	1.85	0.42
1:A:175:PHE:CE2	22:3:605:CLA:H13	2.54	0.42
22:A:1013:CLA:H92	22:A:1013:CLA:H61	1.60	0.42
22:A:1111:CLA:H111	22:A:1111:CLA:H91	1.62	0.42
2:B:556:TYR:CD2	22:B:1226:CLA:HED2	2.54	0.42
17:6:194:ALA:CB	38:6:501:LUT:H7	2.44	0.42
38:6:502:LUT:H183	22:6:606:CLA:C3B	2.49	0.42
22:6:618:CLA:HHC	22:6:618:CLA:HBB1	2.02	0.42
18:7:183:MET:SD	22:7:604:CLA:HAB	2.59	0.42
19:8:85:ALA:HB2	38:8:501:LUT:H401	2.01	0.42
39:8:601:CHL:H72	22:8:602:CLA:HMA1	2.01	0.42
22:A:1119:CLA:H171	24:A:4003:BCR:H23C	2.00	0.42
2:B:79:VAL:HG13	2:B:126:TYR:CE1	2.54	0.42
2:B:632:LEU:HD13	2:B:728:ALA:HB3	2.01	0.42
22:B:1023:CLA:HBD	22:B:1023:CLA:HED2	1.83	0.42
22:B:1212:CLA:H192	24:B:4003:BCR:HC41	2.01	0.42
22:B:1217:CLA:HMA2	7:G:1297:VAL:HG13	2.02	0.42
22:B:1223:CLA:H61	22:B:1223:CLA:H102	1.66	0.42
31:B:5005:PTY:H202	31:B:5005:PTY:H171	1.90	0.42
13:1:55:PHE:HB3	22:1:604:CLA:C3D	2.49	0.42
24:3:505:BCR:H402	22:3:610:CLA:C2D	2.50	0.42
15:4:32:TRP:HH2	25:4:802:LHG:HC42	1.85	0.42
15:4:185:LYS:HD3	22:4:607:CLA:O1D	2.20	0.42
16:5:108:LEU:HD12	16:5:108:LEU:HA	1.77	0.42
17:6:40:LEU:CD1	22:6:609:CLA:CED	2.86	0.42
17:6:189:ARG:HB3	25:6:801:LHG:H251	2.02	0.42
30:6:803:PCW:H83	30:6:803:PCW:H42	1.87	0.42
18:7:113:PHE:CE1	22:7:612:CLA:HMB3	2.54	0.42
22:7:604:CLA:H62	22:7:605:CLA:HMA1	2.00	0.42
19:8:188:ASP:O	19:8:192:TRP:HD1	2.02	0.42
22:8:620:CLA:H61	22:8:620:CLA:H102	1.80	0.42
1:A:357:LEU:HD23	1:A:357:LEU:HA	1.88	0.42
1:A:544:HIS:HA	1:A:547:VAL:HG12	2.01	0.42
22:A:1012:CLA:H122	22:A:1012:CLA:H8	1.72	0.42
22:A:1106:CLA:HBB1	22:A:1126:CLA:H101	2.00	0.42
22:A:1115:CLA:HED2	22:A:1115:CLA:H2A	2.01	0.42
25:A:5003:LHG:HO1	25:A:5003:LHG:P	2.38	0.42
22:B:1209:CLA:H2	22:B:1209:CLA:H61	1.79	0.42
22:B:1239:CLA:H193	24:L:4001:BCR:C14	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:1239:CLA:H202	22:B:1239:CLA:H161	1.83	0.42
24:B:4003:BCR:H351	24:B:4003:BCR:H15C	1.89	0.42
4:D:226:SER:HB3	4:D:243:ARG:O	2.20	0.42
8:J:51:PHE:HE2	22:J:1901:CLA:HMA3	1.84	0.42
9:K:58:PRO:HD3	22:K:1403:CLA:C4A	2.47	0.42
13:1:115:PHE:CE1	22:1:606:CLA:HMD2	2.55	0.42
14:3:417:TRP:HE3	16:5:56:PRO:O	2.02	0.42
22:4:605:CLA:HBC1	22:4:612:CLA:HBC1	2.01	0.42
16:5:87:ILE:HD13	38:5:502:LUT:H41	2.01	0.42
38:5:501:LUT:H15	38:5:501:LUT:H201	1.91	0.42
22:5:609:CLA:HBB1	22:5:609:CLA:HMB1	2.01	0.42
18:7:47:ASN:HB3	22:7:604:CLA:HMA1	2.02	0.42
22:7:617:CLA:CAA	26:8:802:DGD:HA81	2.47	0.42
1:A:307:ILE:HD13	24:K:4001:BCR:H17C	2.01	0.42
22:A:1108:CLA:H93	22:A:1108:CLA:H111	1.86	0.42
22:A:1138:CLA:H202	22:A:1138:CLA:H162	1.75	0.42
22:B:1220:CLA:H52	24:B:4004:BCR:C14	2.50	0.42
22:B:1224:CLA:H141	22:B:1224:CLA:H161	1.76	0.42
22:F:1302:CLA:H51	22:F:1302:CLA:H8	1.81	0.42
7:G:1312:TYR:OH	34:G:5002:ERG:C27	2.68	0.42
34:G:5002:ERG:H272	34:G:5002:ERG:H23	1.65	0.42
22:L:1501:CLA:H12	22:L:1501:CLA:HBA2	1.75	0.42
38:1:503:LUT:H35	38:1:503:LUT:H401	1.72	0.42
22:4:601:CLA:H61	22:4:601:CLA:H41	1.70	0.42
24:5:504:BCR:H24C	39:5:610:CHL:HBA2	2.00	0.42
17:6:218:ASP:OD1	17:6:219:ASN:N	2.53	0.42
22:6:603:CLA:H91	22:6:603:CLA:H112	1.79	0.42
39:6:619:CHL:H61	39:6:619:CHL:H41	1.53	0.42
19:8:84:VAL:HG11	38:8:501:LUT:H12	2.01	0.42
19:8:196:ARG:NH2	26:8:802:DGD:O5E	2.52	0.42
22:8:605:CLA:HAC1	22:8:610:CLA:HBB2	2.02	0.42
2:B:57:ILE:HD11	37:M:4001:ECH:C39	2.42	0.42
6:F:318:ASP:OD1	6:F:322:LEU:N	2.51	0.42
13:1:34:GLY:HA3	13:1:53:TYR:CD2	2.55	0.42
14:3:351:ILE:HG22	14:3:353:PRO:HD2	2.00	0.42
14:3:457:MET:CE	14:3:485:ILE:HG22	2.50	0.42
22:3:612:CLA:H112	22:3:612:CLA:H142	1.79	0.42
25:3:801:LHG:H252	25:3:801:LHG:H282	1.85	0.42
31:5:802:PTY:H382	22:7:603:CLA:H172	2.02	0.42
17:6:75:PHE:HB2	22:6:604:CLA:HMA1	1.97	0.42
17:6:215:GLU:O	17:6:223:THR:HG21	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:6:604:CLA:HMB2	22:6:604:CLA:C4	2.49	0.42
18:7:91:ARG:NH2	22:7:606:CLA:HED1	2.34	0.42
22:7:605:CLA:HMD1	48:7:504:C7Z:O23	2.20	0.42
19:8:138:ARG:O	19:8:141:ASP:HB3	2.20	0.42
47:8:808:4RF:H39	40:8:809:OLA:H52	2.02	0.42
1:A:121:ILE:HG12	8:J:46:ILE:HG23	2.01	0.42
1:A:167:LEU:HD12	1:A:167:LEU:HA	1.88	0.42
22:A:1120:CLA:C4D	24:K:4001:BCR:H271	2.49	0.42
24:A:4003:BCR:H381	24:A:4004:BCR:HC42	2.02	0.42
2:B:48:PHE:CE2	2:B:52:PHE:HE2	2.37	0.42
2:B:158:LEU:HD23	2:B:158:LEU:HA	1.92	0.42
2:B:699:VAL:HG12	3:C:79:LEU:HD21	2.02	0.42
22:B:1209:CLA:H72	22:B:1209:CLA:H111	1.48	0.42
4:D:242:MET:HB2	4:D:247:ASN:ND2	2.35	0.42
22:K:1402:CLA:H91	22:K:1402:CLA:H111	1.72	0.42
24:L:4001:BCR:H382	22:L:1502:CLA:HAC2	2.01	0.42
22:1:602:CLA:HHC	22:1:602:CLA:CBB	2.47	0.42
22:3:610:CLA:O1D	22:3:613:CLA:HMC3	2.20	0.42
16:5:171:PRO:HD2	38:5:501:LUT:H23	2.01	0.42
22:5:602:CLA:H61	22:5:602:CLA:H41	1.74	0.42
17:6:75:PHE:HB2	22:6:604:CLA:CMA	2.50	0.42
19:8:120:PHE:CE1	47:8:808:4RF:H41	2.54	0.42
38:8:501:LUT:H11	38:8:501:LUT:H191	1.96	0.42
1:A:206:LEU:HD23	1:A:206:LEU:HA	2.34	0.41
1:A:395:MET:HE1	22:A:1124:CLA:CMD	2.50	0.41
1:A:441:LEU:HD13	22:A:1137:CLA:C3B	2.49	0.41
1:A:598:TRP:HH2	22:B:1022:CLA:HAB	1.85	0.41
1:A:715:PRO:HB3	22:A:1140:CLA:C2C	2.49	0.41
22:A:1134:CLA:HMB1	24:A:4004:BCR:H282	2.02	0.41
2:B:416:LYS:CB	2:B:540:LEU:HD23	2.49	0.41
2:B:429:PHE:HZ	22:B:1235:CLA:HMC3	1.85	0.41
2:B:727:ILE:O	2:B:731:SER:OG	2.19	0.41
22:B:1021:CLA:O2D	22:B:1021:CLA:HAA2	2.20	0.41
22:B:1227:CLA:HMB2	22:B:1228:CLA:C2D	2.50	0.41
30:B:5004:PCW:O2P	6:F:471:MET:HE1	2.19	0.41
22:B:1207:CLA:H43	12:L:371:ILE:HG23	2.02	0.41
7:G:1253:PHE:CE2	29:1:804:LMT:H2'	2.52	0.41
11:I:30:ILE:HG21	24:L:4001:BCR:H333	2.02	0.41
22:1:606:CLA:HMB1	22:1:606:CLA:HBB1	2.01	0.41
14:3:442:ARG:O	14:3:446:ILE:HG13	2.20	0.41
24:3:504:BCR:H351	24:3:504:BCR:H15C	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:3:601:CLA:H71	22:3:602:CLA:HMA1	2.02	0.41
22:3:607:CLA:H141	22:3:607:CLA:H193	2.02	0.41
16:5:119:GLY:O	17:6:226:PHE:HB3	2.20	0.41
17:6:132:VAL:CG1	39:6:611:CHL:C2B	2.97	0.41
17:6:139:ASP:CB	39:6:611:CHL:HAC2	2.50	0.41
22:7:617:CLA:H62	22:7:617:CLA:H93	1.76	0.41
22:A:1108:CLA:O2D	22:A:1108:CLA:H2A	2.20	0.41
22:A:1139:CLA:HBA2	22:A:1139:CLA:H3A	1.33	0.41
22:B:1226:CLA:CAD	26:B:5003:DGD:HB32	2.50	0.41
22:B:1237:CLA:H62	22:B:1237:CLA:H41	1.66	0.41
22:B:1207:CLA:HHC	22:B:1207:CLA:CBB	2.49	0.41
6:F:319:VAL:HG21	6:F:389:ILE:HD11	2.02	0.41
6:F:329:LYS:HA	6:F:329:LYS:HD3	1.93	0.41
9:K:37:THR:HA	9:K:40:ILE:HG22	2.02	0.41
24:3:503:BCR:H282	22:3:616:CLA:HAB	2.02	0.41
38:4:501:LUT:H15	38:4:501:LUT:H201	1.91	0.41
24:4:503:BCR:H19C	39:4:613:CHL:O1A	2.20	0.41
16:5:91:GLU:OE1	16:5:211:PRO:HG2	2.19	0.41
22:7:612:CLA:H93	22:7:612:CLA:H111	1.95	0.41
39:8:601:CHL:H61	39:8:601:CHL:H41	1.62	0.41
1:A:578:PRO:HG2	3:C:69:LEU:HD11	2.02	0.41
22:A:1125:CLA:HBB	22:A:1133:CLA:H43	2.03	0.41
24:A:4001:BCR:H392	24:A:4001:BCR:H23C	2.03	0.41
2:B:92:ILE:HG21	2:B:97:PHE:CE2	2.54	0.41
2:B:449:THR:OG1	2:B:452:LYS:HE2	2.21	0.41
22:B:1224:CLA:H203	22:B:1224:CLA:H162	1.89	0.41
6:F:409:ILE:HG13	25:F:5002:LHG:C15	2.49	0.41
8:J:31:PRO:O	35:J:4002:RRX:H49	2.20	0.41
22:3:607:CLA:H61	22:3:607:CLA:H102	1.82	0.41
15:4:139:GLN:HA	15:4:142:ILE:HG12	2.02	0.41
15:4:188:ARG:HA	15:4:191:MET:HE2	2.01	0.41
16:5:129:MET:HA	16:5:132:VAL:HG22	2.03	0.41
17:6:182:VAL:CG1	22:6:607:CLA:CED	2.96	0.41
17:6:182:VAL:O	17:6:186:LYS:HG2	2.21	0.41
45:6:806:SPH:H151	45:6:806:SPH:H182	1.56	0.41
25:7:801:LHG:H322	25:7:801:LHG:H351	1.56	0.41
19:8:92:GLU:OE2	19:8:95:ARG:NH2	2.44	0.41
1:A:463:SER:OG	1:A:471:MET:SD	2.77	0.41
22:A:1138:CLA:HBC1	23:A:2001:PQN:H191	2.02	0.41
2:B:251:SER:OG	2:B:252:GLY:N	2.52	0.41
2:B:528:LEU:HD12	2:B:587:THR:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:632:LEU:HD21	2:B:651:PHE:CD1	2.56	0.41
22:B:1205:CLA:CGA	22:B:1205:CLA:C1A	2.98	0.41
22:B:1209:CLA:HBD	7:G:1278:ARG:CD	2.51	0.41
22:B:1210:CLA:H93	22:B:1210:CLA:H61	1.76	0.41
22:B:1230:CLA:H91	22:B:1230:CLA:H112	1.84	0.41
23:B:2002:PQN:H111	23:B:2002:PQN:H2M1	1.89	0.41
22:1:603:CLA:C4A	22:1:603:CLA:HBA2	2.50	0.41
15:4:204:GLN:OE1	22:4:603:CLA:HED3	2.21	0.41
16:5:88:LEU:HD21	16:5:200:PHE:CZ	2.55	0.41
38:5:501:LUT:H35	38:5:501:LUT:H401	1.76	0.41
38:5:505:LUT:H401	38:5:505:LUT:H35	1.75	0.41
38:6:502:LUT:H361	38:6:502:LUT:H28	2.03	0.41
22:6:604:CLA:HMB1	22:6:604:CLA:CBB	2.50	0.41
19:8:80:ALA:CB	19:8:202:MET:HG2	2.50	0.41
26:8:802:DGD:HAN2	26:8:802:DGD:HAW1	1.71	0.41
24:8:503:BCR:H15C	24:8:503:BCR:H351	1.75	0.41
1:A:337:GLY:O	1:A:426:LEU:HG	2.20	0.41
22:A:1117:CLA:HBA2	22:A:1117:CLA:H3A	1.36	0.41
4:D:218:GLU:HG3	4:D:278:PHE:CE1	2.55	0.41
37:M:4001:ECH:H11	37:M:4001:ECH:H34	1.83	0.41
38:1:503:LUT:H31	38:1:503:LUT:H391	1.88	0.41
14:3:315:ARG:HD3	22:3:601:CLA:CHD	2.51	0.41
15:4:167:ASP:HA	38:4:501:LUT:O23	2.19	0.41
15:4:192:LEU:HD23	15:4:192:LEU:HA	1.90	0.41
16:5:51:ASP:CG	22:5:604:CLA:HED2	2.41	0.41
17:6:150:PRO:HD3	22:6:617:CLA:C2C	2.50	0.41
38:6:501:LUT:H15	38:6:501:LUT:H201	1.93	0.41
39:6:611:CHL:HBB1	22:6:617:CLA:HMC3	2.02	0.41
18:7:153:ARG:H	18:7:153:ARG:HG2	1.65	0.41
38:8:501:LUT:H34	39:8:601:CHL:CBB	2.50	0.41
38:8:502:LUT:H15	38:8:502:LUT:H201	1.93	0.41
1:A:313:ARG:HH21	1:A:321:SER:HB2	1.85	0.41
22:A:1108:CLA:C4C	22:A:1111:CLA:H203	2.50	0.41
22:A:1114:CLA:CAD	29:A:5008:LMT:H4'	2.50	0.41
22:A:1130:CLA:H41	22:A:1130:CLA:H61	1.39	0.41
2:B:523:ALA:HB1	22:B:1021:CLA:H171	2.02	0.41
22:B:1212:CLA:O1A	24:B:4001:BCR:H281	2.21	0.41
22:B:1240:CLA:H142	22:B:1240:CLA:H112	1.88	0.41
22:B:1228:CLA:H42	6:F:465:TYR:CD1	2.55	0.41
13:1:57:PRO:HD2	38:1:502:LUT:H23	2.03	0.41
13:1:159:MET:HG2	38:1:501:LUT:H222	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:222:PRO:HG3	22:1:615:CLA:C2B	2.50	0.41
29:1:804:LMT:H1'	22:1:612:CLA:HBA2	2.03	0.41
14:3:264:TYR:O	14:3:265:LYS:HB3	2.21	0.41
14:3:325:LEU:HD12	14:3:325:LEU:HA	1.86	0.41
38:3:502:LUT:H35	38:3:502:LUT:H401	1.83	0.41
24:3:504:BCR:C11	39:3:611:CHL:HBA1	2.51	0.41
16:5:245:LEU:HD23	24:5:504:BCR:H352	2.01	0.41
16:5:251:CYS:O	16:5:252:LEU:HB2	2.21	0.41
17:6:65:LEU:HB3	22:6:604:CLA:H11	2.03	0.41
17:6:90:VAL:CG1	38:6:501:LUT:H14	2.51	0.41
22:6:604:CLA:CB	22:6:609:CLA:HBB2	2.47	0.41
18:7:152:GLY:O	18:7:162:ARG:NH2	2.53	0.41
22:7:612:CLA:H2	48:7:504:C7Z:C38	2.51	0.41
1:A:91:MET:SD	22:A:1106:CLA:HAA2	2.60	0.41
1:A:358:ALA:HB1	24:A:4004:BCR:H10C	2.02	0.41
1:A:481:PRO:HG3	1:A:533:PHE:HB2	2.03	0.41
22:A:1134:CLA:H143	22:A:1134:CLA:H112	1.70	0.41
22:A:1101:CLA:C3D	8:J:31:PRO:HD3	2.50	0.41
2:B:6:PHE:O	2:B:8:LYS:N	2.53	0.41
2:B:391:GLY:HA2	24:B:4005:BCR:H393	2.03	0.41
22:B:1209:CLA:H143	22:B:1217:CLA:C2	2.50	0.41
30:B:5004:PCW:H331	24:F:4001:BCR:H14C	2.03	0.41
6:F:393:GLY:N	6:F:396:LEU:HD12	2.35	0.41
22:F:1302:CLA:C2D	47:7:807:4RF:H35	2.51	0.41
7:G:1247:ARG:HG2	22:G:1602:CLA:C3B	2.50	0.41
14:3:457:MET:HE1	14:3:485:ILE:HG22	2.03	0.41
38:3:501:LUT:H11	38:3:501:LUT:H191	1.93	0.41
39:3:608:CHL:HMA2	39:3:608:CHL:HAA1	1.89	0.41
15:4:119:LYS:HE3	15:4:123:ILE:HD12	2.03	0.41
17:6:97:GLU:HG3	17:6:208:ASN:HB3	2.02	0.41
38:8:501:LUT:H401	38:8:501:LUT:H35	1.89	0.41
1:A:15:ILE:HG23	22:A:1108:CLA:HMA2	2.03	0.41
1:A:453:PHE:CE2	1:A:457:ILE:HD11	2.56	0.41
1:A:713:ILE:CD1	6:F:440:ILE:HG23	2.51	0.41
22:A:1107:CLA:H93	35:J:4002:RRX:H38	2.02	0.41
22:A:1112:CLA:H62	22:A:1112:CLA:H2	1.82	0.41
2:B:141:ILE:HD13	2:B:141:ILE:HA	1.91	0.41
2:B:668:TRP:HA	23:B:2002:PQN:C8	2.50	0.41
22:B:1205:CLA:HAB	22:B:1206:CLA:CBA	2.41	0.41
24:B:4004:BCR:H23C	24:B:4004:BCR:H392	2.02	0.41
14:3:447:ALA:HA	22:3:603:CLA:HBB1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:3:605:CLA:H3A	22:3:605:CLA:HBA1	1.78	0.41
39:5:613:CHL:HMB1	39:5:613:CHL:CBB	2.48	0.41
39:6:619:CHL:HMA2	39:6:619:CHL:HAA1	1.88	0.41
18:7:113:PHE:CD2	22:8:609:CLA:HMA2	2.56	0.41
22:7:615:CLA:HBA1	22:7:615:CLA:H2	2.03	0.41
22:8:606:CLA:H62	22:8:606:CLA:H41	1.64	0.41
1:A:80:GLN:HB2	22:A:1103:CLA:HMB2	2.02	0.41
1:A:444:VAL:HG21	22:A:1137:CLA:HMC3	2.01	0.41
22:A:1013:CLA:H8	22:A:1139:CLA:HMC2	2.02	0.41
22:A:1102:CLA:H61	22:A:1102:CLA:H93	1.83	0.41
22:A:1106:CLA:H142	22:A:1106:CLA:H112	1.79	0.41
22:A:1109:CLA:HBA1	22:A:1109:CLA:CBD	2.51	0.41
22:A:1131:CLA:H172	22:B:1238:CLA:HHB	2.03	0.41
2:B:17:PRO:O	2:B:697:LYS:HG3	2.21	0.41
2:B:92:ILE:HG21	2:B:97:PHE:HE2	1.86	0.41
2:B:184:PHE:CZ	22:B:1210:CLA:H72	2.56	0.41
2:B:349:VAL:CG2	22:B:1225:CLA:HMD3	2.51	0.41
2:B:716:VAL:HG22	26:B:5003:DGD:HGB2	2.03	0.41
22:B:1204:CLA:H111	22:B:1204:CLA:H142	1.74	0.41
3:C:27:GLU:CD	4:D:294:PRO:HA	2.39	0.41
7:G:1248:PHE:CD1	38:1:503:LUT:H221	2.55	0.41
9:K:36:THR:O	9:K:40:ILE:HG22	2.21	0.41
12:L:350:TYR:O	12:L:353:VAL:HG22	2.20	0.41
12:L:356:PHE:CB	12:L:372:VAL:HG13	2.43	0.41
24:L:4003:BCR:H351	24:L:4003:BCR:H15C	1.78	0.41
13:1:126:LEU:HD11	39:1:613:CHL:HMD3	2.02	0.41
14:3:315:ARG:HD3	22:3:601:CLA:C4C	2.51	0.41
14:3:462:PRO:O	38:3:501:LUT:O3	2.37	0.41
22:3:602:CLA:HMD2	22:3:607:CLA:C1D	2.51	0.41
44:5:803:DGA:HB51	44:5:803:DGA:HA32	2.03	0.41
17:6:54:LEU:CD1	22:6:604:CLA:HED1	2.51	0.41
17:6:74:TRP:CZ2	22:6:612:CLA:HED1	2.56	0.41
17:6:81:VAL:HG11	17:6:136:ARG:CZ	2.51	0.41
17:6:195:PHE:CD2	38:6:502:LUT:H12	2.56	0.41
18:7:57:LEU:HD21	22:7:612:CLA:HBC3	2.03	0.41
18:7:192:GLN:NE2	38:7:501:LUT:H42	2.36	0.41
22:8:618:CLA:H3A	22:8:618:CLA:HBA1	1.81	0.41
1:A:13:VAL:HG13	1:A:193:ASN:HD22	1.86	0.41
1:A:680:ALA:CB	22:A:1013:CLA:HBB2	2.51	0.41
22:A:1108:CLA:O1D	14:3:299:GLY:HA3	2.21	0.41
2:B:55:LEU:HD22	2:B:150:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:TRP:HA	22:B:1204:CLA:HAB	2.03	0.41
22:B:1201:CLA:H71	10:M:30:TYR:CE1	2.56	0.41
22:B:1222:CLA:H51	22:B:1234:CLA:H2	2.02	0.41
22:1:608:CLA:H42	39:1:609:CHL:H93	2.03	0.41
15:4:37:GLU:OE1	15:4:37:GLU:HA	2.20	0.41
22:5:609:CLA:CBD	25:5:801:LHG:HC62	2.50	0.41
17:6:125:GLU:OE2	39:6:613:CHL:CMB	2.66	0.41
18:7:121:ASN:ND2	19:8:37:GLY:O	2.54	0.41
26:8:802:DGD:HA91	26:8:802:DGD:C1G	2.50	0.41
22:8:602:CLA:H41	22:8:602:CLA:H61	1.62	0.41
1:A:17:VAL:CG2	14:3:298:GLY:HA3	2.51	0.40
1:A:206:LEU:HD13	1:A:305:PHE:HE2	1.86	0.40
1:A:389:SER:OG	1:A:744:LEU:HD21	2.21	0.40
1:A:712:ALA:O	6:F:436:ILE:HG22	2.21	0.40
22:A:1131:CLA:H193	22:A:1131:CLA:H162	1.82	0.40
22:A:1136:CLA:H3A	22:A:1136:CLA:HBA2	1.79	0.40
22:A:1140:CLA:H92	6:F:451:LEU:HD22	2.03	0.40
22:B:1209:CLA:HED2	22:B:1210:CLA:HAC1	2.03	0.40
7:G:1230:ASP:O	7:G:1234:VAL:HG22	2.22	0.40
7:G:1234:VAL:HG23	7:G:1235:VAL:N	2.35	0.40
8:J:47:GLU:HA	8:J:47:GLU:OE1	2.21	0.40
10:M:14:LEU:HD23	10:M:14:LEU:HA	1.91	0.40
13:1:80:TRP:CE2	22:1:612:CLA:HBC3	2.56	0.40
13:1:122:ASP:O	13:1:126:LEU:HG	2.21	0.40
39:1:609:CHL:HMD2	24:8:503:BCR:HC21	2.03	0.40
15:4:69:TYR:C	22:4:604:CLA:HMA1	2.42	0.40
15:4:215:HIS:CG	22:4:603:CLA:HAA2	2.56	0.40
38:4:502:LUT:H11	38:4:502:LUT:H191	1.97	0.40
22:5:604:CLA:HMD2	22:5:609:CLA:HMD3	2.02	0.40
22:5:607:CLA:HBC1	25:5:801:LHG:H151	2.03	0.40
39:5:610:CHL:HBB2	22:5:612:CLA:CBC	2.50	0.40
17:6:38:ASN:ND2	17:6:43:SER:O	2.55	0.40
17:6:46:PRO:HD2	17:6:49:LEU:HB2	2.02	0.40
19:8:179:LEU:HD23	19:8:179:LEU:HA	1.80	0.40
1:A:198:LEU:HG	22:A:1123:CLA:HMD3	2.03	0.40
2:B:83:LEU:HD23	2:B:83:LEU:HA	1.85	0.40
2:B:423:LEU:HG	22:B:1236:CLA:CAB	2.51	0.40
2:B:524:ILE:HG21	22:B:1234:CLA:HAB	2.03	0.40
22:B:1218:CLA:HBA1	22:B:1218:CLA:H12	1.80	0.40
4:D:254:LYS:HE3	4:D:286:LEU:HD13	2.03	0.40
33:G:5001:SQD:H132	33:G:5001:SQD:H272	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:G:5001:SQD:H461	33:G:5001:SQD:H82	2.02	0.40
12:L:384:LEU:HD11	12:L:431:ALA:HB2	2.03	0.40
22:1:603:CLA:H91	22:1:603:CLA:H111	1.67	0.40
39:1:609:CHL:HMD2	24:8:503:BCR:C2	2.51	0.40
14:3:426:THR:HG22	14:3:428:GLU:H	1.85	0.40
16:5:32:LYS:HD3	16:5:33:LEU:N	2.36	0.40
16:5:252:LEU:HA	31:5:802:PTY:H122	2.04	0.40
17:6:184:GLU:HB2	22:6:601:CLA:C1B	2.51	0.40
17:6:255:PRO:HG2	25:6:802:LHG:H322	2.03	0.40
19:8:67:ASN:O	19:8:71:ASN:ND2	2.54	0.40
22:8:605:CLA:HHC	22:8:605:CLA:CBB	2.50	0.40
1:A:345:LEU:HD11	1:A:355:ILE:CD1	2.51	0.40
23:A:2001:PQN:H111	23:A:2001:PQN:H2M1	1.82	0.40
22:L:1503:CLA:HED2	22:L:1503:CLA:H2A	2.03	0.40
22:1:607:CLA:HAB	24:8:503:BCR:C31	2.51	0.40
22:1:612:CLA:H193	22:1:612:CLA:H161	1.66	0.40
15:4:129:MET:HE1	39:4:613:CHL:HED3	2.03	0.40
16:5:31:ARG:NE	16:5:31:ARG:HA	2.37	0.40
22:A:1119:CLA:H72	24:A:4004:BCR:H14C	2.03	0.40
22:A:1126:CLA:O1D	22:A:1127:CLA:HMA1	2.21	0.40
2:B:66:LEU:HD21	24:B:4003:BCR:H281	2.03	0.40
2:B:372:LEU:HD11	22:B:1225:CLA:HED3	2.03	0.40
22:B:1214:CLA:HBA2	22:B:1214:CLA:H3A	1.78	0.40
22:B:1231:CLA:H142	22:B:1231:CLA:H111	1.87	0.40
15:4:183:GLU:HB2	22:4:601:CLA:CHB	2.52	0.40
22:5:618:CLA:HHC	22:5:618:CLA:CBB	2.49	0.40
17:6:130:HIS:CD2	22:6:612:CLA:HMB1	2.56	0.40
19:8:120:PHE:CE1	47:8:808:4RF:H43	2.56	0.40
22:8:620:CLA:H12	22:8:620:CLA:H203	2.04	0.40
1:A:154:THR:HG21	1:A:228:LEU:HD11	2.03	0.40
1:A:178:TRP:HH2	31:3:802:PTY:H121	1.86	0.40
1:A:444:VAL:CG2	22:A:1137:CLA:HMC3	2.52	0.40
22:A:1121:CLA:H61	22:A:1121:CLA:H41	1.67	0.40
22:A:1131:CLA:H141	22:A:1131:CLA:H161	1.76	0.40
22:A:1133:CLA:C2D	22:A:1134:CLA:HAB	2.52	0.40
22:A:1136:CLA:H51	22:A:1136:CLA:H11	1.79	0.40
25:A:5002:LHG:H151	25:A:5002:LHG:H122	1.75	0.40
2:B:345:ILE:HG23	22:B:1215:CLA:H61	2.03	0.40
2:B:662:PHE:CE1	2:B:714:PHE:HE2	2.39	0.40
4:D:287:HIS:CB	4:D:288:PRO:HD3	2.52	0.40
25:1:801:LHG:HC81	25:1:801:LHG:H111	1.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:3:610:CLA:H62	22:3:610:CLA:H41	1.36	0.40
15:4:119:LYS:CD	22:4:610:CLA:HBC3	2.51	0.40
22:4:607:CLA:H8	22:4:607:CLA:H51	1.58	0.40
16:5:155:LEU:HD13	22:5:618:CLA:HBD	2.04	0.40
17:6:90:VAL:HG23	17:6:198:PHE:CE2	2.56	0.40
22:7:610:CLA:H41	22:7:610:CLA:H61	1.79	0.40
19:8:208:PHE:CE1	38:8:501:LUT:H41	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	739/741 (100%)	702 (95%)	36 (5%)	1 (0%)	51	85
2	B	729/731 (100%)	682 (94%)	47 (6%)	0	100	100
3	C	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
4	D	141/143 (99%)	131 (93%)	10 (7%)	0	100	100
5	E	62/64 (97%)	56 (90%)	6 (10%)	0	100	100
6	F	163/165 (99%)	150 (92%)	13 (8%)	0	100	100
7	G	97/99 (98%)	92 (95%)	4 (4%)	1 (1%)	15	54
8	J	39/41 (95%)	39 (100%)	0	0	100	100
9	K	84/86 (98%)	78 (93%)	6 (7%)	0	100	100
10	M	29/31 (94%)	29 (100%)	0	0	100	100
11	I	33/35 (94%)	31 (94%)	2 (6%)	0	100	100
12	L	136/157 (87%)	129 (95%)	7 (5%)	0	100	100
13	1	190/192 (99%)	167 (88%)	22 (12%)	1 (0%)	29	68
13	a	190/192 (99%)	164 (86%)	25 (13%)	1 (0%)	29	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	3	239/241 (99%)	219 (92%)	19 (8%)	1 (0%)	34	72
15	4	205/207 (99%)	188 (92%)	16 (8%)	1 (0%)	29	68
16	5	225/227 (99%)	201 (89%)	23 (10%)	1 (0%)	34	72
17	6	229/231 (99%)	208 (91%)	19 (8%)	2 (1%)	17	56
18	7	219/221 (99%)	198 (90%)	20 (9%)	1 (0%)	29	68
19	8	217/219 (99%)	194 (89%)	21 (10%)	2 (1%)	17	56
All	All	4044/4103 (99%)	3732 (92%)	300 (7%)	12 (0%)	44	76

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	1	36	TRP
17	6	46	PRO
18	7	131	PRO
19	8	45	ASP
13	a	107	VAL
14	3	280	LEU
15	4	230	SER
17	6	60	PHE
16	5	31	ARG
7	G	1230	ASP
1	A	122	VAL
19	8	46	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	600/600 (100%)	598 (100%)	2 (0%)	92	95
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	70 (99%)	1 (1%)	67	80
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	L	108/122 (88%)	108 (100%)	0	100	100
13	1	134/134 (100%)	134 (100%)	0	100	100
13	a	134/134 (100%)	133 (99%)	1 (1%)	84	90
14	3	186/186 (100%)	186 (100%)	0	100	100
15	4	165/165 (100%)	165 (100%)	0	100	100
16	5	183/183 (100%)	183 (100%)	0	100	100
17	6	187/187 (100%)	187 (100%)	0	100	100
18	7	176/176 (100%)	176 (100%)	0	100	100
19	8	168/168 (100%)	168 (100%)	0	100	100
All	All	3225/3239 (100%)	3221 (100%)	4 (0%)	93	97

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

Mol	Chain	Res	Type
1	A	37	ARG
1	A	421	ASN
7	G	1307	HIS
13	a	35	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	ASN
1	A	442	ASN
2	B	134	GLN
4	D	247	ASN
12	L	396	GLN
14	3	481	ASN

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Mol	Chain	Res	Type
15	4	112	ASN
16	5	107	ASN
16	5	117	ASN
16	5	205	GLN
19	8	76	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

337 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	$\# Z > 2$
39	CHL	4	613	-	52,60,74	1.07	3 (5%)	56,97,114	1.59	12 (21%)
39	CHL	5	613	-	56,64,74	0.90	2 (3%)	61,102,114	1.39	10 (16%)
22	CLA	a	608	-	55,63,73	1.47	8 (14%)	64,101,113	2.03	15 (23%)
24	BCR	A	4005	-	41,41,41	1.85	6 (14%)	56,56,56	4.26	15 (26%)
22	CLA	5	608	-	45,53,73	1.62	8 (17%)	52,89,113	2.19	15 (28%)
22	CLA	B	1216	-	61,69,73	1.41	7 (11%)	71,108,113	1.97	17 (23%)
22	CLA	A	1119	-	65,73,73	1.37	7 (10%)	76,113,113	1.82	16 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	LHG	4	801	22	48,48,48	0.40	0	51,54,54	1.07	3 (5%)
22	CLA	B	1211	-	55,63,73	1.49	7 (12%)	64,101,113	2.13	18 (28%)
22	CLA	K	1402	-	60,68,73	1.41	8 (13%)	70,107,113	2.08	18 (25%)
22	CLA	8	607	25	46,54,73	1.60	7 (15%)	53,90,113	2.11	11 (20%)
22	CLA	4	603	15	56,64,73	1.46	7 (12%)	65,102,113	2.15	17 (26%)
22	CLA	B	1234	-	56,64,73	1.50	7 (12%)	65,102,113	2.26	17 (26%)
22	CLA	5	616	-	46,54,73	1.62	8 (17%)	53,90,113	2.11	13 (24%)
22	CLA	6	603	-	65,73,73	1.37	9 (13%)	76,113,113	2.04	16 (21%)
22	CLA	a	612	13	57,65,73	1.47	6 (10%)	66,103,113	2.02	18 (27%)
22	CLA	1	603	-	65,73,73	1.34	7 (10%)	76,113,113	1.98	17 (22%)
39	CHL	3	608	-	43,51,74	1.07	3 (6%)	45,86,114	1.47	9 (20%)
22	CLA	F	1301	6	50,58,73	1.53	7 (14%)	58,95,113	2.29	17 (29%)
23	PQN	A	2001	-	34,34,34	0.34	0	42,45,45	1.27	4 (9%)
22	CLA	B	1203	-	65,73,73	1.37	7 (10%)	76,113,113	1.96	15 (19%)
25	LHG	7	801	22	48,48,48	0.37	0	51,54,54	1.23	4 (7%)
48	C7Z	7	504	-	43,43,43	5.33	27 (62%)	58,60,60	2.76	26 (44%)
22	CLA	B	1229	-	65,73,73	1.37	7 (10%)	76,113,113	1.98	18 (23%)
22	CLA	8	612	19	46,54,73	1.63	7 (15%)	53,90,113	2.08	12 (22%)
22	CLA	5	612	16	65,73,73	1.36	7 (10%)	76,113,113	1.93	13 (17%)
24	BCR	F	4001	-	41,41,41	1.89	5 (12%)	56,56,56	3.99	16 (28%)
22	CLA	1	601	13	60,68,73	1.41	8 (13%)	70,107,113	2.03	17 (24%)
40	OLA	8	809	-	19,19,19	0.56	0	19,19,19	1.07	0
31	PTY	3	802	-	37,37,49	1.00	4 (10%)	40,42,54	1.09	2 (5%)
22	CLA	6	615	-	65,73,73	1.37	8 (12%)	76,113,113	1.98	18 (23%)
22	CLA	K	1401	-	46,54,73	1.62	8 (17%)	53,90,113	2.05	12 (22%)
25	LHG	3	801	22	48,48,48	0.40	0	51,54,54	1.05	3 (5%)
22	CLA	B	1201	-	65,73,73	1.35	8 (12%)	76,113,113	2.08	23 (30%)
22	CLA	4	605	-	46,54,73	1.60	7 (15%)	53,90,113	2.25	17 (32%)
22	CLA	6	606	-	52,60,73	1.52	7 (13%)	60,97,113	2.15	17 (28%)
22	CLA	3	603	-	65,73,73	1.37	8 (12%)	76,113,113	1.95	14 (18%)
22	CLA	A	1103	-	65,73,73	1.35	7 (10%)	76,113,113	2.07	18 (23%)
22	CLA	A	1137	-	60,68,73	1.40	7 (11%)	70,107,113	2.06	20 (28%)
22	CLA	8	618	-	60,68,73	1.42	7 (11%)	70,107,113	2.08	17 (24%)
30	PCW	6	803	-	35,35,53	1.28	4 (11%)	41,43,61	1.13	2 (4%)
38	LUT	1	501	-	42,43,43	2.40	1 (2%)	51,60,60	2.02	17 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	A	1129	-	50,58,73	1.57	7 (14%)	58,95,113	2.27	17 (29%)
22	CLA	B	1232	-	45,53,73	1.66	8 (17%)	52,89,113	2.07	11 (21%)
22	CLA	A	1104	-	65,73,73	1.36	7 (10%)	76,113,113	2.02	18 (23%)
29	LMT	1	804	-	36,36,36	1.18	6 (16%)	47,47,47	1.05	1 (2%)
24	BCR	4	503	-	41,41,41	1.86	5 (12%)	56,56,56	4.38	12 (21%)
24	BCR	L	4001	-	41,41,41	1.87	4 (9%)	56,56,56	4.26	18 (32%)
22	CLA	1	602	-	45,53,73	1.59	7 (15%)	52,89,113	2.10	12 (23%)
25	LHG	a	801	-	34,34,48	0.47	0	37,40,54	1.31	5 (13%)
22	CLA	1	605	-	65,73,73	1.34	7 (10%)	76,113,113	2.11	20 (26%)
43	PLM	6	804	-	17,17,17	0.56	0	17,17,17	1.12	0
22	CLA	A	1126	-	65,73,73	1.40	8 (12%)	76,113,113	2.00	15 (19%)
22	CLA	8	606	-	57,65,73	1.46	7 (12%)	66,103,113	2.20	18 (27%)
45	SPH	6	806	-	19,20,20	0.61	0	18,21,21	1.13	1 (5%)
36	LPX	J	5001	-	16,16,29	1.32	2 (12%)	18,20,33	1.06	2 (11%)
22	CLA	6	607	25	55,63,73	1.49	8 (14%)	64,101,113	2.07	16 (25%)
25	LHG	F	5002	-	35,35,48	0.45	0	38,41,54	1.22	4 (10%)
22	CLA	A	1138	-	65,73,73	1.37	8 (12%)	76,113,113	2.10	18 (23%)
22	CLA	1	607	-	65,73,73	1.35	7 (10%)	76,113,113	1.94	16 (21%)
22	CLA	K	1403	9	46,54,73	1.63	8 (17%)	53,90,113	2.12	11 (20%)
22	CLA	7	612	-	60,68,73	1.49	8 (13%)	70,107,113	2.03	17 (24%)
22	CLA	A	1125	-	65,73,73	1.43	8 (12%)	76,113,113	2.26	19 (25%)
22	CLA	5	617	-	50,58,73	1.55	7 (14%)	58,95,113	2.31	17 (29%)
22	CLA	7	604	-	65,73,73	1.35	8 (12%)	76,113,113	2.00	22 (28%)
22	CLA	B	1022	-	65,73,73	1.42	7 (10%)	76,113,113	1.90	16 (21%)
22	CLA	4	611	-	56,64,73	1.46	7 (12%)	65,102,113	2.09	17 (26%)
39	CHL	4	618	15	56,64,74	1.07	4 (7%)	61,102,114	1.36	11 (18%)
22	CLA	A	1114	-	65,73,73	1.40	7 (10%)	76,113,113	2.03	20 (26%)
33	SQD	7	805	-	38,39,54	0.90	0	47,50,65	1.01	3 (6%)
33	SQD	G	5001	-	45,46,54	0.82	0	54,57,65	0.95	2 (3%)
22	CLA	B	1231	-	65,73,73	1.38	7 (10%)	76,113,113	2.00	16 (21%)
44	DGA	5	803	-	22,22,43	1.43	3 (13%)	24,24,45	1.38	2 (8%)
22	CLA	4	602	15	52,60,73	1.51	7 (13%)	60,97,113	2.20	18 (30%)
31	PTY	8	810	-	34,34,49	1.02	3 (8%)	37,39,54	1.33	3 (8%)
24	BCR	B	4005	-	41,41,41	1.89	6 (14%)	56,56,56	4.28	20 (35%)
22	CLA	a	605	-	65,73,73	1.33	7 (10%)	76,113,113	2.00	20 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	1222	-	58,66,73	1.45	7 (12%)	67,104,113	2.10	15 (22%)
22	CLA	1	604	-	65,73,73	1.40	8 (12%)	76,113,113	1.98	18 (23%)
22	CLA	A	1105	-	57,65,73	1.46	8 (14%)	66,103,113	2.12	19 (28%)
27	3PH	A	5007	-	32,32,47	1.01	4 (12%)	36,37,52	1.20	2 (5%)
22	CLA	A	1121	-	57,65,73	1.47	8 (14%)	66,103,113	2.25	18 (27%)
26	DGD	A	5005	-	52,52,67	0.92	4 (7%)	66,66,81	1.13	5 (7%)
22	CLA	A	1113	-	52,60,73	1.52	7 (13%)	60,97,113	2.26	19 (31%)
39	CHL	3	611	-	55,63,74	1.15	4 (7%)	59,100,114	1.44	11 (18%)
22	CLA	B	1226	-	65,73,73	1.37	7 (10%)	76,113,113	1.99	14 (18%)
24	BCR	B	4003	-	41,41,41	1.84	5 (12%)	56,56,56	4.49	18 (32%)
22	CLA	a	615	13	46,54,73	1.59	7 (15%)	53,90,113	2.12	16 (30%)
22	CLA	5	614	-	46,54,73	1.59	8 (17%)	53,90,113	2.15	12 (22%)
46	XAT	7	502	-	39,47,47	0.78	1 (2%)	54,74,74	1.98	12 (22%)
22	CLA	7	610	-	55,63,73	1.48	7 (12%)	64,101,113	2.06	18 (28%)
22	CLA	8	610	-	55,63,73	1.48	7 (12%)	64,101,113	2.14	19 (29%)
25	LHG	B	5002	-	48,48,48	0.41	0	51,54,54	0.96	3 (5%)
24	BCR	6	504	-	41,41,41	1.86	6 (14%)	56,56,56	4.27	20 (35%)
31	PTY	B	5005	-	40,40,49	0.94	4 (10%)	43,45,54	1.17	2 (4%)
22	CLA	A	1136	-	65,73,73	1.37	7 (10%)	76,113,113	1.97	15 (19%)
22	CLA	A	1108	-	65,73,73	1.38	7 (10%)	76,113,113	2.10	15 (19%)
22	CLA	B	1209	-	65,73,73	1.37	8 (12%)	76,113,113	2.08	19 (25%)
22	CLA	3	602	14	46,54,73	1.58	7 (15%)	53,90,113	2.22	17 (32%)
31	PTY	7	804	-	32,32,49	1.06	4 (12%)	35,37,54	1.20	2 (5%)
22	CLA	3	604	-	60,68,73	1.42	7 (11%)	70,107,113	2.13	20 (28%)
22	CLA	8	611	-	50,58,73	1.51	7 (14%)	58,95,113	2.32	17 (29%)
22	CLA	A	1135	-	65,73,73	1.36	7 (10%)	76,113,113	1.95	18 (23%)
35	RRX	J	4002	-	42,42,42	4.86	24 (57%)	57,58,58	2.45	20 (35%)
22	CLA	7	603	-	65,73,73	1.37	7 (10%)	76,113,113	1.98	15 (19%)
22	CLA	6	602	17	52,60,73	1.51	8 (15%)	60,97,113	2.21	17 (28%)
24	BCR	B	4004	-	41,41,41	1.85	4 (9%)	56,56,56	4.36	20 (35%)
22	CLA	A	1139	-	55,63,73	1.53	7 (12%)	64,101,113	2.08	17 (26%)
22	CLA	6	604	-	65,73,73	1.33	7 (10%)	76,113,113	2.16	23 (30%)
22	CLA	7	608	-	42,50,73	1.69	7 (16%)	48,85,113	2.28	12 (25%)
22	CLA	5	606	-	50,58,73	1.56	7 (14%)	58,95,113	2.22	18 (31%)
22	CLA	A	1123	-	65,73,73	1.34	7 (10%)	76,113,113	2.05	19 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	L	4002	-	41,41,41	1.81	4 (9%)	56,56,56	4.41	17 (30%)
32	LAP	K	5001	-	28,28,28	1.26	3 (10%)	33,35,35	1.06	2 (6%)
32	LAP	B	5007	-	28,28,28	1.21	3 (10%)	33,35,35	0.96	1 (3%)
21	CL0	A	1011	-	65,73,73	2.31	17 (26%)	76,113,113	2.54	24 (31%)
40	OLA	1	803	-	19,19,19	0.56	0	19,19,19	1.06	1 (5%)
22	CLA	4	612	15	62,70,73	1.39	9 (14%)	72,109,113	2.13	19 (26%)
22	CLA	G	1602	-	46,54,73	1.61	8 (17%)	53,90,113	2.10	15 (28%)
22	CLA	1	606	-	57,65,73	1.45	8 (14%)	66,103,113	2.14	18 (27%)
22	CLA	6	612	-	50,58,73	1.52	7 (14%)	58,95,113	2.30	17 (29%)
26	DGD	8	802	-	67,67,67	1.18	7 (10%)	81,81,81	1.11	5 (6%)
22	CLA	A	1117	-	65,73,73	1.36	7 (10%)	76,113,113	2.00	16 (21%)
22	CLA	B	1206	2	55,63,73	1.51	8 (14%)	64,101,113	2.20	18 (28%)
22	CLA	A	1128	-	65,73,73	1.41	7 (10%)	76,113,113	2.08	18 (23%)
39	CHL	4	609	15	66,74,74	0.90	3 (4%)	73,114,114	1.42	13 (17%)
22	CLA	4	616	-	50,58,73	1.57	8 (16%)	58,95,113	2.22	16 (27%)
24	BCR	A	4003	-	41,41,41	1.85	5 (12%)	56,56,56	4.32	16 (28%)
24	BCR	A	4004	-	41,41,41	1.93	6 (14%)	56,56,56	4.50	15 (26%)
22	CLA	5	602	-	52,60,73	1.54	7 (13%)	60,97,113	2.20	17 (28%)
41	QTB	3	506	-	19,19,19	2.67	6 (31%)	20,26,26	2.78	8 (40%)
26	DGD	B	5003	-	67,67,67	1.18	7 (10%)	81,81,81	1.08	4 (4%)
22	CLA	B	1214	-	62,70,73	1.41	7 (11%)	72,109,113	1.98	18 (25%)
22	CLA	B	1215	-	60,68,73	1.42	7 (11%)	70,107,113	1.94	16 (22%)
22	CLA	A	1130	-	56,64,73	1.46	7 (12%)	65,102,113	2.08	16 (24%)
38	LUT	8	502	-	42,43,43	2.33	1 (2%)	51,60,60	1.91	14 (27%)
22	CLA	5	604	-	65,73,73	1.36	7 (10%)	76,113,113	2.04	20 (26%)
38	LUT	1	503	-	42,43,43	2.41	1 (2%)	51,60,60	2.31	13 (25%)
39	CHL	8	601	19	61,69,74	1.08	6 (9%)	67,108,114	1.30	8 (11%)
39	CHL	8	613	-	51,59,74	1.11	4 (7%)	55,96,114	1.43	8 (14%)
22	CLA	B	1223	-	65,73,73	1.35	8 (12%)	76,113,113	2.00	17 (22%)
22	CLA	B	1213	-	60,68,73	1.46	8 (13%)	70,107,113	2.06	18 (25%)
24	BCR	G	4001	-	41,41,41	1.86	4 (9%)	56,56,56	4.29	19 (33%)
25	LHG	A	5003	-	41,41,48	0.43	0	44,47,54	1.16	3 (6%)
24	BCR	5	504	-	41,41,41	1.85	6 (14%)	56,56,56	4.18	18 (32%)
22	CLA	6	618	-	46,54,73	1.57	7 (15%)	53,90,113	2.20	13 (24%)
24	BCR	B	4006	-	41,41,41	1.81	5 (12%)	56,56,56	4.34	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	CHL	5	611	-	51,59,74	1.13	5 (9%)	55,96,114	1.43	11 (20%)
22	CLA	3	606	-	65,73,73	1.37	7 (10%)	76,113,113	1.99	16 (21%)
24	BCR	6	503	-	41,41,41	1.89	5 (12%)	56,56,56	4.32	15 (26%)
24	BCR	K	4002	-	41,41,41	1.88	5 (12%)	56,56,56	4.14	15 (26%)
22	CLA	B	1023	-	65,73,73	1.35	7 (10%)	76,113,113	2.01	18 (23%)
22	CLA	B	1230	-	58,66,73	1.43	7 (12%)	67,104,113	2.19	19 (28%)
22	CLA	4	615	15	60,68,73	1.42	7 (11%)	70,107,113	2.06	19 (27%)
38	LUT	5	505	-	42,43,43	2.42	2 (4%)	51,60,60	2.72	19 (37%)
22	CLA	A	1109	22	65,73,73	1.33	8 (12%)	76,113,113	2.14	19 (25%)
47	4RF	8	808	-	53,53,56	0.90	5 (9%)	56,56,59	1.04	3 (5%)
22	CLA	A	1116	-	60,68,73	1.45	7 (11%)	70,107,113	2.13	19 (27%)
22	CLA	1	610	-	45,53,73	1.63	7 (15%)	52,89,113	2.16	14 (26%)
24	BCR	A	4001	-	41,41,41	1.79	5 (12%)	56,56,56	4.02	18 (32%)
39	CHL	a	609	13	53,61,74	1.03	4 (7%)	57,98,114	1.42	11 (19%)
25	LHG	A	5002	-	48,48,48	0.39	0	51,54,54	1.04	3 (5%)
22	CLA	B	1237	-	65,73,73	1.39	7 (10%)	76,113,113	1.98	18 (23%)
22	CLA	B	1212	-	65,73,73	1.39	8 (12%)	76,113,113	2.07	19 (25%)
22	CLA	8	608	-	52,60,73	1.53	7 (13%)	60,97,113	2.37	19 (31%)
38	LUT	4	502	-	42,43,43	2.33	1 (2%)	51,60,60	1.92	12 (23%)
22	CLA	5	603	-	56,64,73	1.45	8 (14%)	65,102,113	2.18	17 (26%)
38	LUT	4	501	-	42,43,43	2.28	1 (2%)	51,60,60	1.94	15 (29%)
22	CLA	A	1122	-	65,73,73	1.38	8 (12%)	76,113,113	1.93	14 (18%)
22	CLA	8	620	19	65,73,73	1.34	7 (10%)	76,113,113	1.99	19 (25%)
25	LHG	4	802	-	31,31,48	0.45	0	34,37,54	1.16	2 (5%)
42	GG0	a	805	-	7,8,8	1.37	2 (28%)	6,9,9	0.80	0
25	LHG	B	5001	22	45,45,48	0.41	0	48,51,54	1.05	3 (6%)
28	SF4	A	3001	1,2	0,12,12	-	-	-	-	-
38	LUT	6	502	-	42,43,43	2.32	2 (4%)	51,60,60	2.29	13 (25%)
22	CLA	1	608	-	60,68,73	1.43	8 (13%)	70,107,113	2.02	16 (22%)
22	CLA	1	611	-	55,63,73	1.49	8 (14%)	64,101,113	2.07	18 (28%)
25	LHG	6	802	-	36,36,48	0.43	0	39,42,54	1.17	3 (7%)
39	CHL	6	613	-	51,59,74	0.91	2 (3%)	55,96,114	1.45	11 (20%)
39	CHL	6	610	-	56,64,74	0.92	3 (5%)	61,102,114	1.42	11 (18%)
38	LUT	3	501	-	42,43,43	2.35	1 (2%)	51,60,60	2.08	15 (29%)
22	CLA	3	601	-	65,73,73	1.35	7 (10%)	76,113,113	2.04	18 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	3	613	-	61,69,73	1.41	7 (11%)	71,108,113	2.00	15 (21%)
25	LHG	F	5001	22	42,42,48	0.42	0	45,48,54	1.13	3 (6%)
39	CHL	8	604	19	62,70,74	1.06	5 (8%)	68,109,114	1.32	9 (13%)
22	CLA	B	1218	-	55,63,73	1.47	8 (14%)	64,101,113	2.24	19 (29%)
22	CLA	a	601	13	60,68,73	1.40	7 (11%)	70,107,113	2.07	19 (27%)
24	BCR	J	4001	-	41,41,41	1.84	5 (12%)	56,56,56	4.37	16 (28%)
47	4RF	8	807	-	41,41,56	1.00	6 (14%)	44,44,59	1.08	3 (6%)
22	CLA	3	610	14	60,68,73	1.41	7 (11%)	70,107,113	2.05	17 (24%)
36	LPX	a	804	-	29,29,29	1.01	2 (6%)	31,33,33	0.92	1 (3%)
22	CLA	4	607	25	55,63,73	1.49	8 (14%)	64,101,113	2.10	15 (23%)
38	LUT	a	503	-	42,43,43	2.38	1 (2%)	51,60,60	2.19	15 (29%)
24	BCR	7	503	-	41,41,41	1.83	5 (12%)	56,56,56	4.31	13 (23%)
24	BCR	8	503	-	41,41,41	1.88	4 (9%)	56,56,56	4.25	17 (30%)
22	CLA	B	1227	-	50,58,73	1.52	8 (16%)	58,95,113	2.24	19 (32%)
22	CLA	a	603	-	65,73,73	1.38	7 (10%)	76,113,113	2.03	18 (23%)
22	CLA	A	1133	-	65,73,73	1.37	7 (10%)	76,113,113	1.95	16 (21%)
22	CLA	A	1102	22	65,73,73	1.36	8 (12%)	76,113,113	2.28	18 (23%)
38	LUT	7	501	-	42,43,43	2.37	2 (4%)	51,60,60	1.97	15 (29%)
38	LUT	a	501	-	42,43,43	2.36	1 (2%)	51,60,60	2.24	16 (31%)
22	CLA	B	1208	-	60,68,73	1.41	7 (11%)	70,107,113	2.14	21 (30%)
38	LUT	5	502	-	42,43,43	2.35	2 (4%)	51,60,60	2.05	13 (25%)
22	CLA	A	1134	1	60,68,73	1.41	7 (11%)	70,107,113	2.07	17 (24%)
22	CLA	8	602	19	52,60,73	1.54	7 (13%)	60,97,113	2.13	16 (26%)
32	LAP	F	5003	-	28,28,28	1.24	3 (10%)	33,35,35	0.93	1 (3%)
22	CLA	A	1112	-	55,63,73	1.49	9 (16%)	64,101,113	2.24	19 (29%)
22	CLA	A	1131	-	65,73,73	1.40	7 (10%)	76,113,113	1.96	16 (21%)
22	CLA	6	608	-	45,53,73	1.62	7 (15%)	52,89,113	2.19	15 (28%)
22	CLA	7	607	25	59,67,73	1.45	7 (11%)	68,105,113	2.03	14 (20%)
22	CLA	7	601	-	60,68,73	1.42	8 (13%)	70,107,113	2.05	20 (28%)
22	CLA	B	1219	-	59,67,73	1.44	7 (11%)	68,105,113	2.09	16 (23%)
22	CLA	B	1202	-	65,73,73	1.35	7 (10%)	76,113,113	2.00	15 (19%)
22	CLA	A	1124	-	55,63,73	1.51	7 (12%)	64,101,113	2.07	16 (25%)
22	CLA	B	1240	25	65,73,73	1.39	7 (10%)	76,113,113	1.99	16 (21%)
24	BCR	3	505	-	41,41,41	1.89	4 (9%)	56,56,56	4.12	17 (30%)
22	CLA	6	601	-	60,68,73	1.42	7 (11%)	70,107,113	2.13	17 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	3	607	25	65,73,73	1.33	6 (9%)	76,113,113	2.04	17 (22%)
22	CLA	A	1132	-	65,73,73	1.37	7 (10%)	76,113,113	2.05	18 (23%)
22	CLA	B	1210	-	65,73,73	1.38	8 (12%)	76,113,113	2.18	18 (23%)
38	LUT	3	502	-	42,43,43	2.36	1 (2%)	51,60,60	2.01	12 (23%)
39	CHL	6	619	17	66,74,74	0.89	3 (4%)	73,114,114	1.29	11 (15%)
22	CLA	B	1221	-	65,73,73	1.36	8 (12%)	76,113,113	2.07	17 (22%)
41	QTB	a	504	-	19,19,19	2.62	5 (26%)	20,26,26	2.82	10 (50%)
22	CLA	1	615	13	46,54,73	1.60	7 (15%)	53,90,113	2.12	13 (24%)
22	CLA	B	1236	-	53,61,73	1.52	7 (13%)	61,98,113	2.35	18 (29%)
24	BCR	B	4007	-	41,41,41	1.84	5 (12%)	56,56,56	4.14	16 (28%)
22	CLA	a	604	13	65,73,73	1.36	8 (12%)	76,113,113	2.05	19 (25%)
22	CLA	7	605	-	43,52,73	1.68	8 (18%)	49,88,113	2.13	12 (24%)
22	CLA	5	601	16	60,68,73	1.40	7 (11%)	70,107,113	2.10	21 (30%)
23	PQN	B	2002	-	34,34,34	0.41	0	42,45,45	1.28	4 (9%)
22	CLA	B	1239	-	65,73,73	1.39	7 (10%)	76,113,113	1.95	16 (21%)
22	CLA	B	1217	-	56,64,73	1.45	7 (12%)	65,102,113	2.11	15 (23%)
28	SF4	C	3002	3	0,12,12	-	-	-	-	-
29	LMT	A	5008	-	36,36,36	1.12	5 (13%)	47,47,47	1.04	3 (6%)
22	CLA	A	1140	-	55,63,73	1.50	9 (16%)	64,101,113	2.07	14 (21%)
39	CHL	a	613	-	46,54,74	1.01	3 (6%)	49,90,114	1.52	10 (20%)
22	CLA	5	607	25	55,63,73	1.49	7 (12%)	64,101,113	2.02	15 (23%)
29	LMT	B	5006	-	36,36,36	1.18	5 (13%)	47,47,47	1.01	2 (4%)
22	CLA	A	1101	-	65,73,73	1.36	7 (10%)	76,113,113	2.05	17 (22%)
25	LHG	1	802	-	41,41,48	0.42	0	44,47,54	1.07	4 (9%)
34	ERG	G	5002	-	31,32,32	8.20	18 (58%)	47,50,50	3.19	21 (44%)
49	P5S	8	806	-	35,36,53	1.17	3 (8%)	39,43,60	1.18	3 (7%)
39	CHL	1	613	-	48,56,74	1.00	3 (6%)	51,92,114	1.36	9 (17%)
22	CLA	8	605	-	45,53,73	1.66	7 (15%)	52,89,113	2.09	13 (25%)
22	CLA	A	1127	-	65,73,73	1.40	7 (10%)	76,113,113	1.89	14 (18%)
22	CLA	A	1107	1	55,63,73	1.46	8 (14%)	64,101,113	2.18	18 (28%)
24	BCR	A	4002	-	41,41,41	1.85	6 (14%)	56,56,56	4.31	16 (28%)
22	CLA	L	1502	-	60,68,73	1.41	8 (13%)	70,107,113	2.16	17 (24%)
25	LHG	A	5001	22	28,28,48	0.51	0	31,34,54	1.34	3 (9%)
39	CHL	a	606	-	56,64,74	1.00	3 (5%)	61,102,114	1.32	11 (18%)
25	LHG	6	801	22	48,48,48	0.40	0	51,54,54	1.12	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	A	1111	-	65,73,73	1.37	7 (10%)	76,113,113	2.01	20 (26%)
22	CLA	J	1901	8	42,50,73	1.62	7 (16%)	48,85,113	2.23	13 (27%)
22	CLA	a	607	-	58,66,73	1.44	8 (13%)	67,104,113	2.18	16 (23%)
22	CLA	F	1302	25	55,63,73	1.47	6 (10%)	64,101,113	2.27	20 (31%)
22	CLA	B	1204	-	65,73,73	1.39	7 (10%)	76,113,113	2.01	17 (22%)
22	CLA	A	1110	-	60,68,73	1.43	8 (13%)	70,107,113	2.03	16 (22%)
22	CLA	B	1205	-	65,73,73	1.36	7 (10%)	76,113,113	2.08	16 (21%)
22	CLA	7	609	-	60,68,73	1.41	7 (11%)	70,107,113	2.10	18 (25%)
25	LHG	7	802	-	35,35,48	0.45	0	38,41,54	1.15	3 (7%)
22	CLA	A	1120	-	49,57,73	1.56	8 (16%)	55,93,113	2.35	17 (30%)
22	CLA	4	617	-	45,53,73	1.62	7 (15%)	52,89,113	2.19	15 (28%)
22	CLA	A	1118	-	55,63,73	1.48	7 (12%)	64,101,113	2.16	15 (23%)
39	CHL	7	613	-	66,74,74	0.95	3 (4%)	73,114,114	1.31	13 (17%)
22	CLA	7	602	-	44,52,73	1.66	7 (15%)	49,87,113	2.20	15 (30%)
24	BCR	3	503	-	41,41,41	1.88	6 (14%)	56,56,56	4.07	18 (32%)
22	CLA	B	1220	-	60,68,73	1.45	7 (11%)	70,107,113	2.10	15 (21%)
22	CLA	4	610	-	65,73,73	1.37	8 (12%)	76,113,113	2.02	17 (22%)
22	CLA	3	605	-	65,73,73	1.37	7 (10%)	76,113,113	2.06	17 (22%)
47	4RF	7	807	-	31,31,56	1.16	6 (19%)	34,34,59	1.17	3 (8%)
25	LHG	1	801	-	34,34,48	0.45	0	37,40,54	1.25	4 (10%)
25	LHG	5	801	22	48,48,48	0.39	0	51,54,54	1.04	3 (5%)
22	CLA	6	605	-	46,54,73	1.59	8 (17%)	53,90,113	2.19	14 (26%)
22	CLA	6	617	17	45,53,73	1.60	7 (15%)	52,89,113	2.14	15 (28%)
22	CLA	B	1235	-	65,73,73	1.38	8 (12%)	76,113,113	2.05	16 (21%)
22	CLA	B	1228	-	65,73,73	1.41	10 (15%)	76,113,113	2.89	24 (31%)
22	CLA	4	606	-	50,58,73	1.53	7 (14%)	58,95,113	2.23	17 (29%)
22	CLA	B	1225	-	65,73,73	1.40	7 (10%)	76,113,113	1.90	14 (18%)
24	BCR	K	4001	-	41,41,41	1.86	4 (9%)	56,56,56	4.34	17 (30%)
38	LUT	6	501	-	42,43,43	2.36	1 (2%)	51,60,60	2.26	15 (29%)
22	CLA	5	618	16	52,60,73	1.53	8 (15%)	60,97,113	2.13	19 (31%)
37	ECH	M	4001	-	42,42,42	1.19	3 (7%)	55,58,58	2.03	15 (27%)
22	CLA	B	1021	-	65,73,73	1.41	7 (10%)	76,113,113	1.95	16 (21%)
22	CLA	G	1603	-	45,53,73	1.61	8 (17%)	52,89,113	2.06	12 (23%)
22	CLA	4	601	-	60,68,73	1.42	6 (10%)	70,107,113	2.09	18 (25%)
22	CLA	3	616	-	56,64,73	1.48	7 (12%)	65,102,113	2.05	17 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PTY	5	802	-	37,37,49	0.98	4 (10%)	40,42,54	1.18	2 (5%)
43	PLM	4	803	-	16,16,17	0.44	0	15,15,17	0.69	0
22	CLA	5	605	-	46,54,73	1.63	7 (15%)	53,90,113	2.13	15 (28%)
39	CHL	1	609	13	66,74,74	0.97	6 (9%)	73,114,114	1.33	12 (16%)
22	CLA	8	615	-	46,54,73	1.59	7 (15%)	53,90,113	2.13	15 (28%)
22	CLA	7	611	-	60,68,73	1.37	8 (13%)	70,107,113	2.21	22 (31%)
22	CLA	L	1501	-	50,58,73	1.56	8 (16%)	58,95,113	2.38	18 (31%)
22	CLA	A	1115	-	60,68,73	1.44	8 (13%)	70,107,113	2.06	17 (24%)
22	CLA	L	1503	-	45,53,73	1.65	9 (20%)	52,89,113	2.32	20 (38%)
38	LUT	8	501	-	42,43,43	2.37	2 (4%)	51,60,60	1.83	14 (27%)
22	CLA	1	612	13	65,73,73	1.36	7 (10%)	76,113,113	1.95	15 (19%)
22	CLA	6	609	17	65,73,73	1.34	8 (12%)	76,113,113	1.99	16 (21%)
24	BCR	5	503	-	41,41,41	1.85	5 (12%)	56,56,56	4.32	18 (32%)
25	LHG	8	801	22	36,36,48	0.46	0	39,42,54	1.22	4 (10%)
38	LUT	5	501	-	42,43,43	2.37	1 (2%)	51,60,60	2.03	15 (29%)
22	CLA	B	1224	-	65,73,73	1.38	8 (12%)	76,113,113	1.98	17 (22%)
22	CLA	3	618	-	46,54,73	1.64	8 (17%)	53,90,113	2.12	12 (22%)
22	CLA	8	603	19	65,73,73	1.36	8 (12%)	76,113,113	2.14	19 (25%)
24	BCR	L	4003	-	41,41,41	1.88	4 (9%)	56,56,56	4.35	15 (26%)
28	SF4	C	3003	3	0,12,12	-	-	-	-	-
25	LHG	7	803	-	42,42,48	0.39	0	45,48,54	1.07	2 (4%)
24	BCR	3	504	-	41,41,41	1.85	4 (9%)	56,56,56	4.26	15 (26%)
22	CLA	A	1141	25	45,53,73	1.62	8 (17%)	52,89,113	2.17	12 (23%)
22	CLA	8	609	19	60,68,73	1.42	7 (11%)	70,107,113	2.06	15 (21%)
39	CHL	6	611	-	51,59,74	1.07	3 (5%)	55,96,114	1.46	9 (16%)
22	CLA	A	1106	1	65,73,73	1.34	7 (10%)	76,113,113	2.04	15 (19%)
22	CLA	a	611	-	50,58,73	1.56	7 (14%)	58,95,113	2.18	17 (29%)
22	CLA	5	609	16	51,59,73	1.54	8 (15%)	59,96,113	2.24	17 (28%)
38	LUT	a	502	-	42,43,43	2.37	2 (4%)	51,60,60	1.99	14 (27%)
22	CLA	A	1012	-	65,73,73	1.39	7 (10%)	76,113,113	1.92	14 (18%)
22	CLA	B	1207	-	60,68,73	1.43	7 (11%)	70,107,113	2.02	17 (24%)
44	DGA	8	803	-	29,29,43	1.25	2 (6%)	31,31,45	1.16	2 (6%)
22	CLA	a	602	-	50,58,73	1.56	8 (16%)	58,95,113	2.19	16 (27%)
22	CLA	3	612	-	65,73,73	1.37	7 (10%)	76,113,113	1.94	15 (19%)
38	LUT	1	502	-	42,43,43	2.28	1 (2%)	51,60,60	2.05	16 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	4	608	-	51,59,73	1.54	8 (15%)	59,96,113	2.26	18 (30%)
39	CHL	a	610	-	48,56,74	1.00	3 (6%)	51,92,114	1.45	11 (21%)
22	CLA	K	1404	9	52,60,73	1.53	9 (17%)	60,97,113	2.22	18 (30%)
39	CHL	5	610	-	66,74,74	0.89	3 (4%)	73,114,114	1.28	12 (16%)
22	CLA	G	1601	-	50,58,73	1.56	7 (14%)	58,95,113	2.23	17 (29%)
22	CLA	B	1238	-	65,73,73	1.36	7 (10%)	76,113,113	1.98	16 (21%)
30	PCW	B	5004	-	29,29,53	1.32	3 (10%)	35,37,61	0.95	1 (2%)
24	BCR	B	4002	-	41,41,41	1.86	4 (9%)	56,56,56	4.35	13 (23%)
22	CLA	A	1013	-	65,73,73	1.36	7 (10%)	76,113,113	2.00	20 (26%)
24	BCR	I	4001	-	41,41,41	1.84	4 (9%)	56,56,56	4.21	17 (30%)
22	CLA	7	606	-	55,63,73	1.45	7 (12%)	64,101,113	2.10	19 (29%)
22	CLA	4	604	15	60,68,73	1.44	9 (15%)	70,107,113	2.01	17 (24%)
24	BCR	B	4001	-	41,41,41	1.85	5 (12%)	56,56,56	4.28	16 (28%)
22	CLA	7	617	18	54,62,73	1.49	7 (12%)	63,100,113	2.16	16 (25%)
22	CLA	7	615	18	55,63,73	1.47	7 (12%)	64,101,113	2.02	15 (23%)

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
39	CHL	4	613	-	3/3/17/26	7/23/121/137	-
39	CHL	5	613	-	4/4/18/26	5/27/125/137	-
22	CLA	a	608	-	1/1/13/20	13/25/103/115	-
24	BCR	A	4005	-	-	16/29/63/63	0/2/2/2
22	CLA	5	608	-	1/1/11/20	6/13/91/115	-
22	CLA	B	1216	-	1/1/14/20	21/33/111/115	-
22	CLA	A	1119	-	1/1/15/20	17/37/115/115	-
25	LHG	4	801	22	-	37/53/53/53	-
22	CLA	B	1211	-	1/1/13/20	12/25/103/115	-
22	CLA	K	1402	-	1/1/14/20	13/31/109/115	-
22	CLA	8	607	25	1/1/11/20	6/15/93/115	-
22	CLA	4	603	15	1/1/13/20	14/27/105/115	-
22	CLA	B	1234	-	1/1/13/20	13/27/105/115	-
22	CLA	5	616	-	1/1/11/20	7/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	6	603	-	1/1/15/20	19/37/115/115	-
22	CLA	a	612	13	1/1/13/20	10/28/106/115	-
22	CLA	1	603	-	1/1/15/20	22/37/115/115	-
39	CHL	3	608	-	4/4/15/26	3/12/110/137	-
22	CLA	F	1301	6	1/1/12/20	6/19/97/115	-
23	PQN	A	2001	-	-	9/23/43/43	0/2/2/2
22	CLA	B	1203	-	1/1/15/20	17/37/115/115	-
25	LHG	7	801	22	-	27/53/53/53	-
48	C7Z	7	504	-	1/1/12/26	8/29/67/67	0/2/2/2
22	CLA	B	1229	-	1/1/15/20	11/37/115/115	-
22	CLA	8	612	19	1/1/11/20	8/15/93/115	-
22	CLA	5	612	16	1/1/15/20	20/37/115/115	-
24	BCR	F	4001	-	-	9/29/63/63	0/2/2/2
22	CLA	1	601	13	1/1/14/20	9/31/109/115	-
40	OLA	8	809	-	-	8/17/17/17	-
31	PTY	3	802	-	-	24/41/41/53	-
22	CLA	6	615	-	1/1/15/20	22/37/115/115	-
22	CLA	K	1401	-	1/1/11/20	7/15/93/115	-
25	LHG	3	801	22	-	33/53/53/53	-
22	CLA	B	1201	-	1/1/15/20	17/37/115/115	-
22	CLA	4	605	-	1/1/11/20	6/15/93/115	-
22	CLA	6	606	-	1/1/12/20	12/22/100/115	-
22	CLA	3	603	-	1/1/15/20	19/37/115/115	-
22	CLA	A	1103	-	1/1/15/20	16/37/115/115	-
22	CLA	A	1137	-	1/1/14/20	12/31/109/115	-
22	CLA	8	618	-	1/1/14/20	15/31/109/115	-
30	PCW	6	803	-	-	19/39/39/57	-
38	LUT	1	501	-	-	3/29/67/67	0/2/2/2
22	CLA	A	1129	-	1/1/12/20	12/19/97/115	-
22	CLA	B	1232	-	1/1/11/20	5/13/91/115	-
22	CLA	A	1104	-	1/1/15/20	19/37/115/115	-
29	LMT	1	804	-	-	10/21/61/61	0/2/2/2
24	BCR	4	503	-	-	15/29/63/63	0/2/2/2
24	BCR	L	4001	-	-	13/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	1	602	-	1/1/11/20	7/13/91/115	-
25	LHG	a	801	-	-	25/39/39/53	-
22	CLA	1	605	-	1/1/15/20	16/37/115/115	-
43	PLM	6	804	-	-	6/15/15/15	-
22	CLA	A	1126	-	1/1/15/20	24/37/115/115	-
22	CLA	8	606	-	1/1/13/20	14/28/106/115	-
45	SPH	6	806	-	-	13/21/21/21	-
36	LPX	J	5001	-	-	11/18/18/31	-
22	CLA	6	607	25	1/1/13/20	9/25/103/115	-
25	LHG	F	5002	-	-	28/40/40/53	-
22	CLA	A	1138	-	1/1/15/20	16/37/115/115	-
22	CLA	1	607	-	1/1/15/20	14/37/115/115	-
22	CLA	K	1403	9	1/1/11/20	8/15/93/115	-
22	CLA	7	612	-	1/1/14/20	19/31/109/115	-
22	CLA	A	1125	-	1/1/15/20	22/37/115/115	-
22	CLA	5	617	-	1/1/12/20	11/19/97/115	-
22	CLA	7	604	-	1/1/15/20	18/37/115/115	-
22	CLA	B	1022	-	1/1/15/20	13/37/115/115	-
22	CLA	4	611	-	1/1/13/20	9/27/105/115	-
39	CHL	4	618	15	4/4/18/26	7/27/125/137	-
22	CLA	A	1114	-	1/1/15/20	17/37/115/115	-
33	SQD	7	805	-	-	14/34/54/69	0/1/1/1
33	SQD	G	5001	-	-	21/41/61/69	0/1/1/1
22	CLA	B	1231	-	1/1/15/20	17/37/115/115	-
44	DGA	5	803	-	-	13/24/24/45	-
22	CLA	4	602	15	1/1/12/20	5/22/100/115	-
31	PTY	8	810	-	-	19/38/38/53	-
24	BCR	B	4005	-	-	12/29/63/63	0/2/2/2
22	CLA	a	605	-	1/1/15/20	10/37/115/115	-
22	CLA	B	1222	-	1/1/13/20	5/29/107/115	-
22	CLA	1	604	-	1/1/15/20	20/37/115/115	-
22	CLA	A	1105	-	1/1/13/20	8/28/106/115	-
27	3PH	A	5007	-	-	10/34/34/49	-
22	CLA	A	1121	-	1/1/13/20	14/28/106/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	DGD	A	5005	-	-	20/40/80/95	0/2/2/2
22	CLA	A	1113	-	1/1/12/20	11/22/100/115	-
39	CHL	3	611	-	3/3/17/26	4/26/124/137	-
22	CLA	B	1226	-	1/1/15/20	14/37/115/115	-
24	BCR	B	4003	-	-	7/29/63/63	0/2/2/2
22	CLA	a	615	13	1/1/11/20	5/15/93/115	-
22	CLA	5	614	-	1/1/11/20	4/15/93/115	-
46	XAT	7	502	-	3/3/12/26	1/31/93/93	0/4/4/4
22	CLA	7	610	-	1/1/13/20	10/25/103/115	-
22	CLA	8	610	-	1/1/13/20	15/25/103/115	-
25	LHG	B	5002	-	-	37/53/53/53	-
24	BCR	6	504	-	-	9/29/63/63	0/2/2/2
31	PTY	B	5005	-	-	22/44/44/53	-
22	CLA	A	1136	-	1/1/15/20	18/37/115/115	-
22	CLA	A	1108	-	1/1/15/20	17/37/115/115	-
22	CLA	B	1209	-	1/1/15/20	18/37/115/115	-
22	CLA	3	602	14	1/1/11/20	8/15/93/115	-
31	PTY	7	804	-	-	17/36/36/53	-
22	CLA	3	604	-	1/1/14/20	13/31/109/115	-
22	CLA	8	611	-	1/1/12/20	7/19/97/115	-
22	CLA	A	1135	-	1/1/15/20	20/37/115/115	-
35	RRX	J	4002	-	1/1/11/25	12/29/65/65	0/2/2/2
22	CLA	7	603	-	1/1/15/20	21/37/115/115	-
22	CLA	6	602	17	1/1/12/20	4/22/100/115	-
24	BCR	B	4004	-	-	11/29/63/63	0/2/2/2
22	CLA	A	1139	-	1/1/13/20	15/25/103/115	-
22	CLA	6	604	-	1/1/15/20	21/37/115/115	-
22	CLA	7	608	-	1/1/10/20	7/10/88/115	-
22	CLA	5	606	-	1/1/12/20	7/19/97/115	-
22	CLA	A	1123	-	1/1/15/20	15/37/115/115	-
24	BCR	L	4002	-	-	8/29/63/63	0/2/2/2
32	LAP	K	5001	-	-	19/30/30/30	-
32	LAP	B	5007	-	-	19/30/30/30	-
21	CL0	A	1011	-	3/3/20/25	13/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	OLA	1	803	-	-	8/17/17/17	-
22	CLA	4	612	15	1/1/14/20	16/34/112/115	-
22	CLA	G	1602	-	1/1/11/20	7/15/93/115	-
22	CLA	1	606	-	1/1/13/20	13/28/106/115	-
22	CLA	6	612	-	1/1/12/20	12/19/97/115	-
26	DGD	8	802	-	-	26/55/95/95	0/2/2/2
22	CLA	A	1117	-	1/1/15/20	21/37/115/115	-
22	CLA	B	1206	2	1/1/13/20	13/25/103/115	-
22	CLA	A	1128	-	1/1/15/20	15/37/115/115	-
39	CHL	4	609	15	4/4/20/26	19/39/137/137	-
22	CLA	4	616	-	1/1/12/20	8/19/97/115	-
24	BCR	A	4003	-	-	11/29/63/63	0/2/2/2
24	BCR	A	4004	-	-	12/29/63/63	0/2/2/2
22	CLA	5	602	-	1/1/12/20	8/22/100/115	-
41	QTB	3	506	-	2/2/5/10	3/11/28/28	0/1/1/1
26	DGD	B	5003	-	-	19/55/95/95	0/2/2/2
22	CLA	B	1214	-	1/1/14/20	19/34/112/115	-
22	CLA	B	1215	-	1/1/14/20	20/31/109/115	-
22	CLA	A	1130	-	1/1/13/20	11/27/105/115	-
38	LUT	8	502	-	-	3/29/67/67	0/2/2/2
22	CLA	5	604	-	1/1/15/20	12/37/115/115	-
38	LUT	1	503	-	1/1/12/27	8/29/67/67	0/2/2/2
39	CHL	8	601	19	4/4/19/26	10/33/131/137	-
39	CHL	8	613	-	3/3/17/26	2/21/119/137	-
22	CLA	B	1223	-	1/1/15/20	14/37/115/115	-
22	CLA	B	1213	-	1/1/14/20	17/31/109/115	-
24	BCR	G	4001	-	-	10/29/63/63	0/2/2/2
25	LHG	A	5003	-	-	31/46/46/53	-
24	BCR	5	504	-	-	9/29/63/63	0/2/2/2
22	CLA	6	618	-	1/1/11/20	9/15/93/115	-
24	BCR	B	4006	-	-	13/29/63/63	0/2/2/2
39	CHL	5	611	-	3/3/17/26	6/21/119/137	-
22	CLA	3	606	-	1/1/15/20	12/37/115/115	-
24	BCR	6	503	-	-	14/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	K	4002	-	-	12/29/63/63	0/2/2/2
22	CLA	B	1023	-	1/1/15/20	19/37/115/115	-
22	CLA	B	1230	-	1/1/13/20	13/29/107/115	-
22	CLA	4	615	15	1/1/14/20	14/31/109/115	-
38	LUT	5	505	-	1/1/12/27	9/29/67/67	0/2/2/2
22	CLA	A	1109	22	1/1/15/20	23/37/115/115	-
47	4RF	8	808	-	-	25/56/56/59	-
22	CLA	A	1116	-	1/1/14/20	16/31/109/115	-
22	CLA	1	610	-	1/1/11/20	4/13/91/115	-
24	BCR	A	4001	-	-	10/29/63/63	0/2/2/2
39	CHL	a	609	13	3/3/17/26	4/24/122/137	-
25	LHG	A	5002	-	-	34/53/53/53	-
22	CLA	B	1237	-	1/1/15/20	17/37/115/115	-
22	CLA	B	1212	-	1/1/15/20	21/37/115/115	-
22	CLA	8	608	-	1/1/12/20	12/22/100/115	-
38	LUT	4	502	-	-	3/29/67/67	0/2/2/2
22	CLA	5	603	-	1/1/13/20	16/27/105/115	-
38	LUT	4	501	-	-	2/29/67/67	0/2/2/2
22	CLA	A	1122	-	1/1/15/20	19/37/115/115	-
22	CLA	8	620	19	1/1/15/20	17/37/115/115	-
25	LHG	4	802	-	-	19/36/36/53	-
42	GG0	a	805	-	-	2/7/7/7	-
25	LHG	B	5001	22	-	29/50/50/53	-
28	SF4	A	3001	1,2	-	-	0/6/5/5
38	LUT	6	502	-	1/1/12/27	8/29/67/67	0/2/2/2
22	CLA	1	608	-	1/1/14/20	14/31/109/115	-
22	CLA	1	611	-	1/1/13/20	11/25/103/115	-
25	LHG	6	802	-	-	27/41/41/53	-
39	CHL	6	613	-	3/3/17/26	2/21/119/137	-
39	CHL	6	610	-	4/4/18/26	6/27/125/137	-
38	LUT	3	501	-	-	2/29/67/67	0/2/2/2
22	CLA	3	601	-	1/1/15/20	13/37/115/115	-
22	CLA	3	613	-	1/1/14/20	14/33/111/115	-
25	LHG	F	5001	22	-	31/47/47/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	8	604	19	4/4/19/26	13/35/133/137	-
22	CLA	B	1218	-	1/1/13/20	10/25/103/115	-
22	CLA	a	601	13	1/1/14/20	8/31/109/115	-
24	BCR	J	4001	-	-	13/29/63/63	0/2/2/2
47	4RF	8	807	-	-	23/44/44/59	-
22	CLA	3	610	14	1/1/14/20	15/31/109/115	-
22	CLA	4	607	25	1/1/13/20	11/25/103/115	-
36	LPX	a	804	-	-	14/31/31/31	-
38	LUT	a	503	-	-	4/29/67/67	0/2/2/2
24	BCR	7	503	-	-	16/29/63/63	0/2/2/2
24	BCR	8	503	-	-	10/29/63/63	0/2/2/2
22	CLA	B	1227	-	1/1/12/20	8/19/97/115	-
22	CLA	a	603	-	1/1/15/20	14/37/115/115	-
22	CLA	A	1133	-	1/1/15/20	19/37/115/115	-
22	CLA	A	1102	22	1/1/15/20	18/37/115/115	-
38	LUT	7	501	-	1/1/12/27	6/29/67/67	0/2/2/2
38	LUT	a	501	-	-	7/29/67/67	0/2/2/2
22	CLA	B	1208	-	1/1/14/20	11/31/109/115	-
38	LUT	5	502	-	-	1/29/67/67	0/2/2/2
22	CLA	A	1134	1	1/1/14/20	20/31/109/115	-
22	CLA	8	602	19	1/1/12/20	8/22/100/115	-
32	LAP	F	5003	-	-	20/30/30/30	-
22	CLA	A	1112	-	1/1/13/20	9/25/103/115	-
22	CLA	A	1131	-	1/1/15/20	21/37/115/115	-
22	CLA	6	608	-	1/1/11/20	4/13/91/115	-
22	CLA	7	607	25	1/1/13/20	12/29/107/115	-
22	CLA	7	601	-	1/1/14/20	17/31/109/115	-
22	CLA	B	1219	-	1/1/13/20	10/30/108/115	-
22	CLA	B	1202	-	1/1/15/20	14/37/115/115	-
22	CLA	A	1124	-	1/1/13/20	9/25/103/115	-
22	CLA	B	1240	25	1/1/15/20	9/37/115/115	-
24	BCR	3	505	-	-	13/29/63/63	0/2/2/2
22	CLA	6	601	-	1/1/14/20	14/31/109/115	-
22	CLA	3	607	25	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	1132	-	1/1/15/20	17/37/115/115	-
22	CLA	B	1210	-	1/1/15/20	22/37/115/115	-
39	CHL	6	619	17	5/5/20/26	17/39/137/137	-
38	LUT	3	502	-	-	2/29/67/67	0/2/2/2
22	CLA	B	1221	-	1/1/15/20	13/37/115/115	-
41	QTB	a	504	-	-	6/11/28/28	0/1/1/1
22	CLA	1	615	13	1/1/11/20	8/15/93/115	-
22	CLA	B	1236	-	1/1/12/20	13/23/101/115	-
24	BCR	B	4007	-	-	10/29/63/63	0/2/2/2
22	CLA	a	604	13	1/1/15/20	18/37/115/115	-
22	CLA	7	605	-	1/1/11/20	8/11/89/115	-
22	CLA	5	601	16	1/1/14/20	13/31/109/115	-
23	PQN	B	2002	-	-	5/23/43/43	0/2/2/2
22	CLA	B	1239	-	1/1/15/20	18/37/115/115	-
22	CLA	B	1217	-	1/1/13/20	15/27/105/115	-
28	SF4	C	3002	3	-	-	0/6/5/5
29	LMT	A	5008	-	-	7/21/61/61	0/2/2/2
22	CLA	A	1140	-	1/1/13/20	16/25/103/115	-
39	CHL	a	613	-	3/3/16/26	6/15/113/137	-
22	CLA	5	607	25	1/1/13/20	12/25/103/115	-
29	LMT	B	5006	-	-	10/21/61/61	0/2/2/2
22	CLA	A	1101	-	1/1/15/20	23/37/115/115	-
25	LHG	1	802	-	-	29/46/46/53	-
34	ERG	G	5002	-	4/4/11/15	10/13/71/71	0/4/4/4
49	P5S	8	806	-	-	31/42/42/59	-
39	CHL	1	613	-	3/3/16/26	1/18/116/137	-
22	CLA	8	605	-	1/1/11/20	6/13/91/115	-
22	CLA	A	1127	-	1/1/15/20	13/37/115/115	-
22	CLA	A	1107	1	1/1/13/20	8/25/103/115	-
24	BCR	A	4002	-	-	11/29/63/63	0/2/2/2
22	CLA	L	1502	-	1/1/14/20	13/31/109/115	-
25	LHG	A	5001	22	-	20/33/33/53	-
39	CHL	a	606	-	4/4/18/26	8/27/125/137	-
25	LHG	6	801	22	-	29/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	1111	-	1/1/15/20	25/37/115/115	-
22	CLA	J	1901	8	1/1/10/20	5/10/88/115	-
22	CLA	a	607	-	1/1/13/20	10/29/107/115	-
22	CLA	F	1302	25	1/1/13/20	12/25/103/115	-
22	CLA	B	1204	-	1/1/15/20	25/37/115/115	-
22	CLA	A	1110	-	1/1/14/20	15/31/109/115	-
22	CLA	B	1205	-	1/1/15/20	14/37/115/115	-
22	CLA	7	609	-	1/1/14/20	14/31/109/115	-
25	LHG	7	802	-	-	23/40/40/53	-
22	CLA	A	1120	-	1/1/11/20	9/18/96/115	-
22	CLA	4	617	-	1/1/11/20	5/13/91/115	-
22	CLA	A	1118	-	1/1/13/20	15/25/103/115	-
39	CHL	7	613	-	4/4/20/26	10/39/137/137	-
22	CLA	7	602	-	1/1/10/20	7/11/90/115	-
24	BCR	3	503	-	-	9/29/63/63	0/2/2/2
22	CLA	B	1220	-	1/1/14/20	17/31/109/115	-
22	CLA	4	610	-	1/1/15/20	19/37/115/115	-
22	CLA	3	605	-	1/1/15/20	14/37/115/115	-
47	4RF	7	807	-	-	20/34/34/59	-
25	LHG	1	801	-	-	26/39/39/53	-
25	LHG	5	801	22	-	30/53/53/53	-
22	CLA	6	605	-	1/1/11/20	5/15/93/115	-
22	CLA	6	617	17	1/1/11/20	4/13/91/115	-
22	CLA	B	1235	-	1/1/15/20	21/37/115/115	-
22	CLA	B	1228	-	1/1/15/20	18/37/115/115	-
22	CLA	4	606	-	1/1/12/20	5/19/97/115	-
22	CLA	B	1225	-	1/1/15/20	12/37/115/115	-
24	BCR	K	4001	-	-	12/29/63/63	0/2/2/2
38	LUT	6	501	-	1/1/12/27	7/29/67/67	0/2/2/2
22	CLA	5	618	16	1/1/12/20	4/22/100/115	-
37	ECH	M	4001	-	-	9/29/66/66	0/2/2/2
22	CLA	B	1021	-	1/1/15/20	25/37/115/115	-
22	CLA	G	1603	-	1/1/11/20	6/13/91/115	-
22	CLA	4	601	-	1/1/14/20	8/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	3	616	-	1/1/13/20	17/27/105/115	-
31	PTY	5	802	-	-	19/41/41/53	-
43	PLM	4	803	-	-	8/13/14/15	-
22	CLA	5	605	-	1/1/11/20	6/15/93/115	-
39	CHL	1	609	13	4/4/20/26	14/39/137/137	-
22	CLA	8	615	-	1/1/11/20	6/15/93/115	-
22	CLA	7	611	-	1/1/14/20	10/31/109/115	-
22	CLA	L	1501	-	1/1/12/20	8/19/97/115	-
22	CLA	A	1115	-	1/1/14/20	10/31/109/115	-
22	CLA	L	1503	-	1/1/11/20	8/13/91/115	-
38	LUT	8	501	-	-	2/29/67/67	0/2/2/2
22	CLA	1	612	13	1/1/15/20	16/37/115/115	-
22	CLA	6	609	17	1/1/15/20	22/37/115/115	-
24	BCR	5	503	-	-	16/29/63/63	0/2/2/2
25	LHG	8	801	22	-	27/41/41/53	-
38	LUT	5	501	-	-	1/29/67/67	0/2/2/2
22	CLA	B	1224	-	1/1/15/20	25/37/115/115	-
22	CLA	3	618	-	1/1/11/20	6/15/93/115	-
22	CLA	8	603	19	1/1/15/20	22/37/115/115	-
24	BCR	L	4003	-	-	9/29/63/63	0/2/2/2
28	SF4	C	3003	3	-	-	0/6/5/5
25	LHG	7	803	-	-	28/47/47/53	-
24	BCR	3	504	-	-	12/29/63/63	0/2/2/2
22	CLA	A	1141	25	1/1/11/20	8/13/91/115	-
22	CLA	8	609	19	1/1/14/20	22/31/109/115	-
39	CHL	6	611	-	3/3/17/26	3/21/119/137	-
22	CLA	A	1106	1	1/1/15/20	20/37/115/115	-
22	CLA	a	611	-	1/1/12/20	8/19/97/115	-
22	CLA	5	609	16	1/1/12/20	9/21/99/115	-
38	LUT	a	502	-	1/1/12/27	11/29/67/67	0/2/2/2
22	CLA	A	1012	-	1/1/15/20	12/37/115/115	-
22	CLA	B	1207	-	1/1/14/20	21/31/109/115	-
44	DGA	8	803	-	-	12/31/31/45	-
22	CLA	a	602	-	1/1/12/20	6/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	3	612	-	1/1/15/20	15/37/115/115	-
38	LUT	1	502	-	-	2/29/67/67	0/2/2/2
22	CLA	4	608	-	1/1/12/20	9/21/99/115	-
39	CHL	a	610	-	3/3/16/26	6/18/116/137	-
22	CLA	K	1404	9	1/1/12/20	9/22/100/115	-
39	CHL	5	610	-	4/4/20/26	9/39/137/137	-
22	CLA	G	1601	-	1/1/12/20	12/19/97/115	-
22	CLA	B	1238	-	1/1/15/20	11/37/115/115	-
30	PCW	B	5004	-	-	15/33/33/57	-
24	BCR	B	4002	-	-	13/29/63/63	0/2/2/2
22	CLA	A	1013	-	1/1/15/20	15/37/115/115	-
24	BCR	I	4001	-	-	10/29/63/63	0/2/2/2
22	CLA	7	606	-	1/1/13/20	9/25/103/115	-
22	CLA	4	604	15	1/1/14/20	13/31/109/115	-
24	BCR	B	4001	-	-	15/29/63/63	0/2/2/2
22	CLA	7	617	18	1/1/13/20	13/23/101/115	-
22	CLA	7	615	18	1/1/13/20	13/25/103/115	-

All (1936) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	G	5002	ERG	C1-C10	-24.25	1.08	1.54
34	G	5002	ERG	C10-C9	-22.01	1.26	1.55
48	7	504	C7Z	C25-C26	15.87	1.61	1.34
34	G	5002	ERG	C10-C5	-15.71	1.21	1.52
35	J	4002	RRX	C26-C25	15.66	1.61	1.34
48	7	504	C7Z	C5-C6	15.53	1.61	1.34
38	1	503	LUT	C24-C25	14.75	1.51	1.33
38	5	505	LUT	C24-C25	14.58	1.51	1.33
38	a	503	LUT	C24-C25	14.53	1.51	1.33
38	1	501	LUT	C24-C25	14.50	1.51	1.33
38	6	501	LUT	C24-C25	14.42	1.51	1.33
35	J	4002	RRX	C5-C6	14.42	1.59	1.34
38	7	501	LUT	C24-C25	14.36	1.51	1.33
38	5	501	LUT	C24-C25	14.36	1.51	1.33
38	a	501	LUT	C24-C25	14.31	1.51	1.33
38	3	502	LUT	C24-C25	14.22	1.50	1.33
38	8	501	LUT	C24-C25	14.17	1.50	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	4	502	LUT	C24-C25	14.14	1.50	1.33
38	a	502	LUT	C24-C25	14.13	1.50	1.33
38	3	501	LUT	C24-C25	14.12	1.50	1.33
38	5	502	LUT	C24-C25	14.09	1.50	1.33
34	G	5002	ERG	C4-C3	-14.07	1.27	1.52
38	8	502	LUT	C24-C25	14.04	1.50	1.33
38	6	502	LUT	C24-C25	13.78	1.50	1.33
38	4	501	LUT	C24-C25	13.75	1.50	1.33
38	1	502	LUT	C24-C25	13.66	1.50	1.33
34	G	5002	ERG	C2-C3	-11.45	1.24	1.51
48	7	504	C7Z	C24-C23	10.80	1.71	1.52
48	7	504	C7Z	C22-C23	-10.60	1.37	1.52
35	J	4002	RRX	C29-C28	-10.25	1.37	1.52
48	7	504	C7Z	C2-C3	-9.62	1.38	1.52
34	G	5002	ERG	C12-C13	9.18	1.70	1.54
34	G	5002	ERG	O1-C3	9.17	1.70	1.43
48	7	504	C7Z	C4-C3	9.16	1.68	1.52
34	G	5002	ERG	C6-C5	8.86	1.54	1.33
21	A	1011	CL0	MG-NA	8.72	2.27	2.06
41	3	506	QTB	C11-C12	-8.09	1.36	1.54
41	a	504	QTB	C11-C12	-7.93	1.36	1.54
35	J	4002	RRX	C27-C28	7.81	1.65	1.52
24	3	505	BCR	C10-C9	7.59	1.45	1.35
24	L	4003	BCR	C10-C9	7.33	1.45	1.35
24	G	4001	BCR	C10-C9	7.31	1.45	1.35
24	6	503	BCR	C10-C9	7.20	1.45	1.35
24	F	4001	BCR	C10-C9	7.07	1.45	1.35
24	B	4003	BCR	C10-C9	7.03	1.45	1.35
24	K	4002	BCR	C10-C9	7.01	1.45	1.35
24	8	503	BCR	C10-C9	6.88	1.44	1.35
24	B	4002	BCR	C10-C9	6.87	1.44	1.35
24	4	503	BCR	C10-C9	6.84	1.44	1.35
24	I	4001	BCR	C10-C9	6.77	1.44	1.35
35	J	4002	RRX	C2-C3	-6.77	1.35	1.52
24	A	4003	BCR	C10-C9	6.74	1.44	1.35
24	3	504	BCR	C10-C9	6.74	1.44	1.35
24	L	4001	BCR	C10-C9	6.68	1.44	1.35
24	K	4001	BCR	C10-C9	6.63	1.44	1.35
24	J	4001	BCR	C10-C9	6.62	1.44	1.35
24	B	4001	BCR	C10-C9	6.57	1.44	1.35
24	5	504	BCR	C10-C9	6.57	1.44	1.35
24	B	4004	BCR	C10-C9	6.53	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	503	BCR	C10-C9	6.52	1.44	1.35
24	A	4005	BCR	C10-C9	6.42	1.44	1.35
22	4	615	CLA	MG-NA	6.37	2.21	2.06
22	5	618	CLA	MG-NA	6.36	2.21	2.06
22	5	608	CLA	MG-NA	6.34	2.21	2.06
24	B	4006	BCR	C10-C9	6.34	1.44	1.35
24	L	4002	BCR	C10-C9	6.34	1.44	1.35
24	7	503	BCR	C10-C9	6.33	1.44	1.35
22	B	1240	CLA	MG-NA	6.33	2.21	2.06
22	K	1404	CLA	MG-NA	6.32	2.21	2.06
22	4	617	CLA	MG-NA	6.32	2.21	2.06
22	a	603	CLA	MG-NA	6.32	2.21	2.06
22	a	602	CLA	MG-NA	6.31	2.21	2.06
24	A	4004	BCR	C11-C12	-6.30	1.18	1.34
22	G	1602	CLA	MG-NA	6.30	2.21	2.06
24	A	4002	BCR	C10-C9	6.29	1.44	1.35
24	B	4005	BCR	C10-C9	6.29	1.44	1.35
22	4	610	CLA	MG-NA	6.29	2.21	2.06
22	5	602	CLA	MG-NA	6.28	2.21	2.06
22	5	607	CLA	MG-NA	6.28	2.21	2.06
22	A	1114	CLA	MG-NA	6.27	2.21	2.06
22	5	609	CLA	MG-NA	6.27	2.21	2.06
22	3	618	CLA	MG-NA	6.26	2.21	2.06
22	1	608	CLA	MG-NA	6.26	2.21	2.06
22	4	616	CLA	MG-NA	6.26	2.21	2.06
22	K	1402	CLA	MG-NA	6.25	2.21	2.06
24	B	4007	BCR	C10-C9	6.25	1.44	1.35
22	a	611	CLA	MG-NA	6.24	2.21	2.06
22	8	602	CLA	MG-NA	6.24	2.21	2.06
22	8	605	CLA	MG-NA	6.24	2.21	2.06
22	7	602	CLA	MG-NA	6.24	2.21	2.06
22	3	602	CLA	MG-NA	6.24	2.21	2.06
22	5	614	CLA	MG-NA	6.23	2.21	2.06
22	7	606	CLA	MG-NA	6.23	2.21	2.06
22	A	1139	CLA	MG-NA	6.22	2.21	2.06
22	6	617	CLA	MG-NA	6.22	2.21	2.06
22	A	1101	CLA	MG-NA	6.21	2.21	2.06
24	6	504	BCR	C10-C9	6.21	1.44	1.35
22	3	616	CLA	MG-NA	6.21	2.21	2.06
22	6	601	CLA	MG-NA	6.21	2.21	2.06
22	K	1403	CLA	MG-NA	6.20	2.21	2.06
22	a	608	CLA	MG-NA	6.20	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	605	CLA	MG-NA	6.20	2.21	2.06
22	A	1127	CLA	MG-NA	6.20	2.21	2.06
22	7	603	CLA	MG-NA	6.20	2.21	2.06
22	5	605	CLA	MG-NA	6.19	2.21	2.06
22	a	607	CLA	MG-NA	6.19	2.21	2.06
22	A	1137	CLA	MG-NA	6.19	2.21	2.06
22	A	1141	CLA	MG-NA	6.19	2.21	2.06
22	L	1503	CLA	MG-NA	6.19	2.21	2.06
22	B	1219	CLA	MG-NA	6.19	2.21	2.06
22	1	611	CLA	MG-NA	6.19	2.21	2.06
22	B	1213	CLA	MG-NA	6.19	2.21	2.06
22	6	606	CLA	MG-NA	6.18	2.21	2.06
22	A	1115	CLA	MG-NA	6.18	2.21	2.06
22	6	615	CLA	MG-NA	6.18	2.21	2.06
22	4	602	CLA	MG-NA	6.18	2.20	2.06
22	B	1218	CLA	MG-NA	6.18	2.20	2.06
22	A	1123	CLA	MG-NA	6.18	2.20	2.06
22	6	609	CLA	MG-NA	6.18	2.20	2.06
22	L	1501	CLA	MG-NA	6.17	2.20	2.06
22	G	1601	CLA	MG-NA	6.17	2.20	2.06
22	K	1401	CLA	MG-NA	6.17	2.20	2.06
22	4	608	CLA	MG-NA	6.17	2.20	2.06
22	A	1140	CLA	MG-NA	6.16	2.20	2.06
22	B	1206	CLA	MG-NA	6.16	2.20	2.06
22	A	1012	CLA	MG-NA	6.16	2.20	2.06
22	G	1603	CLA	MG-NA	6.15	2.20	2.06
22	3	603	CLA	MG-NA	6.15	2.20	2.06
22	8	620	CLA	MG-NA	6.15	2.20	2.06
22	A	1110	CLA	MG-NA	6.15	2.20	2.06
22	8	610	CLA	MG-NA	6.15	2.20	2.06
22	A	1134	CLA	MG-NA	6.15	2.20	2.06
22	5	616	CLA	MG-NA	6.15	2.20	2.06
22	A	1121	CLA	MG-NA	6.15	2.20	2.06
22	a	605	CLA	MG-NA	6.14	2.20	2.06
22	B	1229	CLA	MG-NA	6.14	2.20	2.06
22	A	1125	CLA	MG-NA	6.14	2.20	2.06
22	B	1237	CLA	MG-NA	6.14	2.20	2.06
22	1	607	CLA	MG-NA	6.14	2.20	2.06
22	B	1022	CLA	MG-NA	6.13	2.20	2.06
22	a	604	CLA	MG-NA	6.13	2.20	2.06
22	4	605	CLA	MG-NA	6.13	2.20	2.06
22	5	606	CLA	MG-NA	6.13	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	3	503	BCR	C10-C9	6.13	1.43	1.35
22	A	1122	CLA	MG-NA	6.12	2.20	2.06
22	B	1227	CLA	MG-NA	6.12	2.20	2.06
22	F	1302	CLA	MG-NA	6.12	2.20	2.06
22	6	605	CLA	MG-NA	6.12	2.20	2.06
22	8	608	CLA	MG-NA	6.12	2.20	2.06
22	7	615	CLA	MG-NA	6.11	2.20	2.06
22	A	1112	CLA	MG-NA	6.11	2.20	2.06
22	3	607	CLA	MG-NA	6.11	2.20	2.06
22	5	603	CLA	MG-NA	6.11	2.20	2.06
22	8	615	CLA	MG-NA	6.11	2.20	2.06
22	6	607	CLA	MG-NA	6.11	2.20	2.06
22	A	1105	CLA	MG-NA	6.10	2.20	2.06
22	B	1220	CLA	MG-NA	6.10	2.20	2.06
22	3	613	CLA	MG-NA	6.10	2.20	2.06
22	A	1107	CLA	MG-NA	6.10	2.20	2.06
22	B	1209	CLA	MG-NA	6.09	2.20	2.06
22	7	617	CLA	MG-NA	6.09	2.20	2.06
22	4	612	CLA	MG-NA	6.09	2.20	2.06
22	J	1901	CLA	MG-NA	6.09	2.20	2.06
22	7	608	CLA	MG-NA	6.09	2.20	2.06
22	A	1129	CLA	MG-NA	6.08	2.20	2.06
22	B	1238	CLA	MG-NA	6.08	2.20	2.06
22	6	604	CLA	MG-NA	6.08	2.20	2.06
22	8	606	CLA	MG-NA	6.08	2.20	2.06
22	1	601	CLA	MG-NA	6.08	2.20	2.06
22	1	602	CLA	MG-NA	6.08	2.20	2.06
22	A	1124	CLA	MG-NA	6.07	2.20	2.06
22	A	1136	CLA	MG-NA	6.07	2.20	2.06
22	A	1126	CLA	MG-NA	6.07	2.20	2.06
22	1	615	CLA	MG-NA	6.07	2.20	2.06
22	A	1135	CLA	MG-NA	6.07	2.20	2.06
22	B	1223	CLA	MG-NA	6.07	2.20	2.06
22	B	1212	CLA	MG-NA	6.07	2.20	2.06
22	B	1232	CLA	MG-NA	6.07	2.20	2.06
22	A	1113	CLA	MG-NA	6.07	2.20	2.06
22	4	607	CLA	MG-NA	6.06	2.20	2.06
22	F	1301	CLA	MG-NA	6.06	2.20	2.06
22	7	604	CLA	MG-NA	6.06	2.20	2.06
22	6	618	CLA	MG-NA	6.06	2.20	2.06
22	7	610	CLA	MG-NA	6.06	2.20	2.06
22	1	612	CLA	MG-NA	6.06	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	617	CLA	MG-NA	6.06	2.20	2.06
22	8	603	CLA	MG-NA	6.06	2.20	2.06
22	A	1109	CLA	MG-NA	6.06	2.20	2.06
22	3	605	CLA	MG-NA	6.06	2.20	2.06
22	B	1221	CLA	MG-NA	6.05	2.20	2.06
22	1	605	CLA	MG-NA	6.05	2.20	2.06
22	6	602	CLA	MG-NA	6.05	2.20	2.06
22	1	606	CLA	MG-NA	6.05	2.20	2.06
22	4	601	CLA	MG-NA	6.05	2.20	2.06
22	1	603	CLA	MG-NA	6.05	2.20	2.06
22	4	611	CLA	MG-NA	6.05	2.20	2.06
22	4	604	CLA	MG-NA	6.05	2.20	2.06
22	B	1208	CLA	MG-NA	6.05	2.20	2.06
22	A	1116	CLA	MG-NA	6.04	2.20	2.06
22	B	1236	CLA	MG-NA	6.04	2.20	2.06
22	B	1225	CLA	MG-NA	6.04	2.20	2.06
22	A	1118	CLA	MG-NA	6.03	2.20	2.06
22	4	603	CLA	MG-NA	6.03	2.20	2.06
22	5	601	CLA	MG-NA	6.03	2.20	2.06
22	4	606	CLA	MG-NA	6.03	2.20	2.06
22	A	1131	CLA	MG-NA	6.03	2.20	2.06
22	B	1234	CLA	MG-NA	6.03	2.20	2.06
22	1	610	CLA	MG-NA	6.03	2.20	2.06
22	7	607	CLA	MG-NA	6.03	2.20	2.06
22	6	608	CLA	MG-NA	6.03	2.20	2.06
22	B	1207	CLA	MG-NA	6.02	2.20	2.06
22	B	1217	CLA	MG-NA	6.02	2.20	2.06
22	B	1239	CLA	MG-NA	6.02	2.20	2.06
22	A	1111	CLA	MG-NA	6.02	2.20	2.06
22	8	611	CLA	MG-NA	6.02	2.20	2.06
22	3	610	CLA	MG-NA	6.01	2.20	2.06
22	B	1224	CLA	MG-NA	6.01	2.20	2.06
22	8	618	CLA	MG-NA	6.01	2.20	2.06
22	5	612	CLA	MG-NA	6.01	2.20	2.06
22	B	1203	CLA	MG-NA	6.01	2.20	2.06
22	3	601	CLA	MG-NA	6.01	2.20	2.06
22	B	1222	CLA	MG-NA	6.00	2.20	2.06
22	A	1120	CLA	MG-NA	6.00	2.20	2.06
22	A	1104	CLA	MG-NA	6.00	2.20	2.06
22	3	604	CLA	MG-NA	6.00	2.20	2.06
22	A	1119	CLA	MG-NA	6.00	2.20	2.06
22	3	612	CLA	MG-NA	6.00	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	1204	CLA	MG-NA	5.99	2.20	2.06
22	A	1013	CLA	MG-NA	5.99	2.20	2.06
22	B	1211	CLA	MG-NA	5.99	2.20	2.06
22	A	1130	CLA	MG-NA	5.99	2.20	2.06
22	a	612	CLA	MG-NA	5.99	2.20	2.06
22	8	609	CLA	MG-NA	5.98	2.20	2.06
34	G	5002	ERG	C16-C17	-5.98	1.42	1.54
22	B	1214	CLA	MG-NA	5.98	2.20	2.06
22	5	604	CLA	MG-NA	5.98	2.20	2.06
22	1	604	CLA	MG-NA	5.98	2.20	2.06
22	a	601	CLA	MG-NA	5.97	2.20	2.06
22	L	1502	CLA	MG-NA	5.97	2.20	2.06
22	a	615	CLA	MG-NA	5.96	2.20	2.06
22	3	606	CLA	MG-NA	5.95	2.20	2.06
22	B	1230	CLA	MG-NA	5.95	2.20	2.06
22	B	1226	CLA	MG-NA	5.94	2.20	2.06
22	A	1133	CLA	MG-NA	5.94	2.20	2.06
22	B	1202	CLA	MG-NA	5.93	2.20	2.06
22	B	1201	CLA	MG-NA	5.93	2.20	2.06
22	A	1128	CLA	MG-NA	5.93	2.20	2.06
22	7	611	CLA	MG-NA	5.93	2.20	2.06
22	A	1138	CLA	MG-NA	5.93	2.20	2.06
22	A	1117	CLA	MG-NA	5.92	2.20	2.06
22	6	612	CLA	MG-NA	5.92	2.20	2.06
22	8	607	CLA	MG-NA	5.91	2.20	2.06
22	A	1108	CLA	MG-NA	5.90	2.20	2.06
22	B	1235	CLA	MG-NA	5.90	2.20	2.06
22	B	1231	CLA	MG-NA	5.90	2.20	2.06
22	B	1216	CLA	MG-NA	5.90	2.20	2.06
22	B	1023	CLA	MG-NA	5.87	2.20	2.06
22	B	1215	CLA	MG-NA	5.87	2.20	2.06
22	7	612	CLA	MG-NA	5.87	2.20	2.06
35	J	4002	RRX	C1-C6	-5.86	1.45	1.53
22	A	1103	CLA	MG-NA	5.86	2.20	2.06
22	B	1021	CLA	MG-NA	5.86	2.20	2.06
22	A	1132	CLA	MG-NA	5.84	2.20	2.06
22	7	609	CLA	MG-NA	5.83	2.20	2.06
24	L	4003	BCR	C24-C23	5.83	1.50	1.33
24	L	4001	BCR	C24-C23	5.83	1.50	1.33
24	G	4001	BCR	C24-C23	5.82	1.50	1.33
22	B	1205	CLA	MG-NA	5.81	2.20	2.06
22	7	601	CLA	MG-NA	5.80	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1106	CLA	MG-NA	5.79	2.20	2.06
24	6	503	BCR	C24-C23	5.76	1.50	1.33
35	J	4002	RRX	C30-C25	-5.75	1.45	1.53
24	3	504	BCR	C24-C23	5.75	1.50	1.33
22	A	1102	CLA	MG-NA	5.74	2.19	2.06
22	8	612	CLA	MG-NA	5.74	2.19	2.06
24	K	4002	BCR	C24-C23	5.71	1.50	1.33
24	L	4002	BCR	C24-C23	5.70	1.50	1.33
24	8	503	BCR	C24-C23	5.67	1.50	1.33
24	5	503	BCR	C24-C23	5.63	1.50	1.33
24	6	504	BCR	C24-C23	5.63	1.50	1.33
48	7	504	C7Z	C1-C6	-5.62	1.46	1.53
24	3	503	BCR	C24-C23	5.61	1.50	1.33
24	B	4005	BCR	C11-C12	-5.60	1.20	1.34
24	A	4001	BCR	C11-C12	-5.58	1.20	1.34
22	B	1210	CLA	MG-NA	5.58	2.19	2.06
24	6	504	BCR	C11-C12	-5.57	1.20	1.34
22	6	603	CLA	MG-NA	5.57	2.19	2.06
48	7	504	C7Z	C24-C25	-5.56	1.42	1.51
24	A	4001	BCR	C10-C9	5.55	1.43	1.35
24	4	503	BCR	C24-C23	5.55	1.49	1.33
24	F	4001	BCR	C24-C23	5.55	1.49	1.33
24	B	4002	BCR	C24-C23	5.54	1.49	1.33
24	B	4006	BCR	C24-C23	5.54	1.49	1.33
24	3	503	BCR	C11-C12	-5.53	1.20	1.34
24	5	504	BCR	C24-C23	5.53	1.49	1.33
24	B	4001	BCR	C24-C23	5.52	1.49	1.33
24	A	4001	BCR	C24-C23	5.52	1.49	1.33
24	3	505	BCR	C24-C23	5.52	1.49	1.33
24	I	4001	BCR	C24-C23	5.52	1.49	1.33
24	A	4004	BCR	C10-C9	5.51	1.43	1.35
24	B	4007	BCR	C24-C23	5.51	1.49	1.33
24	J	4001	BCR	C24-C23	5.49	1.49	1.33
48	7	504	C7Z	C12-C13	5.49	1.57	1.45
24	A	4003	BCR	C24-C23	5.49	1.49	1.33
24	B	4007	BCR	C11-C12	-5.48	1.20	1.34
24	B	4001	BCR	C11-C12	-5.48	1.20	1.34
24	K	4001	BCR	C24-C23	5.46	1.49	1.33
24	A	4005	BCR	C24-C23	5.46	1.49	1.33
24	5	503	BCR	C11-C12	-5.44	1.20	1.34
24	A	4002	BCR	C11-C12	-5.43	1.20	1.34
34	G	5002	ERG	C13-C14	-5.43	1.47	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	4003	BCR	C24-C23	5.43	1.49	1.33
24	8	503	BCR	C11-C12	-5.42	1.20	1.34
24	A	4002	BCR	C24-C23	5.42	1.49	1.33
24	5	504	BCR	C11-C12	-5.42	1.20	1.34
24	A	4003	BCR	C11-C12	-5.41	1.20	1.34
24	A	4004	BCR	C24-C23	5.41	1.49	1.33
41	a	504	QTB	C17-C11	-5.40	1.50	1.55
24	B	4005	BCR	C24-C23	5.39	1.49	1.33
24	B	4006	BCR	C11-C12	-5.39	1.20	1.34
24	K	4001	BCR	C11-C12	-5.37	1.20	1.34
24	J	4001	BCR	C11-C12	-5.35	1.20	1.34
24	7	503	BCR	C11-C12	-5.35	1.20	1.34
24	B	4004	BCR	C24-C23	5.34	1.49	1.33
24	7	503	BCR	C24-C23	5.33	1.49	1.33
24	A	4005	BCR	C11-C12	-5.31	1.20	1.34
24	4	503	BCR	C11-C12	-5.31	1.20	1.34
24	3	504	BCR	C11-C12	-5.29	1.20	1.34
24	B	4004	BCR	C11-C12	-5.29	1.20	1.34
24	L	4001	BCR	C11-C12	-5.29	1.21	1.34
24	I	4001	BCR	C11-C12	-5.26	1.21	1.34
24	K	4002	BCR	C11-C12	-5.22	1.21	1.34
21	A	1011	CL0	O2A-C1	5.22	1.60	1.46
24	B	4002	BCR	C11-C12	-5.20	1.21	1.34
24	L	4002	BCR	C11-C12	-5.17	1.21	1.34
24	6	503	BCR	C11-C12	-5.17	1.21	1.34
24	F	4001	BCR	C11-C12	-5.14	1.21	1.34
24	L	4003	BCR	C11-C12	-5.08	1.21	1.34
24	B	4003	BCR	C11-C12	-5.08	1.21	1.34
35	J	4002	RRX	C2-C1	5.02	1.65	1.54
24	G	4001	BCR	C11-C12	-5.01	1.21	1.34
35	J	4002	RRX	C19-C18	4.90	1.56	1.45
21	A	1011	CL0	O2D-CGD	4.88	1.45	1.33
34	G	5002	ERG	C12-C11	-4.85	1.43	1.53
34	G	5002	ERG	C1-C2	4.81	1.63	1.53
22	B	1228	CLA	MG-NA	4.78	2.17	2.06
21	A	1011	CL0	CHC-C1C	4.78	1.47	1.35
24	3	505	BCR	C11-C12	-4.77	1.22	1.34
24	B	4005	BCR	C16-C17	-4.76	1.28	1.43
41	3	506	QTB	C17-C11	-4.73	1.50	1.55
34	G	5002	ERG	C7-C6	-4.70	1.27	1.41
24	3	503	BCR	C16-C17	-4.68	1.28	1.43
21	A	1011	CL0	C3D-C4D	-4.68	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	7	503	BCR	C16-C17	-4.60	1.29	1.43
41	3	506	QTB	C11-C10	-4.59	1.44	1.50
24	F	4001	BCR	C16-C17	-4.58	1.29	1.43
24	A	4004	BCR	C16-C17	-4.57	1.29	1.43
22	B	1210	CLA	C1C-NC	-4.57	1.31	1.37
24	K	4001	BCR	C16-C17	-4.53	1.29	1.43
24	B	4004	BCR	C16-C17	-4.53	1.29	1.43
24	A	4005	BCR	C16-C17	-4.53	1.29	1.43
22	a	612	CLA	MG-ND	-4.50	1.96	2.05
24	5	503	BCR	C16-C17	-4.49	1.29	1.43
24	A	4002	BCR	C16-C17	-4.49	1.29	1.43
39	3	611	CHL	C3B-C2B	-4.46	1.34	1.40
24	8	503	BCR	C16-C17	-4.45	1.29	1.43
22	A	1128	CLA	MG-ND	-4.44	1.97	2.05
24	B	4002	BCR	C16-C17	-4.44	1.29	1.43
21	A	1011	CL0	C3C-C2C	4.43	1.46	1.36
24	K	4002	BCR	C16-C17	-4.43	1.29	1.43
24	A	4003	BCR	C16-C17	-4.40	1.29	1.43
24	B	4007	BCR	C16-C17	-4.40	1.29	1.43
22	A	1139	CLA	MG-ND	-4.39	1.97	2.05
21	A	1011	CL0	CHD-C1D	4.39	1.46	1.38
24	J	4001	BCR	C16-C17	-4.39	1.29	1.43
48	7	504	C7Z	C28-C29	4.39	1.55	1.45
24	B	4001	BCR	C16-C17	-4.38	1.29	1.43
24	I	4001	BCR	C16-C17	-4.38	1.29	1.43
41	a	504	QTB	C11-C10	-4.37	1.44	1.50
24	A	4001	BCR	C16-C17	-4.37	1.29	1.43
35	J	4002	RRX	C27-C26	-4.36	1.44	1.51
24	3	505	BCR	C16-C17	-4.36	1.29	1.43
24	4	503	BCR	C16-C17	-4.36	1.29	1.43
24	6	504	BCR	C16-C17	-4.34	1.30	1.43
48	7	504	C7Z	C31-C30	4.34	1.56	1.43
35	J	4002	RRX	C8-C9	4.33	1.55	1.45
24	L	4002	BCR	C16-C17	-4.33	1.30	1.43
24	B	4003	BCR	C16-C17	-4.33	1.30	1.43
24	L	4003	BCR	C16-C17	-4.33	1.30	1.43
34	G	5002	ERG	C13-C17	4.33	1.63	1.55
24	3	504	BCR	C16-C17	-4.32	1.30	1.43
22	A	1131	CLA	MG-ND	-4.31	1.97	2.05
22	B	1022	CLA	MG-ND	-4.30	1.97	2.05
24	B	4006	BCR	C16-C17	-4.30	1.30	1.43
22	B	1021	CLA	MG-ND	-4.28	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	1221	CLA	MG-ND	-4.28	1.97	2.05
22	B	1214	CLA	MG-ND	-4.27	1.97	2.05
26	A	5005	DGD	O1G-C1A	4.27	1.45	1.33
22	7	612	CLA	MG-ND	-4.26	1.97	2.05
22	5	605	CLA	MG-ND	-4.26	1.97	2.05
22	7	607	CLA	MG-ND	-4.25	1.97	2.05
22	B	1023	CLA	MG-ND	-4.25	1.97	2.05
22	A	1126	CLA	MG-ND	-4.24	1.97	2.05
22	B	1239	CLA	MG-ND	-4.24	1.97	2.05
24	5	504	BCR	C16-C17	-4.24	1.30	1.43
22	A	1116	CLA	MG-ND	-4.23	1.97	2.05
24	G	4001	BCR	C16-C17	-4.23	1.30	1.43
22	6	609	CLA	MG-ND	-4.22	1.97	2.05
48	7	504	C7Z	C8-C9	4.22	1.55	1.45
22	B	1206	CLA	MG-ND	-4.22	1.97	2.05
22	B	1225	CLA	MG-ND	-4.22	1.97	2.05
21	A	1011	CL0	C3B-C2B	4.21	1.46	1.40
22	A	1124	CLA	MG-ND	-4.21	1.97	2.05
22	A	1129	CLA	MG-ND	-4.21	1.97	2.05
48	7	504	C7Z	C32-C33	4.20	1.55	1.45
22	8	612	CLA	MG-ND	-4.20	1.97	2.05
22	6	603	CLA	C1C-NC	-4.20	1.31	1.37
22	3	606	CLA	MG-ND	-4.19	1.97	2.05
22	4	610	CLA	MG-ND	-4.19	1.97	2.05
22	8	610	CLA	MG-ND	-4.19	1.97	2.05
24	6	503	BCR	C16-C17	-4.19	1.30	1.43
22	A	1114	CLA	MG-ND	-4.18	1.97	2.05
22	7	608	CLA	MG-ND	-4.18	1.97	2.05
22	5	616	CLA	MG-ND	-4.18	1.97	2.05
22	B	1213	CLA	MG-ND	-4.18	1.97	2.05
22	A	1121	CLA	MG-ND	-4.17	1.97	2.05
22	A	1012	CLA	MG-ND	-4.17	1.97	2.05
22	A	1013	CLA	MG-ND	-4.17	1.97	2.05
22	B	1219	CLA	MG-ND	-4.15	1.97	2.05
22	7	609	CLA	MG-ND	-4.15	1.97	2.05
22	B	1204	CLA	MG-ND	-4.15	1.97	2.05
22	5	609	CLA	MG-ND	-4.15	1.97	2.05
22	A	1117	CLA	MG-ND	-4.13	1.97	2.05
22	B	1237	CLA	MG-ND	-4.13	1.97	2.05
22	a	615	CLA	MG-ND	-4.13	1.97	2.05
22	6	607	CLA	MG-ND	-4.13	1.97	2.05
22	B	1212	CLA	MG-ND	-4.13	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	615	CLA	MG-ND	-4.12	1.97	2.05
22	B	1216	CLA	MG-ND	-4.12	1.97	2.05
24	L	4001	BCR	C16-C17	-4.12	1.30	1.43
22	A	1112	CLA	MG-ND	-4.11	1.97	2.05
26	B	5003	DGD	O1G-C1A	4.11	1.45	1.33
22	B	1220	CLA	MG-ND	-4.11	1.97	2.05
22	B	1232	CLA	MG-ND	-4.11	1.97	2.05
22	B	1235	CLA	MG-ND	-4.11	1.97	2.05
22	4	607	CLA	MG-ND	-4.11	1.97	2.05
22	K	1404	CLA	MG-ND	-4.11	1.97	2.05
22	A	1111	CLA	MG-ND	-4.11	1.97	2.05
22	B	1207	CLA	MG-ND	-4.11	1.97	2.05
22	A	1128	CLA	C1C-NC	-4.10	1.31	1.37
22	B	1202	CLA	MG-ND	-4.10	1.97	2.05
22	B	1223	CLA	MG-ND	-4.10	1.97	2.05
22	5	608	CLA	MG-ND	-4.10	1.97	2.05
35	J	4002	RRX	C23-C22	4.10	1.54	1.45
22	1	608	CLA	MG-ND	-4.10	1.97	2.05
22	4	608	CLA	MG-ND	-4.10	1.97	2.05
22	K	1401	CLA	MG-ND	-4.10	1.97	2.05
22	A	1133	CLA	MG-ND	-4.09	1.97	2.05
22	6	615	CLA	MG-ND	-4.09	1.97	2.05
22	B	1208	CLA	MG-ND	-4.09	1.97	2.05
22	B	1210	CLA	MG-ND	-4.09	1.97	2.05
22	B	1238	CLA	MG-ND	-4.07	1.97	2.05
22	1	615	CLA	MG-ND	-4.07	1.97	2.05
22	3	613	CLA	MG-ND	-4.07	1.97	2.05
22	A	1136	CLA	MG-ND	-4.07	1.97	2.05
22	A	1119	CLA	MG-ND	-4.07	1.97	2.05
22	A	1118	CLA	MG-ND	-4.06	1.97	2.05
22	8	608	CLA	MG-ND	-4.06	1.97	2.05
22	A	1138	CLA	MG-ND	-4.06	1.97	2.05
22	1	610	CLA	MG-ND	-4.06	1.97	2.05
22	B	1211	CLA	MG-ND	-4.06	1.97	2.05
22	A	1108	CLA	C1C-NC	-4.06	1.31	1.37
35	J	4002	RRX	C3-C4	4.06	1.65	1.52
22	B	1209	CLA	MG-ND	-4.06	1.97	2.05
22	5	618	CLA	MG-ND	-4.06	1.97	2.05
22	a	603	CLA	MG-ND	-4.05	1.97	2.05
22	8	609	CLA	MG-ND	-4.05	1.97	2.05
26	8	802	DGD	O1G-C1A	4.05	1.45	1.33
22	A	1141	CLA	MG-ND	-4.05	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	1222	CLA	MG-ND	-4.05	1.97	2.05
22	4	605	CLA	MG-ND	-4.04	1.97	2.05
22	A	1123	CLA	MG-ND	-4.04	1.97	2.05
22	B	1226	CLA	MG-ND	-4.04	1.97	2.05
35	J	4002	RRX	C12-C13	4.04	1.54	1.45
22	B	1240	CLA	MG-ND	-4.04	1.97	2.05
22	4	604	CLA	MG-ND	-4.04	1.97	2.05
22	8	607	CLA	MG-ND	-4.04	1.97	2.05
22	A	1110	CLA	MG-ND	-4.04	1.97	2.05
22	6	605	CLA	MG-ND	-4.04	1.97	2.05
22	A	1135	CLA	MG-ND	-4.03	1.97	2.05
22	6	601	CLA	MG-ND	-4.03	1.97	2.05
22	7	601	CLA	MG-ND	-4.03	1.97	2.05
22	5	612	CLA	MG-ND	-4.03	1.97	2.05
22	8	606	CLA	MG-ND	-4.03	1.97	2.05
34	G	5002	ERG	C16-C15	4.03	1.65	1.54
22	1	612	CLA	MG-ND	-4.03	1.97	2.05
22	7	615	CLA	MG-ND	-4.02	1.97	2.05
22	5	607	CLA	MG-ND	-4.02	1.97	2.05
22	3	603	CLA	MG-ND	-4.02	1.97	2.05
22	3	612	CLA	MG-ND	-4.02	1.97	2.05
22	5	602	CLA	MG-ND	-4.02	1.97	2.05
22	8	602	CLA	MG-ND	-4.02	1.97	2.05
22	7	610	CLA	MG-ND	-4.02	1.97	2.05
22	1	604	CLA	MG-ND	-4.02	1.97	2.05
22	4	606	CLA	MG-ND	-4.02	1.97	2.05
22	a	602	CLA	MG-ND	-4.02	1.97	2.05
22	8	605	CLA	MG-ND	-4.01	1.97	2.05
39	8	601	CHL	C3B-C2B	-4.01	1.34	1.40
22	1	606	CLA	MG-ND	-4.01	1.97	2.05
22	L	1503	CLA	MG-ND	-4.01	1.97	2.05
22	B	1215	CLA	MG-ND	-4.00	1.97	2.05
22	B	1207	CLA	C1C-NC	-4.00	1.31	1.37
22	G	1601	CLA	MG-ND	-4.00	1.97	2.05
22	3	618	CLA	MG-ND	-4.00	1.97	2.05
22	B	1203	CLA	MG-ND	-3.99	1.97	2.05
22	L	1502	CLA	MG-ND	-3.99	1.97	2.05
22	A	1134	CLA	MG-ND	-3.99	1.97	2.05
22	A	1115	CLA	MG-ND	-3.98	1.97	2.05
22	8	618	CLA	MG-ND	-3.98	1.97	2.05
22	A	1113	CLA	MG-ND	-3.98	1.97	2.05
22	B	1212	CLA	C1C-NC	-3.98	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1108	CLA	MG-ND	-3.98	1.97	2.05
22	B	1205	CLA	MG-ND	-3.97	1.97	2.05
22	3	602	CLA	MG-ND	-3.97	1.97	2.05
22	4	601	CLA	MG-ND	-3.97	1.97	2.05
22	4	612	CLA	MG-ND	-3.97	1.97	2.05
22	3	610	CLA	MG-ND	-3.97	1.97	2.05
22	3	604	CLA	MG-ND	-3.97	1.97	2.05
22	8	603	CLA	MG-ND	-3.96	1.97	2.05
22	4	611	CLA	MG-ND	-3.96	1.97	2.05
22	B	1224	CLA	MG-ND	-3.96	1.97	2.05
22	3	616	CLA	MG-ND	-3.96	1.97	2.05
48	7	504	C7Z	C11-C10	3.96	1.55	1.43
22	B	1021	CLA	C1C-NC	-3.96	1.31	1.37
22	L	1501	CLA	MG-ND	-3.96	1.97	2.05
22	3	605	CLA	MG-ND	-3.95	1.97	2.05
22	A	1112	CLA	C1C-NC	-3.95	1.31	1.37
22	B	1229	CLA	MG-ND	-3.95	1.98	2.05
22	a	611	CLA	MG-ND	-3.95	1.98	2.05
22	a	612	CLA	C1C-NC	-3.95	1.31	1.37
22	B	1236	CLA	C1C-NC	-3.95	1.31	1.37
22	A	1102	CLA	MG-ND	-3.95	1.98	2.05
22	8	609	CLA	C1C-NC	-3.95	1.31	1.37
22	A	1132	CLA	MG-ND	-3.95	1.98	2.05
22	A	1127	CLA	MG-ND	-3.94	1.98	2.05
22	7	603	CLA	MG-ND	-3.94	1.98	2.05
22	A	1130	CLA	MG-ND	-3.94	1.98	2.05
22	G	1602	CLA	MG-ND	-3.94	1.98	2.05
22	a	608	CLA	MG-ND	-3.94	1.98	2.05
22	3	607	CLA	MG-ND	-3.94	1.98	2.05
22	A	1104	CLA	MG-ND	-3.93	1.98	2.05
22	8	620	CLA	MG-ND	-3.93	1.98	2.05
22	7	605	CLA	MG-ND	-3.93	1.98	2.05
22	B	1201	CLA	MG-ND	-3.93	1.98	2.05
22	K	1402	CLA	MG-ND	-3.93	1.98	2.05
22	G	1603	CLA	MG-ND	-3.93	1.98	2.05
22	A	1122	CLA	MG-ND	-3.92	1.98	2.05
22	5	604	CLA	MG-ND	-3.92	1.98	2.05
22	a	607	CLA	MG-ND	-3.92	1.98	2.05
35	J	4002	RRX	C20-C21	3.92	1.55	1.43
22	B	1217	CLA	MG-ND	-3.92	1.98	2.05
39	8	604	CHL	C3B-C2B	-3.92	1.34	1.40
22	A	1140	CLA	MG-ND	-3.92	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	606	CLA	MG-ND	-3.92	1.98	2.05
22	3	601	CLA	MG-ND	-3.92	1.98	2.05
22	8	611	CLA	MG-ND	-3.92	1.98	2.05
22	B	1239	CLA	C1C-NC	-3.91	1.32	1.37
22	7	602	CLA	MG-ND	-3.91	1.98	2.05
22	5	614	CLA	MG-ND	-3.91	1.98	2.05
22	1	611	CLA	MG-ND	-3.91	1.98	2.05
22	4	616	CLA	MG-ND	-3.91	1.98	2.05
22	L	1503	CLA	C1C-NC	-3.91	1.32	1.37
22	6	606	CLA	MG-ND	-3.90	1.98	2.05
22	7	601	CLA	C1C-NC	-3.90	1.32	1.37
22	6	608	CLA	MG-ND	-3.90	1.98	2.05
22	B	1231	CLA	MG-ND	-3.90	1.98	2.05
22	A	1139	CLA	C1C-NC	-3.89	1.32	1.37
22	6	602	CLA	MG-ND	-3.89	1.98	2.05
22	B	1209	CLA	C1C-NC	-3.89	1.32	1.37
22	5	601	CLA	MG-ND	-3.88	1.98	2.05
39	5	611	CHL	C3B-C2B	-3.88	1.35	1.40
22	A	1131	CLA	C1C-NC	-3.88	1.32	1.37
22	A	1125	CLA	MG-ND	-3.88	1.98	2.05
22	6	612	CLA	MG-ND	-3.88	1.98	2.05
22	B	1218	CLA	MG-ND	-3.87	1.98	2.05
22	A	1106	CLA	C1C-NC	-3.87	1.32	1.37
22	B	1230	CLA	MG-ND	-3.87	1.98	2.05
22	8	612	CLA	C1C-NC	-3.87	1.32	1.37
22	A	1138	CLA	C1C-NC	-3.87	1.32	1.37
22	B	1228	CLA	MG-ND	-3.87	1.98	2.05
22	8	605	CLA	C1C-NC	-3.87	1.32	1.37
21	A	1011	CL0	C1D-ND	-3.87	1.33	1.37
22	A	1116	CLA	C1C-NC	-3.86	1.32	1.37
22	8	610	CLA	C1C-NC	-3.86	1.32	1.37
22	4	617	CLA	MG-ND	-3.86	1.98	2.05
22	A	1137	CLA	MG-ND	-3.86	1.98	2.05
22	4	603	CLA	MG-ND	-3.86	1.98	2.05
22	K	1403	CLA	MG-ND	-3.86	1.98	2.05
22	A	1103	CLA	MG-ND	-3.85	1.98	2.05
22	B	1222	CLA	C1C-NC	-3.85	1.32	1.37
22	B	1234	CLA	MG-ND	-3.84	1.98	2.05
22	6	617	CLA	MG-ND	-3.84	1.98	2.05
22	A	1117	CLA	C1C-NC	-3.84	1.32	1.37
22	5	617	CLA	C1C-NC	-3.84	1.32	1.37
22	B	1228	CLA	C1C-NC	-3.83	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	610	CLA	C1C-NC	-3.82	1.32	1.37
22	7	612	CLA	C3B-C2B	-3.82	1.35	1.40
22	A	1120	CLA	MG-ND	-3.82	1.98	2.05
22	B	1204	CLA	C1C-NC	-3.82	1.32	1.37
22	1	605	CLA	MG-ND	-3.82	1.98	2.05
22	5	603	CLA	MG-ND	-3.82	1.98	2.05
22	B	1230	CLA	C1C-NC	-3.81	1.32	1.37
22	8	615	CLA	MG-ND	-3.81	1.98	2.05
22	B	1215	CLA	C1C-NC	-3.80	1.32	1.37
22	A	1107	CLA	MG-ND	-3.80	1.98	2.05
22	1	601	CLA	MG-ND	-3.80	1.98	2.05
22	A	1101	CLA	C1C-NC	-3.80	1.32	1.37
21	A	1011	CL0	CHD-C4C	3.79	1.47	1.39
22	4	602	CLA	MG-ND	-3.79	1.98	2.05
22	B	1223	CLA	C1C-NC	-3.79	1.32	1.37
22	B	1201	CLA	C1C-NC	-3.78	1.32	1.37
22	8	602	CLA	C1C-NC	-3.77	1.32	1.37
22	1	607	CLA	MG-ND	-3.77	1.98	2.05
22	3	605	CLA	C1C-NC	-3.77	1.32	1.37
22	7	617	CLA	MG-ND	-3.77	1.98	2.05
22	a	615	CLA	C1C-NC	-3.77	1.32	1.37
22	3	613	CLA	C1C-NC	-3.76	1.32	1.37
22	4	601	CLA	C1C-NC	-3.76	1.32	1.37
22	a	601	CLA	MG-ND	-3.76	1.98	2.05
22	A	1101	CLA	MG-ND	-3.76	1.98	2.05
22	B	1225	CLA	C1C-NC	-3.76	1.32	1.37
22	7	610	CLA	C1C-NC	-3.76	1.32	1.37
22	7	604	CLA	MG-ND	-3.76	1.98	2.05
22	A	1124	CLA	C1C-NC	-3.76	1.32	1.37
22	7	617	CLA	C1C-NC	-3.76	1.32	1.37
22	A	1111	CLA	C1C-NC	-3.76	1.32	1.37
22	B	1234	CLA	C1C-NC	-3.75	1.32	1.37
22	7	609	CLA	C1C-NC	-3.74	1.32	1.37
22	4	604	CLA	C1C-NC	-3.74	1.32	1.37
22	1	602	CLA	C1C-NC	-3.74	1.32	1.37
22	6	604	CLA	MG-ND	-3.74	1.98	2.05
22	A	1133	CLA	C1C-NC	-3.74	1.32	1.37
22	A	1113	CLA	C1C-NC	-3.74	1.32	1.37
22	B	1205	CLA	C1C-NC	-3.74	1.32	1.37
22	A	1132	CLA	C1C-NC	-3.73	1.32	1.37
22	A	1105	CLA	MG-ND	-3.73	1.98	2.05
22	3	618	CLA	C1C-NC	-3.73	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1104	CLA	C1C-NC	-3.73	1.32	1.37
22	a	605	CLA	MG-ND	-3.73	1.98	2.05
22	F	1302	CLA	MG-ND	-3.72	1.98	2.05
22	3	606	CLA	C1C-NC	-3.72	1.32	1.37
22	8	608	CLA	C1C-NC	-3.72	1.32	1.37
22	B	1227	CLA	MG-ND	-3.72	1.98	2.05
39	6	611	CHL	C3B-C2B	-3.71	1.35	1.40
22	B	1211	CLA	C1C-NC	-3.71	1.32	1.37
22	L	1501	CLA	C1C-NC	-3.71	1.32	1.37
22	F	1301	CLA	MG-ND	-3.71	1.98	2.05
48	7	504	C7Z	C15-C14	3.71	1.54	1.43
22	5	607	CLA	C1C-NC	-3.71	1.32	1.37
48	7	504	C7Z	C38-C25	3.71	1.57	1.50
22	B	1206	CLA	C1C-NC	-3.70	1.32	1.37
22	A	1102	CLA	C1C-NC	-3.70	1.32	1.37
22	3	616	CLA	C1C-NC	-3.70	1.32	1.37
32	F	5003	LAP	P9-O6	3.70	1.74	1.59
22	B	1240	CLA	C1C-NC	-3.70	1.32	1.37
22	B	1224	CLA	C1C-NC	-3.70	1.32	1.37
22	5	617	CLA	MG-ND	-3.70	1.98	2.05
22	7	605	CLA	C1C-NC	-3.69	1.32	1.37
22	A	1106	CLA	MG-ND	-3.69	1.98	2.05
22	7	607	CLA	C1C-NC	-3.69	1.32	1.37
22	A	1107	CLA	C1C-NC	-3.69	1.32	1.37
22	A	1121	CLA	C1C-NC	-3.68	1.32	1.37
22	A	1136	CLA	C1C-NC	-3.68	1.32	1.37
22	A	1103	CLA	C1C-NC	-3.68	1.32	1.37
22	B	1202	CLA	C1C-NC	-3.68	1.32	1.37
22	A	1110	CLA	C1C-NC	-3.68	1.32	1.37
22	B	1232	CLA	C1C-NC	-3.67	1.32	1.37
22	1	602	CLA	MG-ND	-3.67	1.98	2.05
22	6	618	CLA	MG-ND	-3.67	1.98	2.05
22	A	1126	CLA	C1C-NC	-3.67	1.32	1.37
22	1	603	CLA	MG-ND	-3.66	1.98	2.05
22	7	611	CLA	MG-ND	-3.66	1.98	2.05
48	7	504	C7Z	C7-C6	3.66	1.58	1.45
22	5	603	CLA	C1C-NC	-3.66	1.32	1.37
35	J	4002	RRX	C24-C25	3.65	1.58	1.45
22	B	1236	CLA	MG-ND	-3.65	1.98	2.05
22	4	611	CLA	C1C-NC	-3.65	1.32	1.37
35	J	4002	RRX	C15-C14	3.65	1.54	1.43
22	4	603	CLA	C1C-NC	-3.65	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	8	606	CLA	C1C-NC	-3.65	1.32	1.37
22	A	1122	CLA	C1C-NC	-3.64	1.32	1.37
22	7	606	CLA	MG-ND	-3.64	1.98	2.05
22	5	604	CLA	C1C-NC	-3.64	1.32	1.37
22	6	603	CLA	MG-ND	-3.64	1.98	2.05
22	8	618	CLA	C1C-NC	-3.64	1.32	1.37
22	A	1013	CLA	C1C-NC	-3.63	1.32	1.37
32	K	5001	LAP	P9-O6	3.62	1.74	1.59
22	A	1137	CLA	C1C-NC	-3.62	1.32	1.37
22	B	1235	CLA	C1C-NC	-3.62	1.32	1.37
22	A	1115	CLA	C1C-NC	-3.62	1.32	1.37
22	5	601	CLA	C1C-NC	-3.61	1.32	1.37
22	1	605	CLA	C1C-NC	-3.61	1.32	1.37
22	B	1219	CLA	C1C-NC	-3.61	1.32	1.37
22	3	607	CLA	C1C-NC	-3.61	1.32	1.37
48	7	504	C7Z	C22-C21	3.60	1.66	1.54
22	4	605	CLA	C1C-NC	-3.60	1.32	1.37
22	3	612	CLA	C1C-NC	-3.60	1.32	1.37
22	A	1114	CLA	C1C-NC	-3.60	1.32	1.37
22	a	611	CLA	C1C-NC	-3.60	1.32	1.37
22	8	607	CLA	C1C-NC	-3.60	1.32	1.37
22	A	1135	CLA	C1C-NC	-3.59	1.32	1.37
22	B	1231	CLA	C1C-NC	-3.59	1.32	1.37
39	8	613	CHL	C3B-C2B	-3.59	1.35	1.40
22	B	1220	CLA	C1C-NC	-3.59	1.32	1.37
22	B	1214	CLA	C1C-NC	-3.59	1.32	1.37
22	3	601	CLA	C1C-NC	-3.59	1.32	1.37
22	J	1901	CLA	MG-ND	-3.59	1.98	2.05
22	3	603	CLA	C1C-NC	-3.58	1.32	1.37
22	B	1208	CLA	C1C-NC	-3.58	1.32	1.37
22	B	1023	CLA	C1C-NC	-3.58	1.32	1.37
22	K	1403	CLA	C1C-NC	-3.58	1.32	1.37
22	A	1114	CLA	C3B-C2B	-3.58	1.35	1.40
22	6	607	CLA	C1C-NC	-3.58	1.32	1.37
22	A	1109	CLA	MG-ND	-3.57	1.98	2.05
22	3	604	CLA	C1C-NC	-3.57	1.32	1.37
22	A	1127	CLA	C1C-NC	-3.57	1.32	1.37
22	A	1140	CLA	C1C-NC	-3.57	1.32	1.37
22	5	609	CLA	C1C-NC	-3.56	1.32	1.37
22	8	603	CLA	C1C-NC	-3.56	1.32	1.37
48	7	504	C7Z	C2-C1	3.56	1.66	1.54
22	1	611	CLA	C1C-NC	-3.56	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1105	CLA	C1C-NC	-3.56	1.32	1.37
22	6	601	CLA	C1C-NC	-3.56	1.32	1.37
22	a	601	CLA	C1C-NC	-3.55	1.32	1.37
22	7	604	CLA	C1C-NC	-3.55	1.32	1.37
22	1	604	CLA	C1C-NC	-3.55	1.32	1.37
22	1	612	CLA	C1C-NC	-3.55	1.32	1.37
22	5	616	CLA	C1C-NC	-3.54	1.32	1.37
44	8	803	DGA	OG2-CB1	3.54	1.44	1.34
22	6	606	CLA	C1C-NC	-3.54	1.32	1.37
39	4	613	CHL	C3B-C2B	-3.54	1.35	1.40
22	B	1237	CLA	C1C-NC	-3.54	1.32	1.37
22	7	603	CLA	C1C-NC	-3.54	1.32	1.37
22	A	1109	CLA	C1C-NC	-3.53	1.32	1.37
22	4	606	CLA	C1C-NC	-3.53	1.32	1.37
22	B	1218	CLA	C1C-NC	-3.52	1.32	1.37
22	B	1229	CLA	C1C-NC	-3.52	1.32	1.37
22	1	615	CLA	C1C-NC	-3.52	1.32	1.37
22	B	1216	CLA	C1C-NC	-3.52	1.32	1.37
44	5	803	DGA	OG2-CB1	3.52	1.44	1.34
22	B	1226	CLA	C1C-NC	-3.52	1.32	1.37
22	A	1134	CLA	C1C-NC	-3.51	1.32	1.37
22	A	1118	CLA	C1C-NC	-3.51	1.32	1.37
22	B	1022	CLA	C1C-NC	-3.51	1.32	1.37
22	B	1221	CLA	C1C-NC	-3.50	1.32	1.37
22	a	602	CLA	C1C-NC	-3.50	1.32	1.37
22	L	1502	CLA	C1C-NC	-3.50	1.32	1.37
22	3	610	CLA	C1C-NC	-3.50	1.32	1.37
22	6	612	CLA	C1C-NC	-3.50	1.32	1.37
22	B	1213	CLA	C1C-NC	-3.50	1.32	1.37
22	K	1401	CLA	C1C-NC	-3.50	1.32	1.37
22	B	1203	CLA	C1C-NC	-3.50	1.32	1.37
39	4	618	CHL	C3B-C2B	-3.50	1.35	1.40
22	5	605	CLA	C1C-NC	-3.49	1.32	1.37
22	A	1130	CLA	C1C-NC	-3.49	1.32	1.37
22	8	620	CLA	C1C-NC	-3.49	1.32	1.37
22	A	1125	CLA	C3B-C2B	-3.49	1.35	1.40
22	6	615	CLA	C1C-NC	-3.49	1.32	1.37
22	5	602	CLA	C1C-NC	-3.48	1.32	1.37
22	B	1217	CLA	C1C-NC	-3.48	1.32	1.37
21	A	1011	CL0	OBD-CAD	3.48	1.28	1.22
22	B	1238	CLA	C1C-NC	-3.48	1.32	1.37
22	G	1603	CLA	C1C-NC	-3.48	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	618	CLA	C1C-NC	-3.47	1.32	1.37
22	1	606	CLA	C1C-NC	-3.47	1.32	1.37
22	7	608	CLA	C1C-NC	-3.46	1.32	1.37
22	6	602	CLA	C1C-NC	-3.46	1.32	1.37
22	A	1123	CLA	C1C-NC	-3.46	1.32	1.37
22	7	612	CLA	C1C-NC	-3.46	1.32	1.37
22	F	1301	CLA	C1C-NC	-3.46	1.32	1.37
22	7	615	CLA	C1C-NC	-3.46	1.32	1.37
22	7	602	CLA	C1C-NC	-3.46	1.32	1.37
22	A	1129	CLA	C1C-NC	-3.45	1.32	1.37
48	7	504	C7Z	C4-C5	-3.45	1.45	1.51
22	4	602	CLA	C1C-NC	-3.45	1.32	1.37
22	A	1127	CLA	C3B-C2B	-3.45	1.35	1.40
22	5	612	CLA	C1C-NC	-3.44	1.32	1.37
22	A	1120	CLA	C1C-NC	-3.44	1.32	1.37
22	A	1125	CLA	C1C-C2C	3.43	1.51	1.44
22	a	604	CLA	MG-ND	-3.43	1.99	2.05
22	4	610	CLA	C1C-NC	-3.43	1.32	1.37
22	4	617	CLA	C1C-NC	-3.43	1.32	1.37
22	A	1119	CLA	C1C-NC	-3.42	1.32	1.37
22	6	604	CLA	C1C-NC	-3.42	1.32	1.37
22	1	603	CLA	C1C-NC	-3.42	1.32	1.37
22	6	605	CLA	C1C-NC	-3.41	1.32	1.37
22	8	611	CLA	C1C-NC	-3.41	1.32	1.37
22	a	605	CLA	C1C-NC	-3.41	1.32	1.37
22	B	1225	CLA	C3B-C2B	-3.41	1.35	1.40
39	3	611	CHL	C4B-NB	3.40	1.38	1.35
22	1	601	CLA	C1C-NC	-3.40	1.32	1.37
22	a	603	CLA	C1C-NC	-3.40	1.32	1.37
22	4	615	CLA	C1C-NC	-3.39	1.32	1.37
22	5	618	CLA	C1C-NC	-3.39	1.32	1.37
22	5	606	CLA	C1C-NC	-3.39	1.32	1.37
22	K	1404	CLA	C1C-NC	-3.39	1.32	1.37
39	7	613	CHL	C3B-C2B	-3.38	1.35	1.40
22	3	602	CLA	C1C-NC	-3.38	1.32	1.37
22	G	1601	CLA	C1C-NC	-3.38	1.32	1.37
22	L	1501	CLA	CBB-CAB	3.38	1.51	1.29
22	a	602	CLA	CBB-CAB	3.38	1.51	1.29
22	4	608	CLA	C1C-NC	-3.37	1.32	1.37
22	J	1901	CLA	C1C-NC	-3.37	1.32	1.37
22	6	618	CLA	CBB-CAB	3.37	1.51	1.29
22	5	608	CLA	CBB-CAB	3.37	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	7	504	C7Z	C35-C34	3.37	1.53	1.43
22	A	1012	CLA	CBB-CAB	3.37	1.51	1.29
22	A	1123	CLA	CBB-CAB	3.36	1.51	1.29
22	6	607	CLA	CBB-CAB	3.36	1.51	1.29
22	B	1219	CLA	CBB-CAB	3.36	1.51	1.29
22	a	608	CLA	CBB-CAB	3.36	1.51	1.29
22	1	615	CLA	CBB-CAB	3.36	1.51	1.29
39	1	613	CHL	CBB-CAB	3.36	1.51	1.29
22	8	620	CLA	CBB-CAB	3.36	1.51	1.29
22	4	615	CLA	CBB-CAB	3.36	1.51	1.29
22	6	615	CLA	CBB-CAB	3.36	1.51	1.29
22	7	611	CLA	C1C-NC	-3.36	1.32	1.37
22	5	617	CLA	CBB-CAB	3.35	1.51	1.29
22	4	612	CLA	C1C-NC	-3.35	1.32	1.37
22	a	608	CLA	C1C-NC	-3.35	1.32	1.37
22	6	608	CLA	CBB-CAB	3.35	1.51	1.29
22	4	602	CLA	CBB-CAB	3.35	1.51	1.29
22	G	1602	CLA	C1C-NC	-3.35	1.32	1.37
22	a	607	CLA	CBB-CAB	3.35	1.51	1.29
22	5	607	CLA	CBB-CAB	3.35	1.51	1.29
44	5	803	DGA	OG1-CA1	3.35	1.43	1.33
22	B	1021	CLA	C3B-C2B	-3.35	1.35	1.40
22	6	602	CLA	CBB-CAB	3.35	1.51	1.29
22	6	608	CLA	C1C-NC	-3.35	1.32	1.37
22	B	1222	CLA	CBB-CAB	3.35	1.51	1.29
22	A	1013	CLA	CBB-CAB	3.35	1.51	1.29
22	B	1221	CLA	CBB-CAB	3.35	1.51	1.29
22	A	1141	CLA	C1C-NC	-3.35	1.32	1.37
22	7	617	CLA	CBB-CAB	3.35	1.51	1.29
22	5	616	CLA	CBB-CAB	3.35	1.51	1.29
22	4	617	CLA	CBB-CAB	3.34	1.51	1.29
22	8	618	CLA	CBB-CAB	3.34	1.51	1.29
22	3	602	CLA	CBB-CAB	3.34	1.51	1.29
22	L	1503	CLA	CBB-CAB	3.34	1.51	1.29
22	F	1301	CLA	CBB-CAB	3.34	1.51	1.29
35	J	4002	RRX	C29-C30	3.34	1.65	1.54
22	8	602	CLA	CBB-CAB	3.34	1.51	1.29
22	8	605	CLA	CBB-CAB	3.34	1.51	1.29
22	6	617	CLA	CBB-CAB	3.34	1.51	1.29
22	3	618	CLA	CBB-CAB	3.34	1.51	1.29
22	B	1231	CLA	CBB-CAB	3.34	1.51	1.29
22	a	604	CLA	C1C-NC	-3.34	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	G	1602	CLA	CBB-CAB	3.34	1.51	1.29
22	6	604	CLA	CBB-CAB	3.34	1.51	1.29
22	5	601	CLA	CBB-CAB	3.34	1.51	1.29
22	8	608	CLA	CBB-CAB	3.34	1.51	1.29
48	7	504	C7Z	C27-C26	3.34	1.56	1.45
22	8	615	CLA	C1C-NC	-3.34	1.32	1.37
22	5	609	CLA	CBB-CAB	3.34	1.51	1.29
22	L	1502	CLA	CBB-CAB	3.33	1.51	1.29
22	5	618	CLA	CBB-CAB	3.33	1.51	1.29
22	6	601	CLA	CBB-CAB	3.33	1.51	1.29
22	B	1206	CLA	CBB-CAB	3.33	1.51	1.29
22	5	603	CLA	CBB-CAB	3.33	1.51	1.29
22	a	612	CLA	CBB-CAB	3.33	1.51	1.29
22	3	616	CLA	CBB-CAB	3.33	1.51	1.29
22	5	602	CLA	CBB-CAB	3.33	1.51	1.29
39	a	610	CHL	CBB-CAB	3.33	1.51	1.29
22	1	607	CLA	CBB-CAB	3.33	1.51	1.29
22	1	612	CLA	CBB-CAB	3.33	1.51	1.29
22	A	1117	CLA	CBB-CAB	3.33	1.51	1.29
22	B	1207	CLA	CBB-CAB	3.33	1.51	1.29
22	a	603	CLA	CBB-CAB	3.33	1.51	1.29
22	A	1137	CLA	CBB-CAB	3.33	1.51	1.29
22	4	607	CLA	CBB-CAB	3.33	1.51	1.29
22	3	607	CLA	CBB-CAB	3.33	1.51	1.29
22	5	612	CLA	CBB-CAB	3.33	1.51	1.29
22	G	1603	CLA	CBB-CAB	3.33	1.51	1.29
22	A	1139	CLA	CBB-CAB	3.33	1.51	1.29
22	1	605	CLA	CBB-CAB	3.33	1.51	1.29
22	1	602	CLA	CBB-CAB	3.33	1.51	1.29
22	B	1205	CLA	CBB-CAB	3.33	1.51	1.29
22	B	1236	CLA	CBB-CAB	3.33	1.51	1.29
22	7	615	CLA	CBB-CAB	3.32	1.51	1.29
22	K	1404	CLA	CBB-CAB	3.32	1.51	1.29
22	F	1302	CLA	CBB-CAB	3.32	1.51	1.29
22	B	1227	CLA	CBB-CAB	3.32	1.51	1.29
22	A	1110	CLA	CBB-CAB	3.32	1.51	1.29
22	A	1132	CLA	CBB-CAB	3.32	1.51	1.29
22	5	614	CLA	CBB-CAB	3.32	1.51	1.29
22	8	615	CLA	CBB-CAB	3.32	1.51	1.29
22	4	607	CLA	C1C-NC	-3.32	1.32	1.37
22	7	610	CLA	CBB-CAB	3.32	1.51	1.29
22	7	607	CLA	CBB-CAB	3.32	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	605	CLA	CBB-CAB	3.32	1.51	1.29
22	J	1901	CLA	CBB-CAB	3.32	1.51	1.29
22	A	1101	CLA	CBB-CAB	3.32	1.51	1.29
22	4	616	CLA	CBB-CAB	3.32	1.51	1.29
22	B	1227	CLA	C1C-NC	-3.32	1.32	1.37
22	A	1140	CLA	CBB-CAB	3.32	1.51	1.29
22	1	611	CLA	CBB-CAB	3.32	1.51	1.29
22	B	1210	CLA	CBB-CAB	3.32	1.51	1.29
22	B	1217	CLA	CBB-CAB	3.32	1.51	1.29
22	3	605	CLA	CBB-CAB	3.32	1.51	1.29
22	1	610	CLA	CBB-CAB	3.32	1.51	1.29
22	a	615	CLA	CBB-CAB	3.32	1.51	1.29
22	B	1201	CLA	CBB-CAB	3.32	1.51	1.29
22	B	1215	CLA	CBB-CAB	3.31	1.51	1.29
22	1	601	CLA	CBB-CAB	3.31	1.51	1.29
22	A	1107	CLA	CBB-CAB	3.31	1.51	1.29
22	B	1211	CLA	CBB-CAB	3.31	1.51	1.29
22	A	1126	CLA	CBB-CAB	3.31	1.51	1.29
22	G	1601	CLA	CBB-CAB	3.31	1.51	1.29
22	7	612	CLA	CBB-CAB	3.31	1.51	1.29
22	4	605	CLA	CBB-CAB	3.31	1.51	1.29
22	8	611	CLA	CBB-CAB	3.31	1.51	1.29
22	K	1401	CLA	CBB-CAB	3.31	1.51	1.29
22	5	606	CLA	CBB-CAB	3.31	1.51	1.29
35	J	4002	RRX	C11-C10	3.31	1.53	1.43
22	4	610	CLA	CBB-CAB	3.31	1.51	1.29
22	B	1216	CLA	CBB-CAB	3.31	1.51	1.29
22	7	603	CLA	CBB-CAB	3.31	1.51	1.29
22	A	1111	CLA	CBB-CAB	3.31	1.51	1.29
22	A	1122	CLA	CBB-CAB	3.31	1.51	1.29
22	3	613	CLA	CBB-CAB	3.31	1.51	1.29
22	a	601	CLA	CBB-CAB	3.31	1.51	1.29
22	8	607	CLA	CBB-CAB	3.31	1.51	1.29
22	A	1120	CLA	CBB-CAB	3.31	1.51	1.29
22	3	601	CLA	CBB-CAB	3.31	1.51	1.29
22	4	601	CLA	CBB-CAB	3.31	1.51	1.29
22	A	1121	CLA	CBB-CAB	3.31	1.51	1.29
22	A	1131	CLA	CBB-CAB	3.31	1.51	1.29
22	1	608	CLA	CBB-CAB	3.31	1.51	1.29
22	7	606	CLA	CBB-CAB	3.31	1.51	1.29
22	6	617	CLA	C1C-NC	-3.31	1.32	1.37
22	A	1119	CLA	CBB-CAB	3.31	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	608	CLA	CBB-CAB	3.31	1.51	1.29
22	A	1012	CLA	C1C-NC	-3.31	1.32	1.37
22	4	612	CLA	CBB-CAB	3.31	1.51	1.29
22	B	1223	CLA	CBB-CAB	3.30	1.51	1.29
22	B	1224	CLA	CBB-CAB	3.30	1.51	1.29
22	B	1023	CLA	CBB-CAB	3.30	1.51	1.29
22	B	1228	CLA	CBB-CAB	3.30	1.51	1.29
22	5	605	CLA	CBB-CAB	3.30	1.51	1.29
22	A	1118	CLA	CBB-CAB	3.30	1.51	1.29
22	K	1402	CLA	CBB-CAB	3.30	1.51	1.29
26	B	5003	DGD	CAA-C9A	-3.30	1.33	1.51
22	1	607	CLA	C1C-NC	-3.30	1.32	1.37
22	3	612	CLA	CBB-CAB	3.30	1.51	1.29
22	4	606	CLA	CBB-CAB	3.30	1.51	1.29
22	B	1229	CLA	CBB-CAB	3.30	1.51	1.29
26	B	5003	DGD	CGB-CFB	-3.30	1.33	1.51
22	B	1226	CLA	CBB-CAB	3.30	1.51	1.29
26	8	802	DGD	CAA-C9A	-3.30	1.33	1.51
22	1	608	CLA	C1C-NC	-3.30	1.32	1.37
22	B	1230	CLA	CBB-CAB	3.30	1.51	1.29
22	A	1108	CLA	CBB-CAB	3.30	1.51	1.29
22	1	606	CLA	CBB-CAB	3.30	1.51	1.29
22	7	606	CLA	C1C-NC	-3.30	1.32	1.37
22	B	1232	CLA	CBB-CAB	3.30	1.51	1.29
22	8	603	CLA	CBB-CAB	3.30	1.51	1.29
22	A	1109	CLA	CBB-CAB	3.30	1.51	1.29
22	7	601	CLA	CBB-CAB	3.30	1.51	1.29
22	K	1402	CLA	C1C-NC	-3.30	1.32	1.37
39	3	608	CHL	CBB-CAB	3.29	1.51	1.29
22	A	1141	CLA	CBB-CAB	3.29	1.51	1.29
22	B	1218	CLA	CBB-CAB	3.29	1.51	1.29
22	a	611	CLA	CBB-CAB	3.29	1.51	1.29
22	B	1239	CLA	CBB-CAB	3.29	1.51	1.29
22	B	1209	CLA	CBB-CAB	3.29	1.51	1.29
22	7	608	CLA	CBB-CAB	3.29	1.51	1.29
22	a	605	CLA	CBB-CAB	3.29	1.51	1.29
22	A	1102	CLA	CBB-CAB	3.29	1.51	1.29
22	K	1403	CLA	CBB-CAB	3.29	1.51	1.29
22	B	1238	CLA	CBB-CAB	3.29	1.51	1.29
22	B	1237	CLA	C3B-C2B	-3.29	1.35	1.40
22	5	604	CLA	CBB-CAB	3.29	1.51	1.29
22	A	1124	CLA	CBB-CAB	3.29	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1113	CLA	CBB-CAB	3.29	1.51	1.29
22	A	1135	CLA	CBB-CAB	3.29	1.51	1.29
22	A	1134	CLA	CBB-CAB	3.29	1.51	1.29
22	7	602	CLA	CBB-CAB	3.29	1.51	1.29
22	4	603	CLA	CBB-CAB	3.29	1.51	1.29
22	8	606	CLA	CBB-CAB	3.29	1.51	1.29
22	A	1105	CLA	CBB-CAB	3.29	1.51	1.29
22	B	1214	CLA	CBB-CAB	3.28	1.51	1.29
22	7	611	CLA	CBB-CAB	3.28	1.51	1.29
22	a	607	CLA	C1C-NC	-3.28	1.32	1.37
39	6	619	CHL	CBB-CAB	3.28	1.51	1.29
22	B	1208	CLA	CBB-CAB	3.28	1.51	1.29
26	B	5003	DGD	CDB-CCB	-3.28	1.33	1.51
22	A	1138	CLA	CBB-CAB	3.28	1.51	1.29
22	A	1136	CLA	CBB-CAB	3.28	1.51	1.29
22	B	1204	CLA	CBB-CAB	3.28	1.51	1.29
22	8	610	CLA	CBB-CAB	3.28	1.51	1.29
22	B	1212	CLA	CBB-CAB	3.28	1.51	1.29
22	4	604	CLA	CBB-CAB	3.28	1.51	1.29
22	7	604	CLA	CBB-CAB	3.28	1.51	1.29
22	3	603	CLA	CBB-CAB	3.28	1.51	1.29
22	A	1127	CLA	CBB-CAB	3.28	1.51	1.29
22	6	606	CLA	CBB-CAB	3.28	1.51	1.29
22	3	610	CLA	CBB-CAB	3.28	1.51	1.29
22	4	611	CLA	CBB-CAB	3.28	1.51	1.29
22	A	1129	CLA	CBB-CAB	3.27	1.51	1.29
22	B	1235	CLA	CBB-CAB	3.27	1.51	1.29
22	3	604	CLA	CBB-CAB	3.27	1.51	1.29
22	B	1213	CLA	CBB-CAB	3.27	1.51	1.29
22	A	1103	CLA	CBB-CAB	3.27	1.51	1.29
39	5	613	CHL	CBB-CAB	3.27	1.51	1.29
22	6	612	CLA	CBB-CAB	3.27	1.51	1.29
22	B	1237	CLA	CBB-CAB	3.27	1.50	1.29
39	a	613	CHL	CBB-CAB	3.26	1.50	1.29
22	A	1115	CLA	CBB-CAB	3.26	1.50	1.29
22	A	1112	CLA	CBB-CAB	3.26	1.50	1.29
22	A	1104	CLA	CBB-CAB	3.26	1.50	1.29
22	A	1106	CLA	CBB-CAB	3.26	1.50	1.29
22	A	1128	CLA	CBB-CAB	3.26	1.50	1.29
22	3	606	CLA	CBB-CAB	3.26	1.50	1.29
22	B	1220	CLA	CBB-CAB	3.26	1.50	1.29
22	1	603	CLA	CBB-CAB	3.26	1.50	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	5003	DGD	CGA-CFA	-3.26	1.33	1.51
22	B	1022	CLA	C3B-C2B	-3.25	1.35	1.40
22	B	1022	CLA	CBB-CAB	3.25	1.50	1.29
22	B	1021	CLA	CBB-CAB	3.25	1.50	1.29
22	A	1130	CLA	CBB-CAB	3.25	1.50	1.29
22	5	608	CLA	C1C-NC	-3.25	1.33	1.37
22	6	603	CLA	CBB-CAB	3.25	1.50	1.29
22	B	1240	CLA	CBB-CAB	3.25	1.50	1.29
22	8	612	CLA	CBB-CAB	3.25	1.50	1.29
22	1	604	CLA	CBB-CAB	3.24	1.50	1.29
22	B	1202	CLA	CBB-CAB	3.24	1.50	1.29
22	8	609	CLA	CBB-CAB	3.24	1.50	1.29
26	8	802	DGD	CGA-CFA	-3.24	1.33	1.51
22	5	614	CLA	C1C-NC	-3.24	1.33	1.37
22	4	616	CLA	C1C-NC	-3.24	1.33	1.37
39	4	613	CHL	CBB-CAB	3.24	1.50	1.29
26	8	802	DGD	CDA-CCA	-3.24	1.33	1.51
26	8	802	DGD	CGB-CFB	-3.24	1.33	1.51
26	8	802	DGD	CAB-C9B	-3.23	1.33	1.51
22	7	605	CLA	CBB-CAB	3.23	1.50	1.29
22	B	1225	CLA	CBB-CAB	3.23	1.50	1.29
39	a	606	CHL	CBB-CAB	3.23	1.50	1.29
26	B	5003	DGD	CAB-C9B	-3.23	1.33	1.51
22	A	1103	CLA	C3B-C2B	-3.23	1.35	1.40
22	A	1114	CLA	CBB-CAB	3.22	1.50	1.29
22	7	609	CLA	CBB-CAB	3.22	1.50	1.29
39	1	609	CHL	CBB-CAB	3.22	1.50	1.29
39	a	609	CHL	C4B-NB	3.22	1.38	1.35
22	A	1133	CLA	CBB-CAB	3.22	1.50	1.29
22	B	1234	CLA	CBB-CAB	3.22	1.50	1.29
22	A	1125	CLA	CBB-CAB	3.22	1.50	1.29
22	A	1116	CLA	CBB-CAB	3.22	1.50	1.29
35	J	4002	RRX	C16-C17	3.21	1.53	1.43
26	B	5003	DGD	CDA-CCA	-3.21	1.33	1.51
22	a	604	CLA	CBB-CAB	3.20	1.50	1.29
39	4	609	CHL	CBB-CAB	3.20	1.50	1.29
39	5	610	CHL	CBB-CAB	3.20	1.50	1.29
39	4	618	CHL	CBB-CAB	3.20	1.50	1.29
30	6	803	PCW	O3-C11	3.20	1.42	1.33
22	B	1203	CLA	C3B-C2B	-3.19	1.35	1.40
22	A	1133	CLA	C3B-C2B	-3.19	1.35	1.40
22	B	1229	CLA	C3B-C2B	-3.18	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	a	606	CHL	C3B-C2B	-3.18	1.36	1.40
22	6	609	CLA	CBB-CAB	3.18	1.50	1.29
39	a	610	CHL	C4B-NB	3.17	1.38	1.35
39	6	610	CHL	CBB-CAB	3.16	1.50	1.29
22	A	1116	CLA	C3B-C2B	-3.16	1.36	1.40
22	B	1234	CLA	C3B-C2B	-3.16	1.36	1.40
22	B	1203	CLA	CBB-CAB	3.16	1.50	1.29
22	A	1125	CLA	C1C-NC	-3.16	1.33	1.37
22	B	1239	CLA	C3B-C2B	-3.16	1.36	1.40
22	8	609	CLA	C3B-C2B	-3.15	1.36	1.40
30	B	5004	PCW	O3-C11	3.15	1.42	1.33
26	8	802	DGD	CDB-CCB	-3.15	1.33	1.51
22	B	1215	CLA	C3B-C2B	-3.14	1.36	1.40
39	a	609	CHL	CBB-CAB	3.14	1.50	1.29
39	8	604	CHL	C4B-NB	3.14	1.38	1.35
21	A	1011	CL0	C1C-NC	-3.14	1.33	1.37
32	B	5007	LAP	P9-O6	3.14	1.72	1.59
37	M	4001	ECH	C30-C25	-3.13	1.49	1.53
39	8	613	CHL	CBB-CAB	3.12	1.50	1.29
22	F	1302	CLA	C1C-NC	-3.12	1.33	1.37
39	6	613	CHL	CBB-CAB	3.12	1.50	1.29
21	A	1011	CL0	MG-NC	3.12	2.13	2.06
39	6	611	CHL	CBB-CAB	3.12	1.50	1.29
41	3	506	QTB	C14-C12	-3.11	1.46	1.53
22	B	1231	CLA	C3B-C2B	-3.11	1.36	1.40
39	a	613	CHL	C4B-NB	3.10	1.38	1.35
39	4	618	CHL	C4B-NB	3.10	1.38	1.35
22	B	1209	CLA	C3B-C2B	-3.09	1.36	1.40
32	K	5001	LAP	P9-O4	3.09	1.71	1.59
39	5	611	CHL	C4B-NB	3.09	1.38	1.35
39	7	613	CHL	CBB-CAB	3.08	1.49	1.29
22	A	1132	CLA	C3B-C2B	-3.08	1.36	1.40
39	a	606	CHL	C4B-NB	3.08	1.38	1.35
22	B	1205	CLA	C3B-C2B	-3.08	1.36	1.40
35	J	4002	RRX	C4-C5	-3.08	1.44	1.51
32	B	5007	LAP	P9-O4	3.07	1.71	1.59
22	8	612	CLA	C3B-C2B	-3.05	1.36	1.40
22	B	1232	CLA	C3B-C2B	-3.05	1.36	1.40
39	5	610	CHL	C3B-C2B	-3.04	1.36	1.40
22	3	616	CLA	C3B-C2B	-3.04	1.36	1.40
35	J	4002	RRX	C7-C6	3.04	1.55	1.45
22	A	1104	CLA	C3B-C2B	-3.04	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	1204	CLA	C3B-C2B	-3.04	1.36	1.40
39	8	613	CHL	C4B-NB	3.04	1.37	1.35
22	A	1130	CLA	C3B-C2B	-3.03	1.36	1.40
22	A	1108	CLA	C3B-C2B	-3.03	1.36	1.40
37	M	4001	ECH	C25-C26	-3.03	1.31	1.35
39	3	608	CHL	C4B-NB	3.03	1.37	1.35
22	A	1115	CLA	C3B-C2B	-3.03	1.36	1.40
39	8	601	CHL	CBB-CAB	3.02	1.49	1.29
48	7	504	C7Z	C21-C26	-3.01	1.49	1.53
22	B	1202	CLA	C3B-C2B	-3.01	1.36	1.40
22	8	618	CLA	C3B-C2B	-3.01	1.36	1.40
39	5	611	CHL	CBB-CAB	3.01	1.49	1.29
49	8	806	P5S	O37-C38	3.01	1.42	1.34
22	A	1101	CLA	C3B-C2B	-3.01	1.36	1.40
39	8	604	CHL	CBB-CAB	3.00	1.49	1.29
22	6	609	CLA	C1C-NC	-2.99	1.33	1.37
22	A	1135	CLA	C3B-C2B	-2.98	1.36	1.40
22	B	1207	CLA	C3B-C2B	-2.98	1.36	1.40
22	7	609	CLA	C3B-C2B	-2.97	1.36	1.40
22	A	1125	CLA	CHC-C1C	2.97	1.42	1.35
22	A	1120	CLA	C3B-C2B	-2.96	1.36	1.40
39	6	611	CHL	C4B-NB	2.96	1.37	1.35
39	8	601	CHL	C4B-NB	2.96	1.37	1.35
22	K	1401	CLA	C3B-C2B	-2.95	1.36	1.40
22	B	1223	CLA	C3B-C2B	-2.94	1.36	1.40
22	A	1106	CLA	C3B-C2B	-2.94	1.36	1.40
22	B	1214	CLA	C3B-C2B	-2.94	1.36	1.40
22	7	602	CLA	C3B-C2B	-2.94	1.36	1.40
22	5	602	CLA	C3B-C2B	-2.94	1.36	1.40
22	1	611	CLA	C3B-C2B	-2.93	1.36	1.40
22	4	603	CLA	C3B-C2B	-2.93	1.36	1.40
22	A	1122	CLA	C3B-C2B	-2.93	1.36	1.40
22	B	1206	CLA	C3B-C2B	-2.93	1.36	1.40
22	1	603	CLA	C3B-C2B	-2.93	1.36	1.40
22	a	604	CLA	C3B-C2B	-2.92	1.36	1.40
22	4	611	CLA	C3B-C2B	-2.92	1.36	1.40
22	A	1134	CLA	C3B-C2B	-2.92	1.36	1.40
22	B	1212	CLA	C3B-C2B	-2.91	1.36	1.40
39	3	611	CHL	CBB-CAB	2.91	1.48	1.29
44	8	803	DGA	OG1-CA1	2.91	1.41	1.33
22	B	1213	CLA	C3B-C2B	-2.91	1.36	1.40
22	3	618	CLA	C3B-C2B	-2.90	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	7	613	CHL	C4B-NB	2.90	1.37	1.35
22	a	604	CLA	CHC-C1C	2.90	1.42	1.35
22	B	1217	CLA	C3B-C2B	-2.90	1.36	1.40
22	A	1118	CLA	C3B-C2B	-2.90	1.36	1.40
22	A	1136	CLA	C3B-C2B	-2.90	1.36	1.40
22	F	1302	CLA	CHC-C1C	2.89	1.42	1.35
22	G	1601	CLA	C3B-C2B	-2.88	1.36	1.40
22	A	1140	CLA	C3B-C2B	-2.88	1.36	1.40
22	B	1220	CLA	C3B-C2B	-2.87	1.36	1.40
22	8	605	CLA	C3B-C2B	-2.87	1.36	1.40
39	5	613	CHL	C4B-NB	2.87	1.37	1.35
22	6	606	CLA	C3B-C2B	-2.87	1.36	1.40
22	3	603	CLA	C3B-C2B	-2.86	1.36	1.40
22	B	1238	CLA	C3B-C2B	-2.86	1.36	1.40
22	1	604	CLA	C1C-C2C	2.86	1.50	1.44
22	1	604	CLA	C3B-C2B	-2.86	1.36	1.40
22	7	610	CLA	C3B-C2B	-2.85	1.36	1.40
22	8	602	CLA	C3B-C2B	-2.85	1.36	1.40
22	5	617	CLA	C3B-C2B	-2.85	1.36	1.40
22	A	1137	CLA	C3B-C2B	-2.84	1.36	1.40
24	A	4004	BCR	C12-C13	-2.84	1.39	1.45
22	A	1105	CLA	C3B-C2B	-2.84	1.36	1.40
36	J	5001	LPX	P1-O1	2.83	1.70	1.59
22	B	1224	CLA	C3B-C2B	-2.82	1.36	1.40
39	4	609	CHL	C4B-NB	2.82	1.37	1.35
39	4	613	CHL	C4B-NB	2.82	1.37	1.35
22	1	604	CLA	CHC-C1C	2.82	1.42	1.35
21	A	1011	CL0	C3D-C2D	2.82	1.46	1.39
22	B	1216	CLA	C3B-C2B	-2.81	1.36	1.40
36	a	804	LPX	P1-O1	2.81	1.70	1.59
39	4	618	CHL	C3A-C2A	-2.81	1.46	1.54
22	A	1139	CLA	C3B-C2B	-2.80	1.36	1.40
39	1	613	CHL	C4B-NB	2.80	1.37	1.35
22	B	1203	CLA	CHC-C1C	2.80	1.42	1.35
22	K	1403	CLA	C3B-C2B	-2.80	1.36	1.40
22	5	605	CLA	C3B-C2B	-2.79	1.36	1.40
22	A	1012	CLA	C3B-C2B	-2.79	1.36	1.40
22	5	616	CLA	C3B-C2B	-2.78	1.36	1.40
22	5	608	CLA	CHC-C1C	2.78	1.42	1.35
22	7	607	CLA	C3B-C2B	-2.77	1.36	1.40
22	1	601	CLA	CHC-C1C	2.77	1.42	1.35
22	A	1109	CLA	C3B-C2B	-2.77	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1128	CLA	C3B-C2B	-2.77	1.36	1.40
29	B	5006	LMT	O3'-C3'	-2.76	1.36	1.43
22	K	1402	CLA	CHC-C1C	2.76	1.42	1.35
39	a	610	CHL	C3B-C2B	-2.76	1.36	1.40
22	8	608	CLA	C3B-C2B	-2.75	1.36	1.40
22	K	1402	CLA	C3B-C2B	-2.75	1.36	1.40
22	5	606	CLA	C3B-C2B	-2.75	1.36	1.40
22	5	614	CLA	C3B-C2B	-2.75	1.36	1.40
22	7	608	CLA	C3B-C2B	-2.75	1.36	1.40
22	B	1240	CLA	C3B-C2B	-2.75	1.36	1.40
22	5	618	CLA	C3B-C2B	-2.74	1.36	1.40
22	4	605	CLA	C3B-C2B	-2.74	1.36	1.40
22	B	1234	CLA	CHC-C1C	2.73	1.42	1.35
22	5	612	CLA	C3B-C2B	-2.73	1.36	1.40
22	7	617	CLA	C3B-C2B	-2.72	1.36	1.40
22	a	607	CLA	C3B-C2B	-2.72	1.36	1.40
22	B	1236	CLA	C3B-C2B	-2.71	1.36	1.40
39	5	610	CHL	C4B-NB	2.71	1.37	1.35
39	4	609	CHL	C3B-C2B	-2.71	1.36	1.40
22	A	1110	CLA	C3B-C2B	-2.71	1.36	1.40
22	7	603	CLA	C3B-C2B	-2.71	1.36	1.40
29	1	804	LMT	O2'-C2'	-2.70	1.36	1.43
22	6	603	CLA	C3D-C4D	-2.70	1.38	1.44
22	G	1602	CLA	CHC-C1C	2.70	1.41	1.35
22	K	1404	CLA	C3B-C2B	-2.70	1.36	1.40
22	5	607	CLA	C3B-C2B	-2.70	1.36	1.40
22	B	1213	CLA	CHC-C1C	2.70	1.41	1.35
39	6	613	CHL	C4B-NB	2.69	1.37	1.35
22	F	1301	CLA	C3B-C2B	-2.69	1.36	1.40
49	8	806	P5S	O19-C17	2.69	1.41	1.33
22	a	602	CLA	C3B-C2B	-2.69	1.36	1.40
39	6	610	CHL	C4B-NB	2.69	1.37	1.35
22	6	609	CLA	CHC-C1C	2.69	1.41	1.35
22	6	618	CLA	CHC-C1C	2.69	1.41	1.35
22	G	1603	CLA	CHC-C1C	2.69	1.41	1.35
22	B	1228	CLA	CAA-C2A	-2.69	1.49	1.54
22	7	605	CLA	CHC-C1C	2.69	1.41	1.35
22	B	1228	CLA	C2A-C1A	-2.68	1.46	1.52
22	B	1231	CLA	CHC-C1C	2.68	1.41	1.35
39	1	609	CHL	C3B-C2B	-2.68	1.36	1.40
22	4	616	CLA	C3B-C2B	-2.68	1.36	1.40
22	B	1227	CLA	CHC-C1C	2.68	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	607	CLA	C3B-C2B	-2.67	1.36	1.40
22	6	602	CLA	CHC-C1C	2.67	1.41	1.35
22	6	602	CLA	C3B-C2B	-2.66	1.36	1.40
22	a	601	CLA	CHC-C1C	2.66	1.41	1.35
22	A	1127	CLA	CHC-C1C	2.66	1.41	1.35
22	4	604	CLA	C3B-C2B	-2.66	1.36	1.40
22	A	1123	CLA	CHC-C1C	2.66	1.41	1.35
22	B	1228	CLA	C3B-C2B	-2.66	1.36	1.40
22	B	1210	CLA	C4B-NB	-2.66	1.32	1.35
22	8	603	CLA	C3B-C2B	-2.66	1.36	1.40
22	B	1023	CLA	CHC-C1C	2.66	1.41	1.35
22	4	602	CLA	C3B-C2B	-2.65	1.36	1.40
22	3	603	CLA	CHC-C1C	2.65	1.41	1.35
22	B	1226	CLA	C3B-C2B	-2.65	1.36	1.40
22	5	604	CLA	C3D-C4D	-2.64	1.38	1.44
22	1	607	CLA	CHC-C1C	2.64	1.41	1.35
22	3	605	CLA	C3B-C2B	-2.64	1.36	1.40
39	6	619	CHL	C3A-C2A	-2.64	1.47	1.54
22	A	1119	CLA	CHC-C1C	2.64	1.41	1.35
22	6	607	CLA	CHC-C1C	2.63	1.41	1.35
22	A	1012	CLA	CHC-C1C	2.63	1.41	1.35
22	A	1120	CLA	CHC-C1C	2.63	1.41	1.35
22	A	1131	CLA	C3B-C2B	-2.63	1.36	1.40
22	8	615	CLA	CHC-C1C	2.63	1.41	1.35
22	A	1141	CLA	C3B-C2B	-2.63	1.36	1.40
22	7	606	CLA	CHC-C1C	2.63	1.41	1.35
22	1	607	CLA	C3B-C2B	-2.63	1.36	1.40
22	1	612	CLA	C3B-C2B	-2.62	1.36	1.40
21	A	1011	CL0	C4D-CHA	2.62	1.47	1.38
22	1	608	CLA	CHC-C1C	2.62	1.41	1.35
22	B	1218	CLA	C3B-C2B	-2.62	1.36	1.40
22	4	604	CLA	CHC-C1C	2.62	1.41	1.35
22	B	1228	CLA	C3D-C4D	-2.62	1.38	1.44
22	5	601	CLA	CHC-C1C	2.61	1.41	1.35
22	1	603	CLA	CHC-C1C	2.61	1.41	1.35
22	K	1404	CLA	CHC-C1C	2.61	1.41	1.35
22	a	607	CLA	CHC-C1C	2.61	1.41	1.35
22	L	1502	CLA	CHC-C1C	2.61	1.41	1.35
22	6	615	CLA	CHC-C1C	2.60	1.41	1.35
22	7	604	CLA	CHC-C1C	2.60	1.41	1.35
22	7	603	CLA	CHC-C1C	2.60	1.41	1.35
26	A	5005	DGD	CAB-C9B	-2.60	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	8	808	4RF	O18-C16	2.60	1.40	1.33
22	1	608	CLA	C3B-C2B	-2.60	1.36	1.40
39	1	609	CHL	C4B-NB	2.60	1.37	1.35
29	1	804	LMT	O3'-C3'	-2.60	1.36	1.43
22	1	606	CLA	CHC-C1C	2.60	1.41	1.35
22	A	1102	CLA	CHC-C1C	2.60	1.41	1.35
22	a	602	CLA	CHC-C1C	2.59	1.41	1.35
22	3	604	CLA	C3B-C2B	-2.59	1.36	1.40
22	a	605	CLA	CHC-C1C	2.59	1.41	1.35
22	5	618	CLA	CHC-C1C	2.59	1.41	1.35
47	7	807	4RF	O21-C20	-2.59	1.40	1.46
22	G	1601	CLA	CHC-C1C	2.59	1.41	1.35
22	B	1238	CLA	CHC-C1C	2.58	1.41	1.35
38	5	505	LUT	C1-C6	-2.58	1.50	1.53
22	4	608	CLA	C3B-C2B	-2.58	1.36	1.40
39	6	619	CHL	C4B-NB	2.58	1.37	1.35
22	A	1105	CLA	CHC-C1C	2.58	1.41	1.35
22	4	615	CLA	CHC-C1C	2.58	1.41	1.35
22	a	608	CLA	CHC-C1C	2.57	1.41	1.35
22	B	1235	CLA	C3B-C2B	-2.57	1.36	1.40
22	L	1501	CLA	C3B-C2B	-2.57	1.36	1.40
22	1	611	CLA	CHC-C1C	2.57	1.41	1.35
22	A	1126	CLA	C3B-C2B	-2.57	1.36	1.40
22	L	1502	CLA	C3B-C2B	-2.57	1.36	1.40
22	K	1401	CLA	CHC-C1C	2.57	1.41	1.35
22	A	1130	CLA	CHC-C1C	2.57	1.41	1.35
22	4	607	CLA	CHC-C1C	2.57	1.41	1.35
22	B	1208	CLA	CHC-C1C	2.57	1.41	1.35
22	7	601	CLA	CHC-C1C	2.57	1.41	1.35
46	7	502	XAT	O24-C25	-2.56	1.42	1.46
22	4	616	CLA	CHC-C1C	2.56	1.41	1.35
22	1	602	CLA	C3B-C2B	-2.56	1.36	1.40
22	3	607	CLA	CHC-C1C	2.56	1.41	1.35
22	6	617	CLA	C3B-C2B	-2.55	1.36	1.40
22	7	605	CLA	C3B-C2B	-2.55	1.36	1.40
22	8	615	CLA	C3B-C2B	-2.55	1.36	1.40
22	A	1116	CLA	CHC-C1C	2.55	1.41	1.35
22	L	1503	CLA	CHC-C1C	2.55	1.41	1.35
22	6	612	CLA	CHC-C1C	2.55	1.41	1.35
22	A	1103	CLA	CHC-C1C	2.55	1.41	1.35
22	4	608	CLA	CHC-C1C	2.55	1.41	1.35
22	a	615	CLA	CHC-C1C	2.55	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	603	CLA	C3B-C2B	-2.55	1.36	1.40
22	B	1218	CLA	CHC-C1C	2.54	1.41	1.35
22	K	1403	CLA	CHC-C1C	2.54	1.41	1.35
22	6	605	CLA	CHC-C1C	2.54	1.41	1.35
22	3	610	CLA	C3B-C2B	-2.54	1.36	1.40
22	a	608	CLA	C3B-C2B	-2.54	1.36	1.40
38	a	502	LUT	C22-C21	-2.54	1.51	1.54
22	A	1107	CLA	CHC-C1C	2.54	1.41	1.35
39	a	613	CHL	C3B-C2B	-2.54	1.36	1.40
22	A	1124	CLA	C3B-C2B	-2.54	1.36	1.40
29	A	5008	LMT	O3'-C3'	-2.53	1.37	1.43
22	A	1013	CLA	C3B-C2B	-2.53	1.36	1.40
22	8	607	CLA	CHC-C1C	2.53	1.41	1.35
22	6	603	CLA	C1D-ND	-2.53	1.34	1.37
22	6	617	CLA	CHC-C1C	2.53	1.41	1.35
22	a	603	CLA	CHC-C1C	2.53	1.41	1.35
22	7	602	CLA	CHC-C1C	2.53	1.41	1.35
22	6	612	CLA	C3B-C2B	-2.53	1.36	1.40
22	B	1224	CLA	CHC-C1C	2.53	1.41	1.35
22	5	606	CLA	CHC-C1C	2.53	1.41	1.35
22	6	601	CLA	C3B-C2B	-2.53	1.36	1.40
22	A	1118	CLA	CHC-C1C	2.52	1.41	1.35
22	B	1219	CLA	CHC-C1C	2.52	1.41	1.35
22	3	602	CLA	CHC-C1C	2.52	1.41	1.35
22	6	604	CLA	CHC-C1C	2.52	1.41	1.35
41	a	504	QTB	C03-C02	-2.52	1.32	1.35
22	4	617	CLA	CHC-C1C	2.52	1.41	1.35
22	B	1230	CLA	CHC-C1C	2.52	1.41	1.35
22	4	612	CLA	CHC-C1C	2.52	1.41	1.35
22	A	1013	CLA	CHC-C1C	2.52	1.41	1.35
22	A	1129	CLA	CHC-C1C	2.51	1.41	1.35
22	A	1129	CLA	C3B-C2B	-2.51	1.36	1.40
22	A	1122	CLA	CHC-C1C	2.51	1.41	1.35
30	B	5004	PCW	O2-C2	-2.51	1.40	1.46
22	J	1901	CLA	CHC-C1C	2.51	1.41	1.35
22	4	612	CLA	C3B-C2B	-2.51	1.36	1.40
22	7	615	CLA	CHC-C1C	2.51	1.41	1.35
22	4	603	CLA	CHC-C1C	2.51	1.41	1.35
22	5	604	CLA	CHC-C1C	2.51	1.41	1.35
22	A	1111	CLA	CHC-C1C	2.51	1.41	1.35
22	8	620	CLA	CHC-C1C	2.51	1.41	1.35
22	B	1222	CLA	C3B-C2B	-2.50	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1140	CLA	CHC-C1C	2.50	1.41	1.35
22	5	607	CLA	CHC-C1C	2.50	1.41	1.35
22	B	1210	CLA	C3B-C2B	-2.50	1.36	1.40
22	A	1126	CLA	CHC-C1C	2.50	1.41	1.35
22	1	605	CLA	CHC-C1C	2.50	1.41	1.35
22	A	1131	CLA	C3D-C4D	-2.50	1.38	1.44
35	J	4002	RRX	C32-C1	2.50	1.58	1.53
22	3	604	CLA	CHC-C1C	2.50	1.41	1.35
22	4	602	CLA	CHC-C1C	2.50	1.41	1.35
39	1	609	CHL	C1B-NB	-2.50	1.33	1.35
22	5	605	CLA	CHC-C1C	2.50	1.41	1.35
21	A	1011	CL0	C1B-CHB	2.50	1.47	1.41
22	5	616	CLA	CHC-C1C	2.50	1.41	1.35
22	B	1229	CLA	CHC-C1C	2.50	1.41	1.35
22	5	612	CLA	CHC-C1C	2.50	1.41	1.35
22	A	1113	CLA	CHC-C1C	2.50	1.41	1.35
22	A	1106	CLA	CHC-C1C	2.50	1.41	1.35
22	6	618	CLA	C3B-C2B	-2.50	1.36	1.40
22	G	1603	CLA	C3B-C2B	-2.49	1.36	1.40
22	4	601	CLA	CHC-C1C	2.49	1.41	1.35
47	8	807	4RF	O18-C16	2.49	1.40	1.33
22	B	1202	CLA	CHC-C1C	2.49	1.41	1.35
22	B	1209	CLA	CHC-C1C	2.49	1.41	1.35
22	A	1121	CLA	CHC-C1C	2.49	1.41	1.35
22	6	608	CLA	CHC-C1C	2.49	1.41	1.35
22	B	1240	CLA	CHC-C1C	2.48	1.41	1.35
22	8	608	CLA	CHC-C1C	2.48	1.41	1.35
22	B	1215	CLA	CHC-C1C	2.48	1.41	1.35
22	A	1141	CLA	CHC-C1C	2.48	1.41	1.35
22	A	1134	CLA	CHC-C1C	2.48	1.41	1.35
22	a	612	CLA	CHC-C1C	2.48	1.41	1.35
22	5	614	CLA	CHC-C1C	2.48	1.41	1.35
22	A	1136	CLA	CHC-C1C	2.48	1.41	1.35
22	6	608	CLA	C3B-C2B	-2.48	1.36	1.40
22	a	611	CLA	C3B-C2B	-2.47	1.36	1.40
31	B	5005	PTY	O7-C6	-2.47	1.40	1.46
30	6	803	PCW	O2-C2	-2.47	1.40	1.46
22	7	609	CLA	CHC-C1C	2.47	1.41	1.35
22	A	1115	CLA	CHC-C1C	2.47	1.41	1.35
22	B	1228	CLA	CHC-C1C	2.47	1.41	1.35
22	6	601	CLA	CHC-C1C	2.47	1.41	1.35
22	a	611	CLA	CHC-C1C	2.47	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	1217	CLA	CHC-C1C	2.47	1.41	1.35
22	B	1235	CLA	CHC-C1C	2.47	1.41	1.35
22	5	609	CLA	CHC-C1C	2.47	1.41	1.35
22	7	611	CLA	CHC-C1C	2.47	1.41	1.35
22	B	1022	CLA	CHC-C1C	2.46	1.41	1.35
22	B	1201	CLA	CHC-C1C	2.46	1.41	1.35
22	3	601	CLA	CHC-C1C	2.46	1.41	1.35
24	A	4004	BCR	C35-C13	-2.46	1.45	1.50
22	1	610	CLA	C3B-C2B	-2.46	1.37	1.40
22	5	603	CLA	CHC-C1C	2.46	1.41	1.35
22	6	606	CLA	CHC-C1C	2.46	1.41	1.35
22	1	615	CLA	C3B-C2B	-2.46	1.37	1.40
27	A	5007	3PH	O21-C2	-2.46	1.40	1.46
22	A	1108	CLA	CHC-C1C	2.46	1.41	1.35
22	3	612	CLA	CHC-C1C	2.46	1.41	1.35
48	7	504	C7Z	C18-C5	2.46	1.55	1.50
39	a	609	CHL	C3A-C2A	-2.46	1.47	1.54
22	A	1124	CLA	C3D-C4D	-2.46	1.38	1.44
22	8	606	CLA	C3B-C2B	-2.46	1.37	1.40
22	5	601	CLA	C3B-C2B	-2.45	1.37	1.40
22	B	1205	CLA	C3D-C4D	-2.45	1.38	1.44
22	4	610	CLA	C3B-C2B	-2.45	1.37	1.40
22	5	602	CLA	CHC-C1C	2.45	1.41	1.35
22	7	617	CLA	CHC-C1C	2.45	1.41	1.35
22	A	1132	CLA	CHC-C1C	2.45	1.41	1.35
22	B	1221	CLA	CHC-C1C	2.45	1.41	1.35
22	1	615	CLA	CHC-C1C	2.45	1.41	1.35
22	A	1124	CLA	CHC-C1C	2.44	1.41	1.35
22	L	1501	CLA	CHC-C1C	2.44	1.41	1.35
31	3	802	PTY	O4-C30	2.44	1.40	1.33
22	A	1135	CLA	CHC-C1C	2.44	1.41	1.35
22	3	610	CLA	CHC-C1C	2.44	1.41	1.35
22	J	1901	CLA	C3B-C2B	-2.44	1.37	1.40
39	a	609	CHL	C3B-C2B	-2.44	1.37	1.40
22	3	606	CLA	CHC-C1C	2.44	1.41	1.35
22	A	1114	CLA	C3D-C4D	-2.44	1.38	1.44
22	A	1101	CLA	CHC-C1C	2.44	1.41	1.35
22	B	1022	CLA	C3D-C4D	-2.44	1.38	1.44
22	8	611	CLA	CHC-C1C	2.44	1.41	1.35
22	8	618	CLA	CHC-C1C	2.43	1.41	1.35
29	B	5006	LMT	O2B-C2B	-2.43	1.37	1.43
22	A	1110	CLA	CHC-C1C	2.43	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	1223	CLA	CHC-C1C	2.43	1.41	1.35
22	F	1301	CLA	CHC-C1C	2.43	1.41	1.35
22	1	610	CLA	CHC-C1C	2.43	1.41	1.35
22	A	1138	CLA	CHC-C1C	2.43	1.41	1.35
22	A	1102	CLA	C4B-NB	-2.43	1.33	1.35
22	6	607	CLA	C3B-C2B	-2.43	1.37	1.40
29	B	5006	LMT	O2'-C2'	-2.43	1.37	1.43
22	7	615	CLA	C3B-C2B	-2.43	1.37	1.40
29	A	5008	LMT	O2B-C2B	-2.43	1.37	1.43
22	B	1232	CLA	CHC-C1C	2.43	1.41	1.35
22	3	618	CLA	CHC-C1C	2.43	1.41	1.35
22	5	617	CLA	CHC-C1C	2.43	1.41	1.35
31	8	810	PTY	O7-C8	2.43	1.41	1.34
22	B	1237	CLA	CHC-C1C	2.43	1.41	1.35
22	B	1214	CLA	CHC-C1C	2.42	1.41	1.35
22	4	611	CLA	CHC-C1C	2.42	1.41	1.35
22	8	609	CLA	CHC-C1C	2.42	1.41	1.35
22	4	617	CLA	C3B-C2B	-2.42	1.37	1.40
22	B	1204	CLA	CHC-C1C	2.42	1.41	1.35
22	3	605	CLA	CHC-C1C	2.42	1.41	1.35
22	7	607	CLA	CHC-C1C	2.42	1.41	1.35
22	1	612	CLA	CHC-C1C	2.42	1.41	1.35
22	B	1225	CLA	C3D-C4D	-2.42	1.38	1.44
22	3	613	CLA	CHC-C1C	2.42	1.41	1.35
22	B	1222	CLA	CHC-C1C	2.42	1.41	1.35
22	5	605	CLA	C3D-C4D	-2.42	1.38	1.44
22	A	1109	CLA	CHC-C1C	2.41	1.41	1.35
30	6	803	PCW	O2-C31	2.41	1.41	1.34
22	7	612	CLA	CMB-C2B	-2.41	1.46	1.51
22	6	605	CLA	C3B-C2B	-2.41	1.37	1.40
22	8	602	CLA	CHC-C1C	2.41	1.41	1.35
29	1	804	LMT	O2B-C2B	-2.41	1.37	1.43
22	B	1225	CLA	CHC-C1C	2.41	1.41	1.35
22	A	1114	CLA	CHC-C1C	2.41	1.41	1.35
22	7	608	CLA	CHC-C1C	2.41	1.41	1.35
22	7	610	CLA	CHC-C1C	2.40	1.41	1.35
22	3	612	CLA	C3D-C4D	-2.40	1.38	1.44
22	4	606	CLA	CHC-C1C	2.40	1.41	1.35
22	B	1212	CLA	CHC-C1C	2.40	1.41	1.35
22	B	1239	CLA	CHC-C1C	2.40	1.41	1.35
22	1	602	CLA	CHC-C1C	2.40	1.41	1.35
22	A	1131	CLA	CHC-C1C	2.40	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	1211	CLA	CHC-C1C	2.40	1.41	1.35
22	6	615	CLA	C3B-C2B	-2.39	1.37	1.40
22	A	1104	CLA	CHC-C1C	2.39	1.41	1.35
22	B	1023	CLA	C3B-C2B	-2.39	1.37	1.40
22	B	1236	CLA	CHC-C1C	2.39	1.41	1.35
22	B	1216	CLA	CHC-C1C	2.39	1.41	1.35
22	A	1119	CLA	C3B-C2B	-2.39	1.37	1.40
22	8	610	CLA	C3B-C2B	-2.39	1.37	1.40
22	7	601	CLA	C3D-C4D	-2.39	1.38	1.44
22	A	1111	CLA	C3D-C4D	-2.39	1.38	1.44
22	A	1137	CLA	CHC-C1C	2.39	1.41	1.35
22	8	605	CLA	C3D-C4D	-2.38	1.38	1.44
29	A	5008	LMT	O2'-C2'	-2.38	1.37	1.43
22	B	1226	CLA	CHC-C1C	2.38	1.41	1.35
22	A	1117	CLA	C3B-C2B	-2.38	1.37	1.40
22	3	606	CLA	C3B-C2B	-2.38	1.37	1.40
47	7	807	4RF	O18-C19	-2.38	1.39	1.45
24	A	4005	BCR	C1-C6	-2.38	1.50	1.53
22	3	616	CLA	CHC-C1C	2.37	1.41	1.35
22	4	605	CLA	CHC-C1C	2.37	1.41	1.35
22	8	612	CLA	CHC-C1C	2.37	1.41	1.35
30	B	5004	PCW	O2-C31	2.37	1.41	1.34
22	8	607	CLA	C3D-C4D	-2.37	1.38	1.44
22	B	1021	CLA	CHC-C1C	2.37	1.41	1.35
22	B	1211	CLA	C3B-C2B	-2.37	1.37	1.40
22	A	1126	CLA	C3D-C4D	-2.36	1.38	1.44
22	B	1227	CLA	C3B-C2B	-2.36	1.37	1.40
22	6	603	CLA	C4B-NB	-2.36	1.33	1.35
22	A	1138	CLA	C3B-C2B	-2.36	1.37	1.40
22	7	612	CLA	C3D-C4D	-2.36	1.38	1.44
22	3	613	CLA	C3B-C2B	-2.36	1.37	1.40
39	8	604	CHL	C3A-C2A	-2.36	1.47	1.54
22	8	607	CLA	C3B-C2B	-2.35	1.37	1.40
22	B	1213	CLA	C3D-C4D	-2.35	1.38	1.44
47	7	807	4RF	O40-C39	-2.35	1.39	1.45
22	8	603	CLA	CHC-C1C	2.35	1.41	1.35
22	G	1602	CLA	C3B-C2B	-2.35	1.37	1.40
22	A	1012	CLA	C3D-C4D	-2.35	1.38	1.44
39	6	610	CHL	C3A-C2A	-2.35	1.47	1.54
22	4	610	CLA	CHC-C1C	2.35	1.41	1.35
32	F	5003	LAP	P9-O4	2.34	1.68	1.59
22	A	1139	CLA	CHC-C1C	2.34	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	604	CLA	C3B-C2B	-2.34	1.37	1.40
22	8	605	CLA	CHC-C1C	2.34	1.41	1.35
22	B	1231	CLA	C3D-C4D	-2.34	1.38	1.44
22	8	610	CLA	CHC-C1C	2.34	1.41	1.35
22	B	1220	CLA	CHC-C1C	2.34	1.41	1.35
22	A	1135	CLA	C3D-C4D	-2.34	1.38	1.44
22	B	1207	CLA	CHC-C1C	2.33	1.41	1.35
22	8	606	CLA	CHC-C1C	2.33	1.40	1.35
47	8	807	4RF	O40-C41	2.33	1.40	1.33
47	7	807	4RF	O21-C22	2.33	1.40	1.34
22	A	1121	CLA	C3B-C2B	-2.33	1.37	1.40
22	B	1219	CLA	C3B-C2B	-2.33	1.37	1.40
22	B	1211	CLA	C3D-C4D	-2.33	1.38	1.44
35	J	4002	RRX	C35-C13	2.33	1.55	1.50
22	A	1127	CLA	C3D-C4D	-2.33	1.38	1.44
24	B	4005	BCR	C12-C13	-2.33	1.40	1.45
22	A	1132	CLA	C3D-C4D	-2.32	1.38	1.44
22	A	1118	CLA	C3D-C4D	-2.32	1.38	1.44
22	B	1224	CLA	C3D-C4D	-2.32	1.38	1.44
22	7	609	CLA	C3D-C4D	-2.32	1.38	1.44
22	1	601	CLA	C3B-C2B	-2.32	1.37	1.40
22	4	605	CLA	C3D-C4D	-2.32	1.38	1.44
22	A	1133	CLA	CHC-C1C	2.31	1.40	1.35
22	B	1237	CLA	C3D-C4D	-2.31	1.39	1.44
22	A	1138	CLA	C3D-C4D	-2.31	1.39	1.44
22	8	611	CLA	C3D-C4D	-2.31	1.39	1.44
22	3	605	CLA	C3D-C4D	-2.31	1.39	1.44
22	B	1236	CLA	C3D-C4D	-2.31	1.39	1.44
34	G	5002	ERG	C9-C8	2.31	1.57	1.51
31	7	804	PTY	O4-C30	2.31	1.40	1.33
22	B	1230	CLA	C3B-C2B	-2.31	1.37	1.40
22	3	606	CLA	C3D-C4D	-2.31	1.39	1.44
22	B	1229	CLA	C3D-C4D	-2.31	1.39	1.44
22	B	1216	CLA	C3D-C4D	-2.31	1.39	1.44
22	A	1117	CLA	CHC-C1C	2.31	1.40	1.35
47	7	807	4RF	O18-C16	2.30	1.40	1.33
22	1	604	CLA	C3D-C4D	-2.30	1.39	1.44
29	1	804	LMT	O4'-C4B	-2.30	1.37	1.43
22	A	1119	CLA	C3D-C4D	-2.30	1.39	1.44
22	6	603	CLA	CHC-C1C	2.30	1.40	1.35
22	A	1112	CLA	C3B-C2B	-2.30	1.37	1.40
22	4	601	CLA	C3B-C2B	-2.30	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1111	CLA	C3B-C2B	-2.30	1.37	1.40
24	A	4002	BCR	C1-C6	-2.29	1.50	1.53
22	8	602	CLA	C3D-C4D	-2.29	1.39	1.44
22	7	608	CLA	C3D-C4D	-2.29	1.39	1.44
24	A	4001	BCR	C12-C13	-2.29	1.41	1.45
22	a	601	CLA	C3D-C4D	-2.29	1.39	1.44
22	A	1140	CLA	C3D-C4D	-2.29	1.39	1.44
22	A	1117	CLA	C3D-C4D	-2.29	1.39	1.44
31	5	802	PTY	O4-C30	2.29	1.40	1.33
47	8	808	4RF	O21-C22	2.29	1.40	1.34
22	6	608	CLA	C3D-C4D	-2.29	1.39	1.44
48	7	504	C7Z	C10-C9	-2.29	1.32	1.35
39	1	613	CHL	C1D-ND	-2.29	1.35	1.37
22	B	1235	CLA	C3D-C4D	-2.28	1.39	1.44
22	B	1238	CLA	C3D-C4D	-2.28	1.39	1.44
22	B	1206	CLA	C3D-C4D	-2.28	1.39	1.44
27	A	5007	3PH	O31-C31	2.28	1.40	1.33
22	6	605	CLA	C3D-C4D	-2.28	1.39	1.44
22	A	1102	CLA	C3B-C2B	-2.28	1.37	1.40
22	A	1113	CLA	C3B-C2B	-2.28	1.37	1.40
22	B	1234	CLA	C3D-C4D	-2.28	1.39	1.44
22	B	1202	CLA	C3D-C4D	-2.28	1.39	1.44
24	B	4007	BCR	C12-C13	-2.28	1.41	1.45
22	A	1106	CLA	C3D-C4D	-2.27	1.39	1.44
22	A	1108	CLA	C3D-C4D	-2.27	1.39	1.44
22	B	1227	CLA	C3D-C4D	-2.27	1.39	1.44
22	5	606	CLA	C3D-C4D	-2.27	1.39	1.44
22	B	1222	CLA	C3D-C4D	-2.27	1.39	1.44
22	B	1239	CLA	C3D-C4D	-2.27	1.39	1.44
42	a	805	GG0	C06-C07	2.27	1.55	1.51
22	1	605	CLA	C3B-C2B	-2.27	1.37	1.40
22	6	603	CLA	C3B-C2B	-2.27	1.37	1.40
22	B	1220	CLA	C3D-C4D	-2.27	1.39	1.44
22	1	607	CLA	C3D-C4D	-2.27	1.39	1.44
22	B	1205	CLA	CHC-C1C	2.27	1.40	1.35
41	a	504	QTB	C14-C12	-2.27	1.48	1.53
31	3	802	PTY	O7-C8	2.27	1.40	1.34
22	A	1112	CLA	CHC-C1C	2.27	1.40	1.35
31	7	804	PTY	O7-C6	-2.27	1.40	1.46
31	5	802	PTY	O7-C8	2.27	1.40	1.34
22	A	1104	CLA	C3D-C4D	-2.27	1.39	1.44
22	A	1128	CLA	CHC-C1C	2.27	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	5005	PTY	O4-C30	2.27	1.39	1.33
47	8	808	4RF	O40-C39	-2.26	1.40	1.45
22	A	1139	CLA	C3D-C4D	-2.26	1.39	1.44
22	B	1208	CLA	C3B-C2B	-2.26	1.37	1.40
24	6	503	BCR	C1-C6	-2.26	1.50	1.53
47	8	808	4RF	O40-C41	2.26	1.39	1.33
36	a	804	LPX	P1-O2	2.26	1.68	1.59
47	8	807	4RF	O21-C22	2.26	1.40	1.34
22	B	1214	CLA	C3D-C4D	-2.26	1.39	1.44
31	5	802	PTY	O7-C6	-2.26	1.40	1.46
22	4	615	CLA	C3B-C2B	-2.26	1.37	1.40
22	7	617	CLA	C3D-C4D	-2.26	1.39	1.44
47	8	807	4RF	O21-C20	-2.26	1.41	1.46
22	a	605	CLA	C3B-C2B	-2.26	1.37	1.40
38	8	501	LUT	C22-C21	-2.26	1.51	1.54
22	A	1101	CLA	C3D-C4D	-2.25	1.39	1.44
22	K	1403	CLA	C3D-C4D	-2.25	1.39	1.44
22	1	606	CLA	C3D-C4D	-2.25	1.39	1.44
22	3	601	CLA	C3B-C2B	-2.25	1.37	1.40
22	5	603	CLA	C3D-C4D	-2.25	1.39	1.44
22	B	1204	CLA	C3D-C4D	-2.25	1.39	1.44
47	8	808	4RF	O21-C20	-2.25	1.41	1.46
22	A	1116	CLA	C3D-C4D	-2.25	1.39	1.44
22	A	1109	CLA	C3D-C4D	-2.25	1.39	1.44
22	A	1133	CLA	C3D-C4D	-2.25	1.39	1.44
22	a	605	CLA	C3D-C4D	-2.25	1.39	1.44
22	3	604	CLA	C3D-C4D	-2.25	1.39	1.44
22	4	616	CLA	C3D-C4D	-2.25	1.39	1.44
24	6	504	BCR	C1-C6	-2.25	1.50	1.53
22	7	601	CLA	C3B-C2B	-2.25	1.37	1.40
22	B	1023	CLA	C3D-C4D	-2.25	1.39	1.44
39	3	608	CHL	C3B-C2B	-2.25	1.37	1.40
22	3	613	CLA	C3D-C4D	-2.24	1.39	1.44
22	A	1128	CLA	C3D-C4D	-2.24	1.39	1.44
22	A	1113	CLA	C3D-C4D	-2.24	1.39	1.44
22	B	1219	CLA	C3D-C4D	-2.24	1.39	1.44
22	4	611	CLA	C3D-C4D	-2.24	1.39	1.44
22	B	1232	CLA	C3D-C4D	-2.24	1.39	1.44
22	K	1402	CLA	C1C-C2C	2.24	1.48	1.44
22	7	604	CLA	C3D-C4D	-2.24	1.39	1.44
24	F	4001	BCR	C1-C6	-2.24	1.50	1.53
22	B	1207	CLA	C3D-C4D	-2.24	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	8	601	CHL	CHC-C1C	2.24	1.40	1.35
22	5	617	CLA	C3D-C4D	-2.23	1.39	1.44
22	8	618	CLA	C3D-C4D	-2.23	1.39	1.44
36	J	5001	LPX	P1-O2	2.23	1.68	1.59
22	6	604	CLA	C3D-C4D	-2.23	1.39	1.44
22	8	609	CLA	C3D-C4D	-2.23	1.39	1.44
22	B	1203	CLA	C3D-C4D	-2.23	1.39	1.44
22	B	1021	CLA	C3D-C4D	-2.23	1.39	1.44
22	A	1107	CLA	C1A-CHA	2.23	1.52	1.43
22	A	1129	CLA	C3D-C4D	-2.23	1.39	1.44
22	B	1210	CLA	C3D-C4D	-2.23	1.39	1.44
22	A	1121	CLA	C3D-C4D	-2.22	1.39	1.44
22	8	612	CLA	C3D-C4D	-2.22	1.39	1.44
22	B	1226	CLA	C3D-C4D	-2.22	1.39	1.44
22	7	615	CLA	C3D-C4D	-2.22	1.39	1.44
22	7	604	CLA	C4B-NB	-2.22	1.33	1.35
39	8	601	CHL	C3A-C2A	-2.22	1.48	1.54
31	3	802	PTY	O7-C6	-2.22	1.41	1.46
22	7	601	CLA	C4B-NB	-2.22	1.33	1.35
22	B	1217	CLA	C3D-C4D	-2.22	1.39	1.44
22	B	1210	CLA	CHC-C1C	2.22	1.40	1.35
24	B	4006	BCR	C12-C13	-2.22	1.41	1.45
22	7	607	CLA	C3D-C4D	-2.21	1.39	1.44
47	7	807	4RF	O40-C41	2.21	1.39	1.33
31	7	804	PTY	O4-C1	-2.21	1.40	1.45
22	A	1140	CLA	C1C-C2C	2.21	1.48	1.44
22	A	1136	CLA	C3D-C4D	-2.21	1.39	1.44
22	3	602	CLA	C3D-C4D	-2.21	1.39	1.44
22	A	1130	CLA	C3D-C4D	-2.21	1.39	1.44
22	4	606	CLA	C3D-C4D	-2.21	1.39	1.44
22	A	1109	CLA	C1A-CHA	2.21	1.52	1.43
22	7	605	CLA	C3D-C4D	-2.21	1.39	1.44
31	8	810	PTY	O4-C30	2.21	1.39	1.33
22	B	1230	CLA	C3D-C4D	-2.21	1.39	1.44
22	3	610	CLA	C3D-C4D	-2.20	1.39	1.44
32	F	5003	LAP	O4-C15	-2.20	1.36	1.44
22	A	1107	CLA	C3D-C4D	-2.20	1.39	1.44
29	A	5008	LMT	O3B-C3B	-2.20	1.37	1.43
27	A	5007	3PH	O31-C3	-2.20	1.40	1.45
22	F	1301	CLA	C3D-C4D	-2.20	1.39	1.44
22	1	610	CLA	C3D-C4D	-2.20	1.39	1.44
22	7	605	CLA	C4B-NB	-2.20	1.33	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	8	807	4RF	O18-C19	-2.20	1.40	1.45
22	A	1103	CLA	C3D-C4D	-2.20	1.39	1.44
22	5	608	CLA	C3B-C2B	-2.20	1.37	1.40
22	4	615	CLA	C3D-C4D	-2.20	1.39	1.44
22	5	618	CLA	C1C-C2C	2.20	1.48	1.44
22	a	611	CLA	C3D-C4D	-2.19	1.39	1.44
34	G	5002	ERG	C14-C8	2.19	1.57	1.51
22	6	618	CLA	C3D-C4D	-2.19	1.39	1.44
22	7	603	CLA	C3D-C4D	-2.19	1.39	1.44
22	B	1215	CLA	C3D-C4D	-2.19	1.39	1.44
22	7	606	CLA	C3D-C4D	-2.19	1.39	1.44
22	4	604	CLA	C3D-C4D	-2.19	1.39	1.44
22	B	1201	CLA	C3B-C2B	-2.19	1.37	1.40
22	A	1112	CLA	C3D-C4D	-2.18	1.39	1.44
22	7	602	CLA	C3D-C4D	-2.18	1.39	1.44
22	B	1201	CLA	C3D-C4D	-2.18	1.39	1.44
22	3	612	CLA	C3B-C2B	-2.18	1.37	1.40
22	G	1601	CLA	C3D-C4D	-2.18	1.39	1.44
22	1	608	CLA	C3D-C4D	-2.18	1.39	1.44
22	B	1221	CLA	C3D-C4D	-2.18	1.39	1.44
22	B	1209	CLA	C1A-CHA	2.18	1.52	1.43
22	3	616	CLA	C3D-C4D	-2.18	1.39	1.44
22	A	1122	CLA	C3D-C4D	-2.18	1.39	1.44
22	1	601	CLA	C3D-C4D	-2.18	1.39	1.44
22	a	604	CLA	C3D-C4D	-2.18	1.39	1.44
22	4	612	CLA	C1A-CHA	2.18	1.52	1.43
22	1	602	CLA	C3D-C4D	-2.17	1.39	1.44
47	8	807	4RF	O40-C39	-2.17	1.40	1.45
22	B	1223	CLA	C3D-C4D	-2.17	1.39	1.44
22	7	611	CLA	C3D-C4D	-2.17	1.39	1.44
39	5	611	CHL	C1D-ND	-2.17	1.35	1.37
32	K	5001	LAP	O1-C13	-2.17	1.40	1.45
22	1	615	CLA	C3D-C4D	-2.17	1.39	1.44
24	5	504	BCR	C12-C13	-2.17	1.41	1.45
22	A	1013	CLA	C3D-C4D	-2.17	1.39	1.44
22	F	1302	CLA	C3D-C4D	-2.17	1.39	1.44
22	L	1501	CLA	C1B-NB	2.16	1.37	1.35
22	8	606	CLA	C3D-C4D	-2.16	1.39	1.44
22	6	609	CLA	C3B-C2B	-2.16	1.37	1.40
22	L	1501	CLA	C1A-CHA	2.16	1.52	1.43
29	B	5006	LMT	O3B-C3B	-2.16	1.37	1.43
22	B	1208	CLA	C3D-C4D	-2.16	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	605	CLA	C3D-C4D	-2.16	1.39	1.44
22	4	602	CLA	C3D-C4D	-2.16	1.39	1.44
22	a	604	CLA	C1C-C2C	2.16	1.48	1.44
29	A	5008	LMT	O4'-C4B	-2.16	1.37	1.43
38	5	502	LUT	C1-C6	-2.16	1.50	1.53
26	A	5005	DGD	O3G-C1D	2.16	1.43	1.40
22	6	604	CLA	C3B-C2B	-2.16	1.37	1.40
22	8	603	CLA	C3D-C4D	-2.16	1.39	1.44
22	1	611	CLA	C3D-C4D	-2.16	1.39	1.44
31	5	802	PTY	O4-C1	-2.16	1.40	1.45
21	A	1011	CL0	C4B-CHC	2.16	1.47	1.41
22	3	601	CLA	C3D-C4D	-2.16	1.39	1.44
22	B	1213	CLA	C1C-C2C	2.15	1.48	1.44
22	1	606	CLA	C3B-C2B	-2.15	1.37	1.40
22	A	1105	CLA	C3D-C4D	-2.15	1.39	1.44
22	B	1206	CLA	CHC-C1C	2.15	1.40	1.35
39	8	601	CHL	C1D-ND	-2.15	1.35	1.37
22	A	1115	CLA	C3D-C4D	-2.15	1.39	1.44
22	8	615	CLA	C3D-C4D	-2.15	1.39	1.44
22	B	1218	CLA	C3D-C4D	-2.15	1.39	1.44
22	A	1102	CLA	C3D-C4D	-2.15	1.39	1.44
22	A	1137	CLA	C3D-C4D	-2.15	1.39	1.44
42	a	805	GG0	C03-N05	2.15	1.38	1.33
39	5	611	CHL	C3A-C2A	-2.15	1.48	1.54
22	8	610	CLA	C3D-C4D	-2.14	1.39	1.44
31	3	802	PTY	O4-C1	-2.14	1.40	1.45
22	4	603	CLA	C3D-C4D	-2.14	1.39	1.44
22	A	1125	CLA	C3D-C4D	-2.14	1.39	1.44
27	A	5007	3PH	O21-C21	2.14	1.40	1.34
22	A	1110	CLA	C3D-C4D	-2.13	1.39	1.44
22	a	615	CLA	C3D-C4D	-2.13	1.39	1.44
39	1	609	CHL	C1D-ND	-2.13	1.35	1.37
22	4	606	CLA	C3B-C2B	-2.13	1.37	1.40
22	4	610	CLA	C3D-C4D	-2.13	1.39	1.44
41	3	506	QTB	C03-C02	-2.13	1.33	1.35
22	A	1120	CLA	C1C-C2C	2.13	1.48	1.44
22	A	1141	CLA	C3D-C4D	-2.12	1.39	1.44
22	B	1212	CLA	C3D-C4D	-2.12	1.39	1.44
22	G	1602	CLA	C3D-C4D	-2.12	1.39	1.44
22	L	1502	CLA	C3D-C4D	-2.12	1.39	1.44
22	6	606	CLA	C3D-C4D	-2.12	1.39	1.44
22	7	610	CLA	C3D-C4D	-2.12	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	8	603	CLA	C1A-CHA	2.12	1.51	1.43
22	L	1503	CLA	C3D-C4D	-2.12	1.39	1.44
39	3	611	CHL	CHC-C1C	2.12	1.40	1.35
30	6	803	PCW	P-O4P	2.12	1.67	1.59
22	a	602	CLA	C1C-C2C	2.11	1.48	1.44
22	6	602	CLA	C3D-C4D	-2.11	1.39	1.44
34	G	5002	ERG	C4-C5	2.11	1.56	1.51
24	B	4001	BCR	C12-C13	-2.11	1.41	1.45
49	8	806	P5S	O37-C2	-2.11	1.41	1.46
22	6	615	CLA	C3D-C4D	-2.11	1.39	1.44
22	A	1107	CLA	C3B-C2B	-2.11	1.37	1.40
41	3	506	QTB	C13-C12	-2.11	1.47	1.53
22	5	608	CLA	C1C-C2C	2.11	1.48	1.44
22	6	615	CLA	C1A-CHA	2.11	1.51	1.43
22	6	609	CLA	C3D-C4D	-2.11	1.39	1.44
22	A	1141	CLA	C1A-CHA	2.10	1.51	1.43
22	K	1404	CLA	C3D-C4D	-2.10	1.39	1.44
22	8	611	CLA	C3B-C2B	-2.10	1.37	1.40
48	7	504	C7Z	C40-C33	2.10	1.55	1.50
31	B	5005	PTY	O7-C8	2.10	1.40	1.34
31	7	804	PTY	O7-C8	2.10	1.40	1.34
22	6	601	CLA	C3D-C4D	-2.10	1.39	1.44
22	4	616	CLA	C1A-CHA	2.10	1.51	1.43
22	A	1134	CLA	C3D-C4D	-2.10	1.39	1.44
22	4	608	CLA	C3D-C4D	-2.10	1.39	1.44
22	3	618	CLA	C3D-C4D	-2.10	1.39	1.44
22	5	612	CLA	C3D-C4D	-2.10	1.39	1.44
22	a	602	CLA	C3D-C4D	-2.10	1.39	1.44
44	5	803	DGA	OG2-CG2	-2.10	1.41	1.46
37	M	4001	ECH	C1-C6	-2.10	1.50	1.53
22	1	603	CLA	C3D-C4D	-2.10	1.39	1.44
39	8	613	CHL	C3A-C2A	-2.10	1.48	1.54
22	4	607	CLA	C3D-C4D	-2.09	1.39	1.44
22	5	603	CLA	C3B-C2B	-2.09	1.37	1.40
22	5	602	CLA	C3D-C4D	-2.09	1.39	1.44
22	5	609	CLA	C3B-C2B	-2.09	1.37	1.40
22	K	1401	CLA	C3D-C4D	-2.09	1.39	1.44
22	B	1228	CLA	C2-C3	-2.09	1.28	1.33
22	A	1123	CLA	C3D-C4D	-2.09	1.39	1.44
24	6	504	BCR	C12-C13	-2.09	1.41	1.45
22	a	612	CLA	C3B-C2B	-2.09	1.37	1.40
22	3	618	CLA	C1A-CHA	2.09	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	603	CLA	C3D-C4D	-2.09	1.39	1.44
22	5	607	CLA	C3D-C4D	-2.09	1.39	1.44
22	5	609	CLA	C1C-C2C	2.09	1.48	1.44
22	7	611	CLA	C4B-NB	-2.09	1.33	1.35
22	G	1602	CLA	C1C-C2C	2.09	1.48	1.44
22	8	620	CLA	C3D-C4D	-2.08	1.39	1.44
22	B	1212	CLA	C1A-CHA	2.08	1.51	1.43
22	B	1240	CLA	C3D-C4D	-2.08	1.39	1.44
24	7	503	BCR	C12-C13	-2.08	1.41	1.45
22	K	1404	CLA	C1C-C2C	2.08	1.48	1.44
22	B	1227	CLA	C4B-NB	-2.08	1.33	1.35
31	B	5005	PTY	O4-C1	-2.08	1.40	1.45
22	6	607	CLA	C1C-C2C	2.08	1.48	1.44
22	B	1232	CLA	C1A-CHA	2.08	1.51	1.43
29	1	804	LMT	O3B-C3B	-2.08	1.38	1.43
29	1	804	LMT	O1'-C1'	-2.08	1.36	1.40
22	L	1502	CLA	C1C-C2C	2.07	1.48	1.44
22	7	611	CLA	C3B-C2B	-2.07	1.37	1.40
22	3	607	CLA	C3D-C4D	-2.07	1.39	1.44
38	6	502	LUT	C22-C21	-2.07	1.52	1.54
22	a	608	CLA	C3D-C4D	-2.07	1.39	1.44
22	a	607	CLA	C3D-C4D	-2.07	1.39	1.44
22	5	601	CLA	C3D-C4D	-2.07	1.39	1.44
22	1	612	CLA	C3D-C4D	-2.07	1.39	1.44
22	5	616	CLA	C3D-C4D	-2.06	1.39	1.44
22	G	1603	CLA	C3D-C4D	-2.06	1.39	1.44
24	3	503	BCR	C12-C13	-2.06	1.41	1.45
22	K	1402	CLA	C1A-CHA	2.06	1.51	1.43
39	8	604	CHL	CHC-C1C	2.06	1.40	1.35
22	4	610	CLA	C1A-CHA	2.06	1.51	1.43
22	A	1122	CLA	C1A-CHA	2.06	1.51	1.43
22	8	620	CLA	C1A-CHA	2.06	1.51	1.43
22	L	1503	CLA	C3B-C2B	-2.06	1.37	1.40
48	7	504	C7Z	C20-C13	2.06	1.55	1.50
22	5	609	CLA	C3D-C4D	-2.06	1.39	1.44
22	8	608	CLA	C3D-C4D	-2.06	1.39	1.44
24	B	4005	BCR	C1-C6	-2.06	1.50	1.53
31	8	810	PTY	O7-C6	-2.06	1.41	1.46
22	5	604	CLA	C3B-C2B	-2.06	1.37	1.40
24	5	504	BCR	C1-C6	-2.05	1.50	1.53
24	J	4001	BCR	C12-C13	-2.05	1.41	1.45
22	G	1603	CLA	C1C-C2C	2.05	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	5006	LMT	O4'-C4B	-2.05	1.38	1.43
22	5	614	CLA	C1A-CHA	2.05	1.51	1.43
22	6	607	CLA	C1A-CHA	2.05	1.51	1.43
22	3	603	CLA	C3D-C4D	-2.05	1.39	1.44
39	1	609	CHL	C3A-C2A	-2.05	1.48	1.54
22	A	1140	CLA	C1A-CHA	2.05	1.51	1.43
22	A	1115	CLA	C1A-CHA	2.04	1.51	1.43
22	a	601	CLA	C3B-C2B	-2.04	1.37	1.40
22	6	612	CLA	C3D-C4D	-2.04	1.39	1.44
24	B	4003	BCR	C1-C6	-2.04	1.51	1.53
22	K	1401	CLA	C1A-CHA	2.04	1.51	1.43
22	A	1120	CLA	C3D-C4D	-2.04	1.39	1.44
22	1	601	CLA	C1C-C2C	2.04	1.48	1.44
22	4	617	CLA	C3D-C4D	-2.04	1.39	1.44
22	6	605	CLA	C1C-C2C	2.04	1.48	1.44
22	a	615	CLA	C3B-C2B	-2.04	1.37	1.40
22	4	604	CLA	C4B-NB	-2.04	1.33	1.35
22	1	608	CLA	C1C-C2C	2.04	1.48	1.44
22	4	608	CLA	C1C-C2C	2.04	1.48	1.44
22	6	617	CLA	C3D-C4D	-2.04	1.39	1.44
22	B	1206	CLA	C1A-CHA	2.04	1.51	1.43
24	3	503	BCR	C1-C6	-2.03	1.51	1.53
22	B	1221	CLA	C1A-CHA	2.03	1.51	1.43
22	7	612	CLA	CHC-C1C	2.03	1.40	1.35
24	A	4003	BCR	C12-C13	-2.03	1.41	1.45
22	7	606	CLA	C3B-C2B	-2.03	1.37	1.40
22	A	1138	CLA	C1A-CHA	2.03	1.51	1.43
22	6	609	CLA	C4B-NB	-2.03	1.33	1.35
22	B	1221	CLA	C1C-C2C	2.03	1.48	1.44
24	A	4005	BCR	C12-C13	-2.03	1.41	1.45
22	1	606	CLA	C1C-C2C	2.03	1.48	1.44
22	B	1209	CLA	C3D-C4D	-2.02	1.39	1.44
24	K	4002	BCR	C12-C13	-2.02	1.41	1.45
22	B	1201	CLA	C1A-CHA	2.02	1.51	1.43
22	5	614	CLA	C3D-C4D	-2.02	1.39	1.44
22	A	1105	CLA	C1C-C2C	2.02	1.48	1.44
22	1	611	CLA	C1C-C2C	2.02	1.48	1.44
22	A	1112	CLA	C1A-CHA	2.02	1.51	1.43
22	3	603	CLA	C1A-CHA	2.02	1.51	1.43
22	a	608	CLA	C1C-C2C	2.02	1.48	1.44
24	4	503	BCR	C12-C13	-2.02	1.41	1.45
22	K	1403	CLA	C1A-CHA	2.02	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	1224	CLA	C1A-CHA	2.02	1.51	1.43
22	K	1404	CLA	C1A-CHA	2.02	1.51	1.43
22	3	602	CLA	C1A-CHA	2.02	1.51	1.43
22	4	604	CLA	C1C-C2C	2.02	1.48	1.44
22	A	1126	CLA	C4B-NB	-2.02	1.33	1.35
22	4	607	CLA	C1C-C2C	2.02	1.48	1.44
38	7	501	LUT	C22-C21	-2.01	1.52	1.54
22	A	1112	CLA	C4B-NB	-2.01	1.33	1.35
22	4	612	CLA	C1C-C2C	2.01	1.48	1.44
22	B	1235	CLA	C1A-CHA	2.01	1.51	1.43
22	6	602	CLA	C1C-C2C	2.01	1.48	1.44
22	5	603	CLA	C1A-CHA	2.01	1.51	1.43
24	A	4002	BCR	C12-C13	-2.01	1.41	1.45
22	a	607	CLA	C1A-CHA	2.01	1.51	1.43
22	A	1121	CLA	C1A-CHA	2.01	1.51	1.43
22	A	1123	CLA	C1A-CHA	2.01	1.51	1.43
26	A	5005	DGD	CAA-C9A	-2.01	1.33	1.49
22	5	616	CLA	C1A-CHA	2.01	1.51	1.43
22	L	1503	CLA	C1A-CHA	2.01	1.51	1.43
22	5	618	CLA	C3D-C4D	-2.01	1.39	1.44
22	B	1223	CLA	C1A-CHA	2.01	1.51	1.43
24	5	503	BCR	C12-C13	-2.01	1.41	1.45
22	A	1110	CLA	C1A-CHA	2.01	1.51	1.43
22	L	1503	CLA	C1C-C2C	2.00	1.48	1.44
22	J	1901	CLA	C3D-C4D	-2.00	1.39	1.44
22	4	612	CLA	C3D-C4D	-2.00	1.39	1.44
32	B	5007	LAP	O1-C13	-2.00	1.40	1.45
22	B	1218	CLA	C1A-CHA	2.00	1.51	1.43
22	5	608	CLA	C1A-CHA	2.00	1.51	1.43

All (4631) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	J	4001	BCR	C10-C11-C12	18.04	179.50	123.22
24	A	4004	BCR	C10-C11-C12	17.82	178.83	123.22
24	A	4002	BCR	C10-C11-C12	17.72	178.51	123.22
24	4	503	BCR	C10-C11-C12	17.70	178.47	123.22
24	F	4001	BCR	C10-C11-C12	17.67	178.36	123.22
24	K	4001	BCR	C10-C11-C12	17.49	177.79	123.22
24	B	4004	BCR	C10-C11-C12	17.46	177.71	123.22
24	7	503	BCR	C10-C11-C12	17.20	176.90	123.22
24	B	4001	BCR	C10-C11-C12	17.16	176.77	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	6	503	BCR	C16-C15-C14	17.01	158.32	123.47
24	8	503	BCR	C10-C11-C12	16.90	175.97	123.22
24	L	4002	BCR	C10-C11-C12	16.88	175.91	123.22
24	I	4001	BCR	C10-C11-C12	16.83	175.75	123.22
24	5	503	BCR	C10-C11-C12	16.75	175.48	123.22
24	B	4002	BCR	C10-C11-C12	16.73	175.44	123.22
24	3	504	BCR	C10-C11-C12	16.71	175.37	123.22
24	B	4007	BCR	C10-C11-C12	16.60	175.03	123.22
24	K	4002	BCR	C10-C11-C12	16.58	174.96	123.22
24	L	4003	BCR	C10-C11-C12	16.52	174.76	123.22
24	6	503	BCR	C10-C11-C12	16.49	174.69	123.22
24	B	4006	BCR	C10-C11-C12	16.48	174.66	123.22
24	A	4003	BCR	C10-C11-C12	16.39	174.36	123.22
24	B	4003	BCR	C10-C11-C12	16.17	173.69	123.22
24	B	4003	BCR	C11-C10-C9	16.10	150.28	127.31
24	L	4001	BCR	C10-C11-C12	16.06	173.35	123.22
24	A	4005	BCR	C10-C11-C12	15.98	173.10	123.22
24	5	504	BCR	C10-C11-C12	15.96	173.02	123.22
24	G	4001	BCR	C10-C11-C12	15.87	172.73	123.22
24	3	503	BCR	C10-C11-C12	15.79	172.50	123.22
24	B	4005	BCR	C10-C11-C12	15.75	172.35	123.22
22	B	1228	CLA	C4A-NA-C1A	15.62	113.73	106.71
24	3	505	BCR	C10-C11-C12	15.54	171.72	123.22
24	5	504	BCR	C16-C15-C14	14.92	154.04	123.47
24	K	4002	BCR	C16-C15-C14	14.15	152.47	123.47
24	J	4001	BCR	C16-C15-C14	13.74	151.63	123.47
24	A	4005	BCR	C11-C10-C9	13.73	146.91	127.31
24	L	4003	BCR	C11-C10-C9	13.71	146.88	127.31
24	B	4006	BCR	C11-C10-C9	13.67	146.82	127.31
24	B	4004	BCR	C11-C10-C9	13.61	146.74	127.31
24	7	503	BCR	C16-C15-C14	13.57	151.28	123.47
24	A	4003	BCR	C11-C10-C9	13.46	146.53	127.31
24	3	504	BCR	C21-C20-C19	13.45	165.20	123.22
24	5	503	BCR	C16-C15-C14	13.44	151.01	123.47
24	6	504	BCR	C10-C11-C12	13.38	164.96	123.22
24	B	4006	BCR	C16-C15-C14	13.36	150.84	123.47
24	L	4001	BCR	C11-C10-C9	13.35	146.36	127.31
24	B	4002	BCR	C11-C10-C9	13.31	146.30	127.31
24	6	504	BCR	C16-C15-C14	13.29	150.69	123.47
24	K	4001	BCR	C11-C10-C9	13.25	146.22	127.31
24	G	4001	BCR	C21-C20-C19	13.19	164.37	123.22
24	K	4001	BCR	C21-C20-C19	13.17	164.30	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	4001	BCR	C10-C11-C12	13.07	164.01	123.22
24	4	503	BCR	C16-C15-C14	12.99	150.09	123.47
24	B	4001	BCR	C21-C20-C19	12.99	163.75	123.22
24	G	4001	BCR	C11-C10-C9	12.96	145.81	127.31
24	A	4001	BCR	C21-C20-C19	12.94	163.59	123.22
24	A	4003	BCR	C21-C20-C19	12.93	163.58	123.22
24	3	504	BCR	C11-C10-C9	12.93	145.77	127.31
24	A	4004	BCR	C11-C10-C9	12.93	145.76	127.31
24	A	4003	BCR	C16-C15-C14	12.87	149.85	123.47
24	L	4002	BCR	C11-C12-C13	12.86	162.55	126.42
24	A	4004	BCR	C16-C15-C14	12.82	149.74	123.47
24	8	503	BCR	C11-C10-C9	12.81	145.59	127.31
24	A	4004	BCR	C11-C12-C13	12.73	162.18	126.42
24	A	4002	BCR	C11-C10-C9	12.70	145.44	127.31
24	B	4003	BCR	C11-C12-C13	12.69	162.07	126.42
24	L	4002	BCR	C11-C10-C9	12.67	145.40	127.31
24	B	4002	BCR	C16-C15-C14	12.59	149.27	123.47
24	5	503	BCR	C11-C10-C9	12.56	145.23	127.31
24	B	4005	BCR	C16-C15-C14	12.54	149.17	123.47
24	7	503	BCR	C11-C10-C9	12.54	145.20	127.31
24	B	4005	BCR	C21-C20-C19	12.51	162.26	123.22
24	3	505	BCR	C16-C15-C14	12.44	148.97	123.47
24	L	4003	BCR	C16-C15-C14	12.39	148.86	123.47
24	A	4004	BCR	C21-C20-C19	12.27	161.52	123.22
24	I	4001	BCR	C11-C12-C13	12.26	160.87	126.42
24	4	503	BCR	C11-C12-C13	12.25	160.84	126.42
24	L	4002	BCR	C16-C15-C14	12.23	148.53	123.47
24	A	4001	BCR	C11-C10-C9	12.19	144.71	127.31
24	3	505	BCR	C21-C20-C19	12.19	161.25	123.22
24	3	504	BCR	C16-C15-C14	12.18	148.43	123.47
24	L	4001	BCR	C16-C15-C14	12.10	148.26	123.47
24	A	4005	BCR	C11-C12-C13	12.09	160.37	126.42
24	8	503	BCR	C21-C20-C19	12.07	160.88	123.22
24	B	4001	BCR	C11-C10-C9	12.06	144.52	127.31
24	L	4002	BCR	C21-C20-C19	12.03	160.76	123.22
24	5	504	BCR	C21-C20-C19	11.88	160.30	123.22
24	B	4005	BCR	C11-C12-C13	11.82	159.63	126.42
24	B	4001	BCR	C11-C12-C13	11.81	159.59	126.42
24	B	4005	BCR	C11-C10-C9	11.79	144.13	127.31
24	8	503	BCR	C16-C15-C14	11.75	147.55	123.47
24	K	4002	BCR	C21-C20-C19	11.73	159.82	123.22
24	B	4004	BCR	C11-C12-C13	11.73	159.36	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	4004	BCR	C21-C20-C19	11.70	159.72	123.22
24	A	4002	BCR	C16-C15-C14	11.67	147.37	123.47
24	A	4001	BCR	C11-C12-C13	11.65	159.13	126.42
24	L	4003	BCR	C11-C12-C13	11.60	159.01	126.42
24	B	4002	BCR	C11-C12-C13	11.58	158.95	126.42
24	K	4001	BCR	C16-C15-C14	11.58	147.19	123.47
24	6	504	BCR	C21-C20-C19	11.58	159.34	123.22
24	G	4001	BCR	C11-C12-C13	11.53	158.82	126.42
24	L	4003	BCR	C21-C20-C19	11.52	159.18	123.22
24	B	4006	BCR	C21-C20-C19	11.51	159.14	123.22
24	3	503	BCR	C11-C12-C13	11.44	158.56	126.42
24	B	4003	BCR	C16-C15-C14	11.36	146.74	123.47
24	I	4001	BCR	C11-C10-C9	11.33	143.48	127.31
24	B	4007	BCR	C11-C10-C9	11.32	143.47	127.31
24	B	4007	BCR	C16-C15-C14	11.32	146.66	123.47
24	J	4001	BCR	C21-C20-C19	11.31	158.52	123.22
24	3	503	BCR	C16-C15-C14	11.27	146.55	123.47
24	4	503	BCR	C11-C10-C9	11.24	143.35	127.31
24	A	4002	BCR	C11-C12-C13	11.22	157.94	126.42
34	G	5002	ERG	C15-C14-C8	-11.11	103.60	120.44
24	3	505	BCR	C11-C10-C9	11.05	143.07	127.31
24	4	503	BCR	C21-C20-C19	11.00	157.56	123.22
24	F	4001	BCR	C21-C20-C19	10.99	157.50	123.22
24	3	503	BCR	C21-C20-C19	10.98	157.49	123.22
24	A	4005	BCR	C16-C15-C14	10.89	145.78	123.47
24	J	4001	BCR	C11-C10-C9	10.88	142.84	127.31
24	B	4002	BCR	C21-C20-C19	10.85	157.09	123.22
24	L	4001	BCR	C21-C20-C19	10.84	157.06	123.22
24	A	4002	BCR	C21-C20-C19	10.83	157.02	123.22
24	B	4007	BCR	C21-C20-C19	10.79	156.90	123.22
24	7	503	BCR	C21-C20-C19	10.75	156.76	123.22
24	A	4005	BCR	C21-C20-C19	10.61	156.32	123.22
24	K	4001	BCR	C11-C12-C13	10.59	156.15	126.42
24	B	4004	BCR	C16-C15-C14	10.59	145.16	123.47
24	F	4001	BCR	C16-C15-C14	10.51	145.00	123.47
24	5	503	BCR	C21-C20-C19	10.49	155.94	123.22
24	B	4007	BCR	C11-C12-C13	10.41	155.67	126.42
24	K	4002	BCR	C11-C12-C13	10.36	155.53	126.42
24	L	4001	BCR	C11-C12-C13	10.36	155.52	126.42
24	B	4006	BCR	C11-C12-C13	10.27	155.26	126.42
24	I	4001	BCR	C16-C15-C14	10.26	144.50	123.47
22	B	1205	CLA	C4A-NA-C1A	10.26	111.32	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	6	503	BCR	C21-C20-C19	10.25	155.20	123.22
22	B	1210	CLA	C4A-NA-C1A	10.24	111.31	106.71
24	8	503	BCR	C11-C12-C13	10.17	154.97	126.42
24	3	504	BCR	C11-C12-C13	10.16	154.96	126.42
24	3	503	BCR	C11-C10-C9	10.05	141.65	127.31
24	I	4001	BCR	C21-C20-C19	10.01	154.45	123.22
22	A	1106	CLA	C4A-NA-C1A	10.01	111.20	106.71
24	5	503	BCR	C11-C12-C13	10.00	154.51	126.42
22	L	1501	CLA	C4A-NA-C1A	9.95	111.18	106.71
24	6	503	BCR	C11-C10-C9	9.94	141.50	127.31
24	G	4001	BCR	C16-C15-C14	9.91	143.78	123.47
24	B	4003	BCR	C21-C20-C19	9.90	154.11	123.22
24	A	4001	BCR	C16-C15-C14	9.89	143.73	123.47
24	J	4001	BCR	C11-C12-C13	9.87	154.16	126.42
22	4	612	CLA	C4A-NA-C1A	9.80	111.11	106.71
22	A	1103	CLA	C4A-NA-C1A	9.78	111.10	106.71
22	F	1301	CLA	C4A-NA-C1A	9.70	111.07	106.71
22	A	1109	CLA	C4A-NA-C1A	9.68	111.06	106.71
24	B	4001	BCR	C16-C15-C14	9.67	143.29	123.47
22	8	611	CLA	C4A-NA-C1A	9.65	111.04	106.71
22	L	1502	CLA	C4A-NA-C1A	9.61	111.03	106.71
22	7	611	CLA	C4A-NA-C1A	9.60	111.02	106.71
22	a	604	CLA	C4A-NA-C1A	9.60	111.02	106.71
24	6	504	BCR	C11-C12-C13	9.58	153.31	126.42
24	3	505	BCR	C11-C12-C13	9.52	153.16	126.42
22	B	1235	CLA	C4A-NA-C1A	9.48	110.97	106.71
22	A	1141	CLA	C4A-NA-C1A	9.46	110.96	106.71
22	6	618	CLA	C4A-NA-C1A	9.45	110.96	106.71
24	6	504	BCR	C33-C5-C6	-9.43	113.94	124.53
22	8	606	CLA	C4A-NA-C1A	9.41	110.94	106.71
22	A	1132	CLA	C4A-NA-C1A	9.39	110.93	106.71
24	7	503	BCR	C11-C12-C13	9.38	152.78	126.42
22	A	1101	CLA	C4A-NA-C1A	9.34	110.91	106.71
22	B	1221	CLA	C4A-NA-C1A	9.33	110.90	106.71
22	B	1237	CLA	C4A-NA-C1A	9.32	110.90	106.71
22	1	612	CLA	C4A-NA-C1A	9.30	110.89	106.71
22	A	1120	CLA	C4A-NA-C1A	9.27	110.88	106.71
22	B	1212	CLA	C4A-NA-C1A	9.26	110.87	106.71
24	6	504	BCR	C11-C10-C9	9.26	140.52	127.31
24	L	4001	BCR	C20-C19-C18	9.25	152.41	126.42
22	a	607	CLA	C4A-NA-C1A	9.24	110.86	106.71
24	5	503	BCR	C20-C19-C18	9.24	152.36	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	605	CLA	C4A-NA-C1A	9.23	110.86	106.71
22	6	603	CLA	C4A-NA-C1A	9.21	110.85	106.71
22	A	1102	CLA	C4A-NA-C1A	9.21	110.85	106.71
22	3	612	CLA	C4A-NA-C1A	9.21	110.85	106.71
24	5	504	BCR	C11-C12-C13	9.20	152.26	126.42
22	6	601	CLA	C4A-NA-C1A	9.20	110.84	106.71
22	5	617	CLA	C4A-NA-C1A	9.19	110.84	106.71
24	A	4005	BCR	C20-C19-C18	9.19	152.23	126.42
22	B	1202	CLA	C4A-NA-C1A	9.18	110.83	106.71
22	a	615	CLA	C4A-NA-C1A	9.17	110.83	106.71
24	B	4003	BCR	C20-C19-C18	9.17	152.16	126.42
22	5	616	CLA	C4A-NA-C1A	9.16	110.83	106.71
22	A	1115	CLA	C4A-NA-C1A	9.16	110.83	106.71
22	3	602	CLA	C4A-NA-C1A	9.16	110.82	106.71
22	4	603	CLA	C4A-NA-C1A	9.15	110.82	106.71
22	A	1121	CLA	C4A-NA-C1A	9.14	110.82	106.71
22	7	608	CLA	C4A-NA-C1A	9.14	110.82	106.71
22	3	605	CLA	C4A-NA-C1A	9.13	110.81	106.71
22	5	603	CLA	C4A-NA-C1A	9.12	110.81	106.71
22	A	1107	CLA	C4A-NA-C1A	9.11	110.80	106.71
22	8	609	CLA	C4A-NA-C1A	9.10	110.80	106.71
24	7	503	BCR	C20-C19-C18	9.10	151.98	126.42
24	I	4001	BCR	C20-C19-C18	9.09	151.96	126.42
22	4	616	CLA	C4A-NA-C1A	9.09	110.79	106.71
24	6	503	BCR	C11-C12-C13	9.08	151.92	126.42
22	A	1113	CLA	C4A-NA-C1A	9.07	110.78	106.71
22	B	1224	CLA	C4A-NA-C1A	9.06	110.78	106.71
22	3	603	CLA	C4A-NA-C1A	9.05	110.77	106.71
22	3	604	CLA	C4A-NA-C1A	9.05	110.77	106.71
22	8	612	CLA	C4A-NA-C1A	9.04	110.77	106.71
22	B	1234	CLA	C4A-NA-C1A	9.04	110.77	106.71
22	B	1206	CLA	C4A-NA-C1A	9.04	110.77	106.71
22	8	620	CLA	C4A-NA-C1A	9.04	110.77	106.71
22	B	1222	CLA	C4A-NA-C1A	9.03	110.77	106.71
22	J	1901	CLA	C4A-NA-C1A	9.03	110.77	106.71
22	8	607	CLA	C4A-NA-C1A	9.03	110.77	106.71
22	A	1117	CLA	C4A-NA-C1A	8.98	110.75	106.71
22	B	1230	CLA	C4A-NA-C1A	8.98	110.75	106.71
24	4	503	BCR	C20-C19-C18	8.97	151.60	126.42
22	4	602	CLA	C4A-NA-C1A	8.96	110.74	106.71
22	6	612	CLA	C4A-NA-C1A	8.96	110.73	106.71
22	8	610	CLA	C4A-NA-C1A	8.96	110.73	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	7	610	CLA	C4A-NA-C1A	8.95	110.73	106.71
22	8	603	CLA	C4A-NA-C1A	8.95	110.73	106.71
22	1	615	CLA	C4A-NA-C1A	8.93	110.72	106.71
22	3	601	CLA	C4A-NA-C1A	8.93	110.72	106.71
22	A	1108	CLA	C4A-NA-C1A	8.93	110.72	106.71
22	A	1126	CLA	C4A-NA-C1A	8.92	110.72	106.71
22	A	1013	CLA	C4A-NA-C1A	8.91	110.71	106.71
22	B	1236	CLA	C4A-NA-C1A	8.91	110.71	106.71
22	4	605	CLA	C4A-NA-C1A	8.91	110.71	106.71
22	7	612	CLA	C4A-NA-C1A	8.91	110.71	106.71
22	A	1118	CLA	C4A-NA-C1A	8.90	110.71	106.71
22	A	1112	CLA	C4A-NA-C1A	8.90	110.71	106.71
22	B	1209	CLA	C4A-NA-C1A	8.89	110.70	106.71
22	3	607	CLA	C4A-NA-C1A	8.89	110.70	106.71
22	B	1211	CLA	C4A-NA-C1A	8.89	110.70	106.71
22	B	1021	CLA	C4A-NA-C1A	8.88	110.70	106.71
22	B	1201	CLA	C4A-NA-C1A	8.88	110.70	106.71
22	1	611	CLA	C4A-NA-C1A	8.88	110.70	106.71
22	4	610	CLA	C4A-NA-C1A	8.87	110.69	106.71
22	6	605	CLA	C4A-NA-C1A	8.87	110.69	106.71
22	6	608	CLA	C4A-NA-C1A	8.86	110.69	106.71
22	A	1111	CLA	C4A-NA-C1A	8.85	110.69	106.71
22	7	607	CLA	C4A-NA-C1A	8.85	110.69	106.71
22	a	608	CLA	C4A-NA-C1A	8.84	110.68	106.71
22	A	1110	CLA	C4A-NA-C1A	8.84	110.68	106.71
24	B	4002	BCR	C20-C19-C18	8.84	151.24	126.42
22	6	607	CLA	C4A-NA-C1A	8.83	110.68	106.71
22	6	617	CLA	C4A-NA-C1A	8.83	110.67	106.71
22	3	606	CLA	C4A-NA-C1A	8.82	110.67	106.71
24	A	4003	BCR	C11-C12-C13	8.82	151.18	126.42
22	8	605	CLA	C4A-NA-C1A	8.81	110.67	106.71
22	5	614	CLA	C4A-NA-C1A	8.80	110.66	106.71
22	1	602	CLA	C4A-NA-C1A	8.80	110.66	106.71
22	7	609	CLA	C4A-NA-C1A	8.80	110.66	106.71
22	a	602	CLA	C4A-NA-C1A	8.79	110.66	106.71
22	7	617	CLA	C4A-NA-C1A	8.79	110.66	106.71
22	4	606	CLA	C4A-NA-C1A	8.79	110.66	106.71
22	A	1140	CLA	C4A-NA-C1A	8.78	110.66	106.71
22	5	604	CLA	C4A-NA-C1A	8.78	110.66	106.71
22	5	612	CLA	C4A-NA-C1A	8.77	110.65	106.71
48	7	504	C7Z	C27-C28-C29	-8.77	112.98	126.23
22	1	603	CLA	C4A-NA-C1A	8.77	110.65	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1226	CLA	C4A-NA-C1A	8.76	110.64	106.71
22	K	1404	CLA	C4A-NA-C1A	8.75	110.64	106.71
22	3	613	CLA	C4A-NA-C1A	8.75	110.64	106.71
22	A	1129	CLA	C4A-NA-C1A	8.75	110.64	106.71
22	5	601	CLA	C4A-NA-C1A	8.73	110.63	106.71
22	A	1104	CLA	C4A-NA-C1A	8.72	110.63	106.71
22	A	1138	CLA	C4A-NA-C1A	8.72	110.62	106.71
22	1	608	CLA	C4A-NA-C1A	8.71	110.62	106.71
22	B	1207	CLA	C4A-NA-C1A	8.71	110.62	106.71
22	G	1601	CLA	C4A-NA-C1A	8.71	110.62	106.71
22	A	1133	CLA	C4A-NA-C1A	8.69	110.61	106.71
22	3	616	CLA	C4A-NA-C1A	8.69	110.61	106.71
22	3	618	CLA	C4A-NA-C1A	8.69	110.61	106.71
22	A	1122	CLA	C4A-NA-C1A	8.68	110.61	106.71
22	B	1223	CLA	C4A-NA-C1A	8.68	110.61	106.71
22	B	1239	CLA	C4A-NA-C1A	8.66	110.60	106.71
22	4	608	CLA	C4A-NA-C1A	8.65	110.60	106.71
22	A	1134	CLA	C4A-NA-C1A	8.65	110.59	106.71
22	B	1219	CLA	C4A-NA-C1A	8.65	110.59	106.71
22	B	1217	CLA	C4A-NA-C1A	8.64	110.59	106.71
22	7	605	CLA	C4A-NA-C1A	8.64	110.59	106.71
22	A	1123	CLA	C4A-NA-C1A	8.63	110.59	106.71
22	8	618	CLA	C4A-NA-C1A	8.63	110.59	106.71
22	1	610	CLA	C4A-NA-C1A	8.63	110.58	106.71
22	6	606	CLA	C4A-NA-C1A	8.63	110.58	106.71
22	B	1218	CLA	C4A-NA-C1A	8.62	110.58	106.71
22	B	1220	CLA	C4A-NA-C1A	8.62	110.58	106.71
22	L	1503	CLA	C4A-NA-C1A	8.62	110.58	106.71
22	a	603	CLA	C4A-NA-C1A	8.61	110.58	106.71
22	4	611	CLA	C4A-NA-C1A	8.61	110.58	106.71
22	B	1023	CLA	C4A-NA-C1A	8.61	110.58	106.71
22	4	601	CLA	C4A-NA-C1A	8.61	110.58	106.71
22	5	609	CLA	C4A-NA-C1A	8.60	110.57	106.71
22	4	604	CLA	C4A-NA-C1A	8.60	110.57	106.71
22	A	1116	CLA	C4A-NA-C1A	8.59	110.57	106.71
22	6	615	CLA	C4A-NA-C1A	8.58	110.56	106.71
22	7	601	CLA	C4A-NA-C1A	8.58	110.56	106.71
22	A	1136	CLA	C4A-NA-C1A	8.58	110.56	106.71
22	A	1139	CLA	C4A-NA-C1A	8.58	110.56	106.71
22	B	1232	CLA	C4A-NA-C1A	8.56	110.55	106.71
22	A	1131	CLA	C4A-NA-C1A	8.55	110.55	106.71
22	5	602	CLA	C4A-NA-C1A	8.55	110.55	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	5	608	CLA	C4A-NA-C1A	8.55	110.55	106.71
24	F	4001	BCR	C20-C19-C18	8.54	150.41	126.42
22	B	1229	CLA	C4A-NA-C1A	8.54	110.55	106.71
22	4	607	CLA	C4A-NA-C1A	8.53	110.54	106.71
22	4	617	CLA	C4A-NA-C1A	8.53	110.54	106.71
24	J	4001	BCR	C20-C19-C18	8.51	150.33	126.42
22	A	1130	CLA	C4A-NA-C1A	8.50	110.53	106.71
22	B	1208	CLA	C4A-NA-C1A	8.50	110.53	106.71
22	8	615	CLA	C4A-NA-C1A	8.50	110.53	106.71
22	A	1124	CLA	C4A-NA-C1A	8.50	110.53	106.71
22	6	602	CLA	C4A-NA-C1A	8.49	110.53	106.71
22	1	607	CLA	C4A-NA-C1A	8.49	110.52	106.71
22	a	605	CLA	C4A-NA-C1A	8.49	110.52	106.71
22	a	612	CLA	C4A-NA-C1A	8.49	110.52	106.71
48	7	504	C7Z	C15-C14-C13	-8.46	115.23	127.31
22	A	1128	CLA	C4A-NA-C1A	8.46	110.51	106.71
22	K	1402	CLA	C4A-NA-C1A	8.45	110.50	106.71
22	a	611	CLA	C4A-NA-C1A	8.42	110.49	106.71
22	B	1240	CLA	C4A-NA-C1A	8.42	110.49	106.71
22	B	1204	CLA	C4A-NA-C1A	8.42	110.49	106.71
22	1	601	CLA	C4A-NA-C1A	8.42	110.49	106.71
22	A	1105	CLA	C4A-NA-C1A	8.41	110.49	106.71
22	B	1213	CLA	C4A-NA-C1A	8.41	110.49	106.71
22	5	606	CLA	C4A-NA-C1A	8.41	110.48	106.71
24	K	4002	BCR	C11-C10-C9	8.39	139.29	127.31
22	K	1401	CLA	C4A-NA-C1A	8.37	110.47	106.71
24	A	4002	BCR	C20-C19-C18	8.37	149.94	126.42
22	A	1114	CLA	C4A-NA-C1A	8.37	110.47	106.71
22	7	606	CLA	C4A-NA-C1A	8.35	110.46	106.71
22	B	1203	CLA	C4A-NA-C1A	8.35	110.46	106.71
22	B	1231	CLA	C4A-NA-C1A	8.35	110.46	106.71
22	1	606	CLA	C4A-NA-C1A	8.35	110.46	106.71
22	1	604	CLA	C4A-NA-C1A	8.34	110.46	106.71
22	B	1215	CLA	C4A-NA-C1A	8.33	110.45	106.71
24	5	504	BCR	C11-C10-C9	8.32	139.19	127.31
22	5	605	CLA	C4A-NA-C1A	8.32	110.44	106.71
24	L	4003	BCR	C20-C19-C18	8.31	149.77	126.42
22	8	602	CLA	C4A-NA-C1A	8.31	110.44	106.71
22	3	610	CLA	C4A-NA-C1A	8.29	110.43	106.71
22	7	603	CLA	C4A-NA-C1A	8.29	110.43	106.71
22	A	1137	CLA	C4A-NA-C1A	8.29	110.43	106.71
22	A	1012	CLA	C4A-NA-C1A	8.28	110.43	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	F	4001	BCR	C11-C10-C9	8.27	139.11	127.31
22	G	1603	CLA	C4A-NA-C1A	8.27	110.42	106.71
22	G	1602	CLA	C4A-NA-C1A	8.27	110.42	106.71
22	7	602	CLA	C4A-NA-C1A	8.25	110.42	106.71
22	B	1216	CLA	C4A-NA-C1A	8.24	110.41	106.71
22	F	1302	CLA	C4A-NA-C1A	8.21	110.40	106.71
22	5	607	CLA	C4A-NA-C1A	8.19	110.39	106.71
22	A	1135	CLA	C4A-NA-C1A	8.18	110.38	106.71
22	4	615	CLA	C4A-NA-C1A	8.17	110.38	106.71
22	A	1125	CLA	C4A-NA-C1A	8.15	110.37	106.71
22	a	601	CLA	C4A-NA-C1A	8.15	110.37	106.71
22	B	1238	CLA	C4A-NA-C1A	8.09	110.34	106.71
24	6	504	BCR	C20-C19-C18	8.09	149.14	126.42
22	B	1214	CLA	C4A-NA-C1A	8.07	110.33	106.71
22	K	1403	CLA	C4A-NA-C1A	8.07	110.33	106.71
24	B	4006	BCR	C20-C19-C18	8.05	149.04	126.42
22	6	604	CLA	C4A-NA-C1A	8.05	110.33	106.71
22	5	618	CLA	C4A-NA-C1A	8.02	110.31	106.71
22	A	1127	CLA	C4A-NA-C1A	8.02	110.31	106.71
22	7	604	CLA	C4A-NA-C1A	7.99	110.30	106.71
22	B	1225	CLA	C4A-NA-C1A	7.93	110.27	106.71
22	B	1227	CLA	C4A-NA-C1A	7.93	110.27	106.71
24	B	4007	BCR	C20-C19-C18	7.88	148.54	126.42
24	3	503	BCR	C20-C19-C18	7.87	148.53	126.42
22	6	609	CLA	C4A-NA-C1A	7.84	110.23	106.71
22	7	615	CLA	C4A-NA-C1A	7.83	110.23	106.71
24	K	4002	BCR	C20-C19-C18	7.83	148.41	126.42
24	L	4002	BCR	C20-C19-C18	7.82	148.39	126.42
22	A	1119	CLA	C4A-NA-C1A	7.77	110.20	106.71
24	3	505	BCR	C20-C19-C18	7.76	148.23	126.42
34	G	5002	ERG	C19-C10-C9	-7.76	98.00	111.03
38	5	505	LUT	C21-C26-C27	7.69	122.42	112.70
24	8	503	BCR	C20-C19-C18	7.56	147.66	126.42
22	B	1022	CLA	C4A-NA-C1A	7.56	110.10	106.71
24	B	4004	BCR	C20-C19-C18	7.51	147.51	126.42
22	8	608	CLA	O2D-CGD-CBD	7.49	124.58	111.27
38	6	502	LUT	C21-C26-C27	7.37	122.02	112.70
38	5	505	LUT	C15-C14-C13	-7.33	116.85	127.31
21	A	1011	CL0	CMD-C2D-C1D	7.25	137.49	124.71
24	B	4005	BCR	C20-C19-C18	7.15	146.51	126.42
24	6	504	BCR	C33-C5-C4	7.11	127.28	113.62
24	F	4001	BCR	C11-C12-C13	7.11	146.38	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	4003	BCR	C20-C19-C18	7.02	146.14	126.42
21	A	1011	CL0	C4A-NA-C1A	7.00	109.86	106.71
35	J	4002	RRX	C38-C26-C25	-6.97	116.71	124.53
22	6	604	CLA	O2D-CGD-CBD	6.93	123.58	111.27
21	A	1011	CL0	C2C-C1C-NC	6.88	116.41	109.97
24	G	4001	BCR	C20-C19-C18	6.86	145.70	126.42
22	8	608	CLA	C4A-NA-C1A	6.85	109.78	106.71
34	G	5002	ERG	C14-C13-C17	6.83	107.00	99.72
22	A	1125	CLA	CMC-C2C-C1C	6.81	135.41	125.04
24	A	4004	BCR	C20-C19-C18	6.78	145.46	126.42
24	6	503	BCR	C15-C14-C13	-6.76	117.67	127.31
22	8	603	CLA	O2A-C1-C2	6.71	126.27	108.64
22	B	1228	CLA	C1-C2-C3	-6.69	114.47	126.04
22	A	1102	CLA	CAC-C3C-C4C	6.67	133.46	124.81
38	1	503	LUT	C21-C26-C27	6.65	121.11	112.70
22	B	1220	CLA	O2A-C1-C2	6.64	126.10	108.64
24	K	4001	BCR	C20-C19-C18	6.62	145.03	126.42
22	4	612	CLA	O2D-CGD-CBD	6.61	123.01	111.27
22	B	1221	CLA	O2D-CGD-CBD	6.55	122.90	111.27
22	B	1218	CLA	O2D-CGD-CBD	6.54	122.88	111.27
22	B	1205	CLA	O2D-CGD-CBD	6.52	122.86	111.27
22	A	1108	CLA	O2D-CGD-CBD	6.50	122.82	111.27
24	A	4001	BCR	C20-C19-C18	6.49	144.65	126.42
24	6	503	BCR	C20-C19-C18	6.47	144.60	126.42
22	B	1023	CLA	O2A-C1-C2	6.47	125.64	108.64
38	6	501	LUT	C21-C26-C27	6.43	120.83	112.70
22	A	1138	CLA	O2D-CGD-CBD	6.41	122.66	111.27
24	5	504	BCR	C20-C19-C18	6.39	144.37	126.42
22	a	607	CLA	O2D-CGD-CBD	6.33	122.52	111.27
22	6	609	CLA	O2D-CGD-CBD	6.28	122.42	111.27
38	6	502	LUT	C31-C30-C29	-6.28	118.35	127.31
41	3	506	QTB	C04-C03-C02	6.23	136.20	127.31
22	B	1210	CLA	O2D-CGD-CBD	6.21	122.30	111.27
38	5	505	LUT	C11-C10-C9	-6.19	118.47	127.31
22	A	1121	CLA	O2D-CGD-CBD	6.19	122.27	111.27
22	B	1231	CLA	CMD-C2D-C1D	6.19	135.62	124.71
22	A	1112	CLA	O2D-CGD-CBD	6.16	122.21	111.27
22	B	1201	CLA	O2D-CGD-CBD	6.15	122.19	111.27
38	7	501	LUT	C21-C26-C27	6.13	120.45	112.70
22	B	1228	CLA	C3A-C2A-C1A	6.13	110.52	101.34
22	A	1121	CLA	CMD-C2D-C1D	6.12	135.50	124.71
34	G	5002	ERG	C12-C13-C14	6.12	116.98	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	5	608	CLA	O2D-CGD-CBD	6.12	122.14	111.27
38	1	502	LUT	C21-C26-C25	6.11	122.37	111.42
22	8	608	CLA	O1D-CGD-CBD	-6.11	111.99	124.48
22	A	1132	CLA	O2D-CGD-CBD	6.10	122.12	111.27
21	A	1011	CL0	C1C-C2C-C3C	-6.09	100.56	106.96
22	4	607	CLA	O2D-CGD-CBD	6.09	122.09	111.27
38	a	503	LUT	C21-C26-C25	6.06	122.27	111.42
48	7	504	C7Z	C18-C5-C6	-6.03	117.75	124.53
22	1	606	CLA	CMD-C2D-C1D	6.00	135.29	124.71
22	B	1228	CLA	C1-O2A-CGA	6.00	132.19	116.44
22	B	1236	CLA	O2D-CGD-CBD	6.00	121.93	111.27
41	a	504	QTB	C09-C02-C03	5.99	128.14	118.94
24	3	504	BCR	C20-C19-C18	5.99	143.25	126.42
22	A	1120	CLA	O2D-CGD-CBD	5.99	121.92	111.27
22	B	1238	CLA	O2A-C1-C2	5.99	124.38	108.64
22	A	1114	CLA	CMD-C2D-C1D	5.98	135.25	124.71
22	7	604	CLA	O2D-CGD-CBD	5.97	121.88	111.27
22	A	1134	CLA	O2D-CGD-CBD	5.96	121.87	111.27
38	3	502	LUT	C21-C26-C25	5.96	122.09	111.42
22	B	1230	CLA	O2D-CGD-CBD	5.94	121.83	111.27
22	A	1137	CLA	O2D-CGD-CBD	5.93	121.81	111.27
22	4	611	CLA	CMD-C2D-C1D	5.93	135.16	124.71
22	A	1131	CLA	CMD-C2D-C1D	5.92	135.15	124.71
22	A	1118	CLA	O2D-CGD-CBD	5.91	121.78	111.27
22	1	605	CLA	O2A-C1-C2	5.91	124.16	108.64
22	A	1101	CLA	O2D-CGD-CBD	5.90	121.75	111.27
22	4	617	CLA	CMD-C2D-C1D	5.90	135.11	124.71
37	M	4001	ECH	C20-C21-C22	-5.90	118.90	127.31
38	5	501	LUT	C21-C26-C25	5.89	121.96	111.42
22	A	1129	CLA	O2D-CGD-CBD	5.89	121.73	111.27
22	B	1227	CLA	O2D-CGD-CBD	5.88	121.72	111.27
22	B	1228	CLA	C4-C3-C5	5.88	125.17	115.27
22	K	1403	CLA	CMD-C2D-C1D	5.88	135.08	124.71
22	A	1120	CLA	O2A-C1-C2	5.88	122.73	108.97
22	A	1128	CLA	O2D-CGD-CBD	5.88	121.71	111.27
22	B	1220	CLA	O2D-CGD-CBD	5.86	121.68	111.27
22	8	611	CLA	CMD-C2D-C1D	5.85	135.03	124.71
22	7	606	CLA	CMD-C2D-C1D	5.85	135.02	124.71
22	7	608	CLA	O2D-CGD-CBD	5.85	121.66	111.27
22	4	605	CLA	O2D-CGD-CBD	5.85	121.66	111.27
22	4	608	CLA	O2D-CGD-CBD	5.83	121.62	111.27
22	5	604	CLA	CMD-C2D-C1D	5.83	134.98	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	7	609	CLA	O2D-CGD-CBD	5.83	121.62	111.27
22	A	1101	CLA	CMD-C2D-C1D	5.83	134.98	124.71
22	8	609	CLA	O2D-CGD-CBD	5.82	121.62	111.27
22	B	1208	CLA	O2D-CGD-CBD	5.82	121.61	111.27
22	7	609	CLA	CMD-C2D-C1D	5.82	134.97	124.71
22	a	611	CLA	CMD-C2D-C1D	5.82	134.97	124.71
24	B	4001	BCR	C20-C19-C18	5.82	142.75	126.42
22	7	607	CLA	O2A-C1-C2	5.81	122.56	108.97
22	A	1115	CLA	O2D-CGD-CBD	5.81	121.59	111.27
22	5	603	CLA	CMD-C2D-C1D	5.79	134.92	124.71
22	A	1116	CLA	O2D-CGD-CBD	5.79	121.56	111.27
22	6	608	CLA	CMD-C2D-C1D	5.79	134.91	124.71
22	A	1139	CLA	O2D-CGD-CBD	5.77	121.53	111.27
22	B	1209	CLA	CMD-C2D-C1D	5.76	134.87	124.71
22	A	1123	CLA	CMD-C2D-C1D	5.76	134.87	124.71
22	3	605	CLA	O2A-C1-C2	5.75	123.75	108.64
22	5	617	CLA	CMD-C2D-C1D	5.75	134.84	124.71
22	1	605	CLA	O2D-CGD-CBD	5.74	121.47	111.27
22	8	618	CLA	O2D-CGD-CBD	5.74	121.47	111.27
22	A	1133	CLA	O2D-CGD-CBD	5.74	121.47	111.27
22	1	604	CLA	O2D-CGD-CBD	5.73	121.45	111.27
22	L	1502	CLA	O2D-CGD-CBD	5.73	121.45	111.27
22	3	604	CLA	O2D-CGD-CBD	5.72	121.44	111.27
22	B	1213	CLA	CMD-C2D-C1D	5.72	134.80	124.71
22	B	1223	CLA	O2D-CGD-CBD	5.72	121.43	111.27
38	6	501	LUT	C21-C26-C25	5.72	121.66	111.42
22	5	601	CLA	CMD-C2D-C1D	5.70	134.76	124.71
22	B	1208	CLA	CMD-C2D-C1D	5.70	134.76	124.71
22	B	1229	CLA	O2D-CGD-CBD	5.70	121.39	111.27
22	8	602	CLA	CMD-C2D-C1D	5.70	134.75	124.71
22	F	1302	CLA	O2D-CGD-CBD	5.70	121.39	111.27
22	B	1202	CLA	O2D-CGD-CBD	5.69	121.39	111.27
35	J	4002	RRX	C11-C10-C9	-5.69	119.18	127.31
22	A	1103	CLA	O2D-CGD-CBD	5.69	121.38	111.27
22	8	608	CLA	O2A-C1-C2	5.69	123.59	108.64
22	A	1104	CLA	CMD-C2D-C1D	5.68	134.73	124.71
22	A	1125	CLA	O2D-CGD-CBD	5.68	121.37	111.27
22	4	608	CLA	CMD-C2D-C1D	5.68	134.73	124.71
22	B	1219	CLA	O2D-CGD-CBD	5.67	121.34	111.27
22	B	1231	CLA	O2A-C1-C2	5.67	123.53	108.64
22	3	602	CLA	CMD-C2D-C1D	5.67	134.70	124.71
22	B	1227	CLA	CMD-C2D-C1D	5.66	134.69	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	8	606	CLA	O2A-C1-C2	5.66	123.51	108.64
38	4	502	LUT	C21-C26-C25	5.65	121.55	111.42
22	4	607	CLA	O2A-C1-C2	5.65	123.48	108.64
22	a	601	CLA	O2A-C1-C2	5.65	123.48	108.64
22	5	614	CLA	CMD-C2D-C1D	5.65	134.66	124.71
22	4	610	CLA	CMD-C2D-C1D	5.64	134.66	124.71
38	8	502	LUT	C21-C26-C25	5.63	121.51	111.42
22	3	602	CLA	O2D-CGD-CBD	5.63	121.27	111.27
22	3	604	CLA	CMD-C2D-C1D	5.63	134.63	124.71
22	3	606	CLA	CMD-C2D-C1D	5.62	134.62	124.71
22	B	1212	CLA	O2D-CGD-CBD	5.62	121.26	111.27
22	L	1502	CLA	O2A-C1-C2	5.62	123.41	108.64
24	4	503	BCR	C15-C14-C13	-5.62	119.29	127.31
22	B	1203	CLA	CMD-C2D-C1D	5.62	134.62	124.71
22	L	1501	CLA	O2D-CGD-CBD	5.62	121.25	111.27
22	7	602	CLA	CMD-C2D-C1D	5.62	134.62	124.71
22	B	1230	CLA	CMD-C2D-C1D	5.60	134.59	124.71
22	3	606	CLA	O2A-C1-C2	5.60	123.36	108.64
22	4	603	CLA	CMD-C2D-C1D	5.60	134.59	124.71
22	K	1402	CLA	CMD-C2D-C1D	5.60	134.58	124.71
22	8	615	CLA	CMD-C2D-C1D	5.60	134.57	124.71
22	B	1230	CLA	O2A-C1-C2	5.59	123.34	108.64
22	L	1501	CLA	CMD-C2D-C1D	5.59	134.57	124.71
22	B	1211	CLA	CMD-C2D-C1D	5.59	134.57	124.71
22	a	604	CLA	CMD-C2D-C1D	5.59	134.57	124.71
22	B	1240	CLA	O2D-CGD-CBD	5.59	121.20	111.27
22	5	609	CLA	O2D-CGD-CBD	5.59	121.20	111.27
22	a	605	CLA	CMD-C2D-C1D	5.58	134.55	124.71
22	8	605	CLA	CMD-C2D-C1D	5.58	134.55	124.71
22	A	1102	CLA	O2D-CGD-CBD	5.58	121.19	111.27
22	A	1115	CLA	O2A-C1-C2	5.58	123.30	108.64
41	a	504	QTB	C04-C03-C02	5.58	135.27	127.31
22	F	1301	CLA	CMD-C2D-C1D	5.58	134.54	124.71
21	A	1011	CL0	O2A-C1-C2	5.57	123.28	108.64
22	B	1231	CLA	O2D-CGD-CBD	5.57	121.16	111.27
22	B	1211	CLA	O2D-CGD-CBD	5.57	121.16	111.27
22	B	1214	CLA	CMD-C2D-C1D	5.56	134.52	124.71
22	A	1117	CLA	O2A-C1-C2	5.56	123.25	108.64
38	3	501	LUT	C21-C26-C27	5.56	119.73	112.70
22	B	1212	CLA	CMD-C2D-C1D	5.56	134.51	124.71
22	A	1126	CLA	CMD-C2D-C1D	5.56	134.51	124.71
22	4	615	CLA	O2A-C1-C2	5.56	123.24	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	7	617	CLA	O2D-CGD-CBD	5.56	121.14	111.27
22	3	605	CLA	CMD-C2D-C1D	5.55	134.50	124.71
22	a	601	CLA	CMD-C2D-C1D	5.55	134.50	124.71
22	A	1109	CLA	O2A-C1-C2	5.55	123.22	108.64
22	6	605	CLA	CMD-C2D-C1D	5.55	134.50	124.71
38	1	501	LUT	C21-C26-C25	5.55	121.36	111.42
22	A	1113	CLA	CMD-C2D-C1D	5.55	134.49	124.71
22	1	604	CLA	O2A-C1-C2	5.55	123.21	108.64
22	B	1217	CLA	O2D-CGD-CBD	5.55	121.12	111.27
22	A	1125	CLA	CMD-C2D-C1D	5.54	134.48	124.71
22	8	606	CLA	O2D-CGD-CBD	5.54	121.11	111.27
22	A	1108	CLA	CMD-C2D-C1D	5.54	134.47	124.71
22	F	1302	CLA	CMD-C2D-C1D	5.53	134.46	124.71
22	7	603	CLA	CMD-C2D-C1D	5.53	134.46	124.71
22	A	1132	CLA	CMD-C2D-C1D	5.53	134.46	124.71
22	7	601	CLA	CMD-C2D-C1D	5.53	134.45	124.71
22	A	1130	CLA	O2D-CGD-CBD	5.53	121.09	111.27
22	L	1503	CLA	CMD-C2D-C1D	5.52	134.45	124.71
22	A	1135	CLA	O2D-CGD-CBD	5.52	121.08	111.27
22	B	1217	CLA	O2A-C1-C2	5.52	123.13	108.64
22	B	1213	CLA	O2D-CGD-CBD	5.52	121.07	111.27
22	A	1111	CLA	CMD-C2D-C1D	5.52	134.43	124.71
22	4	616	CLA	CMD-C2D-C1D	5.52	134.43	124.71
22	7	608	CLA	CMD-C2D-C1D	5.51	134.43	124.71
38	1	503	LUT	C35-C34-C33	-5.51	119.44	127.31
22	5	617	CLA	O2D-CGD-CBD	5.51	121.06	111.27
22	6	602	CLA	O2D-CGD-CBD	5.51	121.06	111.27
22	7	604	CLA	CMD-C2D-C1D	5.51	134.42	124.71
22	4	602	CLA	CMD-C2D-C1D	5.50	134.41	124.71
22	B	1216	CLA	O2D-CGD-CBD	5.50	121.04	111.27
22	A	1124	CLA	O2D-CGD-CBD	5.50	121.04	111.27
22	5	606	CLA	O2D-CGD-CBD	5.50	121.04	111.27
22	K	1404	CLA	CMD-C2D-C1D	5.50	134.40	124.71
22	B	1218	CLA	O2A-C1-C2	5.50	123.08	108.64
22	A	1116	CLA	CMD-C2D-C1D	5.50	134.40	124.71
22	6	617	CLA	CMD-C2D-C1D	5.49	134.40	124.71
22	B	1234	CLA	O2D-CGD-CBD	5.49	121.03	111.27
22	6	604	CLA	CMD-C2D-C1D	5.49	134.40	124.71
22	8	608	CLA	CMD-C2D-C1D	5.49	134.39	124.71
22	B	1239	CLA	O2D-CGD-CBD	5.49	121.02	111.27
22	7	603	CLA	O2D-CGD-CBD	5.49	121.02	111.27
22	8	609	CLA	CMD-C2D-C1D	5.49	134.39	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	4	615	CLA	CMD-C2D-C1D	5.49	134.38	124.71
22	1	608	CLA	O2D-CGD-CBD	5.49	121.02	111.27
22	4	606	CLA	CMD-C2D-C1D	5.49	134.38	124.71
22	1	605	CLA	CMD-C2D-C1D	5.48	134.38	124.71
22	8	603	CLA	CMD-C2D-C1D	5.48	134.38	124.71
22	6	615	CLA	CMD-C2D-C1D	5.48	134.37	124.71
22	7	617	CLA	CMD-C2D-C1D	5.48	134.37	124.71
22	G	1601	CLA	O2A-C1-C2	5.48	123.03	108.64
22	A	1108	CLA	O2A-C1-C2	5.47	123.01	108.64
22	A	1129	CLA	CMD-C2D-C1D	5.47	134.35	124.71
22	B	1223	CLA	CMD-C2D-C1D	5.47	134.35	124.71
22	A	1140	CLA	O2D-CGD-CBD	5.46	120.98	111.27
22	1	610	CLA	O2D-CGD-CBD	5.46	120.98	111.27
38	5	502	LUT	C21-C26-C27	5.46	119.61	112.70
22	A	1137	CLA	CMD-C2D-C1D	5.46	134.34	124.71
22	B	1239	CLA	CMD-C2D-C1D	5.46	134.33	124.71
22	1	602	CLA	CMD-C2D-C1D	5.45	134.32	124.71
22	7	610	CLA	CMD-C2D-C1D	5.45	134.32	124.71
22	A	1135	CLA	CMD-C2D-C1D	5.45	134.32	124.71
22	B	1201	CLA	CMD-C2D-C1D	5.45	134.32	124.71
22	A	1134	CLA	CMD-C2D-C1D	5.45	134.31	124.71
22	A	1106	CLA	O2D-CGD-CBD	5.45	120.95	111.27
22	a	612	CLA	O2A-C1-C2	5.44	122.93	108.64
22	B	1240	CLA	O2A-C1-C2	5.44	122.93	108.64
41	a	504	QTB	C01-C02-C09	-5.44	109.51	118.08
22	1	601	CLA	CMD-C2D-C1D	5.44	134.29	124.71
22	A	1110	CLA	O2D-CGD-CBD	5.43	120.92	111.27
22	1	611	CLA	CMD-C2D-C1D	5.43	134.29	124.71
22	A	1116	CLA	O2A-C1-C2	5.43	122.91	108.64
22	K	1402	CLA	O2A-C1-C2	5.43	122.91	108.64
22	B	1226	CLA	CMD-C2D-C1D	5.43	134.28	124.71
22	4	606	CLA	O2D-CGD-CBD	5.43	120.92	111.27
22	5	606	CLA	CMD-C2D-C1D	5.42	134.27	124.71
22	5	609	CLA	CMD-C2D-C1D	5.42	134.27	124.71
22	5	605	CLA	CMD-C2D-C1D	5.42	134.27	124.71
22	B	1225	CLA	O2A-C1-C2	5.42	122.88	108.64
22	3	610	CLA	CMD-C2D-C1D	5.42	134.26	124.71
25	7	801	LHG	O7-C7-C8	5.42	123.18	111.50
22	3	610	CLA	O2D-CGD-CBD	5.41	120.89	111.27
22	B	1218	CLA	CMD-C2D-C1D	5.41	134.25	124.71
35	J	4002	RRX	C33-C5-C6	-5.41	118.46	124.53
22	A	1103	CLA	CMD-C2D-C1D	5.41	134.24	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	L	1503	CLA	O2D-CGD-CBD	5.40	120.87	111.27
22	B	1229	CLA	CMD-C2D-C1D	5.40	134.24	124.71
22	B	1224	CLA	O2D-CGD-CBD	5.40	120.87	111.27
22	B	1220	CLA	CMD-C2D-C1D	5.40	134.23	124.71
22	A	1128	CLA	O2A-C1-C2	5.40	122.83	108.64
22	A	1113	CLA	O2D-CGD-CBD	5.40	120.86	111.27
22	5	602	CLA	O2A-C1-C2	5.39	122.81	108.64
22	B	1214	CLA	O2D-CGD-CBD	5.39	120.85	111.27
22	a	603	CLA	CMD-C2D-C1D	5.39	134.21	124.71
38	3	501	LUT	C21-C26-C25	5.39	121.07	111.42
22	6	606	CLA	CMD-C2D-C1D	5.39	134.21	124.71
22	1	601	CLA	O2A-C1-C2	5.39	122.79	108.64
22	B	1238	CLA	CMD-C2D-C1D	5.39	134.21	124.71
22	6	601	CLA	O2A-C1-C2	5.38	122.78	108.64
22	B	1232	CLA	CMD-C2D-C1D	5.38	134.20	124.71
22	J	1901	CLA	CMD-C2D-C1D	5.38	134.20	124.71
22	B	1228	CLA	CMD-C2D-C1D	5.38	134.19	124.71
22	A	1109	CLA	CMD-C2D-C1D	5.38	134.19	124.71
22	B	1203	CLA	O2A-C1-C2	5.38	122.77	108.64
22	6	601	CLA	CMD-C2D-C1D	5.38	134.19	124.71
22	6	618	CLA	CMD-C2D-C1D	5.37	134.18	124.71
22	B	1204	CLA	O2D-CGD-CBD	5.37	120.81	111.27
22	B	1217	CLA	CMD-C2D-C1D	5.37	134.17	124.71
22	7	611	CLA	CMD-C2D-C1D	5.37	134.17	124.71
22	3	607	CLA	O2D-CGD-CBD	5.36	120.80	111.27
22	4	605	CLA	CMD-C2D-C1D	5.36	134.16	124.71
22	3	601	CLA	O2A-C1-C2	5.36	122.71	108.64
22	A	1102	CLA	CMD-C2D-C1D	5.35	134.15	124.71
22	A	1139	CLA	CMD-C2D-C1D	5.35	134.15	124.71
22	B	1212	CLA	O2A-C1-C2	5.35	122.70	108.64
22	1	603	CLA	CMD-C2D-C1D	5.35	134.14	124.71
22	B	1207	CLA	O2D-CGD-CBD	5.35	120.77	111.27
22	5	618	CLA	CMD-C2D-C1D	5.35	134.14	124.71
22	K	1402	CLA	O2D-CGD-CBD	5.34	120.76	111.27
22	4	601	CLA	O2D-CGD-CBD	5.34	120.76	111.27
22	5	606	CLA	O2A-C1-C2	5.34	122.67	108.64
22	A	1105	CLA	CMD-C2D-C1D	5.34	134.12	124.71
22	A	1137	CLA	O2A-C1-C2	5.34	122.66	108.64
22	B	1225	CLA	CMD-C2D-C1D	5.34	134.12	124.71
21	A	1011	CL0	O2D-CGD-CBD	5.33	120.74	111.27
22	8	611	CLA	O2A-C1-C2	5.33	122.64	108.64
38	4	501	LUT	C21-C26-C25	5.33	120.96	111.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	615	CLA	O2D-CGD-CBD	5.33	120.73	111.27
22	B	1208	CLA	O2A-C1-C2	5.33	122.63	108.64
37	M	4001	ECH	C15-C14-C13	-5.33	119.71	127.31
22	8	610	CLA	CMD-C2D-C1D	5.32	134.09	124.71
22	B	1226	CLA	O2D-CGD-CBD	5.32	120.72	111.27
22	8	607	CLA	O2D-CGD-CBD	5.32	120.72	111.27
22	8	602	CLA	O2D-CGD-CBD	5.32	120.72	111.27
22	G	1602	CLA	CMD-C2D-C1D	5.32	134.09	124.71
22	6	608	CLA	O2D-CGD-CBD	5.32	120.72	111.27
38	8	501	LUT	C21-C26-C25	5.32	120.94	111.42
22	a	602	CLA	CMD-C2D-C1D	5.31	134.08	124.71
22	B	1223	CLA	O2A-C1-C2	5.31	122.59	108.64
22	a	604	CLA	O2D-CGD-CBD	5.31	120.70	111.27
22	A	1128	CLA	CMD-C2D-C1D	5.31	134.07	124.71
22	6	602	CLA	CMD-C2D-C1D	5.31	134.07	124.71
38	5	505	LUT	C21-C26-C25	5.31	120.92	111.42
22	B	1227	CLA	O2A-C1-C2	5.31	122.58	108.64
22	3	603	CLA	O2D-CGD-CBD	5.31	120.70	111.27
22	B	1215	CLA	CMD-C2D-C1D	5.31	134.06	124.71
22	5	616	CLA	CMD-C2D-C1D	5.30	134.06	124.71
22	B	1210	CLA	CMD-C2D-C1D	5.30	134.06	124.71
22	A	1130	CLA	O2A-C1-C2	5.30	122.57	108.64
22	A	1111	CLA	O2D-CGD-CBD	5.30	120.69	111.27
22	5	602	CLA	CMD-C2D-C1D	5.30	134.06	124.71
22	A	1136	CLA	CMD-C2D-C1D	5.30	134.06	124.71
22	B	1237	CLA	CMD-C2D-C1D	5.30	134.06	124.71
22	B	1222	CLA	CMD-C2D-C1D	5.30	134.05	124.71
22	B	1207	CLA	CMD-C2D-C1D	5.30	134.05	124.71
22	8	620	CLA	CMD-C2D-C1D	5.29	134.04	124.71
22	7	615	CLA	CMD-C2D-C1D	5.29	134.04	124.71
21	A	1011	CL0	C2D-C1D-ND	5.29	114.00	110.10
22	K	1404	CLA	O2D-CGD-CBD	5.29	120.67	111.27
22	B	1234	CLA	CMD-C2D-C1D	5.29	134.03	124.71
22	G	1601	CLA	CMD-C2D-C1D	5.29	134.03	124.71
22	B	1021	CLA	O2D-CGD-CBD	5.29	120.66	111.27
22	B	1226	CLA	O2A-C1-C2	5.29	122.53	108.64
41	3	506	QTB	C09-C02-C03	5.28	127.05	118.94
22	7	601	CLA	O2A-C1-C2	5.28	122.52	108.64
22	B	1237	CLA	O2D-CGD-CBD	5.28	120.65	111.27
22	A	1138	CLA	CMD-C2D-C1D	5.28	134.02	124.71
22	A	1012	CLA	O2D-CGD-CBD	5.28	120.65	111.27
22	A	1119	CLA	CMD-C2D-C1D	5.28	134.01	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	6	612	CLA	CMD-C2D-C1D	5.27	134.00	124.71
22	4	615	CLA	O2D-CGD-CBD	5.27	120.63	111.27
22	5	605	CLA	O2D-CGD-CBD	5.27	120.63	111.27
22	B	1206	CLA	CMD-C2D-C1D	5.27	134.00	124.71
22	a	605	CLA	O2D-CGD-CBD	5.27	120.63	111.27
22	B	1215	CLA	O2D-CGD-CBD	5.26	120.62	111.27
22	1	607	CLA	CMD-C2D-C1D	5.26	133.99	124.71
22	4	601	CLA	O2A-C1-C2	5.26	122.45	108.64
22	B	1216	CLA	CMD-C2D-C1D	5.25	133.97	124.71
22	1	612	CLA	CMD-C2D-C1D	5.25	133.97	124.71
22	A	1134	CLA	O2A-C1-C2	5.24	122.42	108.64
22	5	603	CLA	O2A-C1-C2	5.24	122.41	108.64
22	A	1104	CLA	O2D-CGD-CBD	5.24	120.58	111.27
22	A	1120	CLA	CMD-C2D-C1D	5.24	133.94	124.71
22	a	601	CLA	O2D-CGD-CBD	5.23	120.57	111.27
22	a	607	CLA	O2A-C1-C2	5.23	122.37	108.64
22	A	1140	CLA	O2A-C1-C2	5.22	122.37	108.64
22	A	1125	CLA	O2A-C1-C2	5.22	122.36	108.64
22	3	601	CLA	CMD-C2D-C1D	5.22	133.91	124.71
22	F	1301	CLA	O2A-C1-C2	5.22	122.35	108.64
22	K	1403	CLA	O2D-CGD-CBD	5.22	120.54	111.27
22	3	607	CLA	CMD-C2D-C1D	5.22	133.91	124.71
22	B	1209	CLA	O2D-CGD-CBD	5.22	120.54	111.27
22	A	1114	CLA	O2A-C1-C2	5.21	122.34	108.64
22	A	1141	CLA	CMD-C2D-C1D	5.21	133.89	124.71
22	G	1603	CLA	O2D-CGD-CBD	5.21	120.52	111.27
22	4	610	CLA	O2D-CGD-CBD	5.20	120.52	111.27
22	5	602	CLA	O2D-CGD-CBD	5.20	120.52	111.27
22	B	1201	CLA	O2A-C1-C2	5.20	122.31	108.64
48	7	504	C7Z	C11-C10-C9	-5.20	119.89	127.31
22	A	1109	CLA	O2D-CGD-CBD	5.20	120.51	111.27
22	3	613	CLA	CMD-C2D-C1D	5.20	133.88	124.71
22	B	1224	CLA	CMD-C2D-C1D	5.20	133.87	124.71
22	4	604	CLA	CMD-C2D-C1D	5.20	133.87	124.71
22	A	1118	CLA	CMD-C2D-C1D	5.20	133.87	124.71
22	B	1235	CLA	CMD-C2D-C1D	5.19	133.87	124.71
22	B	1202	CLA	CMD-C2D-C1D	5.19	133.87	124.71
22	A	1123	CLA	O2A-C1-C2	5.19	122.28	108.64
38	6	502	LUT	C35-C34-C33	-5.19	119.90	127.31
22	A	1114	CLA	O2D-CGD-CBD	5.19	120.49	111.27
38	a	503	LUT	C35-C34-C33	-5.19	119.90	127.31
22	8	603	CLA	C1-C2-C3	-5.19	117.07	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	603	CLA	O2D-CGD-CBD	5.19	120.49	111.27
22	1	608	CLA	CMD-C2D-C1D	5.19	133.86	124.71
22	A	1138	CLA	O2A-C1-C2	5.19	122.27	108.64
22	G	1601	CLA	O2D-CGD-CBD	5.19	120.48	111.27
24	6	504	BCR	C15-C14-C13	-5.18	119.91	127.31
22	B	1206	CLA	O2D-CGD-CBD	5.18	120.48	111.27
22	5	614	CLA	O2D-CGD-CBD	5.18	120.48	111.27
22	5	608	CLA	CMD-C2D-C1D	5.18	133.84	124.71
22	4	610	CLA	O2A-C1-C2	5.18	122.25	108.64
22	3	612	CLA	O2D-CGD-CBD	5.18	120.47	111.27
24	B	4007	BCR	C34-C9-C10	-5.18	115.67	122.92
22	B	1210	CLA	O2A-C1-C2	5.18	122.24	108.64
22	1	603	CLA	O2A-C1-C2	5.17	122.23	108.64
22	A	1122	CLA	CMD-C2D-C1D	5.17	133.83	124.71
22	a	608	CLA	CMD-C2D-C1D	5.17	133.83	124.71
22	a	607	CLA	CMD-C2D-C1D	5.17	133.82	124.71
22	A	1130	CLA	CMD-C2D-C1D	5.17	133.82	124.71
22	8	618	CLA	CMD-C2D-C1D	5.17	133.82	124.71
22	8	610	CLA	O2A-C1-C2	5.16	122.20	108.64
22	3	607	CLA	O2A-C1-C2	5.16	122.20	108.64
22	8	606	CLA	CMD-C2D-C1D	5.16	133.80	124.71
22	A	1127	CLA	O2D-CGD-CBD	5.16	120.43	111.27
38	5	502	LUT	C21-C26-C25	5.15	120.65	111.42
22	7	602	CLA	O2D-CGD-CBD	5.15	120.43	111.27
22	A	1122	CLA	O2D-CGD-CBD	5.15	120.42	111.27
22	7	607	CLA	O2D-CGD-CBD	5.15	120.41	111.27
22	3	616	CLA	CMD-C2D-C1D	5.14	133.78	124.71
22	B	1203	CLA	O2D-CGD-CBD	5.14	120.40	111.27
22	7	611	CLA	O2D-CGD-CBD	5.14	120.40	111.27
22	a	603	CLA	O2A-C1-C2	5.14	122.13	108.64
38	5	505	LUT	C22-C23-C24	-5.13	105.90	111.74
22	3	618	CLA	CMD-C2D-C1D	5.13	133.76	124.71
22	5	618	CLA	O2A-C1-C2	5.13	122.12	108.64
22	K	1401	CLA	O2D-CGD-CBD	5.13	120.38	111.27
22	5	612	CLA	CMD-C2D-C1D	5.13	133.75	124.71
22	A	1133	CLA	CMD-C2D-C1D	5.12	133.74	124.71
22	B	1023	CLA	CMD-C2D-C1D	5.12	133.73	124.71
22	A	1133	CLA	O2A-C1-C2	5.12	122.08	108.64
22	5	603	CLA	O2D-CGD-CBD	5.11	120.35	111.27
22	B	1234	CLA	O2A-C1-C2	5.11	122.07	108.64
22	5	607	CLA	CMD-C2D-C1D	5.11	133.72	124.71
22	1	610	CLA	CMD-C2D-C1D	5.11	133.72	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1221	CLA	CMD-C2D-C1D	5.10	133.71	124.71
22	A	1105	CLA	O2D-CGD-CBD	5.10	120.34	111.27
22	B	1236	CLA	CMD-C2D-C1D	5.10	133.70	124.71
22	8	615	CLA	O2D-CGD-CBD	5.10	120.33	111.27
22	A	1013	CLA	CMD-C2D-C1D	5.10	133.70	124.71
22	B	1205	CLA	CMD-C2D-C1D	5.10	133.70	124.71
22	6	615	CLA	O2D-CGD-CBD	5.10	120.32	111.27
22	B	1222	CLA	O2A-C1-C2	5.09	122.02	108.64
22	6	602	CLA	O2A-C1-C2	5.09	122.02	108.64
22	B	1225	CLA	O2D-CGD-CBD	5.09	120.31	111.27
22	3	603	CLA	O2A-C1-C2	5.08	122.00	108.64
22	6	609	CLA	O2A-C1-C2	5.08	122.00	108.64
22	B	1204	CLA	CMD-C2D-C1D	5.08	133.67	124.71
22	A	1112	CLA	CMD-C2D-C1D	5.08	133.67	124.71
22	B	1204	CLA	O2A-C1-C2	5.08	121.98	108.64
22	6	607	CLA	O2A-C1-C2	5.08	121.98	108.64
22	8	610	CLA	O2D-CGD-CBD	5.08	120.29	111.27
22	3	610	CLA	O2A-C1-C2	5.07	121.97	108.64
22	7	615	CLA	O2D-CGD-CBD	5.07	120.28	111.27
22	3	616	CLA	O2A-C1-C2	5.07	121.96	108.64
22	4	606	CLA	O2A-C1-C2	5.07	121.96	108.64
22	6	612	CLA	O2D-CGD-CBD	5.07	120.27	111.27
22	5	601	CLA	O2A-C1-C2	5.06	121.94	108.64
22	8	618	CLA	O2A-C1-C2	5.06	121.94	108.64
22	8	603	CLA	O2D-CGD-CBD	5.06	120.26	111.27
22	K	1404	CLA	O2A-C1-C2	5.06	121.93	108.64
22	A	1131	CLA	O2D-CGD-CBD	5.06	120.26	111.27
24	F	4001	BCR	C12-C13-C14	5.06	126.70	118.94
22	B	1022	CLA	O2A-C1-C2	5.05	121.91	108.64
22	L	1501	CLA	O2A-C1-C2	5.05	121.91	108.64
22	8	611	CLA	O2D-CGD-CBD	5.05	120.24	111.27
22	A	1126	CLA	C1-C2-C3	-5.05	117.31	126.04
37	M	4001	ECH	C11-C10-C9	-5.05	120.11	127.31
22	6	601	CLA	C1-C2-C3	-5.04	117.32	126.04
22	A	1112	CLA	O2A-C1-C2	5.04	121.88	108.64
22	6	601	CLA	O2D-CGD-CBD	5.04	120.22	111.27
22	6	607	CLA	O2D-CGD-CBD	5.04	120.22	111.27
22	A	1105	CLA	O2A-C1-C2	5.04	121.88	108.64
22	4	607	CLA	CMD-C2D-C1D	5.04	133.59	124.71
22	A	1106	CLA	CMD-C2D-C1D	5.03	133.59	124.71
22	B	1021	CLA	O2A-C1-C2	5.03	121.85	108.64
38	1	503	LUT	C21-C26-C25	5.03	120.43	111.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	6	605	CLA	O2D-CGD-CBD	5.03	120.20	111.27
22	4	602	CLA	O2A-C1-C2	5.02	121.83	108.64
41	3	506	QTB	C13-C12-C11	5.02	122.50	112.60
22	A	1117	CLA	CMD-C2D-C1D	5.02	133.56	124.71
22	A	1108	CLA	C1-C2-C3	-5.02	117.36	126.04
35	J	4002	RRX	C20-C21-C22	-5.01	120.15	127.31
22	a	615	CLA	CMD-C2D-C1D	5.01	133.55	124.71
22	B	1238	CLA	O2D-CGD-CBD	5.01	120.16	111.27
22	B	1213	CLA	O2A-C1-C2	5.00	121.78	108.64
22	A	1140	CLA	CMD-C2D-C1D	5.00	133.53	124.71
22	A	1107	CLA	O2D-CGD-CBD	5.00	120.16	111.27
22	A	1127	CLA	CMD-C2D-C1D	5.00	133.52	124.71
22	A	1104	CLA	O2A-C1-C2	5.00	121.77	108.64
22	6	617	CLA	O2D-CGD-CBD	4.99	120.14	111.27
22	K	1401	CLA	CMD-C2D-C1D	4.99	133.51	124.71
22	A	1136	CLA	O2A-C1-C2	4.99	121.75	108.64
22	3	604	CLA	O2A-C1-C2	4.99	121.74	108.64
22	1	606	CLA	O2D-CGD-CBD	4.98	120.12	111.27
22	4	616	CLA	O2A-C1-C2	4.98	121.73	108.64
22	8	612	CLA	CMD-C2D-C1D	4.98	133.49	124.71
22	A	1132	CLA	O2A-C1-C2	4.98	121.71	108.64
22	6	603	CLA	O2A-C1-C2	4.97	121.71	108.64
22	3	605	CLA	O2D-CGD-CBD	4.97	120.11	111.27
38	6	501	LUT	C18-C5-C6	-4.97	118.95	124.53
22	8	607	CLA	CMD-C2D-C1D	4.97	133.47	124.71
22	7	611	CLA	O2A-C1-C2	4.96	121.68	108.64
22	B	1023	CLA	O2D-CGD-CBD	4.96	120.08	111.27
22	3	618	CLA	O2D-CGD-CBD	4.96	120.08	111.27
22	a	612	CLA	CMD-C2D-C1D	4.96	133.45	124.71
22	B	1219	CLA	O2A-C1-C2	4.96	121.66	108.64
22	3	601	CLA	O2D-CGD-CBD	4.96	120.07	111.27
22	4	601	CLA	CMD-C2D-C1D	4.95	133.44	124.71
22	B	1205	CLA	O2A-C1-C2	4.95	121.65	108.64
22	1	612	CLA	O2A-C1-C2	4.95	121.65	108.64
22	3	613	CLA	O2A-C1-C2	4.95	121.63	108.64
22	4	603	CLA	O2D-CGD-CBD	4.94	120.05	111.27
21	A	1011	CL0	O2A-CGA-O1A	-4.93	111.14	123.59
22	a	611	CLA	O2A-C1-C2	4.93	121.60	108.64
22	B	1022	CLA	CMD-C2D-C1D	4.93	133.40	124.71
22	B	1221	CLA	O2A-C1-C2	4.93	121.59	108.64
22	5	607	CLA	O2D-CGD-CBD	4.93	120.02	111.27
22	4	612	CLA	CMD-C2D-C1D	4.93	133.40	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1136	CLA	O2D-CGD-CBD	4.93	120.02	111.27
22	A	1126	CLA	O2D-CGD-CBD	4.92	120.02	111.27
22	B	1228	CLA	O2D-CGD-CBD	4.92	120.01	111.27
38	a	501	LUT	C21-C26-C27	4.91	118.91	112.70
22	1	607	CLA	O2D-CGD-CBD	4.91	120.00	111.27
22	B	1206	CLA	O2A-C1-C2	4.91	121.54	108.64
22	J	1901	CLA	O2D-CGD-CBD	4.91	119.99	111.27
22	4	602	CLA	O2D-CGD-CBD	4.91	119.99	111.27
22	1	611	CLA	O2D-CGD-CBD	4.90	119.98	111.27
22	A	1121	CLA	O2A-C1-C2	4.90	121.51	108.64
22	A	1013	CLA	O2D-CGD-CBD	4.90	119.97	111.27
38	a	501	LUT	C15-C14-C13	-4.90	120.32	127.31
22	7	615	CLA	O2A-C1-C2	4.89	121.50	108.64
22	A	1107	CLA	CMD-C2D-C1D	4.89	133.34	124.71
38	3	502	LUT	C21-C26-C27	4.89	118.89	112.70
22	B	1219	CLA	CMD-C2D-C1D	4.89	133.33	124.71
22	a	602	CLA	O2A-C1-C2	4.89	121.48	108.64
26	8	802	DGD	O2G-C1B-C2B	4.89	122.03	111.50
22	B	1236	CLA	O2A-C1-C2	4.88	121.47	108.64
46	7	502	XAT	C38-C25-C24	4.88	119.77	114.28
22	B	1240	CLA	CMD-C2D-C1D	4.88	133.31	124.71
22	A	1123	CLA	O2D-CGD-CBD	4.88	119.93	111.27
41	3	506	QTB	C01-C02-C09	-4.87	110.40	118.08
22	1	604	CLA	CMD-C2D-C1D	4.87	133.30	124.71
22	5	601	CLA	O2D-CGD-CBD	4.87	119.92	111.27
47	8	808	4RF	O21-C22-C24	4.87	121.99	111.50
22	A	1115	CLA	CMD-C2D-C1D	4.87	133.29	124.71
22	B	1211	CLA	O2A-C1-C2	4.87	121.42	108.64
22	1	615	CLA	CMD-C2D-C1D	4.86	133.28	124.71
22	5	612	CLA	O2A-C1-C2	4.86	121.40	108.64
22	F	1302	CLA	O2A-C1-C2	4.85	121.39	108.64
22	A	1141	CLA	O2D-CGD-CBD	4.85	119.89	111.27
22	6	615	CLA	O2A-C1-C2	4.85	121.38	108.64
22	A	1110	CLA	CMD-C2D-C1D	4.85	133.26	124.71
22	F	1301	CLA	O2D-CGD-CBD	4.84	119.88	111.27
38	a	502	LUT	C21-C26-C25	4.84	120.08	111.42
38	a	501	LUT	C18-C5-C6	-4.83	119.10	124.53
24	I	4001	BCR	C34-C9-C10	-4.83	116.15	122.92
22	a	604	CLA	O2A-C1-C2	4.83	121.33	108.64
38	1	503	LUT	C31-C30-C29	-4.83	120.42	127.31
22	A	1119	CLA	O2D-CGD-CBD	4.83	119.85	111.27
22	6	606	CLA	O2D-CGD-CBD	4.83	119.85	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1107	CLA	O2A-C1-C2	4.82	121.31	108.64
22	3	613	CLA	O2D-CGD-CBD	4.82	119.84	111.27
22	B	1234	CLA	CAC-C3C-C4C	4.82	131.07	124.81
38	1	502	LUT	C21-C26-C27	4.82	118.80	112.70
22	A	1138	CLA	C1-C2-C3	-4.82	117.71	126.04
22	B	1216	CLA	O2A-C1-C2	4.82	121.30	108.64
22	7	601	CLA	O2D-CGD-CBD	4.82	119.83	111.27
22	4	604	CLA	O2D-CGD-CBD	4.81	119.82	111.27
22	1	601	CLA	O2D-CGD-CBD	4.81	119.82	111.27
22	4	611	CLA	O2D-CGD-CBD	4.81	119.81	111.27
22	1	607	CLA	O2A-C1-C2	4.81	121.27	108.64
24	5	504	BCR	C15-C14-C13	-4.80	120.45	127.31
34	G	5002	ERG	C1-C10-C9	4.80	118.23	108.28
22	A	1124	CLA	O2A-C1-C2	4.80	121.25	108.64
22	A	1139	CLA	O2A-C1-C2	4.80	121.25	108.64
22	6	618	CLA	O2D-CGD-CBD	4.79	119.79	111.27
24	7	503	BCR	C15-C14-C13	-4.79	120.47	127.31
22	a	605	CLA	O2A-C1-C2	4.79	121.22	108.64
22	7	607	CLA	CMD-C2D-C1D	4.79	133.15	124.71
22	7	603	CLA	O2A-C1-C2	4.78	121.21	108.64
38	5	505	LUT	C35-C34-C33	-4.78	120.48	127.31
22	A	1127	CLA	O2A-C1-C2	4.78	121.20	108.64
22	A	1117	CLA	O2D-CGD-CBD	4.78	119.76	111.27
22	B	1202	CLA	O2A-C1-C2	4.77	121.18	108.64
22	3	612	CLA	O2A-C1-C2	4.77	121.17	108.64
22	1	608	CLA	O2A-C1-C2	4.77	121.16	108.64
22	8	612	CLA	O2D-CGD-CBD	4.77	119.74	111.27
22	A	1131	CLA	O2A-C1-C2	4.76	121.16	108.64
22	a	615	CLA	O2D-CGD-CBD	4.76	119.73	111.27
38	a	501	LUT	C21-C26-C25	4.76	119.94	111.42
22	A	1129	CLA	O2A-C1-C2	4.76	121.14	108.64
22	6	606	CLA	O2A-C1-C2	4.76	121.14	108.64
22	A	1135	CLA	O2A-C1-C2	4.76	121.14	108.64
22	a	608	CLA	O2A-C1-C2	4.76	121.13	108.64
22	A	1118	CLA	O2A-C1-C2	4.75	121.12	108.64
22	5	612	CLA	O2D-CGD-CBD	4.75	119.71	111.27
22	G	1602	CLA	O2D-CGD-CBD	4.75	119.71	111.27
22	B	1224	CLA	O2A-C1-C2	4.75	121.12	108.64
22	6	612	CLA	O2A-C1-C2	4.75	121.11	108.64
22	7	606	CLA	O2A-C1-C2	4.74	121.09	108.64
38	6	501	LUT	C35-C34-C33	-4.74	120.55	127.31
22	1	602	CLA	O2D-CGD-CBD	4.73	119.68	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	4	611	CLA	O2A-C1-C2	4.73	121.07	108.64
22	7	605	CLA	CMD-C2D-C1D	4.73	133.05	124.71
22	4	608	CLA	O2A-C1-C2	4.73	121.06	108.64
35	J	4002	RRX	C15-C14-C13	-4.72	120.57	127.31
22	8	620	CLA	O2D-CGD-CBD	4.72	119.66	111.27
22	G	1603	CLA	CMD-C2D-C1D	4.72	133.03	124.71
22	7	610	CLA	O2A-C1-C2	4.72	121.04	108.64
34	G	5002	ERG	C19-C10-C1	-4.71	101.98	109.43
22	A	1013	CLA	O2A-C1-C2	4.71	121.02	108.64
22	B	1022	CLA	O2D-CGD-CBD	4.71	119.64	111.27
22	4	604	CLA	O2A-C1-C2	4.70	121.00	108.64
22	5	604	CLA	O2D-CGD-CBD	4.70	119.62	111.27
25	a	801	LHG	O7-C7-C8	4.70	121.62	111.50
41	a	504	QTB	C13-C12-C11	4.69	121.86	112.60
38	5	501	LUT	C35-C34-C33	-4.69	120.61	127.31
22	7	606	CLA	O2D-CGD-CBD	4.69	119.60	111.27
22	A	1111	CLA	O2A-C1-C2	4.69	120.96	108.64
22	5	607	CLA	O2A-C1-C2	4.68	120.95	108.64
22	A	1110	CLA	O2A-C1-C2	4.68	120.94	108.64
22	B	1235	CLA	O2D-CGD-CBD	4.68	119.58	111.27
22	B	1237	CLA	O2A-C1-C2	4.68	120.93	108.64
22	B	1222	CLA	O2D-CGD-CBD	4.68	119.58	111.27
22	A	1122	CLA	O2A-C1-C2	4.67	120.91	108.64
38	8	502	LUT	C21-C26-C27	4.66	118.59	112.70
22	a	611	CLA	O2D-CGD-CBD	4.66	119.54	111.27
22	5	618	CLA	O2D-CGD-CBD	4.66	119.54	111.27
38	a	502	LUT	C35-C34-C33	-4.65	120.67	127.31
22	7	612	CLA	CMD-C2D-C1D	4.65	132.91	124.71
38	5	502	LUT	C7-C8-C9	-4.65	119.21	126.23
24	B	4007	BCR	C8-C9-C10	4.65	126.07	118.94
22	3	606	CLA	O2D-CGD-CBD	4.64	119.52	111.27
22	7	605	CLA	CAC-C3C-C4C	4.63	130.82	124.81
22	A	1124	CLA	CMD-C2D-C1D	4.63	132.87	124.71
22	7	617	CLA	O2A-C1-C2	4.63	120.79	108.64
22	4	616	CLA	O2D-CGD-CBD	4.63	119.49	111.27
22	6	609	CLA	CMD-C2D-C1D	4.62	132.86	124.71
22	a	603	CLA	C1-C2-C3	-4.62	118.05	126.04
22	B	1239	CLA	O2A-C1-C2	4.62	120.78	108.64
25	6	801	LHG	O7-C7-C8	4.62	121.46	111.50
22	4	603	CLA	O2A-C1-C2	4.61	120.74	108.64
22	4	617	CLA	O2D-CGD-CBD	4.60	119.45	111.27
22	5	604	CLA	O2A-C1-C2	4.60	120.73	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	612	CLA	CMD-C2D-C1D	4.60	132.82	124.71
22	L	1502	CLA	CMD-C2D-C1D	4.60	132.82	124.71
22	A	1113	CLA	O2A-C1-C2	4.60	120.72	108.64
22	6	607	CLA	CMD-C2D-C1D	4.60	132.81	124.71
22	B	1229	CLA	O2A-C1-C2	4.59	120.71	108.64
24	F	4001	BCR	C35-C13-C14	-4.59	116.49	122.92
22	B	1209	CLA	O2A-C1-C2	4.59	120.69	108.64
22	1	606	CLA	O2A-C1-C2	4.59	120.69	108.64
22	7	604	CLA	O2A-C1-C2	4.58	120.68	108.64
22	a	602	CLA	C1-C2-C3	-4.57	119.36	126.75
22	8	609	CLA	O2A-C1-C2	4.57	120.64	108.64
22	B	1021	CLA	CMD-C2D-C1D	4.57	132.76	124.71
21	A	1011	CL0	C3D-C2D-C1D	-4.56	99.60	105.83
25	A	5003	LHG	O7-C7-C8	4.56	121.32	111.50
22	5	617	CLA	O2A-C1-C2	4.56	120.61	108.64
38	6	501	LUT	C11-C10-C9	-4.56	120.81	127.31
38	a	503	LUT	C21-C26-C27	4.55	118.46	112.70
22	1	603	CLA	O2D-CGD-CBD	4.55	119.35	111.27
22	B	1021	CLA	C1-C2-C3	-4.55	118.18	126.04
22	5	609	CLA	O2A-C1-C2	4.54	120.56	108.64
25	4	801	LHG	O7-C7-C8	4.53	121.27	111.50
35	J	4002	RRX	C16-C17-C18	-4.53	120.84	127.31
22	B	1235	CLA	O2A-C1-C2	4.53	120.54	108.64
22	a	608	CLA	O2D-CGD-CBD	4.53	119.32	111.27
22	7	609	CLA	O2A-C1-C2	4.53	120.53	108.64
22	a	602	CLA	O2D-CGD-CBD	4.52	119.29	111.27
22	7	612	CLA	O2D-CGD-CBD	4.51	119.29	111.27
22	F	1302	CLA	CAC-C3C-C4C	4.51	130.66	124.81
22	B	1215	CLA	O2A-C1-C2	4.51	120.48	108.64
46	7	502	XAT	C7-C8-C9	-4.50	118.54	125.53
38	7	501	LUT	C21-C26-C25	4.49	119.46	111.42
38	4	501	LUT	C21-C26-C27	4.49	118.37	112.70
22	A	1012	CLA	O2A-C1-C2	4.48	120.42	108.64
22	A	1103	CLA	O2A-C1-C2	4.48	120.40	108.64
22	3	603	CLA	CMD-C2D-C1D	4.47	132.60	124.71
25	F	5001	LHG	O7-C7-C8	4.47	121.13	111.50
46	7	502	XAT	C31-C30-C29	-4.46	120.94	127.31
25	1	801	LHG	O7-C7-C8	4.46	121.12	111.50
22	B	1232	CLA	O2D-CGD-CBD	4.46	119.20	111.27
38	1	501	LUT	C35-C34-C33	-4.46	120.94	127.31
21	A	1011	CL0	CHD-C1D-ND	-4.46	120.36	124.45
39	3	611	CHL	CHD-C1D-ND	-4.45	120.36	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1203	CLA	C1-C2-C3	-4.45	118.35	126.04
22	8	602	CLA	O2A-C1-C2	4.44	120.31	108.64
38	a	501	LUT	C35-C34-C33	-4.44	120.97	127.31
22	6	604	CLA	O2A-C1-C2	4.44	120.30	108.64
22	8	620	CLA	O2A-C1-C2	4.44	120.30	108.64
22	3	616	CLA	O2D-CGD-CBD	4.44	119.15	111.27
48	7	504	C7Z	C31-C30-C29	-4.43	120.98	127.31
22	A	1106	CLA	O2A-C1-C2	4.43	120.27	108.64
22	A	1116	CLA	C1-C2-C3	-4.42	118.39	126.04
25	7	803	LHG	O7-C7-C8	4.42	121.03	111.50
38	a	502	LUT	C38-C25-C24	-4.42	114.10	123.56
22	A	1012	CLA	CMD-C2D-C1D	4.42	132.49	124.71
31	5	802	PTY	O7-C8-C11	4.41	121.01	111.50
22	7	612	CLA	O2A-C1-C2	4.41	120.23	108.64
24	F	4001	BCR	C33-C5-C6	-4.41	119.58	124.53
22	B	1204	CLA	C1-C2-C3	-4.41	118.42	126.04
22	A	1128	CLA	C1-C2-C3	-4.41	118.42	126.04
22	1	612	CLA	O2D-CGD-CBD	4.40	119.09	111.27
22	6	603	CLA	O2D-CGD-CBD	4.40	119.08	111.27
24	G	4001	BCR	C33-C5-C6	-4.39	119.60	124.53
38	1	503	LUT	C18-C5-C6	-4.38	119.61	124.53
24	J	4001	BCR	C15-C14-C13	-4.38	121.06	127.31
24	B	4007	BCR	C33-C5-C6	-4.38	119.61	124.53
22	3	605	CLA	C1-C2-C3	-4.36	118.50	126.04
22	B	1207	CLA	O2A-C1-C2	4.36	120.09	108.64
46	7	502	XAT	C18-C5-C4	4.35	119.17	114.28
31	8	810	PTY	O7-C8-C11	4.35	120.87	111.50
24	I	4001	BCR	C23-C24-C25	-4.34	115.00	127.20
22	8	608	CLA	C1-C2-C3	-4.33	118.55	126.04
38	a	503	LUT	C31-C30-C29	-4.33	121.14	127.31
39	4	613	CHL	CHB-C4A-NA	4.32	130.49	124.51
24	5	504	BCR	C36-C18-C17	-4.32	116.87	122.92
22	B	1214	CLA	O2A-C1-C2	4.32	119.98	108.64
38	a	501	LUT	C11-C10-C9	-4.31	121.16	127.31
26	B	5003	DGD	O2G-C1B-C2B	4.30	120.77	111.50
38	1	503	LUT	C7-C8-C9	-4.30	119.74	126.23
35	J	4002	RRX	C1-C6-C5	-4.29	116.58	122.61
38	7	501	LUT	C7-C8-C9	-4.29	119.76	126.23
30	6	803	PCW	O2-C31-C32	4.29	120.74	111.50
46	7	502	XAT	O4-C5-C18	-4.28	109.92	115.06
22	A	1129	CLA	C1-C2-C3	-4.28	119.82	126.75
38	a	502	LUT	C22-C23-C24	-4.28	106.87	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1136	CLA	C1-C2-C3	-4.28	118.64	126.04
39	6	611	CHL	CHD-C1D-ND	-4.28	120.53	124.45
22	4	612	CLA	O2A-C1-C2	4.27	119.85	108.64
38	1	503	LUT	C15-C14-C13	-4.27	121.22	127.31
22	6	612	CLA	C2D-C1D-ND	4.27	113.25	110.10
22	6	603	CLA	CMA-C3A-C4A	4.26	123.23	111.77
31	B	5005	PTY	O7-C8-C11	4.26	120.69	111.50
38	a	503	LUT	C15-C14-C13	-4.25	121.25	127.31
22	A	1101	CLA	O2A-C1-C2	4.24	119.79	108.64
22	6	603	CLA	CMD-C2D-C1D	4.24	132.19	124.71
38	6	502	LUT	C21-C26-C25	4.24	119.01	111.42
22	A	1102	CLA	CAC-C3C-C2C	-4.23	120.30	127.53
22	A	1118	CLA	C1-C2-C3	-4.23	118.73	126.04
22	3	601	CLA	C1-C2-C3	-4.21	118.76	126.04
39	4	609	CHL	C3C-C4C-NC	-4.21	105.85	110.57
22	A	1102	CLA	O2A-C1-C2	4.21	119.71	108.64
24	A	4003	BCR	C15-C14-C13	-4.20	121.31	127.31
22	7	610	CLA	O2D-CGD-CBD	4.20	118.73	111.27
47	7	807	4RF	O21-C22-C24	4.20	120.55	111.50
39	4	609	CHL	CHD-C4C-C3C	4.19	131.00	124.84
38	5	505	LUT	C8-C7-C6	-4.19	115.44	127.20
47	8	807	4RF	O21-C22-C24	4.18	120.52	111.50
25	A	5001	LHG	O7-C7-C8	4.18	120.51	111.50
38	1	501	LUT	C21-C26-C27	4.18	117.98	112.70
38	a	501	LUT	C7-C8-C9	-4.18	119.92	126.23
22	1	605	CLA	C1-C2-C3	-4.17	118.83	126.04
22	8	618	CLA	C1-C2-C3	-4.16	118.86	126.04
39	8	604	CHL	CHD-C1D-ND	-4.15	120.64	124.45
24	A	4004	BCR	C23-C24-C25	-4.15	115.54	127.20
22	1	611	CLA	O2A-C1-C2	4.15	119.55	108.64
39	6	619	CHL	CHD-C1D-ND	-4.15	120.64	124.45
22	1	606	CLA	C1-C2-C3	-4.15	118.87	126.04
22	5	616	CLA	O2D-CGD-CBD	4.14	118.63	111.27
39	7	613	CHL	CHD-C1D-ND	-4.14	120.65	124.45
24	B	4001	BCR	C12-C13-C14	-4.13	112.60	118.94
39	8	601	CHL	CHD-C1D-ND	-4.13	120.66	124.45
25	8	801	LHG	O7-C7-C8	4.13	120.40	111.50
38	a	502	LUT	C31-C30-C29	-4.13	121.42	127.31
24	A	4001	BCR	C19-C18-C17	4.13	125.27	118.94
22	6	602	CLA	C1-C2-C3	-4.12	118.92	126.04
38	6	501	LUT	C22-C23-C24	-4.12	107.05	111.74
24	L	4003	BCR	C33-C5-C6	-4.12	119.91	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	4001	BCR	C19-C18-C17	4.12	125.26	118.94
22	6	604	CLA	CAC-C3C-C4C	4.11	130.15	124.81
25	4	802	LHG	O7-C7-C8	4.11	120.36	111.50
38	a	502	LUT	C11-C10-C9	-4.10	121.45	127.31
25	3	801	LHG	O7-C7-C8	4.10	120.34	111.50
39	1	609	CHL	C1-C2-C3	-4.10	118.96	126.04
22	A	1125	CLA	C1-C2-C3	-4.09	118.97	126.04
22	A	1112	CLA	C1-C2-C3	-4.09	118.97	126.04
38	4	502	LUT	C22-C23-C24	-4.09	107.09	111.74
22	3	606	CLA	C1-C2-C3	-4.08	118.98	126.04
25	6	802	LHG	O7-C7-C8	4.08	120.29	111.50
22	8	605	CLA	O2D-CGD-CBD	4.08	118.51	111.27
31	7	804	PTY	O7-C8-C11	4.07	120.28	111.50
21	A	1011	CL0	O2A-CGA-CBA	4.07	124.68	111.91
38	3	501	LUT	C22-C23-C24	-4.07	107.11	111.74
38	3	502	LUT	C15-C14-C13	-4.06	121.52	127.31
24	3	505	BCR	C12-C13-C14	-4.06	112.72	118.94
22	A	1109	CLA	C1-C2-C3	-4.06	119.03	126.04
24	A	4001	BCR	C36-C18-C17	-4.04	117.26	122.92
22	A	1128	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
38	5	501	LUT	C7-C8-C9	-4.04	120.14	126.23
22	4	606	CLA	C1-C2-C3	-4.04	120.22	126.75
27	A	5007	3PH	O21-C21-C22	4.03	120.18	111.50
34	G	5002	ERG	C1-C10-C5	4.02	116.12	108.75
25	5	801	LHG	O7-C7-C8	4.02	120.17	111.50
34	G	5002	ERG	C13-C17-C20	-4.01	114.25	119.43
22	B	1236	CLA	C2D-C1D-ND	4.01	113.06	110.10
22	a	612	CLA	O2D-CGD-CBD	4.01	118.40	111.27
24	G	4001	BCR	C27-C26-C25	-4.01	116.91	122.73
24	A	4003	BCR	C34-C9-C10	-4.01	117.31	122.92
22	B	1206	CLA	C1-C2-C3	-4.01	119.11	126.04
22	6	612	CLA	C1-C2-C3	-4.00	120.28	126.75
22	7	612	CLA	CAC-C3C-C4C	4.00	130.00	124.81
25	7	802	LHG	O7-C7-C8	3.99	120.11	111.50
38	5	502	LUT	C35-C34-C33	-3.99	121.62	127.31
25	A	5002	LHG	O7-C7-C8	3.99	120.09	111.50
41	3	506	QTB	C19-C17-C11	-3.98	104.86	110.60
39	a	613	CHL	CHD-C1D-ND	-3.98	120.80	124.45
39	6	613	CHL	CHD-C1D-ND	-3.98	120.80	124.45
24	B	4001	BCR	C33-C5-C6	-3.98	120.06	124.53
38	a	501	LUT	C31-C30-C29	-3.97	121.64	127.31
39	5	613	CHL	CHD-C1D-ND	-3.97	120.81	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	802	LHG	O7-C7-C8	3.96	120.05	111.50
39	a	610	CHL	CHD-C1D-ND	-3.96	120.81	124.45
24	B	4002	BCR	C23-C24-C25	-3.96	116.09	127.20
22	5	617	CLA	C2C-C1C-NC	3.96	113.68	109.97
39	6	610	CHL	C1-O2A-CGA	3.95	126.82	116.44
23	B	2002	PQN	C11-C12-C13	-3.95	120.22	126.79
24	5	504	BCR	C19-C18-C17	3.94	124.99	118.94
24	3	505	BCR	C35-C13-C12	3.94	124.29	118.08
22	6	615	CLA	C1-C2-C3	-3.94	119.23	126.04
22	L	1501	CLA	C1-C2-C3	-3.94	120.38	126.75
39	4	613	CHL	CHD-C1D-ND	-3.93	120.84	124.45
22	A	1109	CLA	O2D-CGD-O1D	-3.93	116.15	123.84
32	F	5003	LAP	O7-P9-O5	3.93	131.67	112.24
22	A	1102	CLA	C2D-C1D-ND	3.93	113.00	110.10
39	6	610	CHL	CHD-C1D-ND	-3.93	120.85	124.45
22	G	1601	CLA	C1-C2-C3	-3.93	120.40	126.75
22	5	601	CLA	C1-C2-C3	-3.93	119.25	126.04
38	8	502	LUT	C35-C34-C33	-3.92	121.71	127.31
38	4	502	LUT	C21-C26-C27	3.92	117.66	112.70
24	B	4005	BCR	C23-C24-C25	-3.92	116.20	127.20
22	A	1125	CLA	C2D-C1D-ND	3.92	112.99	110.10
22	A	1135	CLA	C1-C2-C3	-3.91	119.27	126.04
38	5	501	LUT	C18-C5-C6	-3.91	120.14	124.53
38	6	502	LUT	C18-C5-C6	-3.91	120.14	124.53
22	8	606	CLA	C1-C2-C3	-3.90	119.29	126.04
32	B	5007	LAP	O7-P9-O5	3.90	131.53	112.24
37	M	4001	ECH	C28-C27-C26	-3.90	115.05	118.65
38	7	501	LUT	C35-C34-C33	-3.90	121.75	127.31
22	B	1228	CLA	C5-C3-C2	-3.89	113.24	121.12
22	B	1235	CLA	C1-C2-C3	-3.89	119.32	126.04
22	6	603	CLA	C2C-C1C-NC	3.89	113.61	109.97
24	B	4003	BCR	C23-C22-C21	3.89	124.91	118.94
22	A	1013	CLA	CHD-C1D-ND	-3.89	120.88	124.45
24	B	4004	BCR	C33-C5-C6	-3.88	120.17	124.53
25	B	5001	LHG	O7-C7-C8	3.88	119.86	111.50
22	B	1209	CLA	C1-C2-C3	-3.88	119.34	126.04
22	B	1228	CLA	CMA-C3A-C4A	3.87	122.18	111.77
38	8	501	LUT	C21-C26-C27	3.86	117.58	112.70
24	B	4001	BCR	C28-C27-C26	-3.86	107.19	114.08
38	4	502	LUT	C35-C34-C33	-3.85	121.81	127.31
31	3	802	PTY	O7-C8-C11	3.85	119.79	111.50
38	4	501	LUT	C7-C8-C9	-3.85	120.42	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	5002	LHG	O7-C7-C8	3.84	119.78	111.50
25	F	5002	LHG	O7-C7-C8	3.83	119.77	111.50
22	B	1234	CLA	C2D-C1D-ND	3.83	112.93	110.10
24	B	4001	BCR	C36-C18-C17	-3.82	117.56	122.92
38	4	502	LUT	C18-C5-C6	-3.82	120.23	124.53
24	3	503	BCR	C33-C5-C6	-3.82	120.23	124.53
22	F	1301	CLA	C1-C2-C3	-3.82	120.58	126.75
39	a	609	CHL	CHD-C1D-ND	-3.82	120.95	124.45
22	4	603	CLA	CHD-C1D-ND	-3.81	120.96	124.45
35	J	4002	RRX	C30-C25-C26	-3.81	117.25	122.61
22	A	1114	CLA	C1-C2-C3	-3.80	119.47	126.04
22	A	1123	CLA	C1-C2-C3	-3.80	119.47	126.04
22	F	1302	CLA	C2D-C1D-ND	3.79	112.90	110.10
38	4	502	LUT	C7-C8-C9	-3.79	120.52	126.23
38	a	503	LUT	C11-C10-C9	-3.78	121.92	127.31
24	3	504	BCR	C33-C5-C6	-3.78	120.29	124.53
39	1	609	CHL	CHD-C1D-ND	-3.78	120.98	124.45
44	5	803	DGA	OG2-CB1-CB2	3.78	119.64	111.50
38	a	503	LUT	C7-C8-C9	-3.77	120.53	126.23
22	6	609	CLA	O2D-CGD-O1D	-3.77	116.46	123.84
22	B	1222	CLA	C1-C2-C3	-3.77	119.52	126.04
22	1	603	CLA	C1-C2-C3	-3.77	119.52	126.04
22	A	1105	CLA	C1-C2-C3	-3.77	119.53	126.04
22	5	602	CLA	C1-C2-C3	-3.77	119.53	126.04
22	A	1127	CLA	C1-C2-C3	-3.77	119.53	126.04
22	B	1212	CLA	C1-C2-C3	-3.77	119.53	126.04
22	B	1224	CLA	C1-C2-C3	-3.77	119.53	126.04
32	K	5001	LAP	O7-P9-O5	3.76	130.85	112.24
22	A	1121	CLA	C1-C2-C3	-3.76	119.53	126.04
22	L	1503	CLA	C2C-C1C-NC	3.76	113.50	109.97
24	A	4004	BCR	C34-C9-C10	-3.76	117.65	122.92
34	G	5002	ERG	C18-C13-C14	-3.76	104.15	110.24
39	7	613	CHL	C3C-C4C-NC	-3.76	106.36	110.57
22	B	1226	CLA	CHD-C1D-ND	-3.76	121.00	124.45
38	a	502	LUT	C15-C14-C13	-3.76	121.95	127.31
26	A	5005	DGD	O2G-C1B-C2B	3.76	119.60	111.50
24	B	4002	BCR	C33-C5-C6	-3.76	120.31	124.53
48	7	504	C7Z	C1-C6-C5	-3.75	117.33	122.61
22	A	1126	CLA	O2A-C1-C2	3.75	118.50	108.64
22	B	1228	CLA	CHD-C1D-ND	-3.75	121.01	124.45
39	5	611	CHL	CHD-C1D-ND	-3.75	121.01	124.45
39	a	609	CHL	C3C-C4C-NC	-3.75	106.37	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	1	501	LUT	C22-C23-C24	-3.74	107.48	111.74
24	K	4002	BCR	C34-C9-C10	-3.74	117.69	122.92
24	8	503	BCR	C33-C5-C6	-3.73	120.33	124.53
22	A	1106	CLA	C2D-C1D-ND	3.73	112.85	110.10
22	B	1218	CLA	CHD-C1D-ND	-3.73	121.03	124.45
24	5	504	BCR	C28-C27-C26	-3.73	107.42	114.08
22	B	1210	CLA	C1-C2-C3	-3.73	119.59	126.04
38	3	502	LUT	C7-C8-C9	-3.73	120.61	126.23
22	B	1206	CLA	C2C-C1C-NC	3.72	113.46	109.97
39	4	613	CHL	C3C-C4C-NC	-3.72	106.40	110.57
22	4	608	CLA	C1-C2-C3	-3.72	119.61	126.04
24	G	4001	BCR	C36-C18-C17	-3.71	117.72	122.92
22	B	1225	CLA	C1-C2-C3	-3.71	119.62	126.04
22	8	609	CLA	C1-C2-C3	-3.71	119.62	126.04
38	6	501	LUT	C35-C15-C14	-3.71	115.88	123.47
22	1	603	CLA	CHD-C1D-ND	-3.71	121.05	124.45
22	A	1103	CLA	C1-C2-C3	-3.71	119.63	126.04
39	8	613	CHL	C1-C2-C3	-3.70	120.76	126.75
22	a	607	CLA	C1-C2-C3	-3.70	119.65	126.04
24	5	503	BCR	C36-C18-C17	-3.69	117.75	122.92
24	5	504	BCR	C33-C5-C6	-3.69	120.39	124.53
24	B	4003	BCR	C33-C5-C6	-3.69	120.39	124.53
37	M	4001	ECH	C16-C17-C18	-3.68	122.05	127.31
38	4	501	LUT	C35-C34-C33	-3.68	122.05	127.31
22	4	601	CLA	C1-C2-C3	-3.68	119.67	126.04
46	7	502	XAT	C15-C14-C13	-3.68	122.06	127.31
22	6	603	CLA	O2D-CGD-O1D	-3.67	116.65	123.84
37	M	4001	ECH	C33-C5-C6	-3.67	120.40	124.53
22	B	1236	CLA	CED-O2D-CGD	-3.67	107.64	115.94
48	7	504	C7Z	C20-C13-C14	-3.66	117.79	122.92
48	7	504	C7Z	C30-C31-C32	-3.66	111.79	123.22
38	a	503	LUT	C22-C23-C24	-3.66	107.58	111.74
39	3	611	CHL	C3C-C4C-NC	-3.66	106.47	110.57
22	B	1240	CLA	C1-C2-C3	-3.66	119.72	126.04
22	B	1238	CLA	C1-C2-C3	-3.66	119.72	126.04
38	5	501	LUT	C22-C23-C24	-3.65	107.59	111.74
48	7	504	C7Z	C11-C12-C13	-3.65	116.18	126.42
38	1	501	LUT	C18-C5-C6	-3.64	120.44	124.53
34	G	5002	ERG	C14-C8-C7	-3.64	117.21	124.38
39	5	610	CHL	C1-C2-C3	-3.64	119.75	126.04
38	3	501	LUT	C7-C8-C9	-3.63	120.75	126.23
22	K	1404	CLA	C1-C2-C3	-3.63	119.76	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	1	609	CHL	C3C-C4C-NC	-3.63	106.50	110.57
24	G	4001	BCR	C19-C18-C17	3.63	124.51	118.94
23	A	2001	PQN	C11-C12-C13	-3.63	120.76	126.79
48	7	504	C7Z	O3-C3-C4	3.62	117.44	109.68
22	A	1117	CLA	C1-C2-C3	-3.62	119.78	126.04
24	3	505	BCR	C33-C5-C6	-3.62	120.46	124.53
37	M	4001	ECH	C23-C24-C25	-3.62	117.04	127.20
38	3	502	LUT	C35-C34-C33	-3.62	122.15	127.31
38	1	503	LUT	C11-C10-C9	-3.62	122.15	127.31
33	G	5001	SQD	O7-S-C6	-3.61	102.64	106.94
38	7	501	LUT	C35-C15-C14	-3.61	116.08	123.47
24	A	4004	BCR	C33-C5-C6	-3.61	120.47	124.53
22	a	605	CLA	C1-C2-C3	-3.61	119.81	126.04
24	A	4002	BCR	C36-C18-C17	-3.60	117.88	122.92
22	6	603	CLA	C1-C2-C3	-3.60	119.81	126.04
24	5	503	BCR	C33-C5-C6	-3.60	120.49	124.53
22	A	1131	CLA	C1-C2-C3	-3.60	119.82	126.04
38	4	501	LUT	C18-C5-C6	-3.60	120.49	124.53
39	4	609	CHL	CHD-C1D-ND	-3.59	121.15	124.45
22	L	1502	CLA	C1-C2-C3	-3.59	119.83	126.04
24	B	4003	BCR	C37-C22-C21	-3.59	117.90	122.92
38	8	502	LUT	C7-C8-C9	-3.59	120.81	126.23
39	8	604	CHL	C3C-C4C-NC	-3.59	106.55	110.57
22	B	1230	CLA	C1-C2-C3	-3.58	119.84	126.04
39	5	613	CHL	C2C-C3C-C4C	3.58	109.04	106.49
39	5	611	CHL	C3C-C4C-NC	-3.58	106.56	110.57
24	A	4002	BCR	C23-C24-C25	-3.58	117.15	127.20
22	A	1112	CLA	C2C-C1C-NC	3.58	113.33	109.97
38	3	501	LUT	C35-C34-C33	-3.58	122.20	127.31
39	4	618	CHL	C1-C2-C3	-3.58	119.85	126.04
24	A	4001	BCR	C34-C9-C10	-3.58	117.91	122.92
38	3	501	LUT	C35-C15-C14	-3.58	116.15	123.47
22	B	1209	CLA	C2D-C1D-ND	3.57	112.73	110.10
22	5	606	CLA	C1-C2-C3	-3.57	120.98	126.75
22	K	1403	CLA	CHD-C1D-ND	-3.56	121.18	124.45
48	7	504	C7Z	O3-C3-C2	3.56	116.88	109.80
22	5	604	CLA	CHD-C1D-ND	-3.56	121.18	124.45
39	8	613	CHL	CHD-C1D-ND	-3.56	121.18	124.45
38	6	502	LUT	C11-C10-C9	-3.56	122.23	127.31
22	3	613	CLA	C1-C2-C3	-3.56	119.89	126.04
24	A	4005	BCR	C12-C13-C14	-3.56	113.48	118.94
22	a	601	CLA	C1-C2-C3	-3.55	119.90	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	7	502	XAT	C26-C27-C28	-3.55	118.48	125.99
22	A	1105	CLA	C2D-C1D-ND	3.55	112.72	110.10
22	B	1236	CLA	CAC-C3C-C4C	3.55	129.41	124.81
22	6	618	CLA	C2D-C1D-ND	3.55	112.72	110.10
22	A	1107	CLA	C2D-C1D-ND	3.55	112.72	110.10
34	G	5002	ERG	C18-C13-C12	-3.55	104.99	110.59
22	7	603	CLA	C1-C2-C3	-3.54	119.92	126.04
22	A	1119	CLA	O2A-C1-C2	3.54	117.94	108.64
38	8	501	LUT	C7-C8-C9	-3.54	120.89	126.23
38	5	501	LUT	C21-C26-C27	3.54	117.17	112.70
22	a	611	CLA	C1-C2-C3	-3.54	121.03	126.75
22	B	1235	CLA	CHD-C1D-ND	-3.53	121.21	124.45
39	8	613	CHL	C3C-C4C-NC	-3.53	106.61	110.57
39	8	613	CHL	C2C-C3C-C4C	3.53	109.01	106.49
22	7	612	CLA	C2C-C1C-NC	3.53	113.28	109.97
22	3	603	CLA	C1-C2-C3	-3.53	119.94	126.04
22	B	1213	CLA	C1-C2-C3	-3.53	119.94	126.04
24	L	4002	BCR	C36-C18-C17	-3.53	117.98	122.92
22	7	605	CLA	C2D-C1D-ND	3.52	112.70	110.10
38	5	505	LUT	C11-C12-C13	-3.52	116.52	126.42
22	K	1402	CLA	C1-C2-C3	-3.52	119.95	126.04
39	8	604	CHL	C1-C2-C3	-3.52	119.96	126.04
22	B	1023	CLA	CHD-C1D-ND	-3.52	121.22	124.45
38	6	502	LUT	C15-C14-C13	-3.52	122.29	127.31
22	a	608	CLA	C1-C2-C3	-3.51	119.96	126.04
38	3	502	LUT	C11-C10-C9	-3.51	122.30	127.31
38	3	502	LUT	C22-C23-C24	-3.51	107.75	111.74
22	A	1104	CLA	CHD-C1D-ND	-3.51	121.23	124.45
22	B	1231	CLA	CHD-C1D-ND	-3.51	121.23	124.45
22	4	610	CLA	O1D-CGD-CBD	-3.51	117.30	124.48
38	1	502	LUT	C18-C5-C6	-3.51	120.59	124.53
39	a	613	CHL	C4D-CHA-C1A	3.51	125.52	121.25
22	1	604	CLA	CMC-C2C-C1C	3.51	130.38	125.04
24	B	4003	BCR	C34-C9-C10	-3.51	118.01	122.92
23	A	2001	PQN	C14-C13-C15	3.50	121.17	115.27
24	6	504	BCR	C34-C9-C10	-3.50	118.02	122.92
24	B	4006	BCR	C28-C27-C26	-3.50	107.82	114.08
22	B	1229	CLA	C1-C2-C3	-3.50	119.98	126.04
38	5	505	LUT	C18-C5-C6	-3.50	120.60	124.53
24	B	4007	BCR	C23-C24-C25	-3.50	117.37	127.20
22	7	601	CLA	CHD-C1D-ND	-3.50	121.24	124.45
24	6	504	BCR	C28-C27-C26	-3.50	107.83	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	3	503	BCR	C36-C18-C17	-3.49	118.03	122.92
22	5	612	CLA	C1-C2-C3	-3.49	120.01	126.04
22	3	618	CLA	C2C-C1C-NC	3.49	113.24	109.97
24	B	4002	BCR	C27-C26-C25	-3.49	117.67	122.73
22	5	601	CLA	CHD-C1D-ND	-3.49	121.25	124.45
22	5	612	CLA	CHD-C1D-ND	-3.49	121.25	124.45
39	5	613	CHL	C3C-C4C-NC	-3.48	106.66	110.57
24	L	4002	BCR	C33-C5-C6	-3.48	120.62	124.53
22	B	1205	CLA	C1-C2-C3	-3.48	120.02	126.04
22	4	617	CLA	C2C-C1C-NC	3.48	113.23	109.97
22	A	1141	CLA	C2C-C1C-NC	3.47	113.23	109.97
22	A	1124	CLA	C1-C2-C3	-3.47	120.04	126.04
38	8	501	LUT	C18-C5-C6	-3.47	120.63	124.53
39	6	611	CHL	C3C-C4C-NC	-3.47	106.68	110.57
39	5	611	CHL	C1-C2-C3	-3.46	121.15	126.75
22	K	1402	CLA	C2D-C1D-ND	3.46	112.66	110.10
22	F	1302	CLA	C1D-ND-C4D	-3.46	103.88	106.33
24	G	4001	BCR	C28-C27-C26	-3.46	107.90	114.08
22	3	607	CLA	C1-C2-C3	-3.46	120.07	126.04
39	6	619	CHL	C3C-C4C-NC	-3.46	106.70	110.57
38	5	502	LUT	C11-C10-C9	-3.46	122.38	127.31
38	1	502	LUT	C10-C11-C12	-3.45	112.44	123.22
39	5	610	CHL	CHD-C1D-ND	-3.45	121.28	124.45
24	A	4003	BCR	C33-C5-C6	-3.45	120.65	124.53
33	7	805	SQD	O7-S-C6	-3.45	102.84	106.94
22	6	612	CLA	C1D-ND-C4D	-3.45	103.88	106.33
38	8	502	LUT	C18-C5-C6	-3.45	120.66	124.53
22	7	617	CLA	C2C-C1C-NC	3.44	113.20	109.97
38	3	501	LUT	C18-C5-C6	-3.44	120.66	124.53
22	B	1022	CLA	CHD-C1D-ND	-3.44	121.29	124.45
44	8	803	DGA	OG2-CB1-CB2	3.44	118.92	111.50
38	7	501	LUT	C18-C5-C6	-3.44	120.67	124.53
22	A	1113	CLA	CHD-C1D-ND	-3.43	121.30	124.45
24	K	4002	BCR	C8-C9-C10	3.43	124.21	118.94
22	A	1119	CLA	CHD-C1D-ND	-3.43	121.30	124.45
22	3	610	CLA	CHD-C1D-ND	-3.43	121.30	124.45
24	8	503	BCR	C33-C5-C4	3.43	120.20	113.62
24	J	4001	BCR	C33-C5-C6	-3.43	120.68	124.53
22	B	1207	CLA	C1-C2-C3	-3.43	120.12	126.04
38	1	501	LUT	C15-C14-C13	-3.43	122.42	127.31
48	7	504	C7Z	C22-C23-C24	3.43	114.99	110.30
39	6	611	CHL	C2C-C3C-C4C	3.42	108.93	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	a	503	LUT	C18-C5-C6	-3.42	120.69	124.53
38	5	502	LUT	C18-C5-C6	-3.42	120.69	124.53
22	B	1223	CLA	C1-C2-C3	-3.42	120.13	126.04
22	B	1240	CLA	C2C-C1C-NC	3.42	113.17	109.97
22	4	611	CLA	CHD-C1D-ND	-3.42	121.31	124.45
22	6	604	CLA	CHD-C1D-ND	-3.42	121.31	124.45
24	6	503	BCR	C28-C27-C26	-3.41	107.98	114.08
22	a	612	CLA	C2C-C1C-NC	3.41	113.17	109.97
22	1	601	CLA	C1-C2-C3	-3.41	120.15	126.04
24	B	4005	BCR	C33-C5-C6	-3.41	120.70	124.53
22	3	610	CLA	C1-C2-C3	-3.40	120.15	126.04
39	3	608	CHL	CHD-C1D-ND	-3.40	121.33	124.45
22	B	1236	CLA	C1D-ND-C4D	-3.40	103.92	106.33
22	A	1103	CLA	C2D-C1D-ND	3.40	112.61	110.10
22	1	605	CLA	CHD-C1D-ND	-3.40	121.33	124.45
22	A	1128	CLA	CMB-C2B-C3B	3.40	131.03	124.68
34	G	5002	ERG	C1-C2-C3	3.39	114.82	110.47
22	A	1113	CLA	C6-C5-C3	-3.39	109.07	114.62
22	6	608	CLA	CHD-C1D-ND	-3.39	121.34	124.45
39	8	601	CHL	C1-C2-C3	-3.39	120.18	126.04
22	A	1140	CLA	C1-C2-C3	-3.39	120.19	126.04
22	B	1208	CLA	CHD-C1D-ND	-3.38	121.34	124.45
24	3	504	BCR	C19-C18-C17	3.38	124.13	118.94
26	A	5005	DGD	O6D-C5D-C6D	3.38	113.49	106.67
39	5	610	CHL	C3C-C4C-NC	-3.37	106.79	110.57
22	8	606	CLA	CHD-C1D-ND	-3.37	121.36	124.45
22	A	1120	CLA	CHD-C1D-ND	-3.37	121.36	124.45
38	1	503	LUT	C22-C23-C24	-3.37	107.91	111.74
24	A	4003	BCR	C8-C9-C10	3.36	124.10	118.94
38	5	505	LUT	C18-C5-C4	3.36	120.59	114.36
22	5	602	CLA	C2C-C1C-NC	3.36	113.12	109.97
22	8	603	CLA	CHD-C1D-ND	-3.36	121.36	124.45
22	3	604	CLA	CHD-C1D-ND	-3.36	121.37	124.45
49	8	806	P5S	O37-C38-C39	3.36	118.73	111.50
22	A	1106	CLA	C1-C2-C3	-3.36	120.24	126.04
35	J	4002	RRX	C32-C1-C6	-3.35	104.86	110.30
22	6	602	CLA	C6-C5-C3	-3.35	109.13	114.62
39	6	619	CHL	CMA-C3A-C4A	3.35	120.79	111.77
22	7	601	CLA	CMB-C2B-C3B	3.35	130.94	124.68
39	4	618	CHL	CHD-C1D-ND	-3.35	121.38	124.45
39	a	606	CHL	C4D-CHA-C1A	3.35	125.32	121.25
22	a	604	CLA	C1D-ND-C4D	-3.35	103.96	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	4	613	CHL	C4A-NA-C1A	3.35	108.21	106.71
22	1	612	CLA	CHD-C1D-ND	-3.34	121.38	124.45
22	4	608	CLA	CHD-C1D-ND	-3.34	121.38	124.45
22	B	1212	CLA	C2C-C1C-NC	3.34	113.10	109.97
39	7	613	CHL	C2C-C3C-C4C	3.34	108.87	106.49
22	B	1215	CLA	CHD-C1D-ND	-3.34	121.39	124.45
24	B	4004	BCR	C33-C5-C4	3.33	120.02	113.62
35	J	4002	RRX	C33-C5-C4	3.33	120.01	113.62
24	4	503	BCR	C36-C18-C17	-3.32	118.27	122.92
22	B	1219	CLA	C1-C2-C3	-3.32	120.30	126.04
22	B	1209	CLA	C1-O2A-CGA	3.32	125.16	116.44
22	B	1201	CLA	CHD-C1D-ND	-3.32	121.40	124.45
22	6	604	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
22	4	602	CLA	C6-C5-C3	-3.31	109.20	114.62
39	6	613	CHL	C1-C2-C3	-3.31	121.39	126.75
22	A	1126	CLA	CHD-C1D-ND	-3.31	121.41	124.45
22	4	601	CLA	CHD-C1D-ND	-3.31	121.41	124.45
22	6	602	CLA	C2D-C1D-ND	3.31	112.54	110.10
22	B	1224	CLA	CHD-C1D-ND	-3.31	121.41	124.45
22	4	617	CLA	CHD-C1D-ND	-3.31	121.41	124.45
24	8	503	BCR	C36-C18-C17	-3.31	118.29	122.92
24	J	4001	BCR	C28-C27-C26	-3.31	108.17	114.08
34	G	5002	ERG	C2-C1-C10	3.30	119.90	112.74
24	5	504	BCR	C33-C5-C4	3.30	119.96	113.62
22	A	1117	CLA	CHD-C1D-ND	-3.30	121.42	124.45
38	5	502	LUT	C22-C23-C24	-3.30	107.98	111.74
22	6	618	CLA	C1D-ND-C4D	-3.30	103.99	106.33
22	7	603	CLA	CHD-C1D-ND	-3.30	121.42	124.45
22	7	602	CLA	C2D-C1D-ND	3.30	112.53	110.10
22	a	601	CLA	CHD-C1D-ND	-3.30	121.42	124.45
22	4	605	CLA	C2C-C1C-NC	3.30	113.06	109.97
22	G	1603	CLA	C2D-C1D-ND	3.30	112.53	110.10
22	B	1213	CLA	CHD-C1D-ND	-3.29	121.43	124.45
39	3	611	CHL	C2C-C3C-C4C	3.29	108.84	106.49
24	B	4001	BCR	C35-C13-C12	3.29	123.27	118.08
22	L	1502	CLA	C2D-C1D-ND	3.29	112.53	110.10
22	A	1106	CLA	C1D-ND-C4D	-3.29	104.00	106.33
22	8	611	CLA	C1-C2-C3	-3.29	121.43	126.75
24	7	503	BCR	C23-C24-C25	-3.29	117.96	127.20
22	8	606	CLA	C2C-C1C-NC	3.29	113.05	109.97
22	B	1236	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
48	7	504	C7Z	C15-C35-C34	-3.29	116.74	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	6	604	CLA	CMA-C3A-C4A	3.29	120.60	111.77
22	B	1230	CLA	CHD-C1D-ND	-3.29	121.44	124.45
24	B	4006	BCR	C23-C24-C25	-3.28	117.98	127.20
38	1	502	LUT	C7-C8-C9	-3.28	121.27	126.23
22	B	1234	CLA	C1D-ND-C4D	-3.28	104.00	106.33
24	A	4003	BCR	C28-C27-C26	-3.28	108.22	114.08
24	3	504	BCR	C36-C18-C17	-3.28	118.33	122.92
22	A	1101	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
38	1	501	LUT	C35-C15-C14	-3.28	116.75	123.47
25	A	5001	LHG	C5-O7-C7	-3.28	109.72	117.79
24	B	4005	BCR	C33-C5-C4	3.28	119.91	113.62
39	8	601	CHL	C3C-C4C-NC	-3.28	106.90	110.57
22	A	1109	CLA	C2C-C1C-NC	3.27	113.04	109.97
22	5	616	CLA	C2D-C1D-ND	3.27	112.52	110.10
38	5	501	LUT	C35-C15-C14	-3.27	116.77	123.47
22	7	608	CLA	CHD-C1D-ND	-3.27	121.45	124.45
22	4	602	CLA	C1-C2-C3	-3.27	120.39	126.04
38	8	502	LUT	C22-C23-C24	-3.27	108.02	111.74
46	7	502	XAT	C38-C25-C26	-3.27	116.78	122.26
22	6	601	CLA	CHD-C1D-ND	-3.26	121.45	124.45
22	7	607	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
22	8	618	CLA	C2C-C1C-NC	3.26	113.03	109.97
22	1	606	CLA	CHD-C1D-ND	-3.26	121.46	124.45
22	A	1134	CLA	C1-C2-C3	-3.26	120.40	126.04
22	B	1216	CLA	CHD-C1D-ND	-3.26	121.46	124.45
22	F	1302	CLA	CHD-C1D-ND	-3.26	121.46	124.45
22	a	603	CLA	CHD-C1D-ND	-3.26	121.46	124.45
22	B	1232	CLA	C2C-C1C-NC	3.26	113.02	109.97
39	a	610	CHL	C3C-C4C-NC	-3.26	106.92	110.57
22	4	616	CLA	CHD-C1D-ND	-3.25	121.46	124.45
24	K	4001	BCR	C33-C5-C6	-3.25	120.88	124.53
22	A	1101	CLA	C1-C2-C3	-3.25	120.42	126.04
22	A	1125	CLA	CHC-C1C-NC	-3.25	119.27	124.20
22	A	1130	CLA	CHD-C1D-ND	-3.25	121.47	124.45
22	A	1013	CLA	C2D-C1D-ND	3.25	112.50	110.10
22	4	617	CLA	CMA-C3A-C4A	3.25	120.50	111.77
22	B	1235	CLA	C2D-C1D-ND	3.25	112.50	110.10
22	3	616	CLA	C2C-C1C-NC	3.25	113.01	109.97
22	7	609	CLA	CHD-C1D-ND	-3.25	121.47	124.45
25	F	5002	LHG	O8-C23-C24	3.24	122.09	111.91
22	6	609	CLA	CMB-C2B-C3B	3.24	130.75	124.68
22	7	602	CLA	CHD-C1D-ND	-3.24	121.47	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1236	CLA	C1-C2-C3	-3.24	120.43	126.04
22	K	1402	CLA	CHD-C1D-ND	-3.24	121.47	124.45
24	B	4003	BCR	C33-C5-C4	3.24	119.84	113.62
24	7	503	BCR	C33-C5-C6	-3.24	120.89	124.53
22	A	1104	CLA	C1-C2-C3	-3.24	120.44	126.04
22	1	602	CLA	C2C-C1C-NC	3.24	113.00	109.97
22	4	610	CLA	C2C-C1C-NC	3.24	113.00	109.97
22	A	1107	CLA	C1-C2-C3	-3.24	120.44	126.04
22	5	606	CLA	CHD-C1D-ND	-3.24	121.48	124.45
39	4	613	CHL	C1-C2-C3	-3.23	120.45	126.04
22	K	1403	CLA	C2C-C1C-NC	3.23	113.00	109.97
22	5	609	CLA	C2C-C1C-NC	3.23	113.00	109.97
22	B	1206	CLA	C1C-C2C-C3C	-3.23	103.56	106.96
22	A	1134	CLA	C2C-C1C-NC	3.23	113.00	109.97
22	1	607	CLA	C2C-C1C-NC	3.23	113.00	109.97
22	L	1503	CLA	CAC-C3C-C2C	3.23	133.06	127.53
22	B	1218	CLA	C1-C2-C3	-3.23	120.45	126.04
22	B	1204	CLA	C2C-C1C-NC	3.23	113.00	109.97
22	B	1203	CLA	CHD-C1D-ND	-3.23	121.49	124.45
22	A	1012	CLA	OBD-CAD-C3D	-3.23	120.76	128.52
39	3	608	CHL	C3C-C4C-NC	-3.22	106.95	110.57
22	B	1237	CLA	C1-C2-C3	-3.22	120.47	126.04
22	7	615	CLA	C1-C2-C3	-3.22	120.47	126.04
22	B	1211	CLA	CHD-C1D-ND	-3.22	121.49	124.45
22	8	611	CLA	CHD-C1D-ND	-3.22	121.49	124.45
38	1	502	LUT	C22-C23-C24	-3.22	108.08	111.74
22	F	1301	CLA	C2C-C1C-NC	3.22	112.99	109.97
25	6	801	LHG	O8-C23-C24	3.22	122.00	111.91
22	a	604	CLA	C2D-C1D-ND	3.22	112.47	110.10
24	I	4001	BCR	C34-C9-C8	3.22	123.14	118.08
39	a	613	CHL	C3C-C4C-NC	-3.22	106.96	110.57
24	6	503	BCR	C36-C18-C17	-3.21	118.42	122.92
22	B	1239	CLA	C2C-C1C-NC	3.21	112.98	109.97
22	8	609	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
24	A	4002	BCR	C33-C5-C6	-3.21	120.92	124.53
22	1	601	CLA	CHD-C1D-ND	-3.21	121.50	124.45
22	B	1236	CLA	C2C-C1C-NC	3.21	112.98	109.97
22	G	1601	CLA	C2C-C1C-NC	3.21	112.98	109.97
39	a	613	CHL	C1B-CHB-C4A	-3.21	123.76	130.12
22	6	606	CLA	C1-C2-C3	-3.21	120.49	126.04
24	K	4001	BCR	C36-C18-C17	-3.21	118.42	122.92
38	8	501	LUT	C22-C23-C24	-3.21	108.09	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	F	1301	CLA	C2D-C1D-ND	3.21	112.47	110.10
22	B	1022	CLA	C1-C2-C3	-3.21	120.49	126.04
22	5	603	CLA	C1-C2-C3	-3.21	120.49	126.04
22	3	602	CLA	C2C-C1C-NC	3.21	112.98	109.97
22	7	610	CLA	C2C-C1C-NC	3.21	112.98	109.97
24	B	4005	BCR	C12-C13-C14	-3.21	114.02	118.94
22	G	1602	CLA	CHD-C1D-ND	-3.21	121.51	124.45
22	A	1101	CLA	C2C-C1C-NC	3.21	112.98	109.97
22	A	1121	CLA	C2C-C1C-NC	3.21	112.97	109.97
22	B	1214	CLA	CHD-C1D-ND	-3.20	121.51	124.45
22	8	615	CLA	C1D-ND-C4D	-3.20	104.06	106.33
22	B	1210	CLA	C2C-C1C-NC	3.20	112.97	109.97
38	1	502	LUT	C35-C15-C14	-3.20	116.92	123.47
22	B	1212	CLA	CHD-C1D-ND	-3.20	121.52	124.45
22	5	603	CLA	CHD-C1D-ND	-3.20	121.52	124.45
22	B	1206	CLA	CHD-C1D-ND	-3.20	121.52	124.45
22	5	614	CLA	CHD-C1D-ND	-3.20	121.52	124.45
22	6	612	CLA	CAC-C3C-C4C	3.20	128.96	124.81
24	L	4001	BCR	C33-C5-C6	-3.20	120.94	124.53
38	5	502	LUT	C15-C14-C13	-3.20	122.75	127.31
22	K	1404	CLA	C2C-C1C-NC	3.19	112.96	109.97
22	L	1503	CLA	CHD-C1D-ND	-3.19	121.52	124.45
22	7	608	CLA	C2C-C1C-NC	3.19	112.96	109.97
22	8	610	CLA	C2C-C1C-NC	3.19	112.96	109.97
22	A	1101	CLA	C2D-C1D-ND	3.19	112.46	110.10
22	6	602	CLA	CHD-C1D-ND	-3.19	121.52	124.45
22	A	1118	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
22	A	1134	CLA	CHD-C1D-ND	-3.19	121.52	124.45
22	4	603	CLA	C1-C2-C3	-3.19	120.53	126.04
22	7	611	CLA	C2D-C1D-ND	3.19	112.45	110.10
22	a	607	CLA	C2D-C1D-ND	3.19	112.45	110.10
24	6	504	BCR	C8-C9-C10	3.19	123.83	118.94
39	5	611	CHL	C2C-C3C-C4C	3.18	108.76	106.49
22	A	1135	CLA	CHD-C1D-ND	-3.18	121.53	124.45
24	5	503	BCR	C33-C5-C4	3.18	119.73	113.62
22	A	1137	CLA	C2D-C1D-ND	3.18	112.45	110.10
24	6	503	BCR	C33-C5-C6	-3.18	120.96	124.53
38	3	502	LUT	C18-C5-C6	-3.18	120.96	124.53
22	A	1123	CLA	CHD-C1D-ND	-3.18	121.54	124.45
22	5	609	CLA	C1-C2-C3	-3.17	120.56	126.04
22	A	1102	CLA	CHD-C1D-ND	-3.17	121.54	124.45
22	6	604	CLA	C2D-C1D-ND	3.17	112.44	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1138	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
22	B	1202	CLA	C1-C2-C3	-3.17	120.56	126.04
22	4	615	CLA	CMA-C3A-C4A	3.17	120.30	111.77
41	a	504	QTB	C19-C17-C16	3.17	115.56	109.03
34	G	5002	ERG	C19-C10-C5	-3.17	103.21	108.34
22	B	1202	CLA	C2D-C1D-ND	3.17	112.44	110.10
22	5	618	CLA	C2D-C1D-ND	3.17	112.44	110.10
22	A	1116	CLA	CHD-C1D-ND	-3.17	121.54	124.45
22	4	603	CLA	C2D-C1D-ND	3.17	112.44	110.10
22	A	1139	CLA	C2C-C1C-NC	3.17	112.94	109.97
39	3	608	CHL	C2C-C3C-C4C	3.17	108.75	106.49
22	A	1125	CLA	CHD-C1D-ND	-3.17	121.54	124.45
22	7	609	CLA	O2D-CGD-O1D	-3.17	117.65	123.84
39	6	613	CHL	C3C-C4C-NC	-3.17	107.02	110.57
39	8	604	CHL	C2C-C3C-C4C	3.17	108.75	106.49
22	4	603	CLA	C2C-C1C-NC	3.17	112.94	109.97
22	4	606	CLA	C2C-C1C-NC	3.17	112.94	109.97
22	7	617	CLA	O2D-CGD-O1D	-3.17	117.65	123.84
22	B	1022	CLA	OBD-CAD-C3D	-3.16	120.91	128.52
22	1	608	CLA	C1-C2-C3	-3.16	120.57	126.04
22	3	601	CLA	CHD-C1D-ND	-3.16	121.55	124.45
24	A	4001	BCR	C33-C5-C6	-3.16	120.98	124.53
22	B	1205	CLA	O2D-CGD-O1D	-3.16	117.65	123.84
22	A	1133	CLA	C1-C2-C3	-3.16	120.57	126.04
39	5	613	CHL	C1-O2A-CGA	3.16	124.74	116.44
22	7	611	CLA	CAC-C3C-C4C	3.16	128.91	124.81
22	A	1108	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
22	B	1218	CLA	C2D-C1D-ND	3.16	112.43	110.10
22	A	1132	CLA	CHD-C1D-ND	-3.16	121.55	124.45
22	7	617	CLA	C1C-C2C-C3C	-3.16	104.17	107.07
22	A	1133	CLA	C2C-C1C-NC	3.16	112.93	109.97
22	B	1023	CLA	C2D-C1D-ND	3.16	112.43	110.10
24	I	4001	BCR	C36-C18-C17	-3.16	118.50	122.92
22	8	608	CLA	CHD-C1D-ND	-3.16	121.55	124.45
22	7	607	CLA	C2C-C1C-NC	3.15	112.93	109.97
22	A	1102	CLA	C1D-ND-C4D	-3.15	104.09	106.33
22	8	620	CLA	CMA-C3A-C4A	3.15	120.25	111.77
22	6	615	CLA	CHD-C1D-ND	-3.15	121.56	124.45
22	7	610	CLA	CHD-C1D-ND	-3.15	121.56	124.45
22	B	1227	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
24	6	504	BCR	C31-C1-C6	-3.15	105.19	110.30
22	A	1111	CLA	CHD-C1D-ND	-3.15	121.56	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1130	CLA	C1-C2-C3	-3.15	120.60	126.04
22	A	1115	CLA	C2D-C1D-ND	3.15	112.42	110.10
22	6	606	CLA	CHD-C1D-ND	-3.15	121.56	124.45
22	A	1125	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
22	L	1501	CLA	CMA-C3A-C4A	3.14	120.22	111.77
22	B	1201	CLA	CMB-C2B-C3B	3.14	130.56	124.68
39	4	618	CHL	C3C-C4C-NC	-3.14	107.05	110.57
22	4	603	CLA	CMA-C3A-C4A	3.14	120.22	111.77
22	5	614	CLA	C2C-C1C-NC	3.14	112.92	109.97
22	A	1120	CLA	C2D-C1D-ND	3.14	112.42	110.10
22	7	604	CLA	C1-C2-C3	-3.14	120.61	126.04
22	3	612	CLA	CMB-C2B-C3B	3.14	130.55	124.68
39	a	606	CHL	CHD-C1D-ND	-3.14	121.57	124.45
22	8	612	CLA	CHD-C1D-ND	-3.14	121.57	124.45
24	L	4002	BCR	C8-C7-C6	-3.14	118.39	127.20
24	G	4001	BCR	C12-C13-C14	-3.14	114.13	118.94
22	6	612	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
22	7	606	CLA	C2D-C1D-ND	3.13	112.41	110.10
22	B	1222	CLA	CMA-C3A-C4A	3.13	120.19	111.77
22	6	607	CLA	C2D-C1D-ND	3.13	112.41	110.10
22	A	1110	CLA	C2C-C1C-NC	3.13	112.91	109.97
22	A	1117	CLA	C2C-C1C-NC	3.13	112.91	109.97
22	8	602	CLA	C2C-C1C-NC	3.13	112.91	109.97
22	6	615	CLA	C2D-C1D-ND	3.13	112.41	110.10
22	A	1137	CLA	CHD-C1D-ND	-3.13	121.58	124.45
24	L	4002	BCR	C12-C13-C14	-3.13	114.14	118.94
22	3	613	CLA	C2C-C1C-NC	3.13	112.90	109.97
22	A	1103	CLA	CHD-C1D-ND	-3.13	121.58	124.45
21	A	1011	CL0	C1D-ND-C4D	-3.13	104.11	106.33
39	4	609	CHL	C2C-C3C-C4C	3.13	108.72	106.49
22	8	607	CLA	CHD-C1D-ND	-3.13	121.58	124.45
22	B	1230	CLA	C2D-C1D-ND	3.13	112.41	110.10
22	7	615	CLA	C2C-C1C-NC	3.12	112.90	109.97
38	1	502	LUT	C35-C34-C33	-3.12	122.85	127.31
24	J	4001	BCR	C29-C30-C25	-3.12	105.67	110.48
22	5	607	CLA	C2C-C1C-NC	3.12	112.90	109.97
22	A	1112	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
22	A	1136	CLA	CHD-C1D-ND	-3.12	121.58	124.45
22	a	603	CLA	C2C-C1C-NC	3.12	112.90	109.97
22	6	612	CLA	CHD-C1D-ND	-3.12	121.59	124.45
22	8	620	CLA	CHD-C1D-ND	-3.12	121.59	124.45
22	A	1012	CLA	C1-C2-C3	-3.12	120.65	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	7	503	BCR	C29-C30-C25	-3.12	105.68	110.48
22	L	1502	CLA	CHD-C1D-ND	-3.12	121.59	124.45
22	B	1208	CLA	C1-O2A-CGA	3.12	124.62	116.44
22	B	1229	CLA	CHD-C1D-ND	-3.12	121.59	124.45
22	6	617	CLA	CHD-C1D-ND	-3.12	121.59	124.45
22	a	615	CLA	C2D-C1D-ND	3.12	112.40	110.10
22	7	609	CLA	O2A-CGA-CBA	3.12	121.69	111.91
22	a	611	CLA	CHD-C1D-ND	-3.12	121.59	124.45
24	G	4001	BCR	C30-C25-C26	-3.11	118.23	122.61
24	B	4006	BCR	C33-C5-C6	-3.11	121.03	124.53
22	5	616	CLA	C2C-C1C-NC	3.11	112.89	109.97
24	L	4001	BCR	C33-C5-C4	3.11	119.59	113.62
22	A	1012	CLA	CHD-C1D-ND	-3.11	121.59	124.45
37	M	4001	ECH	C24-C23-C22	-3.11	121.53	126.23
22	A	1102	CLA	CMB-C2B-C3B	3.11	130.50	124.68
22	7	604	CLA	CHD-C1D-ND	-3.11	121.60	124.45
22	B	1022	CLA	C2C-C1C-NC	3.11	112.88	109.97
22	B	1239	CLA	CHD-C1D-ND	-3.11	121.60	124.45
26	B	5003	DGD	C2G-O2G-C1B	-3.11	110.14	117.79
38	8	502	LUT	C10-C11-C12	-3.11	113.53	123.22
22	B	1217	CLA	C1-C2-C3	-3.10	120.67	126.04
39	4	613	CHL	CMA-C3A-C2A	3.10	126.35	113.83
22	4	616	CLA	C2C-C1C-NC	3.10	112.88	109.97
22	8	610	CLA	C1-C2-C3	-3.10	120.67	126.04
22	B	1208	CLA	CAA-C2A-C3A	-3.10	104.28	112.78
22	A	1104	CLA	C2C-C1C-NC	3.10	112.88	109.97
22	4	610	CLA	CHD-C1D-ND	-3.10	121.60	124.45
22	A	1107	CLA	CMB-C2B-C3B	3.10	130.48	124.68
22	a	611	CLA	C2C-C1C-NC	3.10	112.88	109.97
22	B	1220	CLA	C2C-C1C-NC	3.10	112.88	109.97
22	B	1202	CLA	CHD-C1D-ND	-3.10	121.61	124.45
22	3	602	CLA	CHD-C1D-ND	-3.10	121.61	124.45
22	B	1223	CLA	C2D-C1D-ND	3.10	112.39	110.10
22	A	1114	CLA	CMA-C3A-C4A	3.10	120.09	111.77
22	4	604	CLA	CHD-C1D-ND	-3.09	121.61	124.45
22	5	605	CLA	C2C-C1C-NC	3.09	112.87	109.97
31	8	810	PTY	C5-C6-C1	-3.09	104.47	111.79
22	4	602	CLA	C2D-C1D-ND	3.09	112.38	110.10
22	8	605	CLA	C2D-C1D-ND	3.09	112.38	110.10
22	8	615	CLA	C2D-C1D-ND	3.09	112.38	110.10
22	a	608	CLA	CHD-C1D-ND	-3.09	121.62	124.45
24	L	4001	BCR	C27-C26-C25	-3.09	118.25	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1204	CLA	CHD-C1D-ND	-3.09	121.62	124.45
22	8	603	CLA	C2C-C1C-NC	3.09	112.86	109.97
22	8	620	CLA	C2C-C1C-NC	3.09	112.86	109.97
22	B	1227	CLA	C1-C2-C3	-3.09	121.76	126.75
22	B	1214	CLA	C2C-C1C-NC	3.08	112.86	109.97
22	5	609	CLA	CMA-C3A-C4A	3.08	120.06	111.77
39	6	610	CHL	C3C-C4C-NC	-3.08	107.11	110.57
22	B	1224	CLA	C2C-C1C-NC	3.08	112.86	109.97
22	5	617	CLA	C1-C2-C3	-3.08	121.76	126.75
24	B	4005	BCR	C35-C13-C12	3.08	122.93	118.08
22	5	608	CLA	C2D-C1D-ND	3.08	112.37	110.10
38	5	501	LUT	C11-C10-C9	-3.08	122.92	127.31
26	A	5005	DGD	C6D-O5D-C1E	-3.08	107.73	113.74
22	K	1404	CLA	C2D-C1D-ND	3.08	112.37	110.10
22	A	1127	CLA	CHD-C1D-ND	-3.08	121.63	124.45
22	A	1103	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
22	B	1219	CLA	C2C-C1C-NC	3.08	112.85	109.97
22	B	1209	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
22	A	1126	CLA	C2C-C1C-NC	3.07	112.85	109.97
38	6	502	LUT	C36-C21-C26	3.07	114.20	109.55
22	3	606	CLA	CHD-C1D-ND	-3.07	121.63	124.45
22	A	1111	CLA	CMB-C2B-C3B	3.07	130.42	124.68
22	1	612	CLA	C2C-C1C-NC	3.07	112.85	109.97
22	A	1118	CLA	CHD-C1D-ND	-3.07	121.63	124.45
22	B	1205	CLA	CHD-C1D-ND	-3.07	121.63	124.45
22	a	607	CLA	CHD-C1D-ND	-3.07	121.64	124.45
22	3	607	CLA	CHD-C1D-ND	-3.07	121.64	124.45
22	A	1129	CLA	CHD-C1D-ND	-3.07	121.64	124.45
22	A	1114	CLA	CHD-C1D-ND	-3.06	121.64	124.45
38	a	501	LUT	C22-C23-C24	-3.06	108.25	111.74
22	7	602	CLA	C2C-C1C-NC	3.06	112.84	109.97
22	A	1132	CLA	C2C-C1C-NC	3.06	112.84	109.97
22	7	607	CLA	CHD-C1D-ND	-3.06	121.64	124.45
24	B	4003	BCR	C8-C9-C10	3.06	123.63	118.94
22	B	1217	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
22	A	1136	CLA	C2C-C1C-NC	3.06	112.84	109.97
22	4	612	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
22	6	606	CLA	C6-C5-C3	-3.06	109.62	114.62
22	3	616	CLA	C1-C2-C3	-3.06	120.76	126.04
22	6	604	CLA	C2C-C1C-NC	3.06	112.83	109.97
22	A	1109	CLA	C2D-C1D-ND	3.05	112.36	110.10
22	1	615	CLA	C2D-C1D-ND	3.05	112.36	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	4	601	CLA	C2C-C1C-NC	3.05	112.83	109.97
24	3	503	BCR	C34-C9-C10	-3.05	118.65	122.92
39	1	609	CHL	C2C-C3C-C4C	3.05	108.66	106.49
22	1	615	CLA	C2C-C1C-NC	3.05	112.83	109.97
39	6	610	CHL	C1B-CHB-C4A	-3.05	124.08	130.12
22	4	604	CLA	C1-C2-C3	-3.05	120.77	126.04
25	7	801	LHG	C6-C5-C4	-3.05	104.58	111.79
22	3	603	CLA	C2D-C1D-ND	3.05	112.35	110.10
22	1	607	CLA	C2D-C1D-ND	3.05	112.35	110.10
22	A	1132	CLA	C1-C2-C3	-3.05	120.77	126.04
22	3	607	CLA	C2C-C1C-NC	3.05	112.83	109.97
22	A	1123	CLA	CMA-C3A-C4A	3.05	119.96	111.77
24	B	4006	BCR	C12-C13-C14	-3.05	114.27	118.94
22	8	609	CLA	CHD-C1D-ND	-3.05	121.66	124.45
22	1	611	CLA	C2C-C1C-NC	3.05	112.83	109.97
22	5	607	CLA	C1-C2-C3	-3.04	120.78	126.04
24	6	503	BCR	C19-C18-C17	3.04	123.61	118.94
22	B	1226	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
22	A	1102	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
22	B	1239	CLA	C1-C2-C3	-3.04	120.78	126.04
22	B	1217	CLA	C2C-C1C-NC	3.04	112.82	109.97
22	B	1222	CLA	CHD-C1D-ND	-3.04	121.66	124.45
22	1	604	CLA	CHD-C1D-ND	-3.04	121.66	124.45
22	A	1121	CLA	CHD-C1D-ND	-3.04	121.66	124.45
22	1	604	CLA	C1-C2-C3	-3.04	120.79	126.04
22	J	1901	CLA	C2C-C1C-NC	3.04	112.82	109.97
22	a	602	CLA	C2C-C1C-NC	3.04	112.82	109.97
24	3	503	BCR	C38-C26-C25	-3.04	121.12	124.53
22	4	612	CLA	CHD-C1D-ND	-3.04	121.66	124.45
22	B	1221	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
35	J	4002	RRX	C20-C19-C18	-3.03	117.89	126.42
47	8	808	4RF	O18-C16-C15	3.03	121.43	111.91
39	6	611	CHL	C1-C2-C3	-3.03	121.84	126.75
22	a	602	CLA	C2D-C1D-ND	3.03	112.34	110.10
22	B	1222	CLA	C2C-C1C-NC	3.03	112.81	109.97
22	6	606	CLA	C2C-C1C-NC	3.03	112.81	109.97
22	L	1501	CLA	C2C-C1C-NC	3.03	112.81	109.97
22	8	618	CLA	CAC-C3C-C4C	3.03	128.74	124.81
22	4	615	CLA	C2C-C1C-NC	3.03	112.81	109.97
22	J	1901	CLA	C2D-C1D-ND	3.03	112.33	110.10
24	K	4002	BCR	C15-C14-C13	-3.03	122.99	127.31
22	1	608	CLA	C2C-C1C-NC	3.03	112.81	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1102	CLA	C1-C2-C3	-3.02	120.81	126.04
22	A	1110	CLA	CHD-C1D-ND	-3.02	121.68	124.45
22	1	611	CLA	C1-C2-C3	-3.02	120.82	126.04
39	a	610	CHL	C2C-C3C-C4C	3.02	108.64	106.49
22	A	1107	CLA	C2C-C1C-NC	3.02	112.80	109.97
22	4	607	CLA	CHD-C1D-ND	-3.02	121.68	124.45
22	B	1217	CLA	CHD-C1D-ND	-3.02	121.68	124.45
22	A	1139	CLA	C1-C2-C3	-3.02	120.82	126.04
22	K	1402	CLA	CMA-C3A-C4A	3.02	119.89	111.77
39	6	610	CHL	C4D-CHA-C1A	3.02	124.92	121.25
24	F	4001	BCR	C28-C27-C26	-3.02	108.69	114.08
22	A	1104	CLA	C1C-C2C-C3C	-3.02	103.78	106.96
24	3	503	BCR	C33-C5-C4	3.02	119.41	113.62
22	B	1203	CLA	C2D-C1D-ND	3.02	112.33	110.10
22	7	615	CLA	CHD-C1D-ND	-3.02	121.68	124.45
22	a	607	CLA	C2C-C1C-NC	3.01	112.80	109.97
22	a	601	CLA	CMB-C2B-C3B	3.01	130.31	124.68
22	A	1135	CLA	C2C-C1C-NC	3.01	112.79	109.97
22	5	603	CLA	C2C-C1C-NC	3.01	112.79	109.97
38	7	501	LUT	C22-C23-C24	-3.01	108.31	111.74
22	6	609	CLA	C2C-C1C-NC	3.01	112.79	109.97
22	3	612	CLA	CHD-C1D-ND	-3.01	121.69	124.45
22	K	1404	CLA	CHD-C1D-ND	-3.01	121.69	124.45
22	7	611	CLA	C1D-ND-C4D	-3.01	104.20	106.33
22	B	1212	CLA	C2D-C1D-ND	3.01	112.32	110.10
24	A	4005	BCR	C33-C5-C4	3.01	119.39	113.62
22	7	604	CLA	O1D-CGD-CBD	-3.01	118.33	124.48
39	a	610	CHL	C4D-CHA-C1A	3.01	124.91	121.25
39	6	611	CHL	CMA-C3A-C4A	3.01	119.85	111.77
22	6	617	CLA	C2C-C1C-NC	3.01	112.79	109.97
24	G	4001	BCR	C35-C13-C12	3.01	122.81	118.08
22	B	1205	CLA	O2A-CGA-CBA	3.01	121.34	111.91
24	L	4001	BCR	C37-C22-C21	-3.01	118.71	122.92
22	1	605	CLA	C2C-C1C-NC	3.00	112.79	109.97
22	A	1128	CLA	C2C-C1C-NC	3.00	112.78	109.97
24	G	4001	BCR	C37-C22-C21	-3.00	118.72	122.92
39	a	610	CHL	CMA-C3A-C4A	3.00	119.84	111.77
22	7	611	CLA	C2C-C1C-NC	3.00	112.78	109.97
35	J	4002	RRX	C11-C12-C13	-3.00	117.98	126.42
24	A	4005	BCR	C23-C24-C25	-3.00	118.77	127.20
22	8	618	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
38	3	502	LUT	C35-C15-C14	-3.00	117.33	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1220	CLA	CHD-C1D-ND	-3.00	121.70	124.45
22	7	606	CLA	CHD-C1D-ND	-3.00	121.70	124.45
39	1	613	CHL	C3C-C4C-NC	-3.00	107.21	110.57
22	4	615	CLA	O2A-CGA-CBA	3.00	121.31	111.91
22	B	1210	CLA	C2D-C1D-ND	2.99	112.31	110.10
22	A	1135	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
22	8	609	CLA	C2C-C1C-NC	2.99	112.78	109.97
22	4	612	CLA	C2D-C1D-ND	2.99	112.31	110.10
39	a	609	CHL	C2C-C3C-C4C	2.99	108.62	106.49
22	A	1138	CLA	C2C-C1C-NC	2.99	112.77	109.97
22	4	616	CLA	C1-C2-C3	-2.99	121.92	126.75
24	I	4001	BCR	C27-C26-C25	-2.99	118.39	122.73
22	B	1223	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
22	6	608	CLA	C2C-C1C-NC	2.99	112.77	109.97
22	6	607	CLA	C2C-C1C-NC	2.99	112.77	109.97
22	7	611	CLA	CHD-C1D-ND	-2.98	121.71	124.45
22	1	607	CLA	C1-C2-C3	-2.98	120.88	126.04
22	6	601	CLA	C2C-C1C-NC	2.98	112.77	109.97
37	M	4001	ECH	C7-C8-C9	-2.98	121.73	126.23
22	8	609	CLA	C2D-C1D-ND	2.98	112.30	110.10
22	a	608	CLA	C2C-C1C-NC	2.98	112.77	109.97
24	L	4001	BCR	C28-C27-C26	-2.98	108.75	114.08
22	4	602	CLA	C2C-C1C-NC	2.98	112.76	109.97
22	A	1101	CLA	C1D-ND-C4D	-2.98	104.22	106.33
22	7	604	CLA	C2D-C1D-ND	2.98	112.30	110.10
35	J	4002	RRX	C38-C26-C27	-2.98	108.84	114.36
22	B	1201	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
22	B	1226	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
39	1	613	CHL	C4A-NA-C1A	2.98	108.04	106.71
38	5	502	LUT	C10-C11-C12	-2.98	113.93	123.22
22	a	612	CLA	C1-C2-C3	-2.98	120.90	126.04
22	3	613	CLA	CHD-C1D-ND	-2.98	121.72	124.45
22	L	1501	CLA	C2D-C1D-ND	2.97	112.30	110.10
22	a	602	CLA	CMA-C3A-C4A	2.97	119.77	111.77
39	6	619	CHL	C1-O2A-CGA	2.97	124.25	116.44
22	4	605	CLA	CHD-C1D-ND	-2.97	121.72	124.45
39	a	609	CHL	C4D-CHA-C1A	2.97	124.86	121.25
22	6	605	CLA	CHD-C1D-ND	-2.97	121.72	124.45
22	a	607	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
22	4	605	CLA	C1C-C2C-C3C	-2.97	103.84	106.96
22	8	620	CLA	C2D-C1D-ND	2.97	112.29	110.10
22	B	1231	CLA	CMD-C2D-C3D	-2.97	120.79	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1220	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
22	A	1105	CLA	CAC-C3C-C4C	2.97	128.66	124.81
22	4	605	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
22	6	618	CLA	CMA-C3A-C4A	2.96	119.74	111.77
22	A	1133	CLA	CHD-C1D-ND	-2.96	121.73	124.45
22	1	612	CLA	C1-C2-C3	-2.96	120.92	126.04
38	1	501	LUT	C7-C8-C9	-2.96	121.76	126.23
22	A	1123	CLA	C2C-C1C-NC	2.96	112.75	109.97
22	B	1218	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
22	A	1116	CLA	C2D-C1D-ND	2.96	112.29	110.10
22	A	1105	CLA	CHD-C1D-ND	-2.96	121.73	124.45
22	7	609	CLA	C2C-C1C-NC	2.96	112.75	109.97
22	A	1102	CLA	O2A-CGA-CBA	2.96	121.19	111.91
22	A	1122	CLA	CHD-C1D-ND	-2.96	121.73	124.45
22	B	1202	CLA	C2C-C1C-NC	2.96	112.74	109.97
22	5	608	CLA	CHD-C1D-ND	-2.96	121.74	124.45
38	1	502	LUT	C15-C14-C13	-2.96	123.09	127.31
22	5	617	CLA	C1C-C2C-C3C	-2.96	103.85	106.96
22	4	608	CLA	O2A-CGA-CBA	2.96	121.18	111.91
22	A	1121	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
22	F	1302	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
22	B	1209	CLA	C2C-C1C-NC	2.95	112.74	109.97
22	G	1603	CLA	CHD-C1D-ND	-2.95	121.74	124.45
22	5	618	CLA	C6-C5-C3	-2.95	109.79	114.62
22	A	1115	CLA	C1-C2-C3	-2.95	120.94	126.04
22	5	608	CLA	C2C-C1C-NC	2.95	112.74	109.97
22	A	1013	CLA	CMB-C2B-C3B	2.95	130.20	124.68
22	A	1106	CLA	C2C-C1C-NC	2.95	112.74	109.97
22	4	611	CLA	C2C-C1C-NC	2.95	112.74	109.97
22	8	608	CLA	C2C-C1C-NC	2.95	112.73	109.97
22	B	1226	CLA	CMB-C2B-C3B	2.95	130.20	124.68
22	7	605	CLA	C1D-ND-C4D	-2.95	104.24	106.33
22	L	1501	CLA	CHD-C1D-ND	-2.95	121.75	124.45
48	7	504	C7Z	C12-C13-C14	2.95	123.46	118.94
22	A	1123	CLA	CMB-C2B-C3B	2.95	130.19	124.68
22	4	602	CLA	CHD-C1D-ND	-2.95	121.75	124.45
22	1	608	CLA	CHD-C1D-ND	-2.94	121.75	124.45
22	A	1108	CLA	CMA-C3A-C4A	2.94	119.69	111.77
22	A	1110	CLA	C2D-C1D-ND	2.94	112.27	110.10
39	5	610	CHL	C4A-NA-C1A	2.94	108.03	106.71
22	6	604	CLA	C1D-ND-C4D	-2.94	104.25	106.33
22	5	616	CLA	CHD-C1D-ND	-2.94	121.75	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	4	609	CHL	CHB-C4A-NA	2.94	128.58	124.51
22	a	603	CLA	CMA-C3A-C4A	2.94	119.68	111.77
22	A	1129	CLA	C2C-C1C-NC	2.94	112.73	109.97
24	J	4001	BCR	C27-C26-C25	-2.94	118.46	122.73
25	F	5001	LHG	O8-C23-C24	2.93	121.12	111.91
22	A	1125	CLA	CAC-C3C-C4C	2.93	128.62	124.81
22	1	602	CLA	C2D-C1D-ND	2.93	112.27	110.10
22	3	618	CLA	C1C-C2C-C3C	-2.93	103.87	106.96
22	B	1230	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
22	B	1228	CLA	C1D-ND-C4D	-2.93	104.25	106.33
22	1	612	CLA	O2A-CGA-CBA	2.93	121.11	111.91
22	3	618	CLA	CHD-C1D-ND	-2.93	121.76	124.45
22	A	1125	CLA	C1D-ND-C4D	-2.93	104.25	106.33
21	A	1011	CL0	CAA-C2A-C3A	-2.93	104.75	112.78
22	1	615	CLA	CHD-C1D-ND	-2.93	121.76	124.45
22	A	1111	CLA	C1-C2-C3	-2.93	120.98	126.04
22	B	1225	CLA	CHD-C1D-ND	-2.93	121.76	124.45
22	B	1239	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
23	B	2002	PQN	C14-C13-C15	2.93	120.19	115.27
22	A	1136	CLA	CMA-C3A-C4A	2.93	119.64	111.77
22	A	1114	CLA	C2C-C1C-NC	2.92	112.71	109.97
22	A	1124	CLA	C2C-C1C-NC	2.92	112.71	109.97
22	G	1602	CLA	C2D-C1D-ND	2.92	112.26	110.10
22	8	618	CLA	CHD-C1D-ND	-2.92	121.77	124.45
24	3	505	BCR	C36-C18-C17	-2.92	118.83	122.92
22	B	1221	CLA	C2C-C1C-NC	2.92	112.71	109.97
22	A	1110	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
22	A	1115	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
39	4	618	CHL	C4D-CHA-C1A	2.92	124.80	121.25
22	A	1104	CLA	C2D-C1D-ND	2.92	112.25	110.10
22	B	1201	CLA	C2D-C1D-ND	2.92	112.25	110.10
22	7	603	CLA	CMA-C3A-C4A	2.92	119.61	111.77
22	A	1129	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
22	B	1208	CLA	CMB-C2B-C3B	2.92	130.13	124.68
38	6	501	LUT	C15-C14-C13	-2.92	123.15	127.31
22	A	1131	CLA	C2C-C1C-NC	2.92	112.70	109.97
22	A	1105	CLA	C1D-ND-C4D	-2.92	104.26	106.33
22	A	1137	CLA	C1-C2-C3	-2.92	121.00	126.04
22	8	605	CLA	C2C-C1C-NC	2.92	112.70	109.97
38	4	501	LUT	C35-C15-C14	-2.91	117.50	123.47
22	3	601	CLA	C2D-C1D-ND	2.91	112.25	110.10
22	7	617	CLA	C2D-C1D-ND	2.91	112.25	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	8	601	CHL	CHB-C4A-NA	2.91	128.54	124.51
22	A	1105	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
22	B	1207	CLA	C2C-C1C-NC	2.91	112.70	109.97
22	8	602	CLA	CHD-C1D-ND	-2.91	121.78	124.45
22	B	1202	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
22	1	605	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
24	5	504	BCR	C27-C26-C25	-2.91	118.50	122.73
38	4	501	LUT	C15-C14-C13	-2.91	123.16	127.31
22	B	1207	CLA	C2D-C1D-ND	2.91	112.25	110.10
26	B	5003	DGD	O1G-C1A-C2A	2.91	121.04	111.91
22	B	1236	CLA	CHD-C1D-ND	-2.91	121.78	124.45
22	3	604	CLA	C2D-C1D-ND	2.91	112.25	110.10
22	B	1234	CLA	O2A-CGA-CBA	2.91	121.03	111.91
24	B	4006	BCR	C33-C5-C4	2.91	119.20	113.62
22	B	1228	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
22	5	609	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
22	1	606	CLA	C2C-C1C-NC	2.91	112.69	109.97
22	B	1234	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
24	K	4001	BCR	C15-C14-C13	-2.90	123.17	127.31
22	B	1222	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
24	L	4003	BCR	C36-C18-C17	-2.90	118.86	122.92
22	4	611	CLA	CMA-C3A-C4A	2.90	119.57	111.77
22	A	1118	CLA	C2C-C1C-NC	2.90	112.69	109.97
31	8	810	PTY	O4-C30-C31	2.90	121.00	111.91
39	6	619	CHL	C1B-CHB-C4A	-2.90	124.38	130.12
22	A	1013	CLA	C1-C2-C3	-2.90	121.03	126.04
38	a	503	LUT	C31-C32-C33	-2.90	118.28	126.42
22	A	1140	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
22	B	1201	CLA	C1-C2-C3	-2.90	121.03	126.04
22	7	611	CLA	C1-C2-C3	-2.90	121.03	126.04
22	6	617	CLA	C2D-C1D-ND	2.90	112.24	110.10
22	B	1221	CLA	CMB-C2B-C3B	2.90	130.10	124.68
22	4	615	CLA	C1-O2A-CGA	2.90	124.04	116.44
22	B	1210	CLA	CHD-C1D-ND	-2.90	121.79	124.45
22	A	1113	CLA	O2A-CGA-CBA	2.90	121.00	111.91
22	K	1403	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
39	3	611	CHL	CMA-C3A-C4A	2.90	119.56	111.77
22	7	604	CLA	C1D-ND-C4D	-2.90	104.28	106.33
22	5	618	CLA	C2C-C1C-NC	2.89	112.68	109.97
22	G	1602	CLA	C2C-C1C-NC	2.89	112.68	109.97
22	B	1229	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
22	B	1237	CLA	C2D-C1D-ND	2.89	112.24	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1114	CLA	O2A-CGA-CBA	2.89	120.99	111.91
22	6	606	CLA	CMA-C3A-C4A	2.89	119.55	111.77
22	6	615	CLA	C2C-C1C-NC	2.89	112.68	109.97
22	4	607	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
39	a	606	CHL	C1B-CHB-C4A	-2.89	124.39	130.12
22	B	1235	CLA	O2A-CGA-CBA	2.89	120.98	111.91
22	3	602	CLA	C2D-C1D-ND	2.89	112.23	110.10
39	a	613	CHL	C2C-C3C-C4C	2.89	108.55	106.49
22	1	611	CLA	CHD-C1D-ND	-2.89	121.80	124.45
22	A	1132	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
22	3	607	CLA	CMB-C2B-C3B	2.89	130.08	124.68
24	A	4003	BCR	C27-C26-C25	-2.89	118.54	122.73
22	A	1122	CLA	C2C-C1C-NC	2.89	112.68	109.97
22	B	1219	CLA	CHD-C1D-ND	-2.89	121.80	124.45
22	7	606	CLA	C1D-ND-C4D	-2.89	104.28	106.33
22	A	1137	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
22	1	604	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
22	B	1238	CLA	CHD-C1D-ND	-2.88	121.80	124.45
22	4	617	CLA	C1C-C2C-C3C	-2.88	103.92	106.96
39	5	611	CHL	CMA-C3A-C4A	2.88	119.52	111.77
24	3	503	BCR	C19-C18-C17	2.88	123.36	118.94
24	3	505	BCR	C19-C18-C17	2.88	123.36	118.94
22	B	1221	CLA	C2D-C1D-ND	2.88	112.23	110.10
22	A	1112	CLA	CHD-C1D-ND	-2.88	121.81	124.45
22	1	606	CLA	CMD-C2D-C3D	-2.88	120.99	127.61
24	J	4001	BCR	C33-C5-C4	2.88	119.15	113.62
22	A	1113	CLA	C2C-C1C-NC	2.88	112.67	109.97
22	4	606	CLA	CHD-C1D-ND	-2.88	121.81	124.45
49	8	806	P5S	O19-C17-C20	2.88	120.94	111.91
22	6	601	CLA	C2D-C1D-ND	2.88	112.22	110.10
22	8	605	CLA	CHD-C1D-ND	-2.88	121.81	124.45
24	6	504	BCR	C36-C18-C17	-2.88	118.89	122.92
22	F	1302	CLA	C1-C2-C3	-2.88	121.07	126.04
24	B	4002	BCR	C35-C13-C12	2.88	122.61	118.08
22	5	604	CLA	C2C-C1C-NC	2.87	112.67	109.97
22	6	605	CLA	C2C-C1C-NC	2.87	112.67	109.97
25	8	801	LHG	C5-O7-C7	-2.87	110.72	117.79
22	B	1219	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
22	4	601	CLA	CAA-C2A-C3A	-2.87	104.91	112.78
22	B	1215	CLA	C2D-C1D-ND	2.87	112.22	110.10
22	6	605	CLA	C2D-C1D-ND	2.87	112.22	110.10
22	B	1209	CLA	CHD-C1D-ND	-2.87	121.82	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	605	CLA	CHD-C1D-ND	-2.87	121.82	124.45
22	7	612	CLA	CMB-C2B-C1B	-2.87	124.05	128.46
24	B	4006	BCR	C35-C13-C12	2.87	122.60	118.08
22	B	1204	CLA	C2D-C1D-ND	2.87	112.22	110.10
22	1	612	CLA	C2D-C1D-ND	2.87	112.22	110.10
22	6	609	CLA	CMB-C2B-C1B	-2.87	124.06	128.46
39	6	613	CHL	C4D-CHA-C1A	2.87	124.74	121.25
35	J	4002	RRX	C7-C6-C5	-2.87	114.51	121.46
22	a	604	CLA	CHD-C1D-ND	-2.87	121.82	124.45
22	B	1214	CLA	C1C-C2C-C3C	-2.87	103.94	106.96
22	4	602	CLA	CMA-C3A-C4A	2.86	119.47	111.77
22	B	1227	CLA	CMB-C2B-C3B	2.86	130.04	124.68
22	B	1225	CLA	C2C-C1C-NC	2.86	112.66	109.97
22	6	603	CLA	C1-O2A-CGA	2.86	123.96	116.44
22	A	1122	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
22	5	617	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
22	B	1240	CLA	C2D-C1D-ND	2.86	112.21	110.10
22	F	1302	CLA	CMB-C2B-C3B	2.86	130.03	124.68
22	A	1113	CLA	C2D-C1D-ND	2.86	112.21	110.10
22	8	606	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
44	8	803	DGA	CDB-CCB-CBB	-2.86	88.75	115.30
22	4	617	CLA	C2D-C1D-ND	2.86	112.21	110.10
38	7	501	LUT	C31-C30-C29	-2.86	123.23	127.31
22	A	1111	CLA	C2C-C1C-NC	2.86	112.65	109.97
39	a	606	CHL	CMA-C3A-C4A	2.86	119.46	111.77
22	a	611	CLA	CMA-C3A-C4A	2.86	119.45	111.77
22	3	616	CLA	C2D-C1D-ND	2.86	112.21	110.10
38	8	502	LUT	C35-C15-C14	-2.86	117.62	123.47
22	3	601	CLA	C2C-C1C-NC	2.86	112.65	109.97
24	A	4002	BCR	C19-C18-C17	2.86	123.33	118.94
39	1	609	CHL	CMA-C3A-C4A	2.86	119.45	111.77
22	B	1219	CLA	CMB-C2B-C3B	2.86	130.02	124.68
22	7	604	CLA	O2A-CGA-CBA	2.86	120.87	111.91
24	B	4007	BCR	C36-C18-C17	-2.86	118.92	122.92
39	1	613	CHL	C2C-C3C-C4C	2.85	108.52	106.49
22	K	1402	CLA	C1D-ND-C4D	-2.85	104.31	106.33
38	3	501	LUT	C11-C10-C9	-2.85	123.24	127.31
22	6	603	CLA	CHA-C4D-ND	2.85	138.47	132.50
22	B	1239	CLA	C2D-C1D-ND	2.85	112.21	110.10
22	5	602	CLA	CHD-C1D-ND	-2.85	121.83	124.45
22	8	606	CLA	C2D-C1D-ND	2.85	112.21	110.10
22	G	1603	CLA	C2C-C1C-NC	2.85	112.64	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	I	4001	BCR	C12-C13-C14	-2.85	114.56	118.94
22	A	1121	CLA	CMD-C2D-C3D	-2.85	121.05	127.61
25	3	801	LHG	O8-C23-C24	2.85	120.86	111.91
22	6	612	CLA	C2C-C1C-NC	2.85	112.64	109.97
22	a	601	CLA	C2D-C1D-ND	2.85	112.20	110.10
22	a	612	CLA	C2D-C1D-ND	2.85	112.20	110.10
22	4	615	CLA	CHD-C1D-ND	-2.85	121.84	124.45
21	A	1011	CL0	C4-C3-C5	2.85	120.06	115.27
29	1	804	LMT	C1'-O5'-C5'	-2.85	108.10	113.69
22	1	602	CLA	C1D-ND-C4D	-2.85	104.31	106.33
22	3	605	CLA	C2C-C1C-NC	2.85	112.64	109.97
22	1	611	CLA	C1C-C2C-C3C	-2.85	103.97	106.96
22	L	1502	CLA	C2C-C1C-NC	2.84	112.64	109.97
22	1	610	CLA	C2C-C1C-NC	2.84	112.64	109.97
39	4	618	CHL	C1B-CHB-C4A	-2.84	124.48	130.12
39	6	619	CHL	C4D-CHA-C1A	2.84	124.71	121.25
22	6	604	CLA	CAC-C3C-C2C	-2.84	122.67	127.53
22	A	1102	CLA	CHD-C4C-C3C	2.84	129.02	124.84
22	A	1109	CLA	CMA-C3A-C4A	2.84	119.41	111.77
22	B	1227	CLA	CHD-C1D-ND	-2.84	121.84	124.45
22	4	604	CLA	C2C-C1C-NC	2.84	112.63	109.97
22	A	1130	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
22	6	607	CLA	C1-C2-C3	-2.84	121.14	126.04
22	A	1141	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
39	a	609	CHL	C1-O2A-CGA	2.84	123.89	116.44
22	7	610	CLA	C2D-C1D-ND	2.84	112.19	110.10
22	5	618	CLA	CHD-C1D-ND	-2.84	121.85	124.45
39	5	610	CHL	C4D-CHA-C1A	2.84	124.70	121.25
22	7	603	CLA	C2C-C1C-NC	2.84	112.63	109.97
22	F	1301	CLA	C1D-ND-C4D	-2.83	104.32	106.33
24	L	4002	BCR	C34-C9-C10	-2.83	118.95	122.92
22	L	1502	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
22	B	1213	CLA	C2D-C1D-ND	2.83	112.19	110.10
24	3	503	BCR	C35-C13-C12	2.83	122.54	118.08
24	3	503	BCR	C12-C13-C14	-2.83	114.60	118.94
22	B	1214	CLA	C1-C2-C3	-2.83	121.15	126.04
22	B	1208	CLA	C2C-C1C-NC	2.83	112.62	109.97
22	L	1503	CLA	CMA-C3A-C4A	2.83	119.38	111.77
39	4	609	CHL	C1-O2A-CGA	2.83	123.87	116.44
22	3	616	CLA	CMA-C3A-C4A	2.83	119.37	111.77
22	B	1023	CLA	CMB-C2B-C3B	2.83	129.97	124.68
22	A	1118	CLA	C2D-C1D-ND	2.83	112.19	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1117	CLA	CMB-C2B-C3B	2.82	129.96	124.68
22	3	603	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
39	3	611	CHL	C1-C2-C3	-2.82	121.16	126.04
22	5	612	CLA	C2C-C1C-NC	2.82	112.61	109.97
30	B	5004	PCW	O2-C31-C32	2.82	117.58	111.50
48	7	504	C7Z	C7-C8-C9	-2.82	121.97	126.23
22	3	607	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
22	1	607	CLA	CMA-C3A-C4A	2.82	119.35	111.77
38	4	502	LUT	C10-C11-C12	-2.82	114.42	123.22
22	A	1141	CLA	CMA-C3A-C4A	2.82	119.34	111.77
39	6	610	CHL	C2C-C3C-C4C	2.82	108.50	106.49
39	8	613	CHL	CMA-C3A-C4A	2.82	119.34	111.77
22	A	1131	CLA	CHD-C1D-ND	-2.82	121.87	124.45
22	A	1138	CLA	CHD-C1D-ND	-2.81	121.87	124.45
22	5	609	CLA	CHD-C1D-ND	-2.81	121.87	124.45
22	A	1137	CLA	C2C-C1C-NC	2.81	112.61	109.97
22	5	608	CLA	O1D-CGD-CBD	-2.81	118.73	124.48
22	3	605	CLA	C2D-C1D-ND	2.81	112.18	110.10
24	F	4001	BCR	C27-C26-C25	-2.81	118.65	122.73
22	1	604	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
22	A	1106	CLA	CHD-C1D-ND	-2.81	121.87	124.45
22	B	1021	CLA	CHD-C1D-ND	-2.81	121.87	124.45
22	3	607	CLA	CMA-C3A-C4A	2.81	119.33	111.77
22	7	617	CLA	CMA-C3A-C4A	2.81	119.33	111.77
25	A	5001	LHG	O8-C23-C24	2.81	120.72	111.91
22	5	606	CLA	C2D-C1D-ND	2.81	112.17	110.10
22	8	609	CLA	O2A-CGA-CBA	2.81	120.72	111.91
22	B	1239	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
22	B	1240	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
22	L	1503	CLA	CAC-C3C-C4C	-2.81	121.17	124.81
22	A	1107	CLA	C1D-ND-C4D	-2.81	104.34	106.33
24	L	4001	BCR	C38-C26-C27	2.81	119.01	113.62
38	6	502	LUT	C7-C8-C9	-2.81	121.99	126.23
46	7	502	XAT	O4-C5-C4	-2.81	111.27	113.38
22	B	1202	CLA	O2A-CGA-CBA	2.81	120.71	111.91
25	6	802	LHG	O8-C23-C24	2.81	120.71	111.91
22	L	1503	CLA	C2D-C1D-ND	2.80	112.17	110.10
22	6	617	CLA	C1C-C2C-C3C	-2.80	104.01	106.96
22	A	1113	CLA	C1-C2-C3	-2.80	121.19	126.04
22	F	1302	CLA	CMA-C3A-C4A	2.80	119.31	111.77
22	3	603	CLA	CMA-C3A-C4A	2.80	119.31	111.77
29	A	5008	LMT	O1'-C1'-C2'	2.80	112.68	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1240	CLA	CMA-C3A-C4A	2.80	119.31	111.77
22	K	1403	CLA	CMA-C3A-C4A	2.80	119.31	111.77
22	A	1012	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
22	A	1012	CLA	C2D-C1D-ND	2.80	112.17	110.10
38	8	501	LUT	C31-C30-C29	-2.80	123.31	127.31
22	4	610	CLA	C1C-C2C-C3C	-2.80	104.01	106.96
22	B	1226	CLA	C2C-C1C-NC	2.80	112.60	109.97
22	8	610	CLA	CHD-C1D-ND	-2.80	121.88	124.45
22	1	605	CLA	C1C-C2C-C3C	-2.80	104.01	106.96
22	A	1108	CLA	CHD-C1D-ND	-2.80	121.88	124.45
22	6	607	CLA	CHD-C1D-ND	-2.80	121.88	124.45
22	A	1013	CLA	CMB-C2B-C1B	-2.80	124.16	128.46
22	5	601	CLA	C2D-C1D-ND	2.80	112.17	110.10
22	8	602	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
22	A	1141	CLA	CHD-C1D-ND	-2.80	121.88	124.45
38	8	501	LUT	C35-C34-C33	-2.80	123.32	127.31
22	1	607	CLA	C1D-ND-C4D	-2.80	104.35	106.33
24	L	4001	BCR	C34-C9-C10	-2.80	119.00	122.92
22	3	607	CLA	C1C-C2C-C3C	-2.80	104.02	106.96
31	B	5005	PTY	O4-C30-C31	2.80	120.68	111.91
22	A	1107	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
22	5	605	CLA	C1C-C2C-C3C	-2.80	104.02	106.96
22	5	618	CLA	C1C-C2C-C3C	-2.80	104.02	106.96
22	8	612	CLA	C2C-C1C-NC	2.80	112.59	109.97
22	a	602	CLA	CHD-C1D-ND	-2.79	121.89	124.45
22	3	607	CLA	C2D-C1D-ND	2.79	112.16	110.10
22	a	604	CLA	O2A-CGA-CBA	2.79	120.67	111.91
24	F	4001	BCR	C38-C26-C27	2.79	118.98	113.62
22	A	1012	CLA	C2C-C1C-NC	2.79	112.59	109.97
22	1	610	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
24	3	503	BCR	C37-C22-C23	2.79	122.48	118.08
22	B	1211	CLA	C2C-C1C-NC	2.79	112.59	109.97
22	7	612	CLA	CAC-C3C-C2C	-2.79	122.75	127.53
22	4	604	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
22	8	620	CLA	CAA-CBA-CGA	-2.79	105.10	113.25
22	6	618	CLA	C2C-C1C-NC	2.79	112.59	109.97
22	A	1134	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
38	5	505	LUT	C31-C30-C29	-2.79	123.33	127.31
22	6	602	CLA	C2C-C1C-NC	2.79	112.58	109.97
22	A	1133	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
22	7	603	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
39	3	608	CHL	CMA-C3A-C4A	2.79	119.27	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	7	613	CHL	CHB-C4A-NA	2.79	128.37	124.51
22	A	1122	CLA	C1-C2-C3	-2.79	121.22	126.04
22	6	604	CLA	C1-C2-C3	-2.78	121.23	126.04
22	4	605	CLA	C2D-C1D-ND	2.78	112.16	110.10
22	A	1130	CLA	C2D-C1D-ND	2.78	112.15	110.10
22	B	1212	CLA	C1C-C2C-C3C	-2.78	104.03	106.96
22	6	603	CLA	O2A-CGA-CBA	2.78	120.63	111.91
22	L	1502	CLA	CMA-C3A-C4A	2.78	119.24	111.77
22	7	608	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
39	8	604	CHL	C1B-CHB-C4A	-2.78	124.62	130.12
22	B	1232	CLA	CMA-C3A-C4A	2.78	119.24	111.77
22	B	1207	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
22	4	611	CLA	C1C-C2C-C3C	-2.78	104.04	106.96
47	8	807	4RF	O18-C16-C15	2.78	120.62	111.91
39	8	604	CHL	CMA-C3A-C4A	2.78	119.23	111.77
22	6	606	CLA	C2D-C1D-ND	2.77	112.15	110.10
22	5	603	CLA	C1-O2A-CGA	2.77	123.72	116.44
22	A	1115	CLA	C2C-C1C-NC	2.77	112.57	109.97
22	B	1023	CLA	C1-C2-C3	-2.77	121.25	126.04
22	a	607	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
22	B	1237	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
22	3	616	CLA	O2A-CGA-CBA	2.77	120.61	111.91
39	4	613	CHL	C2C-C3C-C4C	2.77	108.47	106.49
22	B	1207	CLA	CHD-C1D-ND	-2.77	121.91	124.45
22	3	613	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
22	6	603	CLA	C4D-C3D-CAD	2.77	111.36	108.10
22	7	615	CLA	O2A-CGA-CBA	2.77	120.60	111.91
22	4	611	CLA	C2D-C1D-ND	2.77	112.14	110.10
22	A	1109	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
22	1	612	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
22	G	1603	CLA	CMA-C3A-C4A	2.77	119.21	111.77
22	5	607	CLA	CHD-C1D-ND	-2.77	121.91	124.45
22	1	607	CLA	CHD-C1D-ND	-2.77	121.91	124.45
22	8	611	CLA	C2C-C1C-NC	2.77	112.56	109.97
22	A	1113	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
22	8	615	CLA	C2C-C1C-NC	2.77	112.56	109.97
25	5	801	LHG	O8-C23-C24	2.77	120.59	111.91
22	A	1120	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
22	8	611	CLA	CMA-C3A-C4A	2.77	119.20	111.77
22	A	1111	CLA	CMB-C2B-C1B	-2.76	124.22	128.46
22	5	602	CLA	C2D-C1D-ND	2.76	112.14	110.10
22	A	1133	CLA	O2D-CGD-O1D	-2.76	118.43	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	606	CLA	CMB-C2B-C3B	2.76	129.85	124.68
22	G	1602	CLA	CMA-C3A-C4A	2.76	119.20	111.77
25	a	801	LHG	O8-C23-C24	2.76	120.58	111.91
22	A	1112	CLA	C2D-C1D-ND	2.76	112.14	110.10
22	7	610	CLA	C1-C2-C3	-2.76	121.27	126.04
22	B	1205	CLA	C2C-C1C-NC	2.76	112.56	109.97
22	A	1114	CLA	OBD-CAD-C3D	-2.76	121.87	128.52
22	K	1404	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
22	A	1119	CLA	CMB-C2B-C3B	2.76	129.84	124.68
22	3	610	CLA	C1C-C2C-C3C	-2.76	104.05	106.96
22	A	1134	CLA	C2D-C1D-ND	2.76	112.14	110.10
22	7	609	CLA	C2D-C1D-ND	2.76	112.14	110.10
22	6	604	CLA	O2A-CGA-CBA	2.76	120.57	111.91
22	6	604	CLA	O1D-CGD-CBD	-2.76	118.84	124.48
22	3	604	CLA	O2A-CGA-CBA	2.76	120.56	111.91
39	1	613	CHL	CHB-C4A-NA	2.76	128.32	124.51
22	6	609	CLA	C2D-C1D-ND	2.76	112.14	110.10
22	3	601	CLA	C1C-C2C-C3C	-2.76	104.06	106.96
22	A	1109	CLA	C1D-ND-C4D	-2.76	104.38	106.33
22	A	1111	CLA	C2D-C1D-ND	2.76	112.14	110.10
44	5	803	DGA	OG1-CA1-CA2	2.76	120.55	111.91
22	A	1107	CLA	CMB-C2B-C1B	-2.75	124.23	128.46
39	1	613	CHL	CHD-C1D-ND	-2.75	121.92	124.45
39	a	609	CHL	C1B-CHB-C4A	-2.75	124.67	130.12
22	A	1134	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
22	3	602	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
22	5	602	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
22	K	1401	CLA	C2C-C1C-NC	2.75	112.55	109.97
22	4	607	CLA	C2C-C1C-NC	2.75	112.55	109.97
39	a	613	CHL	CMA-C3A-C4A	2.75	119.17	111.77
22	7	601	CLA	CMB-C2B-C1B	-2.75	124.23	128.46
22	4	606	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
22	B	1232	CLA	CHD-C1D-ND	-2.75	121.93	124.45
22	6	618	CLA	CHD-C1D-ND	-2.75	121.93	124.45
22	4	605	CLA	OBD-CAD-C3D	-2.75	121.90	128.52
22	J	1901	CLA	C1D-ND-C4D	-2.75	104.38	106.33
22	A	1112	CLA	CMA-C3A-C4A	2.75	119.16	111.77
39	a	606	CHL	C3C-C4C-NC	-2.75	107.49	110.57
22	6	602	CLA	C1D-ND-C4D	-2.75	104.38	106.33
22	A	1131	CLA	CHA-C4D-ND	2.75	138.25	132.50
22	3	610	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
22	4	607	CLA	C1-C2-C3	-2.75	121.29	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	4005	BCR	C35-C13-C12	2.75	122.40	118.08
22	B	1022	CLA	C2D-C1D-ND	2.75	112.13	110.10
22	3	618	CLA	C2D-C1D-ND	2.75	112.13	110.10
22	5	617	CLA	CMA-C3A-C4A	2.74	119.15	111.77
22	5	618	CLA	CMA-C3A-C4A	2.74	119.15	111.77
25	A	5003	LHG	O8-C23-C24	2.74	120.52	111.91
24	6	504	BCR	C27-C26-C25	-2.74	118.75	122.73
22	A	1120	CLA	CMA-C3A-C4A	2.74	119.15	111.77
22	3	604	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
22	A	1116	CLA	C2C-C1C-NC	2.74	112.54	109.97
22	B	1210	CLA	O1D-CGD-CBD	-2.74	118.87	124.48
22	7	606	CLA	C1-C2-C3	-2.74	121.30	126.04
24	A	4002	BCR	C33-C5-C4	2.74	118.88	113.62
22	L	1503	CLA	C1C-C2C-C3C	-2.74	104.08	106.96
22	6	605	CLA	C1C-C2C-C3C	-2.74	104.08	106.96
22	B	1210	CLA	CMB-C2B-C3B	2.74	129.80	124.68
22	4	608	CLA	C2C-C1C-NC	2.74	112.54	109.97
22	5	604	CLA	O2A-CGA-CBA	2.74	120.50	111.91
25	A	5002	LHG	O8-C23-C24	2.74	120.50	111.91
25	7	802	LHG	O8-C23-C24	2.74	120.50	111.91
39	4	609	CHL	C1-C2-C3	-2.74	121.31	126.04
22	4	603	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
24	A	4004	BCR	C36-C18-C17	-2.73	119.09	122.92
22	1	607	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
22	B	1234	CLA	CHD-C1D-ND	-2.73	121.94	124.45
22	A	1123	CLA	CMB-C2B-C1B	-2.73	124.26	128.46
22	B	1222	CLA	C2D-C1D-ND	2.73	112.12	110.10
22	B	1237	CLA	CHD-C1D-ND	-2.73	121.94	124.45
24	B	4007	BCR	C19-C18-C17	2.73	123.13	118.94
22	F	1301	CLA	O2A-CGA-CBA	2.73	120.48	111.91
39	6	610	CHL	CMA-C3A-C4A	2.73	119.11	111.77
22	7	601	CLA	C2D-C1D-ND	2.73	112.12	110.10
22	8	620	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
22	6	608	CLA	C2D-C1D-ND	2.73	112.11	110.10
22	B	1216	CLA	C2C-C1C-NC	2.73	112.53	109.97
22	A	1109	CLA	CHD-C1D-ND	-2.73	121.95	124.45
22	G	1603	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
22	B	1213	CLA	O2A-CGA-CBA	2.73	120.46	111.91
22	B	1230	CLA	C2C-C1C-NC	2.73	112.53	109.97
22	1	610	CLA	C2D-C1D-ND	2.73	112.11	110.10
38	3	501	LUT	C15-C14-C13	-2.72	123.42	127.31
22	B	1238	CLA	CMA-C3A-C4A	2.72	119.10	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	6	504	BCR	C4-C5-C6	-2.72	118.78	122.73
22	7	617	CLA	C1D-ND-C4D	-2.72	104.40	106.33
22	F	1301	CLA	CHD-C1D-ND	-2.72	121.95	124.45
22	4	604	CLA	O2A-CGA-CBA	2.72	120.45	111.91
22	A	1122	CLA	O2A-CGA-CBA	2.72	120.45	111.91
22	a	608	CLA	C1C-C2C-C3C	-2.72	104.09	106.96
22	A	1012	CLA	O2A-CGA-CBA	2.72	120.45	111.91
22	5	605	CLA	CHA-C4D-ND	2.72	138.19	132.50
22	8	607	CLA	C2C-C1C-NC	2.72	112.52	109.97
39	a	609	CHL	CMA-C3A-C4A	2.72	119.08	111.77
22	B	1227	CLA	C2C-C1C-NC	2.72	112.52	109.97
24	L	4002	BCR	C35-C13-C12	2.72	122.36	118.08
22	A	1124	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
22	1	601	CLA	CMB-C2B-C3B	2.72	129.77	124.68
22	5	616	CLA	CMA-C3A-C4A	2.72	119.08	111.77
22	4	601	CLA	C2D-C1D-ND	2.72	112.11	110.10
22	B	1021	CLA	C2C-C1C-NC	2.72	112.52	109.97
39	a	613	CHL	CHD-C4C-C3C	2.72	128.84	124.84
22	A	1121	CLA	CHA-C4D-ND	2.72	138.18	132.50
22	5	604	CLA	C1-C2-C3	-2.72	121.34	126.04
39	3	611	CHL	C4D-CHA-C1A	2.72	124.55	121.25
22	7	604	CLA	CMB-C2B-C3B	2.72	129.76	124.68
22	B	1201	CLA	C2C-C1C-NC	2.72	112.52	109.97
22	3	602	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
22	4	610	CLA	C2D-C1D-ND	2.72	112.11	110.10
24	4	503	BCR	C38-C26-C25	-2.72	121.48	124.53
24	F	4001	BCR	C37-C22-C23	2.72	122.36	118.08
39	3	608	CHL	CHB-C4A-NA	2.71	128.27	124.51
22	5	601	CLA	C2C-C1C-NC	2.71	112.52	109.97
22	B	1023	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
22	A	1138	CLA	CMB-C2B-C3B	2.71	129.75	124.68
22	a	605	CLA	C2C-C1C-NC	2.71	112.51	109.97
22	6	609	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
22	8	603	CLA	CMA-C3A-C4A	2.71	119.06	111.77
22	A	1141	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
22	4	603	CLA	C1-O2A-CGA	2.71	123.56	116.44
22	B	1221	CLA	CHA-C4D-ND	2.71	138.17	132.50
38	3	502	LUT	C10-C11-C12	-2.71	114.76	123.22
22	6	601	CLA	CMA-C3A-C4A	2.71	119.05	111.77
38	4	502	LUT	C15-C14-C13	-2.71	123.44	127.31
38	1	503	LUT	C31-C32-C33	-2.71	118.81	126.42
22	5	617	CLA	CHD-C1D-ND	-2.71	121.97	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	5	502	LUT	C35-C15-C14	-2.71	117.93	123.47
27	A	5007	3PH	O31-C31-C32	2.71	120.40	111.91
22	1	608	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
22	7	612	CLA	CHD-C1D-ND	-2.71	121.97	124.45
22	A	1123	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
22	A	1117	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
22	F	1301	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
22	A	1128	CLA	CHA-C4D-ND	2.70	138.16	132.50
22	8	615	CLA	CHD-C1D-ND	-2.70	121.97	124.45
22	B	1201	CLA	CMB-C2B-C1B	-2.70	124.31	128.46
38	6	501	LUT	C38-C25-C24	-2.70	117.78	123.56
22	4	616	CLA	CMA-C3A-C4A	2.70	119.03	111.77
24	F	4001	BCR	C33-C5-C4	2.70	118.80	113.62
38	5	501	LUT	C15-C14-C13	-2.70	123.46	127.31
36	J	5001	LPX	O3-P1-O4	2.70	125.59	112.24
24	L	4003	BCR	C35-C13-C12	2.70	122.33	118.08
22	3	610	CLA	C2C-C1C-NC	2.70	112.50	109.97
22	A	1131	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
22	B	1229	CLA	C2D-C1D-ND	2.70	112.09	110.10
22	5	609	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
22	A	1124	CLA	CMA-C3A-C4A	2.70	119.02	111.77
22	6	603	CLA	CAC-C3C-C4C	2.70	128.31	124.81
22	7	611	CLA	CMB-C2B-C3B	2.70	129.72	124.68
22	B	1229	CLA	C2C-C1C-NC	2.70	112.50	109.97
22	A	1139	CLA	C2D-C1D-ND	2.70	112.09	110.10
22	B	1228	CLA	C2D-C1D-ND	2.70	112.09	110.10
22	A	1136	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
47	8	808	4RF	O40-C41-C43	2.69	120.36	111.91
22	A	1106	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
22	K	1401	CLA	C2D-C1D-ND	2.69	112.09	110.10
24	6	503	BCR	C35-C13-C14	-2.69	119.15	122.92
22	5	607	CLA	CMA-C3A-C4A	2.69	119.01	111.77
37	M	4001	ECH	C8-C7-C6	-2.69	119.64	127.20
22	8	605	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
22	G	1603	CLA	C1D-ND-C4D	-2.69	104.42	106.33
22	1	611	CLA	C2D-C1D-ND	2.69	112.09	110.10
22	A	1139	CLA	CHA-C4D-ND	2.69	138.12	132.50
22	A	1102	CLA	C2C-C1C-NC	2.69	112.49	109.97
25	4	801	LHG	O8-C23-C24	2.69	120.34	111.91
22	A	1110	CLA	C1-C2-C3	-2.69	121.39	126.04
22	3	616	CLA	CHD-C1D-ND	-2.69	121.98	124.45
22	6	608	CLA	C1C-C2C-C3C	-2.69	104.13	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	8	801	LHG	O8-C23-C24	2.69	120.34	111.91
22	4	608	CLA	C2D-C1D-ND	2.69	112.08	110.10
22	8	602	CLA	CMA-C3A-C4A	2.69	118.99	111.77
22	A	1128	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
31	5	802	PTY	O4-C30-C31	2.69	120.34	111.91
22	3	606	CLA	C2C-C1C-NC	2.69	112.49	109.97
22	a	604	CLA	CMA-C3A-C4A	2.69	118.99	111.77
22	8	603	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
22	5	604	CLA	CMB-C2B-C3B	2.69	129.70	124.68
24	5	504	BCR	C23-C22-C21	-2.68	114.82	118.94
22	6	615	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
38	6	502	LUT	C22-C23-C24	-2.68	108.69	111.74
22	B	1210	CLA	O2A-CGA-CBA	2.68	120.33	111.91
22	1	603	CLA	C2C-C1C-NC	2.68	112.49	109.97
22	B	1223	CLA	OBD-CAD-C3D	-2.68	122.06	128.52
22	1	607	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
22	8	610	CLA	O2A-CGA-CBA	2.68	120.33	111.91
47	7	807	4RF	O18-C16-C15	2.68	120.33	111.91
22	B	1022	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
24	5	503	BCR	C19-C18-C17	2.68	123.06	118.94
22	4	601	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
38	8	501	LUT	C15-C14-C13	-2.68	123.48	127.31
22	A	1127	CLA	C2C-C1C-NC	2.68	112.48	109.97
22	a	601	CLA	O2A-CGA-CBA	2.68	120.32	111.91
22	1	606	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
22	1	611	CLA	CMA-C3A-C4A	2.68	118.98	111.77
22	B	1215	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
24	B	4003	BCR	C35-C13-C12	2.68	122.30	118.08
22	a	602	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
22	A	1129	CLA	C2D-C1D-ND	2.68	112.08	110.10
38	6	501	LUT	C7-C8-C9	-2.68	122.19	126.23
22	5	604	CLA	CED-O2D-CGD	2.68	121.99	115.94
22	1	601	CLA	O2A-CGA-CBA	2.68	120.31	111.91
22	a	615	CLA	CHD-C1D-ND	-2.68	121.99	124.45
22	5	616	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
22	K	1402	CLA	C2C-C1C-NC	2.68	112.48	109.97
22	5	617	CLA	CMC-C2C-C3C	2.68	133.38	126.12
22	A	1132	CLA	C2D-C1D-ND	2.67	112.08	110.10
22	4	604	CLA	C2D-C1D-ND	2.67	112.08	110.10
38	5	501	LUT	C10-C11-C12	-2.67	114.87	123.22
24	B	4005	BCR	C8-C7-C6	-2.67	119.69	127.20
22	A	1128	CLA	CHD-C1D-ND	-2.67	122.00	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1240	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
22	a	607	CLA	CMA-C3A-C4A	2.67	118.96	111.77
22	A	1127	CLA	C2D-C1D-ND	2.67	112.07	110.10
22	a	605	CLA	C2D-C1D-ND	2.67	112.07	110.10
22	B	1230	CLA	CAA-CBA-CGA	-2.67	105.44	113.25
22	a	615	CLA	CMB-C2B-C3B	2.67	129.68	124.68
22	J	1901	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
22	G	1601	CLA	CHD-C1D-ND	-2.67	122.00	124.45
22	4	606	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
22	7	609	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
22	6	605	CLA	OBD-CAD-C3D	-2.67	122.09	128.52
22	7	602	CLA	CMA-C3A-C4A	2.67	118.95	111.77
22	7	608	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
22	B	1228	CLA	C7-C6-C5	-2.67	106.11	113.36
22	7	606	CLA	CMB-C2B-C3B	2.67	129.67	124.68
24	B	4004	BCR	C38-C26-C25	-2.67	121.53	124.53
22	B	1227	CLA	C2D-C1D-ND	2.67	112.07	110.10
22	A	1114	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
31	3	802	PTY	O4-C30-C31	2.67	120.28	111.91
22	7	617	CLA	C1-C2-C3	-2.67	121.43	126.04
22	1	603	CLA	C2D-C1D-ND	2.67	112.07	110.10
29	B	5006	LMT	C1'-O5'-C5'	-2.67	108.46	113.69
25	1	802	LHG	O8-C23-C24	2.67	120.27	111.91
22	A	1135	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
22	A	1139	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
22	7	610	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
22	G	1601	CLA	C2D-C1D-ND	2.66	112.07	110.10
36	a	804	LPX	O3-P1-O4	2.66	125.40	112.24
22	8	612	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
24	8	503	BCR	C19-C18-C17	2.66	123.03	118.94
22	B	1211	CLA	CMB-C2B-C3B	2.66	129.66	124.68
22	8	620	CLA	CMB-C2B-C3B	2.66	129.66	124.68
22	J	1901	CLA	CHD-C1D-ND	-2.66	122.01	124.45
22	B	1218	CLA	O2A-CGA-CBA	2.66	120.26	111.91
39	5	610	CHL	C2C-C3C-C4C	2.66	108.39	106.49
39	6	613	CHL	C2C-C3C-C4C	2.66	108.39	106.49
22	1	602	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
22	3	605	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
22	3	601	CLA	CMB-C2B-C3B	2.66	129.65	124.68
22	7	601	CLA	CAA-C2A-C3A	-2.66	105.50	112.78
22	A	1120	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
39	5	611	CHL	C1B-CHB-C4A	-2.66	124.86	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	K	4001	BCR	C19-C18-C17	2.66	123.02	118.94
22	1	603	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
22	A	1135	CLA	C2D-C1D-ND	2.66	112.06	110.10
22	A	1110	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
24	6	504	BCR	C8-C7-C6	-2.65	119.75	127.20
22	3	612	CLA	C2C-C1C-NC	2.65	112.46	109.97
22	5	606	CLA	C2C-C1C-NC	2.65	112.46	109.97
24	B	4003	BCR	C27-C26-C25	-2.65	118.88	122.73
22	1	610	CLA	CHD-C1D-ND	-2.65	122.02	124.45
22	A	1122	CLA	CMA-C3A-C4A	2.65	118.91	111.77
38	8	501	LUT	C10-C11-C12	-2.65	114.94	123.22
22	6	605	CLA	CMA-C3A-C4A	2.65	118.91	111.77
24	3	503	BCR	C38-C26-C27	2.65	118.71	113.62
22	K	1403	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
24	F	4001	BCR	C34-C9-C10	-2.65	119.21	122.92
22	B	1207	CLA	CAA-C2A-C3A	-2.65	105.52	112.78
39	5	613	CHL	CMA-C3A-C4A	2.65	118.90	111.77
22	3	605	CLA	CHA-C4D-ND	2.65	138.04	132.50
22	B	1230	CLA	O2A-CGA-CBA	2.65	120.22	111.91
22	1	615	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
22	B	1217	CLA	C2D-C1D-ND	2.65	112.06	110.10
22	B	1204	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
22	B	1231	CLA	CHA-C4D-ND	2.65	138.04	132.50
22	B	1218	CLA	O1D-CGD-CBD	-2.65	119.07	124.48
22	a	605	CLA	C1D-ND-C4D	-2.65	104.45	106.33
22	B	1224	CLA	O2A-CGA-CBA	2.65	120.22	111.91
22	5	604	CLA	CMA-C3A-C4A	2.65	118.89	111.77
22	5	607	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
22	6	607	CLA	CMA-C3A-C4A	2.65	118.88	111.77
22	B	1228	CLA	C2C-C1C-NC	2.65	112.45	109.97
22	3	604	CLA	C1-C2-C3	-2.64	121.47	126.04
22	7	606	CLA	C2C-C1C-NC	2.64	112.45	109.97
22	a	612	CLA	CHA-C4D-ND	2.64	138.03	132.50
22	8	607	CLA	C2D-C1D-ND	2.64	112.05	110.10
24	B	4004	BCR	C36-C18-C17	-2.64	119.22	122.92
22	3	604	CLA	CMA-C3A-C4A	2.64	118.87	111.77
22	G	1601	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
22	B	1235	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
22	B	1204	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
22	5	612	CLA	C2D-C1D-ND	2.64	112.05	110.10
22	A	1120	CLA	C2C-C1C-NC	2.64	112.44	109.97
22	G	1601	CLA	C1C-C2C-C3C	-2.64	104.18	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	8	606	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
25	B	5001	LHG	O8-C23-C24	2.64	120.18	111.91
38	1	501	LUT	C11-C10-C9	-2.64	123.55	127.31
22	A	1114	CLA	CHA-C4D-ND	2.63	138.01	132.50
22	B	1219	CLA	CMB-C2B-C1B	-2.63	124.42	128.46
48	7	504	C7Z	C32-C33-C34	-2.63	114.90	118.94
38	6	501	LUT	C1-C6-C7	2.63	123.23	115.78
22	A	1136	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
22	6	607	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
39	5	613	CHL	C4D-CHA-C1A	2.63	124.45	121.25
22	A	1104	CLA	O2A-CGA-CBA	2.63	120.17	111.91
24	L	4001	BCR	C40-C30-C25	-2.63	106.03	110.30
22	A	1138	CLA	CHA-C4D-ND	2.63	138.00	132.50
22	B	1234	CLA	CAC-C3C-C2C	-2.63	123.03	127.53
25	4	802	LHG	O8-C23-C24	2.63	120.16	111.91
22	B	1237	CLA	CMA-C3A-C4A	2.63	118.84	111.77
22	1	603	CLA	CMA-C3A-C4A	2.63	118.84	111.77
22	B	1223	CLA	CHA-C4D-ND	2.63	138.00	132.50
21	A	1011	CL0	O2D-CGD-O1D	-2.63	118.70	123.84
22	7	610	CLA	O2A-CGA-CBA	2.63	120.16	111.91
22	B	1218	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
22	7	607	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
39	4	618	CHL	CMA-C3A-C4A	2.63	118.84	111.77
31	7	804	PTY	O4-C30-C31	2.63	120.16	111.91
22	8	603	CLA	C1-O2A-CGA	2.63	123.34	116.44
39	4	609	CHL	CMA-C3A-C4A	2.63	118.84	111.77
22	4	608	CLA	CHA-C4D-ND	2.63	138.00	132.50
48	7	504	C7Z	C38-C25-C24	2.63	119.22	114.36
22	4	615	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
38	5	505	LUT	C38-C25-C24	-2.63	117.94	123.56
22	8	602	CLA	CHA-C4D-ND	2.63	137.99	132.50
22	6	602	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
22	B	1228	CLA	CMB-C2B-C3B	2.63	129.59	124.68
22	B	1214	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
22	A	1140	CLA	CHA-C4D-ND	2.63	137.99	132.50
22	4	612	CLA	C2C-C1C-NC	2.63	112.43	109.97
22	4	616	CLA	C2D-C1D-ND	2.63	112.04	110.10
22	7	609	CLA	CHA-C4D-ND	2.63	137.99	132.50
22	7	601	CLA	C1-C2-C3	-2.63	121.50	126.04
22	A	1141	CLA	C2D-C1D-ND	2.62	112.04	110.10
41	a	504	QTB	C19-C17-C11	-2.62	106.82	110.60
22	B	1021	CLA	C1C-C2C-C3C	-2.62	104.20	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1217	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
24	A	4005	BCR	C34-C9-C10	-2.62	119.25	122.92
24	3	505	BCR	C38-C26-C25	-2.62	121.58	124.53
22	5	603	CLA	CMA-C3A-C4A	2.62	118.82	111.77
24	B	4004	BCR	C35-C13-C12	2.62	122.21	118.08
22	B	1225	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
38	6	502	LUT	C31-C32-C33	-2.62	119.05	126.42
22	1	606	CLA	O2A-CGA-CBA	2.62	120.14	111.91
38	1	502	LUT	C38-C25-C24	-2.62	117.95	123.56
22	1	601	CLA	CAA-C2A-C3A	-2.62	105.60	112.78
22	B	1208	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
22	4	612	CLA	O1D-CGD-CBD	-2.62	119.12	124.48
22	8	618	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
22	1	615	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
22	6	609	CLA	CHA-C4D-ND	2.62	137.98	132.50
22	1	605	CLA	C2D-C1D-ND	2.62	112.03	110.10
22	8	618	CLA	CMA-C3A-C4A	2.62	118.81	111.77
22	K	1404	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
22	7	612	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
22	J	1901	CLA	CMA-C3A-C4A	2.62	118.81	111.77
22	4	607	CLA	CHA-C4D-ND	2.62	137.97	132.50
22	B	1227	CLA	CMB-C2B-C1B	-2.62	124.44	128.46
24	B	4002	BCR	C38-C26-C27	2.62	118.64	113.62
24	5	504	BCR	C38-C26-C27	2.62	118.64	113.62
22	B	1215	CLA	C1-C2-C3	-2.62	121.52	126.04
22	A	1131	CLA	CMD-C2D-C3D	-2.62	121.60	127.61
22	A	1130	CLA	C2C-C1C-NC	2.62	112.42	109.97
22	B	1238	CLA	C2C-C1C-NC	2.62	112.42	109.97
24	A	4005	BCR	C4-C5-C6	-2.62	118.93	122.73
22	a	611	CLA	C2D-C1D-ND	2.61	112.03	110.10
22	B	1222	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
22	L	1501	CLA	O2A-CGA-CBA	2.61	120.11	111.91
39	4	613	CHL	C1B-CHB-C4A	-2.61	124.94	130.12
22	A	1115	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
22	A	1105	CLA	C2C-C1C-NC	2.61	112.42	109.97
38	a	502	LUT	C21-C26-C27	2.61	116.00	112.70
22	F	1302	CLA	CAC-C3C-C2C	-2.61	123.06	127.53
22	a	605	CLA	CHA-C4D-ND	2.61	137.96	132.50
22	A	1107	CLA	CMA-C3A-C4A	2.61	118.79	111.77
34	G	5002	ERG	C13-C14-C8	2.61	118.54	113.48
24	A	4004	BCR	C33-C5-C4	2.61	118.63	113.62
22	B	1206	CLA	O2D-CGD-O1D	-2.61	118.73	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	6	609	CLA	O2A-CGA-CBA	2.61	120.10	111.91
22	A	1116	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
24	I	4001	BCR	C19-C18-C17	2.61	122.94	118.94
22	5	614	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
22	7	603	CLA	O2A-CGA-CBA	2.61	120.09	111.91
22	A	1104	CLA	CHA-C4D-ND	2.61	137.95	132.50
22	7	604	CLA	CMA-C3A-C4A	2.61	118.78	111.77
39	8	601	CHL	CMA-C3A-C4A	2.61	118.78	111.77
22	B	1220	CLA	CHA-C4D-ND	2.60	137.95	132.50
22	B	1215	CLA	C2C-C1C-NC	2.60	112.41	109.97
22	A	1122	CLA	C2D-C1D-ND	2.60	112.02	110.10
22	8	603	CLA	C2D-C1D-ND	2.60	112.02	110.10
34	G	5002	ERG	C16-C17-C13	2.60	106.98	103.84
22	3	612	CLA	CMB-C2B-C1B	-2.60	124.46	128.46
39	3	608	CHL	C4A-NA-C1A	2.60	107.88	106.71
22	3	603	CLA	C2C-C1C-NC	2.60	112.41	109.97
39	4	609	CHL	CHC-C1C-NC	2.60	128.15	124.20
24	3	504	BCR	C34-C9-C10	-2.60	119.28	122.92
38	5	505	LUT	C7-C8-C9	-2.60	122.31	126.23
22	G	1602	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
22	6	604	CLA	CMB-C2B-C3B	2.60	129.54	124.68
22	4	605	CLA	CBC-CAC-C3C	-2.60	105.27	112.43
22	5	605	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
39	6	613	CHL	C1B-CHB-C4A	-2.60	124.97	130.12
24	7	503	BCR	C27-C26-C25	-2.60	118.96	122.73
22	B	1235	CLA	C2C-C1C-NC	2.60	112.41	109.97
22	6	605	CLA	CHA-C4D-ND	2.60	137.93	132.50
22	B	1211	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
22	K	1404	CLA	C6-C5-C3	-2.60	110.37	114.62
46	7	502	XAT	C6-C7-C8	-2.60	120.50	125.99
22	B	1214	CLA	O2A-CGA-CBA	2.60	120.06	111.91
22	L	1503	CLA	CMB-C2B-C3B	2.60	129.54	124.68
22	B	1231	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
22	B	1208	CLA	C1C-C2C-C3C	-2.60	104.23	106.96
22	B	1221	CLA	CHD-C1D-ND	-2.60	122.07	124.45
22	B	1228	CLA	C2A-C3A-C4A	-2.60	97.68	101.87
38	a	501	LUT	C35-C15-C14	-2.60	118.16	123.47
22	B	1239	CLA	O2A-CGA-CBA	2.59	120.05	111.91
22	B	1208	CLA	CMB-C2B-C1B	-2.59	124.48	128.46
22	8	605	CLA	CHA-C4D-ND	2.59	137.92	132.50
22	A	1102	CLA	CMB-C2B-C1B	-2.59	124.48	128.46
41	3	506	QTB	C03-C04-C05	-2.59	115.13	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	7	601	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
22	B	1216	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
22	3	618	CLA	CMA-C3A-C4A	2.59	118.73	111.77
22	B	1230	CLA	CAA-C2A-C1A	-2.59	103.49	111.97
22	8	607	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
24	K	4002	BCR	C23-C24-C25	-2.59	119.93	127.20
22	a	601	CLA	CAA-C2A-C3A	-2.59	105.69	112.78
22	B	1203	CLA	CHA-C4D-ND	2.59	137.91	132.50
39	8	601	CHL	C1-O2A-CGA	2.59	123.23	116.44
24	L	4002	BCR	C19-C18-C17	2.59	122.91	118.94
22	5	601	CLA	C1C-C2C-C3C	-2.59	104.24	106.96
22	5	604	CLA	C1C-C2C-C3C	-2.59	104.24	106.96
22	B	1223	CLA	CMA-C3A-C4A	2.59	118.73	111.77
22	8	620	CLA	O2A-CGA-CBA	2.59	120.03	111.91
22	a	605	CLA	CHD-C1D-ND	-2.59	122.08	124.45
22	B	1220	CLA	CMA-C3A-C4A	2.59	118.72	111.77
22	L	1502	CLA	C1C-C2C-C3C	-2.59	104.24	106.96
39	6	619	CHL	C2C-C3C-C4C	2.59	108.33	106.49
22	B	1221	CLA	O1D-CGD-CBD	-2.59	119.19	124.48
22	B	1021	CLA	C2D-C1D-ND	2.59	112.01	110.10
24	L	4001	BCR	C29-C30-C25	2.58	114.46	110.48
38	a	502	LUT	C30-C31-C32	-2.58	115.15	123.22
22	B	1202	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
22	A	1119	CLA	C2D-C1D-ND	2.58	112.01	110.10
22	B	1225	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
22	7	602	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
22	3	612	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
39	7	613	CHL	C4A-NA-C1A	2.58	107.87	106.71
22	B	1224	CLA	C2D-C1D-ND	2.58	112.01	110.10
22	5	609	CLA	C2D-C1D-ND	2.58	112.01	110.10
22	3	605	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
22	1	608	CLA	CMA-C3A-C4A	2.58	118.71	111.77
22	a	601	CLA	CMB-C2B-C1B	-2.58	124.50	128.46
22	4	607	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
24	A	4002	BCR	C34-C9-C10	-2.58	119.31	122.92
22	A	1113	CLA	CMA-C3A-C4A	2.58	118.71	111.77
22	A	1138	CLA	C2D-C1D-ND	2.58	112.00	110.10
22	B	1238	CLA	C2D-C1D-ND	2.58	112.00	110.10
22	B	1223	CLA	CHD-C1D-ND	-2.58	122.08	124.45
22	A	1101	CLA	CMA-C3A-C4A	2.58	118.70	111.77
22	A	1114	CLA	CMD-C2D-C3D	-2.58	121.68	127.61
22	1	606	CLA	CHA-C4D-ND	2.58	137.89	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1022	CLA	O2A-CGA-CBA	2.58	120.00	111.91
22	a	603	CLA	C1C-C2C-C3C	-2.58	104.25	106.96
22	a	612	CLA	O2A-CGA-CBA	2.58	120.00	111.91
22	4	611	CLA	C1-C2-C3	-2.58	121.59	126.04
22	3	606	CLA	C2D-C1D-ND	2.58	112.00	110.10
22	A	1115	CLA	CHD-C1D-ND	-2.58	122.09	124.45
38	3	501	LUT	C10-C11-C12	-2.58	115.18	123.22
22	4	615	CLA	CHA-C4D-ND	2.58	137.89	132.50
22	8	611	CLA	CMD-C2D-C3D	-2.58	121.69	127.61
22	A	1133	CLA	C2D-C1D-ND	2.58	112.00	110.10
22	5	604	CLA	C2D-C1D-ND	2.58	112.00	110.10
22	5	605	CLA	OBD-CAD-C3D	-2.58	122.32	128.52
47	8	807	4RF	O40-C41-C43	2.58	119.99	111.91
48	7	504	C7Z	C39-C29-C28	-2.57	114.02	118.08
22	B	1227	CLA	C1D-ND-C4D	-2.57	104.51	106.33
38	4	501	LUT	C22-C23-C24	-2.57	108.81	111.74
22	7	611	CLA	CMA-C3A-C4A	2.57	118.69	111.77
22	8	610	CLA	C2D-C1D-ND	2.57	112.00	110.10
25	a	801	LHG	C6-C5-C4	-2.57	105.70	111.79
22	B	1221	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
22	3	604	CLA	C1D-ND-C4D	-2.57	104.51	106.33
22	1	610	CLA	CMB-C2B-C3B	2.57	129.49	124.68
22	8	609	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
22	G	1601	CLA	CMA-C3A-C4A	2.57	118.68	111.77
22	8	606	CLA	CAA-CBA-CGA	-2.57	105.74	113.25
39	1	613	CHL	CMA-C3A-C4A	2.57	118.68	111.77
22	A	1112	CLA	O2A-CGA-CBA	2.57	119.97	111.91
22	B	1218	CLA	C2C-C1C-NC	2.57	112.38	109.97
22	3	603	CLA	O2A-CGA-CBA	2.57	119.97	111.91
22	A	1116	CLA	C1C-C2C-C3C	-2.57	104.26	106.96
22	A	1103	CLA	C2C-C1C-NC	2.57	112.38	109.97
22	B	1240	CLA	CHD-C1D-ND	-2.57	122.09	124.45
22	A	1138	CLA	C1C-C2C-C3C	-2.57	104.26	106.96
22	B	1221	CLA	O2A-CGA-CBA	2.57	119.96	111.91
39	8	604	CHL	C4D-CHA-C1A	2.57	124.37	121.25
22	5	604	CLA	C1D-ND-C4D	-2.57	104.51	106.33
22	A	1013	CLA	CAA-C2A-C3A	-2.57	105.75	112.78
22	B	1221	CLA	C1-C2-C3	-2.57	121.61	126.04
22	5	602	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
22	A	1111	CLA	O2A-CGA-CBA	2.56	119.96	111.91
22	L	1503	CLA	O2D-CGD-O1D	-2.56	118.82	123.84
26	8	802	DGD	O1G-C1A-C2A	2.56	119.95	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1210	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
22	4	611	CLA	CMD-C2D-C3D	-2.56	121.72	127.61
22	a	605	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
22	5	604	CLA	CHA-C4D-ND	2.56	137.86	132.50
22	B	1226	CLA	CHA-C4D-ND	2.56	137.86	132.50
22	K	1404	CLA	CHA-C4D-ND	2.56	137.86	132.50
22	B	1216	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
22	B	1226	CLA	C1-C2-C3	-2.56	121.61	126.04
22	B	1211	CLA	C1-C2-C3	-2.56	121.61	126.04
22	8	602	CLA	C2D-C1D-ND	2.56	111.99	110.10
22	3	603	CLA	CHD-C1D-ND	-2.56	122.10	124.45
22	1	603	CLA	O2A-CGA-CBA	2.56	119.95	111.91
39	5	610	CHL	CHB-C4A-NA	2.56	128.05	124.51
22	5	618	CLA	C1-C2-C3	-2.56	121.61	126.04
22	B	1229	CLA	CHA-C4D-ND	2.56	137.86	132.50
22	8	611	CLA	O2A-CGA-CBA	2.56	119.94	111.91
22	1	601	CLA	C2D-C1D-ND	2.56	111.99	110.10
22	B	1206	CLA	O2A-CGA-CBA	2.56	119.94	111.91
22	a	612	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
24	6	503	BCR	C33-C5-C4	2.56	118.53	113.62
22	8	611	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
39	3	611	CHL	C1B-CHB-C4A	-2.56	125.05	130.12
22	8	606	CLA	O2A-CGA-CBA	2.56	119.93	111.91
22	B	1213	CLA	CMA-C3A-C4A	2.56	118.64	111.77
22	7	606	CLA	CHA-C4D-ND	2.56	137.85	132.50
22	B	1234	CLA	C1-C2-C3	-2.56	121.62	126.04
22	A	1106	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
22	6	618	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
22	B	1216	CLA	C1-C2-C3	-2.56	121.62	126.04
21	A	1011	CL0	CMC-C2C-C1C	2.56	128.93	125.04
22	K	1401	CLA	CHD-C1D-ND	-2.55	122.11	124.45
22	A	1129	CLA	C1C-C2C-C3C	-2.55	104.27	106.96
22	3	616	CLA	C1C-C2C-C3C	-2.55	104.27	106.96
22	B	1225	CLA	CHA-C4D-ND	2.55	137.84	132.50
39	6	613	CHL	C1-O2A-CGA	2.55	123.14	116.44
22	A	1123	CLA	C1C-C2C-C3C	-2.55	104.27	106.96
22	4	615	CLA	C1-C2-C3	-2.55	121.63	126.04
22	B	1226	CLA	CMD-C2D-C3D	-2.55	121.74	127.61
22	F	1302	CLA	C2C-C1C-NC	2.55	112.36	109.97
22	7	608	CLA	C2D-C1D-ND	2.55	111.98	110.10
22	6	602	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
22	7	617	CLA	CHD-C1D-ND	-2.55	122.11	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1232	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
22	a	602	CLA	CHA-C4D-ND	2.55	137.83	132.50
22	7	617	CLA	CHA-C4D-ND	2.55	137.83	132.50
22	B	1231	CLA	C1-C2-C3	-2.55	121.64	126.04
22	A	1140	CLA	CHD-C1D-ND	-2.55	122.11	124.45
22	B	1228	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
22	B	1235	CLA	CMA-C3A-C4A	2.55	118.62	111.77
22	7	612	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
22	B	1022	CLA	CHA-C4D-ND	2.55	137.83	132.50
22	1	607	CLA	CHA-C4D-ND	2.55	137.83	132.50
22	7	615	CLA	CHA-C4D-ND	2.55	137.82	132.50
22	A	1108	CLA	C2C-C1C-NC	2.55	112.36	109.97
24	B	4002	BCR	C30-C25-C26	-2.55	119.03	122.61
22	4	605	CLA	CHA-C4D-ND	2.55	137.82	132.50
22	8	610	CLA	CMB-C2B-C3B	2.55	129.44	124.68
22	A	1117	CLA	CMB-C2B-C1B	-2.54	124.55	128.46
38	3	501	LUT	C8-C7-C6	-2.54	120.06	127.20
24	A	4005	BCR	C33-C5-C6	-2.54	121.67	124.53
22	4	616	CLA	C1C-C2C-C3C	-2.54	104.28	106.96
22	B	1227	CLA	CHA-C4D-ND	2.54	137.82	132.50
22	5	617	CLA	CHA-C4D-ND	2.54	137.82	132.50
22	L	1501	CLA	C1C-C2C-C3C	-2.54	104.28	106.96
22	F	1301	CLA	CHA-C4D-ND	2.54	137.82	132.50
22	4	610	CLA	CHA-C4D-ND	2.54	137.82	132.50
22	7	608	CLA	CHA-C4D-ND	2.54	137.82	132.50
22	A	1108	CLA	CHA-C4D-ND	2.54	137.81	132.50
41	a	504	QTB	C03-C04-C05	-2.54	115.29	123.22
22	B	1216	CLA	O2A-CGA-CBA	2.54	119.88	111.91
22	a	603	CLA	CHA-C4D-ND	2.54	137.81	132.50
22	B	1206	CLA	CMB-C2B-C1B	-2.54	124.56	128.46
22	A	1012	CLA	CHA-C4D-ND	2.54	137.81	132.50
22	A	1101	CLA	CHA-C4D-ND	2.54	137.81	132.50
25	7	801	LHG	O8-C23-C24	2.54	119.87	111.91
24	B	4005	BCR	C23-C22-C21	-2.54	115.05	118.94
22	1	610	CLA	CMA-C3A-C4A	2.54	118.59	111.77
22	A	1129	CLA	CHA-C4D-ND	2.54	137.81	132.50
22	B	1223	CLA	C2C-C1C-NC	2.54	112.35	109.97
39	6	613	CHL	CMA-C3A-C4A	2.54	118.59	111.77
22	3	602	CLA	CHA-C4D-ND	2.54	137.80	132.50
22	A	1012	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
22	3	607	CLA	O2A-CGA-CBA	2.53	119.86	111.91
22	A	1124	CLA	CHD-C1D-ND	-2.53	122.12	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	5	609	CLA	CHA-C4D-ND	2.53	137.80	132.50
22	4	603	CLA	C1D-ND-C4D	-2.53	104.53	106.33
24	A	4003	BCR	C39-C30-C25	-2.53	106.19	110.30
22	6	615	CLA	CHA-C4D-ND	2.53	137.80	132.50
26	8	802	DGD	C1D-O6D-C5D	-2.53	108.72	113.69
22	B	1218	CLA	C1D-ND-C4D	-2.53	104.54	106.33
22	1	604	CLA	C2D-C1D-ND	2.53	111.97	110.10
22	B	1235	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
22	A	1112	CLA	CMB-C2B-C3B	2.53	129.41	124.68
22	K	1403	CLA	CMD-C2D-C3D	-2.53	121.79	127.61
22	a	611	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
22	A	1110	CLA	O2A-CGA-CBA	2.53	119.84	111.91
22	A	1116	CLA	CHA-C4D-ND	2.53	137.79	132.50
22	7	615	CLA	CMA-C3A-C4A	2.53	118.57	111.77
22	5	614	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
22	8	608	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
22	B	1209	CLA	C3D-C2D-C1D	-2.53	102.38	105.83
22	5	614	CLA	CHA-C4D-ND	2.53	137.78	132.50
22	A	1125	CLA	C3D-C2D-C1D	-2.53	102.38	105.83
24	K	4001	BCR	C34-C9-C10	-2.53	119.38	122.92
24	K	4001	BCR	C33-C5-C4	2.53	118.47	113.62
22	5	608	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
22	5	612	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
22	8	607	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
22	5	602	CLA	CHA-C4D-ND	2.52	137.78	132.50
22	4	612	CLA	C1C-C2C-C3C	-2.52	104.30	106.96
22	8	612	CLA	C1C-C2C-C3C	-2.52	104.30	106.96
22	8	610	CLA	CMA-C3A-C4A	2.52	118.56	111.77
25	3	801	LHG	C5-O7-C7	-2.52	111.58	117.79
22	B	1021	CLA	CHA-C4D-ND	2.52	137.78	132.50
22	8	610	CLA	CHA-C4D-ND	2.52	137.78	132.50
22	A	1135	CLA	O2A-CGA-CBA	2.52	119.83	111.91
22	B	1240	CLA	O2A-CGA-CBA	2.52	119.83	111.91
22	6	606	CLA	C1C-C2C-C3C	-2.52	104.30	106.96
22	7	612	CLA	CHA-C4D-ND	2.52	137.78	132.50
22	B	1221	CLA	CMB-C2B-C1B	-2.52	124.59	128.46
22	A	1131	CLA	CMA-C3A-C4A	2.52	118.55	111.77
22	3	606	CLA	CMB-C2B-C3B	2.52	129.40	124.68
22	B	1219	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
22	8	602	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
22	A	1123	CLA	CHA-C4D-ND	2.52	137.77	132.50
22	4	606	CLA	CHA-C4D-ND	2.52	137.77	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	8	612	CLA	CHA-C4D-ND	2.52	137.77	132.50
24	L	4003	BCR	C8-C7-C6	-2.52	120.12	127.20
24	I	4001	BCR	C38-C26-C27	2.52	118.46	113.62
22	B	1235	CLA	C1D-ND-C4D	-2.52	104.54	106.33
22	L	1502	CLA	C1D-ND-C4D	-2.52	104.54	106.33
22	1	606	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
22	B	1213	CLA	CHA-C4D-ND	2.52	137.77	132.50
22	B	1209	CLA	CHA-C4D-ND	2.52	137.77	132.50
22	5	604	CLA	CMD-C2D-C3D	-2.52	121.82	127.61
22	A	1132	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
24	B	4007	BCR	C33-C5-C4	2.52	118.45	113.62
22	A	1111	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
24	A	4004	BCR	C38-C26-C27	2.52	118.45	113.62
22	B	1228	CLA	CBA-CAA-C2A	-2.52	106.44	113.86
22	1	602	CLA	CHA-C4D-ND	2.52	137.76	132.50
22	4	611	CLA	CHA-C4D-ND	2.52	137.76	132.50
22	4	608	CLA	CMA-C3A-C4A	2.52	118.54	111.77
22	4	617	CLA	CHA-C4D-ND	2.52	137.76	132.50
22	5	602	CLA	C6-C5-C3	-2.52	110.50	114.62
22	A	1140	CLA	C2D-C1D-ND	2.52	111.96	110.10
22	1	603	CLA	C1D-ND-C4D	-2.52	104.55	106.33
29	B	5006	LMT	C3'-C4'-C5'	-2.52	105.16	110.93
22	B	1216	CLA	CHA-C4D-ND	2.52	137.76	132.50
22	B	1211	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
22	7	601	CLA	O2A-CGA-CBA	2.51	119.80	111.91
22	7	605	CLA	C2C-C1C-NC	2.51	112.33	109.97
25	7	803	LHG	O8-C23-C24	2.51	119.80	111.91
22	B	1226	CLA	C1C-C2C-C3C	-2.51	104.31	106.96
48	7	504	C7Z	C1-C6-C7	2.51	122.89	115.78
22	A	1109	CLA	CHA-C4D-ND	2.51	137.76	132.50
22	4	610	CLA	CHA-C1A-NA	-2.51	120.64	126.40
22	5	607	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
38	6	501	LUT	C7-C6-C5	-2.51	115.38	121.46
35	J	4002	RRX	C27-C26-C25	-2.51	115.25	120.85
22	A	1126	CLA	CHA-C4D-ND	2.51	137.75	132.50
39	7	613	CHL	C1B-CHB-C4A	-2.51	125.14	130.12
22	A	1116	CLA	O2A-CGA-CBA	2.51	119.79	111.91
22	B	1211	CLA	CHA-C4D-ND	2.51	137.75	132.50
22	1	611	CLA	CHA-C4D-ND	2.51	137.75	132.50
22	A	1107	CLA	O2A-CGA-CBA	2.51	119.79	111.91
22	7	611	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
22	B	1237	CLA	CHA-C4D-ND	2.51	137.75	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	7	608	CLA	CMA-C3A-C4A	2.51	118.52	111.77
22	A	1113	CLA	CMB-C2B-C3B	2.51	129.37	124.68
22	7	603	CLA	CHA-C4D-ND	2.51	137.75	132.50
24	3	504	BCR	C37-C22-C21	-2.51	119.41	122.92
22	3	601	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
22	5	607	CLA	CHA-C4D-ND	2.51	137.75	132.50
22	7	611	CLA	C1-O2A-CGA	2.51	123.03	116.44
39	1	609	CHL	C4D-CHA-C1A	2.51	124.30	121.25
22	B	1212	CLA	CMA-C3A-C4A	2.51	118.51	111.77
22	5	617	CLA	C2D-C1D-ND	2.51	111.95	110.10
22	B	1231	CLA	C2C-C1C-NC	2.51	112.32	109.97
22	5	603	CLA	CMB-C2B-C3B	2.51	129.37	124.68
22	B	1219	CLA	CMA-C3A-C4A	2.51	118.51	111.77
22	A	1136	CLA	C2D-C1D-ND	2.51	111.95	110.10
22	A	1107	CLA	CHD-C1D-ND	-2.51	122.15	124.45
22	A	1127	CLA	O2A-CGA-CBA	2.51	119.77	111.91
22	B	1220	CLA	O2A-CGA-CBA	2.51	119.77	111.91
22	7	611	CLA	O2A-CGA-CBA	2.51	119.77	111.91
22	7	605	CLA	CHA-C4D-ND	2.51	137.74	132.50
24	L	4003	BCR	C33-C5-C4	2.50	118.43	113.62
22	A	1103	CLA	C1D-ND-C4D	-2.50	104.56	106.33
22	7	602	CLA	C1D-ND-C4D	-2.50	104.56	106.33
22	A	1127	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
22	A	1125	CLA	O2A-CGA-CBA	2.50	119.77	111.91
22	A	1125	CLA	CHA-C4D-ND	2.50	137.74	132.50
22	B	1211	CLA	CMD-C2D-C3D	-2.50	121.85	127.61
22	B	1224	CLA	C1C-C2C-C3C	-2.50	104.32	106.96
22	B	1238	CLA	C1C-C2C-C3C	-2.50	104.32	106.96
22	4	601	CLA	CMB-C2B-C3B	2.50	129.36	124.68
22	B	1219	CLA	CHA-C4D-ND	2.50	137.74	132.50
22	K	1402	CLA	C1C-C2C-C3C	-2.50	104.33	106.96
22	A	1133	CLA	CHA-C4D-ND	2.50	137.73	132.50
22	B	1238	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
22	a	608	CLA	CHA-C4D-ND	2.50	137.73	132.50
22	A	1121	CLA	C1C-C2C-C3C	-2.50	104.33	106.96
22	5	603	CLA	CMD-C2D-C3D	-2.50	121.86	127.61
22	A	1122	CLA	CHA-C4D-ND	2.50	137.73	132.50
22	7	603	CLA	C1C-C2C-C3C	-2.50	104.33	106.96
22	8	611	CLA	CAA-CBA-CGA	-2.50	105.95	113.25
22	B	1203	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
22	B	1021	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
39	5	610	CHL	CHD-C4C-C3C	2.50	128.51	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	4	608	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
22	A	1123	CLA	C2D-C1D-ND	2.50	111.94	110.10
22	A	1013	CLA	C1C-C2C-C3C	-2.50	104.33	106.96
22	8	608	CLA	CHA-C1A-NA	-2.50	120.68	126.40
26	A	5005	DGD	O1G-C1A-C2A	2.50	119.74	111.91
22	B	1231	CLA	O2A-CGA-CBA	2.50	119.74	111.91
22	8	618	CLA	CHA-C4D-ND	2.50	137.72	132.50
22	G	1603	CLA	C1C-C2C-C3C	-2.50	104.33	106.96
22	5	605	CLA	C2D-C1D-ND	2.49	111.94	110.10
30	6	803	PCW	O3-C11-C12	2.49	119.73	111.91
39	5	611	CHL	C4D-CHA-C1A	2.49	124.28	121.25
22	B	1022	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
22	4	615	CLA	C2D-C1D-ND	2.49	111.94	110.10
22	A	1103	CLA	CAA-CBA-CGA	-2.49	105.97	113.25
22	B	1217	CLA	CHA-C4D-ND	2.49	137.71	132.50
39	4	618	CHL	C2C-C3C-C4C	2.49	108.27	106.49
22	B	1227	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
24	G	4001	BCR	C23-C22-C21	2.49	122.76	118.94
22	B	1238	CLA	CHA-C4D-ND	2.49	137.71	132.50
22	7	602	CLA	CHA-C4D-ND	2.49	137.71	132.50
22	K	1403	CLA	CHA-C4D-ND	2.49	137.71	132.50
22	5	603	CLA	CHA-C4D-ND	2.49	137.71	132.50
22	3	613	CLA	C2D-C1D-ND	2.49	111.94	110.10
22	1	615	CLA	CMA-C3A-C4A	2.49	118.47	111.77
22	B	1208	CLA	CMD-C2D-C3D	-2.49	121.89	127.61
22	8	603	CLA	CHA-C4D-ND	2.49	137.71	132.50
22	F	1302	CLA	CMB-C2B-C1B	-2.49	124.64	128.46
22	5	606	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
22	8	615	CLA	CHA-C4D-ND	2.49	137.70	132.50
22	B	1229	CLA	CMA-C3A-C4A	2.49	118.46	111.77
22	3	613	CLA	CHA-C4D-ND	2.49	137.70	132.50
22	A	1137	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
22	B	1204	CLA	CHA-C4D-ND	2.49	137.70	132.50
22	6	608	CLA	CHA-C4D-ND	2.49	137.70	132.50
22	B	1212	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
22	A	1128	CLA	C2D-C1D-ND	2.49	111.94	110.10
22	5	607	CLA	O2A-CGA-CBA	2.49	119.71	111.91
22	4	612	CLA	CHA-C4D-ND	2.49	137.70	132.50
22	B	1201	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
22	B	1239	CLA	CHA-C4D-ND	2.48	137.69	132.50
22	B	1234	CLA	C2C-C1C-NC	2.48	112.30	109.97
22	A	1115	CLA	CMA-C3A-C4A	2.48	118.45	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1111	CLA	CHA-C4D-ND	2.48	137.69	132.50
22	A	1118	CLA	CHA-C4D-ND	2.48	137.69	132.50
22	A	1139	CLA	CHD-C1D-ND	-2.48	122.17	124.45
22	8	608	CLA	C2D-C1D-ND	2.48	111.93	110.10
22	5	617	CLA	CMD-C2D-C3D	-2.48	121.91	127.61
22	4	616	CLA	O2A-CGA-CBA	2.48	119.69	111.91
22	3	610	CLA	CHA-C4D-ND	2.48	137.69	132.50
25	1	802	LHG	C5-O7-C7	-2.48	111.68	117.79
24	5	503	BCR	C35-C13-C12	2.48	121.99	118.08
22	B	1208	CLA	C2D-C1D-ND	2.48	111.93	110.10
22	B	1234	CLA	CHA-C4D-ND	2.48	137.69	132.50
22	B	1220	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
39	a	606	CHL	CHB-C4A-NA	2.48	127.94	124.51
22	A	1117	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
22	A	1110	CLA	CMA-C3A-C4A	2.48	118.44	111.77
22	4	612	CLA	CMB-C2B-C3B	2.48	129.32	124.68
22	B	1215	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
22	a	603	CLA	C2D-C1D-ND	2.48	111.93	110.10
22	7	607	CLA	CMA-C3A-C4A	2.48	118.43	111.77
22	A	1113	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
22	A	1130	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
22	A	1138	CLA	O2A-CGA-CBA	2.48	119.68	111.91
22	G	1601	CLA	CHA-C4D-ND	2.48	137.68	132.50
39	a	610	CHL	C1B-CHB-C4A	-2.47	125.22	130.12
22	4	608	CLA	O1D-CGD-CBD	-2.47	119.42	124.48
22	a	615	CLA	CHA-C4D-ND	2.47	137.68	132.50
24	G	4001	BCR	C33-C5-C4	2.47	118.37	113.62
22	3	602	CLA	CMB-C2B-C3B	2.47	129.31	124.68
22	3	616	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
22	A	1126	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
22	A	1140	CLA	C2C-C1C-NC	2.47	112.29	109.97
22	3	610	CLA	C2D-C1D-ND	2.47	111.93	110.10
26	8	802	DGD	O2G-C1B-O1B	-2.47	117.73	123.70
22	A	1119	CLA	CHA-C4D-ND	2.47	137.67	132.50
24	A	4004	BCR	C27-C26-C25	-2.47	119.14	122.73
22	A	1135	CLA	CHA-C4D-ND	2.47	137.67	132.50
38	3	501	LUT	C39-C29-C28	2.47	121.97	118.08
22	B	1201	CLA	CAA-C2A-C3A	-2.47	106.02	112.78
24	J	4001	BCR	C23-C24-C25	-2.47	120.27	127.20
22	6	617	CLA	CHA-C4D-ND	2.47	137.66	132.50
22	8	609	CLA	CHA-C4D-ND	2.47	137.66	132.50
22	B	1205	CLA	C1C-C2C-C3C	-2.47	104.36	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1011	CL0	C1-C2-C3	-2.47	121.77	126.04
22	5	608	CLA	CHA-C4D-ND	2.47	137.66	132.50
38	5	505	LUT	C20-C13-C14	-2.47	119.47	122.92
22	A	1107	CLA	CHA-C4D-ND	2.47	137.66	132.50
22	B	1209	CLA	CMA-C3A-C4A	2.47	118.41	111.77
22	A	1104	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
22	K	1401	CLA	CHA-C4D-ND	2.47	137.66	132.50
22	B	1209	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
22	8	607	CLA	CMB-C2B-C3B	2.47	129.29	124.68
22	K	1401	CLA	CMA-C3A-C4A	2.47	118.40	111.77
35	J	4002	RRX	C2-C1-C6	2.47	114.28	110.48
22	8	609	CLA	C1D-ND-C4D	-2.47	104.58	106.33
22	A	1114	CLA	C2D-C1D-ND	2.47	111.92	110.10
22	a	607	CLA	O1D-CGD-CBD	-2.47	119.44	124.48
22	A	1134	CLA	CHA-C4D-ND	2.46	137.66	132.50
22	5	614	CLA	C2D-C1D-ND	2.46	111.92	110.10
22	5	606	CLA	CMA-C3A-C4A	2.46	118.39	111.77
22	6	601	CLA	C1C-C2C-C3C	-2.46	104.37	106.96
22	A	1135	CLA	OBD-CAD-C3D	-2.46	122.59	128.52
22	a	601	CLA	C2C-C1C-NC	2.46	112.28	109.97
39	a	609	CHL	CHD-C4C-C3C	2.46	128.46	124.84
22	3	606	CLA	CHA-C4D-ND	2.46	137.65	132.50
22	B	1208	CLA	CMA-C3A-C4A	2.46	118.39	111.77
22	B	1232	CLA	CHA-C4D-ND	2.46	137.65	132.50
22	4	601	CLA	CMA-C3A-C4A	2.46	118.39	111.77
22	A	1137	CLA	CHA-C4D-ND	2.46	137.65	132.50
22	B	1214	CLA	CHA-C4D-ND	2.46	137.65	132.50
24	B	4006	BCR	C36-C18-C17	-2.46	119.47	122.92
39	6	619	CHL	CHD-C4C-C3C	2.46	128.46	124.84
39	a	606	CHL	C1-C2-C3	-2.46	121.78	126.04
22	3	610	CLA	CAA-C2A-C3A	-2.46	106.04	112.78
22	A	1129	CLA	O2A-CGA-CBA	2.46	119.63	111.91
22	A	1128	CLA	CMA-C3A-C4A	2.46	118.38	111.77
22	a	601	CLA	CHA-C4D-ND	2.46	137.64	132.50
22	A	1107	CLA	C1C-C2C-C3C	-2.46	104.37	106.96
24	B	4003	BCR	C12-C13-C14	-2.46	115.17	118.94
22	4	602	CLA	C1C-C2C-C3C	-2.46	104.37	106.96
22	A	1115	CLA	CHA-C4D-ND	2.46	137.64	132.50
22	3	618	CLA	CHA-C4D-ND	2.46	137.64	132.50
24	A	4001	BCR	C37-C22-C21	-2.46	119.48	122.92
22	8	612	CLA	C2D-C1D-ND	2.46	111.92	110.10
22	8	602	CLA	C1-O2A-CGA	2.46	122.89	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1105	CLA	CHA-C4D-ND	2.46	137.63	132.50
22	A	1141	CLA	CHA-C4D-ND	2.46	137.63	132.50
22	A	1124	CLA	CHA-C4D-ND	2.45	137.63	132.50
38	5	505	LUT	C35-C15-C14	-2.45	118.45	123.47
22	B	1206	CLA	CHA-C4D-ND	2.45	137.63	132.50
22	a	601	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
22	a	604	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
22	7	607	CLA	CHA-C4D-ND	2.45	137.63	132.50
38	7	501	LUT	C15-C14-C13	-2.45	123.81	127.31
22	B	1211	CLA	O2A-CGA-CBA	2.45	119.60	111.91
41	3	506	QTB	C13-C12-C14	2.45	115.53	111.04
22	3	607	CLA	CHA-C4D-ND	2.45	137.63	132.50
22	B	1230	CLA	C1D-ND-C4D	-2.45	104.59	106.33
22	A	1118	CLA	CMA-C3A-C4A	2.45	118.36	111.77
38	8	502	LUT	C30-C31-C32	-2.45	115.57	123.22
21	A	1011	CL0	C1-O2A-CGA	2.45	122.87	116.44
22	A	1119	CLA	C2C-C1C-NC	2.45	112.27	109.97
22	J	1901	CLA	CHA-C4D-ND	2.45	137.62	132.50
38	1	502	LUT	C8-C7-C6	-2.45	120.33	127.20
22	B	1240	CLA	CHA-C4D-ND	2.45	137.62	132.50
22	3	612	CLA	CHA-C4D-ND	2.45	137.62	132.50
38	5	501	LUT	C39-C29-C28	2.45	121.93	118.08
22	5	601	CLA	O2A-CGA-CBA	2.45	119.58	111.91
24	K	4001	BCR	C3-C4-C5	-2.45	109.71	114.08
22	6	609	CLA	CHA-C1A-NA	-2.44	120.80	126.40
22	B	1205	CLA	O1D-CGD-CBD	-2.44	119.48	124.48
22	a	611	CLA	CMD-C2D-C3D	-2.44	121.99	127.61
22	a	604	CLA	CHA-C4D-ND	2.44	137.61	132.50
22	B	1205	CLA	CHA-C4D-ND	2.44	137.61	132.50
22	B	1227	CLA	CMD-C2D-C3D	-2.44	122.00	127.61
22	3	612	CLA	C1-C2-C3	-2.44	121.82	126.04
22	B	1207	CLA	CHA-C4D-ND	2.44	137.61	132.50
22	L	1503	CLA	CHA-C4D-ND	2.44	137.61	132.50
22	1	608	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
24	B	4004	BCR	C12-C13-C14	-2.44	115.20	118.94
22	A	1101	CLA	CHD-C1D-ND	-2.44	122.21	124.45
39	4	618	CHL	CHD-C4C-C3C	2.44	128.43	124.84
22	5	608	CLA	CMA-C3A-C4A	2.44	118.33	111.77
38	5	505	LUT	C39-C29-C28	2.44	121.92	118.08
25	F	5002	LHG	O8-C23-O10	-2.44	117.44	123.59
22	B	1202	CLA	CHA-C4D-ND	2.44	137.60	132.50
22	3	613	CLA	O2D-CGD-O1D	-2.44	119.07	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	8	502	LUT	C2-C3-C4	-2.44	106.97	110.30
22	a	612	CLA	CAC-C3C-C4C	2.44	127.97	124.81
22	5	609	CLA	CAA-CBA-CGA	-2.44	106.13	113.25
22	6	605	CLA	O2D-CGD-O1D	-2.44	119.08	123.84
22	1	601	CLA	CHA-C4D-ND	2.44	137.59	132.50
22	a	611	CLA	CHA-C4D-ND	2.44	137.59	132.50
22	3	601	CLA	CHA-C4D-ND	2.44	137.59	132.50
22	5	618	CLA	CHA-C4D-ND	2.44	137.59	132.50
22	A	1128	CLA	C1C-C2C-C3C	-2.44	104.40	106.96
22	B	1231	CLA	C1C-C2C-C3C	-2.44	104.40	106.96
22	4	610	CLA	CMA-C3A-C4A	2.43	118.32	111.77
22	1	612	CLA	CHA-C4D-ND	2.43	137.59	132.50
22	3	604	CLA	CMB-C2B-C3B	2.43	129.23	124.68
22	7	615	CLA	C1C-C2C-C3C	-2.43	104.40	106.96
22	B	1023	CLA	O2A-CGA-CBA	2.43	119.54	111.91
24	5	503	BCR	C37-C22-C23	2.43	121.91	118.08
22	A	1124	CLA	C2D-C1D-ND	2.43	111.90	110.10
22	1	611	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
38	1	501	LUT	C10-C11-C12	-2.43	115.63	123.22
22	A	1138	CLA	CMA-C3A-C4A	2.43	118.30	111.77
22	A	1124	CLA	C1C-C2C-C3C	-2.43	104.40	106.96
22	A	1117	CLA	CMA-C3A-C4A	2.43	118.30	111.77
22	A	1132	CLA	CAA-C2A-C3A	-2.43	106.13	112.78
22	8	615	CLA	CMD-C2D-C3D	-2.43	122.03	127.61
22	A	1108	CLA	O1D-CGD-CBD	-2.43	119.52	124.48
22	3	607	CLA	CMB-C2B-C1B	-2.43	124.73	128.46
22	a	601	CLA	C1D-ND-C4D	-2.43	104.61	106.33
22	A	1123	CLA	CMD-C2D-C3D	-2.43	122.03	127.61
22	B	1210	CLA	CAA-C2A-C1A	-2.43	104.03	111.97
38	5	505	LUT	C1-C6-C5	-2.43	119.20	122.61
22	5	607	CLA	C2D-C1D-ND	2.42	111.89	110.10
22	B	1228	CLA	CAA-C2A-C1A	-2.42	104.03	111.97
38	6	502	LUT	C35-C15-C14	-2.42	118.51	123.47
22	1	615	CLA	CHA-C4D-ND	2.42	137.57	132.50
22	5	603	CLA	C2D-C1D-ND	2.42	111.89	110.10
22	7	606	CLA	CMD-C2D-C3D	-2.42	122.04	127.61
38	1	503	LUT	C35-C15-C14	-2.42	118.51	123.47
22	a	604	CLA	CMC-C2C-C1C	2.42	128.73	125.04
22	5	616	CLA	CHA-C4D-ND	2.42	137.56	132.50
22	5	606	CLA	CHA-C4D-ND	2.42	137.56	132.50
22	1	605	CLA	CHA-C4D-ND	2.42	137.56	132.50
22	B	1203	CLA	C1D-ND-C4D	-2.42	104.62	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1126	CLA	CMB-C2B-C3B	2.42	129.21	124.68
22	B	1216	CLA	C2D-C1D-ND	2.42	111.89	110.10
22	K	1403	CLA	C2D-C1D-ND	2.42	111.89	110.10
22	a	607	CLA	CHA-C4D-ND	2.42	137.56	132.50
22	5	614	CLA	CMD-C2D-C3D	-2.42	122.05	127.61
22	a	611	CLA	O2A-CGA-CBA	2.42	119.50	111.91
22	5	612	CLA	CHA-C4D-ND	2.42	137.56	132.50
22	6	608	CLA	CMD-C2D-C3D	-2.42	122.05	127.61
25	1	801	LHG	O8-C23-C24	2.42	119.49	111.91
22	4	608	CLA	CMD-C2D-C3D	-2.42	122.05	127.61
22	A	1106	CLA	CHA-C4D-ND	2.42	137.55	132.50
22	6	604	CLA	CHA-C4D-ND	2.42	137.55	132.50
22	a	607	CLA	O2A-CGA-CBA	2.42	119.49	111.91
22	B	1218	CLA	CMA-C3A-C4A	2.42	118.27	111.77
22	8	611	CLA	CHA-C4D-ND	2.42	137.55	132.50
22	B	1238	CLA	O2A-CGA-CBA	2.41	119.48	111.91
22	A	1140	CLA	O2A-CGA-CBA	2.41	119.48	111.91
22	5	606	CLA	O2A-CGA-CBA	2.41	119.48	111.91
22	1	605	CLA	CMB-C2B-C3B	2.41	129.19	124.68
24	3	505	BCR	C38-C26-C27	2.41	118.25	113.62
22	A	1132	CLA	CHA-C4D-ND	2.41	137.54	132.50
22	7	604	CLA	CHA-C4D-ND	2.41	137.54	132.50
39	3	608	CHL	C4D-CHA-C1A	2.41	124.18	121.25
22	7	601	CLA	CHA-C4D-ND	2.41	137.54	132.50
22	5	608	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
22	A	1139	CLA	C1C-C2C-C3C	-2.41	104.42	106.96
22	3	604	CLA	C2C-C1C-NC	2.41	112.23	109.97
22	6	618	CLA	CHA-C4D-ND	2.41	137.54	132.50
22	A	1109	CLA	CHA-C1A-NA	-2.41	120.88	126.40
22	A	1132	CLA	CMA-C3A-C4A	2.41	118.25	111.77
22	4	607	CLA	C2D-C1D-ND	2.41	111.88	110.10
22	8	610	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
22	A	1101	CLA	CMD-C2D-C3D	-2.41	122.08	127.61
39	a	609	CHL	CHB-C4A-NA	2.41	127.84	124.51
22	8	602	CLA	C6-C5-C3	-2.41	110.68	114.62
24	B	4004	BCR	C23-C24-C25	-2.41	120.44	127.20
22	A	1102	CLA	CHA-C4D-ND	2.41	137.53	132.50
22	B	1230	CLA	CHA-C4D-ND	2.41	137.53	132.50
22	B	1213	CLA	O1D-CGD-CBD	-2.41	119.56	124.48
24	3	505	BCR	C33-C5-C4	2.41	118.24	113.62
22	4	615	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
22	6	608	CLA	O2D-CGD-O1D	-2.41	119.13	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1127	CLA	C1C-C2C-C3C	-2.41	104.43	106.96
24	L	4003	BCR	C23-C24-C25	-2.41	120.45	127.20
38	4	501	LUT	C11-C10-C9	-2.41	123.88	127.31
21	A	1011	CL0	CMB-C2B-C3B	2.41	129.18	124.68
22	3	604	CLA	CHA-C4D-ND	2.41	137.53	132.50
22	4	608	CLA	C1C-C2C-C3C	-2.40	104.43	106.96
22	3	616	CLA	C1-O2A-CGA	2.40	122.75	116.44
22	B	1201	CLA	CHA-C4D-ND	2.40	137.53	132.50
22	7	605	CLA	CAC-C3C-C2C	-2.40	123.42	127.53
24	B	4001	BCR	C34-C9-C10	-2.40	119.56	122.92
22	4	601	CLA	O1D-CGD-CBD	-2.40	119.57	124.48
22	a	604	CLA	C1-C2-C3	-2.40	121.89	126.04
22	8	611	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
38	6	501	LUT	C31-C32-C33	-2.40	119.67	126.42
22	1	604	CLA	CMA-C3A-C4A	2.40	118.23	111.77
22	8	607	CLA	CHA-C4D-ND	2.40	137.52	132.50
39	7	613	CHL	C1-O2A-CGA	2.40	122.75	116.44
24	A	4001	BCR	C3-C4-C5	-2.40	109.79	114.08
38	8	501	LUT	C30-C31-C32	-2.40	115.72	123.22
22	A	1112	CLA	CHA-C4D-ND	2.40	137.52	132.50
22	B	1215	CLA	CHA-C4D-ND	2.40	137.52	132.50
22	A	1120	CLA	CHA-C4D-ND	2.40	137.52	132.50
22	G	1602	CLA	CHA-C4D-ND	2.40	137.52	132.50
39	8	604	CHL	CHB-C4A-NA	2.40	127.83	124.51
39	8	613	CHL	CHB-C4A-NA	2.40	127.83	124.51
22	7	610	CLA	CHA-C4D-ND	2.40	137.52	132.50
22	A	1111	CLA	C1C-C2C-C3C	-2.40	104.43	106.96
24	3	504	BCR	C8-C9-C10	2.40	122.62	118.94
22	L	1501	CLA	O1D-CGD-CBD	-2.40	119.58	124.48
22	7	602	CLA	CAC-C3C-C4C	2.40	127.92	124.81
24	6	504	BCR	C38-C26-C27	2.40	118.22	113.62
22	A	1136	CLA	CHA-C4D-ND	2.40	137.51	132.50
22	5	601	CLA	CHA-C4D-ND	2.40	137.51	132.50
22	K	1401	CLA	C1C-C2C-C3C	-2.40	104.44	106.96
24	K	4002	BCR	C33-C5-C6	-2.39	121.84	124.53
37	M	4001	ECH	C11-C12-C13	-2.39	119.69	126.42
24	K	4001	BCR	C2-C1-C6	2.39	114.17	110.48
22	A	1131	CLA	O2A-CGA-CBA	2.39	119.42	111.91
22	7	611	CLA	CHA-C4D-ND	2.39	137.51	132.50
38	1	502	LUT	C30-C31-C32	-2.39	115.75	123.22
22	4	617	CLA	CMD-C2D-C3D	-2.39	122.11	127.61
22	8	602	CLA	CMD-C2D-C3D	-2.39	122.11	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	8	806	P5S	OG-CB-CA	2.39	110.14	108.06
22	B	1212	CLA	CHA-C4D-ND	2.39	137.50	132.50
24	A	4002	BCR	C38-C26-C27	2.39	118.21	113.62
24	5	503	BCR	C38-C26-C27	2.39	118.21	113.62
22	L	1501	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
38	a	501	LUT	C36-C21-C26	-2.39	105.92	109.55
22	4	603	CLA	CHA-C4D-ND	2.39	137.50	132.50
38	8	501	LUT	C35-C15-C14	-2.39	118.58	123.47
22	3	606	CLA	CMD-C2D-C3D	-2.39	122.12	127.61
24	K	4002	BCR	C37-C22-C21	-2.39	119.58	122.92
25	7	802	LHG	C5-O7-C7	-2.39	111.91	117.79
22	B	1217	CLA	CMA-C3A-C4A	2.39	118.19	111.77
22	A	1013	CLA	CHA-C4D-ND	2.39	137.49	132.50
22	1	604	CLA	C1-O2A-CGA	2.39	122.71	116.44
38	1	501	LUT	C8-C7-C6	-2.39	120.50	127.20
22	7	604	CLA	C6-C5-C3	-2.39	107.20	113.45
22	A	1124	CLA	O2A-CGA-CBA	2.39	119.40	111.91
22	B	1220	CLA	C1-O2A-CGA	2.39	122.70	116.44
22	8	615	CLA	C1C-C2C-C3C	-2.39	104.45	106.96
22	a	615	CLA	C2C-C1C-NC	2.39	112.21	109.97
38	4	501	LUT	C10-C11-C12	-2.39	115.77	123.22
24	5	503	BCR	C12-C13-C14	-2.39	115.28	118.94
22	4	616	CLA	CHA-C4D-ND	2.38	137.49	132.50
22	B	1208	CLA	CHA-C4D-ND	2.38	137.49	132.50
22	B	1225	CLA	CMD-C2D-C3D	-2.38	122.13	127.61
22	L	1501	CLA	CHA-C4D-ND	2.38	137.49	132.50
22	B	1212	CLA	O2A-CGA-CBA	2.38	119.39	111.91
38	4	502	LUT	C35-C15-C14	-2.38	118.59	123.47
22	7	607	CLA	CAA-C2A-C3A	-2.38	106.25	112.78
22	B	1224	CLA	CHA-C4D-ND	2.38	137.48	132.50
22	a	608	CLA	C2D-C1D-ND	2.38	111.86	110.10
22	A	1105	CLA	CMA-C3A-C4A	2.38	118.17	111.77
22	A	1114	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
22	A	1139	CLA	CMA-C3A-C4A	2.38	118.17	111.77
39	4	613	CHL	C1-O2A-CGA	2.38	122.69	116.44
22	8	611	CLA	C2D-C1D-ND	2.38	111.86	110.10
22	L	1501	CLA	C1-O2A-CGA	2.38	122.69	116.44
22	4	602	CLA	CHA-C4D-ND	2.38	137.47	132.50
22	a	605	CLA	CMD-C2D-C3D	-2.38	122.14	127.61
22	B	1217	CLA	O2A-CGA-CBA	2.38	119.37	111.91
22	K	1402	CLA	CHA-C4D-ND	2.38	137.47	132.50
24	A	4004	BCR	C34-C9-C8	2.38	121.82	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	7	609	CLA	CMD-C2D-C3D	-2.38	122.14	127.61
22	A	1126	CLA	C6-C5-C3	-2.38	107.22	113.45
22	4	604	CLA	CHA-C4D-ND	2.38	137.47	132.50
25	6	802	LHG	C5-O7-C7	-2.38	111.94	117.79
47	7	807	4RF	O40-C41-C43	2.38	119.37	111.91
22	A	1117	CLA	CHA-C4D-ND	2.38	137.47	132.50
22	6	604	CLA	C1C-C2C-C3C	-2.38	104.46	106.96
22	5	606	CLA	C1D-ND-C4D	-2.38	104.65	106.33
22	1	602	CLA	CHD-C1D-ND	-2.38	122.27	124.45
22	B	1222	CLA	CHA-C4D-ND	2.38	137.47	132.50
22	5	609	CLA	CHA-C1A-NA	-2.37	120.96	126.40
22	4	608	CLA	CAA-C2A-C3A	-2.37	106.28	112.78
24	A	4003	BCR	C33-C5-C4	2.37	118.18	113.62
22	B	1224	CLA	O1D-CGD-CBD	-2.37	119.63	124.48
22	F	1301	CLA	CHA-C1A-NA	-2.37	120.96	126.40
22	1	604	CLA	CHA-C4D-ND	2.37	137.46	132.50
22	1	608	CLA	CHA-C4D-ND	2.37	137.46	132.50
22	A	1125	CLA	CMA-C3A-C4A	2.37	118.15	111.77
22	6	607	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
39	5	610	CHL	C1B-CHB-C4A	-2.37	125.42	130.12
22	A	1108	CLA	O2A-CGA-CBA	2.37	119.35	111.91
22	6	603	CLA	CMD-C2D-C3D	-2.37	122.16	127.61
22	A	1120	CLA	C1D-ND-C4D	-2.37	104.65	106.33
22	5	618	CLA	CMC-C2C-C1C	2.37	128.65	125.04
22	F	1302	CLA	CHA-C4D-ND	2.37	137.46	132.50
24	I	4001	BCR	C35-C13-C12	2.37	121.81	118.08
39	5	613	CHL	C4A-NA-C1A	2.37	107.77	106.71
22	6	617	CLA	CBC-CAC-C3C	-2.37	105.89	112.43
22	4	601	CLA	O2A-CGA-CBA	2.37	119.35	111.91
22	3	603	CLA	CHA-C4D-ND	2.37	137.46	132.50
22	5	603	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
24	3	505	BCR	C34-C9-C10	-2.37	119.60	122.92
22	K	1402	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
22	A	1106	CLA	CMA-C3A-C4A	2.37	118.14	111.77
22	J	1901	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
22	a	604	CLA	CMD-C2D-C3D	-2.37	122.17	127.61
48	7	504	C7Z	C3-C4-C5	2.37	116.57	111.85
22	3	616	CLA	CHA-C4D-ND	2.37	137.45	132.50
22	A	1121	CLA	O1D-CGD-CBD	-2.37	119.64	124.48
35	J	4002	RRX	C4-C5-C6	-2.37	119.30	122.73
22	4	611	CLA	C1D-ND-C4D	-2.37	104.65	106.33
24	8	503	BCR	C15-C14-C13	-2.37	123.93	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1210	CLA	CMB-C2B-C1B	-2.37	124.83	128.46
22	7	615	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
24	B	4001	BCR	C33-C5-C4	2.36	118.16	113.62
22	a	602	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
22	A	1103	CLA	CHA-C4D-ND	2.36	137.44	132.50
22	L	1503	CLA	CMC-C2C-C3C	2.36	132.53	126.12
22	5	603	CLA	C1C-C2C-C3C	-2.36	104.47	106.96
22	A	1120	CLA	O1D-CGD-CBD	-2.36	119.65	124.48
38	a	501	LUT	C31-C32-C33	-2.36	119.78	126.42
22	6	601	CLA	CHA-C4D-ND	2.36	137.44	132.50
22	7	609	CLA	OBD-CAD-C3D	-2.36	122.84	128.52
22	6	612	CLA	CHA-C4D-ND	2.36	137.44	132.50
38	7	501	LUT	C11-C10-C9	-2.36	123.94	127.31
22	4	602	CLA	C1D-ND-C4D	-2.36	104.66	106.33
22	B	1214	CLA	CMD-C2D-C3D	-2.36	122.19	127.61
22	6	606	CLA	CHA-C4D-ND	2.36	137.43	132.50
22	B	1207	CLA	C1C-C2C-C3C	-2.36	104.48	106.96
22	3	612	CLA	O2A-CGA-CBA	2.36	119.31	111.91
24	L	4001	BCR	C36-C18-C17	-2.36	119.62	122.92
22	B	1023	CLA	CHA-C4D-ND	2.36	137.43	132.50
24	5	504	BCR	C37-C22-C23	2.36	121.79	118.08
22	A	1108	CLA	C2D-C1D-ND	2.36	111.84	110.10
22	A	1121	CLA	C2D-C1D-ND	2.36	111.84	110.10
22	7	603	CLA	C2D-C1D-ND	2.36	111.84	110.10
24	A	4002	BCR	C15-C14-C13	-2.36	123.95	127.31
22	4	604	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
22	A	1101	CLA	C1C-C2C-C3C	-2.36	104.48	106.96
22	a	605	CLA	CMB-C2B-C3B	2.35	129.08	124.68
22	A	1103	CLA	C1-O2A-CGA	2.35	122.62	116.44
22	B	1204	CLA	O2A-CGA-CBA	2.35	119.30	111.91
24	B	4005	BCR	C37-C22-C23	2.35	121.79	118.08
24	B	4003	BCR	C29-C28-C27	2.35	116.64	111.38
22	B	1208	CLA	O1D-CGD-CBD	-2.35	119.67	124.48
22	A	1130	CLA	CHA-C4D-ND	2.35	137.42	132.50
22	B	1236	CLA	C1C-C2C-C3C	-2.35	104.48	106.96
22	5	602	CLA	CMA-C3A-C4A	2.35	118.10	111.77
22	8	603	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
32	K	5001	LAP	O1-C1-O2	-2.35	117.65	123.59
22	L	1502	CLA	O2A-CGA-CBA	2.35	119.29	111.91
22	A	1134	CLA	O1D-CGD-CBD	-2.35	119.67	124.48
22	3	603	CLA	C1C-C2C-C3C	-2.35	104.48	106.96
22	A	1139	CLA	C1-O2A-CGA	2.35	122.61	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	a	502	LUT	C35-C15-C14	-2.35	118.66	123.47
22	B	1236	CLA	CHA-C4D-ND	2.35	137.42	132.50
22	B	1221	CLA	CHA-C1A-NA	-2.35	121.02	126.40
22	B	1222	CLA	C1D-ND-C4D	-2.35	104.67	106.33
22	8	605	CLA	C1D-ND-C4D	-2.35	104.67	106.33
24	4	503	BCR	C33-C5-C6	-2.35	121.89	124.53
22	B	1228	CLA	C6-C7-C8	-2.35	108.33	115.92
38	a	503	LUT	C38-C25-C24	-2.35	118.53	123.56
24	A	4001	BCR	C30-C25-C24	2.35	122.42	115.78
22	B	1208	CLA	C1D-ND-C4D	-2.35	104.67	106.33
25	B	5002	LHG	O8-C23-C24	2.35	119.28	111.91
22	1	601	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
22	a	601	CLA	C1C-C2C-C3C	-2.35	104.49	106.96
21	A	1011	CL0	CBC-CAC-C3C	-2.35	105.96	112.43
23	A	2001	PQN	C2M-C2-C3	-2.35	120.57	124.40
22	4	604	CLA	CMA-C3A-C4A	2.35	118.08	111.77
22	4	607	CLA	CMA-C3A-C4A	2.35	118.08	111.77
22	7	606	CLA	CMB-C2B-C1B	-2.35	124.86	128.46
22	A	1101	CLA	CHA-C1A-NA	-2.34	121.03	126.40
22	a	608	CLA	CMA-C3A-C4A	2.34	118.07	111.77
22	A	1132	CLA	O1D-CGD-CBD	-2.34	119.69	124.48
22	6	607	CLA	CHA-C4D-ND	2.34	137.40	132.50
39	6	611	CHL	C4D-CHA-C1A	2.34	124.10	121.25
22	7	603	CLA	CMD-C2D-C3D	-2.34	122.23	127.61
22	A	1108	CLA	CMD-C2D-C3D	-2.34	122.23	127.61
22	A	1119	CLA	CMB-C2B-C1B	-2.34	124.86	128.46
22	1	601	CLA	C1C-C2C-C3C	-2.34	104.50	106.96
22	B	1229	CLA	C1C-C2C-C3C	-2.34	104.50	106.96
22	A	1128	CLA	O1D-CGD-CBD	-2.34	119.70	124.48
22	B	1223	CLA	O2A-CGA-CBA	2.34	119.25	111.91
22	B	1213	CLA	CMD-C2D-C3D	-2.34	122.23	127.61
22	B	1214	CLA	C6-C5-C3	-2.34	107.32	113.45
22	7	611	CLA	CMB-C2B-C1B	-2.34	124.87	128.46
25	A	5002	LHG	C5-O7-C7	-2.34	112.04	117.79
22	6	602	CLA	CHA-C4D-ND	2.34	137.39	132.50
22	3	606	CLA	C1C-C2C-C3C	-2.34	104.50	106.96
22	8	603	CLA	CMD-C2D-C3D	-2.34	122.24	127.61
22	A	1125	CLA	C1C-C2C-C3C	-2.34	104.50	106.96
39	1	609	CHL	CGD-CBD-CAD	-2.34	103.17	110.73
22	A	1116	CLA	O1D-CGD-CBD	-2.34	119.71	124.48
22	A	1138	CLA	O1D-CGD-CBD	-2.34	119.71	124.48
39	4	609	CHL	C1B-CHB-C4A	-2.34	125.49	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1201	CLA	C6-C5-C3	-2.34	107.33	113.45
22	B	1218	CLA	CHA-C4D-ND	2.33	137.38	132.50
24	6	503	BCR	C34-C9-C10	-2.33	119.65	122.92
22	7	607	CLA	O2A-CGA-CBA	2.33	119.23	111.91
22	a	615	CLA	CAC-C3C-C4C	2.33	127.84	124.81
22	A	1127	CLA	CHA-C4D-ND	2.33	137.38	132.50
22	4	605	CLA	C1D-ND-C4D	-2.33	104.68	106.33
22	5	617	CLA	C1D-ND-C4D	-2.33	104.68	106.33
34	G	5002	ERG	C16-C15-C14	-2.33	101.46	105.30
22	5	606	CLA	C1C-C2C-C3C	-2.33	104.50	106.96
22	G	1603	CLA	CHA-C4D-ND	2.33	137.37	132.50
22	6	601	CLA	C1D-ND-C4D	-2.33	104.68	106.33
22	A	1118	CLA	C1C-C2C-C3C	-2.33	104.51	106.96
22	6	615	CLA	C1C-C2C-C3C	-2.33	104.51	106.96
34	G	5002	ERG	C7-C6-C5	-2.33	119.11	123.20
22	B	1226	CLA	O2A-CGA-CBA	2.33	119.22	111.91
24	G	4001	BCR	C15-C14-C13	2.33	130.63	127.31
22	8	606	CLA	CHA-C4D-ND	2.33	137.37	132.50
22	4	607	CLA	O1D-CGD-CBD	-2.33	119.72	124.48
24	A	4001	BCR	C38-C26-C25	-2.33	121.91	124.53
22	A	1122	CLA	C1C-C2C-C3C	-2.33	104.51	106.96
22	A	1107	CLA	CHA-C1A-NA	-2.33	121.06	126.40
38	4	502	LUT	C38-C25-C24	-2.33	118.58	123.56
22	B	1202	CLA	C1D-ND-C4D	-2.33	104.68	106.33
22	a	603	CLA	C1-O2A-CGA	2.33	122.55	116.44
22	6	612	CLA	C3D-C2D-C1D	-2.33	102.65	105.83
38	1	502	LUT	C39-C29-C28	2.33	121.75	118.08
22	B	1216	CLA	CAA-C2A-C3A	-2.33	106.40	112.78
22	5	605	CLA	CHD-C1D-ND	-2.33	122.31	124.45
22	5	601	CLA	CMD-C2D-C3D	-2.33	122.26	127.61
39	7	613	CHL	C4D-CHA-C1A	2.33	124.08	121.25
22	8	620	CLA	C1D-ND-C4D	-2.33	104.68	106.33
22	A	1113	CLA	CHA-C4D-ND	2.33	137.37	132.50
22	8	610	CLA	CHA-C1A-NA	-2.33	121.07	126.40
22	1	608	CLA	C2D-C1D-ND	2.33	111.82	110.10
22	a	605	CLA	O2A-CGA-CBA	2.33	119.20	111.91
24	7	503	BCR	C31-C1-C6	-2.32	106.53	110.30
22	B	1232	CLA	C2D-C1D-ND	2.32	111.82	110.10
24	J	4001	BCR	C38-C26-C27	2.32	118.08	113.62
22	7	612	CLA	C2D-C1D-ND	2.32	111.82	110.10
22	A	1131	CLA	C1C-C2C-C3C	-2.32	104.51	106.96
22	8	620	CLA	CHA-C4D-ND	2.32	137.36	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1236	CLA	C3D-C2D-C1D	-2.32	102.66	105.83
22	4	611	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
22	4	606	CLA	CMD-C2D-C3D	-2.32	122.27	127.61
22	B	1237	CLA	C1D-ND-C4D	-2.32	104.69	106.33
24	3	505	BCR	C31-C1-C6	-2.32	106.53	110.30
22	B	1210	CLA	CHA-C4D-ND	2.32	137.35	132.50
22	8	611	CLA	CMB-C2B-C3B	2.32	129.02	124.68
39	4	613	CHL	CHC-C1C-NC	2.32	127.72	124.20
39	6	613	CHL	CHB-C4A-NA	2.32	127.72	124.51
22	7	611	CLA	CAA-CBA-CGA	-2.32	106.47	113.25
22	B	1215	CLA	CMA-C3A-C4A	2.32	118.01	111.77
22	B	1231	CLA	C1-O2A-CGA	2.32	122.53	116.44
22	A	1121	CLA	CMA-C3A-C4A	2.32	118.01	111.77
22	4	615	CLA	CHA-C1A-NA	-2.32	121.09	126.40
22	3	610	CLA	CMB-C2B-C3B	2.32	129.02	124.68
22	5	618	CLA	C1D-ND-C4D	-2.32	104.69	106.33
22	B	1207	CLA	O2A-CGA-CBA	2.32	119.18	111.91
22	A	1112	CLA	C1C-C2C-C3C	-2.32	104.52	106.96
38	3	501	LUT	C38-C25-C24	-2.32	118.60	123.56
22	3	612	CLA	C1C-C2C-C3C	-2.32	104.52	106.96
39	a	606	CHL	CHD-C4C-C3C	2.32	128.25	124.84
22	A	1110	CLA	CHA-C4D-ND	2.32	137.35	132.50
22	3	604	CLA	CAA-C2A-C3A	-2.32	106.43	112.78
48	7	504	C7Z	C21-C26-C25	-2.32	119.35	122.61
38	a	501	LUT	C8-C7-C6	-2.32	120.70	127.20
22	6	608	CLA	CAA-C2A-C3A	-2.32	106.44	112.78
22	L	1502	CLA	CHA-C4D-ND	2.32	137.34	132.50
22	A	1126	CLA	CMD-C2D-C3D	-2.31	122.29	127.61
24	K	4002	BCR	C28-C27-C26	-2.31	109.94	114.08
22	5	612	CLA	O2D-CGD-O1D	-2.31	119.31	123.84
22	4	610	CLA	C1-O2A-CGA	2.31	122.52	116.44
22	6	618	CLA	O2D-CGD-O1D	-2.31	119.31	123.84
22	8	620	CLA	CMB-C2B-C1B	-2.31	124.91	128.46
24	B	4001	BCR	C23-C24-C25	-2.31	120.71	127.20
22	5	602	CLA	CHA-C1A-NA	-2.31	121.11	126.40
22	A	1013	CLA	O2A-CGA-CBA	2.31	119.16	111.91
22	7	603	CLA	C1-O2A-CGA	2.31	122.51	116.44
39	1	609	CHL	CMB-C2B-C1B	-2.31	124.91	128.46
22	A	1133	CLA	CAA-C2A-C3A	-2.31	106.45	112.78
22	A	1119	CLA	OBD-CAD-C3D	-2.31	122.96	128.52
24	B	4005	BCR	C15-C14-C13	-2.31	124.02	127.31
22	6	603	CLA	C1C-C2C-C3C	-2.31	104.53	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	602	CLA	CHA-C1A-NA	-2.31	121.11	126.40
22	B	1201	CLA	O2A-CGA-CBA	2.31	119.15	111.91
22	7	609	CLA	C1-C2-C3	-2.31	122.05	126.04
22	6	604	CLA	CHA-C1A-NA	-2.31	121.11	126.40
22	A	1013	CLA	C1D-ND-C4D	-2.31	104.70	106.33
22	B	1212	CLA	O1D-CGD-CBD	-2.31	119.76	124.48
24	4	503	BCR	C38-C26-C27	2.31	118.05	113.62
22	5	601	CLA	CAA-C2A-C3A	-2.31	106.46	112.78
24	B	4005	BCR	C4-C5-C6	-2.31	119.38	122.73
22	8	620	CLA	CAA-C2A-C1A	-2.31	104.42	111.97
22	A	1134	CLA	CMA-C3A-C4A	2.31	117.97	111.77
22	B	1021	CLA	O2A-CGA-CBA	2.30	119.14	111.91
22	7	601	CLA	C2C-C1C-NC	2.30	112.13	109.97
22	B	1223	CLA	C3D-C2D-C1D	-2.30	102.69	105.83
22	8	618	CLA	O2A-CGA-CBA	2.30	119.14	111.91
22	B	1240	CLA	CHA-C1A-NA	-2.30	121.12	126.40
22	B	1203	CLA	CMD-C2D-C3D	-2.30	122.31	127.61
33	7	805	SQD	O3-C3-C2	-2.30	105.02	110.35
39	8	601	CHL	C2C-C3C-C4C	2.30	108.13	106.49
22	K	1404	CLA	O2A-CGA-CBA	2.30	119.14	111.91
22	A	1137	CLA	C3D-C2D-C1D	-2.30	102.69	105.83
22	B	1022	CLA	CHA-C1A-NA	-2.30	121.12	126.40
22	B	1235	CLA	CHA-C4D-ND	2.30	137.32	132.50
25	B	5002	LHG	C5-O7-C7	-2.30	112.12	117.79
22	G	1601	CLA	C1-O2A-CGA	2.30	122.48	116.44
22	B	1206	CLA	CHA-C1A-NA	-2.30	121.12	126.40
38	3	501	LUT	C31-C30-C29	-2.30	124.02	127.31
22	4	612	CLA	CMC-C2C-C1C	2.30	128.54	125.04
22	4	612	CLA	CAA-C2A-C3A	-2.30	106.47	112.78
24	5	504	BCR	C8-C7-C6	-2.30	120.74	127.20
22	5	617	CLA	CAC-C3C-C2C	2.30	131.47	127.53
22	5	608	CLA	CMB-C2B-C3B	2.30	128.98	124.68
24	B	4005	BCR	C34-C9-C8	2.30	121.70	118.08
22	B	1231	CLA	C1D-ND-C4D	-2.30	104.70	106.33
22	5	601	CLA	CMA-C3A-C4A	2.30	117.95	111.77
22	A	1126	CLA	C2D-C1D-ND	2.30	111.80	110.10
22	3	604	CLA	CMD-C2D-C3D	-2.30	122.32	127.61
22	B	1201	CLA	O1D-CGD-CBD	-2.30	119.78	124.48
22	5	604	CLA	CMB-C2B-C1B	-2.30	124.93	128.46
22	B	1223	CLA	CHA-C1A-NA	-2.30	121.13	126.40
48	7	504	C7Z	C24-C25-C26	-2.30	115.72	120.85
22	1	606	CLA	CMB-C2B-C1B	-2.30	124.93	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	4002	BCR	C36-C18-C17	-2.30	119.70	122.92
24	K	4002	BCR	C36-C18-C17	-2.30	119.71	122.92
22	a	615	CLA	CMB-C2B-C1B	-2.30	124.94	128.46
22	K	1404	CLA	C3D-C2D-C1D	-2.30	102.70	105.83
22	4	602	CLA	O2D-CGD-O1D	-2.29	119.35	123.84
22	4	616	CLA	CMD-C2D-C3D	-2.29	122.33	127.61
22	3	618	CLA	CHA-C1A-NA	-2.29	121.14	126.40
41	3	506	QTB	C11-C10-C09	2.29	130.45	125.47
22	1	603	CLA	O2D-CGD-O1D	-2.29	119.35	123.84
24	L	4003	BCR	C27-C26-C25	-2.29	119.40	122.73
22	L	1503	CLA	CMB-C2B-C1B	-2.29	124.94	128.46
22	5	604	CLA	O2D-CGD-O1D	-2.29	119.35	123.84
38	5	501	LUT	C38-C25-C24	-2.29	118.65	123.56
24	6	503	BCR	C38-C26-C25	-2.29	121.95	124.53
22	8	615	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
22	1	607	CLA	O2A-CGA-CBA	2.29	119.10	111.91
22	B	1229	CLA	C1-O2A-CGA	2.29	122.46	116.44
22	B	1237	CLA	C2C-C1C-NC	2.29	112.12	109.97
24	B	4004	BCR	C19-C18-C17	2.29	122.46	118.94
24	B	4004	BCR	C8-C7-C6	-2.29	120.77	127.20
22	A	1137	CLA	O2A-CGA-CBA	2.29	119.09	111.91
26	8	802	DGD	O6D-C5D-C6D	2.29	111.29	106.67
22	a	608	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
22	A	1121	CLA	O2A-CGA-CBA	2.29	119.09	111.91
22	L	1502	CLA	C1-O2A-CGA	2.29	122.45	116.44
22	7	601	CLA	C1-O2A-CGA	2.29	122.45	116.44
22	1	601	CLA	CMD-C2D-C3D	-2.29	122.35	127.61
22	8	603	CLA	C6-C5-C3	-2.29	107.46	113.45
22	1	610	CLA	CMB-C2B-C1B	-2.29	124.95	128.46
22	6	604	CLA	CMB-C2B-C1B	-2.29	124.95	128.46
22	B	1213	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
22	B	1222	CLA	O2A-CGA-CBA	2.29	119.08	111.91
22	7	604	CLA	C2C-C1C-NC	2.29	112.11	109.97
22	4	603	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
22	4	601	CLA	CHA-C4D-ND	2.29	137.28	132.50
22	8	608	CLA	CHA-C4D-ND	2.29	137.28	132.50
22	F	1302	CLA	O2A-CGA-CBA	2.29	119.08	111.91
23	B	2002	PQN	C2M-C2-C3	-2.28	120.67	124.40
22	3	606	CLA	O2D-CGD-O1D	-2.28	119.37	123.84
24	L	4002	BCR	C33-C5-C4	2.28	118.00	113.62
22	7	605	CLA	CMA-C3A-C4A	2.28	117.91	111.77
22	A	1104	CLA	CMD-C2D-C3D	-2.28	122.36	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	4	610	CLA	CMD-C2D-C3D	-2.28	122.36	127.61
22	3	604	CLA	C1C-C2C-C3C	-2.28	104.56	106.96
22	a	605	CLA	CMA-C3A-C4A	2.28	117.91	111.77
26	B	5003	DGD	O2G-C1B-O1B	-2.28	118.19	123.70
22	1	610	CLA	CHA-C4D-ND	2.28	137.27	132.50
22	A	1128	CLA	O2A-CGA-CBA	2.28	119.07	111.91
22	4	617	CLA	OBD-CAD-C3D	-2.28	123.03	128.52
35	J	4002	RRX	C16-C15-C14	-2.28	118.80	123.47
24	B	4005	BCR	C29-C28-C27	2.28	116.47	111.38
39	a	610	CHL	CHD-C4C-C3C	2.28	128.19	124.84
25	1	801	LHG	C6-C5-C4	-2.28	106.40	111.79
22	6	617	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
22	A	1102	CLA	C3D-C2D-C1D	-2.28	102.72	105.83
38	a	503	LUT	C35-C15-C14	-2.28	118.81	123.47
39	6	611	CHL	CHB-C4A-NA	2.28	127.66	124.51
22	B	1220	CLA	C2D-C1D-ND	2.28	111.78	110.10
22	7	606	CLA	C1C-C2C-C3C	-2.28	104.56	106.96
39	5	610	CHL	CHC-C1C-NC	2.28	127.66	124.20
22	1	605	CLA	CMD-C2D-C3D	-2.28	122.38	127.61
22	B	1210	CLA	CAA-C2A-C3A	-2.27	106.55	112.78
39	5	610	CHL	CMA-C3A-C4A	2.27	117.89	111.77
22	B	1209	CLA	O2A-CGA-CBA	2.27	119.04	111.91
22	1	608	CLA	O2A-CGA-CBA	2.27	119.04	111.91
39	4	609	CHL	C4A-NA-C1A	2.27	107.73	106.71
22	B	1021	CLA	CAA-C2A-C3A	-2.27	106.56	112.78
38	a	502	LUT	C7-C8-C9	-2.27	122.80	126.23
22	4	603	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
22	1	601	CLA	C1D-ND-C4D	-2.27	104.72	106.33
22	3	602	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
39	6	610	CHL	CHD-C4C-C3C	2.27	128.18	124.84
22	A	1116	CLA	C1D-ND-C4D	-2.27	104.72	106.33
22	a	607	CLA	C1D-ND-C4D	-2.27	104.72	106.33
22	6	609	CLA	C1-O2A-CGA	2.27	122.39	116.44
22	A	1139	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
22	6	601	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
22	B	1219	CLA	C2D-C1D-ND	2.27	111.77	110.10
39	6	619	CHL	CMB-C2B-C1B	-2.27	124.98	128.46
22	5	601	CLA	C1D-ND-C4D	-2.26	104.73	106.33
22	1	602	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
34	G	5002	ERG	C20-C22-C23	-2.26	118.65	125.67
22	B	1220	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
22	A	1109	CLA	CAA-C2A-C3A	-2.26	106.58	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1212	CLA	C1-O2A-CGA	2.26	122.38	116.44
22	8	608	CLA	CMA-C3A-C4A	2.26	117.85	111.77
22	4	606	CLA	C2D-C1D-ND	2.26	111.77	110.10
38	1	501	LUT	C38-C25-C24	-2.26	118.72	123.56
22	1	604	CLA	C2C-C1C-NC	2.26	112.09	109.97
38	5	505	LUT	C31-C32-C33	-2.26	120.06	126.42
22	a	612	CLA	C1D-ND-C4D	-2.26	104.73	106.33
22	4	616	CLA	C1D-ND-C4D	-2.26	104.73	106.33
37	M	4001	ECH	C37-C22-C23	-2.26	114.52	118.08
22	A	1138	CLA	CMB-C2B-C1B	-2.26	124.99	128.46
37	M	4001	ECH	C15-C16-C17	-2.26	118.84	123.47
22	7	615	CLA	C1-O2A-CGA	2.26	122.37	116.44
22	7	606	CLA	CHA-C1A-NA	-2.26	121.22	126.40
38	1	501	LUT	C3-C4-C5	-2.26	107.35	111.85
39	1	609	CHL	CHC-C1C-NC	2.26	127.63	124.20
22	4	603	CLA	O2A-CGA-CBA	2.26	119.00	111.91
22	B	1225	CLA	O2A-CGA-CBA	2.26	119.00	111.91
22	B	1214	CLA	CMB-C2B-C3B	2.26	128.90	124.68
22	A	1132	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
22	a	605	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
22	B	1211	CLA	C2D-C1D-ND	2.26	111.77	110.10
22	8	608	CLA	CAA-C2A-C3A	-2.26	106.59	112.78
24	8	503	BCR	C4-C5-C6	-2.26	119.45	122.73
22	A	1105	CLA	C1C-C2C-C3C	-2.26	104.58	106.96
39	4	609	CHL	C4D-CHA-C1A	2.26	124.00	121.25
22	5	616	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
38	8	502	LUT	C38-C25-C24	-2.26	118.73	123.56
22	K	1402	CLA	CHA-C1A-NA	-2.26	121.23	126.40
22	1	608	CLA	CHA-C1A-NA	-2.26	121.23	126.40
22	B	1228	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
39	7	613	CHL	C1-C2-C3	-2.25	122.14	126.04
22	A	1121	CLA	CED-O2D-CGD	-2.25	110.84	115.94
22	7	608	CLA	CMD-C2D-C3D	-2.25	122.43	127.61
22	B	1212	CLA	C1D-ND-C4D	-2.25	104.73	106.33
22	B	1235	CLA	CMB-C2B-C3B	2.25	128.89	124.68
22	A	1116	CLA	CMB-C2B-C3B	2.25	128.89	124.68
22	B	1230	CLA	CMD-C2D-C3D	-2.25	122.43	127.61
22	7	611	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
22	6	602	CLA	CMA-C3A-C4A	2.25	117.83	111.77
22	A	1119	CLA	C1C-C2C-C3C	-2.25	104.59	106.96
22	B	1204	CLA	CAC-C3C-C4C	2.25	127.73	124.81
40	1	803	OLA	C3-C2-C1	-2.25	108.80	114.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	L	4001	BCR	C4-C5-C6	-2.25	119.46	122.73
39	1	609	CHL	C1B-CHB-C4A	-2.25	125.66	130.12
39	a	610	CHL	C1-O2A-CGA	2.25	123.27	116.73
22	1	601	CLA	CMB-C2B-C1B	-2.25	125.01	128.46
38	3	502	LUT	C30-C31-C32	-2.25	116.20	123.22
21	A	1011	CL0	C3D-C4D-ND	2.25	113.88	110.24
22	7	604	CLA	CMB-C2B-C1B	-2.25	125.01	128.46
22	5	609	CLA	CMB-C2B-C3B	2.25	128.89	124.68
38	1	501	LUT	C39-C29-C28	2.25	121.62	118.08
22	A	1118	CLA	C1D-ND-C4D	-2.25	104.74	106.33
22	1	605	CLA	C1D-ND-C4D	-2.25	104.74	106.33
38	a	503	LUT	C8-C7-C6	-2.25	120.89	127.20
22	7	617	CLA	O2A-CGA-CBA	2.25	118.96	111.91
38	5	502	LUT	C16-C1-C6	-2.25	106.65	110.30
22	8	608	CLA	C1-O2A-CGA	2.25	122.34	116.44
39	5	613	CHL	CMB-C2B-C1B	-2.25	125.01	128.46
22	K	1404	CLA	CHA-C1A-NA	-2.25	121.25	126.40
39	4	618	CHL	CHB-C4A-NA	2.25	127.62	124.51
22	3	613	CLA	CMB-C2B-C3B	2.25	128.88	124.68
22	3	605	CLA	CMD-C2D-C3D	-2.25	122.45	127.61
22	B	1201	CLA	CMA-C3A-C4A	2.25	117.81	111.77
22	5	609	CLA	CMD-C2D-C3D	-2.24	122.45	127.61
25	A	5003	LHG	C5-O7-C7	-2.24	112.27	117.79
39	a	610	CHL	CHB-C4A-NA	2.24	127.61	124.51
22	G	1601	CLA	C1D-ND-C4D	-2.24	104.74	106.33
22	A	1109	CLA	O2A-CGA-CBA	2.24	118.95	111.91
22	8	603	CLA	O2A-CGA-CBA	2.24	118.95	111.91
22	B	1228	CLA	CHA-C4D-ND	2.24	137.19	132.50
22	7	602	CLA	C1C-C2C-C3C	-2.24	104.60	106.96
22	6	617	CLA	C1D-ND-C4D	-2.24	104.74	106.33
22	5	614	CLA	CHA-C1A-NA	-2.24	121.27	126.40
22	a	603	CLA	CMD-C2D-C3D	-2.24	122.46	127.61
22	a	612	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
24	B	4001	BCR	C27-C26-C25	-2.24	119.48	122.73
22	3	618	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
22	8	615	CLA	CAC-C3C-C4C	2.24	127.72	124.81
22	B	1205	CLA	C2D-C1D-ND	2.24	111.75	110.10
22	5	605	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
22	A	1126	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
22	K	1401	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
22	a	603	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
22	1	608	CLA	O1D-CGD-CBD	-2.24	119.91	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	7	617	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
38	a	502	LUT	C2-C3-C4	-2.24	107.24	110.30
22	1	605	CLA	CMA-C3A-C4A	2.24	117.78	111.77
22	4	617	CLA	CHA-C1A-NA	-2.24	121.28	126.40
41	a	504	QTB	C11-C10-C09	2.23	130.32	125.47
24	G	4001	BCR	C38-C26-C27	2.23	117.91	113.62
38	3	501	LUT	C30-C31-C32	-2.23	116.25	123.22
22	1	610	CLA	C1D-ND-C4D	-2.23	104.75	106.33
22	A	1125	CLA	CMC-C2C-C3C	-2.23	120.06	126.12
22	G	1602	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
22	B	1214	CLA	CMB-C2B-C1B	-2.23	125.03	128.46
22	4	617	CLA	C3D-C2D-C1D	-2.23	102.79	105.83
22	8	605	CLA	C3D-C2D-C1D	-2.23	102.79	105.83
38	4	501	LUT	C30-C31-C32	-2.23	116.25	123.22
22	8	608	CLA	C4D-CHA-C1A	2.23	123.96	121.25
22	1	603	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
22	B	1210	CLA	C3D-C2D-C1D	-2.23	102.79	105.83
22	4	611	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
39	1	613	CHL	CMB-C2B-C1B	-2.23	125.04	128.46
24	3	504	BCR	C33-C5-C4	2.23	117.90	113.62
22	a	605	CLA	CHA-C1A-NA	-2.23	121.29	126.40
22	5	616	CLA	C3D-C2D-C1D	-2.23	102.79	105.83
22	F	1301	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
22	7	602	CLA	C3D-C2D-C1D	-2.23	102.79	105.83
22	7	608	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
22	1	604	CLA	C1D-ND-C4D	-2.23	104.75	106.33
22	A	1130	CLA	CMA-C3A-C4A	2.23	117.76	111.77
38	5	505	LUT	C1-C6-C7	2.23	122.08	115.78
22	B	1232	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
22	3	605	CLA	OBD-CAD-C3D	-2.23	123.16	128.52
22	J	1901	CLA	CHA-C1A-NA	-2.23	121.30	126.40
22	1	603	CLA	CHA-C4D-ND	2.23	137.16	132.50
22	6	615	CLA	CMB-C2B-C3B	2.23	128.84	124.68
22	A	1101	CLA	O2A-CGA-CBA	2.23	118.90	111.91
24	K	4002	BCR	C38-C26-C25	-2.23	122.03	124.53
24	F	4001	BCR	C8-C9-C10	2.23	122.36	118.94
22	3	601	CLA	CMB-C2B-C1B	-2.23	125.04	128.46
22	8	608	CLA	C6-C5-C3	-2.23	110.98	114.62
22	8	610	CLA	C1C-C2C-C3C	-2.23	104.62	106.96
22	1	602	CLA	O2D-CGD-O1D	-2.22	119.49	123.84
39	6	611	CHL	C1-O2A-CGA	2.22	122.28	116.44
38	4	502	LUT	C11-C10-C9	-2.22	124.14	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1129	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
22	6	606	CLA	O2D-CGD-O1D	-2.22	119.49	123.84
22	F	1301	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
22	L	1501	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
24	B	4003	BCR	C36-C18-C17	-2.22	119.81	122.92
22	K	1402	CLA	O2A-CGA-CBA	2.22	118.88	111.91
22	4	612	CLA	CMA-C3A-C4A	2.22	117.75	111.77
22	B	1207	CLA	CMA-C3A-C4A	2.22	117.74	111.77
22	A	1112	CLA	CAC-C3C-C4C	2.22	127.69	124.81
22	A	1134	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
39	a	609	CHL	CHC-C1C-NC	2.22	127.57	124.20
22	A	1103	CLA	CMA-C3A-C4A	2.22	117.74	111.77
22	6	609	CLA	CMA-C3A-C4A	2.22	117.74	111.77
22	F	1301	CLA	C2A-C1A-CHA	2.22	127.74	123.86
39	6	613	CHL	CMB-C2B-C1B	-2.22	125.05	128.46
22	3	602	CLA	C1D-ND-C4D	-2.22	104.76	106.33
22	A	1125	CLA	C1-O2A-CGA	2.22	122.27	116.44
22	A	1103	CLA	C3D-C2D-C1D	-2.22	102.80	105.83
22	8	606	CLA	C1D-ND-C4D	-2.22	104.76	106.33
22	A	1111	CLA	CAA-C2A-C3A	-2.22	106.70	112.78
38	5	501	LUT	C20-C13-C12	2.22	121.57	118.08
38	1	502	LUT	C18-C5-C4	2.22	118.46	114.36
22	6	605	CLA	C3D-C2D-C1D	-2.22	102.81	105.83
39	4	613	CHL	CHD-C4C-C3C	2.22	128.10	124.84
22	a	615	CLA	C1D-ND-C4D	-2.22	104.76	106.33
22	7	601	CLA	C1D-ND-C4D	-2.22	104.76	106.33
22	A	1115	CLA	O2A-CGA-CBA	2.22	118.86	111.91
22	B	1239	CLA	CMA-C3A-C4A	2.22	117.73	111.77
22	a	605	CLA	O1D-CGD-CBD	-2.22	119.95	124.48
22	B	1224	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
21	A	1011	CL0	C4D-C3D-CAD	2.22	110.71	108.10
22	B	1204	CLA	CAA-CBA-CGA	-2.22	106.78	113.25
39	6	619	CHL	CHC-C1C-NC	2.22	127.56	124.20
22	7	615	CLA	CHA-C1A-NA	-2.21	121.33	126.40
22	A	1111	CLA	CMD-C2D-C3D	-2.21	122.52	127.61
24	B	4004	BCR	C37-C22-C23	2.21	121.56	118.08
22	6	615	CLA	C3D-C2D-C1D	-2.21	102.81	105.83
22	7	606	CLA	CMA-C3A-C4A	2.21	117.72	111.77
22	B	1209	CLA	CHA-C1A-NA	-2.21	121.33	126.40
22	K	1402	CLA	C3D-C2D-C1D	-2.21	102.81	105.83
24	A	4005	BCR	C38-C26-C27	2.21	117.87	113.62
24	L	4003	BCR	C30-C25-C26	-2.21	119.50	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	4001	BCR	C38-C26-C27	2.21	117.86	113.62
22	a	604	CLA	C2C-C1C-NC	2.21	112.04	109.97
22	B	1202	CLA	C3D-C2D-C1D	-2.21	102.81	105.83
25	5	801	LHG	C5-O7-C7	-2.21	112.35	117.79
22	B	1212	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
22	5	606	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
22	6	615	CLA	O2A-CGA-CBA	2.21	118.84	111.91
22	B	1206	CLA	CMB-C2B-C3B	2.21	128.81	124.68
39	6	610	CHL	CMB-C2B-C1B	-2.21	125.07	128.46
22	6	617	CLA	CHA-C1A-NA	-2.21	121.34	126.40
22	L	1501	CLA	C1D-ND-C4D	-2.21	104.77	106.33
38	1	502	LUT	C16-C1-C6	-2.21	106.72	110.30
22	A	1116	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
22	4	607	CLA	O2A-CGA-CBA	2.21	118.84	111.91
22	6	612	CLA	C1C-C2C-C3C	-2.21	104.64	106.96
24	8	503	BCR	C8-C7-C6	-2.21	121.00	127.20
22	a	601	CLA	CMD-C2D-C3D	-2.21	122.54	127.61
22	A	1140	CLA	C1C-C2C-C3C	-2.21	104.64	106.96
22	A	1107	CLA	C2A-C1A-CHA	2.21	127.72	123.86
22	5	608	CLA	CHA-C1A-NA	-2.21	121.35	126.40
22	B	1238	CLA	CMD-C2D-C3D	-2.20	122.54	127.61
22	1	606	CLA	C1D-ND-C4D	-2.20	104.77	106.33
22	3	610	CLA	CMD-C2D-C3D	-2.20	122.54	127.61
22	B	1206	CLA	C2D-C1D-ND	2.20	111.73	110.10
24	6	504	BCR	C37-C22-C23	2.20	121.55	118.08
22	A	1112	CLA	CHA-C1A-NA	-2.20	121.35	126.40
22	B	1203	CLA	C1C-C2C-C3C	-2.20	104.64	106.96
22	a	603	CLA	C6-C5-C3	-2.20	107.68	113.45
22	6	604	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
22	A	1113	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
22	6	617	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
24	A	4003	BCR	C38-C26-C27	2.20	117.84	113.62
22	7	605	CLA	CHA-C1A-NA	-2.20	121.36	126.40
22	7	601	CLA	CMA-C3A-C4A	2.20	117.69	111.77
22	B	1214	CLA	C2D-C1D-ND	2.20	111.73	110.10
38	7	501	LUT	C31-C32-C33	-2.20	120.23	126.42
38	a	501	LUT	C18-C5-C4	2.20	118.43	114.36
38	5	502	LUT	C40-C33-C32	2.20	121.54	118.08
22	7	604	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
25	7	801	LHG	O7-C7-O9	-2.20	118.39	123.70
38	1	502	LUT	C20-C13-C12	2.20	121.54	118.08
46	7	502	XAT	O24-C25-C24	2.20	115.03	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	5008	LMT	O5'-C5'-C6'	2.20	111.90	106.44
22	a	601	CLA	CMA-C3A-C4A	2.20	117.68	111.77
24	B	4007	BCR	C38-C26-C25	-2.20	122.06	124.53
22	a	605	CLA	OBD-CAD-C3D	-2.20	123.23	128.52
22	5	603	CLA	O2A-CGA-CBA	2.20	118.81	111.91
36	J	5001	LPX	O6-C6-C7	2.20	117.14	111.38
22	8	609	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
22	5	605	CLA	CMA-C3A-C4A	2.20	117.68	111.77
22	B	1023	CLA	C1D-ND-C4D	-2.20	104.77	106.33
22	8	603	CLA	C6-C7-C8	-2.20	108.82	115.92
22	5	606	CLA	O1D-CGD-CBD	-2.20	119.99	124.48
38	4	502	LUT	C31-C30-C29	-2.20	124.17	127.31
22	A	1137	CLA	O1D-CGD-CBD	-2.20	119.99	124.48
24	A	4002	BCR	C38-C26-C25	-2.20	122.06	124.53
24	3	505	BCR	C23-C24-C25	-2.20	121.03	127.20
22	A	1123	CLA	O2A-CGA-CBA	2.20	118.80	111.91
22	K	1401	CLA	CHA-C1A-NA	-2.20	121.37	126.40
22	B	1227	CLA	C1-O2A-CGA	2.20	122.20	116.44
22	F	1302	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
22	4	602	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
33	G	5001	SQD	O3-C3-C2	-2.19	105.28	110.35
22	A	1114	CLA	CHA-C1A-NA	-2.19	121.37	126.40
22	4	617	CLA	C1D-ND-C4D	-2.19	104.78	106.33
22	8	611	CLA	C1D-ND-C4D	-2.19	104.78	106.33
22	A	1123	CLA	C1-O2A-CGA	2.19	122.20	116.44
22	B	1222	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
22	L	1503	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
22	B	1209	CLA	C1D-ND-C4D	-2.19	104.78	106.33
22	3	605	CLA	C1D-ND-C4D	-2.19	104.78	106.33
22	B	1219	CLA	CHA-C1A-NA	-2.19	121.38	126.40
22	B	1023	CLA	CMB-C2B-C1B	-2.19	125.10	128.46
22	J	1901	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
22	G	1602	CLA	CMB-C2B-C3B	2.19	128.78	124.68
22	A	1131	CLA	CHA-C1A-NA	-2.19	121.38	126.40
22	A	1110	CLA	C1-O2A-CGA	2.19	122.19	116.44
22	5	612	CLA	CMB-C2B-C3B	2.19	128.77	124.68
22	B	1214	CLA	CMA-C3A-C4A	2.19	117.66	111.77
38	8	502	LUT	C20-C13-C12	2.19	121.53	118.08
22	B	1213	CLA	C1D-ND-C4D	-2.19	104.78	106.33
22	7	611	CLA	CAC-C3C-C2C	-2.19	123.79	127.53
22	A	1129	CLA	CMB-C2B-C3B	2.19	128.77	124.68
22	A	1137	CLA	CHA-C1A-NA	-2.19	121.39	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	5	601	CLA	C6-C5-C3	-2.19	107.72	113.45
22	4	615	CLA	CMD-C2D-C3D	-2.19	122.59	127.61
22	6	603	CLA	CAA-C2A-C1A	-2.19	104.81	111.97
22	5	616	CLA	C1D-ND-C4D	-2.18	104.78	106.33
22	K	1402	CLA	O1D-CGD-CBD	-2.18	120.02	124.48
22	a	604	CLA	C1C-C2C-C3C	-2.18	104.66	106.96
22	B	1218	CLA	CMB-C2B-C3B	2.18	128.76	124.68
22	B	1202	CLA	C11-C12-C13	-2.18	108.86	115.92
22	B	1236	CLA	CHA-C1A-NA	-2.18	121.40	126.40
22	6	607	CLA	O2A-CGA-CBA	2.18	118.76	111.91
22	B	1224	CLA	CMB-C2B-C3B	2.18	128.76	124.68
22	7	602	CLA	CMD-C2D-C3D	-2.18	122.59	127.61
22	A	1130	CLA	O2A-CGA-CBA	2.18	118.75	111.91
22	B	1023	CLA	CHA-C1A-NA	-2.18	121.40	126.40
22	1	607	CLA	CHA-C1A-NA	-2.18	121.40	126.40
22	7	612	CLA	CHA-C1A-NA	-2.18	121.40	126.40
39	3	608	CHL	CMB-C2B-C1B	-2.18	125.11	128.46
22	B	1231	CLA	C2D-C1D-ND	2.18	111.71	110.10
22	7	601	CLA	CMD-C2D-C3D	-2.18	122.60	127.61
24	A	4005	BCR	C38-C26-C25	-2.18	122.08	124.53
22	8	615	CLA	CMA-C3A-C4A	2.18	117.63	111.77
22	a	612	CLA	CMA-C3A-C4A	2.18	117.63	111.77
22	B	1221	CLA	C3D-C2D-C1D	-2.18	102.86	105.83
24	8	503	BCR	C35-C13-C12	2.18	121.51	118.08
22	6	615	CLA	CMA-C3A-C4A	2.18	117.63	111.77
22	A	1121	CLA	CHA-C1A-NA	-2.18	121.41	126.40
22	5	605	CLA	CBC-CAC-C3C	-2.18	106.43	112.43
22	L	1503	CLA	C1D-ND-C4D	-2.18	104.79	106.33
22	K	1402	CLA	CMD-C2D-C3D	-2.18	122.61	127.61
22	3	605	CLA	CAA-CBA-CGA	-2.18	106.89	113.25
22	6	617	CLA	CMA-C3A-C4A	2.18	117.62	111.77
46	7	502	XAT	C35-C15-C14	-2.18	119.02	123.47
22	4	610	CLA	C2A-C1A-CHA	2.17	127.66	123.86
22	3	603	CLA	C1D-ND-C4D	-2.17	104.79	106.33
22	4	611	CLA	O2A-CGA-CBA	2.17	118.73	111.91
22	B	1021	CLA	C2A-C3A-C4A	2.17	105.38	101.87
22	6	618	CLA	CHA-C1A-NA	-2.17	121.42	126.40
24	B	4004	BCR	C31-C1-C6	-2.17	106.77	110.30
22	8	605	CLA	CMA-C3A-C4A	2.17	117.61	111.77
25	1	801	LHG	C5-O7-C7	-2.17	112.44	117.79
22	5	603	CLA	C1D-ND-C4D	-2.17	104.79	106.33
22	7	604	CLA	CHA-C1A-NA	-2.17	121.42	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	6	612	CLA	CMA-C3A-C4A	2.17	117.61	111.77
22	A	1112	CLA	O1D-CGD-CBD	-2.17	120.04	124.48
22	6	605	CLA	CHA-C1A-NA	-2.17	121.42	126.40
22	7	611	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
22	4	604	CLA	C1D-ND-C4D	-2.17	104.79	106.33
39	1	609	CHL	CHD-C4C-C3C	2.17	128.03	124.84
22	a	611	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
22	B	1215	CLA	O2A-CGA-CBA	2.17	118.72	111.91
22	A	1127	CLA	C1D-ND-C4D	-2.17	104.79	106.33
22	A	1012	CLA	CHA-C1A-NA	-2.17	121.43	126.40
39	6	610	CHL	C3A-C2A-C1A	2.17	104.59	101.34
39	6	610	CHL	CHB-C4A-NA	2.17	127.51	124.51
22	4	601	CLA	CHA-C1A-NA	-2.17	121.43	126.40
24	K	4001	BCR	C29-C28-C27	2.17	116.23	111.38
34	G	5002	ERG	C11-C12-C13	2.17	116.50	112.78
22	5	605	CLA	CHA-C1A-NA	-2.17	121.43	126.40
22	a	603	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
22	a	612	CLA	CHD-C1D-ND	-2.17	122.46	124.45
39	7	613	CHL	C3A-C2A-C1A	2.17	104.58	101.34
22	8	618	CLA	CMD-C2D-C3D	-2.17	122.63	127.61
22	3	601	CLA	CMC-C2C-C1C	2.17	128.34	125.04
22	A	1109	CLA	C2A-C1A-CHA	2.17	127.64	123.86
35	J	4002	RRX	C8-C7-C6	-2.16	121.12	127.20
22	5	604	CLA	C1-O2A-CGA	2.16	122.12	116.44
22	1	611	CLA	C6-C5-C3	-2.16	107.78	113.45
22	B	1021	CLA	CHA-C1A-NA	-2.16	121.44	126.40
22	B	1211	CLA	CMB-C2B-C1B	-2.16	125.14	128.46
22	A	1104	CLA	C1D-ND-C4D	-2.16	104.80	106.33
22	1	610	CLA	CHA-C1A-NA	-2.16	121.45	126.40
22	B	1230	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
24	8	503	BCR	C38-C26-C25	-2.16	122.10	124.53
22	6	601	CLA	CHA-C1A-NA	-2.16	121.45	126.40
22	A	1103	CLA	C1C-C2C-C3C	-2.16	104.69	106.96
22	A	1123	CLA	CHA-C1A-NA	-2.16	121.45	126.40
22	3	610	CLA	CHA-C1A-NA	-2.16	121.45	126.40
24	5	503	BCR	C3-C4-C5	-2.16	110.22	114.08
22	A	1109	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
22	A	1136	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
22	B	1207	CLA	C1D-ND-C4D	-2.16	104.80	106.33
38	5	501	LUT	C8-C7-C6	-2.16	121.14	127.20
24	A	4001	BCR	C33-C5-C4	2.16	117.76	113.62
22	4	617	CLA	O2D-CGD-O1D	-2.16	119.62	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	3	611	CHL	CHC-C1C-NC	2.16	127.48	124.20
22	7	609	CLA	C3D-C2D-C1D	-2.16	102.89	105.83
39	5	611	CHL	CHB-C4A-NA	2.16	127.49	124.51
22	B	1211	CLA	O1D-CGD-CBD	-2.16	120.07	124.48
22	5	607	CLA	CHA-C1A-NA	-2.16	121.46	126.40
22	4	610	CLA	OBD-CAD-C3D	-2.16	123.33	128.52
24	4	503	BCR	C31-C1-C6	-2.16	106.80	110.30
22	5	601	CLA	CHA-C1A-NA	-2.15	121.46	126.40
22	3	612	CLA	C2D-C1D-ND	2.15	111.69	110.10
22	6	606	CLA	CMD-C2D-C3D	-2.15	122.66	127.61
22	B	1207	CLA	CHA-C1A-NA	-2.15	121.47	126.40
22	8	602	CLA	CHA-C1A-NA	-2.15	121.47	126.40
22	8	605	CLA	CMD-C2D-C3D	-2.15	122.66	127.61
22	8	606	CLA	CMB-C2B-C3B	2.15	128.71	124.68
22	A	1134	CLA	O2A-CGA-CBA	2.15	118.67	111.91
22	B	1231	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
22	A	1137	CLA	C1D-ND-C4D	-2.15	104.81	106.33
22	6	608	CLA	C1D-ND-C4D	-2.15	104.81	106.33
22	7	610	CLA	CMD-C2D-C3D	-2.15	122.66	127.61
22	1	606	CLA	C2D-C1D-ND	2.15	111.69	110.10
22	3	604	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
22	3	601	CLA	O2A-CGA-CBA	2.15	118.67	111.91
22	A	1119	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
48	7	504	C7Z	C40-C33-C32	2.15	121.47	118.08
22	1	601	CLA	C2C-C1C-NC	2.15	111.99	109.97
22	B	1023	CLA	C1-O2A-CGA	2.15	122.09	116.44
22	6	615	CLA	CHA-C1A-NA	-2.15	121.47	126.40
22	B	1204	CLA	CMA-C3A-C4A	2.15	117.56	111.77
22	a	615	CLA	CMA-C3A-C4A	2.15	117.55	111.77
22	8	605	CLA	CHA-C1A-NA	-2.15	121.47	126.40
22	7	615	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
22	1	611	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
22	B	1239	CLA	C1D-ND-C4D	-2.15	104.81	106.33
23	B	2002	PQN	C16-C15-C13	-2.15	107.82	113.45
22	4	604	CLA	CMB-C2B-C3B	2.15	128.70	124.68
22	6	602	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
38	7	501	LUT	C10-C11-C12	-2.15	116.52	123.22
22	4	606	CLA	CMB-C2B-C3B	2.15	128.69	124.68
22	6	608	CLA	CMA-C3A-C4A	2.15	117.54	111.77
24	A	4003	BCR	C36-C18-C17	-2.15	119.92	122.92
22	A	1105	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
22	F	1302	CLA	CHA-C1A-NA	-2.15	121.48	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1116	CLA	CMB-C2B-C1B	-2.15	125.17	128.46
22	3	616	CLA	CHA-C1A-NA	-2.14	121.49	126.40
38	4	501	LUT	C8-C7-C6	-2.14	121.18	127.20
22	B	1237	CLA	CMD-C2D-C3D	-2.14	122.68	127.61
22	7	610	CLA	CAA-C2A-C3A	-2.14	106.91	112.78
22	A	1104	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
22	3	604	CLA	OBD-CAD-C3D	-2.14	123.36	128.52
22	7	617	CLA	CHA-C1A-NA	-2.14	121.49	126.40
22	B	1205	CLA	CAA-C2A-C3A	-2.14	106.91	112.78
22	A	1131	CLA	CMB-C2B-C3B	2.14	128.69	124.68
22	A	1133	CLA	O1D-CGD-CBD	-2.14	120.10	124.48
24	5	503	BCR	C38-C26-C25	-2.14	122.12	124.53
22	A	1131	CLA	C2D-C1D-ND	2.14	111.68	110.10
22	A	1135	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
22	B	1203	CLA	C2C-C1C-NC	2.14	111.98	109.97
22	8	610	CLA	C1-O2A-CGA	2.14	122.06	116.44
22	a	607	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
22	3	602	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
22	B	1206	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
22	1	608	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
22	8	608	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
22	1	615	CLA	CHA-C1A-NA	-2.14	121.50	126.40
39	4	613	CHL	CMB-C2B-C1B	-2.14	125.18	128.46
22	B	1234	CLA	O1A-CGA-CBA	-2.14	115.39	123.73
22	B	1227	CLA	CMA-C3A-C4A	2.14	117.52	111.77
22	4	605	CLA	CMA-C3A-C4A	2.14	117.52	111.77
24	K	4001	BCR	C37-C22-C21	-2.14	119.93	122.92
22	B	1201	CLA	CMD-C2D-C3D	-2.14	122.70	127.61
22	4	601	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
22	A	1132	CLA	C1D-ND-C4D	-2.14	104.82	106.33
22	3	618	CLA	C1D-ND-C4D	-2.14	104.82	106.33
22	6	605	CLA	CMD-C2D-C3D	-2.14	122.70	127.61
22	B	1234	CLA	C3D-C2D-C1D	-2.14	102.92	105.83
22	F	1302	CLA	CMD-C2D-C3D	-2.14	122.70	127.61
22	5	608	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
22	B	1217	CLA	CMD-C2D-C3D	-2.13	122.70	127.61
22	B	1229	CLA	CMD-C2D-C3D	-2.13	122.70	127.61
22	a	611	CLA	CHA-C1A-NA	-2.13	121.51	126.40
22	5	616	CLA	CHA-C1A-NA	-2.13	121.51	126.40
24	I	4001	BCR	C33-C5-C6	-2.13	122.13	124.53
38	6	502	LUT	C19-C9-C10	-2.13	119.94	122.92
22	4	604	CLA	CMC-C2C-C1C	2.13	128.29	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	8	608	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
22	B	1239	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
25	B	5001	LHG	C5-O7-C7	-2.13	112.54	117.79
22	1	612	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
22	1	611	CLA	CHA-C1A-NA	-2.13	121.52	126.40
22	A	1112	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
22	3	607	CLA	CHA-C1A-NA	-2.13	121.52	126.40
22	3	606	CLA	C1D-ND-C4D	-2.13	104.82	106.33
22	6	606	CLA	C1D-ND-C4D	-2.13	104.82	106.33
24	J	4001	BCR	C31-C1-C6	-2.13	106.84	110.30
22	6	618	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
37	M	4001	ECH	C20-C19-C18	-2.13	120.44	126.42
22	B	1205	CLA	CMA-C3A-C4A	2.13	117.49	111.77
22	4	605	CLA	CHA-C1A-NA	-2.13	121.53	126.40
22	A	1013	CLA	C1-O2A-CGA	2.13	122.03	116.44
22	4	606	CLA	CAA-C2A-C3A	-2.13	106.95	112.78
22	B	1227	CLA	CHA-C1A-NA	-2.13	121.53	126.40
22	L	1501	CLA	C3D-C2D-C1D	-2.13	102.93	105.83
22	A	1119	CLA	C1D-ND-C4D	-2.13	104.82	106.33
22	a	611	CLA	C1D-ND-C4D	-2.13	104.82	106.33
22	6	615	CLA	C1D-ND-C4D	-2.13	104.82	106.33
22	7	606	CLA	O2A-CGA-CBA	2.13	118.58	111.91
39	a	613	CHL	CHB-C4A-NA	2.13	127.45	124.51
22	6	604	CLA	CHD-C4C-C3C	2.13	127.97	124.84
38	8	502	LUT	C15-C14-C13	-2.13	124.28	127.31
22	B	1207	CLA	C3D-C2D-C1D	-2.13	102.93	105.83
22	3	607	CLA	C3D-C2D-C1D	-2.13	102.93	105.83
22	A	1129	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
22	B	1237	CLA	O2A-CGA-CBA	2.13	118.58	111.91
24	3	504	BCR	C15-C14-C13	-2.13	124.28	127.31
22	7	606	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
22	4	602	CLA	O2A-CGA-CBA	2.12	118.58	111.91
22	6	601	CLA	CMD-C2D-C3D	-2.12	122.73	127.61
39	7	613	CHL	CMB-C2B-C1B	-2.12	125.20	128.46
22	B	1229	CLA	O2A-CGA-CBA	2.12	118.57	111.91
22	G	1601	CLA	CMD-C2D-C3D	-2.12	122.73	127.61
22	A	1116	CLA	CHA-C1A-NA	-2.12	121.53	126.40
24	A	4001	BCR	C31-C1-C6	-2.12	106.86	110.30
48	7	504	C7Z	C19-C9-C10	-2.12	119.95	122.92
25	F	5002	LHG	O8-C6-C5	2.12	114.61	108.43
39	8	604	CHL	CMB-C2B-C1B	-2.12	125.20	128.46
22	5	618	CLA	O2D-CGD-O1D	-2.12	119.69	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1117	CLA	O2A-CGA-CBA	2.12	118.57	111.91
22	B	1022	CLA	CMA-C3A-C4A	2.12	117.47	111.77
39	5	613	CHL	C1B-CHB-C4A	-2.12	125.92	130.12
22	1	606	CLA	C1-O2A-CGA	2.12	122.01	116.44
22	5	601	CLA	O1D-CGD-CBD	-2.12	120.15	124.48
22	A	1115	CLA	C1D-ND-C4D	-2.12	104.83	106.33
22	7	606	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
22	3	605	CLA	CAA-C2A-C1A	-2.12	105.03	111.97
22	6	608	CLA	O1D-CGD-CBD	-2.12	120.15	124.48
22	6	606	CLA	CHA-C1A-NA	-2.12	121.54	126.40
29	A	5008	LMT	O5'-C5'-C4'	2.12	114.22	109.75
38	1	501	LUT	C30-C31-C32	-2.12	116.60	123.22
24	5	504	BCR	C4-C5-C6	-2.12	119.66	122.73
22	8	620	CLA	O2D-CGD-O1D	-2.12	119.70	123.84
22	G	1602	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
25	a	801	LHG	C5-O7-C7	-2.12	112.58	117.79
35	J	4002	RRX	C24-C23-C22	-2.12	123.04	126.23
22	1	603	CLA	C1-O2A-CGA	2.12	122.00	116.44
22	A	1113	CLA	C1D-ND-C4D	-2.12	104.83	106.33
22	B	1209	CLA	CMD-C2D-C3D	-2.12	122.75	127.61
22	A	1132	CLA	O2A-CGA-CBA	2.12	118.55	111.91
22	A	1101	CLA	C3D-C2D-C1D	-2.11	102.94	105.83
22	B	1218	CLA	C3D-C2D-C1D	-2.11	102.94	105.83
22	K	1401	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
39	a	606	CHL	CHC-C1C-NC	2.11	127.41	124.20
22	B	1232	CLA	O2D-CGD-O1D	-2.11	119.70	123.84
22	a	612	CLA	CMB-C2B-C3B	2.11	128.63	124.68
22	7	604	CLA	O2D-CGD-O1D	-2.11	119.70	123.84
38	1	503	LUT	C38-C25-C24	-2.11	119.04	123.56
24	8	503	BCR	C30-C25-C24	2.11	121.76	115.78
22	A	1135	CLA	CMA-C3A-C4A	2.11	117.45	111.77
22	7	601	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
26	A	5005	DGD	C3G-C2G-C1G	-2.11	106.79	111.79
24	5	503	BCR	C27-C26-C25	-2.11	119.67	122.73
39	1	613	CHL	C1-O2A-CGA	2.11	122.86	116.73
22	A	1110	CLA	C1D-ND-C4D	-2.11	104.83	106.33
22	A	1109	CLA	C6-C7-C8	-2.11	109.09	115.92
38	8	501	LUT	C15-C35-C34	-2.11	119.15	123.47
22	4	602	CLA	CMD-C2D-C3D	-2.11	122.76	127.61
22	a	608	CLA	CMD-C2D-C3D	-2.11	122.76	127.61
22	A	1115	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
22	B	1212	CLA	CHA-C1A-NA	-2.11	121.56	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1238	CLA	CHA-C1A-NA	-2.11	121.56	126.40
39	8	613	CHL	C1-O2A-CGA	2.11	121.98	116.44
39	a	606	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
22	7	611	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
22	5	609	CLA	O2A-CGA-CBA	2.11	118.53	111.91
22	4	616	CLA	O2D-CGD-O1D	-2.11	119.72	123.84
22	A	1119	CLA	CMD-C2D-C3D	-2.11	122.76	127.61
22	8	607	CLA	CAA-C2A-C3A	-2.11	107.01	112.78
22	A	1124	CLA	CAA-C2A-C1A	-2.11	105.07	111.97
22	B	1215	CLA	C1D-ND-C4D	-2.11	104.84	106.33
22	G	1602	CLA	CHA-C1A-NA	-2.11	121.57	126.40
22	B	1230	CLA	C1C-C2C-C3C	-2.11	104.74	106.96
24	L	4001	BCR	C23-C22-C21	2.11	122.17	118.94
22	4	605	CLA	C3D-C2D-C1D	-2.11	102.96	105.83
22	A	1121	CLA	CMB-C2B-C3B	2.11	128.62	124.68
39	7	613	CHL	CHD-C4C-C3C	2.11	127.94	124.84
22	3	612	CLA	CHA-C1A-NA	-2.11	121.58	126.40
22	7	610	CLA	C1D-ND-C4D	-2.11	104.84	106.33
22	A	1140	CLA	CHA-C1A-NA	-2.11	121.58	126.40
22	5	617	CLA	CHA-C1A-NA	-2.11	121.58	126.40
22	B	1216	CLA	CMD-C2D-C3D	-2.10	122.77	127.61
39	5	611	CHL	C1-O2A-CGA	2.10	121.97	116.44
22	A	1113	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
22	3	616	CLA	C1D-ND-C4D	-2.10	104.84	106.33
38	5	501	LUT	C30-C31-C32	-2.10	116.65	123.22
39	a	610	CHL	CHC-C1C-NC	2.10	127.39	124.20
22	B	1239	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
22	F	1301	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
22	B	1218	CLA	CHA-C1A-NA	-2.10	121.58	126.40
22	B	1201	CLA	C1D-ND-C4D	-2.10	104.84	106.33
22	A	1129	CLA	CMA-C3A-C4A	2.10	117.42	111.77
22	B	1235	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
38	a	501	LUT	C15-C35-C34	-2.10	119.17	123.47
22	A	1013	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
22	B	1216	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
22	B	1240	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
22	B	1212	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
39	a	610	CHL	CMB-C2B-C1B	-2.10	125.23	128.46
22	K	1404	CLA	OBD-CAD-C3D	-2.10	123.46	128.52
24	B	4005	BCR	C36-C18-C17	-2.10	119.98	122.92
22	6	602	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
39	5	611	CHL	CHD-C4C-C3C	2.10	127.93	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1137	CLA	CMA-C3A-C4A	2.10	117.42	111.77
22	A	1129	CLA	CHA-C1A-NA	-2.10	121.59	126.40
22	4	608	CLA	C1D-ND-C4D	-2.10	104.84	106.33
39	4	609	CHL	CMB-C2B-C1B	-2.10	125.24	128.46
22	8	610	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
22	1	604	CLA	CHC-C1C-NC	-2.10	121.02	124.20
39	4	618	CHL	CHC-C1C-NC	2.10	127.39	124.20
22	A	1120	CLA	CMC-C2C-C1C	2.10	128.24	125.04
39	5	610	CHL	CMB-C2B-C1B	-2.10	125.24	128.46
22	L	1503	CLA	CBC-CAC-C3C	2.10	118.22	112.43
22	a	601	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
22	A	1106	CLA	CAC-C3C-C4C	2.10	127.53	124.81
22	7	604	CLA	CAC-C3C-C4C	2.10	127.53	124.81
22	B	1234	CLA	C1-O2A-CGA	2.10	121.95	116.44
22	7	602	CLA	CHA-C1A-NA	-2.10	121.59	126.40
22	7	604	CLA	C1C-C2C-C3C	-2.10	104.75	106.96
22	B	1228	CLA	C6-C5-C3	-2.10	107.95	113.45
39	6	613	CHL	CHD-C4C-C3C	2.10	127.92	124.84
22	B	1213	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
22	a	603	CLA	CAC-C3C-C4C	2.10	127.53	124.81
39	5	611	CHL	CMB-C2B-C1B	-2.10	125.24	128.46
38	a	503	LUT	C18-C5-C4	2.10	118.24	114.36
22	5	601	CLA	CMB-C2B-C3B	2.10	128.60	124.68
22	3	601	CLA	C1D-ND-C4D	-2.10	104.85	106.33
38	a	502	LUT	C11-C12-C13	-2.10	120.53	126.42
22	7	605	CLA	CHD-C1D-ND	-2.10	122.53	124.45
22	3	602	CLA	O1D-CGD-CBD	-2.10	120.20	124.48
22	4	616	CLA	CHA-C1A-NA	-2.10	121.60	126.40
22	5	618	CLA	O2A-CGA-CBA	2.09	118.48	111.91
39	6	611	CHL	CMB-C2B-C1B	-2.09	125.25	128.46
22	7	612	CLA	CHD-C4C-C3C	2.09	127.92	124.84
22	6	607	CLA	CHA-C1A-NA	-2.09	121.60	126.40
22	B	1208	CLA	C1-C2-C3	-2.09	122.42	126.04
22	A	1013	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
22	6	606	CLA	O2A-CGA-CBA	2.09	118.47	111.91
22	G	1601	CLA	O2A-CGA-CBA	2.09	118.47	111.91
22	G	1601	CLA	CHA-C1A-NA	-2.09	121.61	126.40
22	A	1126	CLA	CHA-C1A-NA	-2.09	121.61	126.40
22	B	1230	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
22	a	602	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
22	5	601	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
22	A	1117	CLA	C2D-C1D-ND	2.09	111.64	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	a	504	QTB	C13-C12-C14	2.09	114.87	111.04
22	B	1218	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
24	3	503	BCR	C23-C22-C21	-2.09	115.73	118.94
22	L	1503	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
22	B	1216	CLA	CMB-C2B-C3B	2.09	128.59	124.68
22	8	606	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
22	B	1215	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
22	A	1013	CLA	C2C-C1C-NC	2.09	111.93	109.97
22	3	613	CLA	CHA-C1A-NA	-2.09	121.61	126.40
22	5	618	CLA	CHA-C1A-NA	-2.09	121.61	126.40
22	A	1137	CLA	CAA-CBA-CGA	-2.09	107.15	113.25
22	B	1205	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
22	A	1137	CLA	C6-C5-C3	-2.09	107.98	113.45
22	5	618	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
22	B	1238	CLA	CMB-C2B-C3B	2.09	128.59	124.68
22	A	1112	CLA	CMB-C2B-C1B	-2.09	125.26	128.46
22	7	601	CLA	C1C-C2C-C3C	-2.09	104.76	106.96
22	3	610	CLA	O2A-CGA-CBA	2.09	118.46	111.91
22	4	610	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
22	A	1133	CLA	O2A-CGA-CBA	2.09	118.46	111.91
22	A	1135	CLA	CHA-C1A-NA	-2.09	121.62	126.40
22	A	1134	CLA	C1D-ND-C4D	-2.09	104.85	106.33
22	6	615	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
25	1	802	LHG	O7-C7-O9	-2.09	118.66	123.70
39	1	613	CHL	CHD-C4C-C3C	2.09	127.91	124.84
22	7	610	CLA	CHA-C1A-NA	-2.09	121.62	126.40
22	1	615	CLA	C1D-ND-C4D	-2.08	104.85	106.33
22	B	1201	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
22	6	609	CLA	CHD-C1D-ND	-2.08	122.54	124.45
22	A	1132	CLA	C1-O2A-CGA	2.08	121.91	116.44
22	7	607	CLA	C2D-C1D-ND	2.08	111.64	110.10
22	6	612	CLA	O2A-CGA-CBA	2.08	118.44	111.91
22	A	1130	CLA	C1D-ND-C4D	-2.08	104.86	106.33
22	B	1229	CLA	CHA-C1A-NA	-2.08	121.63	126.40
22	A	1128	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
22	8	603	CLA	CAA-C2A-C3A	-2.08	107.08	112.78
22	3	606	CLA	O2A-CGA-CBA	2.08	118.44	111.91
22	B	1213	CLA	CAA-C2A-C3A	-2.08	107.08	112.78
22	8	618	CLA	CHA-C1A-NA	-2.08	121.63	126.40
22	A	1139	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
22	A	1106	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
22	A	1135	CLA	C3D-C2D-C1D	-2.08	102.99	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	6	607	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
24	B	4005	BCR	C34-C9-C10	-2.08	120.01	122.92
34	G	5002	ERG	C18-C13-C17	-2.08	107.83	111.71
22	7	609	CLA	CAA-CBA-CGA	-2.08	107.18	113.25
22	1	607	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
25	4	801	LHG	C5-O7-C7	-2.08	112.67	117.79
22	4	615	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
25	6	801	LHG	C5-O7-C7	-2.08	112.68	117.79
39	8	601	CHL	CMB-C2B-C1B	-2.08	125.27	128.46
38	1	501	LUT	C31-C30-C29	-2.08	124.35	127.31
24	L	4002	BCR	C37-C22-C23	2.08	121.35	118.08
22	B	1236	CLA	OBD-CAD-C3D	-2.08	123.52	128.52
22	3	601	CLA	C3D-C2D-C1D	-2.08	103.00	105.83
22	B	1211	CLA	CMA-C3A-C4A	2.08	117.35	111.77
39	5	613	CHL	CHB-C4A-NA	2.08	127.38	124.51
39	a	613	CHL	CHC-C1C-NC	2.07	127.35	124.20
38	6	501	LUT	C11-C12-C13	-2.07	120.59	126.42
38	a	503	LUT	C10-C11-C12	-2.07	116.75	123.22
22	a	602	CLA	C1D-ND-C4D	-2.07	104.86	106.33
39	4	618	CHL	CMB-C2B-C1B	-2.07	125.28	128.46
22	A	1134	CLA	CHA-C1A-NA	-2.07	121.65	126.40
24	A	4002	BCR	C27-C26-C25	-2.07	119.72	122.73
22	3	616	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
22	4	608	CLA	CHA-C1A-NA	-2.07	121.65	126.40
22	A	1105	CLA	CMC-C2C-C1C	2.07	128.19	125.04
38	1	501	LUT	C18-C5-C4	2.07	118.19	114.36
22	B	1217	CLA	CHA-C1A-NA	-2.07	121.66	126.40
22	8	615	CLA	CHA-C1A-NA	-2.07	121.66	126.40
38	7	501	LUT	C18-C5-C4	2.07	118.19	114.36
38	8	501	LUT	C11-C10-C9	-2.07	124.36	127.31
39	a	613	CHL	CMB-C2B-C1B	-2.07	125.28	128.46
22	8	602	CLA	OBD-CAD-C3D	-2.07	123.54	128.52
38	3	502	LUT	C38-C25-C24	-2.07	119.13	123.56
22	4	612	CLA	CHA-C1A-NA	-2.07	121.66	126.40
24	6	504	BCR	C23-C24-C25	-2.07	121.39	127.20
22	3	602	CLA	CMA-C3A-C4A	2.07	117.33	111.77
22	B	1211	CLA	C1D-ND-C4D	-2.07	104.87	106.33
22	a	604	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
22	a	605	CLA	CMB-C2B-C1B	-2.07	125.29	128.46
22	L	1502	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
22	1	610	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
24	B	4007	BCR	C37-C22-C23	2.07	121.33	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	501	LUT	C39-C29-C28	2.07	121.33	118.08
22	A	1104	CLA	CHA-C1A-NA	-2.07	121.66	126.40
22	B	1225	CLA	CHA-C1A-NA	-2.07	121.66	126.40
22	4	612	CLA	O2A-CGA-CBA	2.07	118.39	111.91
22	B	1203	CLA	O2A-CGA-CBA	2.07	118.39	111.91
22	B	1224	CLA	CHA-C1A-NA	-2.07	121.67	126.40
22	A	1120	CLA	O2A-CGA-CBA	2.07	118.39	111.91
22	7	609	CLA	C1-O2A-CGA	2.07	121.86	116.44
39	8	613	CHL	CMB-C2B-C1B	-2.07	125.29	128.46
22	B	1240	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
22	5	604	CLA	OBD-CAD-C3D	-2.07	123.55	128.52
38	6	501	LUT	C2-C3-C4	-2.07	107.48	110.30
22	A	1124	CLA	CMB-C2B-C3B	2.06	128.54	124.68
22	1	611	CLA	O2A-CGA-CBA	2.06	118.38	111.91
22	a	604	CLA	C3A-C2A-C1A	2.06	104.43	101.34
22	L	1502	CLA	CAA-C2A-C3A	-2.06	107.13	112.78
22	4	611	CLA	CHA-C1A-NA	-2.06	121.67	126.40
22	7	607	CLA	CHA-C1A-NA	-2.06	121.68	126.40
39	a	609	CHL	CMB-C2B-C1B	-2.06	125.30	128.46
22	5	606	CLA	CAA-C2A-C3A	-2.06	107.13	112.78
24	3	503	BCR	C29-C28-C27	2.06	115.98	111.38
22	A	1104	CLA	CBC-CAC-C3C	-2.06	106.75	112.43
22	8	603	CLA	C1D-ND-C4D	-2.06	104.87	106.33
22	5	602	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
39	3	611	CHL	CMB-C2B-C1B	-2.06	125.30	128.46
22	7	610	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
22	B	1213	CLA	C2C-C1C-NC	2.06	111.90	109.97
22	a	615	CLA	CHA-C1A-NA	-2.06	121.68	126.40
22	8	620	CLA	CMD-C2D-C3D	-2.06	122.88	127.61
24	B	4006	BCR	C19-C18-C17	2.06	122.10	118.94
22	B	1237	CLA	CAC-C3C-C4C	2.06	127.48	124.81
22	4	603	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
22	K	1404	CLA	C1D-ND-C4D	-2.06	104.87	106.33
22	5	618	CLA	CMD-C2D-C3D	-2.06	122.88	127.61
22	4	605	CLA	CMD-C2D-C3D	-2.06	122.88	127.61
39	3	611	CHL	CHB-C4A-NA	2.06	127.36	124.51
22	1	603	CLA	CAA-C2A-C3A	-2.06	107.15	112.78
22	7	604	CLA	C3D-C2D-C1D	-2.06	103.03	105.83
22	A	1115	CLA	O1D-CGD-CBD	-2.06	120.28	124.48
22	A	1139	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
22	A	1113	CLA	CMB-C2B-C1B	-2.05	125.31	128.46
22	A	1136	CLA	C1D-ND-C4D	-2.05	104.88	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	4004	BCR	C39-C30-C25	-2.05	106.97	110.30
22	4	615	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
22	B	1220	CLA	O1D-CGD-CBD	-2.05	120.28	124.48
22	B	1230	CLA	CMB-C2B-C3B	2.05	128.52	124.68
22	A	1114	CLA	C1D-ND-C4D	-2.05	104.88	106.33
22	4	601	CLA	C1D-ND-C4D	-2.05	104.88	106.33
22	a	608	CLA	O2A-CGA-CBA	2.05	118.34	111.91
22	B	1229	CLA	C1D-ND-C4D	-2.05	104.88	106.33
22	6	608	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
24	5	503	BCR	C4-C5-C6	-2.05	119.75	122.73
22	K	1404	CLA	CMD-C2D-C3D	-2.05	122.90	127.61
22	A	1127	CLA	CHA-C1A-NA	-2.05	121.70	126.40
37	M	4001	ECH	O27-C27-C26	2.05	122.78	120.96
21	A	1011	CL0	CMD-C2D-C3D	-2.05	122.91	127.61
24	L	4002	BCR	C38-C26-C27	2.05	117.55	113.62
22	A	1138	CLA	CMD-C2D-C3D	-2.05	122.91	127.61
22	A	1111	CLA	CHA-C1A-NA	-2.05	121.71	126.40
21	A	1011	CL0	CHC-C1C-C2C	-2.05	121.06	126.72
22	B	1223	CLA	C1D-ND-C4D	-2.05	104.88	106.33
22	B	1022	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
22	A	1117	CLA	CMD-C2D-C3D	-2.04	122.91	127.61
22	4	605	CLA	O1D-CGD-CBD	-2.04	120.30	124.48
22	A	1139	CLA	CHA-C1A-NA	-2.04	121.72	126.40
39	a	606	CHL	C4A-NA-C1A	2.04	107.62	106.71
22	4	612	CLA	CMB-C2B-C1B	-2.04	125.32	128.46
22	3	613	CLA	CMD-C2D-C3D	-2.04	122.91	127.61
22	A	1013	CLA	O2D-CGD-O1D	-2.04	119.84	123.84
22	1	606	CLA	CAA-CBA-CGA	-2.04	107.28	113.25
39	7	613	CHL	CMA-C3A-C4A	2.04	117.26	111.77
22	a	611	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
24	7	503	BCR	C38-C26-C27	2.04	117.54	113.62
33	7	805	SQD	O8-S-C6	-2.04	102.48	105.74
22	7	612	CLA	O2A-CGA-CBA	2.04	118.32	111.91
22	1	605	CLA	CBC-CAC-C3C	-2.04	106.80	112.43
22	B	1023	CLA	C2C-C1C-NC	2.04	111.89	109.97
22	L	1503	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
22	A	1111	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
24	B	4006	BCR	C4-C5-C6	-2.04	119.77	122.73
22	3	613	CLA	O2A-CGA-CBA	2.04	118.31	111.91
22	1	611	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
22	A	1110	CLA	CHA-C1A-NA	-2.04	121.72	126.40
22	8	615	CLA	O1D-CGD-CBD	-2.04	120.31	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1219	CLA	O2A-CGA-CBA	2.04	118.31	111.91
22	8	610	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
39	3	608	CHL	C1B-CHB-C4A	-2.04	126.08	130.12
22	A	1133	CLA	C1-O2A-CGA	2.04	121.80	116.44
22	G	1603	CLA	CHA-C1A-NA	-2.04	121.73	126.40
24	A	4001	BCR	C2-C1-C6	2.04	113.62	110.48
24	B	4007	BCR	C15-C14-C13	-2.04	124.40	127.31
22	5	602	CLA	CMD-C2D-C3D	-2.04	122.92	127.61
24	B	4003	BCR	C4-C5-C6	-2.04	119.77	122.73
22	A	1118	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
22	3	604	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
22	B	1237	CLA	C1C-C2C-C3C	-2.04	104.81	106.96
22	1	612	CLA	C1D-ND-C4D	-2.04	104.89	106.33
22	B	1208	CLA	O2A-CGA-CBA	2.04	118.30	111.91
22	A	1118	CLA	CHA-C1A-NA	-2.04	121.73	126.40
22	5	606	CLA	CHA-C1A-NA	-2.04	121.73	126.40
22	3	605	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
22	3	602	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
22	5	602	CLA	C1-O2A-CGA	2.04	121.79	116.44
38	4	501	LUT	C20-C13-C12	2.04	121.29	118.08
22	B	1023	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
22	8	606	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
38	7	501	LUT	C38-C25-C24	-2.04	119.20	123.56
22	6	617	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
22	a	608	CLA	CHA-C1A-NA	-2.04	121.74	126.40
22	1	605	CLA	CMB-C2B-C1B	-2.03	125.34	128.46
24	L	4002	BCR	C34-C9-C8	2.03	121.28	118.08
24	I	4001	BCR	C30-C25-C26	-2.03	119.75	122.61
22	A	1114	CLA	C1-O2A-CGA	2.03	121.78	116.44
24	K	4001	BCR	C38-C26-C25	-2.03	122.25	124.53
22	B	1236	CLA	CAC-C3C-C2C	-2.03	124.05	127.53
22	6	604	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
22	8	609	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
22	A	1114	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
22	A	1128	CLA	CMD-C2D-C3D	-2.03	122.94	127.61
22	8	618	CLA	CAC-C3C-C2C	-2.03	124.05	127.53
22	B	1204	CLA	C1D-ND-C4D	-2.03	104.89	106.33
22	B	1229	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
22	8	610	CLA	CMD-C2D-C3D	-2.03	122.94	127.61
22	a	604	CLA	CAC-C3C-C4C	2.03	127.44	124.81
22	8	606	CLA	C1-O2A-CGA	2.03	121.77	116.44
22	B	1224	CLA	CAA-C2A-C3A	-2.03	107.22	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1136	CLA	C1-O2A-CGA	2.03	121.77	116.44
22	a	602	CLA	CMD-C2D-C3D	-2.03	122.94	127.61
22	A	1111	CLA	CMA-C3A-C4A	2.03	117.23	111.77
38	4	501	LUT	C18-C5-C4	2.03	118.11	114.36
22	4	606	CLA	CHA-C1A-NA	-2.03	121.75	126.40
22	8	618	CLA	C2D-C1D-ND	2.03	111.60	110.10
22	A	1105	CLA	CHA-C1A-NA	-2.03	121.76	126.40
22	B	1203	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
38	1	503	LUT	C18-C5-C4	2.03	118.11	114.36
22	8	612	CLA	OBD-CAD-C3D	-2.03	123.64	128.52
22	A	1116	CLA	C3D-C2D-C1D	-2.03	103.07	105.83
22	A	1124	CLA	O1D-CGD-CBD	-2.03	120.34	124.48
22	A	1103	CLA	CMD-C2D-C3D	-2.02	122.96	127.61
22	A	1114	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
24	L	4003	BCR	C38-C26-C27	2.02	117.50	113.62
22	1	612	CLA	CMD-C2D-C3D	-2.02	122.96	127.61
22	a	615	CLA	O2D-CGD-O1D	-2.02	119.88	123.84
22	4	602	CLA	CHA-C1A-NA	-2.02	121.76	126.40
22	B	1237	CLA	C11-C10-C8	-2.02	109.38	115.92
25	F	5001	LHG	O7-C7-O9	-2.02	118.81	123.70
22	5	607	CLA	CMD-C2D-C3D	-2.02	122.96	127.61
39	1	609	CHL	CHA-C1A-NA	-2.02	121.77	126.40
22	a	615	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
22	4	604	CLA	CMD-C2D-C3D	-2.02	122.96	127.61
22	A	1141	CLA	CHA-C1A-NA	-2.02	121.77	126.40
22	B	1206	CLA	CAA-C2A-C3A	-2.02	107.24	112.78
22	1	604	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
22	B	1209	CLA	C16-C15-C13	-2.02	109.38	115.92
22	5	612	CLA	CHA-C1A-NA	-2.02	121.77	126.40
22	5	614	CLA	CMA-C3A-C4A	2.02	117.20	111.77
22	A	1120	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
22	a	603	CLA	C5-C3-C2	2.02	125.20	121.12
22	3	610	CLA	CMA-C3A-C4A	2.02	117.20	111.77
22	6	612	CLA	CHA-C1A-NA	-2.02	121.77	126.40
22	A	1103	CLA	CAA-C2A-C1A	-2.02	105.36	111.97
22	B	1223	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
24	B	4004	BCR	C4-C5-C6	-2.02	119.80	122.73
22	6	602	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
22	a	602	CLA	CHA-C1A-NA	-2.02	121.78	126.40
22	1	612	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
24	8	503	BCR	C3-C4-C5	-2.02	110.47	114.08
24	A	4004	BCR	C8-C7-C6	-2.02	121.53	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	4	615	CLA	CMB-C2B-C3B	2.02	128.45	124.68
22	G	1602	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
22	A	1130	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
22	A	1138	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
22	B	1216	CLA	CHA-C1A-NA	-2.02	121.78	126.40
22	5	605	CLA	C1D-ND-C4D	-2.02	104.90	106.33
22	A	1115	CLA	CHA-C1A-NA	-2.02	121.78	126.40
22	3	602	CLA	CHA-C1A-NA	-2.02	121.78	126.40
48	7	504	C7Z	C1-C2-C3	2.02	118.20	113.64
22	8	620	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
22	A	1105	CLA	CMD-C2D-C3D	-2.02	122.98	127.61
22	A	1013	CLA	CHA-C1A-NA	-2.02	121.78	126.40
22	A	1137	CLA	CMD-C2D-C3D	-2.02	122.98	127.61
22	A	1130	CLA	CHA-C1A-NA	-2.02	121.78	126.40
38	8	502	LUT	C19-C9-C8	2.02	121.25	118.08
22	A	1105	CLA	O2A-CGA-CBA	2.02	118.23	111.91
22	B	1023	CLA	CAA-C2A-C3A	-2.01	107.26	112.78
22	A	1133	CLA	CMD-C2D-C3D	-2.01	122.98	127.61
22	B	1227	CLA	O2A-CGA-CBA	2.01	118.23	111.91
24	B	4004	BCR	C38-C26-C27	2.01	117.48	113.62
22	7	612	CLA	CMA-C3A-C4A	2.01	117.19	111.77
39	3	611	CHL	C1-O2A-CGA	2.01	121.73	116.44
22	A	1140	CLA	CMC-C2C-C1C	2.01	128.10	125.04
22	B	1201	CLA	C16-C15-C13	-2.01	109.41	115.92
25	a	801	LHG	O7-C7-O9	-2.01	118.84	123.70
22	7	610	CLA	CMA-C3A-C4A	2.01	117.18	111.77
39	6	619	CHL	CHB-C4A-NA	2.01	127.30	124.51
22	B	1201	CLA	CHA-C1A-NA	-2.01	121.79	126.40
22	6	607	CLA	CMB-C2B-C3B	2.01	128.44	124.68
22	4	606	CLA	CMA-C3A-C4A	2.01	117.18	111.77
48	7	504	C7Z	C35-C34-C33	-2.01	124.44	127.31
22	G	1602	CLA	C1D-ND-C4D	-2.01	104.91	106.33
22	3	601	CLA	CMA-C3A-C4A	2.01	117.18	111.77
22	B	1224	CLA	CMD-C2D-C3D	-2.01	122.99	127.61
38	a	501	LUT	C11-C12-C13	-2.01	120.77	126.42
22	A	1141	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
22	4	612	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
22	6	601	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
22	A	1122	CLA	CMD-C2D-C3D	-2.01	122.99	127.61
22	8	612	CLA	CHA-C1A-NA	-2.01	121.79	126.40
22	A	1104	CLA	C1-O2A-CGA	2.01	121.72	116.44
22	A	1111	CLA	C1D-ND-C4D	-2.01	104.91	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	611	CLA	C1D-ND-C4D	-2.01	104.91	106.33
22	5	608	CLA	C1D-ND-C4D	-2.01	104.91	106.33
22	a	612	CLA	CHA-C1A-NA	-2.01	121.80	126.40
22	A	1120	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
38	8	501	LUT	C36-C21-C26	-2.01	106.50	109.55
22	B	1225	CLA	CMA-C3A-C4A	2.01	117.17	111.77
38	a	502	LUT	C15-C35-C34	-2.01	119.36	123.47
22	B	1208	CLA	CHA-C1A-NA	-2.01	121.80	126.40
22	A	1108	CLA	CAC-C3C-C4C	2.01	127.42	124.81
22	8	612	CLA	CMD-C2D-C3D	-2.01	123.00	127.61
38	5	502	LUT	C38-C25-C24	-2.01	119.26	123.56
22	4	606	CLA	O2A-CGA-CBA	2.01	118.20	111.91
22	1	605	CLA	OBD-CAD-C3D	-2.01	123.69	128.52
22	3	606	CLA	C1-O2A-CGA	2.01	121.71	116.44
24	J	4001	BCR	C37-C22-C21	-2.01	120.11	122.92
22	B	1214	CLA	CHA-C1A-NA	-2.01	121.80	126.40
22	A	1135	CLA	C1D-ND-C4D	-2.01	104.91	106.33
22	7	609	CLA	C1D-ND-C4D	-2.01	104.91	106.33
22	1	605	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
22	a	612	CLA	CMD-C2D-C3D	-2.01	123.00	127.61
38	7	501	LUT	C8-C7-C6	-2.01	121.57	127.20
22	B	1206	CLA	CBC-CAC-C3C	-2.01	106.90	112.43
22	7	605	CLA	CMB-C2B-C3B	2.00	128.43	124.68
45	6	806	SPH	C3-C4-C5	-2.00	120.32	124.79
22	A	1119	CLA	CHA-C1A-NA	-2.00	121.81	126.40
22	4	607	CLA	CAA-C2A-C3A	-2.00	107.29	112.78
22	B	1210	CLA	CAA-CBA-CGA	-2.00	107.40	113.25
22	7	610	CLA	O2D-CGD-O1D	-2.00	119.92	123.84
22	B	1021	CLA	O1D-CGD-CBD	-2.00	120.38	124.48
22	a	615	CLA	O1D-CGD-CBD	-2.00	120.38	124.48
22	B	1237	CLA	CMC-C2C-C1C	2.00	128.09	125.04
22	1	605	CLA	CAA-C2A-C1A	-2.00	105.41	111.97
22	5	601	CLA	O2D-CGD-O1D	-2.00	119.92	123.84
22	6	601	CLA	O2D-CGD-O1D	-2.00	119.92	123.84
22	B	1204	CLA	CAA-C2A-C3A	-2.00	107.30	112.78
25	8	801	LHG	O8-C23-O10	-2.00	118.54	123.59
22	1	604	CLA	C6-C5-C3	-2.00	108.20	113.45
22	A	1123	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
22	1	615	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
41	a	504	QTB	C16-C15-C14	2.00	114.64	111.38
23	A	2001	PQN	C12-C11-C3	-2.00	106.65	112.05
22	B	1215	CLA	O1D-CGD-CBD	-2.00	120.39	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	3	504	BCR	C23-C24-C25	-2.00	121.58	127.20
22	B	1213	CLA	CHA-C1A-NA	-2.00	121.82	126.40

All (299) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	A	1011	CL0	NA
21	A	1011	CL0	NC
21	A	1011	CL0	ND
22	A	1012	CLA	ND
22	A	1013	CLA	ND
22	A	1102	CLA	ND
22	A	1103	CLA	ND
22	A	1104	CLA	ND
22	A	1105	CLA	ND
22	A	1106	CLA	ND
22	A	1107	CLA	ND
22	A	1108	CLA	ND
22	A	1109	CLA	ND
22	A	1110	CLA	ND
22	A	1111	CLA	ND
22	A	1112	CLA	ND
22	A	1113	CLA	ND
22	A	1114	CLA	ND
22	A	1115	CLA	ND
22	A	1116	CLA	ND
22	A	1117	CLA	ND
22	A	1118	CLA	ND
22	A	1119	CLA	ND
22	A	1120	CLA	ND
22	A	1121	CLA	ND
22	A	1122	CLA	ND
22	A	1123	CLA	ND
22	A	1124	CLA	ND
22	A	1125	CLA	ND
22	A	1126	CLA	ND
22	A	1127	CLA	ND
22	A	1128	CLA	ND
22	A	1129	CLA	ND
22	A	1130	CLA	ND
22	A	1131	CLA	ND
22	A	1132	CLA	ND

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Mol	Chain	Res	Type	Atom
22	A	1133	CLA	ND
22	A	1134	CLA	ND
22	A	1135	CLA	ND
22	A	1136	CLA	ND
22	A	1137	CLA	ND
22	A	1138	CLA	ND
22	A	1139	CLA	ND
22	A	1141	CLA	ND
22	A	1140	CLA	ND
22	A	1101	CLA	ND
22	B	1022	CLA	ND
22	B	1021	CLA	ND
22	B	1023	CLA	ND
22	B	1201	CLA	ND
22	B	1202	CLA	ND
22	B	1203	CLA	ND
22	B	1205	CLA	ND
22	B	1206	CLA	ND
22	B	1208	CLA	ND
22	B	1209	CLA	ND
22	B	1210	CLA	ND
22	B	1211	CLA	ND
22	B	1212	CLA	ND
22	B	1213	CLA	ND
22	B	1214	CLA	ND
22	B	1215	CLA	ND
22	B	1216	CLA	ND
22	B	1217	CLA	ND
22	B	1218	CLA	ND
22	B	1219	CLA	ND
22	B	1220	CLA	ND
22	B	1221	CLA	ND
22	B	1222	CLA	ND
22	B	1223	CLA	ND
22	B	1224	CLA	ND
22	B	1225	CLA	ND
22	B	1226	CLA	ND
22	B	1227	CLA	ND
22	B	1230	CLA	ND
22	B	1231	CLA	ND
22	B	1232	CLA	ND
22	B	1234	CLA	ND

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Mol	Chain	Res	Type	Atom
22	B	1235	CLA	ND
22	B	1236	CLA	ND
22	B	1237	CLA	ND
22	B	1238	CLA	ND
22	B	1239	CLA	ND
22	B	1240	CLA	ND
22	B	1228	CLA	ND
22	B	1229	CLA	ND
22	B	1204	CLA	ND
22	B	1207	CLA	ND
22	F	1301	CLA	ND
22	F	1302	CLA	ND
22	G	1601	CLA	ND
22	G	1602	CLA	ND
22	G	1603	CLA	ND
22	J	1901	CLA	ND
22	K	1401	CLA	ND
22	K	1402	CLA	ND
22	K	1403	CLA	ND
22	K	1404	CLA	ND
22	L	1501	CLA	ND
22	L	1502	CLA	ND
22	L	1503	CLA	ND
22	1	601	CLA	ND
22	1	602	CLA	ND
22	1	603	CLA	ND
22	1	604	CLA	ND
22	1	605	CLA	ND
22	1	606	CLA	ND
22	1	607	CLA	ND
22	1	608	CLA	ND
22	1	610	CLA	ND
22	1	611	CLA	ND
22	1	612	CLA	ND
22	1	615	CLA	ND
22	a	601	CLA	ND
22	a	602	CLA	ND
22	a	603	CLA	ND
22	a	604	CLA	ND
22	a	605	CLA	ND
22	a	607	CLA	ND
22	a	608	CLA	ND

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Mol	Chain	Res	Type	Atom
22	a	611	CLA	ND
22	a	612	CLA	ND
22	a	615	CLA	ND
22	3	601	CLA	ND
22	3	602	CLA	ND
22	3	603	CLA	ND
22	3	604	CLA	ND
22	3	605	CLA	ND
22	3	606	CLA	ND
22	3	607	CLA	ND
22	3	610	CLA	ND
22	3	612	CLA	ND
22	3	613	CLA	ND
22	3	616	CLA	ND
22	3	618	CLA	ND
22	4	601	CLA	ND
22	4	602	CLA	ND
22	4	603	CLA	ND
22	4	604	CLA	ND
22	4	605	CLA	ND
22	4	606	CLA	ND
22	4	607	CLA	ND
22	4	610	CLA	ND
22	4	611	CLA	ND
22	4	612	CLA	ND
22	4	615	CLA	ND
22	4	616	CLA	ND
22	4	617	CLA	ND
22	4	608	CLA	ND
22	5	601	CLA	ND
22	5	602	CLA	ND
22	5	603	CLA	ND
22	5	604	CLA	ND
22	5	605	CLA	ND
22	5	606	CLA	ND
22	5	607	CLA	ND
22	5	608	CLA	ND
22	5	609	CLA	ND
22	5	612	CLA	ND
22	5	614	CLA	ND
22	5	616	CLA	ND
22	5	617	CLA	ND

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Mol	Chain	Res	Type	Atom
22	5	618	CLA	ND
22	6	608	CLA	ND
22	6	601	CLA	ND
22	6	602	CLA	ND
22	6	603	CLA	ND
22	6	604	CLA	ND
22	6	605	CLA	ND
22	6	606	CLA	ND
22	6	607	CLA	ND
22	6	609	CLA	ND
22	6	612	CLA	ND
22	6	615	CLA	ND
22	6	617	CLA	ND
22	6	618	CLA	ND
22	7	609	CLA	ND
22	7	601	CLA	ND
22	7	602	CLA	ND
22	7	603	CLA	ND
22	7	604	CLA	ND
22	7	605	CLA	ND
22	7	606	CLA	ND
22	7	607	CLA	ND
22	7	608	CLA	ND
22	7	610	CLA	ND
22	7	611	CLA	ND
22	7	612	CLA	ND
22	7	615	CLA	ND
22	7	617	CLA	ND
22	8	609	CLA	ND
22	8	602	CLA	ND
22	8	603	CLA	ND
22	8	605	CLA	ND
22	8	606	CLA	ND
22	8	607	CLA	ND
22	8	608	CLA	ND
22	8	610	CLA	ND
22	8	611	CLA	ND
22	8	612	CLA	ND
22	8	615	CLA	ND
22	8	618	CLA	ND
22	8	620	CLA	ND
34	G	5002	ERG	C24

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Mol	Chain	Res	Type	Atom
34	G	5002	ERG	C14
34	G	5002	ERG	C20
34	G	5002	ERG	C9
35	J	4002	RRX	C28
38	1	503	LUT	C26
38	a	502	LUT	C26
38	5	505	LUT	C26
38	6	501	LUT	C26
38	6	502	LUT	C26
38	7	501	LUT	C26
39	1	613	CHL	NA
39	1	613	CHL	NC
39	1	613	CHL	ND
39	1	609	CHL	C8
39	1	609	CHL	NA
39	1	609	CHL	NC
39	1	609	CHL	ND
39	a	606	CHL	C8
39	a	606	CHL	NA
39	a	606	CHL	NC
39	a	606	CHL	ND
39	a	609	CHL	NA
39	a	609	CHL	NC
39	a	609	CHL	ND
39	a	610	CHL	NA
39	a	610	CHL	NC
39	a	610	CHL	ND
39	a	613	CHL	NA
39	a	613	CHL	NC
39	a	613	CHL	ND
39	3	608	CHL	NA
39	3	608	CHL	NC
39	3	608	CHL	ND
39	3	608	CHL	C3A
39	3	611	CHL	NA
39	3	611	CHL	NC
39	3	611	CHL	ND
39	4	609	CHL	C8
39	4	609	CHL	NA
39	4	609	CHL	NC
39	4	609	CHL	ND
39	4	613	CHL	NA

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Mol	Chain	Res	Type	Atom
39	4	613	CHL	NC
39	4	613	CHL	ND
39	4	618	CHL	C8
39	4	618	CHL	NA
39	4	618	CHL	NC
39	4	618	CHL	ND
39	5	610	CHL	C8
39	5	610	CHL	NA
39	5	610	CHL	NC
39	5	610	CHL	ND
39	5	611	CHL	NA
39	5	611	CHL	NC
39	5	611	CHL	ND
39	5	613	CHL	C8
39	5	613	CHL	NA
39	5	613	CHL	NC
39	5	613	CHL	ND
39	6	610	CHL	C8
39	6	610	CHL	NA
39	6	610	CHL	NC
39	6	610	CHL	ND
39	6	611	CHL	NA
39	6	611	CHL	NC
39	6	611	CHL	ND
39	6	613	CHL	NA
39	6	613	CHL	NC
39	6	613	CHL	ND
39	6	619	CHL	NC
39	6	619	CHL	C3A
39	6	619	CHL	NA
39	6	619	CHL	C8
39	6	619	CHL	ND
39	7	613	CHL	C8
39	7	613	CHL	NA
39	7	613	CHL	NC
39	7	613	CHL	ND
39	8	601	CHL	C8
39	8	601	CHL	NA
39	8	601	CHL	NC
39	8	601	CHL	ND
39	8	604	CHL	C8
39	8	604	CHL	NA

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Mol	Chain	Res	Type	Atom
39	8	604	CHL	NC
39	8	604	CHL	ND
39	8	613	CHL	NA
39	8	613	CHL	NC
39	8	613	CHL	ND
41	3	506	QTB	C12
41	3	506	QTB	C11
46	7	502	XAT	C26
46	7	502	XAT	C6
46	7	502	XAT	C5
48	7	504	C7Z	C3

All (4397) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	1011	CL0	C2-C1-O2A-CGA
22	A	1013	CLA	CHA-CBD-CGD-O1D
22	A	1013	CLA	CHA-CBD-CGD-O2D
22	A	1013	CLA	CBD-CGD-O2D-CED
22	A	1102	CLA	C1A-C2A-CAA-CBA
22	A	1102	CLA	C3A-C2A-CAA-CBA
22	A	1102	CLA	C2C-C3C-CAC-CBC
22	A	1102	CLA	C4C-C3C-CAC-CBC
22	A	1103	CLA	C1A-C2A-CAA-CBA
22	A	1103	CLA	C3A-C2A-CAA-CBA
22	A	1106	CLA	C3A-C2A-CAA-CBA
22	A	1106	CLA	CHA-CBD-CGD-O1D
22	A	1106	CLA	CHA-CBD-CGD-O2D
22	A	1107	CLA	C1A-C2A-CAA-CBA
22	A	1107	CLA	CBD-CGD-O2D-CED
22	A	1108	CLA	C1A-C2A-CAA-CBA
22	A	1108	CLA	C3A-C2A-CAA-CBA
22	A	1109	CLA	C1A-C2A-CAA-CBA
22	A	1109	CLA	C3A-C2A-CAA-CBA
22	A	1109	CLA	C2-C1-O2A-CGA
22	A	1109	CLA	CBD-CGD-O2D-CED
22	A	1110	CLA	CBA-CGA-O2A-C1
22	A	1110	CLA	O1A-CGA-O2A-C1
22	A	1111	CLA	C1A-C2A-CAA-CBA
22	A	1111	CLA	C3A-C2A-CAA-CBA
22	A	1111	CLA	CBD-CGD-O2D-CED
22	A	1112	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	A	1114	CLA	CBA-CGA-O2A-C1
22	A	1114	CLA	O1A-CGA-O2A-C1
22	A	1114	CLA	CBD-CGD-O2D-CED
22	A	1115	CLA	C2-C3-C5-C6
22	A	1115	CLA	C4-C3-C5-C6
22	A	1116	CLA	C3A-C2A-CAA-CBA
22	A	1116	CLA	CBD-CGD-O2D-CED
22	A	1117	CLA	C1A-C2A-CAA-CBA
22	A	1117	CLA	C3A-C2A-CAA-CBA
22	A	1117	CLA	CHA-CBD-CGD-O1D
22	A	1117	CLA	CHA-CBD-CGD-O2D
22	A	1118	CLA	C1A-C2A-CAA-CBA
22	A	1118	CLA	C3A-C2A-CAA-CBA
22	A	1118	CLA	CHA-CBD-CGD-O1D
22	A	1118	CLA	CHA-CBD-CGD-O2D
22	A	1119	CLA	CHA-CBD-CGD-O1D
22	A	1119	CLA	CHA-CBD-CGD-O2D
22	A	1119	CLA	CBD-CGD-O2D-CED
22	A	1120	CLA	CHA-CBD-CGD-O1D
22	A	1120	CLA	CHA-CBD-CGD-O2D
22	A	1121	CLA	CBD-CGD-O2D-CED
22	A	1122	CLA	CHA-CBD-CGD-O1D
22	A	1122	CLA	C6-C7-C8-C9
22	A	1123	CLA	CHA-CBD-CGD-O1D
22	A	1123	CLA	CHA-CBD-CGD-O2D
22	A	1123	CLA	CAD-CBD-CGD-O1D
22	A	1123	CLA	CAD-CBD-CGD-O2D
22	A	1124	CLA	C1A-C2A-CAA-CBA
22	A	1124	CLA	C3A-C2A-CAA-CBA
22	A	1125	CLA	CHA-CBD-CGD-O1D
22	A	1125	CLA	CHA-CBD-CGD-O2D
22	A	1125	CLA	CAD-CBD-CGD-O1D
22	A	1126	CLA	C1A-C2A-CAA-CBA
22	A	1126	CLA	C3A-C2A-CAA-CBA
22	A	1126	CLA	C2-C1-O2A-CGA
22	A	1126	CLA	CHA-CBD-CGD-O1D
22	A	1126	CLA	CHA-CBD-CGD-O2D
22	A	1128	CLA	CHA-CBD-CGD-O1D
22	A	1128	CLA	CHA-CBD-CGD-O2D
22	A	1129	CLA	CHA-CBD-CGD-O1D
22	A	1129	CLA	CHA-CBD-CGD-O2D
22	A	1129	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	A	1130	CLA	C1A-C2A-CAA-CBA
22	A	1130	CLA	C3A-C2A-CAA-CBA
22	A	1130	CLA	C4-C3-C5-C6
22	A	1133	CLA	C2-C3-C5-C6
22	A	1133	CLA	C4-C3-C5-C6
22	A	1133	CLA	C12-C13-C15-C16
22	A	1134	CLA	C1A-C2A-CAA-CBA
22	A	1134	CLA	C3A-C2A-CAA-CBA
22	A	1134	CLA	CHA-CBD-CGD-O1D
22	A	1134	CLA	CHA-CBD-CGD-O2D
22	A	1135	CLA	C2-C3-C5-C6
22	A	1135	CLA	C4-C3-C5-C6
22	A	1135	CLA	C6-C7-C8-C10
22	A	1136	CLA	CHA-CBD-CGD-O1D
22	A	1136	CLA	CHA-CBD-CGD-O2D
22	A	1136	CLA	CAD-CBD-CGD-O1D
22	A	1136	CLA	C2-C3-C5-C6
22	A	1136	CLA	C4-C3-C5-C6
22	A	1138	CLA	C1A-C2A-CAA-CBA
22	A	1138	CLA	C3A-C2A-CAA-CBA
22	A	1138	CLA	CAD-CBD-CGD-O2D
22	A	1139	CLA	C3A-C2A-CAA-CBA
22	A	1141	CLA	CAD-CBD-CGD-O1D
22	A	1141	CLA	CAD-CBD-CGD-O2D
22	A	1140	CLA	CHA-CBD-CGD-O1D
22	A	1140	CLA	CHA-CBD-CGD-O2D
22	A	1140	CLA	CBD-CGD-O2D-CED
22	A	1101	CLA	C1A-C2A-CAA-CBA
22	B	1022	CLA	CBD-CGD-O2D-CED
22	B	1021	CLA	CHA-CBD-CGD-O1D
22	B	1021	CLA	CHA-CBD-CGD-O2D
22	B	1023	CLA	C2-C1-O2A-CGA
22	B	1023	CLA	CBD-CGD-O2D-CED
22	B	1201	CLA	C1A-C2A-CAA-CBA
22	B	1201	CLA	CHA-CBD-CGD-O1D
22	B	1201	CLA	CHA-CBD-CGD-O2D
22	B	1202	CLA	C1A-C2A-CAA-CBA
22	B	1202	CLA	C3A-C2A-CAA-CBA
22	B	1205	CLA	CHA-CBD-CGD-O1D
22	B	1205	CLA	CHA-CBD-CGD-O2D
22	B	1206	CLA	CBD-CGD-O2D-CED
22	B	1206	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	B	1206	CLA	C4-C3-C5-C6
22	B	1208	CLA	C1A-C2A-CAA-CBA
22	B	1210	CLA	C1A-C2A-CAA-CBA
22	B	1210	CLA	C3A-C2A-CAA-CBA
22	B	1212	CLA	C1A-C2A-CAA-CBA
22	B	1212	CLA	C3A-C2A-CAA-CBA
22	B	1214	CLA	C1A-C2A-CAA-CBA
22	B	1214	CLA	C3A-C2A-CAA-CBA
22	B	1215	CLA	C3A-C2A-CAA-CBA
22	B	1215	CLA	C2-C3-C5-C6
22	B	1215	CLA	C4-C3-C5-C6
22	B	1216	CLA	CHA-CBD-CGD-O1D
22	B	1216	CLA	CHA-CBD-CGD-O2D
22	B	1217	CLA	CHA-CBD-CGD-O1D
22	B	1217	CLA	CHA-CBD-CGD-O2D
22	B	1217	CLA	CAD-CBD-CGD-O1D
22	B	1217	CLA	C4-C3-C5-C6
22	B	1218	CLA	CBA-CGA-O2A-C1
22	B	1218	CLA	O1A-CGA-O2A-C1
22	B	1218	CLA	C4-C3-C5-C6
22	B	1220	CLA	CBD-CGD-O2D-CED
22	B	1221	CLA	CHA-CBD-CGD-O1D
22	B	1221	CLA	CHA-CBD-CGD-O2D
22	B	1223	CLA	C1A-C2A-CAA-CBA
22	B	1223	CLA	C3A-C2A-CAA-CBA
22	B	1224	CLA	C1A-C2A-CAA-CBA
22	B	1224	CLA	CHA-CBD-CGD-O1D
22	B	1224	CLA	CHA-CBD-CGD-O2D
22	B	1224	CLA	CBD-CGD-O2D-CED
22	B	1224	CLA	C11-C10-C8-C9
22	B	1225	CLA	C1A-C2A-CAA-CBA
22	B	1225	CLA	C3A-C2A-CAA-CBA
22	B	1225	CLA	CHA-CBD-CGD-O1D
22	B	1226	CLA	C2-C3-C5-C6
22	B	1226	CLA	C4-C3-C5-C6
22	B	1226	CLA	C6-C7-C8-C9
22	B	1227	CLA	C2-C1-O2A-CGA
22	B	1227	CLA	CHA-CBD-CGD-O1D
22	B	1227	CLA	CAD-CBD-CGD-O1D
22	B	1230	CLA	CHA-CBD-CGD-O1D
22	B	1230	CLA	CHA-CBD-CGD-O2D
22	B	1231	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
22	B	1232	CLA	C3A-C2A-CAA-CBA
22	B	1234	CLA	C2A-CAA-CBA-CGA
22	B	1236	CLA	C1A-C2A-CAA-CBA
22	B	1236	CLA	C3A-C2A-CAA-CBA
22	B	1236	CLA	C4-C3-C5-C6
22	B	1237	CLA	C2-C1-O2A-CGA
22	B	1228	CLA	C1A-C2A-CAA-CBA
22	B	1228	CLA	C2A-CAA-CBA-CGA
22	B	1229	CLA	CBD-CGD-O2D-CED
22	B	1204	CLA	CHA-CBD-CGD-O1D
22	B	1204	CLA	CHA-CBD-CGD-O2D
22	B	1207	CLA	C2-C1-O2A-CGA
22	B	1207	CLA	CHA-CBD-CGD-O1D
22	B	1207	CLA	CHA-CBD-CGD-O2D
22	B	1207	CLA	CAD-CBD-CGD-O1D
22	B	1207	CLA	CBD-CGD-O2D-CED
22	F	1301	CLA	CHA-CBD-CGD-O1D
22	F	1301	CLA	CHA-CBD-CGD-O2D
22	F	1302	CLA	CBD-CGD-O2D-CED
22	G	1601	CLA	C1A-C2A-CAA-CBA
22	G	1601	CLA	CBD-CGD-O2D-CED
22	G	1603	CLA	CBD-CGD-O2D-CED
22	J	1901	CLA	C1A-C2A-CAA-CBA
22	J	1901	CLA	CBD-CGD-O2D-CED
22	K	1401	CLA	CBA-CGA-O2A-C1
22	K	1402	CLA	CBD-CGD-O2D-CED
22	K	1403	CLA	CBA-CGA-O2A-C1
22	K	1403	CLA	CHA-CBD-CGD-O1D
22	K	1403	CLA	CHA-CBD-CGD-O2D
22	K	1403	CLA	CAD-CBD-CGD-O1D
22	L	1501	CLA	CBA-CGA-O2A-C1
22	L	1501	CLA	O1A-CGA-O2A-C1
22	1	602	CLA	C1A-C2A-CAA-CBA
22	1	603	CLA	CBD-CGD-O2D-CED
22	1	603	CLA	C2-C3-C5-C6
22	1	603	CLA	C4-C3-C5-C6
22	1	604	CLA	C3A-C2A-CAA-CBA
22	1	605	CLA	C2-C3-C5-C6
22	1	605	CLA	C4-C3-C5-C6
22	1	606	CLA	CHA-CBD-CGD-O1D
22	1	606	CLA	CHA-CBD-CGD-O2D
22	1	608	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	1	608	CLA	CHA-CBD-CGD-O2D
22	1	611	CLA	CBD-CGD-O2D-CED
22	1	612	CLA	C3A-C2A-CAA-CBA
22	1	615	CLA	CBA-CGA-O2A-C1
22	1	615	CLA	CBD-CGD-O2D-CED
22	a	601	CLA	CHA-CBD-CGD-O1D
22	a	601	CLA	CHA-CBD-CGD-O2D
22	a	602	CLA	C1A-C2A-CAA-CBA
22	a	603	CLA	CBD-CGD-O2D-CED
22	a	604	CLA	C1A-C2A-CAA-CBA
22	a	604	CLA	C3A-C2A-CAA-CBA
22	a	605	CLA	C2-C3-C5-C6
22	a	605	CLA	C4-C3-C5-C6
22	a	608	CLA	C1A-C2A-CAA-CBA
22	a	608	CLA	C3A-C2A-CAA-CBA
22	a	608	CLA	CHA-CBD-CGD-O1D
22	a	608	CLA	CHA-CBD-CGD-O2D
22	a	611	CLA	C1A-C2A-CAA-CBA
22	a	611	CLA	C3A-C2A-CAA-CBA
22	a	611	CLA	C2-C1-O2A-CGA
22	a	611	CLA	CBD-CGD-O2D-CED
22	a	612	CLA	C1A-C2A-CAA-CBA
22	a	612	CLA	C3A-C2A-CAA-CBA
22	a	612	CLA	CBD-CGD-O2D-CED
22	a	615	CLA	CBD-CGD-O2D-CED
22	3	601	CLA	C3A-C2A-CAA-CBA
22	3	603	CLA	CHA-CBD-CGD-O1D
22	3	603	CLA	CHA-CBD-CGD-O2D
22	3	603	CLA	C4-C3-C5-C6
22	3	605	CLA	CBD-CGD-O2D-CED
22	3	606	CLA	C1A-C2A-CAA-CBA
22	3	606	CLA	C3A-C2A-CAA-CBA
22	3	606	CLA	CHA-CBD-CGD-O1D
22	3	606	CLA	CHA-CBD-CGD-O2D
22	3	610	CLA	C1A-C2A-CAA-CBA
22	3	610	CLA	C2A-CAA-CBA-CGA
22	3	616	CLA	C2-C3-C5-C6
22	3	616	CLA	C4-C3-C5-C6
22	3	618	CLA	CBA-CGA-O2A-C1
22	3	618	CLA	CBD-CGD-O2D-CED
22	4	602	CLA	CBD-CGD-O2D-CED
22	4	603	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	4	607	CLA	CBD-CGD-O2D-CED
22	4	610	CLA	CBD-CGD-O2D-CED
22	4	611	CLA	CBD-CGD-O2D-CED
22	4	612	CLA	CHA-CBD-CGD-O1D
22	4	612	CLA	CHA-CBD-CGD-O2D
22	4	615	CLA	CBA-CGA-O2A-C1
22	4	615	CLA	O1A-CGA-O2A-C1
22	4	615	CLA	CHA-CBD-CGD-O1D
22	4	615	CLA	CHA-CBD-CGD-O2D
22	4	615	CLA	CBD-CGD-O2D-CED
22	4	616	CLA	C2-C1-O2A-CGA
22	4	616	CLA	CHA-CBD-CGD-O1D
22	4	616	CLA	CHA-CBD-CGD-O2D
22	4	608	CLA	CHA-CBD-CGD-O1D
22	4	608	CLA	CHA-CBD-CGD-O2D
22	4	608	CLA	C2-C3-C5-C6
22	5	602	CLA	CBD-CGD-O2D-CED
22	5	602	CLA	C2-C3-C5-C6
22	5	602	CLA	C4-C3-C5-C6
22	5	603	CLA	CHA-CBD-CGD-O1D
22	5	603	CLA	CHA-CBD-CGD-O2D
22	5	603	CLA	CBD-CGD-O2D-CED
22	5	603	CLA	C11-C10-C8-C7
22	5	604	CLA	CHA-CBD-CGD-O1D
22	5	604	CLA	CHA-CBD-CGD-O2D
22	5	606	CLA	CHA-CBD-CGD-O1D
22	5	606	CLA	CHA-CBD-CGD-O2D
22	5	608	CLA	C1A-C2A-CAA-CBA
22	5	608	CLA	C3A-C2A-CAA-CBA
22	5	608	CLA	CHA-CBD-CGD-O1D
22	5	608	CLA	CHA-CBD-CGD-O2D
22	5	609	CLA	C2-C3-C5-C6
22	5	609	CLA	C4-C3-C5-C6
22	5	612	CLA	C2-C1-O2A-CGA
22	5	612	CLA	C11-C10-C8-C7
22	5	614	CLA	CBD-CGD-O2D-CED
22	5	616	CLA	C1A-C2A-CAA-CBA
22	5	616	CLA	C3A-C2A-CAA-CBA
22	5	616	CLA	CBD-CGD-O2D-CED
22	5	617	CLA	C3A-C2A-CAA-CBA
22	5	617	CLA	C2-C1-O2A-CGA
22	5	617	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	5	618	CLA	C3-C5-C6-C7
22	6	608	CLA	CBD-CGD-O2D-CED
22	6	605	CLA	CBA-CGA-O2A-C1
22	6	606	CLA	CHA-CBD-CGD-O1D
22	6	606	CLA	CHA-CBD-CGD-O2D
22	6	606	CLA	CBD-CGD-O2D-CED
22	6	606	CLA	C3-C5-C6-C7
22	6	607	CLA	CHA-CBD-CGD-O1D
22	6	607	CLA	CHA-CBD-CGD-O2D
22	6	609	CLA	C1A-C2A-CAA-CBA
22	6	609	CLA	C3A-C2A-CAA-CBA
22	6	609	CLA	C2-C1-O2A-CGA
22	6	609	CLA	CHA-CBD-CGD-O1D
22	6	609	CLA	CHA-CBD-CGD-O2D
22	6	609	CLA	CAD-CBD-CGD-O1D
22	6	609	CLA	CAD-CBD-CGD-O2D
22	6	612	CLA	C1A-C2A-CAA-CBA
22	6	612	CLA	C3A-C2A-CAA-CBA
22	6	612	CLA	CHA-CBD-CGD-O1D
22	6	612	CLA	CHA-CBD-CGD-O2D
22	6	615	CLA	CHA-CBD-CGD-O1D
22	6	615	CLA	CAD-CBD-CGD-O1D
22	6	615	CLA	CAD-CBD-CGD-O2D
22	6	615	CLA	C2-C3-C5-C6
22	6	615	CLA	C4-C3-C5-C6
22	6	617	CLA	C3A-C2A-CAA-CBA
22	6	618	CLA	C1A-C2A-CAA-CBA
22	6	618	CLA	CBA-CGA-O2A-C1
22	6	618	CLA	CBD-CGD-O2D-CED
22	7	609	CLA	CHA-CBD-CGD-O1D
22	7	609	CLA	CHA-CBD-CGD-O2D
22	7	609	CLA	CAD-CBD-CGD-O1D
22	7	603	CLA	CHA-CBD-CGD-O1D
22	7	603	CLA	CHA-CBD-CGD-O2D
22	7	603	CLA	CBD-CGD-O2D-CED
22	7	604	CLA	CHA-CBD-CGD-O1D
22	7	604	CLA	CHA-CBD-CGD-O2D
22	7	606	CLA	CBD-CGD-O2D-CED
22	7	607	CLA	CHA-CBD-CGD-O1D
22	7	607	CLA	CHA-CBD-CGD-O2D
22	7	608	CLA	C1A-C2A-CAA-CBA
22	7	608	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	7	610	CLA	CBD-CGD-O2D-CED
22	7	611	CLA	C2-C1-O2A-CGA
22	7	611	CLA	C4-C3-C5-C6
22	7	612	CLA	C11-C10-C8-C9
22	7	615	CLA	C2A-CAA-CBA-CGA
22	7	615	CLA	CHA-CBD-CGD-O1D
22	7	615	CLA	CHA-CBD-CGD-O2D
22	7	617	CLA	CHA-CBD-CGD-O1D
22	8	609	CLA	C1A-C2A-CAA-CBA
22	8	602	CLA	C2-C3-C5-C6
22	8	602	CLA	C4-C3-C5-C6
22	8	603	CLA	CHA-CBD-CGD-O1D
22	8	603	CLA	CHA-CBD-CGD-O2D
22	8	603	CLA	CBD-CGD-O2D-CED
22	8	606	CLA	CHA-CBD-CGD-O1D
22	8	606	CLA	CHA-CBD-CGD-O2D
22	8	606	CLA	CBD-CGD-O2D-CED
22	8	608	CLA	C2-C1-O2A-CGA
22	8	610	CLA	C1A-C2A-CAA-CBA
22	8	610	CLA	C3A-C2A-CAA-CBA
22	8	610	CLA	CHA-CBD-CGD-O1D
22	8	611	CLA	C2-C1-O2A-CGA
22	8	611	CLA	CHA-CBD-CGD-O1D
22	8	611	CLA	CHA-CBD-CGD-O2D
22	8	611	CLA	CBD-CGD-O2D-CED
22	8	612	CLA	C3A-C2A-CAA-CBA
22	8	615	CLA	CHA-CBD-CGD-O1D
22	8	615	CLA	CHA-CBD-CGD-O2D
22	8	620	CLA	C2-C1-O2A-CGA
24	A	4001	BCR	C1-C6-C7-C8
24	A	4001	BCR	C23-C24-C25-C26
24	A	4001	BCR	C23-C24-C25-C30
24	A	4002	BCR	C7-C8-C9-C10
24	A	4002	BCR	C7-C8-C9-C34
24	A	4002	BCR	C11-C10-C9-C8
24	A	4002	BCR	C11-C10-C9-C34
24	A	4003	BCR	C11-C10-C9-C8
24	A	4003	BCR	C11-C10-C9-C34
24	A	4003	BCR	C10-C11-C12-C13
24	A	4003	BCR	C11-C12-C13-C14
24	A	4003	BCR	C11-C12-C13-C35
24	A	4003	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
24	A	4003	BCR	C36-C18-C19-C20
24	A	4004	BCR	C11-C10-C9-C8
24	A	4004	BCR	C11-C10-C9-C34
24	A	4004	BCR	C11-C12-C13-C35
24	A	4004	BCR	C17-C18-C19-C20
24	A	4004	BCR	C36-C18-C19-C20
24	A	4005	BCR	C1-C6-C7-C8
24	A	4005	BCR	C7-C8-C9-C10
24	A	4005	BCR	C7-C8-C9-C34
24	A	4005	BCR	C17-C18-C19-C20
24	A	4005	BCR	C36-C18-C19-C20
24	A	4005	BCR	C21-C22-C23-C24
24	A	4005	BCR	C37-C22-C23-C24
24	B	4002	BCR	C7-C8-C9-C10
24	B	4002	BCR	C7-C8-C9-C34
24	B	4002	BCR	C17-C18-C19-C20
24	B	4002	BCR	C36-C18-C19-C20
24	B	4002	BCR	C21-C22-C23-C24
24	B	4002	BCR	C37-C22-C23-C24
24	B	4003	BCR	C21-C22-C23-C24
24	B	4003	BCR	C37-C22-C23-C24
24	B	4004	BCR	C11-C10-C9-C8
24	B	4004	BCR	C11-C10-C9-C34
24	B	4004	BCR	C10-C11-C12-C13
24	B	4004	BCR	C21-C22-C23-C24
24	B	4004	BCR	C37-C22-C23-C24
24	B	4004	BCR	C23-C24-C25-C26
24	B	4004	BCR	C23-C24-C25-C30
24	B	4005	BCR	C7-C8-C9-C10
24	B	4005	BCR	C7-C8-C9-C34
24	B	4005	BCR	C19-C20-C21-C22
24	B	4007	BCR	C11-C10-C9-C8
24	B	4007	BCR	C11-C10-C9-C34
24	B	4007	BCR	C10-C11-C12-C13
24	B	4007	BCR	C36-C18-C19-C20
24	B	4006	BCR	C11-C10-C9-C8
24	B	4006	BCR	C11-C10-C9-C34
24	B	4006	BCR	C10-C11-C12-C13
24	B	4006	BCR	C17-C18-C19-C20
24	B	4006	BCR	C36-C18-C19-C20
24	B	4006	BCR	C21-C22-C23-C24
24	B	4006	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
24	B	4001	BCR	C7-C8-C9-C10
24	B	4001	BCR	C7-C8-C9-C34
24	B	4001	BCR	C11-C10-C9-C8
24	B	4001	BCR	C11-C10-C9-C34
24	B	4001	BCR	C11-C12-C13-C14
24	B	4001	BCR	C11-C12-C13-C35
24	B	4001	BCR	C23-C24-C25-C30
24	F	4001	BCR	C23-C24-C25-C26
24	G	4001	BCR	C1-C6-C7-C8
24	G	4001	BCR	C11-C10-C9-C8
24	G	4001	BCR	C11-C10-C9-C34
24	G	4001	BCR	C17-C18-C19-C20
24	G	4001	BCR	C36-C18-C19-C20
24	J	4001	BCR	C11-C10-C9-C8
24	J	4001	BCR	C11-C10-C9-C34
24	J	4001	BCR	C10-C11-C12-C13
24	J	4001	BCR	C17-C18-C19-C20
24	J	4001	BCR	C36-C18-C19-C20
24	K	4001	BCR	C7-C8-C9-C10
24	K	4001	BCR	C7-C8-C9-C34
24	K	4001	BCR	C11-C10-C9-C8
24	K	4001	BCR	C11-C10-C9-C34
24	K	4001	BCR	C11-C12-C13-C14
24	K	4001	BCR	C11-C12-C13-C35
24	K	4001	BCR	C21-C22-C23-C24
24	K	4001	BCR	C37-C22-C23-C24
24	K	4002	BCR	C10-C11-C12-C13
24	K	4002	BCR	C11-C12-C13-C14
24	K	4002	BCR	C11-C12-C13-C35
24	K	4002	BCR	C17-C18-C19-C20
24	K	4002	BCR	C36-C18-C19-C20
24	I	4001	BCR	C7-C8-C9-C10
24	I	4001	BCR	C7-C8-C9-C34
24	I	4001	BCR	C11-C10-C9-C8
24	I	4001	BCR	C11-C10-C9-C34
24	I	4001	BCR	C10-C11-C12-C13
24	I	4001	BCR	C11-C12-C13-C35
24	L	4002	BCR	C11-C10-C9-C8
24	L	4002	BCR	C11-C10-C9-C34
24	L	4002	BCR	C13-C14-C15-C16
24	L	4002	BCR	C21-C22-C23-C24
24	L	4002	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
24	L	4001	BCR	C1-C6-C7-C8
24	L	4001	BCR	C11-C10-C9-C8
24	L	4001	BCR	C11-C10-C9-C34
24	L	4001	BCR	C10-C11-C12-C13
24	L	4001	BCR	C13-C14-C15-C16
24	L	4001	BCR	C21-C22-C23-C24
24	L	4001	BCR	C37-C22-C23-C24
24	L	4001	BCR	C23-C24-C25-C26
24	L	4001	BCR	C23-C24-C25-C30
24	3	503	BCR	C23-C24-C25-C26
24	3	503	BCR	C23-C24-C25-C30
24	3	504	BCR	C7-C8-C9-C10
24	3	504	BCR	C7-C8-C9-C34
24	3	504	BCR	C11-C10-C9-C8
24	3	504	BCR	C11-C10-C9-C34
24	3	504	BCR	C9-C10-C11-C12
24	3	504	BCR	C10-C11-C12-C13
24	3	504	BCR	C36-C18-C19-C20
24	3	504	BCR	C21-C22-C23-C24
24	3	504	BCR	C37-C22-C23-C24
24	3	505	BCR	C11-C10-C9-C8
24	3	505	BCR	C11-C10-C9-C34
24	3	505	BCR	C17-C18-C19-C20
24	3	505	BCR	C36-C18-C19-C20
24	3	505	BCR	C21-C22-C23-C24
24	3	505	BCR	C37-C22-C23-C24
24	3	505	BCR	C23-C24-C25-C26
24	3	505	BCR	C23-C24-C25-C30
24	4	503	BCR	C7-C8-C9-C10
24	4	503	BCR	C7-C8-C9-C34
24	4	503	BCR	C11-C10-C9-C8
24	4	503	BCR	C11-C10-C9-C34
24	4	503	BCR	C9-C10-C11-C12
24	4	503	BCR	C11-C12-C13-C14
24	4	503	BCR	C11-C12-C13-C35
24	4	503	BCR	C19-C20-C21-C22
24	4	503	BCR	C21-C22-C23-C24
24	4	503	BCR	C37-C22-C23-C24
24	4	503	BCR	C23-C24-C25-C26
24	4	503	BCR	C23-C24-C25-C30
24	5	503	BCR	C11-C10-C9-C8
24	5	503	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
24	5	503	BCR	C10-C11-C12-C13
24	5	503	BCR	C11-C12-C13-C14
24	5	503	BCR	C11-C12-C13-C35
24	5	503	BCR	C17-C18-C19-C20
24	5	503	BCR	C36-C18-C19-C20
24	5	504	BCR	C10-C11-C12-C13
24	5	504	BCR	C13-C14-C15-C16
24	6	504	BCR	C17-C18-C19-C20
24	6	504	BCR	C36-C18-C19-C20
24	6	503	BCR	C17-C18-C19-C20
24	6	503	BCR	C36-C18-C19-C20
24	6	503	BCR	C23-C24-C25-C30
24	7	503	BCR	C7-C8-C9-C10
24	7	503	BCR	C7-C8-C9-C34
24	7	503	BCR	C11-C10-C9-C8
24	7	503	BCR	C11-C10-C9-C34
24	7	503	BCR	C11-C12-C13-C35
24	7	503	BCR	C21-C22-C23-C24
24	7	503	BCR	C37-C22-C23-C24
24	8	503	BCR	C7-C8-C9-C10
24	8	503	BCR	C7-C8-C9-C34
24	8	503	BCR	C11-C10-C9-C8
24	8	503	BCR	C11-C10-C9-C34
24	8	503	BCR	C10-C11-C12-C13
24	8	503	BCR	C21-C22-C23-C24
24	8	503	BCR	C37-C22-C23-C24
24	8	503	BCR	C23-C24-C25-C26
24	8	503	BCR	C23-C24-C25-C30
25	A	5001	LHG	O1-C1-C2-C3
25	A	5001	LHG	C4-O6-P-O3
25	A	5001	LHG	C4-O6-P-O4
25	A	5001	LHG	C4-O6-P-O5
25	A	5001	LHG	O6-C4-C5-O7
25	A	5002	LHG	O1-C1-C2-O2
25	A	5002	LHG	O1-C1-C2-C3
25	A	5002	LHG	C3-O3-P-O4
25	A	5002	LHG	C4-O6-P-O4
25	A	5002	LHG	C4-O6-P-O5
25	A	5003	LHG	O1-C1-C2-C3
25	A	5003	LHG	C3-O3-P-O4
25	A	5003	LHG	C4-O6-P-O3
25	A	5003	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
25	A	5003	LHG	C4-O6-P-O5
25	A	5003	LHG	C8-C7-O7-C5
25	B	5002	LHG	O1-C1-C2-C3
25	B	5002	LHG	C4-O6-P-O4
25	B	5001	LHG	C3-O3-P-O4
25	B	5001	LHG	C3-O3-P-O5
25	B	5001	LHG	C3-O3-P-O6
25	B	5001	LHG	C4-O6-P-O5
25	F	5002	LHG	O2-C2-C3-O3
25	F	5002	LHG	C3-O3-P-O5
25	F	5002	LHG	C4-O6-P-O3
25	F	5002	LHG	C4-O6-P-O4
25	F	5002	LHG	C4-O6-P-O5
25	F	5002	LHG	C8-C7-O7-C5
25	F	5001	LHG	O1-C1-C2-O2
25	F	5001	LHG	O1-C1-C2-C3
25	F	5001	LHG	C4-O6-P-O4
25	F	5001	LHG	C8-C7-O7-C5
25	1	801	LHG	C1-C2-C3-O3
25	1	801	LHG	C3-O3-P-O5
25	1	801	LHG	C4-O6-P-O5
25	1	802	LHG	O1-C1-C2-C3
25	1	802	LHG	O7-C5-C6-O8
25	1	802	LHG	C8-C7-O7-C5
25	a	801	LHG	C3-O3-P-O4
25	a	801	LHG	C3-O3-P-O5
25	a	801	LHG	C3-O3-P-O6
25	a	801	LHG	C4-O6-P-O3
25	a	801	LHG	C4-O6-P-O5
25	a	801	LHG	C8-C7-O7-C5
25	3	801	LHG	O1-C1-C2-C3
25	3	801	LHG	C1-C2-C3-O3
25	3	801	LHG	C3-O3-P-O4
25	3	801	LHG	C3-O3-P-O5
25	3	801	LHG	C3-O3-P-O6
25	3	801	LHG	O9-C7-O7-C5
25	4	802	LHG	C3-O3-P-O4
25	4	802	LHG	C3-O3-P-O5
25	4	802	LHG	C3-O3-P-O6
25	4	802	LHG	C4-O6-P-O5
25	4	802	LHG	C8-C7-O7-C5
25	5	801	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
25	5	801	LHG	C4-O6-P-O3
25	6	802	LHG	O1-C1-C2-C3
25	6	802	LHG	C1-C2-C3-O3
25	6	801	LHG	C3-O3-P-O4
25	6	801	LHG	C3-O3-P-O5
25	6	801	LHG	C3-O3-P-O6
25	6	801	LHG	C4-O6-P-O5
25	7	801	LHG	O1-C1-C2-C3
25	7	801	LHG	C3-O3-P-O4
25	7	801	LHG	C3-O3-P-O5
25	7	801	LHG	C3-O3-P-O6
25	7	801	LHG	C4-O6-P-O4
25	7	801	LHG	C4-O6-P-O5
25	7	801	LHG	O9-C7-O7-C5
25	7	801	LHG	C8-C7-O7-C5
25	7	802	LHG	O2-C2-C3-O3
25	7	802	LHG	C2-C3-O3-P
25	7	803	LHG	O1-C1-C2-C3
25	7	803	LHG	C3-O3-P-O4
25	7	803	LHG	C4-O6-P-O3
25	7	803	LHG	C4-O6-P-O5
25	8	801	LHG	C4-O6-P-O3
25	8	801	LHG	C4-O6-P-O4
25	8	801	LHG	C4-O6-P-O5
26	A	5005	DGD	C2A-C1A-O1G-C1G
26	A	5005	DGD	O1A-C1A-O1G-C1G
26	A	5005	DGD	O6D-C1D-O3G-C3G
26	8	802	DGD	C2B-C1B-O2G-C2G
26	8	802	DGD	C2G-C3G-O3G-C1D
26	8	802	DGD	C5D-C6D-O5D-C1E
26	8	802	DGD	C2E-C1E-O5D-C6D
26	8	802	DGD	O6E-C1E-O5D-C6D
27	A	5007	3PH	C22-C21-O21-C2
29	A	5008	LMT	C2'-C1'-O1'-C1
29	A	5008	LMT	O5'-C1'-O1'-C1
29	B	5006	LMT	O5'-C1'-O1'-C1
29	1	804	LMT	C2-C1-O1'-C1'
30	B	5004	PCW	C2-C1-O3P-P
30	6	803	PCW	O4P-C4-C5-N
30	6	803	PCW	C1-O3P-P-O2P
30	6	803	PCW	C4-O4P-P-O1P
30	6	803	PCW	C4-O4P-P-O2P

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Mol	Chain	Res	Type	Atoms
30	6	803	PCW	C4-O4P-P-O3P
31	B	5005	PTY	N1-C2-C3-O11
31	B	5005	PTY	C3-O11-P1-O14
31	B	5005	PTY	C5-O14-P1-O12
31	B	5005	PTY	C5-O14-P1-O13
31	3	802	PTY	N1-C2-C3-O11
31	3	802	PTY	O10-C8-O7-C6
31	3	802	PTY	C11-C8-O7-C6
31	5	802	PTY	C11-C8-O7-C6
31	7	804	PTY	C11-C8-O7-C6
31	8	810	PTY	O10-C8-O7-C6
32	B	5007	LAP	C14-C15-O4-P9
32	B	5007	LAP	O6-C16-C17-N8
32	F	5003	LAP	C16-O6-P9-O4
32	F	5003	LAP	C16-O6-P9-O5
32	K	5001	LAP	C13-C14-C15-O4
32	K	5001	LAP	C14-C15-O4-P9
32	K	5001	LAP	C15-O4-P9-O7
33	G	5001	SQD	C8-C7-O47-C45
33	G	5001	SQD	C5-C6-S-O7
33	G	5001	SQD	C5-C6-S-O8
33	G	5001	SQD	C5-C6-S-O9
33	7	805	SQD	C2-C1-O6-C44
33	7	805	SQD	O5-C1-O6-C44
33	7	805	SQD	O5-C5-C6-S
34	G	5002	ERG	C13-C17-C20-C21
34	G	5002	ERG	C13-C17-C20-C22
34	G	5002	ERG	C16-C17-C20-C21
34	G	5002	ERG	C16-C17-C20-C22
34	G	5002	ERG	C22-C23-C24-C25
34	G	5002	ERG	C23-C24-C25-C26
34	G	5002	ERG	C23-C24-C25-C27
35	J	4002	RRX	C36-C18-C19-C20
35	J	4002	RRX	C17-C18-C19-C20
35	J	4002	RRX	C7-C8-C9-C10
35	J	4002	RRX	C7-C8-C9-C34
35	J	4002	RRX	C1-C6-C7-C8
36	J	5001	LPX	O1-C3-C4-C5
36	J	5001	LPX	C3-O1-P1-O3
36	J	5001	LPX	O2-C1-C2-N1
36	a	804	LPX	O2-C1-C2-N1
37	M	4001	ECH	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
37	M	4001	ECH	C11-C12-C13-C35
38	1	501	LUT	C1-C6-C7-C8
38	1	503	LUT	C1-C6-C7-C8
38	1	503	LUT	C21-C26-C27-C28
38	1	503	LUT	C27-C28-C29-C30
38	1	503	LUT	C27-C28-C29-C39
38	1	503	LUT	C31-C32-C33-C34
38	1	503	LUT	C31-C32-C33-C40
38	a	501	LUT	C5-C6-C7-C8
38	a	501	LUT	C31-C32-C33-C34
38	a	501	LUT	C31-C32-C33-C40
38	a	502	LUT	C7-C8-C9-C10
38	a	502	LUT	C7-C8-C9-C19
38	a	502	LUT	C21-C26-C27-C28
38	a	502	LUT	C25-C26-C27-C28
38	a	503	LUT	C21-C26-C27-C28
38	a	503	LUT	C31-C32-C33-C34
38	a	503	LUT	C31-C32-C33-C40
38	5	505	LUT	C7-C8-C9-C10
38	5	505	LUT	C7-C8-C9-C19
38	5	505	LUT	C21-C26-C27-C28
38	5	505	LUT	C25-C26-C27-C28
38	6	501	LUT	C7-C8-C9-C10
38	6	501	LUT	C7-C8-C9-C19
38	6	501	LUT	C21-C26-C27-C28
38	6	501	LUT	C25-C26-C27-C28
38	6	502	LUT	C1-C6-C7-C8
38	6	502	LUT	C21-C26-C27-C28
38	7	501	LUT	C21-C26-C27-C28
39	1	609	CHL	C1A-C2A-CAA-CBA
39	1	609	CHL	C3A-C2A-CAA-CBA
39	a	606	CHL	C1A-C2A-CAA-CBA
39	a	606	CHL	C3A-C2A-CAA-CBA
39	3	608	CHL	C1A-C2A-CAA-CBA
39	4	609	CHL	C3A-C2A-CAA-CBA
39	4	609	CHL	C4C-C3C-CAC-CBC
39	4	609	CHL	C4-C3-C5-C6
39	4	613	CHL	C2A-CAA-CBA-CGA
39	4	613	CHL	C2-C3-C5-C6
39	4	613	CHL	C4-C3-C5-C6
39	4	618	CHL	C1A-C2A-CAA-CBA
39	4	618	CHL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
39	4	618	CHL	C4-C3-C5-C6
39	5	610	CHL	C1A-C2A-CAA-CBA
39	5	610	CHL	C2-C3-C5-C6
39	5	610	CHL	C4-C3-C5-C6
39	6	611	CHL	C1A-C2A-CAA-CBA
39	6	619	CHL	CHA-CBD-CGD-O1D
39	6	619	CHL	CHA-CBD-CGD-O2D
39	6	619	CHL	C2-C3-C5-C6
39	6	619	CHL	C4-C3-C5-C6
39	8	601	CHL	C1A-C2A-CAA-CBA
39	8	604	CHL	C3A-C2A-CAA-CBA
41	a	504	QTB	C01-C02-C09-C10
41	a	504	QTB	C03-C02-C09-C10
41	a	504	QTB	C04-C05-C06-C08
41	a	504	QTB	C04-C05-C06-O07
41	a	504	QTB	C09-C10-C11-C12
41	3	506	QTB	C04-C05-C06-O07
42	a	805	GG0	N05-C06-C07-O08
42	a	805	GG0	N05-C06-C07-O09
43	4	803	PLM	C1-C2-C3-C4
44	5	803	DGA	CB2-CB1-OG2-CG2
44	8	803	DGA	CB2-CB1-OG2-CG2
45	6	806	SPH	C2-C3-C4-C5
45	6	806	SPH	O3-C3-C4-C5
47	8	808	4RF	O42-C41-O40-C39
47	8	808	4RF	C43-C41-O40-C39
48	7	504	C7Z	C9-C10-C11-C12
48	7	504	C7Z	C29-C30-C31-C32
49	8	806	P5S	C-CA-CB-OG
49	8	806	P5S	N-CA-CB-OG
49	8	806	P5S	CA-CB-OG-P12
49	8	806	P5S	CB-OG-P12-O15
49	8	806	P5S	C3-O16-P12-O13
22	7	605	CLA	C2C-C3C-CAC-CBC
39	4	609	CHL	C2C-C3C-CAC-CBC
22	A	1138	CLA	O1D-CGD-O2D-CED
22	B	1021	CLA	O1D-CGD-O2D-CED
22	B	1232	CLA	O1D-CGD-O2D-CED
22	L	1501	CLA	O1D-CGD-O2D-CED
22	a	602	CLA	O1D-CGD-O2D-CED
22	a	608	CLA	O1D-CGD-O2D-CED
22	a	615	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	4	603	CLA	O1D-CGD-O2D-CED
22	4	610	CLA	O1D-CGD-O2D-CED
22	5	618	CLA	O1D-CGD-O2D-CED
22	6	606	CLA	O1D-CGD-O2D-CED
22	6	617	CLA	O1D-CGD-O2D-CED
22	8	605	CLA	O1D-CGD-O2D-CED
22	5	612	CLA	C13-C15-C16-C17
22	B	1234	CLA	C2C-C3C-CAC-CBC
22	F	1302	CLA	C2C-C3C-CAC-CBC
22	5	617	CLA	C2C-C3C-CAC-CBC
22	5	617	CLA	C4C-C3C-CAC-CBC
22	A	1108	CLA	O1D-CGD-O2D-CED
22	A	1109	CLA	O1D-CGD-O2D-CED
22	B	1023	CLA	O1D-CGD-O2D-CED
22	F	1302	CLA	O1D-CGD-O2D-CED
22	a	612	CLA	O1D-CGD-O2D-CED
22	3	606	CLA	O1D-CGD-O2D-CED
22	5	616	CLA	O1D-CGD-O2D-CED
22	7	606	CLA	O1D-CGD-O2D-CED
22	7	615	CLA	O1D-CGD-O2D-CED
21	A	1011	CL0	CBD-CGD-O2D-CED
22	A	1012	CLA	CBD-CGD-O2D-CED
22	A	1108	CLA	CBD-CGD-O2D-CED
22	A	1115	CLA	CBD-CGD-O2D-CED
22	A	1122	CLA	CBD-CGD-O2D-CED
22	A	1123	CLA	CBD-CGD-O2D-CED
22	A	1125	CLA	CBD-CGD-O2D-CED
22	A	1126	CLA	CBD-CGD-O2D-CED
22	A	1127	CLA	CBD-CGD-O2D-CED
22	A	1131	CLA	CBD-CGD-O2D-CED
22	A	1132	CLA	CBD-CGD-O2D-CED
22	A	1134	CLA	CBD-CGD-O2D-CED
22	A	1135	CLA	CBD-CGD-O2D-CED
22	A	1138	CLA	CBD-CGD-O2D-CED
22	A	1139	CLA	CBD-CGD-O2D-CED
22	B	1021	CLA	CBD-CGD-O2D-CED
22	B	1203	CLA	CBD-CGD-O2D-CED
22	B	1210	CLA	CBD-CGD-O2D-CED
22	B	1211	CLA	CBD-CGD-O2D-CED
22	B	1212	CLA	CBD-CGD-O2D-CED
22	B	1213	CLA	CBD-CGD-O2D-CED
22	B	1215	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	B	1216	CLA	CBD-CGD-O2D-CED
22	B	1217	CLA	CBD-CGD-O2D-CED
22	B	1219	CLA	CBD-CGD-O2D-CED
22	B	1222	CLA	CBD-CGD-O2D-CED
22	B	1226	CLA	CBD-CGD-O2D-CED
22	B	1227	CLA	CBD-CGD-O2D-CED
22	B	1231	CLA	CBD-CGD-O2D-CED
22	B	1232	CLA	CBD-CGD-O2D-CED
22	B	1237	CLA	CBD-CGD-O2D-CED
22	B	1239	CLA	CBD-CGD-O2D-CED
22	G	1602	CLA	CBD-CGD-O2D-CED
22	K	1401	CLA	CBD-CGD-O2D-CED
22	K	1404	CLA	CBD-CGD-O2D-CED
22	L	1501	CLA	CBD-CGD-O2D-CED
22	L	1503	CLA	CBD-CGD-O2D-CED
22	1	601	CLA	CBD-CGD-O2D-CED
22	1	602	CLA	CBD-CGD-O2D-CED
22	1	605	CLA	CBD-CGD-O2D-CED
22	1	606	CLA	CBD-CGD-O2D-CED
22	1	612	CLA	CBD-CGD-O2D-CED
22	a	602	CLA	CBD-CGD-O2D-CED
22	a	605	CLA	CBD-CGD-O2D-CED
22	a	607	CLA	CBD-CGD-O2D-CED
22	a	608	CLA	CBD-CGD-O2D-CED
22	3	602	CLA	CBD-CGD-O2D-CED
22	3	606	CLA	CBD-CGD-O2D-CED
22	3	612	CLA	CBD-CGD-O2D-CED
22	3	613	CLA	CBD-CGD-O2D-CED
22	3	616	CLA	CBD-CGD-O2D-CED
22	4	603	CLA	CBD-CGD-O2D-CED
22	4	604	CLA	CBD-CGD-O2D-CED
22	4	606	CLA	CBD-CGD-O2D-CED
22	4	612	CLA	CBD-CGD-O2D-CED
22	4	616	CLA	CBD-CGD-O2D-CED
22	4	617	CLA	CBD-CGD-O2D-CED
22	5	601	CLA	CBD-CGD-O2D-CED
22	5	606	CLA	CBD-CGD-O2D-CED
22	5	607	CLA	CBD-CGD-O2D-CED
22	5	608	CLA	CBD-CGD-O2D-CED
22	5	609	CLA	CBD-CGD-O2D-CED
22	5	612	CLA	CBD-CGD-O2D-CED
22	5	618	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	6	602	CLA	CBD-CGD-O2D-CED
22	6	603	CLA	CBD-CGD-O2D-CED
22	6	605	CLA	CBD-CGD-O2D-CED
22	6	617	CLA	CBD-CGD-O2D-CED
22	7	601	CLA	CBD-CGD-O2D-CED
22	7	602	CLA	CBD-CGD-O2D-CED
22	7	608	CLA	CBD-CGD-O2D-CED
22	7	612	CLA	CBD-CGD-O2D-CED
22	7	615	CLA	CBD-CGD-O2D-CED
22	8	605	CLA	CBD-CGD-O2D-CED
22	8	608	CLA	CBD-CGD-O2D-CED
22	8	610	CLA	CBD-CGD-O2D-CED
22	8	615	CLA	CBD-CGD-O2D-CED
22	8	620	CLA	CBD-CGD-O2D-CED
39	4	609	CHL	CBD-CGD-O2D-CED
22	A	1118	CLA	O1A-CGA-O2A-C1
22	F	1301	CLA	O1A-CGA-O2A-C1
22	K	1404	CLA	O1A-CGA-O2A-C1
22	4	607	CLA	O1A-CGA-O2A-C1
22	8	606	CLA	O1A-CGA-O2A-C1
30	6	803	PCW	O11-C11-O3-C3
31	B	5005	PTY	O30-C30-O4-C1
32	F	5003	LAP	O2-C1-O1-C13
47	7	807	4RF	O42-C41-O40-C39
47	8	807	4RF	O17-C16-O18-C19
49	8	806	P5S	O18-C17-O19-C1
22	K	1401	CLA	O1A-CGA-O2A-C1
22	1	615	CLA	O1A-CGA-O2A-C1
22	3	618	CLA	O1A-CGA-O2A-C1
22	6	618	CLA	O1A-CGA-O2A-C1
22	7	605	CLA	C4C-C3C-CAC-CBC
22	A	1126	CLA	O1D-CGD-O2D-CED
22	A	1131	CLA	O1D-CGD-O2D-CED
22	B	1206	CLA	O1D-CGD-O2D-CED
22	B	1224	CLA	O1D-CGD-O2D-CED
22	1	602	CLA	O1D-CGD-O2D-CED
22	1	612	CLA	O1D-CGD-O2D-CED
22	4	616	CLA	O1D-CGD-O2D-CED
22	4	617	CLA	O1D-CGD-O2D-CED
22	7	612	CLA	O1D-CGD-O2D-CED
22	8	610	CLA	O1D-CGD-O2D-CED
22	8	615	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	A	1109	CLA	C15-C16-C17-C18
22	B	1234	CLA	C4C-C3C-CAC-CBC
25	F	5002	LHG	C5-C6-O8-C23
26	B	5003	DGD	C2G-C1G-O1G-C1A
32	F	5003	LAP	C14-C13-O1-C1
22	A	1107	CLA	O1D-CGD-O2D-CED
22	A	1111	CLA	O1D-CGD-O2D-CED
22	A	1114	CLA	O1D-CGD-O2D-CED
22	A	1140	CLA	O1D-CGD-O2D-CED
22	B	1207	CLA	O1D-CGD-O2D-CED
22	G	1603	CLA	O1D-CGD-O2D-CED
22	J	1901	CLA	O1D-CGD-O2D-CED
22	K	1402	CLA	O1D-CGD-O2D-CED
22	1	603	CLA	O1D-CGD-O2D-CED
22	1	611	CLA	O1D-CGD-O2D-CED
22	a	611	CLA	O1D-CGD-O2D-CED
22	3	605	CLA	O1D-CGD-O2D-CED
22	4	607	CLA	O1D-CGD-O2D-CED
22	4	615	CLA	O1D-CGD-O2D-CED
22	5	602	CLA	O1D-CGD-O2D-CED
22	5	603	CLA	O1D-CGD-O2D-CED
22	5	617	CLA	O1D-CGD-O2D-CED
22	6	608	CLA	O1D-CGD-O2D-CED
22	6	603	CLA	O1D-CGD-O2D-CED
22	8	603	CLA	O1D-CGD-O2D-CED
22	8	611	CLA	O1D-CGD-O2D-CED
22	8	620	CLA	O1D-CGD-O2D-CED
22	A	1118	CLA	CBA-CGA-O2A-C1
22	F	1301	CLA	CBA-CGA-O2A-C1
22	K	1404	CLA	CBA-CGA-O2A-C1
22	4	607	CLA	CBA-CGA-O2A-C1
22	7	615	CLA	CBA-CGA-O2A-C1
22	8	606	CLA	CBA-CGA-O2A-C1
31	B	5005	PTY	C31-C30-O4-C1
47	7	807	4RF	C43-C41-O40-C39
47	8	807	4RF	C15-C16-O18-C19
49	8	806	P5S	C20-C17-O19-C1
22	A	1103	CLA	CBD-CGD-O2D-CED
22	A	1104	CLA	CBD-CGD-O2D-CED
22	A	1106	CLA	CBD-CGD-O2D-CED
22	A	1110	CLA	CBD-CGD-O2D-CED
22	A	1113	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	A	1118	CLA	CBD-CGD-O2D-CED
22	A	1128	CLA	CBD-CGD-O2D-CED
22	A	1129	CLA	CBD-CGD-O2D-CED
22	A	1130	CLA	CBD-CGD-O2D-CED
22	B	1201	CLA	CBD-CGD-O2D-CED
22	B	1205	CLA	CBD-CGD-O2D-CED
22	B	1209	CLA	CBD-CGD-O2D-CED
22	B	1225	CLA	CBD-CGD-O2D-CED
22	B	1230	CLA	CBD-CGD-O2D-CED
22	B	1234	CLA	CBD-CGD-O2D-CED
22	B	1238	CLA	CBD-CGD-O2D-CED
22	B	1228	CLA	CBD-CGD-O2D-CED
22	K	1403	CLA	CBD-CGD-O2D-CED
22	L	1502	CLA	CBD-CGD-O2D-CED
22	1	604	CLA	CBD-CGD-O2D-CED
22	1	608	CLA	CBD-CGD-O2D-CED
22	1	610	CLA	CBD-CGD-O2D-CED
22	a	601	CLA	CBD-CGD-O2D-CED
22	3	604	CLA	CBD-CGD-O2D-CED
22	3	610	CLA	CBD-CGD-O2D-CED
22	6	601	CLA	CBD-CGD-O2D-CED
22	6	615	CLA	CBD-CGD-O2D-CED
22	7	609	CLA	CBD-CGD-O2D-CED
22	8	609	CLA	CBD-CGD-O2D-CED
22	8	602	CLA	CBD-CGD-O2D-CED
22	8	618	CLA	CBD-CGD-O2D-CED
39	a	610	CHL	CBD-CGD-O2D-CED
22	A	1122	CLA	O1A-CGA-O2A-C1
22	A	1101	CLA	O1A-CGA-O2A-C1
22	B	1201	CLA	O1A-CGA-O2A-C1
22	B	1206	CLA	O1A-CGA-O2A-C1
22	B	1219	CLA	O1A-CGA-O2A-C1
22	1	607	CLA	O1A-CGA-O2A-C1
22	3	603	CLA	O1A-CGA-O2A-C1
22	3	610	CLA	O1A-CGA-O2A-C1
22	3	612	CLA	O1A-CGA-O2A-C1
22	6	607	CLA	O1A-CGA-O2A-C1
22	6	615	CLA	O1A-CGA-O2A-C1
22	7	610	CLA	O1A-CGA-O2A-C1
22	7	615	CLA	O1A-CGA-O2A-C1
22	8	609	CLA	O1A-CGA-O2A-C1
30	B	5004	PCW	O11-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
33	G	5001	SQD	O10-C23-O48-C46
33	7	805	SQD	O10-C23-O48-C46
44	5	803	DGA	OA1-CA1-OG1-CG1
47	8	807	4RF	O42-C41-O40-C39
22	K	1403	CLA	O1A-CGA-O2A-C1
22	6	605	CLA	O1A-CGA-O2A-C1
22	A	1013	CLA	O1D-CGD-O2D-CED
22	A	1116	CLA	O1D-CGD-O2D-CED
22	A	1119	CLA	O1D-CGD-O2D-CED
22	B	1022	CLA	O1D-CGD-O2D-CED
22	1	615	CLA	O1D-CGD-O2D-CED
22	a	603	CLA	O1D-CGD-O2D-CED
22	4	602	CLA	O1D-CGD-O2D-CED
22	4	611	CLA	O1D-CGD-O2D-CED
22	7	610	CLA	O1D-CGD-O2D-CED
22	A	1121	CLA	O1D-CGD-O2D-CED
22	B	1220	CLA	O1D-CGD-O2D-CED
22	B	1229	CLA	O1D-CGD-O2D-CED
22	G	1601	CLA	O1D-CGD-O2D-CED
22	a	607	CLA	O1D-CGD-O2D-CED
22	3	618	CLA	O1D-CGD-O2D-CED
22	5	614	CLA	O1D-CGD-O2D-CED
22	6	618	CLA	O1D-CGD-O2D-CED
22	7	603	CLA	O1D-CGD-O2D-CED
22	8	606	CLA	O1D-CGD-O2D-CED
22	L	1503	CLA	C2C-C3C-CAC-CBC
22	L	1503	CLA	C4C-C3C-CAC-CBC
22	A	1102	CLA	CBD-CGD-O2D-CED
22	B	1214	CLA	CBD-CGD-O2D-CED
22	B	1240	CLA	CBD-CGD-O2D-CED
22	3	601	CLA	CBD-CGD-O2D-CED
22	5	605	CLA	CBD-CGD-O2D-CED
22	6	612	CLA	CBD-CGD-O2D-CED
22	7	617	CLA	CBD-CGD-O2D-CED
22	A	1135	CLA	C8-C10-C11-C12
22	B	1021	CLA	C5-C6-C7-C8
22	F	1302	CLA	C5-C6-C7-C8
22	A	1112	CLA	O1D-CGD-O2D-CED
22	B	1226	CLA	O1D-CGD-O2D-CED
22	6	605	CLA	O1D-CGD-O2D-CED
22	7	601	CLA	O1D-CGD-O2D-CED
25	A	5003	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
25	F	5002	LHG	O9-C7-O7-C5
25	F	5001	LHG	O9-C7-O7-C5
25	1	802	LHG	O9-C7-O7-C5
25	a	801	LHG	O9-C7-O7-C5
25	4	802	LHG	O9-C7-O7-C5
26	8	802	DGD	O1B-C1B-O2G-C2G
27	A	5007	3PH	O22-C21-O21-C2
31	5	802	PTY	O10-C8-O7-C6
31	7	804	PTY	O10-C8-O7-C6
44	8	803	DGA	OB1-CB1-OG2-CG2
47	8	807	4RF	O23-C22-O21-C20
47	8	808	4RF	O23-C22-O21-C20
25	F	5002	LHG	O10-C23-O8-C6
47	8	808	4RF	O17-C16-O18-C19
22	5	616	CLA	CBA-CGA-O2A-C1
22	F	1302	CLA	C4C-C3C-CAC-CBC
22	A	1013	CLA	C3-C5-C6-C7
22	A	1109	CLA	C3-C5-C6-C7
22	A	1110	CLA	C3-C5-C6-C7
22	A	1114	CLA	C3-C5-C6-C7
22	A	1131	CLA	C3-C5-C6-C7
22	A	1133	CLA	C3-C5-C6-C7
22	A	1135	CLA	C3-C5-C6-C7
22	B	1203	CLA	C3-C5-C6-C7
22	B	1205	CLA	C3-C5-C6-C7
22	B	1206	CLA	C3-C5-C6-C7
22	B	1211	CLA	C3-C5-C6-C7
22	B	1218	CLA	C3-C5-C6-C7
22	B	1234	CLA	C3-C5-C6-C7
22	B	1204	CLA	C3-C5-C6-C7
22	1	604	CLA	C3-C5-C6-C7
22	1	612	CLA	C3-C5-C6-C7
22	a	603	CLA	C3-C5-C6-C7
22	3	603	CLA	C3-C5-C6-C7
22	3	605	CLA	C3-C5-C6-C7
22	3	613	CLA	C3-C5-C6-C7
22	3	616	CLA	C3-C5-C6-C7
22	4	612	CLA	C3-C5-C6-C7
22	6	601	CLA	C3-C5-C6-C7
22	7	609	CLA	C3-C5-C6-C7
22	8	618	CLA	C3-C5-C6-C7
39	4	609	CHL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	A	1122	CLA	CBA-CGA-O2A-C1
22	A	1126	CLA	CBA-CGA-O2A-C1
22	B	1023	CLA	CBA-CGA-O2A-C1
22	B	1201	CLA	CBA-CGA-O2A-C1
22	B	1230	CLA	CBA-CGA-O2A-C1
22	B	1237	CLA	CBA-CGA-O2A-C1
22	B	1228	CLA	CBA-CGA-O2A-C1
22	1	603	CLA	CBA-CGA-O2A-C1
22	3	603	CLA	CBA-CGA-O2A-C1
22	3	610	CLA	CBA-CGA-O2A-C1
22	4	606	CLA	CBA-CGA-O2A-C1
22	6	607	CLA	CBA-CGA-O2A-C1
22	6	615	CLA	CBA-CGA-O2A-C1
22	7	610	CLA	CBA-CGA-O2A-C1
30	B	5004	PCW	C12-C11-O3-C3
30	6	803	PCW	C12-C11-O3-C3
32	F	5003	LAP	C2-C1-O1-C13
33	G	5001	SQD	C24-C23-O48-C46
33	7	805	SQD	C24-C23-O48-C46
44	5	803	DGA	CA2-CA1-OG1-CG1
22	6	612	CLA	C2C-C3C-CAC-CBC
29	B	5006	LMT	O5'-C5'-C6'-O6'
22	1	603	CLA	C5-C6-C7-C8
25	3	801	LHG	C8-C7-O7-C5
31	8	810	PTY	C11-C8-O7-C6
47	8	807	4RF	C24-C22-O21-C20
47	8	808	4RF	C24-C22-O21-C20
22	B	1211	CLA	O1D-CGD-O2D-CED
22	B	1239	CLA	O1D-CGD-O2D-CED
22	4	606	CLA	O1D-CGD-O2D-CED
22	5	609	CLA	O1D-CGD-O2D-CED
22	7	608	CLA	O1D-CGD-O2D-CED
22	B	1202	CLA	CBD-CGD-O2D-CED
22	6	609	CLA	CBD-CGD-O2D-CED
39	a	613	CHL	CBD-CGD-O2D-CED
22	5	607	CLA	O1A-CGA-O2A-C1
22	5	609	CLA	O1A-CGA-O2A-C1
22	4	604	CLA	O1D-CGD-O2D-CED
22	B	1236	CLA	C2C-C3C-CAC-CBC
22	a	615	CLA	CBA-CGA-O2A-C1
22	K	1404	CLA	C3-C5-C6-C7
22	4	602	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	8	602	CLA	C3-C5-C6-C7
22	A	1110	CLA	C4-C3-C5-C6
22	A	1128	CLA	C4-C3-C5-C6
22	A	1132	CLA	C4-C3-C5-C6
22	a	607	CLA	C4-C3-C5-C6
22	5	603	CLA	C4-C3-C5-C6
22	6	601	CLA	C4-C3-C5-C6
22	8	606	CLA	C4-C3-C5-C6
39	5	613	CHL	C4-C3-C5-C6
22	A	1130	CLA	C2-C3-C5-C6
22	B	1217	CLA	C2-C3-C5-C6
22	B	1218	CLA	C2-C3-C5-C6
22	3	603	CLA	C2-C3-C5-C6
22	7	611	CLA	C2-C3-C5-C6
22	8	606	CLA	C2-C3-C5-C6
39	4	609	CHL	C2-C3-C5-C6
39	5	613	CHL	C2-C3-C5-C6
22	A	1137	CLA	CBD-CGD-O2D-CED
22	B	1223	CLA	CBD-CGD-O2D-CED
22	3	603	CLA	CBD-CGD-O2D-CED
22	4	601	CLA	CBD-CGD-O2D-CED
22	A	1110	CLA	C2A-CAA-CBA-CGA
22	A	1114	CLA	C2A-CAA-CBA-CGA
22	A	1125	CLA	C2A-CAA-CBA-CGA
22	A	1129	CLA	C2A-CAA-CBA-CGA
22	B	1225	CLA	C2A-CAA-CBA-CGA
22	B	1232	CLA	C2A-CAA-CBA-CGA
22	B	1237	CLA	C2A-CAA-CBA-CGA
22	B	1204	CLA	C2A-CAA-CBA-CGA
22	1	610	CLA	C2A-CAA-CBA-CGA
22	a	611	CLA	C2A-CAA-CBA-CGA
22	3	603	CLA	C2A-CAA-CBA-CGA
22	3	612	CLA	C2A-CAA-CBA-CGA
22	5	609	CLA	C2A-CAA-CBA-CGA
22	5	616	CLA	C2A-CAA-CBA-CGA
22	7	612	CLA	C2A-CAA-CBA-CGA
22	8	612	CLA	C2A-CAA-CBA-CGA
39	1	609	CHL	C2A-CAA-CBA-CGA
39	a	613	CHL	C2A-CAA-CBA-CGA
22	B	1212	CLA	O1A-CGA-O2A-C1
22	B	1207	CLA	O1A-CGA-O2A-C1
22	a	611	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	a	605	CLA	O1D-CGD-O2D-CED
26	B	5003	DGD	C8A-C9A-CAA-CBA
26	B	5003	DGD	CBA-CCA-CDA-CEA
26	8	802	DGD	CEA-CFA-CGA-CHA
26	8	802	DGD	CEB-CFB-CGB-CHB
22	5	616	CLA	O1A-CGA-O2A-C1
22	A	1111	CLA	C3-C5-C6-C7
22	A	1130	CLA	C3-C5-C6-C7
22	A	1134	CLA	C3-C5-C6-C7
22	B	1214	CLA	C3-C5-C6-C7
22	B	1220	CLA	C3-C5-C6-C7
22	a	605	CLA	C3-C5-C6-C7
22	3	610	CLA	C3-C5-C6-C7
22	7	601	CLA	C3-C5-C6-C7
22	7	615	CLA	C3-C5-C6-C7
22	8	606	CLA	C3-C5-C6-C7
22	A	1117	CLA	CBA-CGA-O2A-C1
22	A	1119	CLA	CBA-CGA-O2A-C1
22	A	1125	CLA	CBA-CGA-O2A-C1
22	A	1101	CLA	CBA-CGA-O2A-C1
22	B	1206	CLA	CBA-CGA-O2A-C1
22	B	1219	CLA	CBA-CGA-O2A-C1
22	1	607	CLA	CBA-CGA-O2A-C1
22	1	611	CLA	CBA-CGA-O2A-C1
22	3	604	CLA	CBA-CGA-O2A-C1
22	3	607	CLA	CBA-CGA-O2A-C1
22	3	612	CLA	CBA-CGA-O2A-C1
22	4	604	CLA	CBA-CGA-O2A-C1
22	4	611	CLA	CBA-CGA-O2A-C1
22	8	609	CLA	CBA-CGA-O2A-C1
22	8	603	CLA	CBA-CGA-O2A-C1
25	F	5002	LHG	C24-C23-O8-C6
36	a	804	LPX	C7-C6-O6-C5
47	8	807	4RF	C43-C41-O40-C39
47	8	808	4RF	C15-C16-O18-C19
32	F	5003	LAP	C5-C6-C7-C8
22	B	1219	CLA	O1D-CGD-O2D-CED
22	K	1404	CLA	O1D-CGD-O2D-CED
22	3	613	CLA	O1D-CGD-O2D-CED
22	3	616	CLA	O1D-CGD-O2D-CED
22	A	1105	CLA	CBD-CGD-O2D-CED
22	A	1117	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	A	1122	CLA	O1D-CGD-O2D-CED
22	A	1135	CLA	O1D-CGD-O2D-CED
22	B	1210	CLA	O1D-CGD-O2D-CED
22	B	1212	CLA	O1D-CGD-O2D-CED
22	B	1215	CLA	O1D-CGD-O2D-CED
22	G	1602	CLA	O1D-CGD-O2D-CED
22	1	605	CLA	O1D-CGD-O2D-CED
22	5	601	CLA	O1D-CGD-O2D-CED
22	5	606	CLA	O1D-CGD-O2D-CED
22	5	607	CLA	O1D-CGD-O2D-CED
22	5	608	CLA	O1D-CGD-O2D-CED
22	7	602	CLA	O1D-CGD-O2D-CED
33	G	5001	SQD	O49-C7-O47-C45
44	5	803	DGA	OB1-CB1-OG2-CG2
22	A	1104	CLA	O1A-CGA-O2A-C1
22	A	1119	CLA	O1A-CGA-O2A-C1
22	B	1237	CLA	O1A-CGA-O2A-C1
22	B	1228	CLA	O1A-CGA-O2A-C1
22	1	603	CLA	O1A-CGA-O2A-C1
22	1	606	CLA	O1A-CGA-O2A-C1
22	1	611	CLA	O1A-CGA-O2A-C1
22	4	606	CLA	O1A-CGA-O2A-C1
22	4	611	CLA	O1A-CGA-O2A-C1
22	7	603	CLA	O1A-CGA-O2A-C1
22	8	620	CLA	O1A-CGA-O2A-C1
31	5	802	PTY	O30-C30-O4-C1
22	B	1216	CLA	O1D-CGD-O2D-CED
22	3	612	CLA	O1D-CGD-O2D-CED
22	6	602	CLA	O1D-CGD-O2D-CED
24	B	4006	BCR	C9-C10-C11-C12
24	7	503	BCR	C13-C14-C15-C16
24	7	503	BCR	C19-C20-C21-C22
38	5	505	LUT	C29-C30-C31-C32
22	A	1120	CLA	CBD-CGD-O2D-CED
22	A	1133	CLA	CBD-CGD-O2D-CED
22	A	1101	CLA	CBD-CGD-O2D-CED
22	3	607	CLA	CBD-CGD-O2D-CED
22	4	605	CLA	CBD-CGD-O2D-CED
22	5	604	CLA	CBD-CGD-O2D-CED
22	7	611	CLA	CBD-CGD-O2D-CED
21	A	1011	CL0	O1D-CGD-O2D-CED
22	A	1123	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	A	1127	CLA	O1D-CGD-O2D-CED
22	A	1132	CLA	O1D-CGD-O2D-CED
22	B	1203	CLA	O1D-CGD-O2D-CED
22	B	1213	CLA	O1D-CGD-O2D-CED
22	3	602	CLA	O1D-CGD-O2D-CED
25	A	5001	LHG	O2-C2-C3-O3
25	A	5003	LHG	O2-C2-C3-O3
25	1	801	LHG	O2-C2-C3-O3
25	a	801	LHG	O2-C2-C3-O3
25	3	801	LHG	O2-C2-C3-O3
25	4	801	LHG	O2-C2-C3-O3
25	5	801	LHG	O2-C2-C3-O3
25	6	801	LHG	O2-C2-C3-O3
25	8	801	LHG	O2-C2-C3-O3
32	F	5003	LAP	O3-C14-C15-O4
32	K	5001	LAP	O3-C14-C15-O4
36	J	5001	LPX	O1-C3-C4-O5
22	B	1208	CLA	C3-C5-C6-C7
22	B	1212	CLA	C3-C5-C6-C7
22	B	1207	CLA	C3-C5-C6-C7
22	K	1402	CLA	C3-C5-C6-C7
22	L	1502	CLA	C3-C5-C6-C7
22	1	603	CLA	C3-C5-C6-C7
22	3	601	CLA	C3-C5-C6-C7
22	4	601	CLA	C3-C5-C6-C7
22	4	615	CLA	C3-C5-C6-C7
22	8	603	CLA	C3-C5-C6-C7
22	8	610	CLA	C3-C5-C6-C7
22	A	1104	CLA	CBA-CGA-O2A-C1
22	B	1217	CLA	CBA-CGA-O2A-C1
22	B	1204	CLA	CBA-CGA-O2A-C1
22	1	606	CLA	CBA-CGA-O2A-C1
22	a	604	CLA	CBA-CGA-O2A-C1
22	a	607	CLA	CBA-CGA-O2A-C1
22	a	611	CLA	CBA-CGA-O2A-C1
22	4	616	CLA	CBA-CGA-O2A-C1
22	5	604	CLA	CBA-CGA-O2A-C1
22	5	607	CLA	CBA-CGA-O2A-C1
22	5	609	CLA	CBA-CGA-O2A-C1
22	5	612	CLA	CBA-CGA-O2A-C1
22	7	609	CLA	CBA-CGA-O2A-C1
22	7	607	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	8	620	CLA	CBA-CGA-O2A-C1
31	5	802	PTY	C31-C30-O4-C1
25	F	5002	LHG	C11-C12-C13-C14
25	5	801	LHG	C28-C29-C30-C31
22	A	1125	CLA	O1A-CGA-O2A-C1
22	A	1126	CLA	O1A-CGA-O2A-C1
22	B	1023	CLA	O1A-CGA-O2A-C1
22	B	1230	CLA	O1A-CGA-O2A-C1
22	5	604	CLA	O1A-CGA-O2A-C1
22	8	603	CLA	O1A-CGA-O2A-C1
22	A	1012	CLA	O1D-CGD-O2D-CED
22	A	1115	CLA	O1D-CGD-O2D-CED
22	A	1139	CLA	O1D-CGD-O2D-CED
22	B	1222	CLA	O1D-CGD-O2D-CED
22	B	1227	CLA	O1D-CGD-O2D-CED
39	4	609	CHL	O1D-CGD-O2D-CED
32	B	5007	LAP	O1-C13-C14-O3
25	A	5002	LHG	C8-C7-O7-C5
49	8	806	P5S	C39-C38-O37-C2
22	B	1236	CLA	CBD-CGD-O2D-CED
22	7	604	CLA	CBD-CGD-O2D-CED
25	7	801	LHG	C11-C12-C13-C14
25	7	801	LHG	C24-C25-C26-C27
32	F	5003	LAP	C7-C8-C9-C10
22	A	1117	CLA	O1A-CGA-O2A-C1
22	3	607	CLA	O1A-CGA-O2A-C1
22	4	616	CLA	O1A-CGA-O2A-C1
22	5	612	CLA	O1A-CGA-O2A-C1
36	a	804	LPX	O7-C6-O6-C5
25	4	801	LHG	C34-C35-C36-C37
29	A	5008	LMT	C5'-C4'-O1B-C1B
29	B	5006	LMT	C4'-C5'-C6'-O6'
22	A	1125	CLA	O1D-CGD-O2D-CED
22	A	1134	CLA	O1D-CGD-O2D-CED
22	1	601	CLA	O1D-CGD-O2D-CED
22	1	606	CLA	O1D-CGD-O2D-CED
22	5	612	CLA	O1D-CGD-O2D-CED
44	8	803	DGA	CB9-CAB-CBB-CCB
22	A	1103	CLA	C3-C5-C6-C7
22	7	617	CLA	C3-C5-C6-C7
22	A	1106	CLA	CBA-CGA-O2A-C1
22	B	1212	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	B	1207	CLA	CBA-CGA-O2A-C1
22	4	612	CLA	CBA-CGA-O2A-C1
22	7	603	CLA	CBA-CGA-O2A-C1
22	B	1231	CLA	O1D-CGD-O2D-CED
29	A	5008	LMT	O5'-C5'-C6'-O6'
49	8	806	P5S	O47-C38-O37-C2
25	6	801	LHG	C2-C3-O3-P
49	8	806	P5S	C2-C3-O16-P12
22	B	1217	CLA	O1A-CGA-O2A-C1
22	3	604	CLA	O1A-CGA-O2A-C1
22	4	604	CLA	O1A-CGA-O2A-C1
22	7	609	CLA	O1A-CGA-O2A-C1
22	7	607	CLA	O1A-CGA-O2A-C1
22	K	1401	CLA	O1D-CGD-O2D-CED
22	a	615	CLA	O1A-CGA-O2A-C1
22	A	1123	CLA	C8-C10-C11-C12
22	B	1228	CLA	C4-C3-C5-C6
22	3	610	CLA	C4-C3-C5-C6
22	4	612	CLA	C4-C3-C5-C6
22	A	1128	CLA	C2-C3-C5-C6
22	B	1236	CLA	C2-C3-C5-C6
22	B	1228	CLA	C2-C3-C5-C6
22	3	610	CLA	C2-C3-C5-C6
22	4	612	CLA	C2-C3-C5-C6
25	6	801	LHG	C23-C24-C25-C26
22	A	1127	CLA	C2A-CAA-CBA-CGA
22	A	1134	CLA	C2A-CAA-CBA-CGA
22	A	1139	CLA	C2A-CAA-CBA-CGA
22	B	1227	CLA	C2A-CAA-CBA-CGA
22	G	1602	CLA	C2A-CAA-CBA-CGA
22	K	1404	CLA	C2A-CAA-CBA-CGA
22	1	611	CLA	C2A-CAA-CBA-CGA
22	A	1104	CLA	O1D-CGD-O2D-CED
22	B	1237	CLA	O1D-CGD-O2D-CED
36	a	804	LPX	C12-C13-C14-C15
22	B	1204	CLA	O1A-CGA-O2A-C1
22	a	607	CLA	O1A-CGA-O2A-C1
22	A	1120	CLA	CBA-CGA-O2A-C1
22	4	603	CLA	CBA-CGA-O2A-C1
22	7	601	CLA	CBA-CGA-O2A-C1
22	8	618	CLA	CBA-CGA-O2A-C1
25	6	802	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
32	K	5001	LAP	C2-C1-O1-C13
31	8	810	PTY	C14-C15-C16-C17
22	L	1503	CLA	O1D-CGD-O2D-CED
22	B	1217	CLA	O1D-CGD-O2D-CED
22	1	604	CLA	O1D-CGD-O2D-CED
22	1	610	CLA	O1D-CGD-O2D-CED
22	4	612	CLA	O1D-CGD-O2D-CED
22	a	604	CLA	O1A-CGA-O2A-C1
22	4	612	CLA	O1A-CGA-O2A-C1
25	7	803	LHG	C8-C7-O7-C5
22	A	1118	CLA	O1D-CGD-O2D-CED
22	B	1225	CLA	O1D-CGD-O2D-CED
22	1	608	CLA	O1D-CGD-O2D-CED
22	a	601	CLA	O1D-CGD-O2D-CED
22	8	602	CLA	O1D-CGD-O2D-CED
22	1	607	CLA	CBD-CGD-O2D-CED
25	5	801	LHG	C7-C8-C9-C10
22	B	1205	CLA	O1D-CGD-O2D-CED
22	3	604	CLA	O1D-CGD-O2D-CED
25	A	5003	LHG	C1-C2-C3-O3
25	4	801	LHG	C1-C2-C3-O3
25	5	801	LHG	C1-C2-C3-O3
32	F	5003	LAP	C13-C14-C15-O4
25	7	803	LHG	O9-C7-O7-C5
22	A	1106	CLA	O1A-CGA-O2A-C1
22	A	1120	CLA	O1A-CGA-O2A-C1
32	K	5001	LAP	O2-C1-O1-C13
25	1	802	LHG	C9-C10-C11-C12
22	A	1106	CLA	O1D-CGD-O2D-CED
22	A	1129	CLA	O1D-CGD-O2D-CED
22	B	1230	CLA	O1D-CGD-O2D-CED
22	B	1228	CLA	O1D-CGD-O2D-CED
22	L	1502	CLA	O1D-CGD-O2D-CED
22	A	1102	CLA	CBA-CGA-O2A-C1
22	A	1113	CLA	CBA-CGA-O2A-C1
22	A	1121	CLA	CBA-CGA-O2A-C1
22	A	1124	CLA	CBA-CGA-O2A-C1
22	A	1136	CLA	CBA-CGA-O2A-C1
22	A	1139	CLA	CBA-CGA-O2A-C1
22	A	1140	CLA	CBA-CGA-O2A-C1
22	B	1213	CLA	CBA-CGA-O2A-C1
22	B	1215	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	B	1231	CLA	CBA-CGA-O2A-C1
22	F	1302	CLA	CBA-CGA-O2A-C1
22	3	616	CLA	CBA-CGA-O2A-C1
22	4	608	CLA	CBA-CGA-O2A-C1
22	6	603	CLA	CBA-CGA-O2A-C1
22	7	606	CLA	CBA-CGA-O2A-C1
22	8	602	CLA	CBA-CGA-O2A-C1
22	8	610	CLA	CBA-CGA-O2A-C1
22	8	611	CLA	CBA-CGA-O2A-C1
25	7	803	LHG	C24-C23-O8-C6
26	B	5003	DGD	C2A-C1A-O1G-C1G
27	A	5007	3PH	C32-C31-O31-C3
22	A	1141	CLA	CBD-CGD-O2D-CED
22	a	604	CLA	CBD-CGD-O2D-CED
22	7	607	CLA	CBD-CGD-O2D-CED
22	8	612	CLA	CBD-CGD-O2D-CED
24	A	4002	BCR	C13-C14-C15-C16
24	J	4001	BCR	C9-C10-C11-C12
24	7	503	BCR	C9-C10-C11-C12
35	J	4002	RRX	C9-C10-C11-C12
22	6	612	CLA	C4C-C3C-CAC-CBC
22	A	1102	CLA	C10-C11-C12-C13
22	B	1214	CLA	C8-C10-C11-C12
22	7	606	CLA	O1A-CGA-O2A-C1
25	5	801	LHG	C31-C32-C33-C34
49	8	806	P5S	C41-C42-C43-C44
22	B	1201	CLA	O1D-CGD-O2D-CED
29	1	804	LMT	O5B-C5B-C6B-O6B
36	a	804	LPX	C16-C17-C18-C19
22	A	1013	CLA	C8-C10-C11-C12
22	B	1224	CLA	C8-C10-C11-C12
22	B	1231	CLA	C10-C11-C12-C13
22	3	616	CLA	C5-C6-C7-C8
22	5	607	CLA	C5-C6-C7-C8
22	5	614	CLA	CBA-CGA-O2A-C1
30	B	5004	PCW	C31-C32-C33-C34
31	7	804	PTY	C8-C11-C12-C13
22	A	1113	CLA	C3-C5-C6-C7
29	B	5006	LMT	C2'-C1'-O1'-C1
25	A	5002	LHG	O7-C5-C6-O8
25	1	801	LHG	O7-C5-C6-O8
22	A	1113	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	A	1124	CLA	O1A-CGA-O2A-C1
22	B	1215	CLA	O1A-CGA-O2A-C1
22	B	1231	CLA	O1A-CGA-O2A-C1
39	8	601	CHL	C4-C3-C5-C6
22	A	1110	CLA	C2-C3-C5-C6
22	A	1132	CLA	C2-C3-C5-C6
22	a	607	CLA	C2-C3-C5-C6
22	5	603	CLA	C2-C3-C5-C6
22	6	601	CLA	C2-C3-C5-C6
22	A	1013	CLA	C6-C7-C8-C9
22	A	1106	CLA	C6-C7-C8-C9
22	A	1111	CLA	C11-C10-C8-C9
22	A	1121	CLA	C6-C7-C8-C9
22	A	1122	CLA	C11-C10-C8-C9
22	A	1125	CLA	C14-C13-C15-C16
22	A	1126	CLA	C14-C13-C15-C16
22	A	1131	CLA	C11-C12-C13-C14
22	A	1133	CLA	C6-C7-C8-C9
22	B	1021	CLA	C11-C12-C13-C14
22	B	1023	CLA	C6-C7-C8-C9
22	B	1201	CLA	C11-C10-C8-C9
22	B	1202	CLA	C6-C7-C8-C9
22	B	1205	CLA	C14-C13-C15-C16
22	B	1210	CLA	C11-C12-C13-C14
22	B	1234	CLA	C6-C7-C8-C9
22	B	1238	CLA	C11-C10-C8-C9
22	B	1239	CLA	C14-C13-C15-C16
22	B	1204	CLA	C11-C10-C8-C9
22	L	1502	CLA	C11-C10-C8-C9
22	1	603	CLA	C11-C10-C8-C9
22	3	601	CLA	C11-C12-C13-C14
22	3	607	CLA	C14-C13-C15-C16
22	4	610	CLA	C11-C12-C13-C14
22	6	601	CLA	C6-C7-C8-C9
22	6	604	CLA	C14-C13-C15-C16
22	6	609	CLA	C6-C7-C8-C9
22	7	601	CLA	C11-C10-C8-C9
22	7	603	CLA	C14-C13-C15-C16
22	8	603	CLA	C11-C10-C8-C9
39	1	609	CHL	C6-C7-C8-C9
39	8	604	CHL	C11-C12-C13-C14
22	A	1103	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	K	1403	CLA	O1D-CGD-O2D-CED
22	B	1212	CLA	C2C-C3C-CAC-CBC
25	F	5002	LHG	C24-C25-C26-C27
25	3	801	LHG	C25-C26-C27-C28
22	A	1105	CLA	C5-C6-C7-C8
22	B	1201	CLA	C15-C16-C17-C18
22	B	1221	CLA	C15-C16-C17-C18
22	B	1228	CLA	C15-C16-C17-C18
22	7	612	CLA	C10-C11-C12-C13
22	B	1214	CLA	C2A-CAA-CBA-CGA
22	6	606	CLA	C2A-CAA-CBA-CGA
22	8	603	CLA	C2A-CAA-CBA-CGA
22	8	618	CLA	C2A-CAA-CBA-CGA
39	8	613	CHL	C2A-CAA-CBA-CGA
24	A	4002	BCR	C36-C18-C19-C20
24	A	4004	BCR	C7-C8-C9-C34
24	B	4005	BCR	C36-C18-C19-C20
24	B	4007	BCR	C11-C12-C13-C35
24	B	4006	BCR	C11-C12-C13-C35
24	F	4001	BCR	C36-C18-C19-C20
24	F	4001	BCR	C37-C22-C23-C24
24	J	4001	BCR	C7-C8-C9-C34
24	5	503	BCR	C37-C22-C23-C24
24	5	504	BCR	C37-C22-C23-C24
24	6	503	BCR	C37-C22-C23-C24
24	7	503	BCR	C36-C18-C19-C20
35	J	4002	RRX	C37-C22-C23-C24
35	J	4002	RRX	C11-C12-C13-C35
37	M	4001	ECH	C36-C18-C19-C20
38	a	502	LUT	C11-C12-C13-C20
38	5	505	LUT	C31-C32-C33-C40
38	6	502	LUT	C27-C28-C29-C39
24	A	4004	BCR	C7-C8-C9-C10
24	B	4005	BCR	C17-C18-C19-C20
24	B	4007	BCR	C11-C12-C13-C14
24	B	4006	BCR	C11-C12-C13-C14
24	F	4001	BCR	C21-C22-C23-C24
24	J	4001	BCR	C7-C8-C9-C10
24	5	503	BCR	C21-C22-C23-C24
24	5	504	BCR	C21-C22-C23-C24
24	6	504	BCR	C21-C22-C23-C24
24	6	503	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
24	7	503	BCR	C17-C18-C19-C20
35	J	4002	RRX	C11-C12-C13-C14
38	a	502	LUT	C11-C12-C13-C14
38	6	502	LUT	C27-C28-C29-C30
22	6	615	CLA	O1D-CGD-O2D-CED
22	8	609	CLA	O1D-CGD-O2D-CED
25	A	5002	LHG	O9-C7-O7-C5
25	F	5001	LHG	C23-C24-C25-C26
22	A	1102	CLA	O1A-CGA-O2A-C1
22	A	1121	CLA	O1A-CGA-O2A-C1
22	A	1139	CLA	O1A-CGA-O2A-C1
22	3	616	CLA	O1A-CGA-O2A-C1
22	6	603	CLA	O1A-CGA-O2A-C1
22	8	602	CLA	O1A-CGA-O2A-C1
22	8	610	CLA	O1A-CGA-O2A-C1
22	A	1112	CLA	C5-C6-C7-C8
22	A	1134	CLA	C8-C10-C11-C12
22	B	1022	CLA	C13-C15-C16-C17
22	B	1021	CLA	C10-C11-C12-C13
22	B	1205	CLA	C15-C16-C17-C18
22	B	1210	CLA	C15-C16-C17-C18
22	B	1215	CLA	C5-C6-C7-C8
22	B	1216	CLA	C5-C6-C7-C8
22	B	1231	CLA	C15-C16-C17-C18
22	B	1235	CLA	C5-C6-C7-C8
22	3	606	CLA	C5-C6-C7-C8
22	6	604	CLA	C5-C6-C7-C8
39	7	613	CHL	C10-C11-C12-C13
22	3	602	CLA	CBA-CGA-O2A-C1
22	A	1136	CLA	CBD-CGD-O2D-CED
45	6	806	SPH	C13-C14-C15-C16
22	A	1113	CLA	O1D-CGD-O2D-CED
22	6	601	CLA	O1D-CGD-O2D-CED
22	B	1021	CLA	C3-C5-C6-C7
22	7	610	CLA	C3-C5-C6-C7
22	A	1112	CLA	CBA-CGA-O2A-C1
22	A	1135	CLA	CBA-CGA-O2A-C1
22	4	610	CLA	CBA-CGA-O2A-C1
22	5	606	CLA	CBA-CGA-O2A-C1
22	7	604	CLA	CBA-CGA-O2A-C1
22	A	1013	CLA	C5-C6-C7-C8
22	A	1127	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	A	1133	CLA	C8-C10-C11-C12
22	A	1101	CLA	C15-C16-C17-C18
22	B	1021	CLA	C8-C10-C11-C12
22	B	1023	CLA	C8-C10-C11-C12
22	B	1201	CLA	C5-C6-C7-C8
22	B	1203	CLA	C8-C10-C11-C12
22	B	1208	CLA	C10-C11-C12-C13
22	B	1210	CLA	C8-C10-C11-C12
22	B	1212	CLA	C10-C11-C12-C13
22	B	1226	CLA	C10-C11-C12-C13
22	B	1226	CLA	C15-C16-C17-C18
22	1	605	CLA	C15-C16-C17-C18
22	3	604	CLA	C10-C11-C12-C13
22	3	605	CLA	C13-C15-C16-C17
22	3	607	CLA	C13-C15-C16-C17
22	4	610	CLA	C8-C10-C11-C12
22	5	612	CLA	C5-C6-C7-C8
22	7	603	CLA	C5-C6-C7-C8
22	7	604	CLA	C10-C11-C12-C13
25	7	801	LHG	C23-C24-C25-C26
26	A	5005	DGD	C1A-C2A-C3A-C4A
31	8	810	PTY	C30-C31-C32-C33
44	8	803	DGA	CB1-CB2-CB3-CB4
47	8	808	4RF	C13-C14-C15-C16
22	A	1110	CLA	O1D-CGD-O2D-CED
22	3	610	CLA	O1D-CGD-O2D-CED
22	5	604	CLA	O1D-CGD-O2D-CED
22	7	609	CLA	O1D-CGD-O2D-CED
22	4	608	CLA	CBD-CGD-O2D-CED
22	B	1234	CLA	O1D-CGD-O2D-CED
22	8	608	CLA	O1D-CGD-O2D-CED
26	8	802	DGD	O6E-C5E-C6E-O5E
22	A	1104	CLA	C8-C10-C11-C12
22	A	1106	CLA	C10-C11-C12-C13
22	A	1106	CLA	C15-C16-C17-C18
22	A	1109	CLA	C13-C15-C16-C17
22	A	1110	CLA	C5-C6-C7-C8
22	A	1114	CLA	C10-C11-C12-C13
22	A	1126	CLA	C10-C11-C12-C13
22	A	1131	CLA	C5-C6-C7-C8
22	B	1021	CLA	C13-C15-C16-C17
22	B	1209	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	B	1214	CLA	C5-C6-C7-C8
22	B	1223	CLA	C8-C10-C11-C12
22	B	1231	CLA	C13-C15-C16-C17
22	B	1239	CLA	C5-C6-C7-C8
22	B	1228	CLA	C13-C15-C16-C17
22	B	1229	CLA	C13-C15-C16-C17
22	1	608	CLA	C5-C6-C7-C8
22	1	612	CLA	C15-C16-C17-C18
22	3	601	CLA	C10-C11-C12-C13
22	3	605	CLA	C5-C6-C7-C8
22	3	605	CLA	C15-C16-C17-C18
22	7	603	CLA	C8-C10-C11-C12
22	7	603	CLA	C13-C15-C16-C17
22	8	603	CLA	C5-C6-C7-C8
22	8	620	CLA	C10-C11-C12-C13
22	8	620	CLA	C15-C16-C17-C18
25	A	5003	LHG	O1-C1-C2-O2
25	a	801	LHG	O1-C1-C2-O2
25	7	802	LHG	O1-C1-C2-O2
22	B	1213	CLA	O1A-CGA-O2A-C1
22	F	1302	CLA	O1A-CGA-O2A-C1
25	A	5002	LHG	C23-C24-C25-C26
25	5	801	LHG	C23-C24-C25-C26
25	6	802	LHG	C7-C8-C9-C10
25	7	803	LHG	C23-C24-C25-C26
25	8	801	LHG	C23-C24-C25-C26
30	B	5004	PCW	C11-C12-C13-C14
31	8	810	PTY	C8-C11-C12-C13
47	7	807	4RF	C41-C43-C44-C45
22	B	1238	CLA	O1D-CGD-O2D-CED
22	A	1130	CLA	C5-C6-C7-C8
22	A	1135	CLA	C13-C15-C16-C17
22	B	1206	CLA	C5-C6-C7-C8
22	B	1210	CLA	C13-C15-C16-C17
22	B	1212	CLA	C5-C6-C7-C8
22	B	1213	CLA	C5-C6-C7-C8
22	B	1216	CLA	C10-C11-C12-C13
22	1	606	CLA	C5-C6-C7-C8
22	a	601	CLA	C5-C6-C7-C8
22	3	601	CLA	C15-C16-C17-C18
22	3	610	CLA	C5-C6-C7-C8
22	4	610	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	7	601	CLA	C10-C11-C12-C13
22	B	1210	CLA	CBA-CGA-O2A-C1
22	a	602	CLA	CBA-CGA-O2A-C1
26	8	802	DGD	C2A-C1A-O1G-C1G
25	4	802	LHG	C11-C12-C13-C14
25	7	801	LHG	C26-C27-C28-C29
22	A	1128	CLA	O1D-CGD-O2D-CED
22	A	1130	CLA	O1D-CGD-O2D-CED
22	5	605	CLA	O1D-CGD-O2D-CED
22	8	618	CLA	O1D-CGD-O2D-CED
39	a	610	CHL	O1D-CGD-O2D-CED
29	1	804	LMT	O5'-C5'-C6'-O6'
22	A	1111	CLA	C2-C1-O2A-CGA
22	A	1120	CLA	C2-C1-O2A-CGA
22	A	1133	CLA	C2-C1-O2A-CGA
22	B	1022	CLA	C2-C1-O2A-CGA
22	B	1220	CLA	C2-C1-O2A-CGA
22	B	1236	CLA	C2-C1-O2A-CGA
22	B	1238	CLA	C2-C1-O2A-CGA
22	B	1228	CLA	C2-C1-O2A-CGA
22	B	1229	CLA	C2-C1-O2A-CGA
22	1	608	CLA	C2-C1-O2A-CGA
22	1	611	CLA	C2-C1-O2A-CGA
22	4	610	CLA	C2-C1-O2A-CGA
22	4	611	CLA	C2-C1-O2A-CGA
22	4	612	CLA	C2-C1-O2A-CGA
22	6	606	CLA	C2-C1-O2A-CGA
22	6	607	CLA	C2-C1-O2A-CGA
22	7	612	CLA	C2-C1-O2A-CGA
22	A	1122	CLA	C8-C10-C11-C12
22	A	1136	CLA	C5-C6-C7-C8
22	B	1204	CLA	C10-C11-C12-C13
22	4	604	CLA	C8-C10-C11-C12
22	B	1214	CLA	O1D-CGD-O2D-CED
31	B	5005	PTY	C8-C11-C12-C13
47	7	807	4RF	C22-C24-C25-C26
22	B	1236	CLA	C4C-C3C-CAC-CBC
22	A	1108	CLA	C10-C11-C12-C13
22	A	1122	CLA	C15-C16-C17-C18
22	3	603	CLA	C5-C6-C7-C8
22	7	617	CLA	O1D-CGD-O2D-CED
22	A	1012	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	A	1103	CLA	C6-C7-C8-C10
22	A	1104	CLA	C6-C7-C8-C10
22	A	1108	CLA	C12-C13-C15-C16
22	A	1121	CLA	C6-C7-C8-C10
22	A	1126	CLA	C6-C7-C8-C10
22	B	1021	CLA	C12-C13-C15-C16
22	B	1203	CLA	C11-C10-C8-C7
22	B	1213	CLA	C6-C7-C8-C10
22	B	1214	CLA	C6-C7-C8-C10
22	B	1216	CLA	C11-C12-C13-C15
22	B	1220	CLA	C6-C7-C8-C10
22	B	1240	CLA	C12-C13-C15-C16
22	B	1204	CLA	C12-C13-C15-C16
22	3	613	CLA	C6-C7-C8-C10
22	3	616	CLA	C6-C7-C8-C10
22	6	604	CLA	C11-C10-C8-C7
22	7	604	CLA	C11-C12-C13-C15
39	6	619	CHL	C12-C13-C15-C16
39	7	613	CHL	C11-C10-C8-C7
39	7	613	CHL	C11-C12-C13-C15
22	B	1201	CLA	C3-C5-C6-C7
22	1	606	CLA	C3-C5-C6-C7
22	4	608	CLA	O1A-CGA-O2A-C1
27	A	5007	3PH	O32-C31-O31-C3
24	B	4007	BCR	C9-C10-C11-C12
24	K	4002	BCR	C9-C10-C11-C12
24	K	4002	BCR	C13-C14-C15-C16
24	3	505	BCR	C13-C14-C15-C16
24	5	503	BCR	C13-C14-C15-C16
24	5	504	BCR	C9-C10-C11-C12
24	5	504	BCR	C15-C16-C17-C18
22	B	1236	CLA	CBA-CGA-O2A-C1
22	A	1130	CLA	C2A-CAA-CBA-CGA
22	A	1140	CLA	C2A-CAA-CBA-CGA
22	B	1212	CLA	C2A-CAA-CBA-CGA
22	F	1302	CLA	C2A-CAA-CBA-CGA
22	1	612	CLA	C2A-CAA-CBA-CGA
22	4	604	CLA	C2A-CAA-CBA-CGA
39	5	613	CHL	C2A-CAA-CBA-CGA
22	B	1202	CLA	O1D-CGD-O2D-CED
22	3	601	CLA	O1D-CGD-O2D-CED
22	A	1111	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	B	1202	CLA	C8-C10-C11-C12
22	B	1212	CLA	C15-C16-C17-C18
22	B	1226	CLA	C13-C15-C16-C17
22	B	1231	CLA	C5-C6-C7-C8
22	1	601	CLA	C5-C6-C7-C8
22	a	604	CLA	C15-C16-C17-C18
22	3	607	CLA	C15-C16-C17-C18
22	3	612	CLA	C10-C11-C12-C13
39	4	609	CHL	C5-C6-C7-C8
22	A	1136	CLA	O1A-CGA-O2A-C1
22	4	603	CLA	O1A-CGA-O2A-C1
22	7	601	CLA	O1A-CGA-O2A-C1
22	8	611	CLA	O1A-CGA-O2A-C1
25	6	802	LHG	O10-C23-O8-C6
25	7	803	LHG	O10-C23-O8-C6
26	B	5003	DGD	O1A-C1A-O1G-C1G
22	4	601	CLA	O1D-CGD-O2D-CED
25	A	5001	LHG	C23-C24-C25-C26
25	B	5001	LHG	C23-C24-C25-C26
24	A	4001	BCR	C10-C11-C12-C13
24	A	4002	BCR	C10-C11-C12-C13
24	G	4001	BCR	C10-C11-C12-C13
24	3	505	BCR	C10-C11-C12-C13
24	4	503	BCR	C10-C11-C12-C13
26	A	5005	DGD	C8B-C9B-CAB-CBB
25	B	5002	LHG	O2-C2-C3-O3
25	6	802	LHG	O2-C2-C3-O3
32	B	5007	LAP	O3-C14-C15-O4
22	A	1122	CLA	C3-C5-C6-C7
22	A	1125	CLA	C3-C5-C6-C7
22	8	609	CLA	C3-C5-C6-C7
22	A	1012	CLA	C13-C15-C16-C17
22	A	1102	CLA	C15-C16-C17-C18
22	B	1023	CLA	C10-C11-C12-C13
22	B	1220	CLA	C8-C10-C11-C12
22	B	1238	CLA	C15-C16-C17-C18
22	B	1228	CLA	C5-C6-C7-C8
22	B	1207	CLA	C8-C10-C11-C12
22	1	603	CLA	C13-C15-C16-C17
22	4	604	CLA	C5-C6-C7-C8
22	4	612	CLA	C10-C11-C12-C13
22	7	603	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	B	1211	CLA	CBA-CGA-O2A-C1
25	7	801	LHG	C32-C33-C34-C35
22	A	1135	CLA	O1A-CGA-O2A-C1
22	A	1140	CLA	O1A-CGA-O2A-C1
22	B	1210	CLA	O1A-CGA-O2A-C1
22	8	618	CLA	O1A-CGA-O2A-C1
25	B	5002	LHG	C7-C8-C9-C10
22	A	1128	CLA	C15-C16-C17-C18
22	A	1134	CLA	C10-C11-C12-C13
22	A	1136	CLA	C15-C16-C17-C18
22	B	1023	CLA	C13-C15-C16-C17
22	B	1215	CLA	C10-C11-C12-C13
22	B	1239	CLA	C13-C15-C16-C17
22	B	1204	CLA	C15-C16-C17-C18
22	3	603	CLA	C10-C11-C12-C13
22	3	606	CLA	C13-C15-C16-C17
22	4	603	CLA	C5-C6-C7-C8
22	5	604	CLA	C15-C16-C17-C18
22	6	601	CLA	C8-C10-C11-C12
22	6	603	CLA	C15-C16-C17-C18
22	8	618	CLA	C5-C6-C7-C8
39	8	601	CHL	C5-C6-C7-C8
25	7	803	LHG	C18-C19-C20-C21
22	B	1209	CLA	O1D-CGD-O2D-CED
22	B	1240	CLA	O1D-CGD-O2D-CED
39	a	613	CHL	O1D-CGD-O2D-CED
22	5	606	CLA	O1A-CGA-O2A-C1
25	1	801	LHG	C8-C7-O7-C5
22	A	1102	CLA	O1D-CGD-O2D-CED
22	A	1111	CLA	C10-C11-C12-C13
22	A	1133	CLA	C13-C15-C16-C17
22	A	1138	CLA	C8-C10-C11-C12
22	B	1240	CLA	C5-C6-C7-C8
22	K	1402	CLA	C8-C10-C11-C12
22	7	609	CLA	C10-C11-C12-C13
22	8	609	CLA	C5-C6-C7-C8
22	8	603	CLA	C10-C11-C12-C13
39	6	619	CHL	C10-C11-C12-C13
25	A	5001	LHG	C3-O3-P-O6
25	A	5002	LHG	C3-O3-P-O6
25	A	5002	LHG	C4-O6-P-O3
25	A	5003	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
25	B	5002	LHG	C3-O3-P-O6
25	B	5002	LHG	C4-O6-P-O3
25	B	5001	LHG	C4-O6-P-O3
25	F	5001	LHG	C4-O6-P-O3
25	1	801	LHG	C4-O6-P-O3
25	1	802	LHG	C4-O6-P-O3
25	4	802	LHG	C4-O6-P-O3
25	6	802	LHG	C4-O6-P-O3
25	7	801	LHG	C4-O6-P-O3
25	7	803	LHG	C3-O3-P-O6
31	B	5005	PTY	C5-O14-P1-O11
31	3	802	PTY	C3-O11-P1-O14
31	3	802	PTY	C5-O14-P1-O11
32	F	5003	LAP	C15-O4-P9-O6
32	K	5001	LAP	C15-O4-P9-O6
32	K	5001	LAP	C16-O6-P9-O4
36	J	5001	LPX	C1-O2-P1-O1
49	8	806	P5S	C3-O16-P12-OG
22	A	1012	CLA	C3-C5-C6-C7
22	5	612	CLA	C3-C5-C6-C7
22	7	603	CLA	C3-C5-C6-C7
39	8	601	CHL	C3-C5-C6-C7
34	G	5002	ERG	C28-C24-C25-C26
22	A	1131	CLA	CBA-CGA-O2A-C1
22	5	603	CLA	CBA-CGA-O2A-C1
31	8	810	PTY	C31-C30-O4-C1
22	B	1223	CLA	O1D-CGD-O2D-CED
22	A	1136	CLA	C13-C15-C16-C17
22	B	1210	CLA	C10-C11-C12-C13
22	B	1224	CLA	C13-C15-C16-C17
22	4	601	CLA	C5-C6-C7-C8
39	7	613	CHL	C5-C6-C7-C8
22	3	603	CLA	O1D-CGD-O2D-CED
22	4	612	CLA	C13-C15-C16-C17
25	A	5003	LHG	C23-C24-C25-C26
40	8	809	OLA	C1-C2-C3-C4
47	8	808	4RF	C41-C43-C44-C45
22	6	612	CLA	O1D-CGD-O2D-CED
25	A	5001	LHG	C1-C2-C3-O3
25	B	5002	LHG	C1-C2-C3-O3
25	F	5002	LHG	C1-C2-C3-O3
25	a	801	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
25	7	802	LHG	C1-C2-C3-O3
32	B	5007	LAP	C13-C14-C15-O4
25	1	801	LHG	O9-C7-O7-C5
21	A	1011	CL0	C4-C3-C5-C6
22	A	1108	CLA	C8-C10-C11-C12
22	A	1125	CLA	C13-C15-C16-C17
22	A	1132	CLA	C13-C15-C16-C17
22	1	604	CLA	C5-C6-C7-C8
22	6	615	CLA	C10-C11-C12-C13
32	F	5003	LAP	C16-C17-N8-C18
32	F	5003	LAP	C16-C17-N8-C19
32	F	5003	LAP	C16-C17-N8-C20
22	A	1113	CLA	C2A-CAA-CBA-CGA
22	1	603	CLA	C2A-CAA-CBA-CGA
22	a	608	CLA	C2A-CAA-CBA-CGA
22	3	604	CLA	C2A-CAA-CBA-CGA
22	5	607	CLA	C2A-CAA-CBA-CGA
22	7	603	CLA	C2A-CAA-CBA-CGA
22	B	1219	CLA	C3-C5-C6-C7
22	6	609	CLA	O1D-CGD-O2D-CED
22	A	1115	CLA	CBA-CGA-O2A-C1
22	B	1221	CLA	CBA-CGA-O2A-C1
31	5	802	PTY	C30-C31-C32-C33
22	A	1102	CLA	C5-C6-C7-C8
22	A	1117	CLA	C13-C15-C16-C17
22	8	609	CLA	C8-C10-C11-C12
25	6	802	LHG	C29-C30-C31-C32
47	8	808	4RF	C02-C03-C04-C05
24	A	4003	BCR	C9-C10-C11-C12
24	L	4001	BCR	C19-C20-C21-C22
24	5	503	BCR	C15-C16-C17-C18
38	a	502	LUT	C9-C10-C11-C12
25	F	5002	LHG	C7-C8-C9-C10
25	5	801	LHG	C12-C13-C14-C15
30	B	5004	PCW	C13-C14-C15-C16
25	B	5001	LHG	C8-C7-O7-C5
30	6	803	PCW	C32-C31-O2-C2
22	B	1235	CLA	C8-C10-C11-C12
22	1	605	CLA	C13-C15-C16-C17
22	4	607	CLA	C5-C6-C7-C8
24	A	4001	BCR	C11-C10-C9-C34
24	A	4005	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
24	K	4002	BCR	C11-C10-C9-C34
24	3	503	BCR	C11-C10-C9-C34
24	6	504	BCR	C11-C10-C9-C34
22	1	605	CLA	C3-C5-C6-C7
39	5	613	CHL	C3-C5-C6-C7
25	B	5002	LHG	C34-C35-C36-C37
25	B	5001	LHG	C29-C30-C31-C32
25	4	801	LHG	C28-C29-C30-C31
25	7	801	LHG	C30-C31-C32-C33
26	B	5003	DGD	C3A-C4A-C5A-C6A
30	6	803	PCW	C12-C13-C14-C15
31	5	802	PTY	C11-C12-C13-C14
31	8	810	PTY	C17-C18-C19-C20
49	8	806	P5S	C39-C40-C41-C42
22	A	1112	CLA	O1A-CGA-O2A-C1
22	a	602	CLA	O1A-CGA-O2A-C1
22	A	1137	CLA	O1D-CGD-O2D-CED
22	A	1117	CLA	C16-C17-C18-C20
22	B	1231	CLA	C16-C17-C18-C19
22	B	1235	CLA	C16-C17-C18-C19
22	B	1239	CLA	C16-C17-C18-C19
22	a	604	CLA	C16-C17-C18-C20
22	4	607	CLA	C6-C7-C8-C10
22	6	615	CLA	C16-C17-C18-C19
22	8	609	CLA	C11-C12-C13-C14
22	8	620	CLA	C16-C17-C18-C19
22	A	1133	CLA	CBA-CGA-O2A-C1
22	B	1220	CLA	CBA-CGA-O2A-C1
22	1	607	CLA	C2C-C3C-CAC-CBC
25	4	801	LHG	C27-C28-C29-C30
25	5	801	LHG	C16-C17-C18-C19
25	7	801	LHG	C25-C26-C27-C28
25	7	802	LHG	C27-C28-C29-C30
26	8	802	DGD	C3A-C4A-C5A-C6A
44	5	803	DGA	CB2-CB3-CB4-CB5
33	G	5001	SQD	C44-C45-O47-C7
44	8	803	DGA	CG1-CG2-OG2-CB1
22	A	1117	CLA	O1D-CGD-O2D-CED
25	4	801	LHG	O9-C7-O7-C5
30	6	803	PCW	O31-C31-O2-C2
22	B	1208	CLA	C5-C6-C7-C8
22	a	605	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	6	601	CLA	C5-C6-C7-C8
32	F	5003	LAP	C1-C2-C3-C4
25	A	5003	LHG	C16-C17-C18-C19
25	4	801	LHG	C29-C30-C31-C32
25	6	801	LHG	C11-C12-C13-C14
29	1	804	LMT	C7-C8-C9-C10
43	4	803	PLM	C9-CA-CB-CC
22	7	604	CLA	O1D-CGD-O2D-CED
36	a	804	LPX	C4-C3-O1-P1
26	8	802	DGD	O1A-C1A-O1G-C1G
25	A	5002	LHG	C34-C35-C36-C37
32	K	5001	LAP	C3-C4-C5-C6
44	5	803	DGA	CA4-CA5-CA6-CA7
22	A	1125	CLA	C8-C10-C11-C12
22	B	1203	CLA	C10-C11-C12-C13
25	4	802	LHG	O2-C2-C3-O3
25	4	801	LHG	C13-C14-C15-C16
25	5	801	LHG	C9-C10-C11-C12
25	6	802	LHG	C11-C12-C13-C14
25	6	802	LHG	C28-C29-C30-C31
45	6	806	SPH	C14-C15-C16-C17
22	B	1221	CLA	C3-C5-C6-C7
25	3	801	LHG	C7-C8-C9-C10
25	4	801	LHG	C23-C24-C25-C26
36	a	804	LPX	C6-C7-C8-C9
22	A	1133	CLA	O1D-CGD-O2D-CED
22	A	1101	CLA	O1D-CGD-O2D-CED
22	B	1236	CLA	O1D-CGD-O2D-CED
22	3	607	CLA	O1D-CGD-O2D-CED
24	A	4001	BCR	C11-C10-C9-C8
24	A	4005	BCR	C11-C10-C9-C8
24	K	4002	BCR	C11-C10-C9-C8
24	3	503	BCR	C11-C10-C9-C8
24	6	504	BCR	C11-C10-C9-C8
24	6	503	BCR	C11-C10-C9-C8
22	7	612	CLA	CBA-CGA-O2A-C1
22	B	1219	CLA	C10-C11-C12-C13
25	B	5002	LHG	C13-C14-C15-C16
25	F	5002	LHG	C25-C26-C27-C28
25	3	801	LHG	C31-C32-C33-C34
25	7	801	LHG	C33-C34-C35-C36
25	7	803	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
27	A	5007	3PH	C22-C23-C24-C25
30	6	803	PCW	C14-C15-C16-C17
43	4	803	PLM	C5-C6-C7-C8
47	7	807	4RF	C08-C09-C10-C11
47	7	807	4RF	C12-C13-C14-C15
22	A	1101	CLA	C8-C10-C11-C12
22	B	1213	CLA	C10-C11-C12-C13
22	B	1236	CLA	O1A-CGA-O2A-C1
21	A	1011	CL0	C16-C17-C18-C20
22	A	1109	CLA	C16-C17-C18-C19
22	A	1118	CLA	C6-C7-C8-C10
22	A	1132	CLA	C16-C17-C18-C19
22	A	1139	CLA	C6-C7-C8-C10
22	B	1218	CLA	C6-C7-C8-C9
22	B	1224	CLA	C16-C17-C18-C19
22	1	605	CLA	C16-C17-C18-C19
22	3	603	CLA	C16-C17-C18-C19
22	8	603	CLA	C16-C17-C18-C20
39	4	609	CHL	C16-C17-C18-C20
22	A	1105	CLA	O1D-CGD-O2D-CED
22	A	1125	CLA	C4-C3-C5-C6
22	B	1229	CLA	C4-C3-C5-C6
25	A	5003	LHG	C13-C14-C15-C16
25	A	5003	LHG	C17-C18-C19-C20
25	3	801	LHG	C27-C28-C29-C30
25	5	801	LHG	C13-C14-C15-C16
29	B	5006	LMT	C5-C6-C7-C8
31	5	802	PTY	C32-C33-C34-C35
33	G	5001	SQD	C11-C10-C9-C8
45	6	806	SPH	C7-C8-C9-C10
39	8	601	CHL	C2-C3-C5-C6
22	A	1126	CLA	C6-C7-C8-C9
22	A	1138	CLA	C11-C10-C8-C9
22	B	1021	CLA	C11-C10-C8-C9
22	B	1212	CLA	C11-C12-C13-C14
22	B	1225	CLA	C14-C13-C15-C16
22	B	1237	CLA	C11-C10-C8-C9
22	1	603	CLA	C11-C12-C13-C14
22	1	604	CLA	C11-C10-C8-C9
22	7	604	CLA	C11-C10-C8-C9
39	4	609	CHL	C11-C12-C13-C14
39	7	613	CHL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	A	1105	CLA	C8-C10-C11-C12
49	8	806	P5S	OXT-C-CA-N
25	1	801	LHG	C23-C24-C25-C26
25	A	5003	LHG	C11-C12-C13-C14
25	B	5002	LHG	C31-C32-C33-C34
25	4	801	LHG	C26-C27-C28-C29
32	K	5001	LAP	C2-C3-C4-C5
36	a	804	LPX	C7-C8-C9-C10
45	6	806	SPH	C10-C11-C12-C13
22	A	1108	CLA	C13-C15-C16-C17
22	B	1201	CLA	C13-C15-C16-C17
22	8	610	CLA	C5-C6-C7-C8
22	8	607	CLA	CBA-CGA-O2A-C1
22	A	1118	CLA	C2A-CAA-CBA-CGA
22	A	1138	CLA	C2A-CAA-CBA-CGA
22	A	1141	CLA	C2A-CAA-CBA-CGA
22	B	1023	CLA	C2A-CAA-CBA-CGA
22	B	1239	CLA	C2A-CAA-CBA-CGA
22	1	602	CLA	C2A-CAA-CBA-CGA
22	5	603	CLA	C2A-CAA-CBA-CGA
22	5	604	CLA	C2A-CAA-CBA-CGA
22	6	603	CLA	C2A-CAA-CBA-CGA
39	3	611	CHL	C2A-CAA-CBA-CGA
39	6	611	CHL	C2A-CAA-CBA-CGA
39	8	604	CHL	C2A-CAA-CBA-CGA
22	B	1211	CLA	O1A-CGA-O2A-C1
22	B	1221	CLA	O1A-CGA-O2A-C1
22	4	610	CLA	O1A-CGA-O2A-C1
24	G	4001	BCR	C37-C22-C23-C24
38	a	502	LUT	C27-C28-C29-C39
48	7	504	C7Z	C27-C28-C29-C39
25	F	5001	LHG	C13-C14-C15-C16
25	3	801	LHG	C26-C27-C28-C29
25	6	801	LHG	C13-C14-C15-C16
25	6	801	LHG	C31-C32-C33-C34
32	F	5003	LAP	C3-C4-C5-C6
33	G	5001	SQD	C13-C14-C15-C16
36	a	804	LPX	C15-C16-C17-C18
25	F	5002	LHG	O1-C1-C2-C3
25	1	801	LHG	O1-C1-C2-C3
25	a	801	LHG	O1-C1-C2-C3
25	7	802	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
25	8	801	LHG	O1-C1-C2-C3
24	A	4004	BCR	C11-C12-C13-C14
24	B	4007	BCR	C17-C18-C19-C20
24	G	4001	BCR	C21-C22-C23-C24
24	3	504	BCR	C17-C18-C19-C20
24	7	503	BCR	C11-C12-C13-C14
35	J	4002	RRX	C21-C22-C23-C24
38	7	501	LUT	C27-C28-C29-C30
48	7	504	C7Z	C27-C28-C29-C30
32	K	5001	LAP	O1-C13-C14-O3
25	B	5001	LHG	O9-C7-O7-C5
22	B	1224	CLA	C10-C11-C12-C13
22	6	603	CLA	C10-C11-C12-C13
25	B	5002	LHG	C8-C7-O7-C5
22	B	1212	CLA	C4C-C3C-CAC-CBC
25	A	5003	LHG	C12-C13-C14-C15
25	a	801	LHG	C28-C29-C30-C31
25	8	801	LHG	C26-C27-C28-C29
31	8	810	PTY	C13-C14-C15-C16
31	8	810	PTY	C32-C33-C34-C35
43	4	803	PLM	CA-CB-CC-CD
47	8	807	4RF	C27-C28-C29-C30
25	6	802	LHG	C23-C24-C25-C26
32	B	5007	LAP	C1-C2-C3-C4
22	4	605	CLA	O1D-CGD-O2D-CED
25	B	5001	LHG	C9-C10-C11-C12
25	F	5001	LHG	C11-C12-C13-C14
25	F	5001	LHG	C16-C17-C18-C19
25	1	802	LHG	C11-C12-C13-C14
25	1	802	LHG	C14-C15-C16-C17
25	a	801	LHG	C30-C31-C32-C33
25	4	801	LHG	C11-C12-C13-C14
25	4	801	LHG	C31-C32-C33-C34
25	5	801	LHG	C34-C35-C36-C37
25	7	801	LHG	C28-C29-C30-C31
25	8	801	LHG	C11-C12-C13-C14
26	B	5003	DGD	C6A-C7A-C8A-C9A
26	B	5003	DGD	C9A-CAA-CBA-CCA
29	1	804	LMT	C3-C4-C5-C6
31	B	5005	PTY	C15-C16-C17-C18
32	B	5007	LAP	C3-C4-C5-C6
45	6	806	SPH	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
47	8	808	4RF	C45-C46-C47-C48
22	A	1136	CLA	C16-C17-C18-C19
22	B	1022	CLA	C16-C17-C18-C19
22	B	1021	CLA	C16-C17-C18-C19
22	B	1206	CLA	C6-C7-C8-C10
22	B	1211	CLA	C6-C7-C8-C9
22	B	1215	CLA	C11-C12-C13-C14
22	B	1238	CLA	C16-C17-C18-C19
22	B	1238	CLA	C16-C17-C18-C20
22	F	1302	CLA	C6-C7-C8-C9
22	F	1302	CLA	C6-C7-C8-C10
22	6	603	CLA	C16-C17-C18-C19
22	6	603	CLA	C16-C17-C18-C20
22	6	607	CLA	C6-C7-C8-C9
22	6	607	CLA	C6-C7-C8-C10
22	6	615	CLA	C16-C17-C18-C20
22	7	612	CLA	C11-C12-C13-C14
22	7	615	CLA	C6-C7-C8-C9
22	7	615	CLA	C6-C7-C8-C10
22	8	609	CLA	C11-C12-C13-C15
22	8	620	CLA	C16-C17-C18-C20
39	7	613	CHL	C16-C17-C18-C20
29	1	804	LMT	O5'-C1'-O1'-C1
39	6	619	CHL	C13-C15-C16-C17
25	B	5002	LHG	C33-C34-C35-C36
25	1	801	LHG	C28-C29-C30-C31
25	7	802	LHG	C28-C29-C30-C31
25	7	803	LHG	C10-C11-C12-C13
29	B	5006	LMT	C4-C5-C6-C7
31	B	5005	PTY	C24-C25-C26-C27
22	4	605	CLA	CBA-CGA-O2A-C1
22	7	611	CLA	O1D-CGD-O2D-CED
25	B	5002	LHG	C11-C10-C9-C8
25	1	802	LHG	C10-C11-C12-C13
25	3	801	LHG	C13-C14-C15-C16
25	3	801	LHG	C16-C17-C18-C19
25	6	801	LHG	C27-C28-C29-C30
25	7	803	LHG	C17-C18-C19-C20
25	8	801	LHG	C25-C26-C27-C28
25	8	801	LHG	C29-C30-C31-C32
31	3	802	PTY	C16-C17-C18-C19
33	G	5001	SQD	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
25	a	801	LHG	C23-C24-C25-C26
25	7	803	LHG	C7-C8-C9-C10
22	A	1134	CLA	C5-C6-C7-C8
22	B	1237	CLA	C10-C11-C12-C13
22	5	603	CLA	O1A-CGA-O2A-C1
31	8	810	PTY	O30-C30-O4-C1
25	F	5001	LHG	C28-C29-C30-C31
30	B	5004	PCW	C12-C13-C14-C15
31	5	802	PTY	C33-C34-C35-C36
44	8	803	DGA	CB7-CB8-CB9-CAB
22	A	1120	CLA	O1D-CGD-O2D-CED
22	B	1216	CLA	C3-C5-C6-C7
22	5	607	CLA	C3-C5-C6-C7
22	6	606	CLA	CBA-CGA-O2A-C1
25	A	5002	LHG	C27-C28-C29-C30
25	A	5003	LHG	C26-C27-C28-C29
25	4	802	LHG	C9-C10-C11-C12
25	7	802	LHG	C11-C12-C13-C14
22	6	604	CLA	O1D-CGD-O2D-CED
22	A	1104	CLA	C3A-C2A-CAA-CBA
22	A	1107	CLA	C3A-C2A-CAA-CBA
22	A	1131	CLA	C3A-C2A-CAA-CBA
22	B	1201	CLA	C3A-C2A-CAA-CBA
22	B	1206	CLA	C3A-C2A-CAA-CBA
22	B	1208	CLA	C3A-C2A-CAA-CBA
22	B	1224	CLA	C3A-C2A-CAA-CBA
22	B	1228	CLA	C3A-C2A-CAA-CBA
22	B	1207	CLA	C3A-C2A-CAA-CBA
22	1	602	CLA	C3A-C2A-CAA-CBA
22	a	602	CLA	C3A-C2A-CAA-CBA
22	4	610	CLA	C3A-C2A-CAA-CBA
22	7	602	CLA	C3A-C2A-CAA-CBA
39	4	613	CHL	C3A-C2A-CAA-CBA
39	4	618	CHL	C3A-C2A-CAA-CBA
39	6	611	CHL	C3A-C2A-CAA-CBA
39	6	619	CHL	C3A-C2A-CAA-CBA
38	3	502	LUT	C29-C30-C31-C32
25	A	5002	LHG	C13-C14-C15-C16
44	5	803	DGA	CB1-CB2-CB3-CB4
22	7	604	CLA	O1A-CGA-O2A-C1
21	A	1011	CL0	C16-C17-C18-C19
22	A	1117	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
22	A	1136	CLA	C16-C17-C18-C20
22	B	1211	CLA	C6-C7-C8-C10
22	B	1218	CLA	C6-C7-C8-C10
22	B	1231	CLA	C16-C17-C18-C20
22	1	605	CLA	C16-C17-C18-C20
22	1	607	CLA	C16-C17-C18-C19
22	1	607	CLA	C16-C17-C18-C20
22	a	604	CLA	C16-C17-C18-C19
22	3	601	CLA	C16-C17-C18-C20
22	7	601	CLA	C11-C12-C13-C14
22	7	601	CLA	C11-C12-C13-C15
22	8	603	CLA	C16-C17-C18-C19
25	7	801	LHG	C11-C10-C9-C8
25	7	803	LHG	C16-C17-C18-C19
26	A	5005	DGD	C2A-C3A-C4A-C5A
29	B	5006	LMT	C11-C10-C9-C8
25	5	801	LHG	C4-C5-C6-O8
22	4	610	CLA	C3-C5-C6-C7
25	A	5003	LHG	C7-C8-C9-C10
25	a	801	LHG	C7-C8-C9-C10
22	7	602	CLA	C2C-C3C-CAC-CBC
47	7	807	4RF	C10-C11-C12-C13
22	A	1131	CLA	O1A-CGA-O2A-C1
22	B	1220	CLA	O1A-CGA-O2A-C1
22	A	1103	CLA	C4-C3-C5-C6
22	B	1205	CLA	C4-C3-C5-C6
22	B	1231	CLA	C4-C3-C5-C6
22	B	1234	CLA	C4-C3-C5-C6
22	4	603	CLA	C4-C3-C5-C6
22	B	1202	CLA	CBA-CGA-O2A-C1
22	1	604	CLA	CBA-CGA-O2A-C1
22	A	1103	CLA	C2-C3-C5-C6
22	A	1125	CLA	C2-C3-C5-C6
22	A	1101	CLA	C2-C3-C5-C6
22	B	1205	CLA	C2-C3-C5-C6
22	B	1231	CLA	C2-C3-C5-C6
22	B	1234	CLA	C2-C3-C5-C6
22	4	603	CLA	C2-C3-C5-C6
25	4	801	LHG	C8-C7-O7-C5
25	6	801	LHG	C8-C7-O7-C5
25	7	802	LHG	C8-C7-O7-C5
25	8	801	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
22	1	607	CLA	O1D-CGD-O2D-CED
22	A	1106	CLA	C2A-CAA-CBA-CGA
22	A	1101	CLA	C2A-CAA-CBA-CGA
25	B	5002	LHG	O1-C1-C2-O2
25	1	802	LHG	O1-C1-C2-O2
25	6	802	LHG	O1-C1-C2-O2
25	7	803	LHG	O1-C1-C2-O2
25	8	801	LHG	O1-C1-C2-O2
22	6	604	CLA	C8-C10-C11-C12
25	A	5002	LHG	C30-C31-C32-C33
25	B	5001	LHG	C28-C29-C30-C31
25	B	5001	LHG	C33-C34-C35-C36
25	4	801	LHG	C15-C16-C17-C18
36	a	804	LPX	C14-C15-C16-C17
45	6	806	SPH	C11-C12-C13-C14
22	a	612	CLA	C8-C10-C11-C12
22	A	1115	CLA	O1A-CGA-O2A-C1
22	7	604	CLA	C16-C17-C18-C20
22	A	1124	CLA	C5-C6-C7-C8
22	1	604	CLA	C15-C16-C17-C18
22	B	1215	CLA	C3-C5-C6-C7
41	3	506	QTB	C04-C05-C06-C08
25	A	5003	LHG	C14-C15-C16-C17
22	A	1133	CLA	O1A-CGA-O2A-C1
39	1	609	CHL	C5-C6-C7-C8
22	5	614	CLA	O1A-CGA-O2A-C1
25	A	5002	LHG	C9-C10-C11-C12
25	6	802	LHG	C26-C27-C28-C29
29	A	5008	LMT	C5-C6-C7-C8
31	7	804	PTY	C14-C15-C16-C17
32	B	5007	LAP	C5-C6-C7-C8
44	8	803	DGA	CAB-CBB-CCB-CDB
47	8	808	4RF	C08-C09-C10-C11
25	B	5002	LHG	O9-C7-O7-C5
25	7	802	LHG	O9-C7-O7-C5
22	A	1012	CLA	C2-C1-O2A-CGA
22	A	1107	CLA	C2-C1-O2A-CGA
22	A	1121	CLA	C2-C1-O2A-CGA
22	A	1123	CLA	C2-C1-O2A-CGA
22	A	1124	CLA	C2-C1-O2A-CGA
22	A	1137	CLA	C2-C1-O2A-CGA
22	A	1139	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
22	A	1140	CLA	C2-C1-O2A-CGA
22	B	1203	CLA	C2-C1-O2A-CGA
22	B	1208	CLA	C2-C1-O2A-CGA
22	B	1214	CLA	C2-C1-O2A-CGA
22	B	1216	CLA	C2-C1-O2A-CGA
22	G	1601	CLA	C2-C1-O2A-CGA
22	1	605	CLA	C2-C1-O2A-CGA
22	a	608	CLA	C2-C1-O2A-CGA
22	4	615	CLA	C2-C1-O2A-CGA
22	5	607	CLA	C2-C1-O2A-CGA
22	5	618	CLA	C2-C1-O2A-CGA
22	8	609	CLA	C2-C1-O2A-CGA
22	8	606	CLA	C2-C1-O2A-CGA
22	8	610	CLA	C2-C1-O2A-CGA
25	B	5002	LHG	C26-C27-C28-C29
25	B	5001	LHG	C31-C32-C33-C34
25	F	5002	LHG	C28-C29-C30-C31
26	B	5003	DGD	CCA-CDA-CEA-CFA
47	8	807	4RF	C32-C33-C34-C35
22	1	605	CLA	C5-C6-C7-C8
22	7	604	CLA	C15-C16-C17-C18
25	A	5002	LHG	C11-C12-C13-C14
22	A	1109	CLA	C16-C17-C18-C20
22	A	1140	CLA	C6-C7-C8-C9
22	4	607	CLA	C6-C7-C8-C9
25	F	5001	LHG	C7-C8-C9-C10
31	3	802	PTY	C8-C11-C12-C13
22	a	612	CLA	C3-C5-C6-C7
22	3	604	CLA	C3-C5-C6-C7
24	A	4001	BCR	C5-C6-C7-C8
24	A	4003	BCR	C1-C6-C7-C8
24	A	4003	BCR	C5-C6-C7-C8
24	A	4004	BCR	C1-C6-C7-C8
24	A	4004	BCR	C5-C6-C7-C8
24	A	4005	BCR	C5-C6-C7-C8
24	B	4002	BCR	C1-C6-C7-C8
24	B	4002	BCR	C5-C6-C7-C8
24	B	4001	BCR	C23-C24-C25-C26
24	F	4001	BCR	C23-C24-C25-C30
24	G	4001	BCR	C5-C6-C7-C8
24	J	4001	BCR	C1-C6-C7-C8
24	J	4001	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	K	4002	BCR	C23-C24-C25-C26
24	K	4002	BCR	C23-C24-C25-C30
24	L	4002	BCR	C1-C6-C7-C8
24	L	4002	BCR	C5-C6-C7-C8
24	L	4001	BCR	C5-C6-C7-C8
24	L	4003	BCR	C23-C24-C25-C26
24	L	4003	BCR	C23-C24-C25-C30
24	5	503	BCR	C1-C6-C7-C8
24	5	503	BCR	C5-C6-C7-C8
24	5	504	BCR	C23-C24-C25-C26
24	5	504	BCR	C23-C24-C25-C30
24	6	504	BCR	C23-C24-C25-C26
24	6	504	BCR	C23-C24-C25-C30
24	6	503	BCR	C1-C6-C7-C8
24	6	503	BCR	C5-C6-C7-C8
24	6	503	BCR	C23-C24-C25-C26
24	7	503	BCR	C1-C6-C7-C8
24	7	503	BCR	C5-C6-C7-C8
35	J	4002	RRX	C23-C24-C25-C26
37	M	4001	ECH	C5-C6-C7-C8
37	M	4001	ECH	C23-C24-C25-C26
38	1	501	LUT	C5-C6-C7-C8
38	1	503	LUT	C5-C6-C7-C8
38	a	501	LUT	C1-C6-C7-C8
38	6	502	LUT	C5-C6-C7-C8
48	7	504	C7Z	C1-C6-C7-C8
48	7	504	C7Z	C5-C6-C7-C8
25	5	801	LHG	C15-C16-C17-C18
29	A	5008	LMT	C3'-C4'-O1B-C1B
31	8	810	PTY	C12-C13-C14-C15
22	B	1209	CLA	CBA-CGA-O2A-C1
22	B	1226	CLA	CBA-CGA-O2A-C1
22	6	612	CLA	CBA-CGA-O2A-C1
25	A	5002	LHG	C24-C23-O8-C6
22	A	1103	CLA	C8-C10-C11-C12
22	A	1140	CLA	C5-C6-C7-C8
22	B	1022	CLA	C8-C10-C11-C12
22	B	1205	CLA	C13-C15-C16-C17
22	1	604	CLA	C8-C10-C11-C12
22	6	615	CLA	C8-C10-C11-C12
22	7	603	CLA	C15-C16-C17-C18
25	F	5001	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
25	6	801	LHG	C12-C13-C14-C15
40	1	803	OLA	C12-C13-C14-C15
25	F	5002	LHG	C23-C24-C25-C26
25	5	801	LHG	C24-C25-C26-C27
25	6	802	LHG	C11-C10-C9-C8
22	A	1116	CLA	C10-C11-C12-C13
22	L	1502	CLA	C8-C10-C11-C12
22	4	610	CLA	C5-C6-C7-C8
25	B	5002	LHG	C16-C17-C18-C19
22	A	1109	CLA	C4-C3-C5-C6
22	A	1101	CLA	C4-C3-C5-C6
22	B	1204	CLA	C4-C3-C5-C6
22	A	1105	CLA	C6-C7-C8-C10
22	A	1106	CLA	C6-C7-C8-C10
22	A	1109	CLA	C2-C3-C5-C6
22	A	1115	CLA	C6-C7-C8-C10
22	A	1138	CLA	C11-C10-C8-C7
22	B	1021	CLA	C11-C10-C8-C7
22	B	1205	CLA	C11-C10-C8-C7
22	B	1205	CLA	C12-C13-C15-C16
22	B	1209	CLA	C2-C3-C5-C6
22	B	1212	CLA	C11-C12-C13-C15
22	B	1229	CLA	C2-C3-C5-C6
22	B	1204	CLA	C2-C3-C5-C6
22	1	604	CLA	C11-C10-C8-C7
22	1	607	CLA	C11-C12-C13-C15
22	1	608	CLA	C11-C10-C8-C7
22	1	612	CLA	C11-C12-C13-C15
22	5	612	CLA	C12-C13-C15-C16
22	6	609	CLA	C6-C7-C8-C10
22	7	603	CLA	C12-C13-C15-C16
22	7	604	CLA	C11-C10-C8-C7
22	8	603	CLA	C11-C10-C8-C7
23	B	2002	PQN	C21-C22-C23-C25
39	1	609	CHL	C6-C7-C8-C10
39	1	609	CHL	C11-C12-C13-C15
39	5	610	CHL	C12-C13-C15-C16
22	B	1224	CLA	C3-C5-C6-C7
22	6	603	CLA	C3-C5-C6-C7
22	B	1202	CLA	O1A-CGA-O2A-C1
22	B	1209	CLA	O1A-CGA-O2A-C1
22	1	604	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	6	606	CLA	O1A-CGA-O2A-C1
22	7	612	CLA	O1A-CGA-O2A-C1
22	B	1239	CLA	C2C-C3C-CAC-CBC
25	B	5001	LHG	C11-C12-C13-C14
25	4	801	LHG	C18-C19-C20-C21
22	B	1220	CLA	C10-C11-C12-C13
22	1	603	CLA	C8-C10-C11-C12
22	1	608	CLA	C8-C10-C11-C12
24	5	503	BCR	C9-C10-C11-C12
24	8	503	BCR	C9-C10-C11-C12
38	a	503	LUT	C29-C30-C31-C32
38	3	501	LUT	C29-C30-C31-C32
22	A	1118	CLA	C6-C7-C8-C9
22	B	1235	CLA	C16-C17-C18-C20
22	B	1239	CLA	C16-C17-C18-C20
22	5	601	CLA	C11-C12-C13-C14
40	1	803	OLA	C10-C11-C12-C13
25	8	801	LHG	O9-C7-O7-C5
25	4	802	LHG	C7-C8-C9-C10
22	3	602	CLA	O1A-CGA-O2A-C1
21	A	1011	CL0	CBA-CGA-O2A-C1
39	a	606	CHL	CBA-CGA-O2A-C1
26	A	5005	DGD	C4B-C5B-C6B-C7B
44	8	803	DGA	CA5-CA6-CA7-CA8
45	6	806	SPH	C15-C16-C17-C18
22	A	1012	CLA	C2A-CAA-CBA-CGA
22	A	1109	CLA	C2A-CAA-CBA-CGA
22	A	1116	CLA	C2A-CAA-CBA-CGA
22	B	1213	CLA	C2A-CAA-CBA-CGA
22	B	1217	CLA	C2A-CAA-CBA-CGA
22	7	605	CLA	C2A-CAA-CBA-CGA
39	4	618	CHL	C2A-CAA-CBA-CGA
22	A	1106	CLA	C13-C15-C16-C17
22	3	603	CLA	C8-C10-C11-C12
23	B	2002	PQN	C23-C25-C26-C27
26	B	5003	DGD	C3B-C4B-C5B-C6B
22	A	1125	CLA	C15-C16-C17-C18
22	1	605	CLA	C8-C10-C11-C12
47	7	807	4RF	C24-C25-C26-C27
25	6	801	LHG	C10-C11-C12-C13
31	7	804	PTY	C13-C14-C15-C16
47	8	807	4RF	C09-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	A	1116	CLA	C11-C12-C13-C14
22	A	1139	CLA	C6-C7-C8-C9
22	B	1209	CLA	C16-C17-C18-C20
26	A	5005	DGD	O6E-C1E-O5D-C6D
22	A	1108	CLA	C5-C6-C7-C8
22	a	603	CLA	C10-C11-C12-C13
22	a	603	CLA	C15-C16-C17-C18
22	A	1141	CLA	O1D-CGD-O2D-CED
22	A	1105	CLA	C2C-C3C-CAC-CBC
25	F	5001	LHG	C26-C27-C28-C29
25	3	801	LHG	C11-C12-C13-C14
43	6	804	PLM	C1-C2-C3-C4
49	8	806	P5S	O37-C2-C3-O16
24	3	503	BCR	C10-C11-C12-C13
22	1	607	CLA	C10-C11-C12-C13
25	8	801	LHG	C28-C29-C30-C31
25	6	801	LHG	O9-C7-O7-C5
39	6	619	CHL	C3-C5-C6-C7
22	6	602	CLA	C3-C5-C6-C7
26	A	5005	DGD	C2E-C1E-O5D-C6D
29	1	804	LMT	C2'-C1'-O1'-C1
25	5	801	LHG	O7-C5-C6-O8
25	A	5002	LHG	C31-C32-C33-C34
33	7	805	SQD	C10-C11-C12-C13
22	A	1135	CLA	C10-C11-C12-C13
22	B	1202	CLA	C15-C16-C17-C18
22	A	1012	CLA	C4-C3-C5-C6
22	B	1209	CLA	C4-C3-C5-C6
22	B	1239	CLA	C4-C3-C5-C6
39	6	610	CHL	C4-C3-C5-C6
22	8	612	CLA	CBA-CGA-O2A-C1
22	A	1012	CLA	C2-C3-C5-C6
22	A	1119	CLA	C2-C3-C5-C6
26	B	5003	DGD	C4B-C5B-C6B-C7B
31	3	802	PTY	C15-C16-C17-C18
22	A	1012	CLA	C6-C7-C8-C9
22	A	1103	CLA	C6-C7-C8-C9
22	A	1105	CLA	C6-C7-C8-C9
22	A	1108	CLA	C14-C13-C15-C16
22	A	1115	CLA	C6-C7-C8-C9
22	A	1116	CLA	C6-C7-C8-C9
22	A	1117	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	B	1205	CLA	C11-C10-C8-C9
22	B	1215	CLA	C11-C10-C8-C9
22	B	1216	CLA	C11-C12-C13-C14
22	B	1240	CLA	C14-C13-C15-C16
22	B	1204	CLA	C14-C13-C15-C16
22	1	612	CLA	C11-C12-C13-C14
22	3	612	CLA	C6-C7-C8-C9
22	5	612	CLA	C14-C13-C15-C16
22	6	604	CLA	C11-C10-C8-C9
39	1	609	CHL	C11-C12-C13-C14
39	6	619	CHL	C14-C13-C15-C16
26	B	5003	DGD	C2B-C3B-C4B-C5B
27	A	5007	3PH	C33-C34-C35-C36
22	A	1104	CLA	C2A-CAA-CBA-CGA
22	A	1135	CLA	C2A-CAA-CBA-CGA
22	B	1224	CLA	C2A-CAA-CBA-CGA
22	4	612	CLA	C2A-CAA-CBA-CGA
24	A	4001	BCR	C37-C22-C23-C24
24	6	504	BCR	C37-C22-C23-C24
38	a	501	LUT	C7-C8-C9-C19
38	7	501	LUT	C27-C28-C29-C39
22	A	1110	CLA	C10-C11-C12-C13
25	6	802	LHG	C25-C26-C27-C28
25	6	801	LHG	C16-C17-C18-C19
24	A	4001	BCR	C21-C22-C23-C24
38	a	501	LUT	C7-C8-C9-C10
48	7	504	C7Z	C7-C8-C9-C10
22	B	1226	CLA	O1A-CGA-O2A-C1
22	6	612	CLA	O1A-CGA-O2A-C1
22	A	1104	CLA	C1A-C2A-CAA-CBA
22	A	1106	CLA	C1A-C2A-CAA-CBA
22	A	1116	CLA	C1A-C2A-CAA-CBA
22	A	1131	CLA	C1A-C2A-CAA-CBA
22	A	1132	CLA	C1A-C2A-CAA-CBA
22	A	1139	CLA	C1A-C2A-CAA-CBA
22	B	1021	CLA	C1A-C2A-CAA-CBA
22	B	1206	CLA	C1A-C2A-CAA-CBA
22	B	1211	CLA	C1A-C2A-CAA-CBA
22	B	1215	CLA	C1A-C2A-CAA-CBA
22	B	1216	CLA	C1A-C2A-CAA-CBA
22	B	1217	CLA	C1A-C2A-CAA-CBA
22	B	1218	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	B	1219	CLA	C1A-C2A-CAA-CBA
22	B	1220	CLA	C1A-C2A-CAA-CBA
22	B	1232	CLA	C1A-C2A-CAA-CBA
22	B	1234	CLA	C1A-C2A-CAA-CBA
22	B	1207	CLA	C1A-C2A-CAA-CBA
22	F	1301	CLA	C1A-C2A-CAA-CBA
22	K	1402	CLA	C1A-C2A-CAA-CBA
22	1	601	CLA	C1A-C2A-CAA-CBA
22	1	604	CLA	C1A-C2A-CAA-CBA
22	1	608	CLA	C1A-C2A-CAA-CBA
22	1	612	CLA	C1A-C2A-CAA-CBA
22	a	601	CLA	C1A-C2A-CAA-CBA
22	a	607	CLA	C1A-C2A-CAA-CBA
22	3	601	CLA	C1A-C2A-CAA-CBA
22	3	607	CLA	C1A-C2A-CAA-CBA
22	3	618	CLA	C1A-C2A-CAA-CBA
22	4	601	CLA	C1A-C2A-CAA-CBA
22	4	610	CLA	C1A-C2A-CAA-CBA
22	4	611	CLA	C1A-C2A-CAA-CBA
22	4	612	CLA	C1A-C2A-CAA-CBA
22	4	616	CLA	C1A-C2A-CAA-CBA
22	4	617	CLA	C1A-C2A-CAA-CBA
22	4	608	CLA	C1A-C2A-CAA-CBA
22	5	601	CLA	C1A-C2A-CAA-CBA
22	5	606	CLA	C1A-C2A-CAA-CBA
22	5	617	CLA	C1A-C2A-CAA-CBA
22	6	601	CLA	C1A-C2A-CAA-CBA
22	6	606	CLA	C1A-C2A-CAA-CBA
22	6	617	CLA	C1A-C2A-CAA-CBA
22	7	602	CLA	C1A-C2A-CAA-CBA
22	7	605	CLA	C1A-C2A-CAA-CBA
22	7	606	CLA	C1A-C2A-CAA-CBA
22	7	607	CLA	C1A-C2A-CAA-CBA
22	7	610	CLA	C1A-C2A-CAA-CBA
22	7	612	CLA	C1A-C2A-CAA-CBA
22	8	608	CLA	C1A-C2A-CAA-CBA
22	8	612	CLA	C1A-C2A-CAA-CBA
39	4	609	CHL	C1A-C2A-CAA-CBA
39	4	613	CHL	C1A-C2A-CAA-CBA
39	6	619	CHL	C1A-C2A-CAA-CBA
39	8	604	CHL	C1A-C2A-CAA-CBA
22	B	1209	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
22	3	603	CLA	C16-C17-C18-C20
22	5	601	CLA	C11-C12-C13-C15
25	A	5003	LHG	C10-C11-C12-C13
25	B	5002	LHG	C11-C12-C13-C14
25	1	802	LHG	C13-C14-C15-C16
25	6	801	LHG	C30-C31-C32-C33
36	a	804	LPX	C17-C18-C19-C20
22	A	1108	CLA	C15-C16-C17-C18
22	A	1114	CLA	C13-C15-C16-C17
22	B	1223	CLA	C10-C11-C12-C13
22	1	612	CLA	C8-C10-C11-C12
22	3	610	CLA	C10-C11-C12-C13
22	7	601	CLA	C8-C10-C11-C12
31	8	810	PTY	C3-O11-P1-O14
49	8	806	P5S	CB-OG-P12-O16
25	F	5001	LHG	C14-C15-C16-C17
22	6	604	CLA	CBD-CGD-O2D-CED
22	A	1112	CLA	C3-C5-C6-C7
22	8	620	CLA	C8-C10-C11-C12
25	7	802	LHG	O6-C4-C5-C6
22	7	607	CLA	O1D-CGD-O2D-CED
22	G	1602	CLA	CBA-CGA-O2A-C1
25	7	802	LHG	C23-C24-C25-C26
22	8	612	CLA	O1D-CGD-O2D-CED
25	A	5002	LHG	C28-C29-C30-C31
22	3	605	CLA	C8-C10-C11-C12
22	A	1116	CLA	C11-C12-C13-C15
22	B	1224	CLA	C16-C17-C18-C20
25	A	5002	LHG	C12-C13-C14-C15
25	3	801	LHG	C23-C24-C25-C26
31	8	810	PTY	C33-C34-C35-C36
22	A	1119	CLA	C4-C3-C5-C6
39	3	608	CHL	C3A-C2A-CAA-CBA
25	A	5003	LHG	C11-C10-C9-C8
25	4	801	LHG	C12-C13-C14-C15
25	A	5002	LHG	C16-C17-C18-C19
39	a	606	CHL	O1A-CGA-O2A-C1
25	B	5002	LHG	C9-C10-C11-C12
33	7	805	SQD	C15-C16-C17-C18
22	B	1235	CLA	C2A-CAA-CBA-CGA
22	6	615	CLA	C2A-CAA-CBA-CGA
39	a	610	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	B	1206	CLA	C6-C7-C8-C9
22	B	1207	CLA	C11-C12-C13-C15
22	3	604	CLA	C11-C12-C13-C15
39	4	609	CHL	C16-C17-C18-C19
22	a	604	CLA	O1D-CGD-O2D-CED
22	4	608	CLA	O1D-CGD-O2D-CED
25	A	5001	LHG	C4-C5-C6-O8
25	1	801	LHG	C4-C5-C6-O8
25	a	801	LHG	C4-C5-C6-O8
25	8	801	LHG	C4-C5-C6-O8
31	5	802	PTY	O4-C1-C6-C5
31	7	804	PTY	O4-C1-C6-C5
31	8	810	PTY	O4-C1-C6-C5
44	5	803	DGA	OG1-CG1-CG2-CG3
22	a	601	CLA	C10-C11-C12-C13
25	F	5001	LHG	C10-C11-C12-C13
25	A	5002	LHG	O10-C23-O8-C6
32	K	5001	LAP	C6-C7-C8-C9
47	8	808	4RF	C46-C47-C48-C49
22	A	1126	CLA	C15-C16-C17-C18
25	6	802	LHG	C30-C31-C32-C33
32	F	5003	LAP	C9-C10-C11-C12
22	A	1124	CLA	O1D-CGD-O2D-CED
22	A	1136	CLA	O1D-CGD-O2D-CED
47	8	808	4RF	C22-C24-C25-C26
21	A	1011	CL0	O1A-CGA-O2A-C1
25	4	801	LHG	C16-C17-C18-C19
25	5	801	LHG	C19-C20-C21-C22
47	7	807	4RF	C25-C26-C27-C28
22	1	604	CLA	C2C-C3C-CAC-CBC
25	1	802	LHG	C19-C20-C21-C22
25	1	802	LHG	C27-C28-C29-C30
25	3	801	LHG	O1-C1-C2-O2
25	7	801	LHG	O1-C1-C2-O2
25	B	5001	LHG	C25-C26-C27-C28
43	4	803	PLM	C7-C8-C9-CA
25	4	802	LHG	C23-C24-C25-C26
25	8	801	LHG	C24-C25-C26-C27
25	4	801	LHG	C19-C20-C21-C22
22	6	604	CLA	C15-C16-C17-C18
24	B	4003	BCR	C11-C10-C9-C34
24	L	4003	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
24	6	503	BCR	C11-C10-C9-C34
22	A	1113	CLA	C4-C3-C5-C6
22	B	1203	CLA	C4-C3-C5-C6
22	B	1225	CLA	C4-C3-C5-C6
22	5	612	CLA	C4-C3-C5-C6
22	6	604	CLA	C4-C3-C5-C6
22	8	603	CLA	C4-C3-C5-C6
22	8	610	CLA	C4-C3-C5-C6
47	8	808	4RF	C31-C32-C33-C34
25	1	802	LHG	C23-C24-C25-C26
22	7	617	CLA	C6-C7-C8-C10
22	1	608	CLA	CBA-CGA-O2A-C1
22	A	1132	CLA	C5-C6-C7-C8
22	B	1204	CLA	C13-C15-C16-C17
29	1	804	LMT	C4B-C5B-C6B-O6B
32	B	5007	LAP	O1-C13-C14-C15
25	7	803	LHG	C25-C26-C27-C28
26	8	802	DGD	C3G-C2G-O2G-C1B
31	3	802	PTY	C5-C6-O7-C8
31	7	804	PTY	C1-C6-O7-C8
47	8	807	4RF	C39-C20-O21-C22
47	8	808	4RF	C39-C20-O21-C22
22	7	609	CLA	C2A-CAA-CBA-CGA
22	8	609	CLA	C2A-CAA-CBA-CGA
22	B	1215	CLA	C8-C10-C11-C12
22	B	1211	CLA	C2-C1-O2A-CGA
22	B	1235	CLA	C2-C1-O2A-CGA
22	B	1239	CLA	C2-C1-O2A-CGA
22	3	612	CLA	C2-C1-O2A-CGA
22	3	613	CLA	C2-C1-O2A-CGA
22	7	607	CLA	C2-C1-O2A-CGA
25	B	5001	LHG	C27-C28-C29-C30
25	5	801	LHG	C29-C30-C31-C32
22	B	1231	CLA	C3-C5-C6-C7
22	7	611	CLA	C3-C5-C6-C7
25	1	801	LHG	C9-C10-C11-C12
25	1	801	LHG	C30-C31-C32-C33
21	A	1011	CL0	C13-C15-C16-C17
22	B	1223	CLA	C5-C6-C7-C8
22	B	1226	CLA	C5-C6-C7-C8
25	4	801	LHG	C35-C36-C37-C38
29	A	5008	LMT	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
22	5	617	CLA	CBA-CGA-O2A-C1
25	3	801	LHG	C24-C23-O8-C6
49	8	806	P5S	O37-C38-C39-C40
22	B	1204	CLA	C16-C17-C18-C20
22	6	604	CLA	C16-C17-C18-C20
22	B	1239	CLA	C4C-C3C-CAC-CBC
25	B	5002	LHG	C27-C28-C29-C30
47	8	807	4RF	C25-C26-C27-C28
31	B	5005	PTY	C11-C12-C13-C14
31	7	804	PTY	C11-C12-C13-C14
25	F	5001	LHG	C25-C26-C27-C28
25	6	801	LHG	C26-C27-C28-C29
43	6	804	PLM	CA-CB-CC-CD
44	5	803	DGA	CA6-CA7-CA8-CA9
22	a	604	CLA	C10-C11-C12-C13
26	A	5005	DGD	C2D-C1D-O3G-C3G
25	8	801	LHG	O7-C5-C6-O8
47	8	808	4RF	O18-C19-C20-O21
22	A	1128	CLA	C10-C11-C12-C13
22	B	1219	CLA	C5-C6-C7-C8
22	4	611	CLA	C5-C6-C7-C8
22	A	1132	CLA	C16-C17-C18-C20
25	3	801	LHG	C9-C10-C11-C12
32	F	5003	LAP	C2-C3-C4-C5
22	A	1118	CLA	C4-C3-C5-C6
22	A	1127	CLA	C15-C16-C17-C18
22	A	1102	CLA	C11-C12-C13-C15
22	A	1106	CLA	C12-C13-C15-C16
22	A	1109	CLA	C11-C12-C13-C15
22	A	1110	CLA	C11-C10-C8-C7
22	A	1111	CLA	C12-C13-C15-C16
22	A	1117	CLA	C6-C7-C8-C10
22	A	1123	CLA	C11-C10-C8-C7
22	A	1126	CLA	C11-C10-C8-C7
22	A	1135	CLA	C11-C10-C8-C7
22	B	1023	CLA	C12-C13-C15-C16
22	B	1209	CLA	C6-C7-C8-C10
22	B	1209	CLA	C11-C10-C8-C7
22	B	1210	CLA	C11-C12-C13-C15
22	B	1214	CLA	C12-C13-C15-C16
22	B	1215	CLA	C11-C10-C8-C7
22	B	1223	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	B	1224	CLA	C11-C10-C8-C7
22	B	1225	CLA	C2-C3-C5-C6
22	B	1231	CLA	C11-C10-C8-C7
22	B	1234	CLA	C6-C7-C8-C10
22	1	606	CLA	C11-C10-C8-C7
22	1	607	CLA	C11-C10-C8-C7
22	a	604	CLA	C12-C13-C15-C16
22	3	603	CLA	C11-C10-C8-C7
22	3	610	CLA	C6-C7-C8-C10
22	3	612	CLA	C11-C10-C8-C7
22	4	610	CLA	C6-C7-C8-C10
22	4	611	CLA	C6-C7-C8-C10
22	6	604	CLA	C12-C13-C15-C16
22	6	615	CLA	C11-C10-C8-C7
22	8	618	CLA	C11-C10-C8-C7
22	8	620	CLA	C11-C12-C13-C15
39	4	609	CHL	C12-C13-C15-C16
39	8	604	CHL	C11-C10-C8-C7
22	G	1601	CLA	CAA-CBA-CGA-O2A
22	A	1109	CLA	C11-C10-C8-C9
22	A	1109	CLA	C11-C12-C13-C14
22	A	1114	CLA	C11-C10-C8-C9
22	A	1122	CLA	C14-C13-C15-C16
22	A	1123	CLA	C11-C10-C8-C9
22	A	1126	CLA	C11-C10-C8-C9
22	A	1133	CLA	C11-C12-C13-C14
22	A	1134	CLA	C11-C10-C8-C9
22	A	1135	CLA	C11-C10-C8-C9
22	A	1101	CLA	C11-C12-C13-C14
22	B	1022	CLA	C6-C7-C8-C9
22	B	1202	CLA	C11-C10-C8-C9
22	B	1203	CLA	C11-C10-C8-C9
22	B	1214	CLA	C6-C7-C8-C9
22	B	1214	CLA	C14-C13-C15-C16
22	B	1221	CLA	C14-C13-C15-C16
22	B	1223	CLA	C11-C10-C8-C9
22	B	1230	CLA	C6-C7-C8-C9
22	B	1231	CLA	C11-C10-C8-C9
22	B	1237	CLA	C14-C13-C15-C16
22	B	1228	CLA	C6-C7-C8-C9
22	B	1204	CLA	C6-C7-C8-C9
22	B	1207	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	1	604	CLA	C6-C7-C8-C9
22	1	606	CLA	C11-C10-C8-C9
22	a	604	CLA	C14-C13-C15-C16
22	3	612	CLA	C11-C10-C8-C9
22	4	604	CLA	C6-C7-C8-C9
22	4	610	CLA	C6-C7-C8-C9
22	5	601	CLA	C11-C10-C8-C9
22	5	603	CLA	C6-C7-C8-C9
22	6	603	CLA	C6-C7-C8-C9
22	6	609	CLA	C11-C10-C8-C9
22	6	615	CLA	C11-C10-C8-C9
22	7	609	CLA	C11-C10-C8-C9
22	7	603	CLA	C11-C10-C8-C9
22	7	603	CLA	C11-C12-C13-C14
22	7	611	CLA	C11-C10-C8-C9
22	8	609	CLA	C6-C7-C8-C9
22	8	609	CLA	C11-C10-C8-C9
22	8	606	CLA	C11-C10-C8-C9
22	8	620	CLA	C11-C12-C13-C14
39	1	609	CHL	C14-C13-C15-C16
39	7	613	CHL	C11-C12-C13-C14
39	8	604	CHL	C11-C10-C8-C9
38	5	505	LUT	C13-C14-C15-C35
22	A	1013	CLA	CBA-CGA-O2A-C1
25	a	801	LHG	C24-C23-O8-C6
22	A	1013	CLA	C15-C16-C17-C18
22	A	1131	CLA	C10-C11-C12-C13
23	A	2001	PQN	C25-C26-C27-C28
22	B	1238	CLA	C2A-CAA-CBA-CGA
22	6	609	CLA	C2A-CAA-CBA-CGA
24	B	4004	BCR	C7-C8-C9-C34
24	B	4001	BCR	C37-C22-C23-C24
24	J	4001	BCR	C11-C12-C13-C35
24	3	503	BCR	C37-C22-C23-C24
48	7	504	C7Z	C7-C8-C9-C19
22	3	605	CLA	C10-C11-C12-C13
22	B	1207	CLA	C11-C12-C13-C14
22	3	604	CLA	C11-C12-C13-C14
22	5	607	CLA	C6-C7-C8-C9
25	7	803	LHG	C27-C28-C29-C30
24	B	4001	BCR	C21-C22-C23-C24
24	J	4001	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	I	4001	BCR	C11-C12-C13-C14
24	3	503	BCR	C21-C22-C23-C24
37	M	4001	ECH	C21-C22-C23-C24
38	5	505	LUT	C31-C32-C33-C34
25	1	801	LHG	C31-C32-C33-C34
25	1	802	LHG	C28-C29-C30-C31
31	5	802	PTY	C34-C35-C36-C37
32	B	5007	LAP	C9-C10-C11-C12
22	B	1228	CLA	C3-C5-C6-C7
22	6	609	CLA	C3-C5-C6-C7
25	6	801	LHG	C1-C2-C3-O3
22	A	1114	CLA	C5-C6-C7-C8
22	A	1117	CLA	C10-C11-C12-C13
22	A	1135	CLA	C15-C16-C17-C18
22	K	1402	CLA	C5-C6-C7-C8
22	7	617	CLA	C5-C6-C7-C8
23	A	2001	PQN	C15-C16-C17-C18
47	7	807	4RF	C24-C22-O21-C20
25	B	5001	LHG	C35-C36-C37-C38
31	5	802	PTY	C38-C39-C40-C41
47	8	808	4RF	C50-C51-C52-C53
22	A	1116	CLA	CBA-CGA-O2A-C1
22	G	1601	CLA	CBA-CGA-O2A-C1
22	4	602	CLA	CBA-CGA-O2A-C1
47	7	807	4RF	C15-C16-O18-C19
25	B	5001	LHG	C16-C17-C18-C19
25	A	5002	LHG	C7-C8-C9-C10
33	G	5001	SQD	C23-C24-C25-C26
22	7	611	CLA	C8-C10-C11-C12
22	8	603	CLA	C13-C15-C16-C17
25	7	803	LHG	C13-C14-C15-C16
25	F	5002	LHG	C9-C10-C11-C12
22	B	1220	CLA	C11-C12-C13-C15
22	A	1126	CLA	C5-C6-C7-C8
22	1	611	CLA	C5-C6-C7-C8
22	a	603	CLA	C13-C15-C16-C17
22	5	601	CLA	C8-C10-C11-C12
22	7	612	CLA	C8-C10-C11-C12
25	4	801	LHG	O6-C4-C5-C6
25	6	802	LHG	O6-C4-C5-C6
31	B	5005	PTY	O14-C5-C6-C1
31	3	802	PTY	O14-C5-C6-C1

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Mol	Chain	Res	Type	Atoms
31	7	804	PTY	O14-C5-C6-C1
49	8	806	P5S	C1-C2-C3-O16
25	7	803	LHG	C24-C25-C26-C27
22	A	1137	CLA	C10-C11-C12-C13
22	a	605	CLA	C5-C6-C7-C8
22	8	603	CLA	C15-C16-C17-C18
31	3	802	PTY	C12-C13-C14-C15
40	1	803	OLA	C3-C4-C5-C6
47	8	808	4RF	C44-C45-C46-C47
22	A	1139	CLA	C4-C3-C5-C6
22	B	1216	CLA	C4-C3-C5-C6
22	B	1230	CLA	C4-C3-C5-C6
21	A	1011	CL0	C2-C3-C5-C6
22	A	1113	CLA	C2-C3-C5-C6
22	A	1118	CLA	C2-C3-C5-C6
22	B	1203	CLA	C2-C3-C5-C6
22	8	603	CLA	C2-C3-C5-C6
22	8	610	CLA	C2-C3-C5-C6
22	5	603	CLA	C11-C10-C8-C9
31	B	5005	PTY	C13-C14-C15-C16
22	A	1101	CLA	C5-C6-C7-C8
26	8	802	DGD	C4E-C5E-C6E-O5E
22	A	1127	CLA	CBA-CGA-O2A-C1
22	A	1129	CLA	CBA-CGA-O2A-C1
22	7	617	CLA	CBA-CGA-O2A-C1
32	B	5007	LAP	C2-C1-O1-C13
39	6	610	CHL	CAA-CBA-CGA-O2A
33	G	5001	SQD	C7-C8-C9-C10
25	B	5001	LHG	C30-C31-C32-C33
25	F	5001	LHG	C11-C10-C9-C8
40	1	803	OLA	C13-C14-C15-C16
22	A	1127	CLA	C3A-C2A-CAA-CBA
22	A	1101	CLA	C3A-C2A-CAA-CBA
22	B	1021	CLA	C3A-C2A-CAA-CBA
22	B	1234	CLA	C3A-C2A-CAA-CBA
22	B	1239	CLA	C3A-C2A-CAA-CBA
22	F	1301	CLA	C3A-C2A-CAA-CBA
22	G	1601	CLA	C3A-C2A-CAA-CBA
22	L	1501	CLA	C3A-C2A-CAA-CBA
22	7	605	CLA	C3A-C2A-CAA-CBA
22	8	609	CLA	C3A-C2A-CAA-CBA
22	8	607	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	A	1102	CLA	C13-C15-C16-C17
22	7	611	CLA	C2C-C3C-CAC-CBC
25	A	5003	LHG	C15-C16-C17-C18
24	B	4005	BCR	C13-C14-C15-C16
24	B	4006	BCR	C13-C14-C15-C16
24	I	4001	BCR	C9-C10-C11-C12
24	L	4003	BCR	C19-C20-C21-C22
35	J	4002	RRX	C19-C20-C21-C22
38	a	501	LUT	C29-C30-C31-C32
47	8	807	4RF	C11-C12-C13-C14
40	8	809	OLA	C6-C7-C8-C9
31	5	802	PTY	C15-C16-C17-C18
22	8	618	CLA	C11-C12-C13-C15
22	B	1216	CLA	CBA-CGA-O2A-C1
22	B	1235	CLA	CBA-CGA-O2A-C1
22	L	1502	CLA	CBA-CGA-O2A-C1
36	J	5001	LPX	C7-C6-O6-C5
22	1	604	CLA	C10-C11-C12-C13
22	a	612	CLA	C5-C6-C7-C8
25	A	5002	LHG	C4-C5-C6-O8
25	A	5003	LHG	C4-C5-C6-O8
25	B	5001	LHG	C4-C5-C6-O8
25	F	5001	LHG	C4-C5-C6-O8
25	1	802	LHG	C4-C5-C6-O8
25	4	802	LHG	C4-C5-C6-O8
25	6	802	LHG	C4-C5-C6-O8
26	B	5003	DGD	O1G-C1G-C2G-C3G
33	7	805	SQD	C44-C45-C46-O48
22	A	1127	CLA	C5-C6-C7-C8
22	A	1138	CLA	C5-C6-C7-C8
26	8	802	DGD	O6D-C5D-C6D-O5D
27	A	5007	3PH	O21-C21-C22-C23
25	5	801	LHG	C10-C11-C12-C13
25	6	801	LHG	C35-C36-C37-C38
22	A	1124	CLA	C3-C5-C6-C7
22	A	1132	CLA	C3-C5-C6-C7
32	K	5001	LAP	O1-C13-C14-C15
22	A	1121	CLA	C4-C3-C5-C6
22	A	1134	CLA	C4-C3-C5-C6
22	1	607	CLA	C4-C3-C5-C6
22	8	618	CLA	C11-C12-C13-C14
22	5	612	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
30	6	803	PCW	C1-O3P-P-O4P
36	J	5001	LPX	C3-O1-P1-O2
22	1	608	CLA	O1A-CGA-O2A-C1
22	A	1140	CLA	C3-C5-C6-C7
22	7	606	CLA	C3-C5-C6-C7
22	A	1119	CLA	C2A-CAA-CBA-CGA
22	3	616	CLA	C2A-CAA-CBA-CGA
25	A	5001	LHG	O1-C1-C2-O2
22	A	1104	CLA	C10-C11-C12-C13
22	1	612	CLA	C10-C11-C12-C13
36	a	804	LPX	C13-C14-C15-C16
25	A	5002	LHG	O6-C4-C5-O7
25	6	802	LHG	O6-C4-C5-O7
34	G	5002	ERG	C28-C24-C25-C27
22	B	1201	CLA	C16-C17-C18-C19
22	7	604	CLA	C16-C17-C18-C19
22	A	1111	CLA	C15-C16-C17-C18
25	7	801	LHG	O2-C2-C3-O3
22	A	1013	CLA	O1A-CGA-O2A-C1
22	4	602	CLA	O1A-CGA-O2A-C1
30	6	803	PCW	C34-C35-C36-C37
33	G	5001	SQD	C16-C17-C18-C19
39	8	601	CHL	C2C-C3C-CAC-CBC
22	4	605	CLA	O1A-CGA-O2A-C1
25	A	5003	LHG	O7-C5-C6-O8
25	B	5002	LHG	O7-C5-C6-O8
25	6	802	LHG	O7-C5-C6-O8
25	6	801	LHG	O7-C5-C6-O8
30	B	5004	PCW	O2-C2-C3-O3
33	G	5001	SQD	O6-C44-C45-O47
47	8	807	4RF	O18-C19-C20-O21
47	8	808	4RF	O21-C20-C39-O40
38	1	502	LUT	C29-C30-C31-C32
22	A	1110	CLA	C11-C12-C13-C14
22	5	607	CLA	C6-C7-C8-C10
22	6	604	CLA	C16-C17-C18-C19
22	7	612	CLA	C11-C12-C13-C15
22	7	617	CLA	C6-C7-C8-C9
25	F	5001	LHG	C1-C2-C3-O3
25	8	801	LHG	C1-C2-C3-O3
49	8	806	P5S	O-C-CA-N
25	B	5001	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
25	7	803	LHG	C11-C12-C13-C14
32	B	5007	LAP	C11-C10-C9-C8
44	5	803	DGA	CB3-CB4-CB5-CB6
22	1	601	CLA	C2-C1-O2A-CGA
22	4	604	CLA	C2-C1-O2A-CGA
22	7	609	CLA	C2-C1-O2A-CGA
22	7	604	CLA	C2-C1-O2A-CGA
22	A	1139	CLA	C2-C3-C5-C6
22	B	1224	CLA	C15-C16-C17-C18
22	B	1228	CLA	C8-C10-C11-C12
22	5	604	CLA	C10-C11-C12-C13
22	A	1138	CLA	C14-C13-C15-C16
22	B	1023	CLA	C14-C13-C15-C16
22	B	1209	CLA	C6-C7-C8-C9
22	B	1213	CLA	C11-C10-C8-C9
22	B	1217	CLA	C6-C7-C8-C9
22	B	1224	CLA	C14-C13-C15-C16
22	K	1402	CLA	C6-C7-C8-C9
22	3	606	CLA	C14-C13-C15-C16
22	4	610	CLA	C14-C13-C15-C16
22	6	609	CLA	C14-C13-C15-C16
22	7	604	CLA	C6-C7-C8-C9
39	5	610	CHL	C11-C10-C8-C9
39	6	619	CHL	C11-C10-C8-C9
39	8	604	CHL	C6-C7-C8-C9
22	a	608	CLA	CBA-CGA-O2A-C1
25	A	5002	LHG	C18-C19-C20-C21
22	A	1109	CLA	C5-C6-C7-C8
22	4	610	CLA	C10-C11-C12-C13
22	4	608	CLA	C4-C3-C5-C6
25	A	5003	LHG	C2-C3-O3-P
25	1	802	LHG	C5-C4-O6-P
25	3	801	LHG	C2-C3-O3-P
25	3	801	LHG	O10-C23-O8-C6
25	A	5002	LHG	C11-C10-C9-C8
25	B	5002	LHG	C25-C26-C27-C28
40	8	809	OLA	C15-C16-C17-C18
47	8	807	4RF	C10-C11-C12-C13
22	A	1111	CLA	C2A-CAA-CBA-CGA
22	B	1201	CLA	C2A-CAA-CBA-CGA
22	5	602	CLA	C2A-CAA-CBA-CGA
22	B	1021	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
22	B	1215	CLA	C11-C12-C13-C15
22	1	612	CLA	C16-C17-C18-C19
22	3	601	CLA	C16-C17-C18-C19
39	7	613	CHL	C16-C17-C18-C19
24	B	4005	BCR	C23-C24-C25-C26
24	B	4005	BCR	C23-C24-C25-C30
24	B	4001	BCR	C1-C6-C7-C8
24	B	4001	BCR	C5-C6-C7-C8
24	3	504	BCR	C23-C24-C25-C30
24	5	503	BCR	C23-C24-C25-C26
37	M	4001	ECH	C23-C24-C25-C30
22	8	620	CLA	C13-C15-C16-C17
22	1	607	CLA	C4C-C3C-CAC-CBC
22	a	608	CLA	CAA-CBA-CGA-O2A
22	3	602	CLA	CAA-CBA-CGA-O2A
24	B	4001	BCR	C36-C18-C19-C20
25	7	802	LHG	C10-C11-C12-C13
47	7	807	4RF	O17-C16-O18-C19
24	B	4004	BCR	C7-C8-C9-C10
24	F	4001	BCR	C17-C18-C19-C20
37	M	4001	ECH	C17-C18-C19-C20
22	A	1128	CLA	C8-C10-C11-C12
22	8	606	CLA	C5-C6-C7-C8
25	4	801	LHG	C25-C26-C27-C28
25	8	801	LHG	C30-C31-C32-C33
47	7	807	4RF	O23-C22-O21-C20
25	A	5001	LHG	C8-C7-O7-C5
43	4	803	PLM	CD-CE-CF-CG
22	1	604	CLA	C4C-C3C-CAC-CBC
22	B	1201	CLA	C16-C17-C18-C20
22	B	1220	CLA	C11-C12-C13-C14
39	8	601	CHL	C11-C12-C13-C14
22	B	1216	CLA	C14-C13-C15-C16
22	3	616	CLA	C11-C10-C8-C9
41	3	506	QTB	C09-C10-C11-C17
40	1	803	OLA	C4-C5-C6-C7
22	A	1101	CLA	C13-C15-C16-C17
25	A	5001	LHG	O6-C4-C5-C6
25	B	5002	LHG	O6-C4-C5-C6
25	F	5002	LHG	O6-C4-C5-C6
30	6	803	PCW	O3P-C1-C2-C3
25	1	802	LHG	O8-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
22	7	612	CLA	C4-C3-C5-C6
22	A	1106	CLA	C11-C10-C8-C7
22	A	1114	CLA	C11-C10-C8-C7
22	A	1117	CLA	C11-C12-C13-C15
22	A	1119	CLA	C6-C7-C8-C10
22	A	1122	CLA	C12-C13-C15-C16
22	A	1125	CLA	C12-C13-C15-C16
22	A	1126	CLA	C12-C13-C15-C16
22	A	1131	CLA	C6-C7-C8-C10
22	A	1131	CLA	C11-C12-C13-C15
22	A	1132	CLA	C6-C7-C8-C10
22	A	1136	CLA	C12-C13-C15-C16
22	A	1137	CLA	C6-C7-C8-C10
22	A	1138	CLA	C12-C13-C15-C16
22	B	1201	CLA	C11-C10-C8-C7
22	B	1202	CLA	C11-C10-C8-C7
22	B	1213	CLA	C11-C10-C8-C7
22	B	1217	CLA	C6-C7-C8-C10
22	B	1219	CLA	C6-C7-C8-C10
22	B	1230	CLA	C6-C7-C8-C10
22	B	1237	CLA	C11-C10-C8-C7
22	B	1237	CLA	C12-C13-C15-C16
22	B	1239	CLA	C12-C13-C15-C16
22	B	1228	CLA	C6-C7-C8-C10
22	B	1204	CLA	C6-C7-C8-C10
22	B	1207	CLA	C6-C7-C8-C10
22	K	1402	CLA	C6-C7-C8-C10
22	1	604	CLA	C6-C7-C8-C10
22	a	604	CLA	C11-C10-C8-C7
22	a	604	CLA	C11-C12-C13-C15
22	4	604	CLA	C6-C7-C8-C10
22	4	610	CLA	C12-C13-C15-C16
22	5	601	CLA	C11-C10-C8-C7
22	5	603	CLA	C6-C7-C8-C10
22	6	603	CLA	C6-C7-C8-C10
22	6	603	CLA	C12-C13-C15-C16
22	6	609	CLA	C11-C10-C8-C7
22	7	609	CLA	C11-C10-C8-C7
22	7	603	CLA	C11-C10-C8-C7
22	7	603	CLA	C11-C12-C13-C15
22	7	611	CLA	C11-C10-C8-C7
22	7	612	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	8	609	CLA	C11-C10-C8-C7
22	8	606	CLA	C11-C10-C8-C7
22	8	620	CLA	C11-C10-C8-C7
23	A	2001	PQN	C21-C22-C23-C25
39	1	609	CHL	C12-C13-C15-C16
39	5	610	CHL	C11-C10-C8-C7
39	8	604	CHL	C11-C12-C13-C15
22	A	1116	CLA	O1A-CGA-O2A-C1
25	7	803	LHG	C15-C16-C17-C18
26	A	5005	DGD	C7B-C8B-C9B-CAB
26	8	802	DGD	C5A-C6A-C7A-C8A
26	8	802	DGD	C2B-C3B-C4B-C5B
22	7	604	CLA	C8-C10-C11-C12
24	A	4004	BCR	C13-C14-C15-C16
24	A	4005	BCR	C19-C20-C21-C22
24	B	4002	BCR	C15-C16-C17-C18
24	B	4003	BCR	C19-C20-C21-C22
24	K	4001	BCR	C13-C14-C15-C16
24	K	4002	BCR	C19-C20-C21-C22
24	I	4001	BCR	C19-C20-C21-C22
24	3	503	BCR	C13-C14-C15-C16
24	6	503	BCR	C19-C20-C21-C22
24	7	503	BCR	C15-C16-C17-C18
38	a	502	LUT	C29-C30-C31-C32
38	6	501	LUT	C29-C30-C31-C32
38	6	502	LUT	C29-C30-C31-C32
38	7	501	LUT	C29-C30-C31-C32
38	8	502	LUT	C29-C30-C31-C32
22	A	1110	CLA	C11-C12-C13-C15
22	A	1114	CLA	C16-C17-C18-C19
22	A	1140	CLA	C6-C7-C8-C10
22	B	1022	CLA	C16-C17-C18-C20
31	B	5005	PTY	C30-C31-C32-C33
29	B	5006	LMT	C5'-C4'-O1B-C1B
22	B	1235	CLA	C15-C16-C17-C18
22	5	612	CLA	C10-C11-C12-C13
26	A	5005	DGD	O6E-C5E-C6E-O5E
22	G	1603	CLA	C2A-CAA-CBA-CGA
22	1	615	CLA	C2A-CAA-CBA-CGA
22	4	607	CLA	C2A-CAA-CBA-CGA
39	5	611	CHL	C2A-CAA-CBA-CGA
40	1	803	OLA	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
22	6	607	CLA	C5-C6-C7-C8
24	B	4005	BCR	C11-C10-C9-C34
22	B	1223	CLA	C3-C5-C6-C7
25	6	801	LHG	C18-C19-C20-C21
22	B	1204	CLA	C16-C17-C18-C19
22	A	1111	CLA	CBA-CGA-O2A-C1
22	B	1021	CLA	CBA-CGA-O2A-C1
22	B	1203	CLA	CBA-CGA-O2A-C1
22	B	1222	CLA	CBA-CGA-O2A-C1
22	B	1225	CLA	CBA-CGA-O2A-C1
31	3	802	PTY	C31-C30-O4-C1
31	7	804	PTY	C31-C30-O4-C1
39	7	613	CHL	CBA-CGA-O2A-C1
39	a	609	CHL	C3-C5-C6-C7
22	3	616	CLA	C11-C10-C8-C7
31	3	802	PTY	C36-C37-C38-C39
22	A	1127	CLA	O1A-CGA-O2A-C1
22	G	1601	CLA	O1A-CGA-O2A-C1
22	5	617	CLA	O1A-CGA-O2A-C1
22	A	1124	CLA	CBD-CGD-O2D-CED
22	B	1204	CLA	C2C-C3C-CAC-CBC
22	A	1108	CLA	CAD-CBD-CGD-O2D
22	A	1115	CLA	CAD-CBD-CGD-O2D
22	B	1202	CLA	CAD-CBD-CGD-O2D
22	B	1212	CLA	CAD-CBD-CGD-O2D
22	B	1217	CLA	CAD-CBD-CGD-O2D
22	B	1207	CLA	CAD-CBD-CGD-O2D
22	K	1402	CLA	CAD-CBD-CGD-O2D
22	K	1403	CLA	CAD-CBD-CGD-O2D
22	L	1501	CLA	CAD-CBD-CGD-O2D
22	a	605	CLA	CAD-CBD-CGD-O2D
22	4	604	CLA	CAD-CBD-CGD-O2D
22	4	607	CLA	CAD-CBD-CGD-O2D
22	7	609	CLA	CAD-CBD-CGD-O2D
22	7	602	CLA	CAD-CBD-CGD-O2D
22	8	608	CLA	CAD-CBD-CGD-O2D
25	4	801	LHG	C4-C5-O7-C7
31	5	802	PTY	C1-C6-O7-C8
49	8	806	P5S	C1-C2-O37-C38
25	B	5002	LHG	C28-C29-C30-C31
22	3	612	CLA	C15-C16-C17-C18
22	4	604	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
25	8	801	LHG	C27-C28-C29-C30
22	B	1224	CLA	CBA-CGA-O2A-C1
22	6	609	CLA	C4-C3-C5-C6
22	a	603	CLA	C16-C17-C18-C20
49	8	806	P5S	C45-C46-C48-C49
25	A	5003	LHG	C5-C4-O6-P
25	a	801	LHG	C2-C3-O3-P
25	6	801	LHG	C4-C5-C6-O8
25	7	803	LHG	C2-C3-O3-P
30	6	803	PCW	C2-C1-O3P-P
33	G	5001	SQD	O6-C44-C45-C46
33	7	805	SQD	O6-C44-C45-C46
47	7	807	4RF	C19-C20-C39-O40
47	8	808	4RF	C19-C20-C39-O40
49	8	806	P5S	O19-C1-C2-C3
22	a	608	CLA	O1A-CGA-O2A-C1
25	a	801	LHG	O10-C23-O8-C6
31	3	802	PTY	O30-C30-O4-C1
25	F	5001	LHG	C24-C25-C26-C27
25	6	802	LHG	C10-C11-C12-C13
25	F	5002	LHG	O6-C4-C5-O7
25	4	801	LHG	O6-C4-C5-O7
25	7	802	LHG	O6-C4-C5-O7
31	B	5005	PTY	O14-C5-C6-O7
22	A	1102	CLA	C8-C10-C11-C12
22	A	1131	CLA	C15-C16-C17-C18
22	B	1209	CLA	C8-C10-C11-C12
22	4	615	CLA	C5-C6-C7-C8
22	B	1209	CLA	C2A-CAA-CBA-CGA
22	1	604	CLA	C2A-CAA-CBA-CGA
22	3	606	CLA	C2A-CAA-CBA-CGA
22	B	1222	CLA	C10-C11-C12-C13
30	6	803	PCW	C13-C14-C15-C16
47	8	808	4RF	C10-C11-C12-C13
22	A	1134	CLA	C11-C12-C13-C14
25	A	5001	LHG	O9-C7-O7-C5
22	A	1102	CLA	CHA-CBD-CGD-O1D
22	A	1111	CLA	CHA-CBD-CGD-O1D
22	A	1111	CLA	CHA-CBD-CGD-O2D
22	A	1113	CLA	CHA-CBD-CGD-O1D
22	A	1113	CLA	CHA-CBD-CGD-O2D
22	A	1121	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	A	1122	CLA	CHA-CBD-CGD-O2D
22	A	1132	CLA	CHA-CBD-CGD-O1D
22	A	1132	CLA	CHA-CBD-CGD-O2D
22	A	1137	CLA	CHA-CBD-CGD-O1D
22	A	1137	CLA	CHA-CBD-CGD-O2D
22	A	1101	CLA	CHA-CBD-CGD-O1D
22	A	1101	CLA	CHA-CBD-CGD-O2D
22	B	1210	CLA	CHA-CBD-CGD-O1D
22	B	1210	CLA	CHA-CBD-CGD-O2D
22	B	1220	CLA	CHA-CBD-CGD-O1D
22	B	1220	CLA	CHA-CBD-CGD-O2D
22	B	1225	CLA	CHA-CBD-CGD-O2D
22	B	1227	CLA	CHA-CBD-CGD-O2D
22	B	1235	CLA	CHA-CBD-CGD-O1D
22	G	1602	CLA	CHA-CBD-CGD-O1D
22	G	1602	CLA	CHA-CBD-CGD-O2D
22	K	1402	CLA	CHA-CBD-CGD-O1D
22	K	1404	CLA	CHA-CBD-CGD-O1D
22	K	1404	CLA	CHA-CBD-CGD-O2D
22	L	1502	CLA	CHA-CBD-CGD-O1D
22	L	1502	CLA	CHA-CBD-CGD-O2D
22	3	604	CLA	CHA-CBD-CGD-O1D
22	4	603	CLA	CHA-CBD-CGD-O2D
22	6	603	CLA	CHA-CBD-CGD-O1D
22	6	604	CLA	CHA-CBD-CGD-O1D
22	6	604	CLA	CHA-CBD-CGD-O2D
22	6	615	CLA	CHA-CBD-CGD-O2D
22	7	608	CLA	CHA-CBD-CGD-O1D
22	7	617	CLA	CHA-CBD-CGD-O2D
22	8	609	CLA	CHA-CBD-CGD-O1D
22	8	609	CLA	CHA-CBD-CGD-O2D
22	8	607	CLA	CHA-CBD-CGD-O1D
22	8	607	CLA	CHA-CBD-CGD-O2D
22	8	610	CLA	CHA-CBD-CGD-O2D
39	1	609	CHL	CHA-CBD-CGD-O1D
39	1	609	CHL	CHA-CBD-CGD-O2D
39	a	609	CHL	CHA-CBD-CGD-O1D
39	a	609	CHL	CHA-CBD-CGD-O2D
39	8	604	CHL	CHA-CBD-CGD-O1D
39	8	604	CHL	CHA-CBD-CGD-O2D
25	B	5002	LHG	O8-C23-C24-C25
25	1	801	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
22	A	1129	CLA	O1A-CGA-O2A-C1
22	B	1021	CLA	O1A-CGA-O2A-C1
22	B	1203	CLA	O1A-CGA-O2A-C1
22	L	1502	CLA	O1A-CGA-O2A-C1
22	7	617	CLA	O1A-CGA-O2A-C1
31	7	804	PTY	O30-C30-O4-C1
36	J	5001	LPX	O7-C6-O6-C5
25	6	801	LHG	C25-C26-C27-C28
24	L	4003	BCR	C11-C10-C9-C8
25	A	5001	LHG	O7-C5-C6-O8
25	a	801	LHG	O7-C5-C6-O8
25	4	802	LHG	O7-C5-C6-O8
31	5	802	PTY	O4-C1-C6-O7
31	7	804	PTY	O4-C1-C6-O7
44	5	803	DGA	OG1-CG1-CG2-OG2
47	7	807	4RF	O21-C20-C39-O40
47	8	807	4RF	O21-C20-C39-O40
25	7	801	LHG	C31-C32-C33-C34
47	7	807	4RF	C45-C46-C47-C48
32	B	5007	LAP	O2-C1-O1-C13
25	6	801	LHG	C19-C20-C21-C22
22	6	604	CLA	C2C-C3C-CAC-CBC
25	F	5001	LHG	C29-C30-C31-C32
36	a	804	LPX	C9-C10-C11-C12
22	A	1139	CLA	C3-C5-C6-C7
22	a	601	CLA	C3-C5-C6-C7
22	7	612	CLA	C3-C5-C6-C7
22	A	1117	CLA	C4-C3-C5-C6
22	B	1212	CLA	C4-C3-C5-C6
22	B	1207	CLA	C4-C3-C5-C6
22	1	611	CLA	C4-C3-C5-C6
25	3	801	LHG	C11-C10-C9-C8
22	B	1216	CLA	O1A-CGA-O2A-C1
22	B	1235	CLA	O1A-CGA-O2A-C1
49	8	806	P5S	C17-C20-C21-C22
22	1	611	CLA	C2-C3-C5-C6
22	A	1117	CLA	C11-C12-C13-C14
22	A	1119	CLA	C6-C7-C8-C9
22	A	1133	CLA	C14-C13-C15-C16
22	B	1229	CLA	C6-C7-C8-C9
22	5	612	CLA	C11-C10-C8-C9
23	A	2001	PQN	C19-C18-C20-C21

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Mol	Chain	Res	Type	Atoms
23	A	2001	PQN	C21-C22-C23-C24
26	8	802	DGD	C2G-C1G-O1G-C1A
22	7	612	CLA	C2C-C3C-CAC-CBC
25	5	801	LHG	C27-C28-C29-C30
39	a	613	CHL	C2C-C3C-CAC-CBC
22	A	1110	CLA	C8-C10-C11-C12
22	A	1128	CLA	C16-C17-C18-C19
22	1	611	CLA	C6-C7-C8-C9
49	8	806	P5S	C43-C44-C45-C46
22	A	1123	CLA	C2A-CAA-CBA-CGA
22	A	1111	CLA	O1A-CGA-O2A-C1
37	M	4001	ECH	C37-C22-C23-C24
25	5	801	LHG	C33-C34-C35-C36
32	K	5001	LAP	C11-C10-C9-C8
24	A	4002	BCR	C17-C18-C19-C20
25	7	803	LHG	C28-C29-C30-C31
47	8	808	4RF	C28-C29-C30-C31
22	A	1121	CLA	C1A-C2A-CAA-CBA
22	B	1239	CLA	C1A-C2A-CAA-CBA
22	1	606	CLA	C1A-C2A-CAA-CBA
22	1	610	CLA	C1A-C2A-CAA-CBA
25	A	5001	LHG	C7-C8-C9-C10
22	A	1109	CLA	C10-C11-C12-C13
22	6	601	CLA	C10-C11-C12-C13
22	B	1230	CLA	C2-C1-O2A-CGA
22	6	602	CLA	C2-C1-O2A-CGA
22	6	604	CLA	CBA-CGA-O2A-C1
25	3	801	LHG	C34-C35-C36-C37
24	B	4006	BCR	C15-C16-C17-C18
24	L	4001	BCR	C9-C10-C11-C12
38	1	503	LUT	C29-C30-C31-C32
38	5	502	LUT	C29-C30-C31-C32
25	6	801	LHG	C4-O6-P-O3
25	3	801	LHG	C30-C31-C32-C33
27	A	5007	3PH	C31-C32-C33-C34
45	6	806	SPH	C9-C10-C11-C12
22	B	1023	CLA	C4-C3-C5-C6
22	4	601	CLA	C4-C3-C5-C6
22	5	601	CLA	C3-C5-C6-C7
25	F	5002	LHG	C2-C3-O3-P
25	1	802	LHG	C2-C3-O3-P
22	7	607	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
22	B	1225	CLA	O1A-CGA-O2A-C1
39	7	613	CHL	O1A-CGA-O2A-C1
25	A	5001	LHG	C3-O3-P-O5
25	B	5002	LHG	C3-O3-P-O5
25	B	5001	LHG	C4-O6-P-O4
25	1	801	LHG	C4-O6-P-O4
25	1	802	LHG	C4-O6-P-O5
25	4	802	LHG	C4-O6-P-O4
25	5	801	LHG	C4-O6-P-O4
25	6	802	LHG	C4-O6-P-O5
25	7	803	LHG	C3-O3-P-O5
31	3	802	PTY	C3-O11-P1-O13
31	3	802	PTY	C5-O14-P1-O13
31	7	804	PTY	C5-O14-P1-O12
31	8	810	PTY	C3-O11-P1-O12
32	B	5007	LAP	C15-O4-P9-O7
32	F	5003	LAP	C15-O4-P9-O5
32	K	5001	LAP	C16-O6-P9-O5
36	J	5001	LPX	C3-O1-P1-O4
36	J	5001	LPX	C1-O2-P1-O3
36	J	5001	LPX	C1-O2-P1-O4
49	8	806	P5S	CB-OG-P12-O13
22	B	1213	CLA	C11-C12-C13-C14
25	7	801	LHG	C18-C19-C20-C21
25	A	5002	LHG	O6-C4-C5-C6
25	A	5003	LHG	O6-C4-C5-C6
25	1	801	LHG	O6-C4-C5-C6
25	8	801	LHG	O6-C4-C5-C6
22	A	1103	CLA	CAA-CBA-CGA-O2A
47	8	807	4RF	C34-C35-C36-C37
22	A	1108	CLA	C2A-CAA-CBA-CGA
22	A	1128	CLA	C3-C5-C6-C7
40	8	809	OLA	C4-C5-C6-C7
26	B	5003	DGD	C4A-C5A-C6A-C7A
43	6	804	PLM	C6-C7-C8-C9
22	A	1134	CLA	C11-C12-C13-C15
25	4	801	LHG	C9-C10-C11-C12
47	7	807	4RF	C43-C44-C45-C46
22	A	1102	CLA	CAD-CBD-CGD-O1D
22	A	1111	CLA	CAD-CBD-CGD-O1D
22	A	1113	CLA	CAD-CBD-CGD-O1D
22	A	1138	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	B	1210	CLA	CAD-CBD-CGD-O1D
22	B	1235	CLA	CAD-CBD-CGD-O1D
22	7	617	CLA	CAD-CBD-CGD-O1D
22	8	609	CLA	CAD-CBD-CGD-O1D
32	F	5003	LAP	C17-C16-O6-P9
32	K	5001	LAP	C17-C16-O6-P9
39	a	609	CHL	CAD-CBD-CGD-O1D
22	6	609	CLA	C15-C16-C17-C18
22	B	1224	CLA	O1A-CGA-O2A-C1
39	3	611	CHL	C3-C5-C6-C7
22	A	1128	CLA	CBA-CGA-O2A-C1
22	8	615	CLA	CBA-CGA-O2A-C1
22	8	612	CLA	O1A-CGA-O2A-C1
22	A	1140	CLA	C4-C3-C5-C6
22	A	1104	CLA	C11-C10-C8-C7
22	A	1104	CLA	C11-C12-C13-C15
22	A	1120	CLA	C3A-C2A-CAA-CBA
22	A	1122	CLA	C11-C10-C8-C7
22	A	1101	CLA	C6-C7-C8-C10
22	B	1021	CLA	C6-C7-C8-C10
22	B	1021	CLA	C11-C12-C13-C15
22	B	1202	CLA	C6-C7-C8-C10
22	B	1208	CLA	C6-C7-C8-C10
22	B	1210	CLA	C12-C13-C15-C16
22	B	1221	CLA	C12-C13-C15-C16
22	B	1235	CLA	C3A-C2A-CAA-CBA
22	B	1235	CLA	C11-C10-C8-C7
22	B	1235	CLA	C12-C13-C15-C16
22	L	1502	CLA	C11-C10-C8-C7
22	1	603	CLA	C6-C7-C8-C10
22	3	605	CLA	C11-C10-C8-C7
22	4	610	CLA	C11-C12-C13-C15
22	5	604	CLA	C12-C13-C15-C16
22	7	601	CLA	C11-C10-C8-C7
25	A	5003	LHG	O6-C4-C5-O7
25	F	5001	LHG	O6-C4-C5-O7
25	1	801	LHG	O6-C4-C5-O7
25	8	801	LHG	O6-C4-C5-O7
31	3	802	PTY	O14-C5-C6-O7
31	5	802	PTY	O14-C5-C6-O7
31	5	802	PTY	C8-C11-C12-C13
31	7	804	PTY	O14-C5-C6-O7

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Mol	Chain	Res	Type	Atoms
39	4	609	CHL	C11-C10-C8-C7
39	6	619	CHL	C11-C10-C8-C7
47	8	807	4RF	C41-C43-C44-C45
47	8	807	4RF	C24-C25-C26-C27
38	1	501	LUT	C29-C30-C31-C32
38	a	502	LUT	C13-C14-C15-C35
38	6	502	LUT	C9-C10-C11-C12
25	B	5002	LHG	C15-C16-C17-C18
26	8	802	DGD	CAB-CBB-CCB-CDB
22	B	1222	CLA	O1A-CGA-O2A-C1
22	B	1236	CLA	C5-C6-C7-C8
26	B	5003	DGD	C7A-C8A-C9A-CAA
22	A	1103	CLA	C2A-CAA-CBA-CGA
25	F	5002	LHG	C26-C27-C28-C29
30	B	5004	PCW	C1-C2-C3-O3
31	B	5005	PTY	O4-C1-C6-C5
32	F	5003	LAP	O6-C16-C17-N8
32	K	5001	LAP	O6-C16-C17-N8
45	6	806	SPH	O1-C1-C2-N2
47	8	807	4RF	O18-C19-C20-C39
47	8	808	4RF	O18-C19-C20-C39
25	B	5001	LHG	O7-C5-C6-O8
25	F	5001	LHG	O7-C5-C6-O8
26	B	5003	DGD	O1G-C1G-C2G-O2G
26	8	802	DGD	O1G-C1G-C2G-O2G
31	B	5005	PTY	O4-C1-C6-O7
31	8	810	PTY	O4-C1-C6-O7
33	7	805	SQD	O47-C45-C46-O48
49	8	806	P5S	O19-C1-C2-O37
31	B	5005	PTY	C25-C26-C27-C28
25	A	5002	LHG	C32-C33-C34-C35
31	8	810	PTY	C16-C17-C18-C19
22	A	1132	CLA	O1A-CGA-O2A-C1
26	B	5003	DGD	C5A-C6A-C7A-C8A
26	A	5005	DGD	C2G-C3G-O3G-C1D
31	8	810	PTY	C11-C12-C13-C14
22	A	1132	CLA	C15-C16-C17-C18
22	B	1212	CLA	C2-C3-C5-C6
22	B	1239	CLA	C2-C3-C5-C6
22	6	609	CLA	C2-C3-C5-C6
39	6	610	CHL	C2-C3-C5-C6
25	1	802	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
22	A	1104	CLA	C6-C7-C8-C9
22	A	1104	CLA	C11-C10-C8-C9
22	A	1131	CLA	C6-C7-C8-C9
22	A	1131	CLA	C14-C13-C15-C16
22	A	1132	CLA	C6-C7-C8-C9
22	A	1135	CLA	C6-C7-C8-C9
22	A	1136	CLA	C14-C13-C15-C16
22	A	1137	CLA	C6-C7-C8-C9
22	B	1210	CLA	C6-C7-C8-C9
22	B	1219	CLA	C6-C7-C8-C9
22	a	604	CLA	C11-C12-C13-C14
22	3	605	CLA	C11-C10-C8-C9
22	3	610	CLA	C6-C7-C8-C9
22	3	613	CLA	C6-C7-C8-C9
22	4	611	CLA	C6-C7-C8-C9
22	6	603	CLA	C14-C13-C15-C16
22	7	604	CLA	C11-C12-C13-C14
22	8	620	CLA	C11-C10-C8-C9
25	5	801	LHG	C26-C27-C28-C29
25	6	801	LHG	C9-C10-C11-C12
22	B	1237	CLA	C3-C5-C6-C7
25	5	801	LHG	C11-C10-C9-C8
25	B	5001	LHG	C12-C13-C14-C15
26	A	5005	DGD	C3B-C4B-C5B-C6B
24	6	503	BCR	C18-C19-C20-C21
24	A	4003	BCR	C19-C20-C21-C22
25	1	801	LHG	C11-C10-C9-C8
25	4	801	LHG	C33-C34-C35-C36
25	4	802	LHG	C10-C11-C12-C13
25	4	802	LHG	C14-C15-C16-C17
26	A	5005	DGD	O6D-C5D-C6D-O5D
25	1	802	LHG	C24-C25-C26-C27
22	A	1128	CLA	C16-C17-C18-C20
22	B	1203	CLA	C16-C17-C18-C19
22	B	1213	CLA	C11-C12-C13-C15
22	B	1221	CLA	C16-C17-C18-C19
22	A	1120	CLA	C1-C2-C3-C4
22	A	1128	CLA	O1A-CGA-O2A-C1
22	A	1127	CLA	CAA-CBA-CGA-O2A
22	B	1224	CLA	CAA-CBA-CGA-O2A
22	G	1602	CLA	O1A-CGA-O2A-C1
25	4	802	LHG	C6-C5-O7-C7

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Mol	Chain	Res	Type	Atoms
22	G	1601	CLA	C2A-CAA-CBA-CGA
43	6	804	PLM	C9-CA-CB-CC
22	B	1202	CLA	C2-C1-O2A-CGA
22	B	1212	CLA	C2-C1-O2A-CGA
22	1	603	CLA	C2-C1-O2A-CGA
22	4	603	CLA	C2-C1-O2A-CGA
39	3	611	CHL	C2-C1-O2A-CGA
22	7	607	CLA	C4C-C3C-CAC-CBC
22	B	1021	CLA	CAA-CBA-CGA-O2A
22	A	1104	CLA	C3-C5-C6-C7
25	5	801	LHG	C35-C36-C37-C38
31	7	804	PTY	C12-C13-C14-C15
25	5	801	LHG	C2-C3-O3-P
47	8	807	4RF	C12-C13-C14-C15
22	A	1132	CLA	CBA-CGA-O2A-C1
25	B	5002	LHG	O6-C4-C5-O7
30	6	803	PCW	O3P-C1-C2-O2
22	3	613	CLA	CAA-CBA-CGA-O2A
22	B	1226	CLA	C16-C17-C18-C19
22	B	1237	CLA	C4-C3-C5-C6
22	7	601	CLA	C4-C3-C5-C6
25	6	801	LHG	C15-C16-C17-C18
24	3	504	BCR	C23-C24-C25-C26
24	5	503	BCR	C23-C24-C25-C30
39	1	609	CHL	C3-C5-C6-C7
22	A	1117	CLA	C2-C3-C5-C6
22	B	1216	CLA	C2-C3-C5-C6
22	B	1207	CLA	C2-C3-C5-C6
25	7	801	LHG	C15-C16-C17-C18
22	B	1204	CLA	O1D-CGD-O2D-CED
25	A	5003	LHG	C27-C28-C29-C30
25	F	5002	LHG	C29-C30-C31-C32
47	7	807	4RF	C44-C45-C46-C47
22	A	1111	CLA	CAA-CBA-CGA-O2A
47	8	808	4RF	C12-C13-C14-C15
47	8	807	4RF	C28-C29-C30-C31
22	1	612	CLA	C16-C17-C18-C20
22	7	617	CLA	C2A-CAA-CBA-CGA
22	B	1235	CLA	O1D-CGD-O2D-CED
24	B	4003	BCR	C11-C10-C9-C8
22	A	1126	CLA	CAA-CBA-CGA-O2A
39	8	601	CHL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
25	F	5002	LHG	C3-O3-P-O6
25	F	5001	LHG	C3-O3-P-O6
25	1	801	LHG	C3-O3-P-O6
25	1	802	LHG	C3-O3-P-O6
25	3	801	LHG	C4-O6-P-O3
25	4	801	LHG	C4-O6-P-O3
25	5	801	LHG	C3-O3-P-O6
25	6	802	LHG	C3-O3-P-O6
25	7	802	LHG	C3-O3-P-O6
25	7	802	LHG	C4-O6-P-O3
25	8	801	LHG	C3-O3-P-O6
30	B	5004	PCW	C1-O3P-P-O4P
32	B	5007	LAP	C15-O4-P9-O6
32	B	5007	LAP	C16-O6-P9-O4
36	a	804	LPX	C3-O1-P1-O2
21	A	1011	CL0	C5-C6-C7-C8
33	7	805	SQD	C14-C15-C16-C17
25	B	5002	LHG	C4-C5-C6-O8
33	G	5001	SQD	C44-C45-C46-O48
26	8	802	DGD	C4D-C5D-C6D-O5D
22	A	1111	CLA	C11-C12-C13-C15
22	A	1101	CLA	C11-C12-C13-C15
22	B	1023	CLA	C6-C7-C8-C10
22	B	1230	CLA	C2-C3-C5-C6
22	B	1229	CLA	C6-C7-C8-C10
22	a	607	CLA	C6-C7-C8-C10
23	A	2001	PQN	C17-C18-C20-C21
39	6	619	CHL	C11-C12-C13-C15
39	a	606	CHL	C3-C5-C6-C7
22	A	1106	CLA	C11-C10-C8-C9
22	A	1106	CLA	C14-C13-C15-C16
22	A	1110	CLA	C11-C10-C8-C9
22	A	1111	CLA	C14-C13-C15-C16
22	B	1021	CLA	C6-C7-C8-C9
22	B	1220	CLA	C6-C7-C8-C9
22	a	604	CLA	C11-C10-C8-C9
22	3	616	CLA	C6-C7-C8-C9
22	5	604	CLA	C14-C13-C15-C16
22	8	618	CLA	C11-C10-C8-C9
39	4	609	CHL	C11-C10-C8-C9
39	5	610	CHL	C14-C13-C15-C16
24	3	505	BCR	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
38	4	501	LUT	C29-C30-C31-C32
38	4	502	LUT	C29-C30-C31-C32
38	5	505	LUT	C9-C10-C11-C12
22	1	611	CLA	C6-C7-C8-C10
22	a	603	CLA	C16-C17-C18-C19
22	B	1218	CLA	C2A-CAA-CBA-CGA
30	6	803	PCW	C33-C34-C35-C36
24	B	4002	BCR	C11-C12-C13-C35
22	B	1238	CLA	CBA-CGA-O2A-C1
22	A	1133	CLA	C10-C11-C12-C13
22	8	618	CLA	C10-C11-C12-C13
22	B	1204	CLA	CBD-CGD-O2D-CED
25	6	802	LHG	C9-C10-C11-C12
22	B	1216	CLA	C12-C13-C15-C16
22	A	1131	CLA	C4-C3-C5-C6
22	8	608	CLA	C4-C3-C5-C6
25	F	5002	LHG	O1-C1-C2-O2
25	1	801	LHG	O1-C1-C2-O2
22	B	1023	CLA	C2-C3-C5-C6
22	1	607	CLA	C2-C3-C5-C6
22	6	604	CLA	C2-C3-C5-C6
25	4	801	LHG	C24-C23-O8-C6
39	4	609	CHL	CBA-CGA-O2A-C1
22	A	1131	CLA	C13-C15-C16-C17
22	B	1203	CLA	C5-C6-C7-C8
25	4	801	LHG	O10-C23-O8-C6
26	A	5005	DGD	C4D-C5D-C6D-O5D
22	B	1022	CLA	C2A-CAA-CBA-CGA
24	B	4004	BCR	C19-C20-C21-C22
24	F	4001	BCR	C19-C20-C21-C22
24	I	4001	BCR	C13-C14-C15-C16
24	L	4002	BCR	C15-C16-C17-C18
24	4	503	BCR	C13-C14-C15-C16
38	1	502	LUT	C33-C34-C35-C15
38	5	501	LUT	C29-C30-C31-C32
25	A	5002	LHG	C10-C11-C12-C13
47	7	807	4RF	C11-C12-C13-C14
22	A	1116	CLA	C3-C5-C6-C7
22	A	1117	CLA	C3-C5-C6-C7
22	B	1213	CLA	C3-C5-C6-C7
22	B	1235	CLA	CBD-CGD-O2D-CED
22	A	1114	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
47	8	807	4RF	C30-C31-C32-C33
25	B	5001	LHG	O6-C4-C5-O7
44	8	803	DGA	CA4-CA5-CA6-CA7
24	B	4002	BCR	C10-C11-C12-C13
24	6	504	BCR	C10-C11-C12-C13
46	7	502	XAT	C10-C11-C12-C13
22	6	615	CLA	C15-C16-C17-C18
33	7	805	SQD	C9-C10-C11-C12
22	B	1239	CLA	C15-C16-C17-C18
22	8	608	CLA	C2-C3-C5-C6
22	A	1115	CLA	C8-C10-C11-C12
22	K	1402	CLA	C10-C11-C12-C13
22	3	603	CLA	C15-C16-C17-C18
25	B	5001	LHG	O2-C2-C3-O3
25	B	5002	LHG	C12-C13-C14-C15
31	B	5005	PTY	C12-C13-C14-C15
32	B	5007	LAP	C6-C7-C8-C9
40	1	803	OLA	O1-C1-C2-C3
40	8	809	OLA	O1-C1-C2-C3
22	B	1210	CLA	C2-C1-O2A-CGA
22	8	602	CLA	C2-C1-O2A-CGA
25	A	5001	LHG	C9-C10-C11-C12
22	A	1119	CLA	C13-C15-C16-C17
22	A	1013	CLA	C16-C17-C18-C19
22	3	601	CLA	C2A-CAA-CBA-CGA
22	4	603	CLA	C2A-CAA-CBA-CGA
22	7	601	CLA	C2A-CAA-CBA-CGA
26	8	802	DGD	CAA-CBA-CCA-CDA
44	5	803	DGA	CA5-CA6-CA7-CA8
33	7	805	SQD	C11-C12-C13-C14
25	B	5002	LHG	C2-C3-O3-P
25	4	801	LHG	C2-C3-O3-P
22	5	609	CLA	C3A-C2A-CAA-CBA
39	5	610	CHL	C3A-C2A-CAA-CBA
39	5	611	CHL	C3A-C2A-CAA-CBA
24	3	505	BCR	C19-C20-C21-C22
24	6	503	BCR	C9-C10-C11-C12
27	A	5007	3PH	C29-C2A-C2B-C2C
43	4	803	PLM	C4-C5-C6-C7
31	3	802	PTY	C32-C33-C34-C35
22	7	612	CLA	C2-C3-C5-C6
31	3	802	PTY	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
31	3	802	PTY	C12-C11-C8-O7
22	A	1102	CLA	C11-C12-C13-C14
22	A	1109	CLA	C14-C13-C15-C16
22	A	1119	CLA	C11-C10-C8-C9
22	A	1138	CLA	C6-C7-C8-C9
22	A	1138	CLA	C11-C12-C13-C14
22	B	1203	CLA	C6-C7-C8-C9
22	B	1224	CLA	C11-C12-C13-C14
22	1	601	CLA	C6-C7-C8-C9
22	a	605	CLA	C11-C12-C13-C14
22	a	612	CLA	C6-C7-C8-C9
39	6	619	CHL	C6-C7-C8-C9
22	8	610	CLA	C6-C7-C8-C9
25	7	801	LHG	C16-C17-C18-C19
22	8	605	CLA	CAA-CBA-CGA-O1A
44	5	803	DGA	CA1-CA2-CA3-CA4
22	8	608	CLA	CBA-CGA-O2A-C1
25	a	801	LHG	C27-C28-C29-C30
47	8	807	4RF	C33-C34-C35-C36
22	7	604	CLA	C13-C15-C16-C17
24	A	4005	BCR	C16-C17-C18-C36
24	B	4003	BCR	C20-C21-C22-C37
24	F	4001	BCR	C35-C13-C14-C15
25	A	5002	LHG	C25-C26-C27-C28
25	F	5001	LHG	O2-C2-C3-O3
24	B	4005	BCR	C11-C12-C13-C35
24	L	4003	BCR	C36-C18-C19-C20
39	4	609	CHL	O1A-CGA-O2A-C1
30	B	5004	PCW	C3-C2-O2-C31
22	6	604	CLA	C10-C11-C12-C13
22	A	1127	CLA	C1A-C2A-CAA-CBA
22	A	1129	CLA	C1A-C2A-CAA-CBA
22	A	1140	CLA	C1A-C2A-CAA-CBA
22	B	1230	CLA	C1A-C2A-CAA-CBA
22	B	1240	CLA	C1A-C2A-CAA-CBA
22	3	613	CLA	C1A-C2A-CAA-CBA
22	4	606	CLA	C1A-C2A-CAA-CBA
39	5	611	CHL	C1A-C2A-CAA-CBA
22	A	1103	CLA	CBA-CGA-O2A-C1
22	A	1108	CLA	C11-C12-C13-C15
22	A	1111	CLA	C11-C10-C8-C7
22	A	1114	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	A	1125	CLA	C6-C7-C8-C10
22	A	1133	CLA	C6-C7-C8-C10
22	A	1101	CLA	C12-C13-C15-C16
22	B	1203	CLA	C11-C12-C13-C15
22	B	1223	CLA	C11-C12-C13-C15
22	B	1237	CLA	C6-C7-C8-C10
22	B	1240	CLA	C6-C7-C8-C10
22	B	1204	CLA	C11-C10-C8-C7
22	a	603	CLA	C6-C7-C8-C10
22	a	605	CLA	C6-C7-C8-C10
22	3	605	CLA	C12-C13-C15-C16
22	3	612	CLA	C6-C7-C8-C10
22	4	603	CLA	C6-C7-C8-C10
22	8	606	CLA	C6-C7-C8-C10
23	B	2002	PQN	C16-C17-C18-C20
25	A	5003	LHG	C9-C10-C11-C12
22	6	604	CLA	C3-C5-C6-C7
22	8	605	CLA	CAA-CBA-CGA-O2A
40	8	809	OLA	O2-C1-C2-C3
25	6	802	LHG	C24-C25-C26-C27
24	5	504	BCR	C19-C20-C21-C22
22	8	607	CLA	CBD-CGD-O2D-CED
25	F	5001	LHG	C27-C28-C29-C30
25	7	801	LHG	C10-C11-C12-C13
44	8	803	DGA	CBB-CAB-CB9-CB8
22	A	1103	CLA	O1A-CGA-O2A-C1
22	A	1125	CLA	C16-C17-C18-C20
25	4	801	LHG	C30-C31-C32-C33
22	A	1131	CLA	C2A-CAA-CBA-CGA
22	A	1101	CLA	C10-C11-C12-C13
22	B	1217	CLA	C5-C6-C7-C8
22	4	610	CLA	C13-C15-C16-C17
25	a	801	LHG	C11-C10-C9-C8
25	a	801	LHG	C9-C10-C11-C12
32	K	5001	LAP	C5-C6-C7-C8
25	F	5001	LHG	O6-C4-C5-C6
31	3	802	PTY	C33-C34-C35-C36
22	B	1212	CLA	C8-C10-C11-C12
40	1	803	OLA	O2-C1-C2-C3
22	A	1126	CLA	C4-C3-C5-C6
22	B	1022	CLA	C4-C3-C5-C6
22	3	607	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	a	607	CLA	C8-C10-C11-C12
22	3	612	CLA	C8-C10-C11-C12
22	4	612	CLA	C5-C6-C7-C8
22	4	612	CLA	C8-C10-C11-C12
31	5	802	PTY	C12-C13-C14-C15
25	4	801	LHG	C17-C18-C19-C20
25	7	802	LHG	C29-C30-C31-C32
25	7	803	LHG	C19-C20-C21-C22
22	A	1133	CLA	C5-C6-C7-C8
22	B	1023	CLA	C5-C6-C7-C8
22	4	615	CLA	C8-C10-C11-C12
22	8	609	CLA	C10-C11-C12-C13
22	B	1238	CLA	O1A-CGA-O2A-C1
33	G	5001	SQD	C26-C27-C28-C29
26	A	5005	DGD	O1B-C1B-O2G-C2G
30	B	5004	PCW	O31-C31-O2-C2
24	A	4005	BCR	C16-C17-C18-C19
24	B	4003	BCR	C20-C21-C22-C23
24	F	4001	BCR	C12-C13-C14-C15
31	3	802	PTY	C11-C12-C13-C14
25	4	801	LHG	O7-C5-C6-O8
25	7	802	LHG	O7-C5-C6-O8
31	3	802	PTY	O4-C1-C6-O7
33	7	805	SQD	O6-C44-C45-O47
25	B	5002	LHG	C24-C23-O8-C6
25	a	801	LHG	C29-C30-C31-C32
39	4	618	CHL	C4C-C3C-CAC-CBC
49	8	806	P5S	O47-C38-C39-C40
24	A	4001	BCR	C19-C20-C21-C22
24	A	4005	BCR	C13-C14-C15-C16
24	B	4002	BCR	C13-C14-C15-C16
24	B	4001	BCR	C13-C14-C15-C16
24	G	4001	BCR	C13-C14-C15-C16
24	J	4001	BCR	C13-C14-C15-C16
24	L	4001	BCR	C15-C16-C17-C18
38	7	501	LUT	C33-C34-C35-C15
22	6	608	CLA	CAA-CBA-CGA-O2A
22	B	1207	CLA	C5-C6-C7-C8
22	8	608	CLA	O1A-CGA-O2A-C1
22	A	1126	CLA	C3-C5-C6-C7
22	B	1214	CLA	C4-C3-C5-C6
22	B	1221	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	3	613	CLA	C4-C3-C5-C6
22	A	1134	CLA	C2-C1-O2A-CGA
22	B	1209	CLA	C2-C1-O2A-CGA
22	B	1215	CLA	C2-C1-O2A-CGA
22	B	1224	CLA	C2-C1-O2A-CGA
22	B	1204	CLA	C2-C1-O2A-CGA
22	3	604	CLA	C2-C1-O2A-CGA
22	4	601	CLA	C2-C1-O2A-CGA
22	5	601	CLA	C2-C1-O2A-CGA
22	6	603	CLA	C2-C1-O2A-CGA
39	4	618	CHL	C2-C1-O2A-CGA
39	6	619	CHL	C8-C10-C11-C12
24	K	4001	BCR	C10-C11-C12-C13
22	A	1116	CLA	CAA-CBA-CGA-O2A
22	B	1221	CLA	C16-C17-C18-C20
22	A	1111	CLA	C6-C7-C8-C9
22	B	1213	CLA	C6-C7-C8-C9
22	A	1107	CLA	C3-C5-C6-C7
49	8	806	P5S	C42-C43-C44-C45
22	A	1013	CLA	C2A-CAA-CBA-CGA
22	7	606	CLA	C2A-CAA-CBA-CGA
23	A	2001	PQN	C26-C27-C28-C29
39	a	610	CHL	C2-C1-O2A-CGA
24	A	4004	BCR	C23-C24-C25-C30
24	B	4007	BCR	C1-C6-C7-C8
24	K	4001	BCR	C23-C24-C25-C30
24	L	4003	BCR	C1-C6-C7-C8
38	3	501	LUT	C1-C6-C7-C8
38	4	501	LUT	C1-C6-C7-C8
38	4	502	LUT	C1-C6-C7-C8
38	7	501	LUT	C1-C6-C7-C8
38	8	501	LUT	C1-C6-C7-C8
38	8	502	LUT	C1-C6-C7-C8
22	7	602	CLA	C4C-C3C-CAC-CBC
22	1	612	CLA	CAA-CBA-CGA-O2A
25	3	801	LHG	C4-C5-C6-O8
22	1	604	CLA	C13-C15-C16-C17
24	A	4002	BCR	C15-C16-C17-C18
24	B	4007	BCR	C19-C20-C21-C22
22	B	1224	CLA	C4-C3-C5-C6
22	L	1502	CLA	C4-C3-C5-C6
22	4	615	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
39	a	606	CHL	C4-C3-C5-C6
24	B	4001	BCR	C17-C18-C19-C20
24	L	4003	BCR	C17-C18-C19-C20
22	B	1229	CLA	C8-C10-C11-C12
22	A	1121	CLA	C2-C3-C5-C6
22	A	1134	CLA	C2-C3-C5-C6
22	1	602	CLA	CAA-CBA-CGA-O2A
22	1	606	CLA	C8-C10-C11-C12
22	5	612	CLA	C16-C17-C18-C20
26	8	802	DGD	CDA-CEA-CFA-CGA
22	B	1208	CLA	C8-C10-C11-C12
25	7	803	LHG	O6-C4-C5-O7
29	B	5006	LMT	C1-C2-C3-C4
22	G	1601	CLA	CAA-CBA-CGA-O1A
22	L	1503	CLA	CAA-CBA-CGA-O2A
22	L	1501	CLA	C2A-CAA-CBA-CGA
22	3	613	CLA	C8-C10-C11-C12
22	A	1122	CLA	C10-C11-C12-C13
29	1	804	LMT	C6-C7-C8-C9
29	1	804	LMT	C5'-C4'-O1B-C1B
31	5	802	PTY	O14-C5-C6-C1
22	F	1302	CLA	C4-C3-C5-C6
22	5	604	CLA	C4-C3-C5-C6
39	6	610	CHL	CAA-CBA-CGA-O1A
25	B	5002	LHG	C35-C36-C37-C38
22	A	1119	CLA	C11-C12-C13-C15
22	B	1224	CLA	C11-C12-C13-C15
22	1	603	CLA	C11-C10-C8-C7
22	3	604	CLA	C11-C10-C8-C7
23	A	2001	PQN	C22-C23-C25-C26
39	4	609	CHL	C11-C12-C13-C15
22	A	1134	CLA	CBA-CGA-O2A-C1
22	A	1111	CLA	C13-C15-C16-C17
24	A	4002	BCR	C19-C20-C21-C22
22	7	612	CLA	CAA-CBA-CGA-O2A
25	B	5002	LHG	O7-C7-C8-C9
25	7	802	LHG	O8-C23-C24-C25
22	6	608	CLA	CAA-CBA-CGA-O1A
26	8	802	DGD	CCA-CDA-CEA-CFA
31	7	804	PTY	C33-C34-C35-C36
22	6	607	CLA	C3-C5-C6-C7
22	4	617	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	3	616	CLA	CAA-CBA-CGA-O2A
25	F	5002	LHG	O8-C23-C24-C25
25	6	802	LHG	O8-C23-C24-C25
31	B	5005	PTY	C12-C11-C8-O7
22	5	612	CLA	C2A-CAA-CBA-CGA
25	1	802	LHG	C17-C18-C19-C20
22	7	615	CLA	C2C-C3C-CAC-CBC
29	B	5006	LMT	C3'-C4'-O1B-C1B
22	B	1023	CLA	C2C-C3C-CAC-CBC
22	8	620	CLA	CAA-CBA-CGA-O2A
22	8	607	CLA	O1D-CGD-O2D-CED
22	A	1104	CLA	C4-C3-C5-C6
22	A	1122	CLA	C4-C3-C5-C6
22	B	1220	CLA	C4-C3-C5-C6
22	B	1235	CLA	C4-C3-C5-C6
22	1	612	CLA	C4-C3-C5-C6
22	7	606	CLA	C4-C3-C5-C6
22	7	610	CLA	C4-C3-C5-C6
22	B	1211	CLA	C5-C6-C7-C8
22	A	1140	CLA	C2-C3-C5-C6
22	B	1221	CLA	C2-C3-C5-C6
22	4	601	CLA	C2-C3-C5-C6
22	4	615	CLA	C2-C3-C5-C6
22	7	601	CLA	C2-C3-C5-C6
39	a	606	CHL	C2-C3-C5-C6
22	3	610	CLA	C11-C12-C13-C14
22	6	601	CLA	C11-C12-C13-C14
22	A	1109	CLA	CAA-CBA-CGA-O2A
22	A	1104	CLA	C11-C12-C13-C14
22	A	1111	CLA	C11-C12-C13-C14
22	A	1136	CLA	C11-C10-C8-C9
22	A	1101	CLA	C6-C7-C8-C9
22	B	1203	CLA	C11-C12-C13-C14
22	B	1208	CLA	C6-C7-C8-C9
22	B	1235	CLA	C11-C10-C8-C9
22	B	1235	CLA	C14-C13-C15-C16
22	B	1237	CLA	C6-C7-C8-C9
22	B	1240	CLA	C6-C7-C8-C9
22	B	1207	CLA	C11-C10-C8-C9
22	1	603	CLA	C6-C7-C8-C9
22	1	607	CLA	C11-C12-C13-C14
22	8	603	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	B	2002	PQN	C16-C17-C18-C19
39	5	610	CHL	C6-C7-C8-C9
22	G	1603	CLA	CAA-CBA-CGA-O2A
22	L	1503	CLA	CAA-CBA-CGA-O1A
43	6	804	PLM	C7-C8-C9-CA
22	A	1141	CLA	C3A-C2A-CAA-CBA
22	A	1140	CLA	C3A-C2A-CAA-CBA
22	B	1230	CLA	C3A-C2A-CAA-CBA
22	3	613	CLA	C3A-C2A-CAA-CBA
22	8	618	CLA	C3A-C2A-CAA-CBA
39	6	613	CHL	C3A-C2A-CAA-CBA
39	8	601	CHL	C3A-C2A-CAA-CBA
22	A	1134	CLA	O1A-CGA-O2A-C1
22	6	604	CLA	O1A-CGA-O2A-C1
22	B	1204	CLA	CAA-CBA-CGA-O2A
25	4	801	LHG	O7-C7-C8-C9
40	8	809	OLA	C7-C8-C9-C10
22	A	1103	CLA	CAD-CBD-CGD-O2D
22	A	1104	CLA	CAD-CBD-CGD-O2D
22	A	1125	CLA	CAD-CBD-CGD-O2D
22	A	1129	CLA	CAD-CBD-CGD-O2D
22	B	1211	CLA	CAD-CBD-CGD-O2D
22	B	1223	CLA	CAD-CBD-CGD-O2D
22	B	1226	CLA	CAD-CBD-CGD-O2D
22	B	1240	CLA	CAD-CBD-CGD-O2D
22	L	1502	CLA	CAD-CBD-CGD-O2D
22	1	604	CLA	CAD-CBD-CGD-O2D
22	1	605	CLA	CAD-CBD-CGD-O2D
22	7	608	CLA	CAD-CBD-CGD-O2D
39	1	613	CHL	CAD-CBD-CGD-O2D
39	1	609	CHL	CAD-CBD-CGD-O2D
39	a	606	CHL	CAD-CBD-CGD-O2D
39	3	608	CHL	CAD-CBD-CGD-O2D
39	8	601	CHL	C11-C12-C13-C15
25	B	5001	LHG	C32-C33-C34-C35
22	B	1216	CLA	C2A-CAA-CBA-CGA
26	B	5003	DGD	O1B-C1B-O2G-C2G
43	6	804	PLM	CC-CD-CE-CF
22	A	1129	CLA	CAA-CBA-CGA-O2A
25	7	802	LHG	O7-C7-C8-C9
25	8	801	LHG	O8-C23-C24-C25
22	B	1021	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
39	a	613	CHL	CAA-CBA-CGA-O2A
27	A	5007	3PH	O22-C21-C22-C23
22	A	1122	CLA	C2-C3-C5-C6
22	A	1126	CLA	C2-C3-C5-C6
22	B	1022	CLA	C2-C3-C5-C6
22	B	1214	CLA	C2-C3-C5-C6
22	L	1502	CLA	C2-C3-C5-C6
22	1	612	CLA	C2-C3-C5-C6
22	3	607	CLA	C2-C3-C5-C6
22	B	1209	CLA	CAA-CBA-CGA-O2A
22	5	612	CLA	CAA-CBA-CGA-O2A
24	B	4002	BCR	C11-C12-C13-C14
24	B	4005	BCR	C11-C12-C13-C14
38	a	502	LUT	C27-C28-C29-C30
22	B	1231	CLA	C8-C10-C11-C12
22	G	1603	CLA	CAA-CBA-CGA-O1A
22	5	601	CLA	O1A-CGA-O2A-C1
25	1	802	LHG	C25-C26-C27-C28
25	a	801	LHG	O6-C4-C5-O7
22	B	1214	CLA	CAA-CBA-CGA-O2A
22	3	605	CLA	CAA-CBA-CGA-O2A
22	5	617	CLA	CAA-CBA-CGA-O2A
22	8	608	CLA	CAA-CBA-CGA-O2A
39	a	610	CHL	CAA-CBA-CGA-O2A
22	7	615	CLA	C4C-C3C-CAC-CBC
47	8	808	4RF	C32-C33-C34-C35
22	A	1126	CLA	O2A-C1-C2-C3
22	B	1213	CLA	O2A-C1-C2-C3
39	5	613	CHL	O2A-C1-C2-C3
22	B	1214	CLA	O1A-CGA-O2A-C1
25	4	802	LHG	C13-C14-C15-C16
22	5	601	CLA	C2A-CAA-CBA-CGA
22	A	1103	CLA	C10-C11-C12-C13
22	7	615	CLA	C5-C6-C7-C8
43	4	803	PLM	C3-C4-C5-C6
22	8	609	CLA	CAA-CBA-CGA-O2A
22	7	607	CLA	C2-C3-C5-C6
22	A	1102	CLA	CHA-CBD-CGD-O2D
22	A	1109	CLA	CHA-CBD-CGD-O1D
22	A	1109	CLA	CHA-CBD-CGD-O2D
22	A	1116	CLA	CHA-CBD-CGD-O1D
22	A	1116	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	A	1121	CLA	CHA-CBD-CGD-O2D
22	A	1127	CLA	CHA-CBD-CGD-O1D
22	A	1127	CLA	CHA-CBD-CGD-O2D
22	A	1133	CLA	CHA-CBD-CGD-O2D
22	A	1135	CLA	CHA-CBD-CGD-O1D
22	A	1135	CLA	CHA-CBD-CGD-O2D
22	B	1022	CLA	CHA-CBD-CGD-O1D
22	B	1022	CLA	CHA-CBD-CGD-O2D
22	B	1023	CLA	CHA-CBD-CGD-O1D
22	B	1023	CLA	CHA-CBD-CGD-O2D
22	B	1215	CLA	CHA-CBD-CGD-O1D
22	B	1215	CLA	CHA-CBD-CGD-O2D
22	B	1235	CLA	CHA-CBD-CGD-O2D
22	B	1236	CLA	CHA-CBD-CGD-O2D
22	G	1601	CLA	CHA-CBD-CGD-O1D
22	G	1601	CLA	CHA-CBD-CGD-O2D
22	J	1901	CLA	CHA-CBD-CGD-O1D
22	J	1901	CLA	CHA-CBD-CGD-O2D
22	K	1401	CLA	CHA-CBD-CGD-O1D
22	K	1401	CLA	CHA-CBD-CGD-O2D
22	L	1503	CLA	CHA-CBD-CGD-O1D
22	L	1503	CLA	CHA-CBD-CGD-O2D
22	1	601	CLA	CHA-CBD-CGD-O2D
22	1	603	CLA	CHA-CBD-CGD-O1D
22	1	603	CLA	CHA-CBD-CGD-O2D
22	1	615	CLA	CHA-CBD-CGD-O1D
22	1	615	CLA	CHA-CBD-CGD-O2D
22	a	603	CLA	CHA-CBD-CGD-O2D
22	a	604	CLA	CHA-CBD-CGD-O1D
22	a	604	CLA	CHA-CBD-CGD-O2D
22	a	607	CLA	CHA-CBD-CGD-O1D
22	a	612	CLA	CHA-CBD-CGD-O2D
22	3	602	CLA	CHA-CBD-CGD-O1D
22	3	602	CLA	CHA-CBD-CGD-O2D
22	3	604	CLA	CHA-CBD-CGD-O2D
22	3	612	CLA	CHA-CBD-CGD-O1D
22	3	612	CLA	CHA-CBD-CGD-O2D
22	3	613	CLA	CHA-CBD-CGD-O1D
22	3	613	CLA	CHA-CBD-CGD-O2D
22	3	616	CLA	CHA-CBD-CGD-O1D
22	3	616	CLA	CHA-CBD-CGD-O2D
22	4	605	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	5	602	CLA	CHA-CBD-CGD-O2D
22	5	605	CLA	CHA-CBD-CGD-O1D
22	5	605	CLA	CHA-CBD-CGD-O2D
22	5	607	CLA	CHA-CBD-CGD-O1D
22	5	607	CLA	CHA-CBD-CGD-O2D
22	5	612	CLA	CHA-CBD-CGD-O2D
22	6	603	CLA	CHA-CBD-CGD-O2D
22	6	618	CLA	CHA-CBD-CGD-O1D
22	6	618	CLA	CHA-CBD-CGD-O2D
22	7	601	CLA	CHA-CBD-CGD-O1D
22	7	601	CLA	CHA-CBD-CGD-O2D
22	7	608	CLA	CHA-CBD-CGD-O2D
22	7	610	CLA	CHA-CBD-CGD-O1D
22	7	610	CLA	CHA-CBD-CGD-O2D
22	8	605	CLA	CHA-CBD-CGD-O1D
22	8	605	CLA	CHA-CBD-CGD-O2D
22	8	618	CLA	CHA-CBD-CGD-O1D
22	8	618	CLA	CHA-CBD-CGD-O2D
24	B	4004	BCR	C9-C10-C11-C12
38	3	502	LUT	C13-C14-C15-C35
39	5	611	CHL	CHA-CBD-CGD-O1D
39	5	611	CHL	CHA-CBD-CGD-O2D
39	6	610	CHL	CHA-CBD-CGD-O1D
39	6	610	CHL	CHA-CBD-CGD-O2D
41	a	504	QTB	C02-C03-C04-C05
22	A	1125	CLA	CAA-CBA-CGA-O2A
22	B	1208	CLA	CAA-CBA-CGA-O2A
22	8	603	CLA	CAA-CBA-CGA-O2A
39	4	613	CHL	CAA-CBA-CGA-O2A
22	B	1224	CLA	C2-C3-C5-C6
25	3	801	LHG	C28-C29-C30-C31
25	1	802	LHG	O6-C4-C5-C6
25	3	801	LHG	O6-C4-C5-C6
22	1	602	CLA	CAA-CBA-CGA-O1A
22	A	1122	CLA	C13-C15-C16-C17
22	A	1112	CLA	CAA-CBA-CGA-O2A
22	1	605	CLA	CAA-CBA-CGA-O2A
22	5	603	CLA	CAA-CBA-CGA-O2A
25	3	801	LHG	O7-C5-C6-O8
30	6	803	PCW	C32-C33-C34-C35
25	B	5002	LHG	O10-C23-O8-C6
22	A	1107	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	A	1121	CLA	CAA-CBA-CGA-O2A
22	A	1131	CLA	CAA-CBA-CGA-O2A
22	B	1210	CLA	CAA-CBA-CGA-O2A
22	1	603	CLA	CAA-CBA-CGA-O2A
22	a	603	CLA	CAA-CBA-CGA-O2A
22	4	603	CLA	CAA-CBA-CGA-O2A
22	6	603	CLA	CAA-CBA-CGA-O2A
22	A	1117	CLA	C2A-CAA-CBA-CGA
21	A	1011	CL0	CAA-CBA-CGA-O2A
22	7	603	CLA	CAA-CBA-CGA-O2A
45	6	806	SPH	C6-C7-C8-C9
22	8	615	CLA	O1A-CGA-O2A-C1
22	4	617	CLA	CAA-CBA-CGA-O1A
22	A	1013	CLA	C11-C10-C8-C7
22	A	1104	CLA	C2-C3-C5-C6
22	A	1111	CLA	C6-C7-C8-C10
22	A	1122	CLA	C6-C7-C8-C10
22	A	1136	CLA	C11-C10-C8-C7
22	A	1137	CLA	C11-C10-C8-C7
22	B	1216	CLA	C6-C7-C8-C10
22	B	1226	CLA	C6-C7-C8-C10
22	B	1237	CLA	C2-C3-C5-C6
22	6	615	CLA	C11-C12-C13-C15
22	8	603	CLA	C11-C12-C13-C15
49	8	806	P5S	OXT-C-CA-CB
45	6	806	SPH	C4-C5-C6-C7
22	4	615	CLA	CAA-CBA-CGA-O2A
25	1	801	LHG	O7-C7-C8-C9
22	A	1013	CLA	C11-C10-C8-C9
22	A	1108	CLA	C11-C12-C13-C14
22	A	1114	CLA	C6-C7-C8-C9
22	A	1119	CLA	C11-C12-C13-C14
22	A	1101	CLA	C14-C13-C15-C16
22	B	1021	CLA	C14-C13-C15-C16
22	B	1210	CLA	C14-C13-C15-C16
22	B	1216	CLA	C6-C7-C8-C9
22	B	1223	CLA	C11-C12-C13-C14
22	3	605	CLA	C14-C13-C15-C16
22	6	601	CLA	C11-C10-C8-C9
24	A	4002	BCR	C9-C10-C11-C12
38	6	502	LUT	C33-C34-C35-C15
22	A	1130	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	6	606	CLA	CAA-CBA-CGA-O2A
22	a	603	CLA	C2A-CAA-CBA-CGA
31	B	5005	PTY	C16-C17-C18-C19
25	A	5002	LHG	O7-C7-C8-C9
25	1	801	LHG	O8-C23-C24-C25
25	8	801	LHG	O7-C7-C8-C9
26	A	5005	DGD	O1G-C1A-C2A-C3A
22	3	616	CLA	CAA-CBA-CGA-O1A
22	5	612	CLA	CAA-CBA-CGA-O1A
22	5	617	CLA	CAA-CBA-CGA-O1A
22	8	609	CLA	CAA-CBA-CGA-O1A
22	8	620	CLA	CAA-CBA-CGA-O1A
22	A	1125	CLA	C16-C17-C18-C19
22	A	1138	CLA	C16-C17-C18-C20
22	1	601	CLA	C11-C12-C13-C14
22	3	610	CLA	C11-C12-C13-C15
22	8	610	CLA	C6-C7-C8-C10
23	A	2001	PQN	C26-C27-C28-C30
25	B	5001	LHG	C14-C15-C16-C17
22	7	606	CLA	C2-C3-C5-C6
33	G	5001	SQD	C14-C15-C16-C17
25	4	801	LHG	O9-C7-C8-C9
25	6	802	LHG	O10-C23-C24-C25
25	7	802	LHG	O9-C7-C8-C9
24	4	503	BCR	C17-C18-C19-C20
22	A	1105	CLA	C4C-C3C-CAC-CBC
22	A	1012	CLA	C1A-C2A-CAA-CBA
22	A	1135	CLA	C1A-C2A-CAA-CBA
22	B	1227	CLA	C1A-C2A-CAA-CBA
22	B	1235	CLA	C1A-C2A-CAA-CBA
22	G	1603	CLA	C1A-C2A-CAA-CBA
22	K	1401	CLA	C1A-C2A-CAA-CBA
22	L	1501	CLA	C1A-C2A-CAA-CBA
22	5	609	CLA	C1A-C2A-CAA-CBA
22	7	605	CLA	CHA-CBD-CGD-O2D
22	7	617	CLA	C1A-C2A-CAA-CBA
39	6	613	CHL	C1A-C2A-CAA-CBA
22	B	1208	CLA	CAA-CBA-CGA-O1A
22	8	608	CLA	CAA-CBA-CGA-O1A
25	1	801	LHG	O9-C7-C8-C9
30	B	5004	PCW	C32-C31-O2-C2
33	G	5001	SQD	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
22	B	1214	CLA	CBA-CGA-O2A-C1
22	5	601	CLA	CBA-CGA-O2A-C1
22	7	612	CLA	CAA-CBA-CGA-O1A
25	7	802	LHG	O10-C23-C24-C25
39	4	613	CHL	CAA-CBA-CGA-O1A
39	a	613	CHL	CAA-CBA-CGA-O1A
39	3	611	CHL	CAA-CBA-CGA-O2A
22	B	1215	CLA	C2A-CAA-CBA-CGA
22	a	612	CLA	C2A-CAA-CBA-CGA
25	1	802	LHG	C12-C13-C14-C15
22	A	1119	CLA	C16-C17-C18-C20
22	6	609	CLA	C16-C17-C18-C19
22	A	1112	CLA	CAA-CBA-CGA-O1A
22	B	1210	CLA	CAA-CBA-CGA-O1A
22	a	608	CLA	CAA-CBA-CGA-O1A
22	3	605	CLA	CAA-CBA-CGA-O1A
25	F	5002	LHG	O10-C23-C24-C25
31	B	5005	PTY	C12-C11-C8-O10
22	3	603	CLA	CAA-CBA-CGA-O2A
22	5	605	CLA	CAA-CBA-CGA-O2A
22	A	1130	CLA	CAA-CBA-CGA-O1A
22	1	603	CLA	CAA-CBA-CGA-O1A
25	B	5002	LHG	O9-C7-C8-C9
22	3	613	CLA	C2-C3-C5-C6
22	A	1141	CLA	CAA-CBA-CGA-O2A
22	3	606	CLA	C15-C16-C17-C18
25	3	801	LHG	C35-C36-C37-C38
25	A	5001	LHG	C3-O3-P-O4
25	F	5001	LHG	C3-O3-P-O5
25	1	802	LHG	C3-O3-P-O5
25	3	801	LHG	C4-O6-P-O5
25	8	801	LHG	C3-O3-P-O5
30	B	5004	PCW	C1-O3P-P-O2P
32	B	5007	LAP	C16-O6-P9-O5
49	8	806	P5S	C40-C41-C42-C43
22	A	1107	CLA	CAA-CBA-CGA-O1A
22	B	1209	CLA	CAA-CBA-CGA-O1A
22	3	602	CLA	CAA-CBA-CGA-O1A
22	4	615	CLA	CAA-CBA-CGA-O1A
25	A	5002	LHG	O9-C7-C8-C9
22	B	1211	CLA	CAA-CBA-CGA-O2A
22	1	608	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	A	1123	CLA	O1A-CGA-O2A-C1
25	B	5001	LHG	O6-C4-C5-C6
25	A	5001	LHG	C10-C11-C12-C13
24	A	4005	BCR	C23-C24-C25-C30
24	K	4001	BCR	C23-C24-C25-C26
24	L	4003	BCR	C5-C6-C7-C8
38	4	502	LUT	C5-C6-C7-C8
38	6	501	LUT	C1-C6-C7-C8
38	6	501	LUT	C5-C6-C7-C8
38	8	501	LUT	C5-C6-C7-C8
38	8	502	LUT	C5-C6-C7-C8
22	1	605	CLA	C10-C11-C12-C13
22	A	1121	CLA	CAA-CBA-CGA-O1A
22	A	1125	CLA	CAA-CBA-CGA-O1A
22	A	1129	CLA	CAA-CBA-CGA-O1A
22	B	1214	CLA	CAA-CBA-CGA-O1A
22	6	603	CLA	CAA-CBA-CGA-O1A
22	8	603	CLA	CAA-CBA-CGA-O1A
25	1	801	LHG	O10-C23-C24-C25
25	8	801	LHG	O10-C23-C24-C25
22	F	1302	CLA	CAA-CBA-CGA-O2A
32	B	5007	LAP	O1-C1-C2-C3
39	a	610	CHL	C2C-C3C-CAC-CBC
34	G	5002	ERG	C22-C23-C24-C28
24	A	4005	BCR	C10-C11-C12-C13
22	5	603	CLA	CAA-CBA-CGA-O1A
25	1	802	LHG	O10-C23-C24-C25
25	7	802	LHG	C25-C26-C27-C28
22	7	605	CLA	CAA-CBA-CGA-O2A
22	5	602	CLA	CAA-CBA-CGA-O2A
22	5	603	CLA	C5-C6-C7-C8
22	A	1118	CLA	C2C-C3C-CAC-CBC
22	A	1131	CLA	C2-C3-C5-C6
22	B	1228	CLA	C10-C11-C12-C13
22	A	1114	CLA	C16-C17-C18-C20
22	A	1108	CLA	CAD-CBD-CGD-O1D
22	A	1112	CLA	CAD-CBD-CGD-O1D
22	A	1114	CLA	CAD-CBD-CGD-O1D
22	A	1134	CLA	CAD-CBD-CGD-O1D
22	B	1234	CLA	CAD-CBD-CGD-O1D
22	B	1239	CLA	CAD-CBD-CGD-O1D
22	B	1229	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	1	601	CLA	CAD-CBD-CGD-O1D
22	a	603	CLA	CAD-CBD-CGD-O1D
22	a	615	CLA	CAD-CBD-CGD-O1D
22	3	618	CLA	CAD-CBD-CGD-O1D
22	4	607	CLA	CAD-CBD-CGD-O1D
22	6	604	CLA	CAD-CBD-CGD-O1D
22	6	605	CLA	CAD-CBD-CGD-O1D
22	7	601	CLA	CAD-CBD-CGD-O1D
22	7	610	CLA	CAD-CBD-CGD-O1D
22	8	608	CLA	CAD-CBD-CGD-O1D
30	B	5004	PCW	C1-C2-O2-C31
31	3	802	PTY	C2-C3-O11-P1
31	5	802	PTY	C2-C3-O11-P1
39	8	613	CHL	CAD-CBD-CGD-O1D
22	B	1204	CLA	CAA-CBA-CGA-O1A
44	8	803	DGA	CB2-CB3-CB4-CB5
22	K	1402	CLA	CAA-CBA-CGA-O2A
22	3	601	CLA	CAA-CBA-CGA-O2A
22	A	1106	CLA	C8-C10-C11-C12
22	A	1135	CLA	C14-C13-C15-C16
22	A	1137	CLA	C11-C10-C8-C9
22	B	1216	CLA	C11-C10-C8-C9
22	6	615	CLA	C11-C12-C13-C14
39	6	619	CHL	C11-C12-C13-C14
22	6	606	CLA	CAA-CBA-CGA-O1A
22	A	1123	CLA	C3-C5-C6-C7
22	A	1137	CLA	C11-C12-C13-C14
22	A	1123	CLA	CAA-CBA-CGA-O2A
22	K	1404	CLA	CAA-CBA-CGA-O2A
22	1	608	CLA	CAA-CBA-CGA-O2A
39	8	604	CHL	CAA-CBA-CGA-O2A
22	B	1229	CLA	C10-C11-C12-C13
22	a	603	CLA	CAA-CBA-CGA-O1A
22	A	1106	CLA	CAA-CBA-CGA-O2A
22	A	1119	CLA	CAA-CBA-CGA-O2A
22	A	1137	CLA	CAA-CBA-CGA-O2A
22	A	1139	CLA	CAA-CBA-CGA-O2A
22	B	1212	CLA	CAA-CBA-CGA-O2A
22	4	607	CLA	CAA-CBA-CGA-O2A
22	6	615	CLA	CAA-CBA-CGA-O2A
22	6	618	CLA	CAA-CBA-CGA-O2A
44	8	803	DGA	OG2-CB1-CB2-CB3

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Mol	Chain	Res	Type	Atoms
25	7	801	LHG	C1-C2-C3-O3
22	A	1131	CLA	CAA-CBA-CGA-O1A
22	1	605	CLA	CAA-CBA-CGA-O1A
26	A	5005	DGD	O1A-C1A-C2A-C3A
25	6	801	LHG	C29-C30-C31-C32
22	a	608	CLA	C6-C7-C8-C10
25	4	801	LHG	C5-C4-O6-P
22	B	1205	CLA	C8-C10-C11-C12
22	A	1012	CLA	C3A-C2A-CAA-CBA
22	A	1117	CLA	C11-C10-C8-C7
22	A	1101	CLA	C11-C10-C8-C7
22	B	1210	CLA	C6-C7-C8-C10
22	B	1223	CLA	C6-C7-C8-C10
22	B	1237	CLA	C11-C12-C13-C15
22	1	603	CLA	C12-C13-C15-C16
22	1	606	CLA	C6-C7-C8-C10
22	6	601	CLA	C6-C7-C8-C10
22	6	601	CLA	C11-C10-C8-C7
23	B	2002	PQN	C17-C18-C20-C21
39	8	604	CHL	C6-C7-C8-C10
21	A	1011	CL0	CAA-CBA-CGA-O1A
22	B	1213	CLA	CAA-CBA-CGA-O1A
22	4	603	CLA	CAA-CBA-CGA-O1A
39	8	604	CHL	CAA-CBA-CGA-O1A
22	7	605	CLA	CAA-CBA-CGA-O1A
49	8	806	P5S	C20-C21-C22-C23
22	A	1118	CLA	CAA-CBA-CGA-O2A
22	B	1213	CLA	CAA-CBA-CGA-O2A
22	B	1238	CLA	CAA-CBA-CGA-O2A
22	1	615	CLA	CAA-CBA-CGA-O2A
22	4	605	CLA	CAA-CBA-CGA-O2A
22	6	609	CLA	CAA-CBA-CGA-O2A
22	6	612	CLA	CAA-CBA-CGA-O2A
22	8	612	CLA	CAA-CBA-CGA-O2A
25	4	801	LHG	O8-C23-C24-C25
25	5	801	LHG	O8-C23-C24-C25
26	A	5005	DGD	O2G-C1B-C2B-C3B
39	5	611	CHL	CAA-CBA-CGA-O2A
40	8	809	OLA	C9-C10-C11-C12
33	G	5001	SQD	C28-C29-C30-C31
24	B	4005	BCR	C21-C22-C23-C24
22	A	1123	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
22	K	1402	CLA	CAA-CBA-CGA-O1A
22	1	608	CLA	CAA-CBA-CGA-O1A
22	3	601	CLA	CAA-CBA-CGA-O1A
22	5	605	CLA	CAA-CBA-CGA-O1A
22	6	609	CLA	CAA-CBA-CGA-O1A
22	7	603	CLA	CAA-CBA-CGA-O1A
25	5	801	LHG	O10-C23-C24-C25
22	A	1141	CLA	CAA-CBA-CGA-O1A
24	B	4006	BCR	C19-C20-C21-C22
24	3	503	BCR	C19-C20-C21-C22
24	3	505	BCR	C9-C10-C11-C12
24	6	503	BCR	C13-C14-C15-C16
22	A	1108	CLA	CAA-CBA-CGA-O2A
22	B	1206	CLA	CAA-CBA-CGA-O2A
22	7	607	CLA	CAA-CBA-CGA-O2A
31	8	810	PTY	O4-C30-C31-C32
26	8	802	DGD	C4A-C5A-C6A-C7A
22	B	1209	CLA	C13-C15-C16-C17
22	A	1109	CLA	CAA-CBA-CGA-O1A
22	A	1139	CLA	CAA-CBA-CGA-O1A
22	5	602	CLA	CAA-CBA-CGA-O1A
22	6	612	CLA	CAA-CBA-CGA-O1A
25	4	801	LHG	O10-C23-C24-C25
22	A	1133	CLA	C15-C16-C17-C18
22	B	1218	CLA	CAA-CBA-CGA-O2A
25	F	5001	LHG	O8-C23-C24-C25
25	3	801	LHG	O8-C23-C24-C25
26	8	802	DGD	O1G-C1A-C2A-C3A
47	7	807	4RF	O21-C22-C24-C25
22	A	1126	CLA	C8-C10-C11-C12
22	3	603	CLA	CAA-CBA-CGA-O1A
22	B	1221	CLA	CBD-CGD-O2D-CED
32	K	5001	LAP	C16-C17-N8-C20
22	A	1116	CLA	C8-C10-C11-C12
22	B	1220	CLA	C5-C6-C7-C8
26	B	5003	DGD	C1B-C2B-C3B-C4B
22	6	615	CLA	CAA-CBA-CGA-O1A
22	6	618	CLA	CAA-CBA-CGA-O1A
25	F	5001	LHG	O10-C23-C24-C25
22	4	604	CLA	C4-C3-C5-C6
25	B	5002	LHG	C29-C30-C31-C32
22	A	1128	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	3	606	CLA	CAA-CBA-CGA-O2A
31	7	804	PTY	C12-C11-C8-O7

There are no ring outliers.

307 monomers are involved in 1582 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	4	613	CHL	3	0
39	5	613	CHL	4	0
24	A	4005	BCR	3	0
22	5	608	CLA	3	0
22	B	1216	CLA	5	0
22	A	1119	CLA	6	0
25	4	801	LHG	15	0
22	B	1211	CLA	4	0
22	K	1402	CLA	6	0
22	8	607	CLA	2	0
22	4	603	CLA	4	0
22	B	1234	CLA	10	0
22	5	616	CLA	2	0
22	6	603	CLA	6	0
22	1	603	CLA	8	0
39	3	608	CHL	2	0
22	F	1301	CLA	5	0
23	A	2001	PQN	6	0
22	B	1203	CLA	7	0
25	7	801	LHG	6	0
48	7	504	C7Z	4	0
22	B	1229	CLA	5	0
22	8	612	CLA	6	0
22	5	612	CLA	11	0
24	F	4001	BCR	5	0
22	1	601	CLA	7	0
40	8	809	OLA	4	0
31	3	802	PTY	5	0
22	6	615	CLA	4	0
22	K	1401	CLA	3	0
25	3	801	LHG	5	0
22	B	1201	CLA	19	0
22	4	605	CLA	3	0
22	6	606	CLA	2	0
22	3	603	CLA	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	1103	CLA	11	0
22	A	1137	CLA	7	0
22	8	618	CLA	8	0
30	6	803	PCW	3	0
38	1	501	LUT	5	0
22	A	1129	CLA	2	0
22	B	1232	CLA	6	0
22	A	1104	CLA	6	0
29	1	804	LMT	8	0
24	4	503	BCR	3	0
24	L	4001	BCR	16	0
22	1	602	CLA	6	0
22	1	605	CLA	10	0
43	6	804	PLM	1	0
22	A	1126	CLA	12	0
22	8	606	CLA	4	0
45	6	806	SPH	7	0
36	J	5001	LPX	3	0
22	6	607	CLA	11	0
25	F	5002	LHG	3	0
22	A	1138	CLA	8	0
22	1	607	CLA	8	0
22	K	1403	CLA	30	0
22	7	612	CLA	10	0
22	A	1125	CLA	8	0
22	5	617	CLA	6	0
22	7	604	CLA	9	0
22	B	1022	CLA	7	0
22	4	611	CLA	1	0
39	4	618	CHL	6	0
22	A	1114	CLA	8	0
33	7	805	SQD	1	0
33	G	5001	SQD	4	0
22	B	1231	CLA	8	0
44	5	803	DGA	3	0
22	4	602	CLA	1	0
31	8	810	PTY	6	0
24	B	4005	BCR	6	0
22	B	1222	CLA	6	0
22	1	604	CLA	12	0
22	A	1105	CLA	4	0
27	A	5007	3PH	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	1121	CLA	7	0
26	A	5005	DGD	3	0
22	A	1113	CLA	4	0
39	3	611	CHL	9	0
22	B	1226	CLA	9	0
24	B	4003	BCR	5	0
46	7	502	XAT	5	0
22	7	610	CLA	4	0
22	8	610	CLA	8	0
25	B	5002	LHG	2	0
24	6	504	BCR	5	0
31	B	5005	PTY	6	0
22	A	1136	CLA	11	0
22	A	1108	CLA	12	0
22	B	1209	CLA	15	0
22	3	602	CLA	4	0
31	7	804	PTY	3	0
22	3	604	CLA	3	0
22	8	611	CLA	3	0
22	A	1135	CLA	5	0
35	J	4002	RRX	10	0
22	7	603	CLA	5	0
22	6	602	CLA	4	0
24	B	4004	BCR	9	0
22	A	1139	CLA	5	0
22	6	604	CLA	23	0
22	7	608	CLA	5	0
22	5	606	CLA	2	0
22	A	1123	CLA	8	0
24	L	4002	BCR	5	0
32	K	5001	LAP	3	0
32	B	5007	LAP	3	0
21	A	1011	CL0	3	0
40	1	803	OLA	2	0
22	4	612	CLA	5	0
22	G	1602	CLA	4	0
22	1	606	CLA	4	0
22	6	612	CLA	3	0
26	8	802	DGD	13	0
22	A	1117	CLA	6	0
22	B	1206	CLA	7	0
22	A	1128	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	4	609	CHL	9	0
22	4	616	CLA	2	0
24	A	4003	BCR	5	0
24	A	4004	BCR	7	0
22	5	602	CLA	2	0
26	B	5003	DGD	10	0
22	B	1214	CLA	7	0
22	B	1215	CLA	6	0
22	A	1130	CLA	8	0
38	8	502	LUT	5	0
22	5	604	CLA	10	0
38	1	503	LUT	8	0
39	8	601	CHL	9	0
39	8	613	CHL	3	0
22	B	1223	CLA	5	0
22	B	1213	CLA	6	0
24	G	4001	BCR	3	0
25	A	5003	LHG	7	0
24	5	504	BCR	5	0
22	6	618	CLA	4	0
24	B	4006	BCR	1	0
39	5	611	CHL	8	0
22	3	606	CLA	4	0
24	6	503	BCR	11	0
24	K	4002	BCR	1	0
22	B	1023	CLA	14	0
22	B	1230	CLA	5	0
22	4	615	CLA	3	0
38	5	505	LUT	7	0
22	A	1109	CLA	13	0
47	8	808	4RF	13	0
22	A	1116	CLA	8	0
22	1	610	CLA	4	0
24	A	4001	BCR	5	0
25	A	5002	LHG	8	0
22	B	1237	CLA	8	0
22	B	1212	CLA	10	0
22	8	608	CLA	6	0
38	4	502	LUT	4	0
22	5	603	CLA	5	0
38	4	501	LUT	5	0
22	A	1122	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	8	620	CLA	6	0
25	4	802	LHG	5	0
25	B	5001	LHG	7	0
38	6	502	LUT	13	0
22	1	608	CLA	4	0
22	1	611	CLA	4	0
25	6	802	LHG	4	0
39	6	613	CHL	19	0
39	6	610	CHL	9	0
38	3	501	LUT	6	0
22	3	601	CLA	13	0
22	3	613	CLA	4	0
25	F	5001	LHG	5	0
39	8	604	CHL	8	0
22	B	1218	CLA	9	0
24	J	4001	BCR	3	0
47	8	807	4RF	3	0
22	3	610	CLA	5	0
22	4	607	CLA	5	0
24	7	503	BCR	9	0
24	8	503	BCR	5	0
22	B	1227	CLA	5	0
22	A	1133	CLA	7	0
22	A	1102	CLA	7	0
38	7	501	LUT	4	0
22	B	1208	CLA	8	0
38	5	502	LUT	5	0
22	A	1134	CLA	8	0
22	8	602	CLA	4	0
32	F	5003	LAP	6	0
22	A	1112	CLA	3	0
22	A	1131	CLA	12	0
22	7	601	CLA	6	0
22	B	1219	CLA	5	0
22	B	1202	CLA	6	0
22	A	1124	CLA	4	0
22	B	1240	CLA	7	0
24	3	505	BCR	1	0
22	6	601	CLA	24	0
22	3	607	CLA	8	0
22	A	1132	CLA	4	0
22	B	1210	CLA	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	3	502	LUT	4	0
39	6	619	CHL	10	0
22	B	1221	CLA	8	0
22	1	615	CLA	4	0
22	B	1236	CLA	7	0
24	B	4007	BCR	3	0
22	7	605	CLA	7	0
22	5	601	CLA	5	0
23	B	2002	PQN	8	0
22	B	1239	CLA	7	0
22	B	1217	CLA	5	0
28	C	3002	SF4	1	0
29	A	5008	LMT	4	0
22	A	1140	CLA	8	0
22	5	607	CLA	3	0
29	B	5006	LMT	2	0
22	A	1101	CLA	7	0
25	1	802	LHG	2	0
34	G	5002	ERG	16	0
39	1	613	CHL	6	0
22	8	605	CLA	5	0
22	A	1127	CLA	6	0
22	A	1107	CLA	8	0
24	A	4002	BCR	4	0
22	L	1502	CLA	15	0
25	A	5001	LHG	1	0
25	6	801	LHG	15	0
22	A	1111	CLA	11	0
22	J	1901	CLA	1	0
22	F	1302	CLA	8	0
22	B	1204	CLA	11	0
22	A	1110	CLA	2	0
22	B	1205	CLA	6	0
22	7	609	CLA	5	0
25	7	802	LHG	1	0
22	A	1120	CLA	6	0
22	4	617	CLA	2	0
22	A	1118	CLA	6	0
39	7	613	CHL	6	0
22	7	602	CLA	2	0
24	3	503	BCR	3	0
22	B	1220	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	4	610	CLA	8	0
22	3	605	CLA	6	0
47	7	807	4RF	6	0
25	1	801	LHG	3	0
25	5	801	LHG	9	0
22	6	605	CLA	2	0
22	6	617	CLA	14	0
22	B	1235	CLA	10	0
22	B	1228	CLA	9	0
22	4	606	CLA	3	0
22	B	1225	CLA	8	0
24	K	4001	BCR	6	0
38	6	501	LUT	16	0
22	5	618	CLA	9	0
37	M	4001	ECH	6	0
22	B	1021	CLA	13	0
22	G	1603	CLA	7	0
22	4	601	CLA	9	0
22	3	616	CLA	11	0
31	5	802	PTY	2	0
22	5	605	CLA	2	0
39	1	609	CHL	10	0
22	8	615	CLA	3	0
22	7	611	CLA	7	0
22	L	1501	CLA	3	0
22	A	1115	CLA	5	0
22	L	1503	CLA	5	0
38	8	501	LUT	12	0
22	1	612	CLA	10	0
22	6	609	CLA	24	0
24	5	503	BCR	5	0
25	8	801	LHG	5	0
38	5	501	LUT	8	0
22	B	1224	CLA	7	0
22	3	618	CLA	1	0
22	8	603	CLA	4	0
24	L	4003	BCR	2	0
28	C	3003	SF4	1	0
25	7	803	LHG	5	0
24	3	504	BCR	10	0
22	8	609	CLA	8	0
39	6	611	CHL	22	0

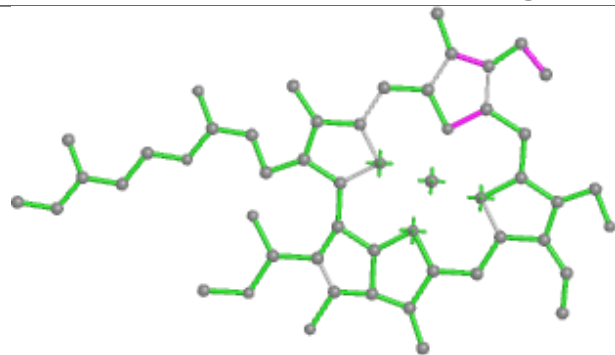
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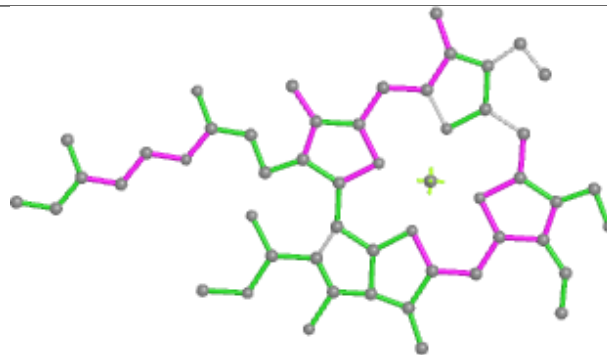
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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22	5	609	CLA	11	0
22	A	1012	CLA	15	0
22	B	1207	CLA	8	0
44	8	803	DGA	5	0
22	3	612	CLA	5	0
38	1	502	LUT	3	0
22	4	608	CLA	5	0
22	K	1404	CLA	2	0
39	5	610	CHL	10	0
22	B	1238	CLA	5	0
30	B	5004	PCW	6	0
24	B	4002	BCR	4	0
22	A	1013	CLA	10	0
24	I	4001	BCR	8	0
22	7	606	CLA	6	0
22	4	604	CLA	8	0
24	B	4001	BCR	7	0
22	7	617	CLA	7	0
22	7	615	CLA	1	0

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

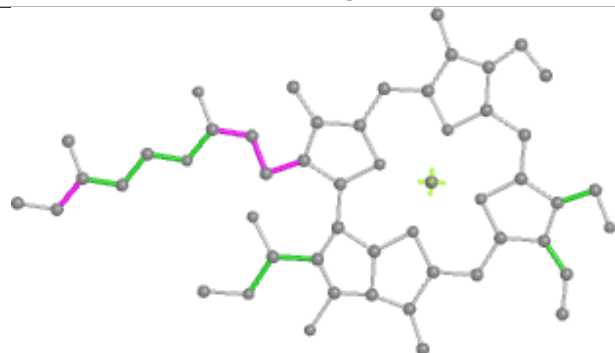
Ligand CHL 4 613



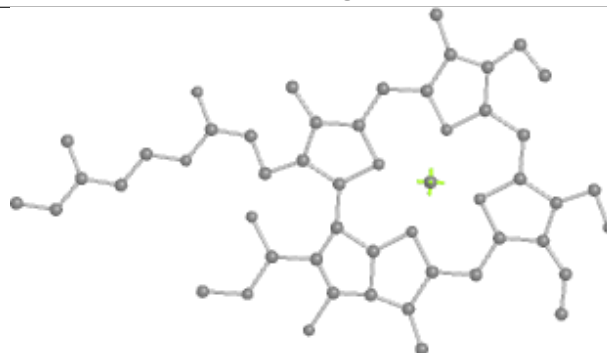
Bond lengths



Bond angles

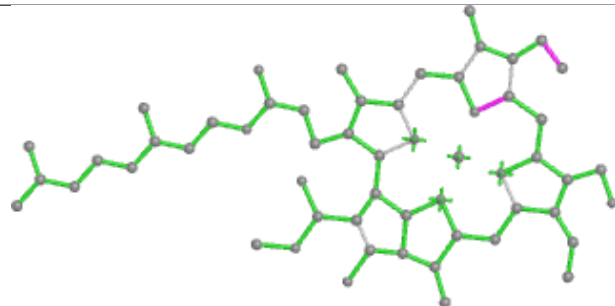


Torsions

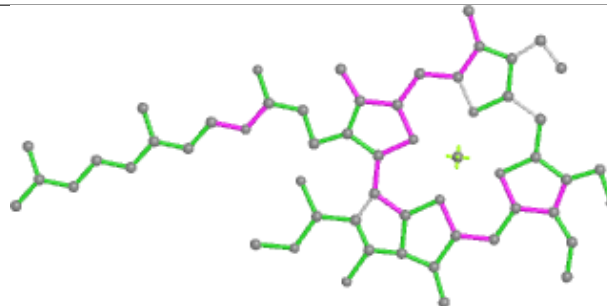


Rings

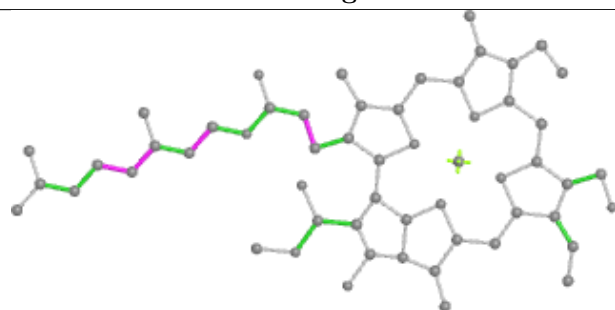
Ligand CHL 5 613



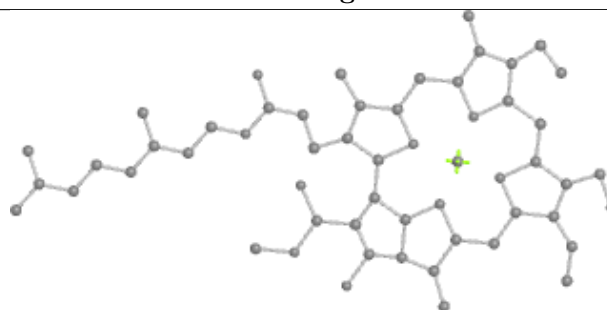
Bond lengths



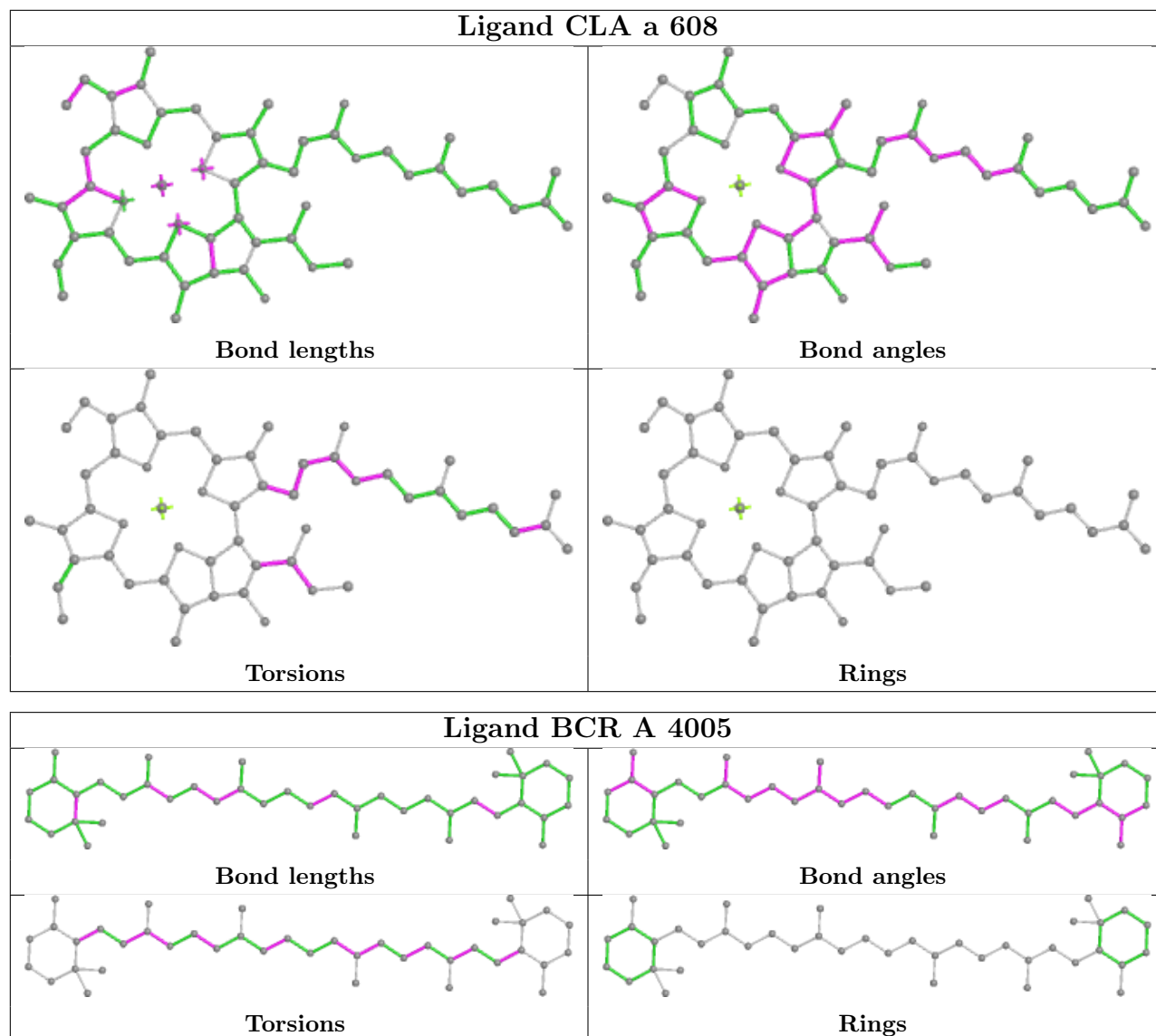
Bond angles



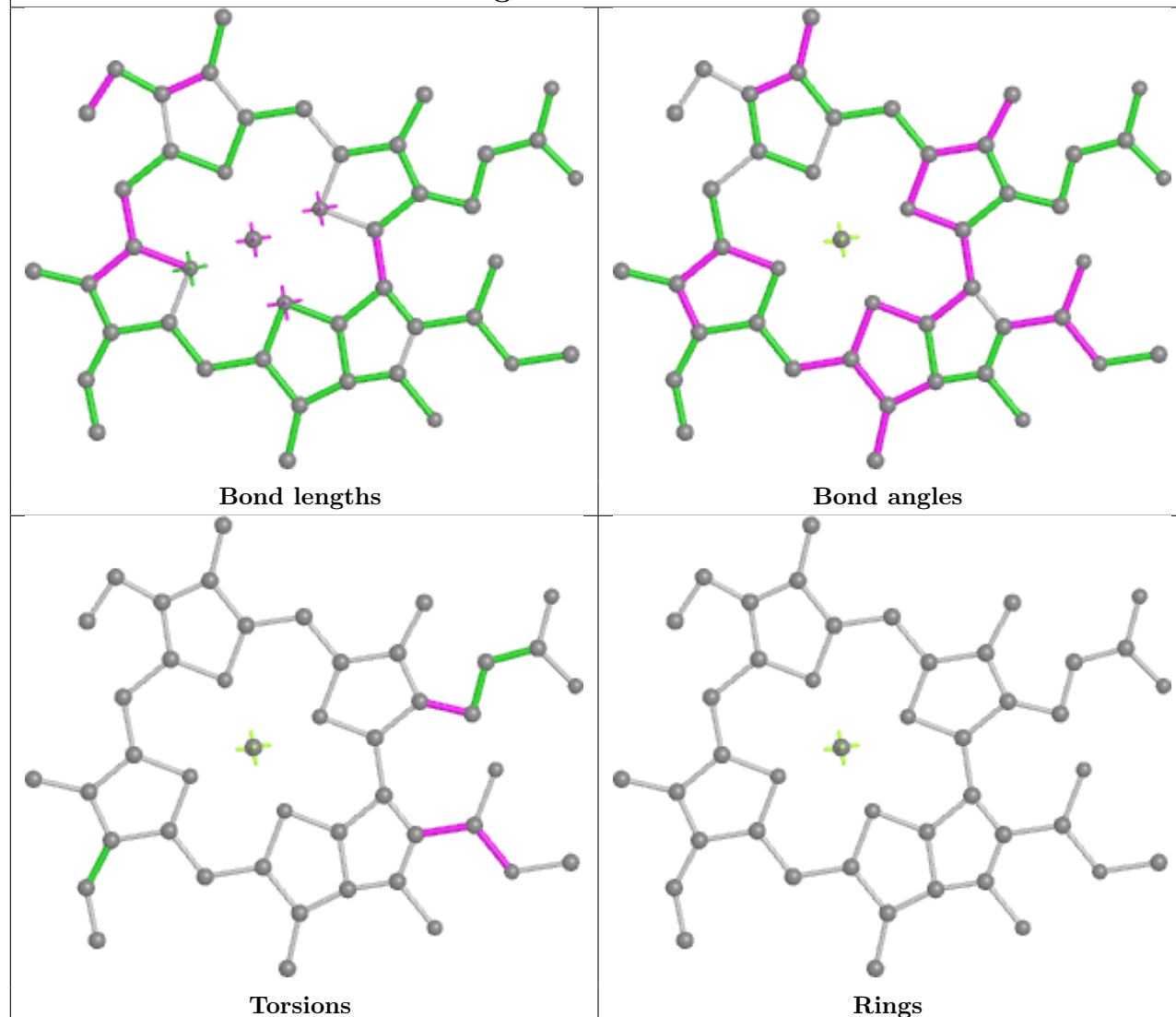
Torsions



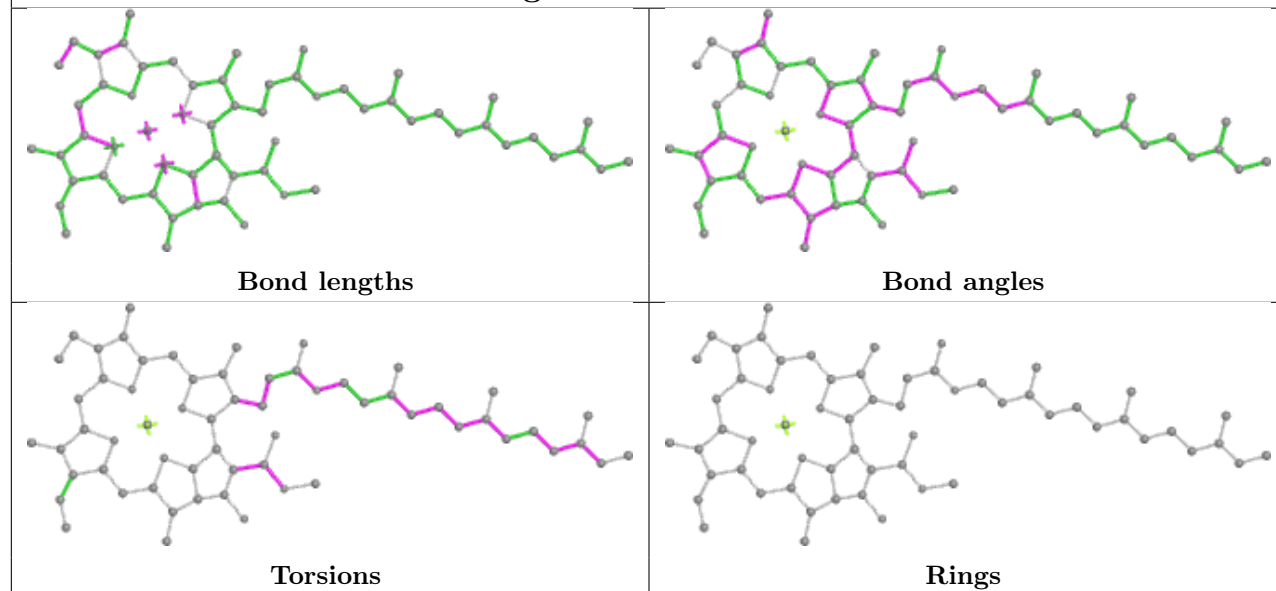
Rings

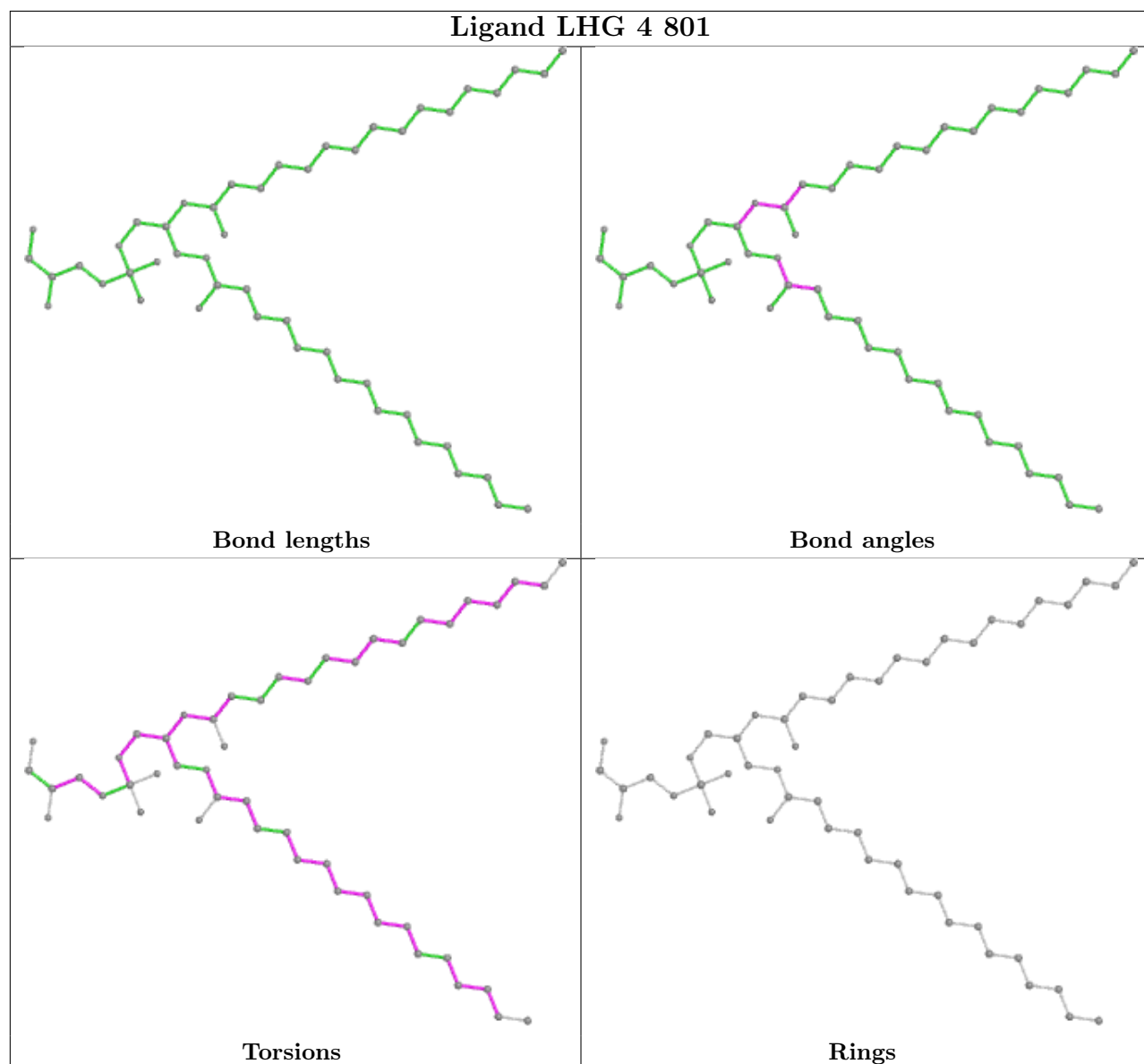
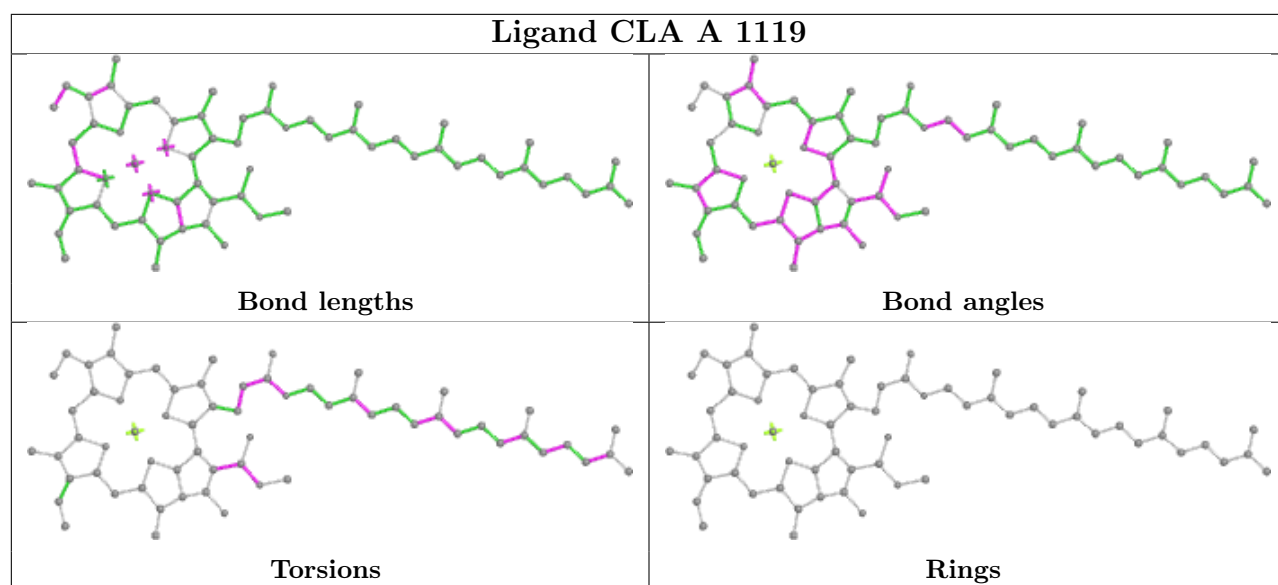


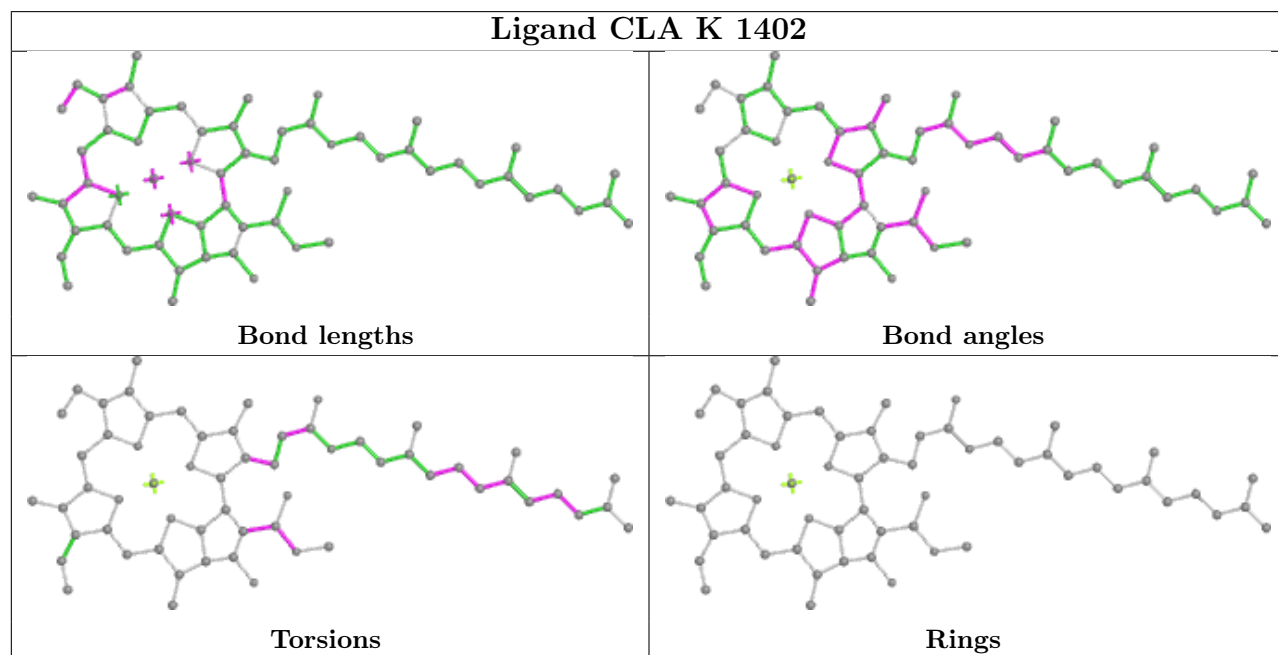
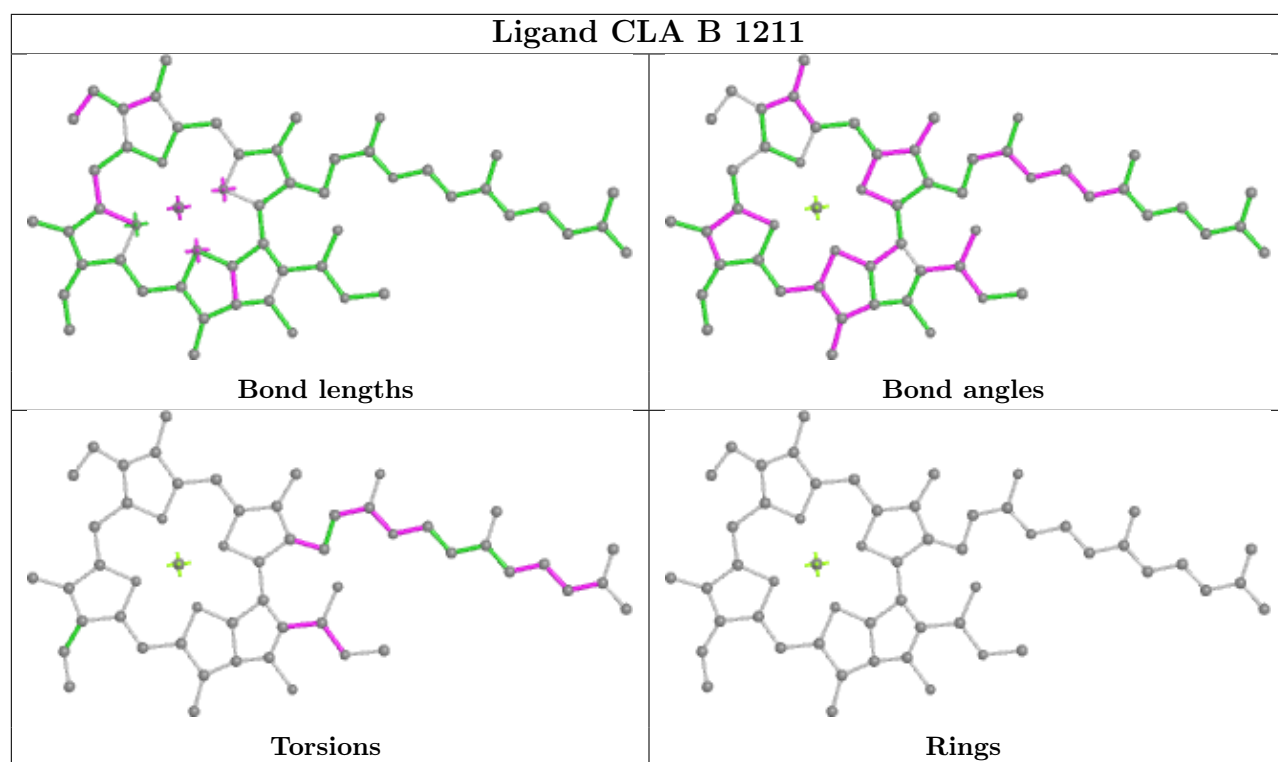
Ligand CLA 5 608



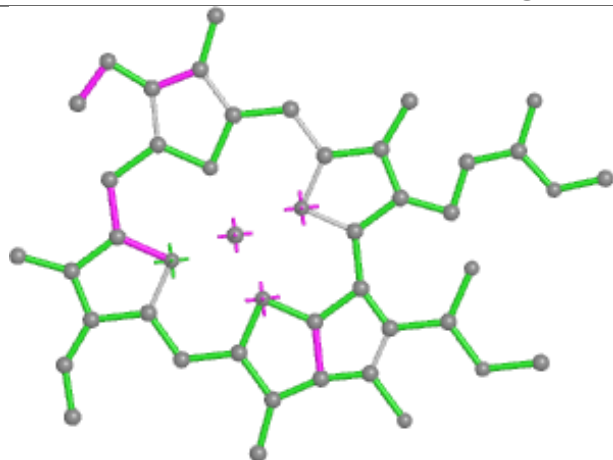
Ligand CLA B 1216



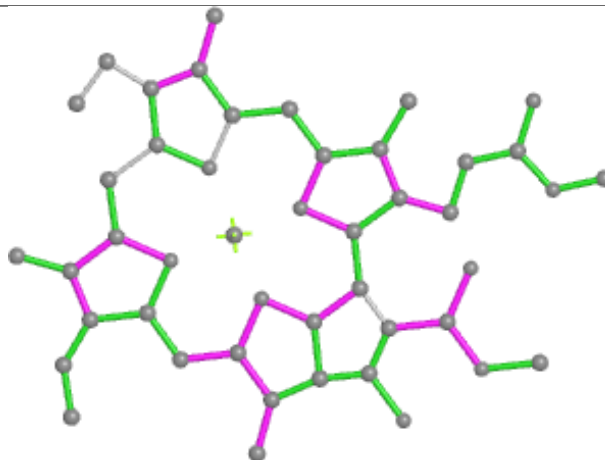




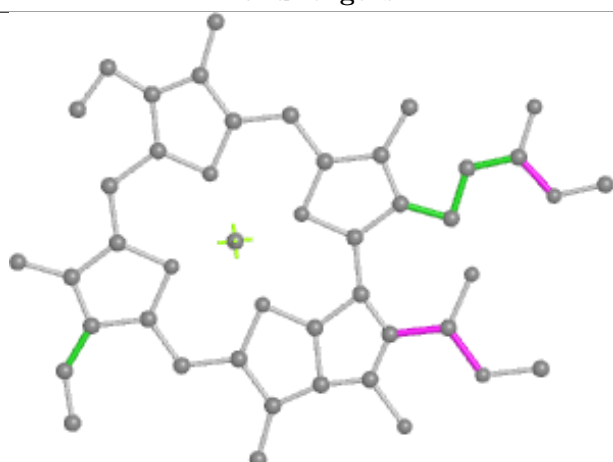
Ligand CLA 8 607



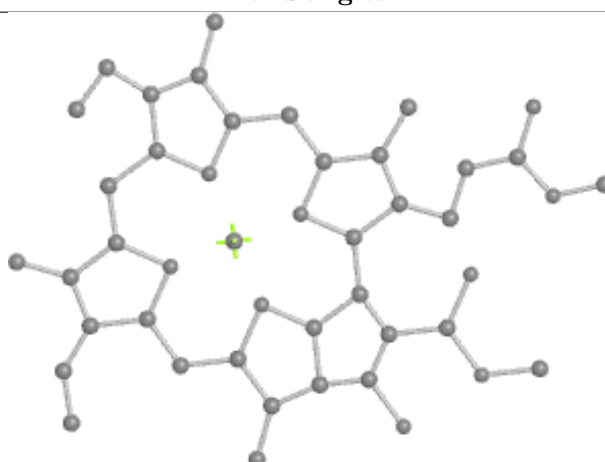
Bond lengths



Bond angles

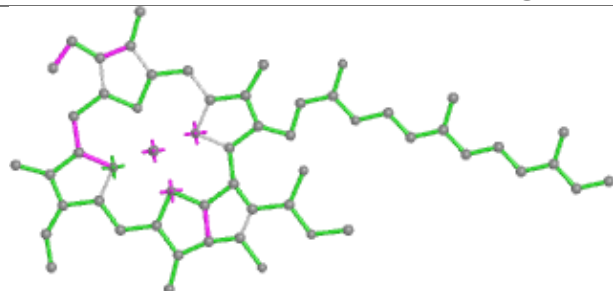


Torsions

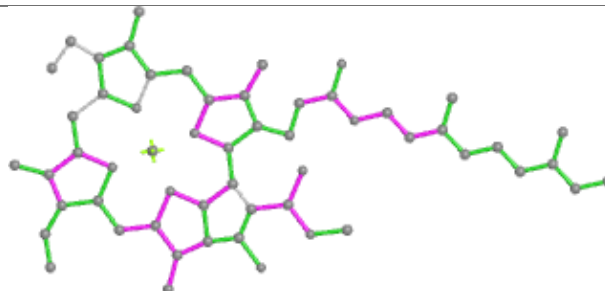


Rings

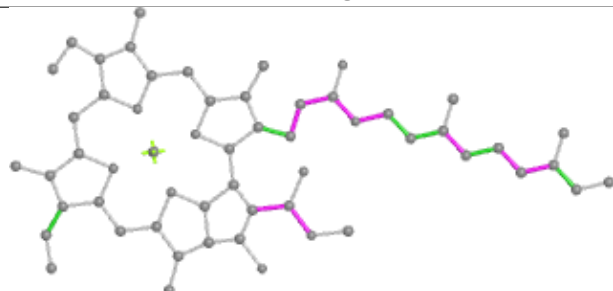
Ligand CLA 4 603



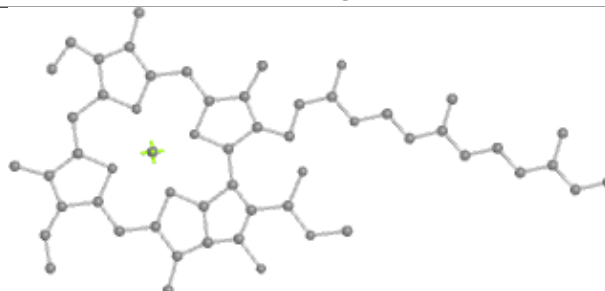
Bond lengths



Bond angles

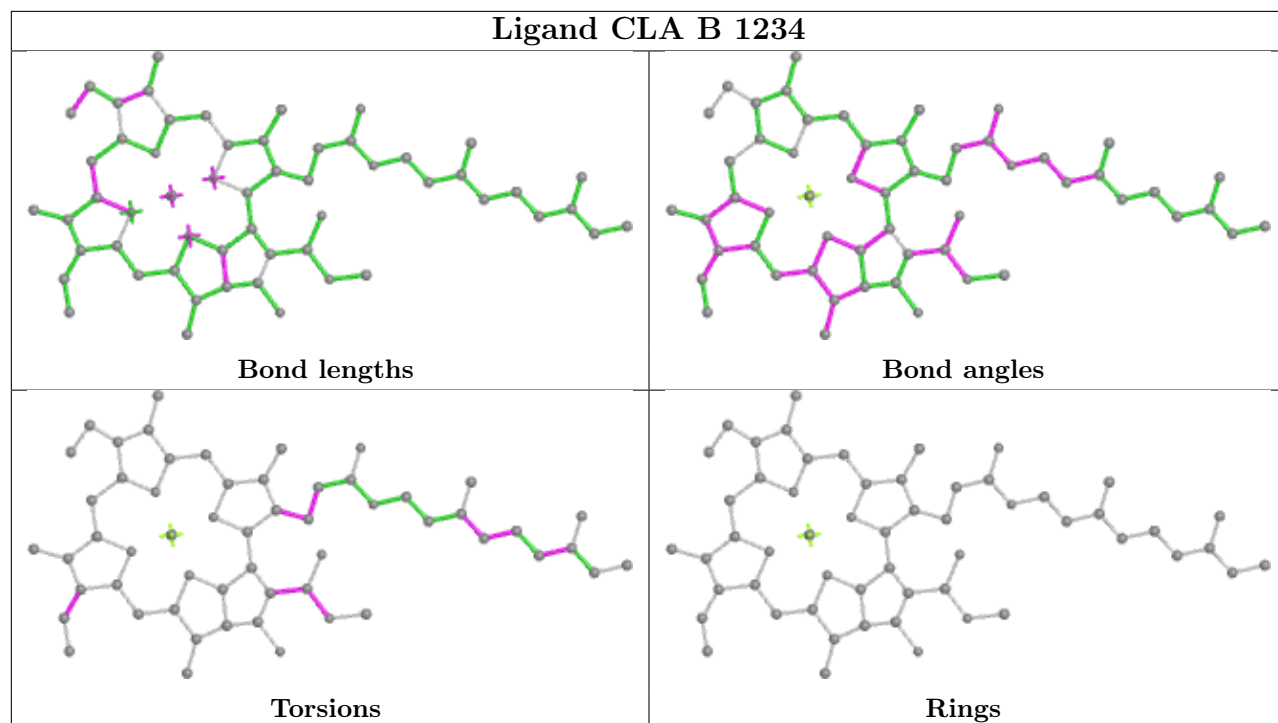


Torsions

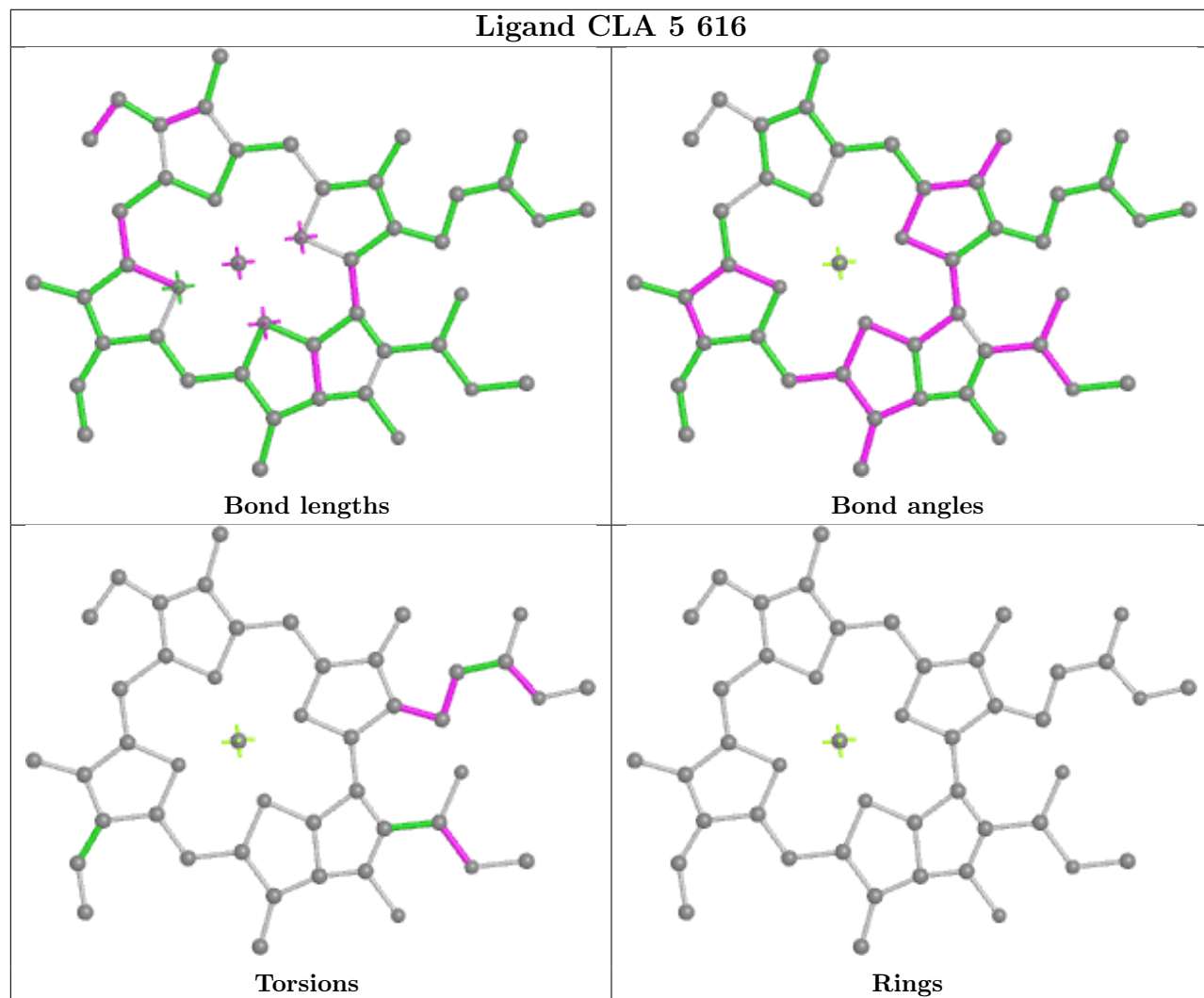


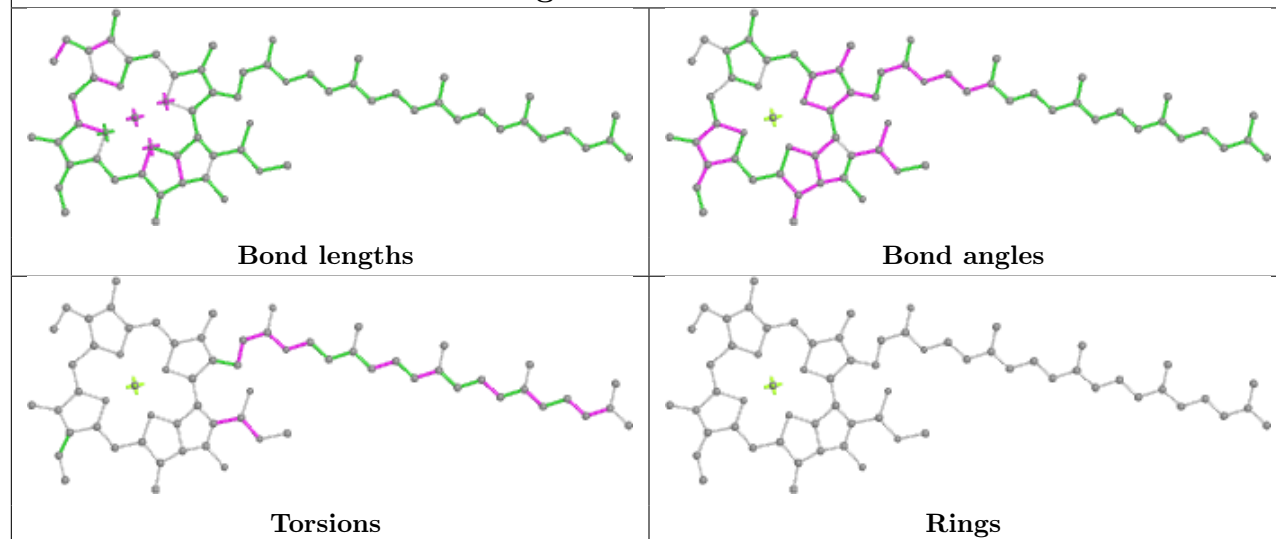
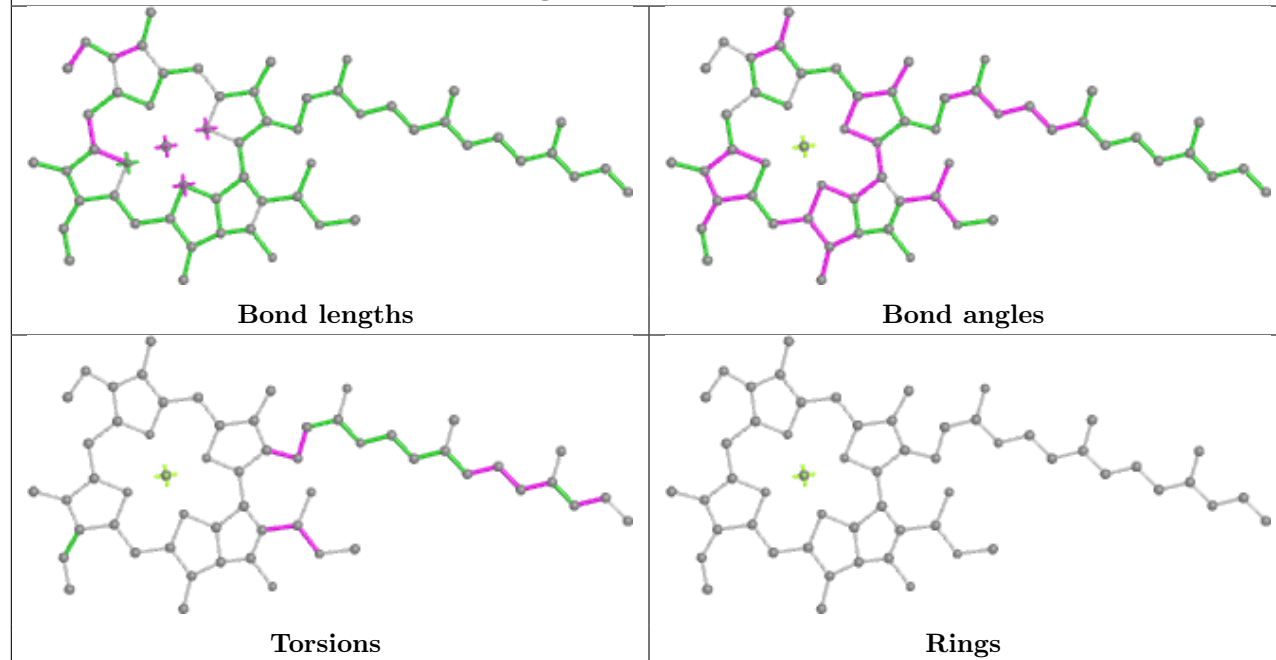
Rings

Ligand CLA B 1234

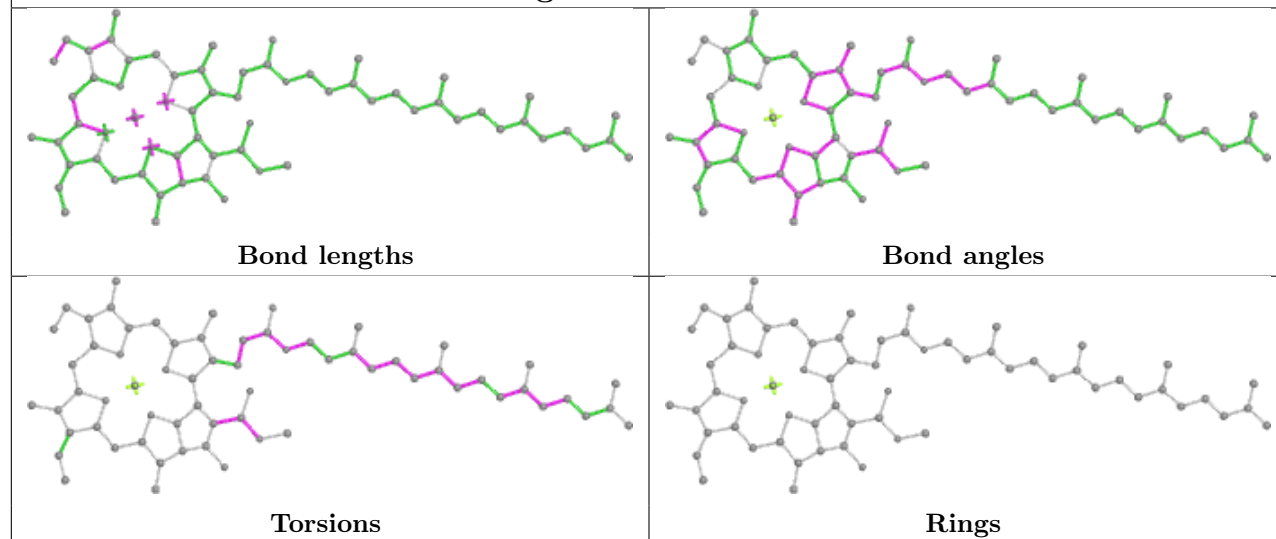


Ligand CLA 5 616

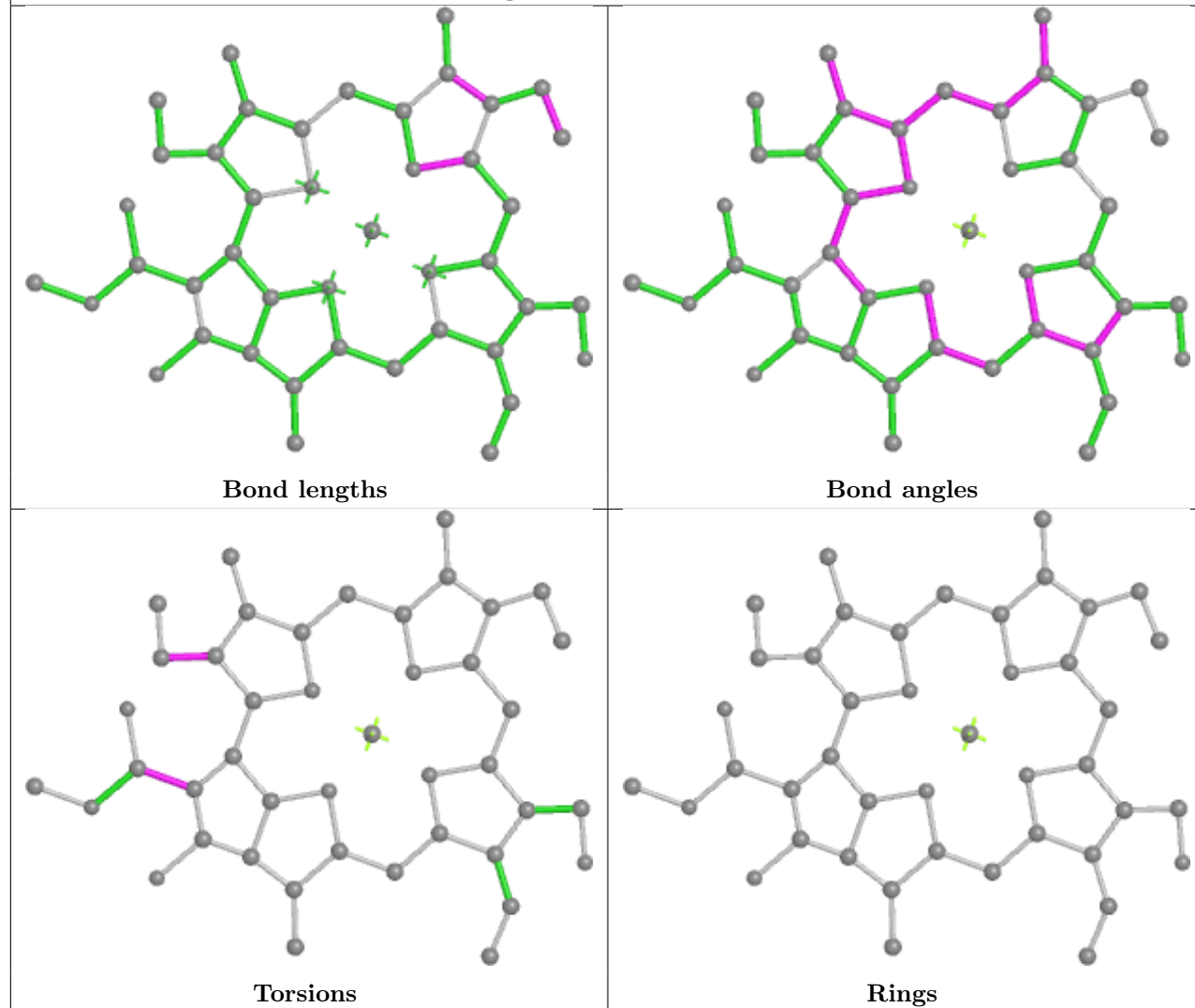


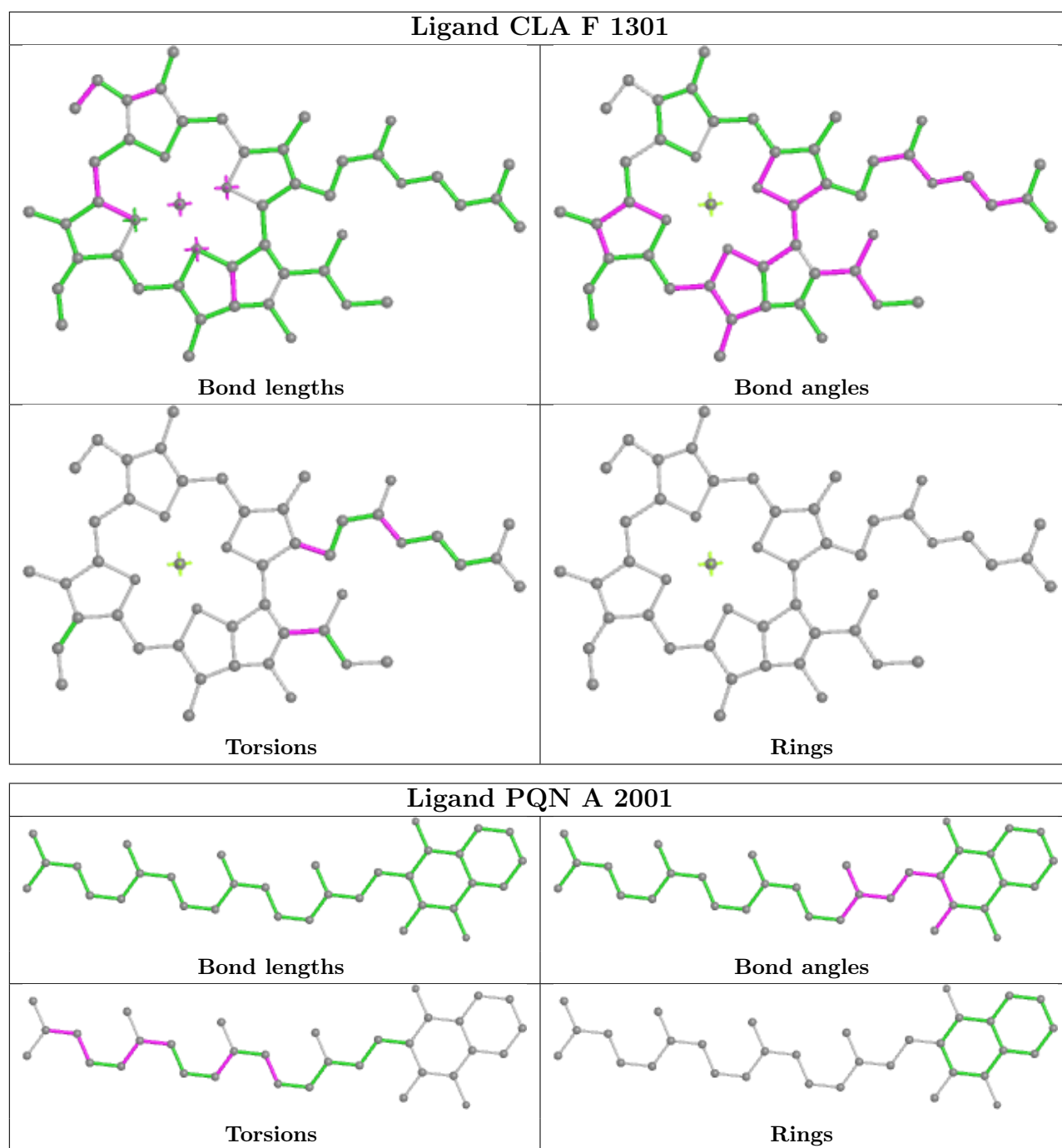
Ligand CLA 6 603**Ligand CLA a 612**

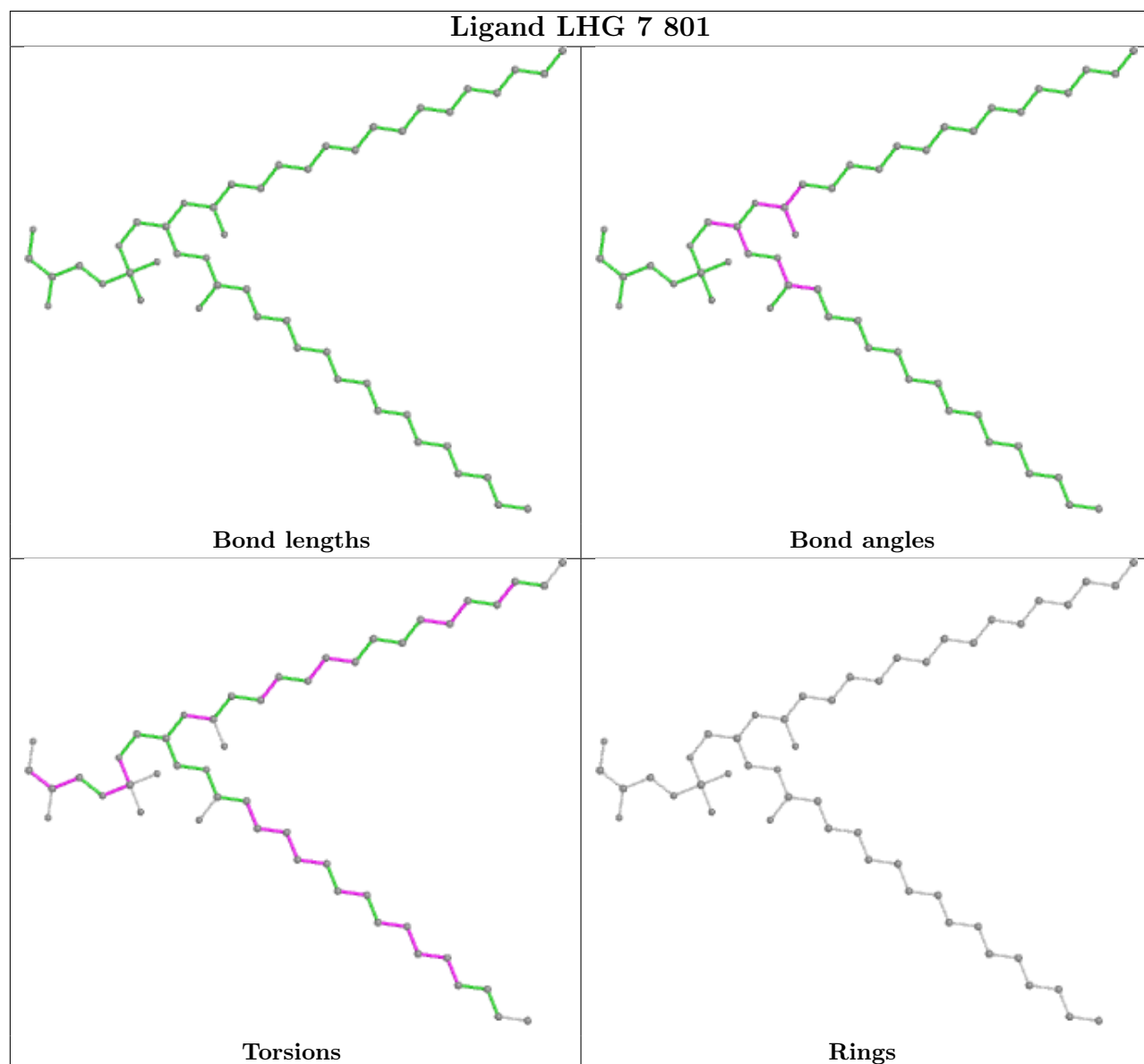
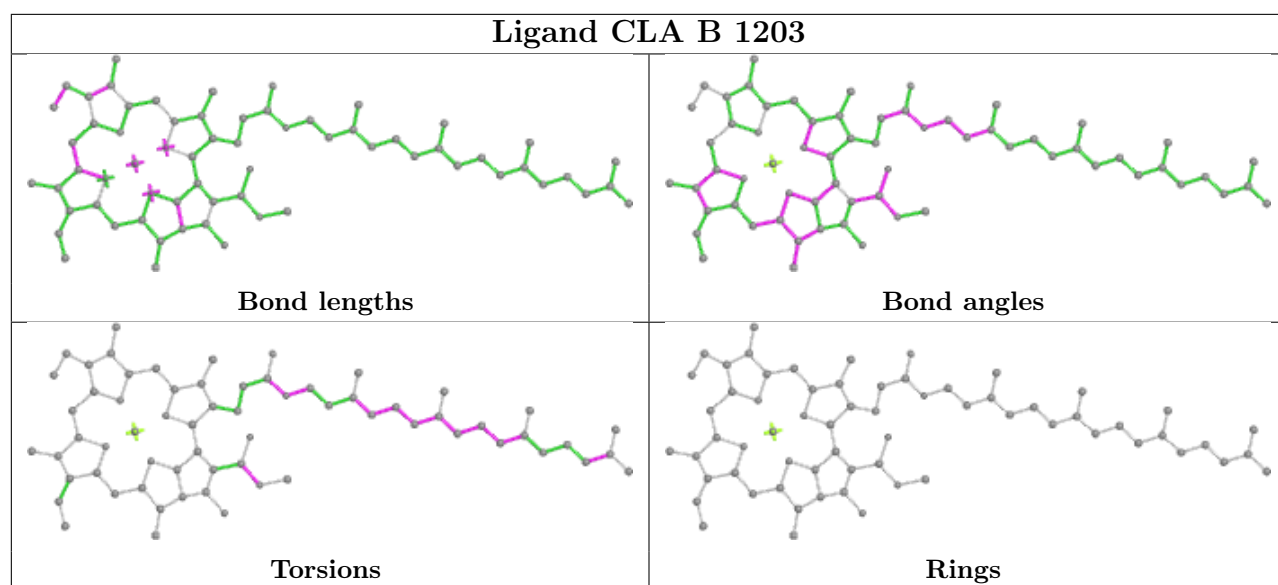
Ligand CLA 1 603

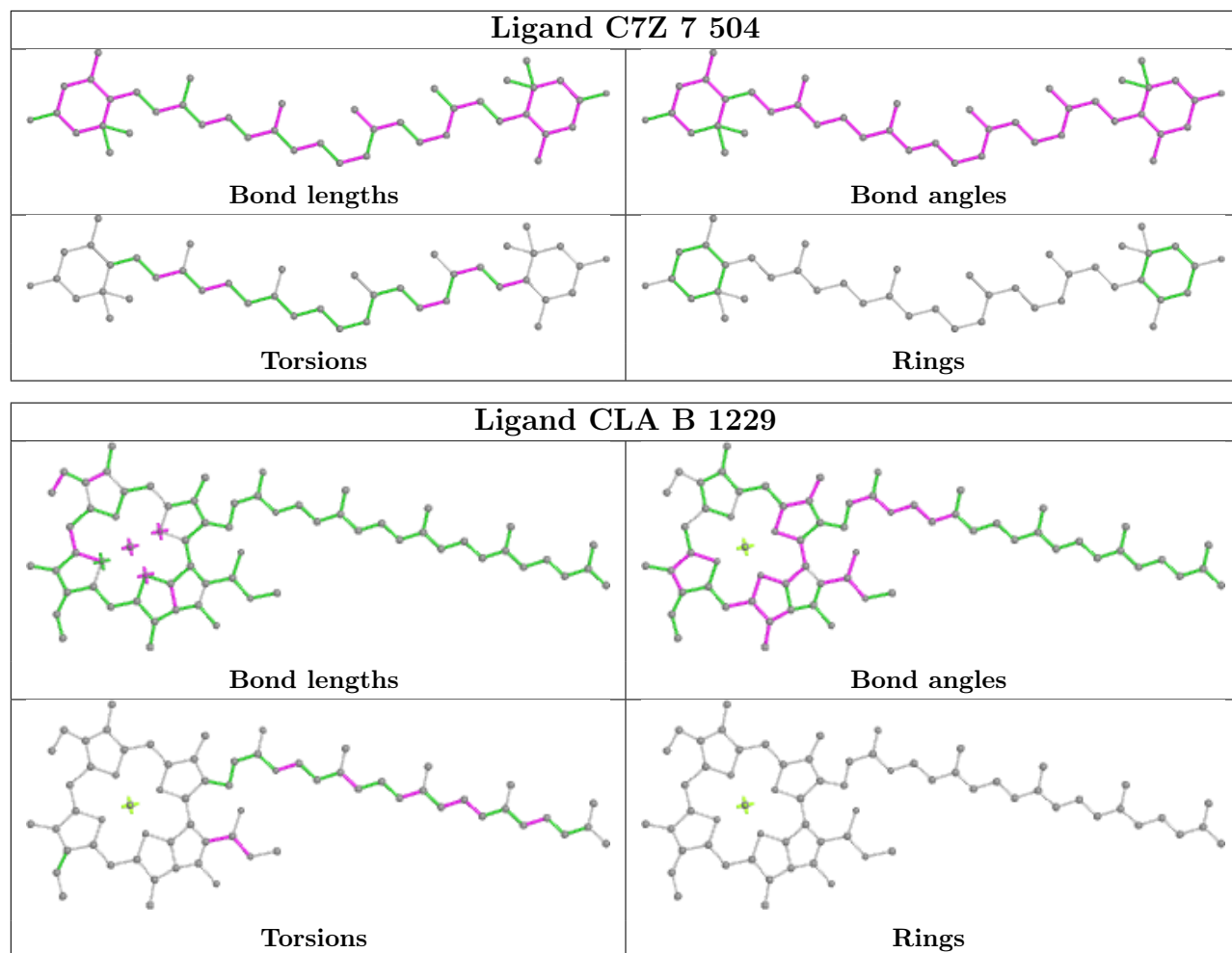


Ligand CHL 3 608

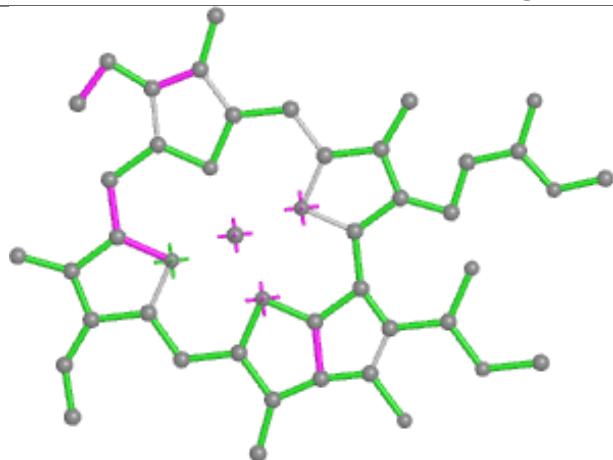




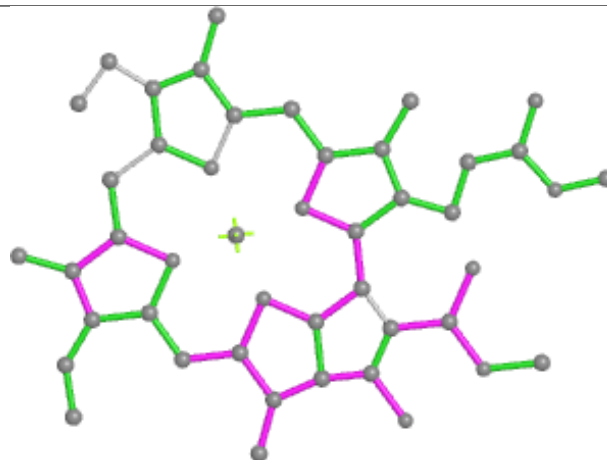




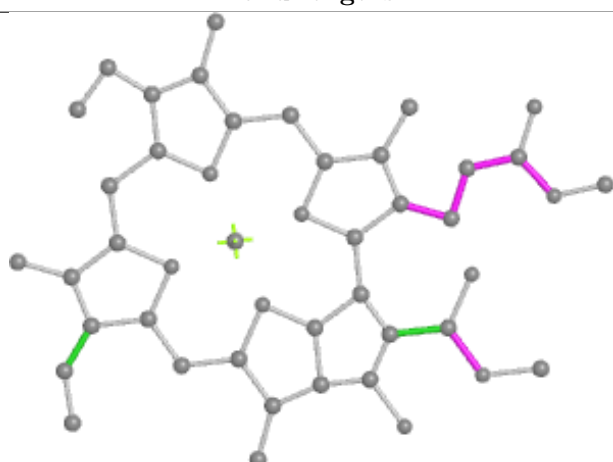
Ligand CLA 8 612



Bond lengths



Bond angles

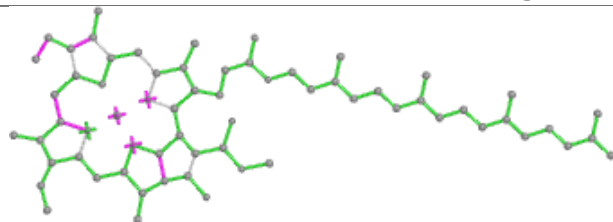


Torsions

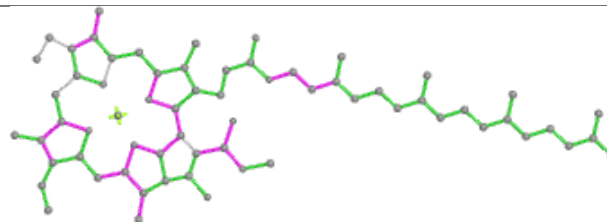


Rings

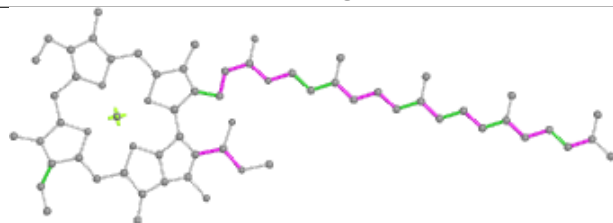
Ligand CLA 5 612



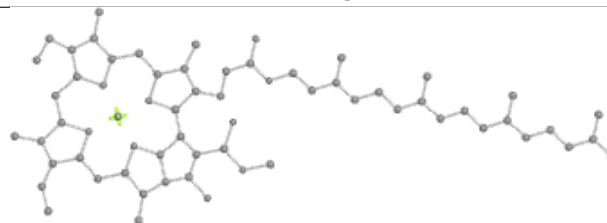
Bond lengths



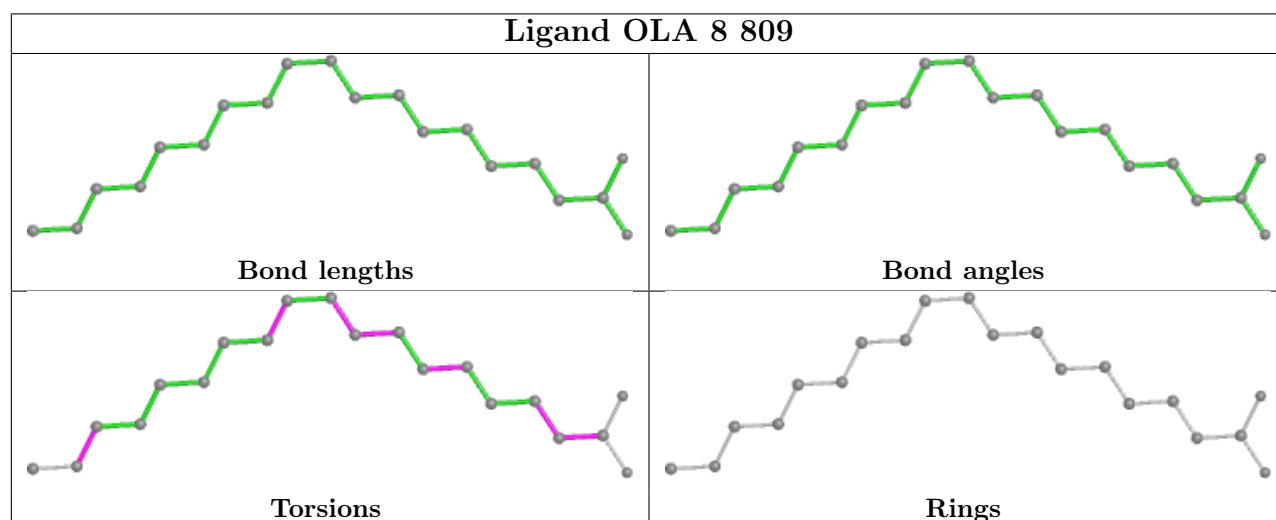
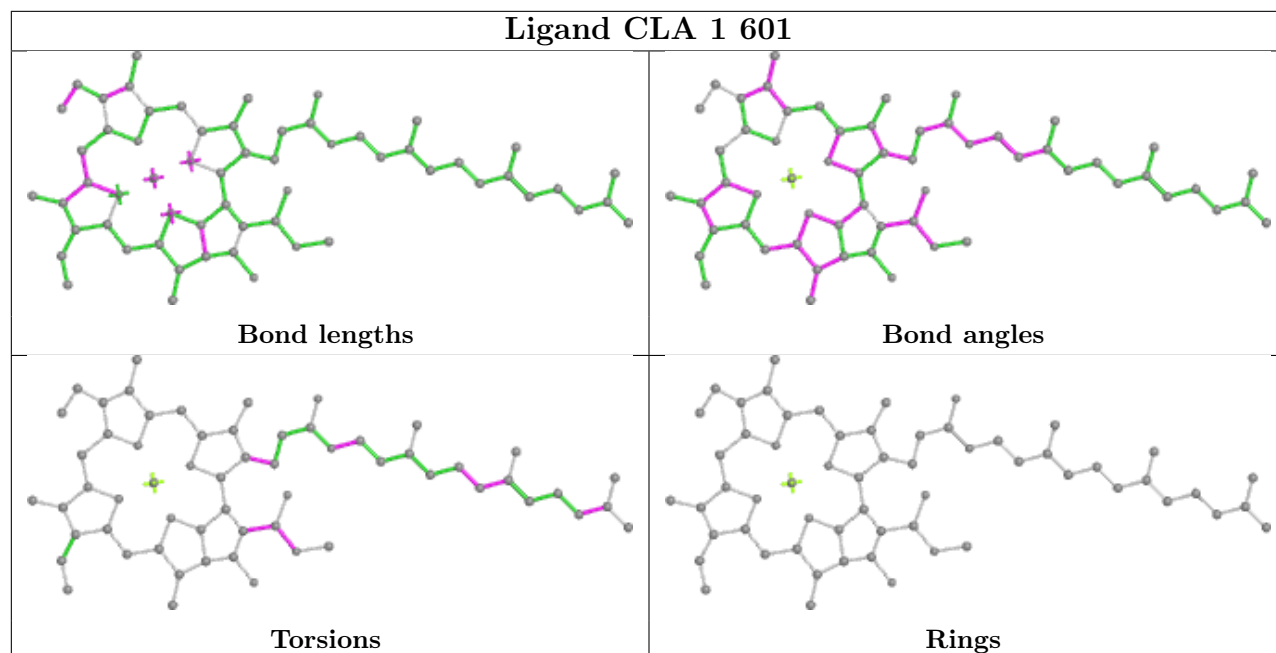
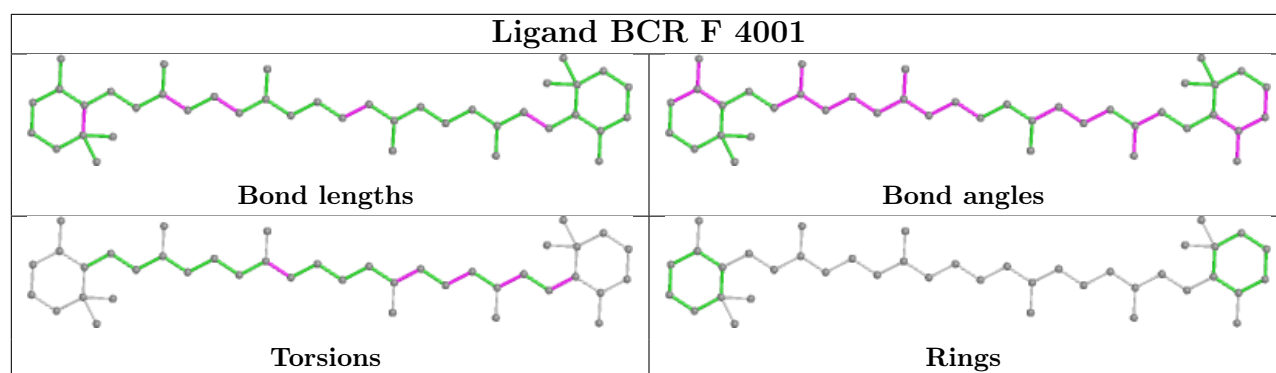
Bond angles

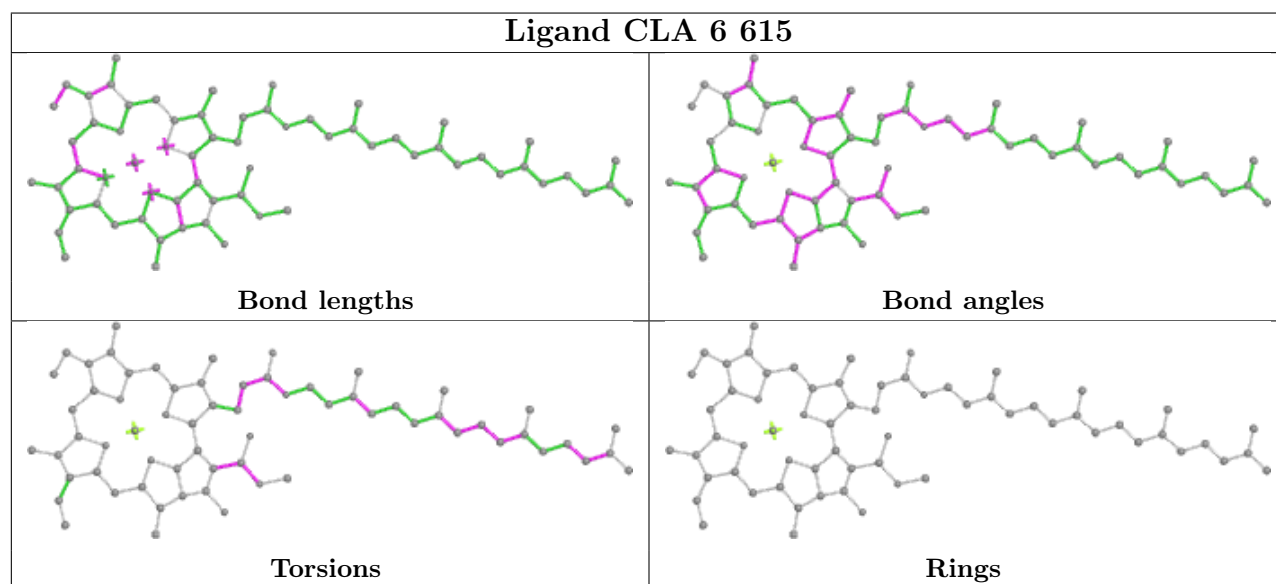
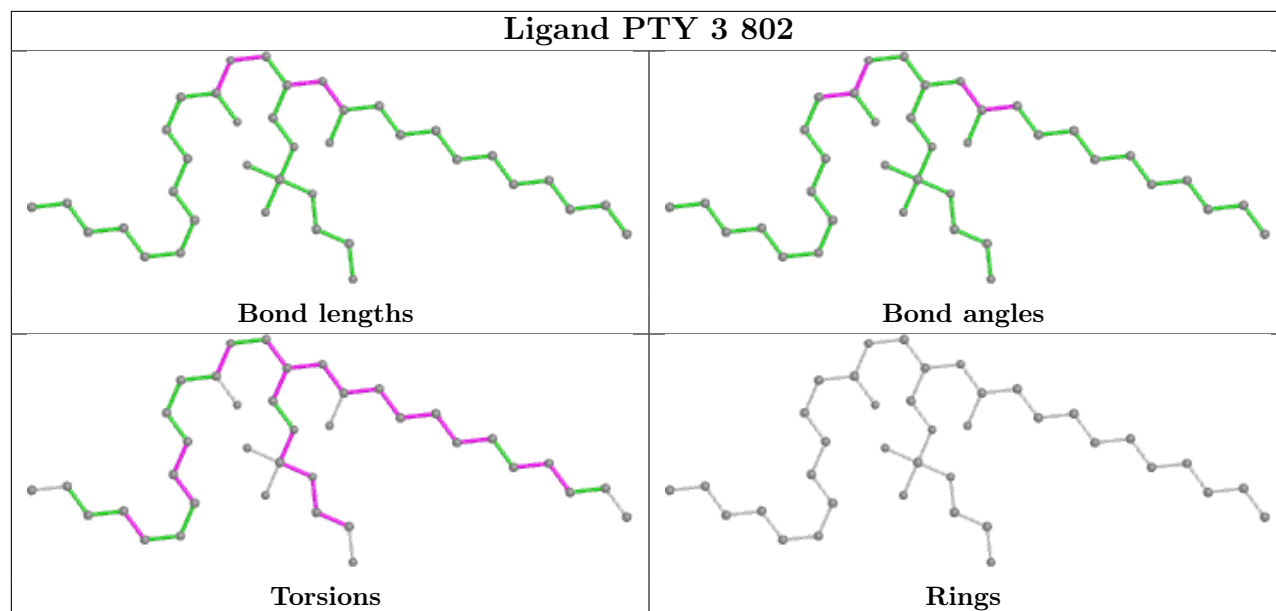


Torsions

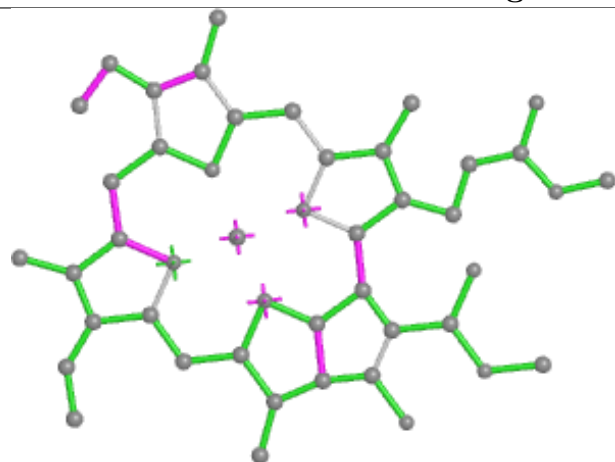


Rings

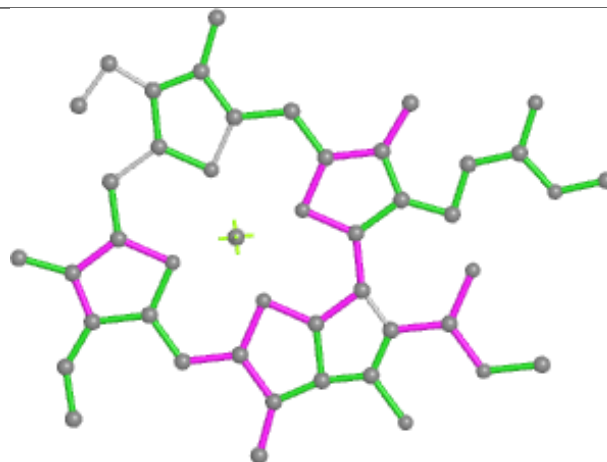




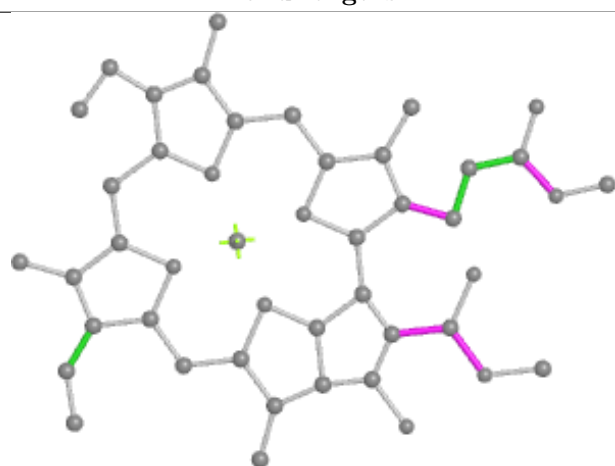
Ligand CLA K 1401



Bond lengths



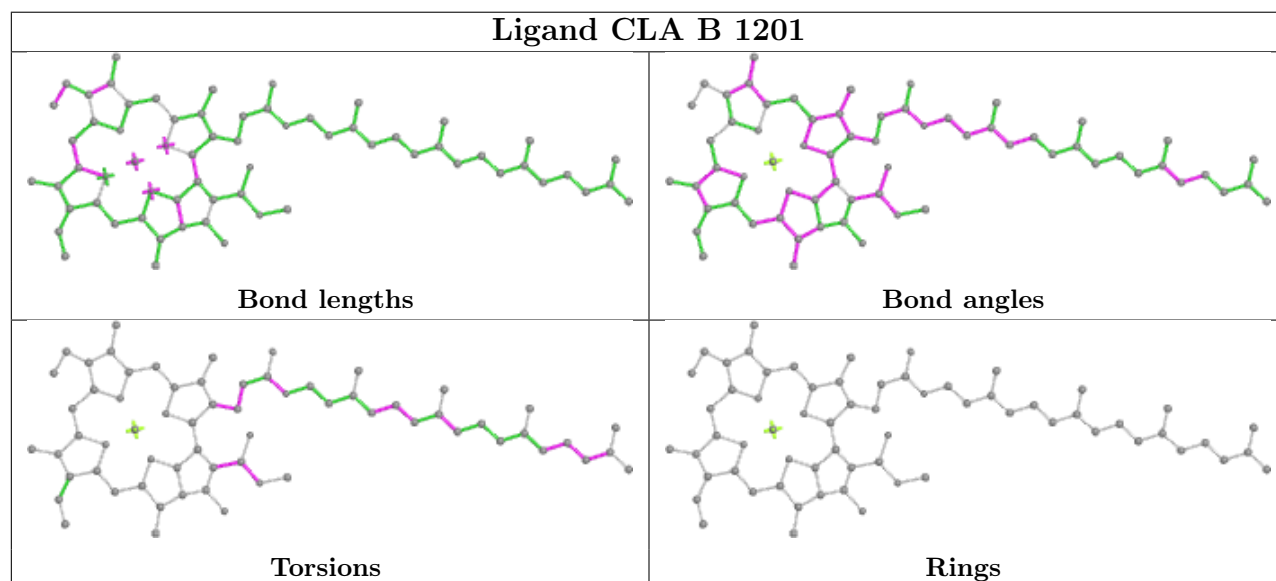
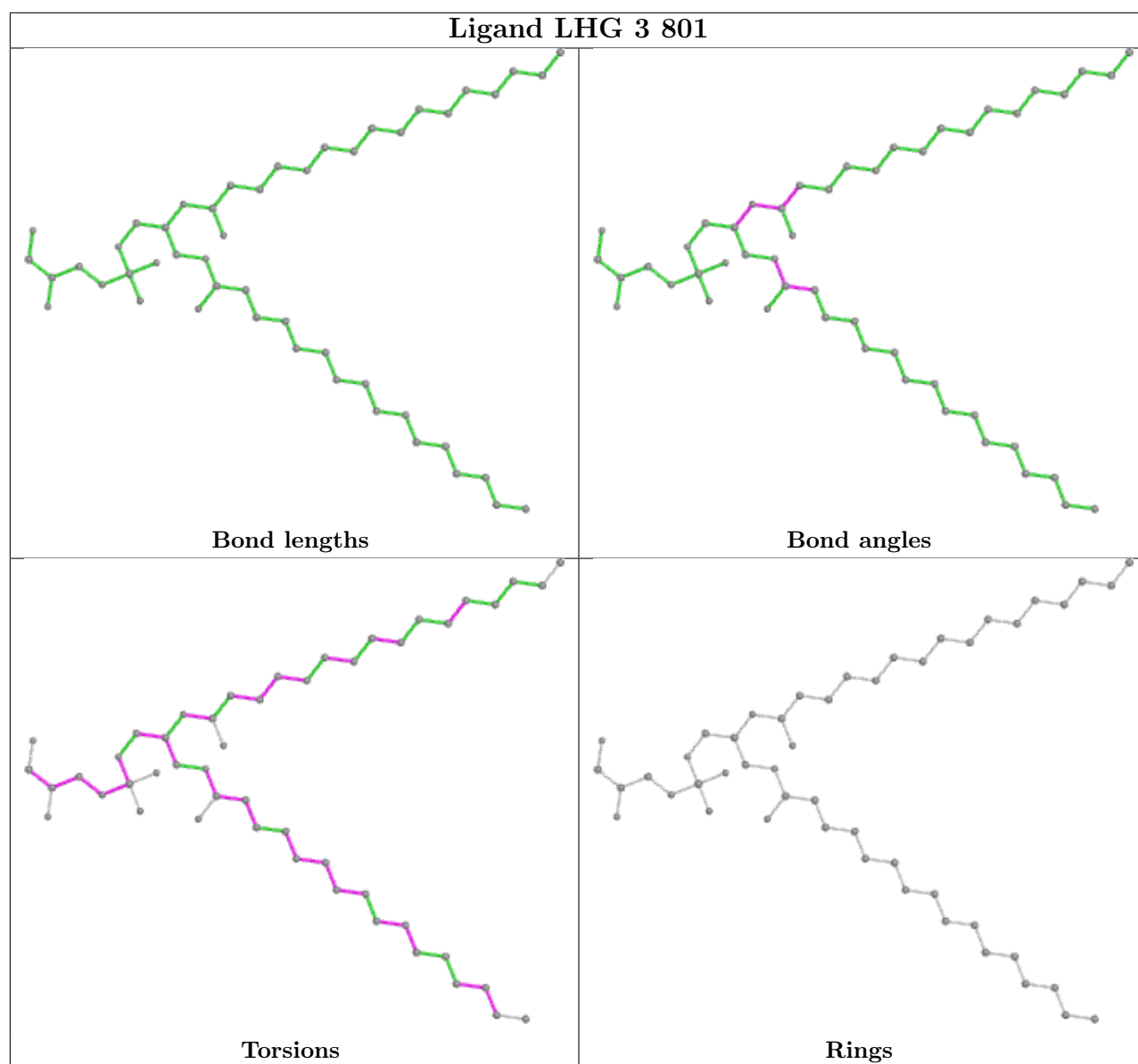
Bond angles



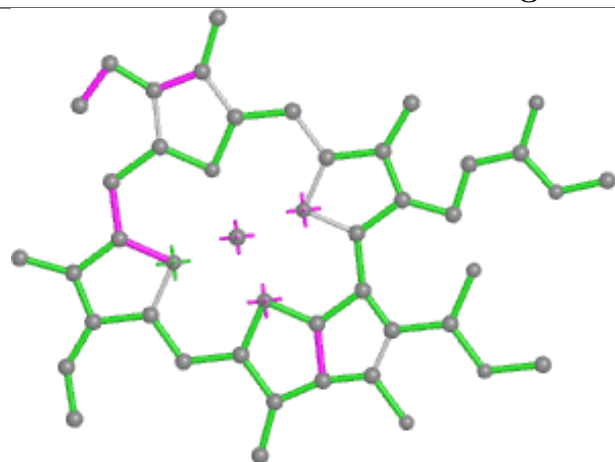
Torsions



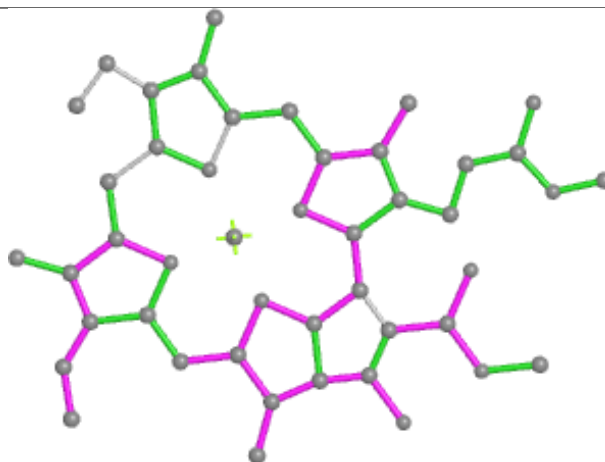
Rings



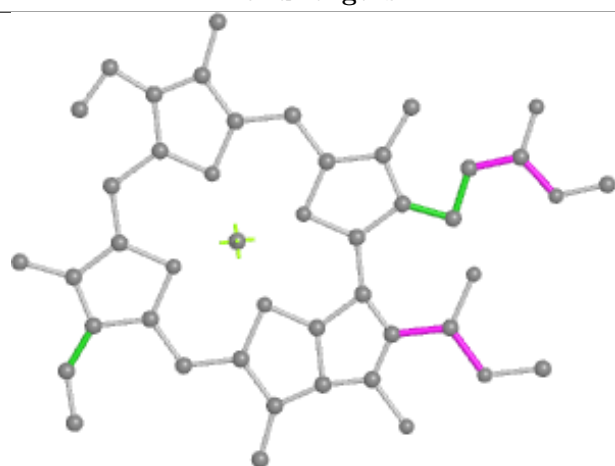
Ligand CLA 4 605



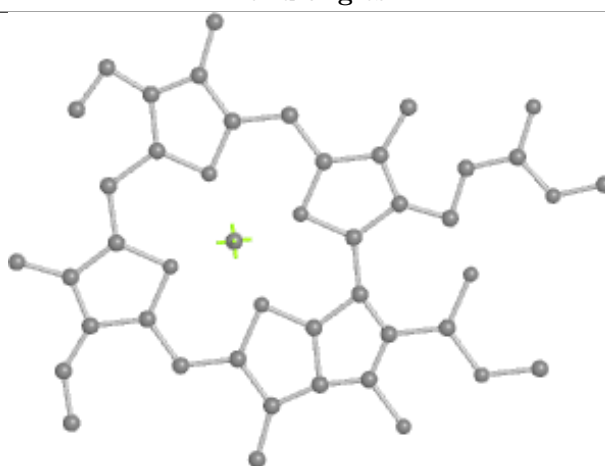
Bond lengths



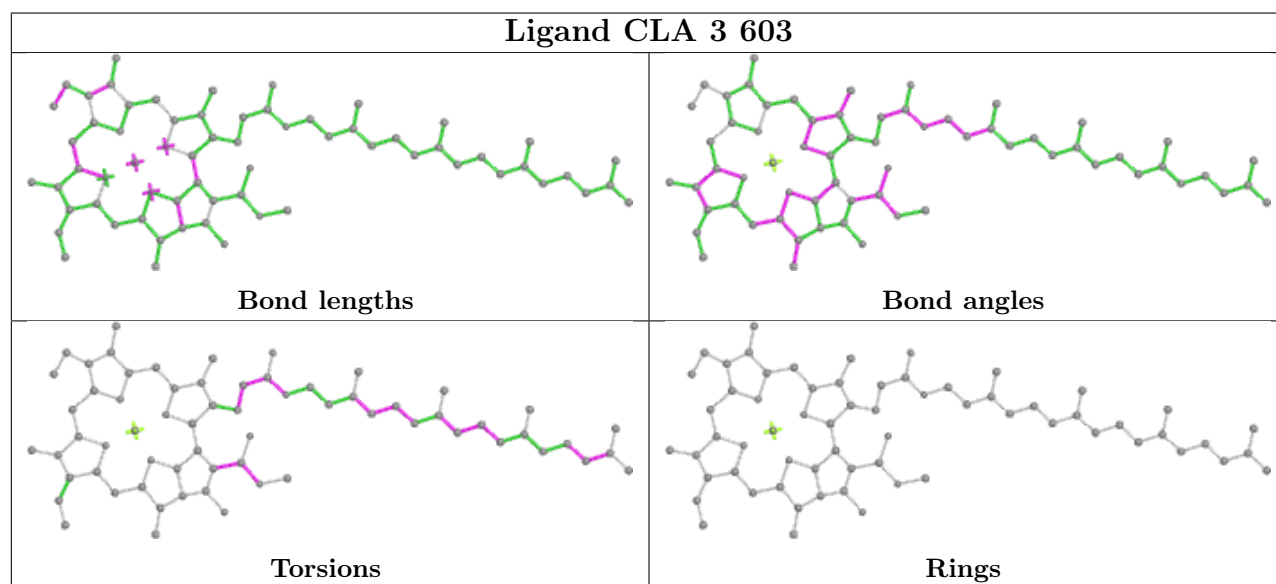
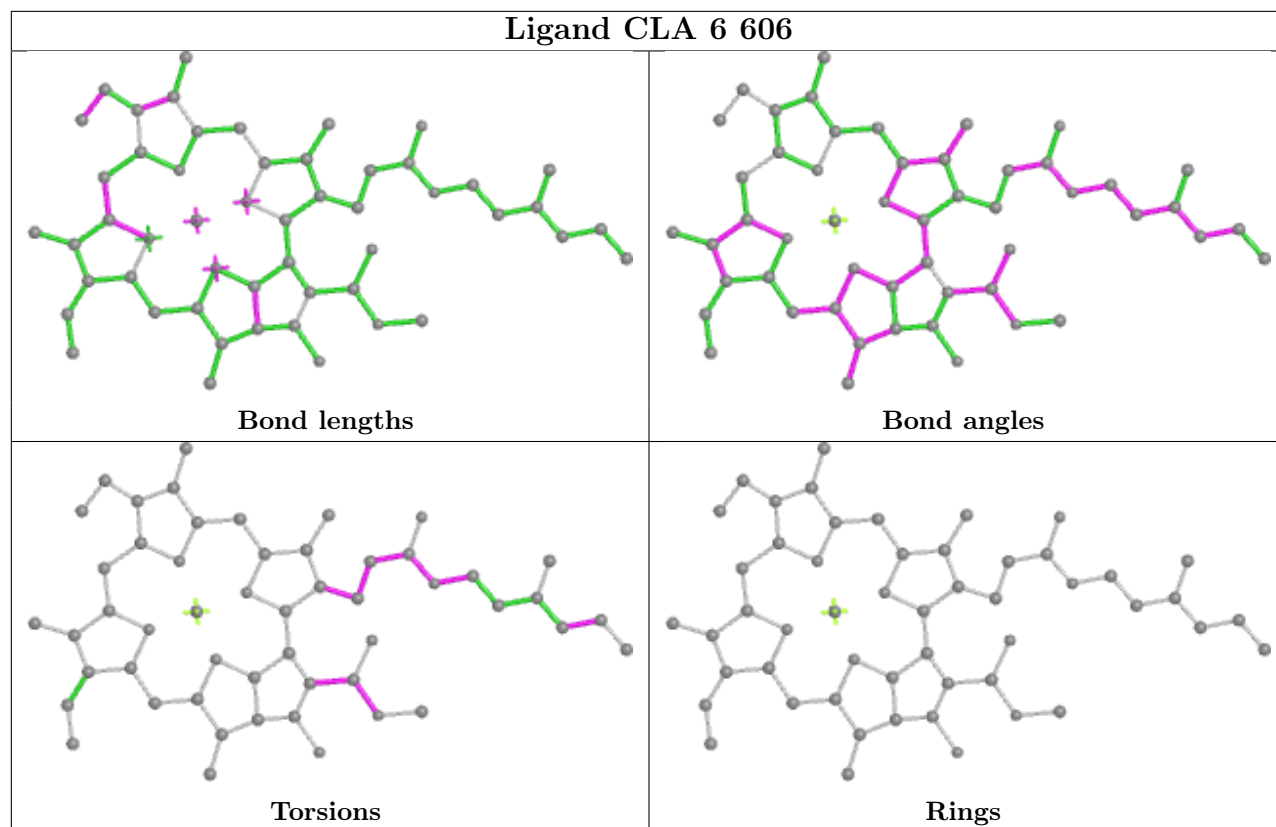
Bond angles

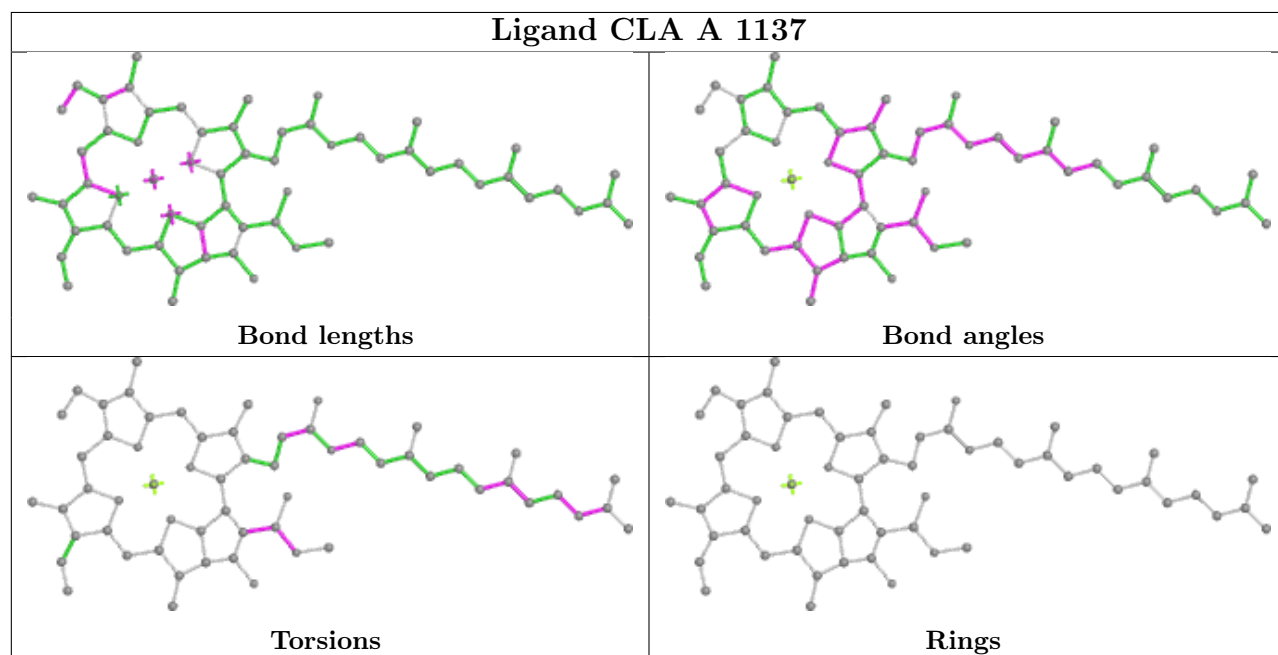
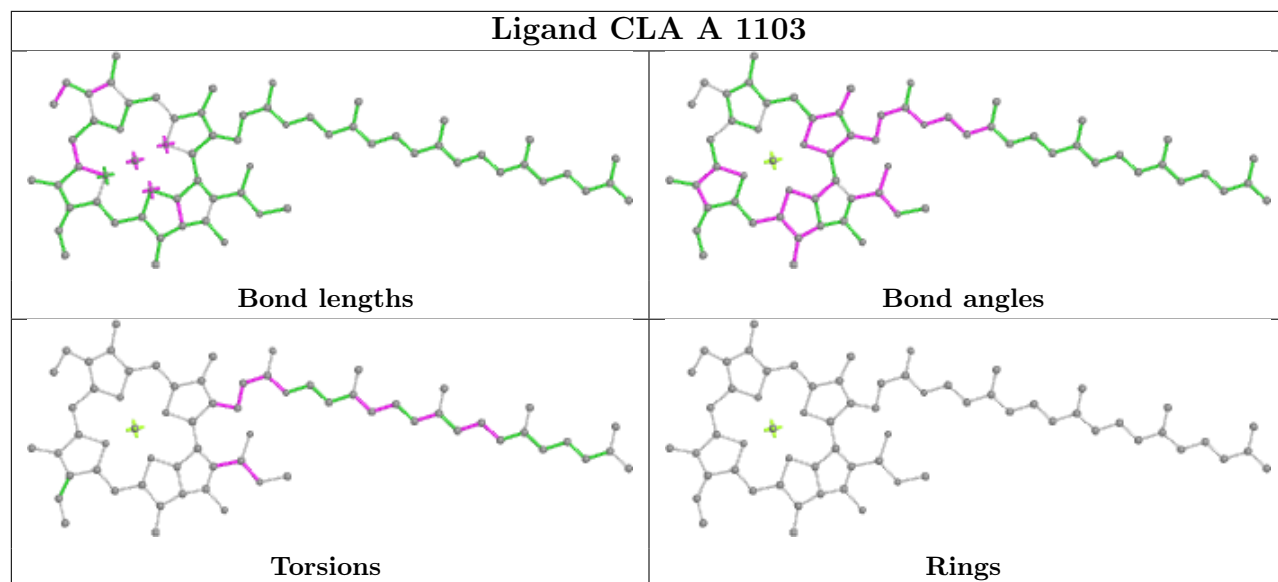


Torsions

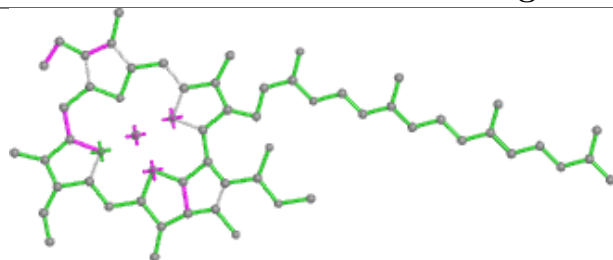


Rings

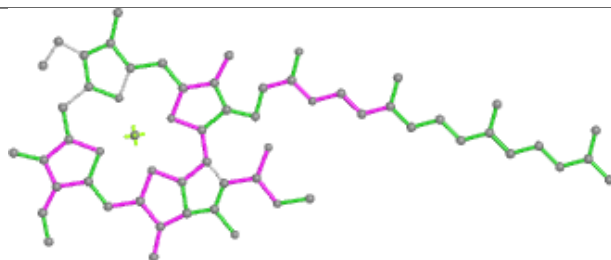




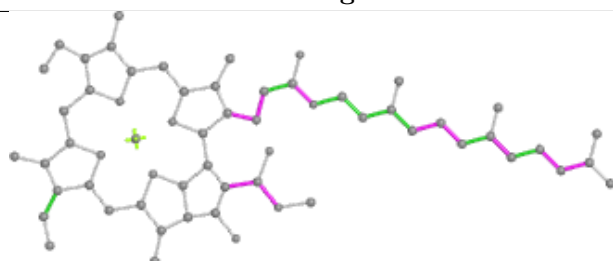
Ligand CLA 8 618



Bond lengths



Bond angles

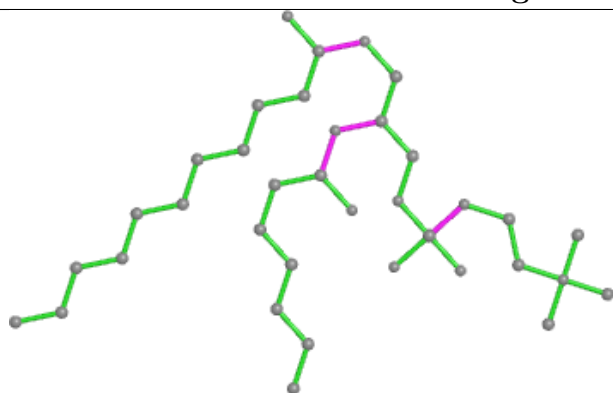


Torsions

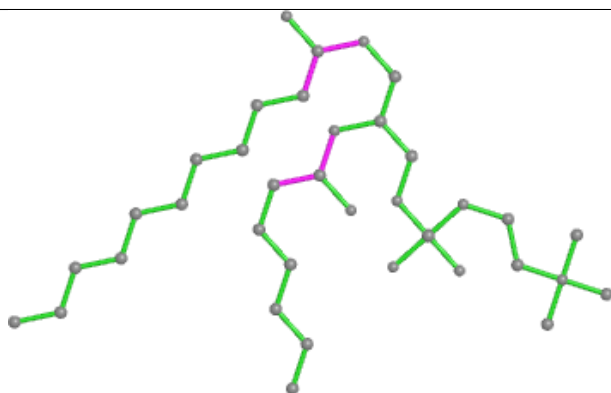


Rings

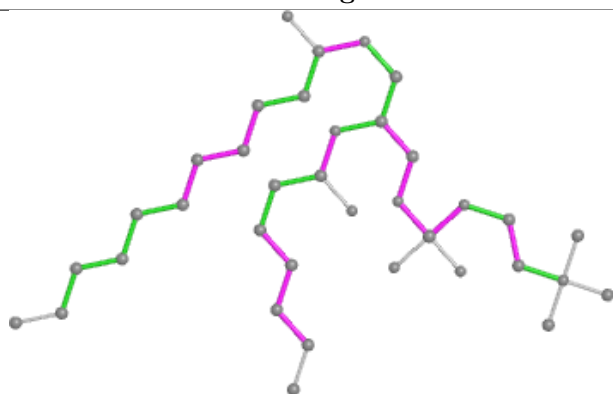
Ligand PCW 6 803



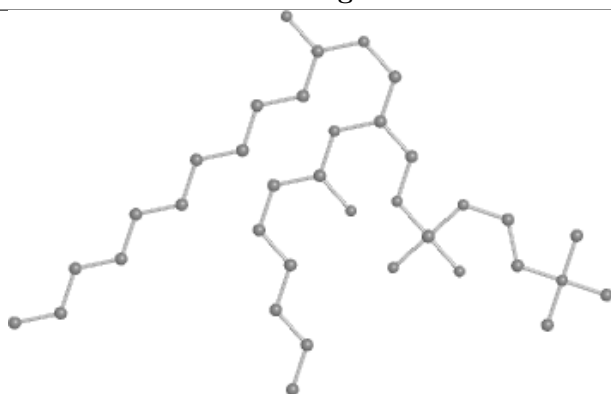
Bond lengths



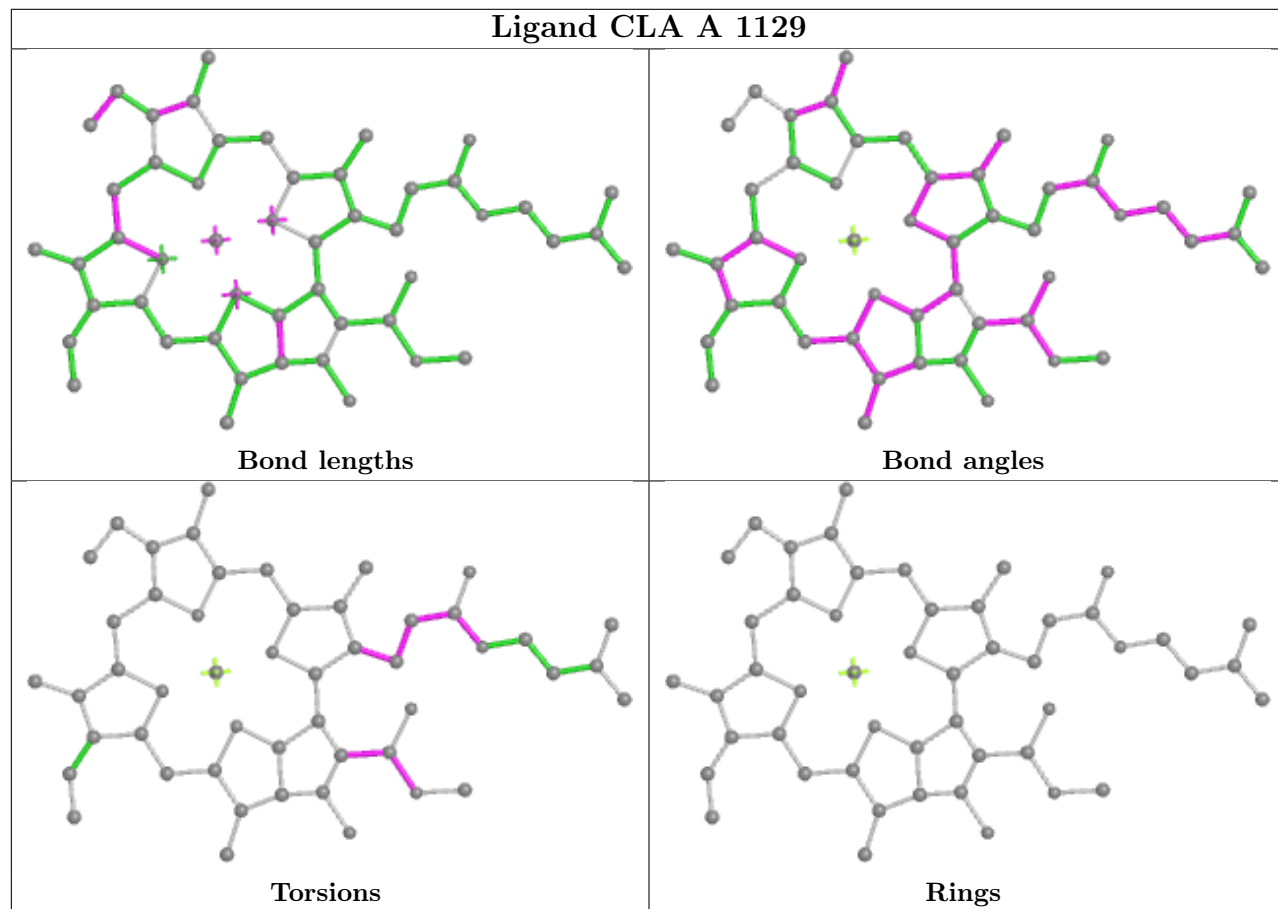
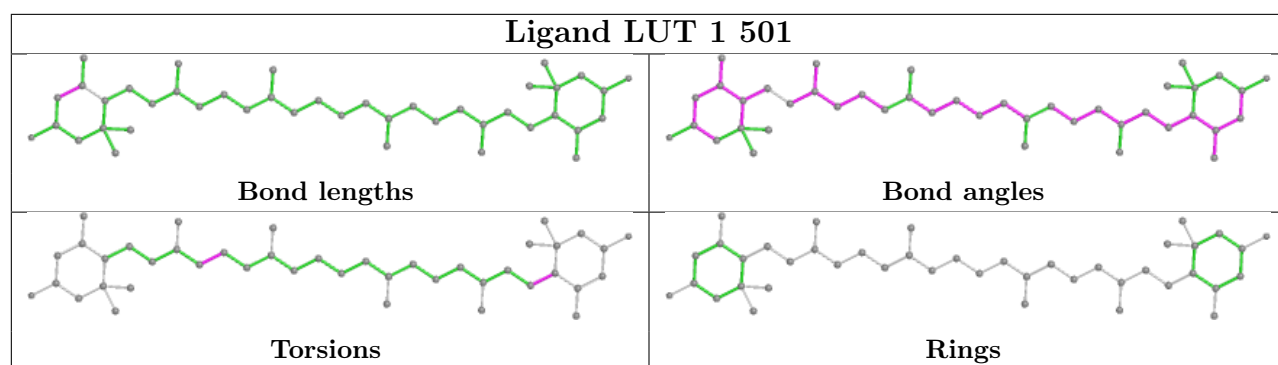
Bond angles



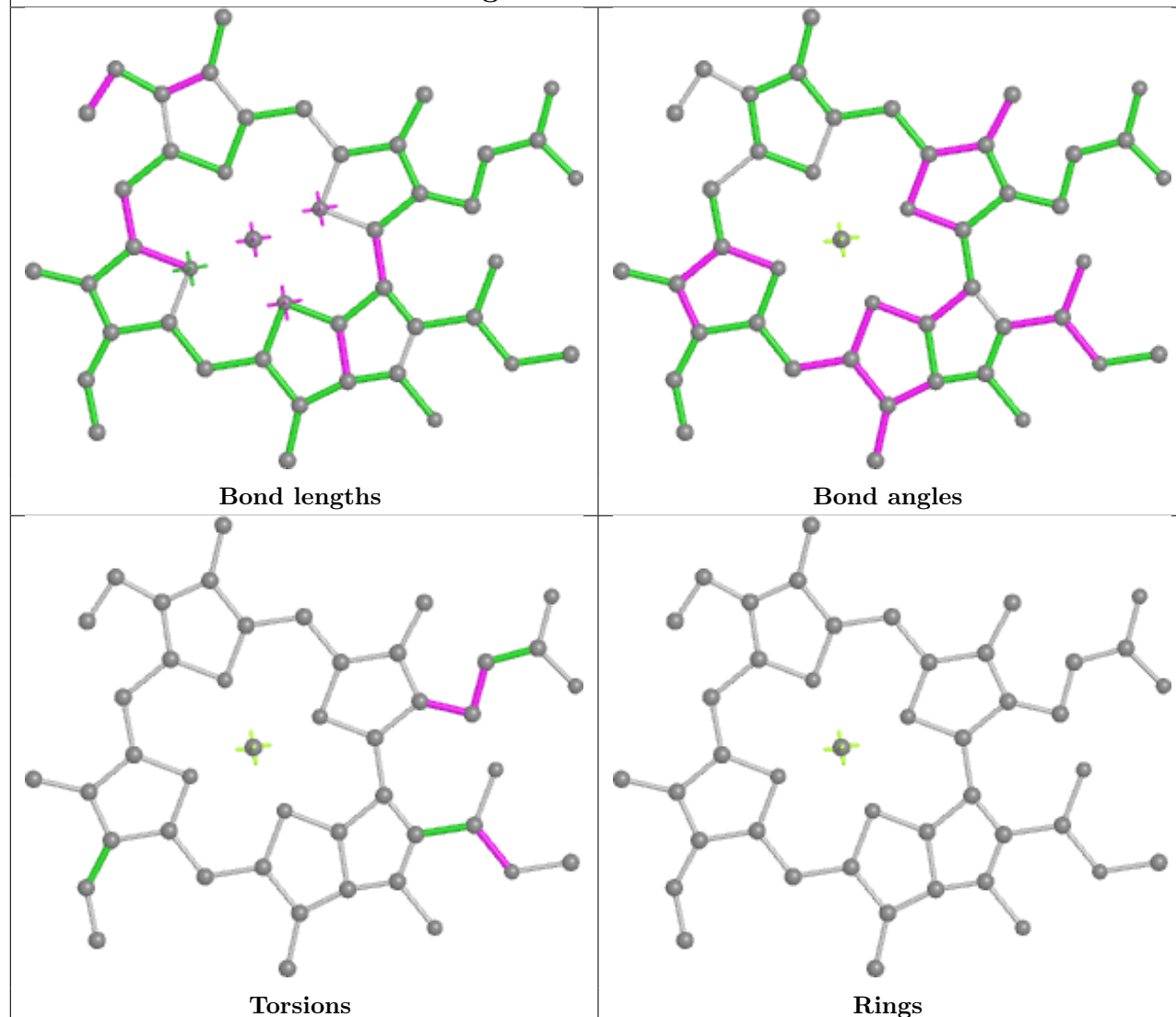
Torsions



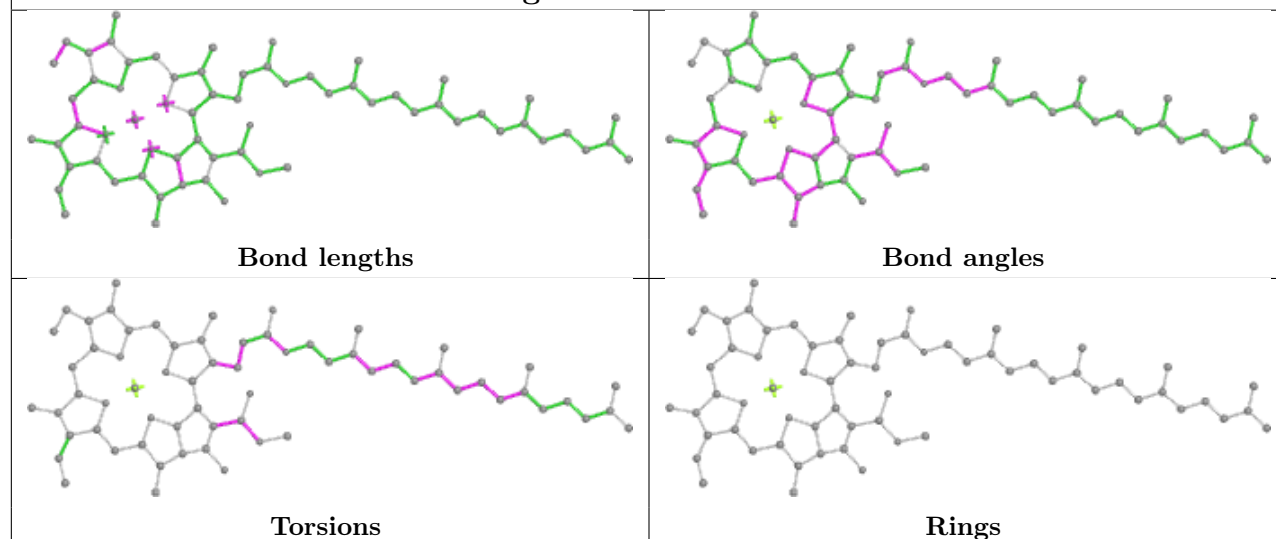
Rings

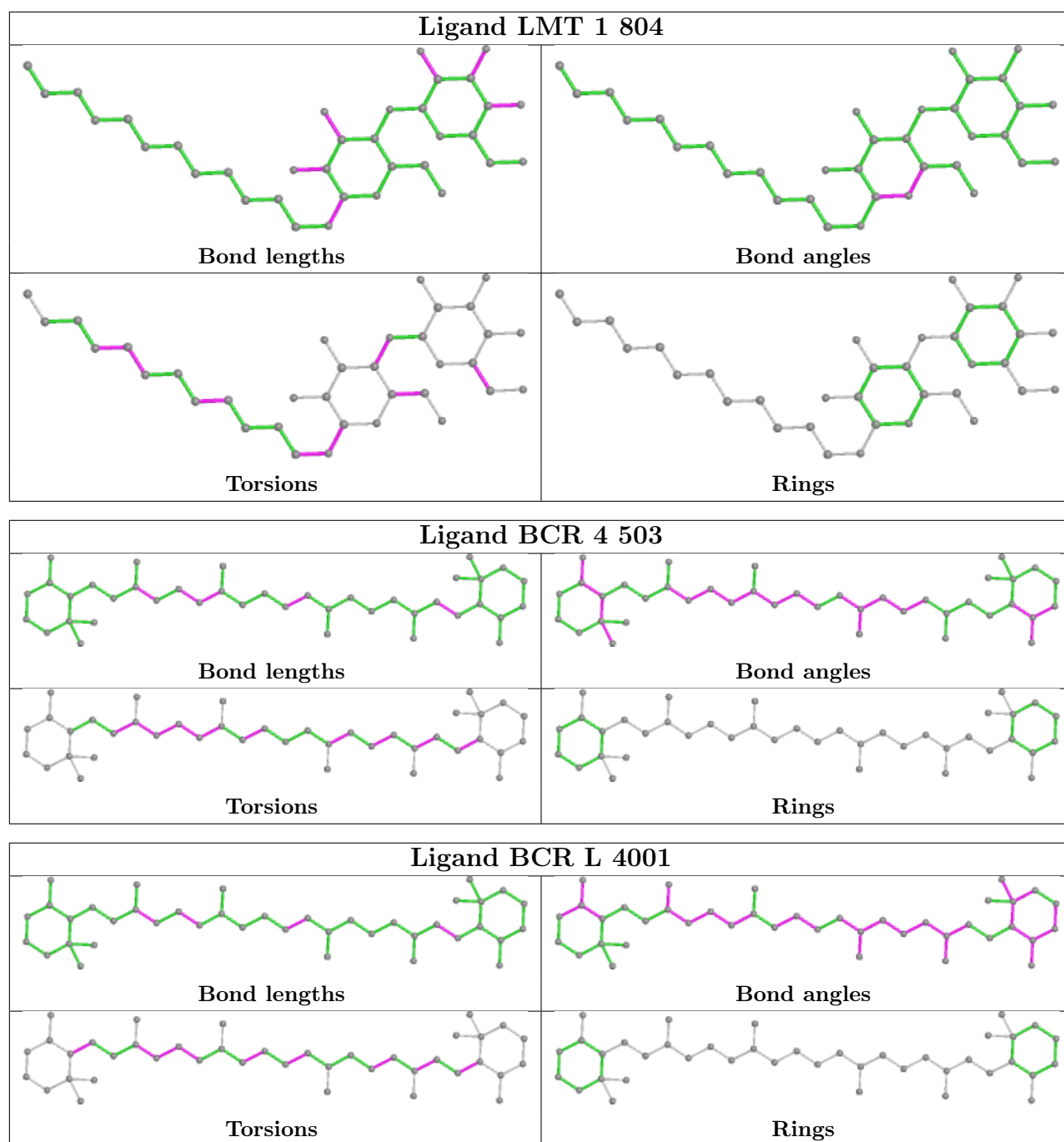


Ligand CLA B 1232

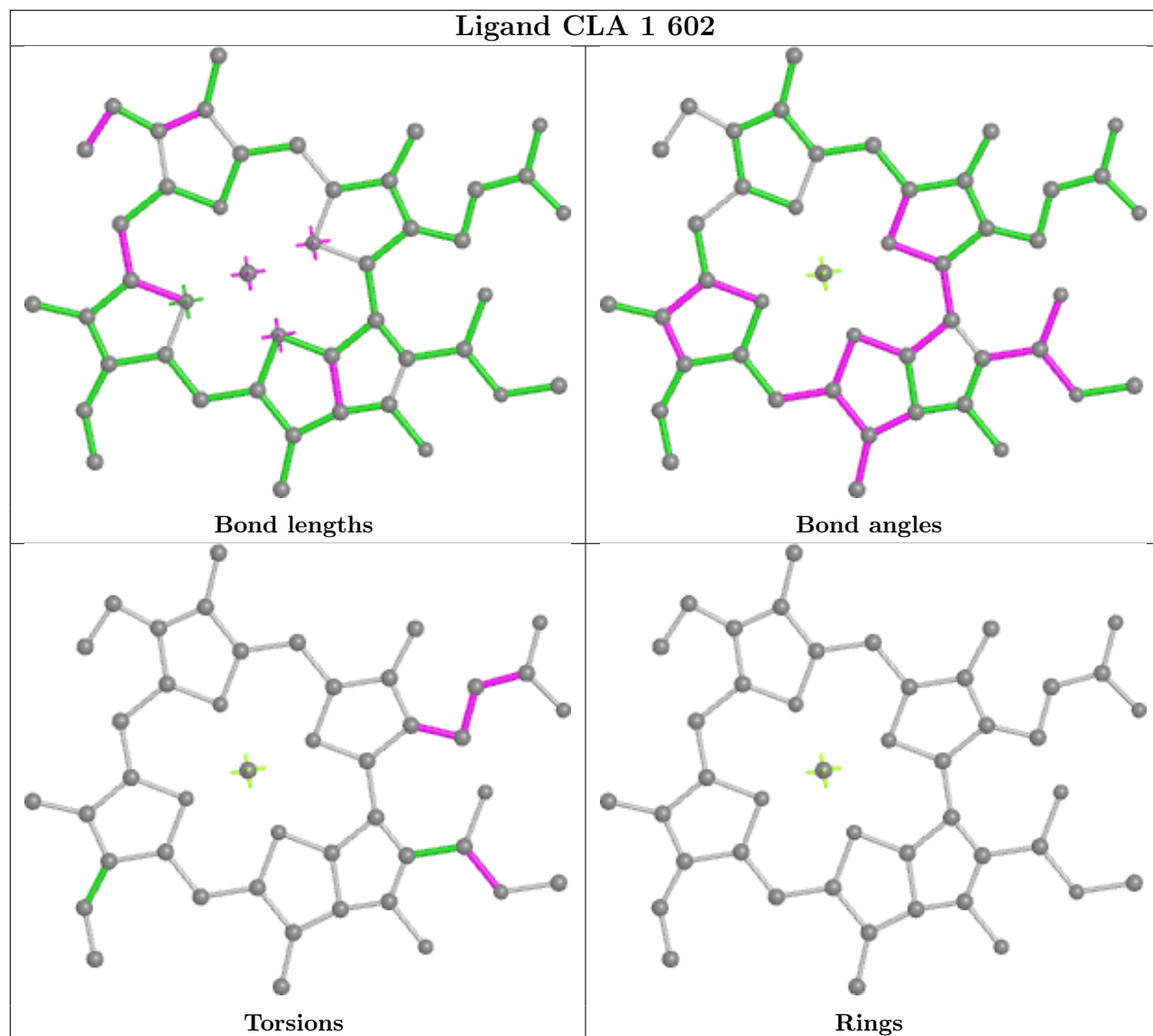


Ligand CLA A 1104

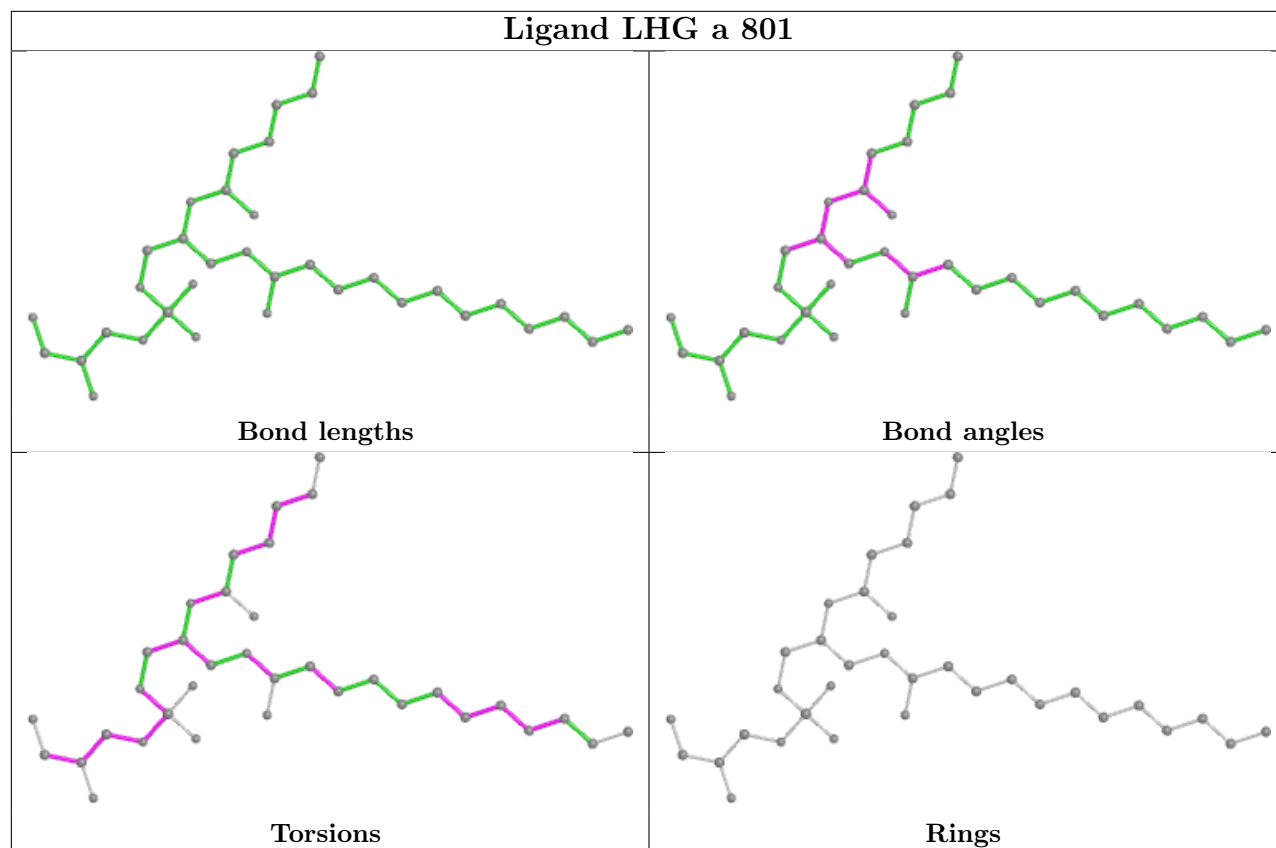




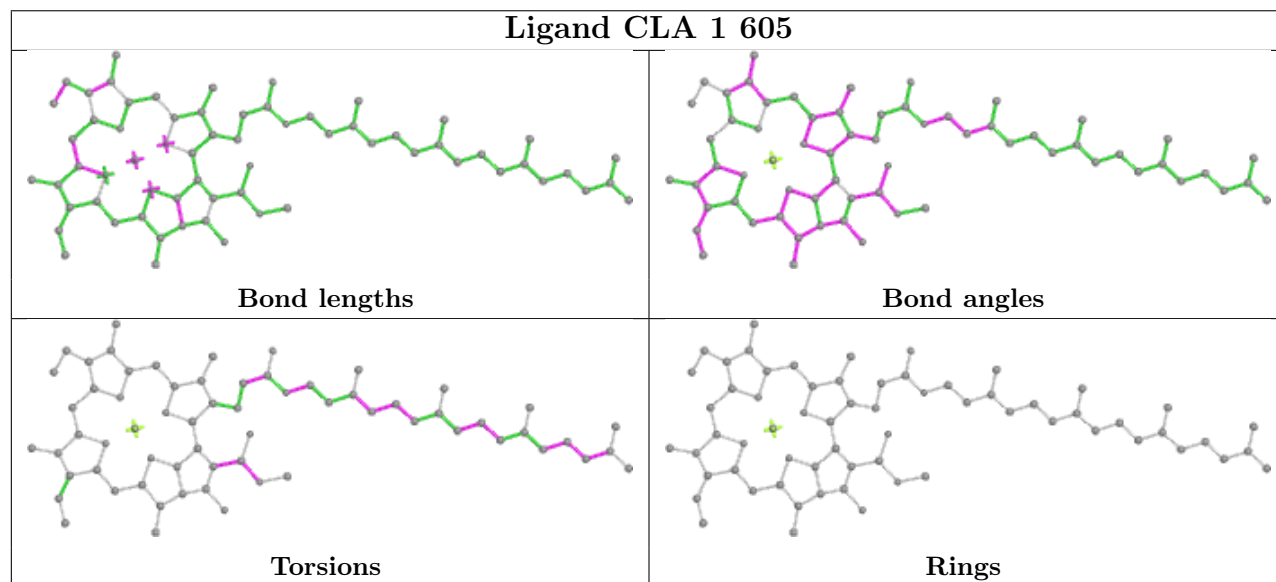
Ligand CLA 1 602

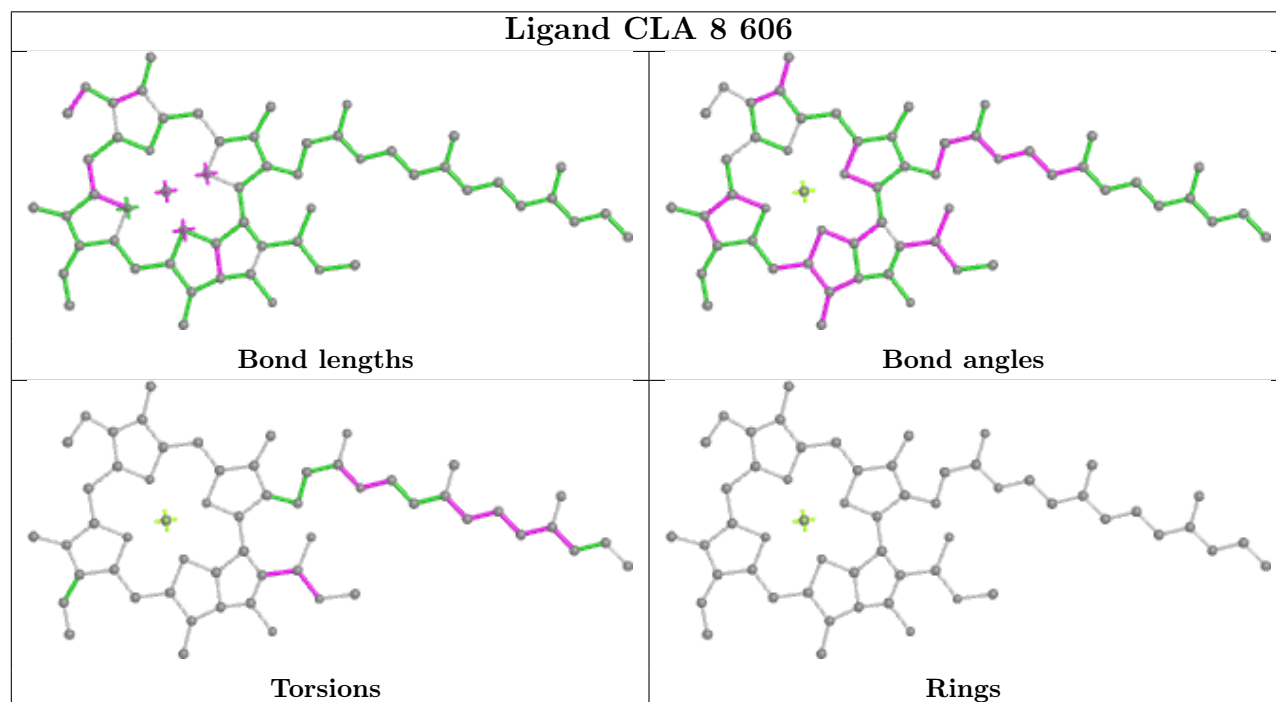
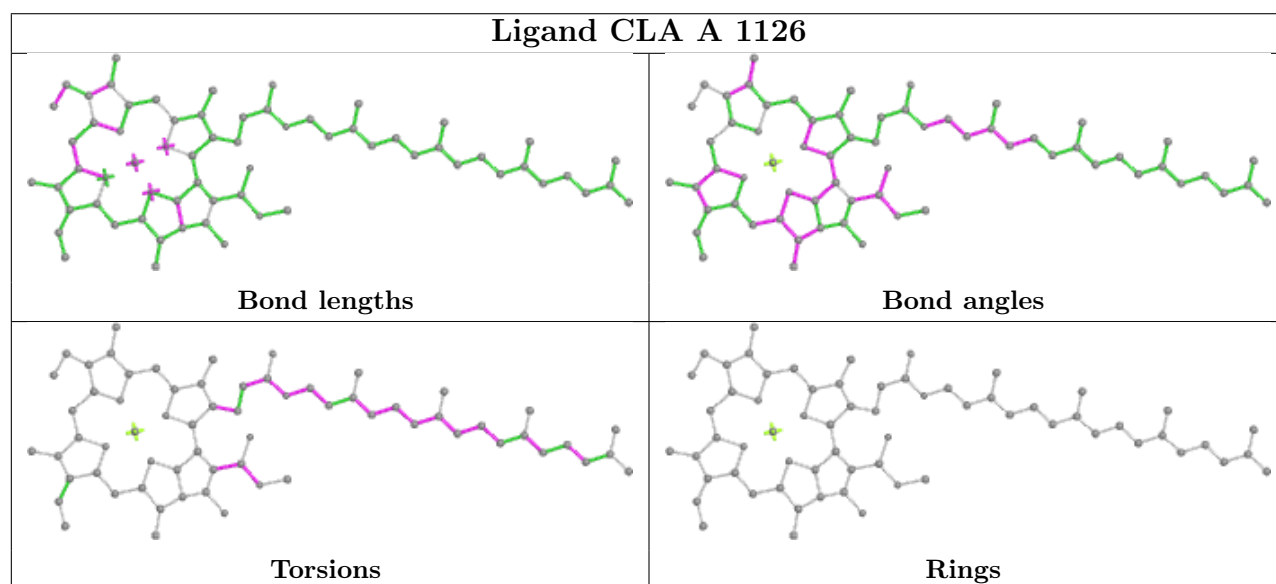
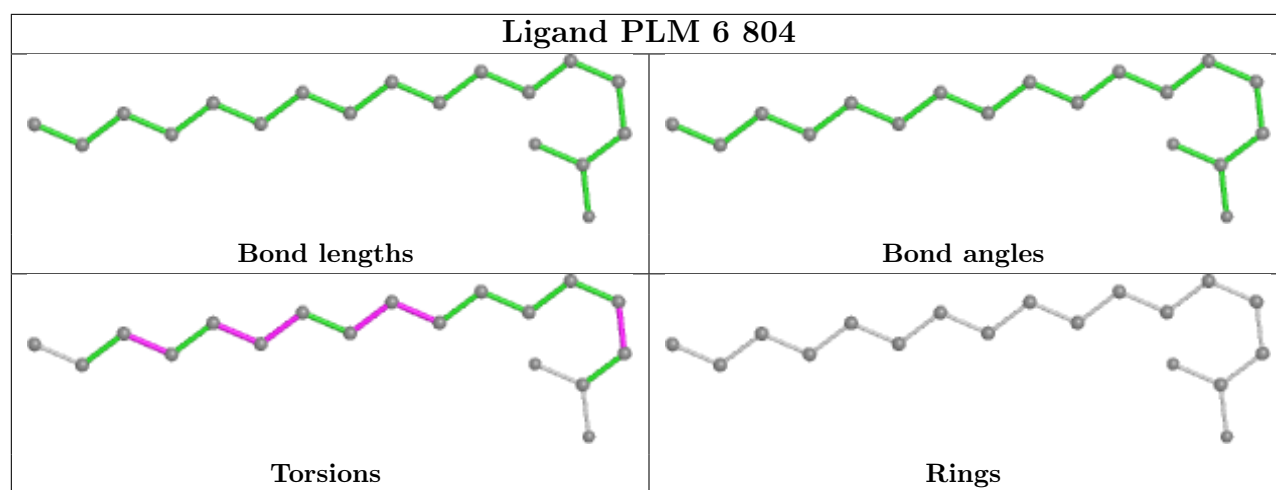


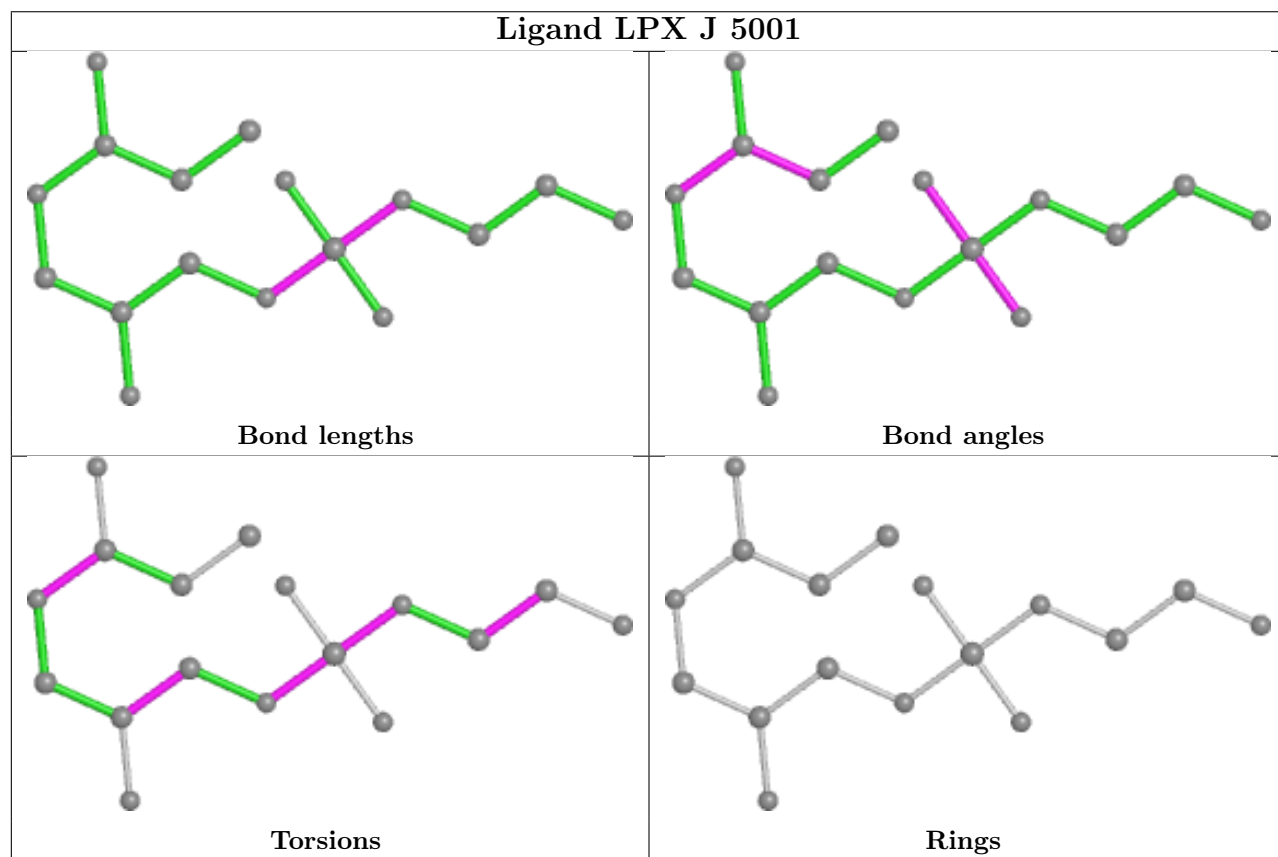
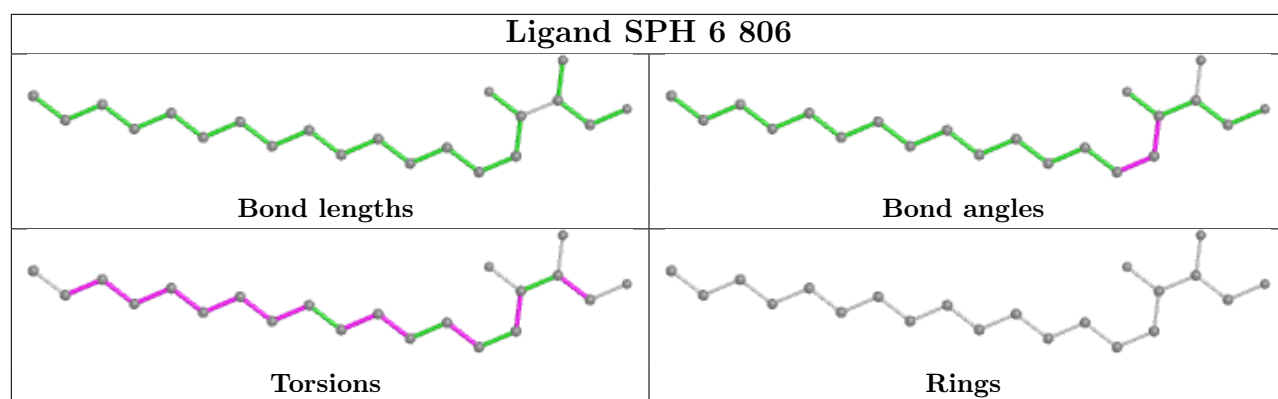
Ligand LHG a 801



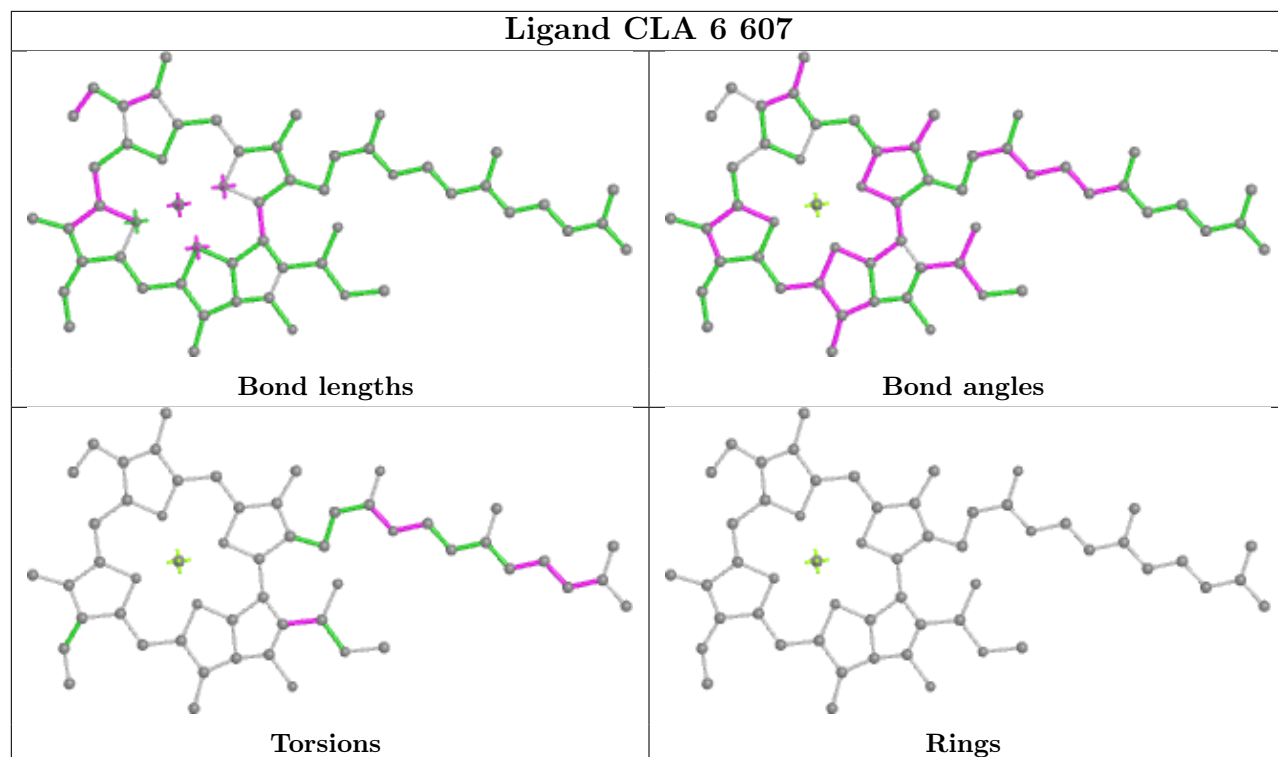
Ligand CLA 1 605



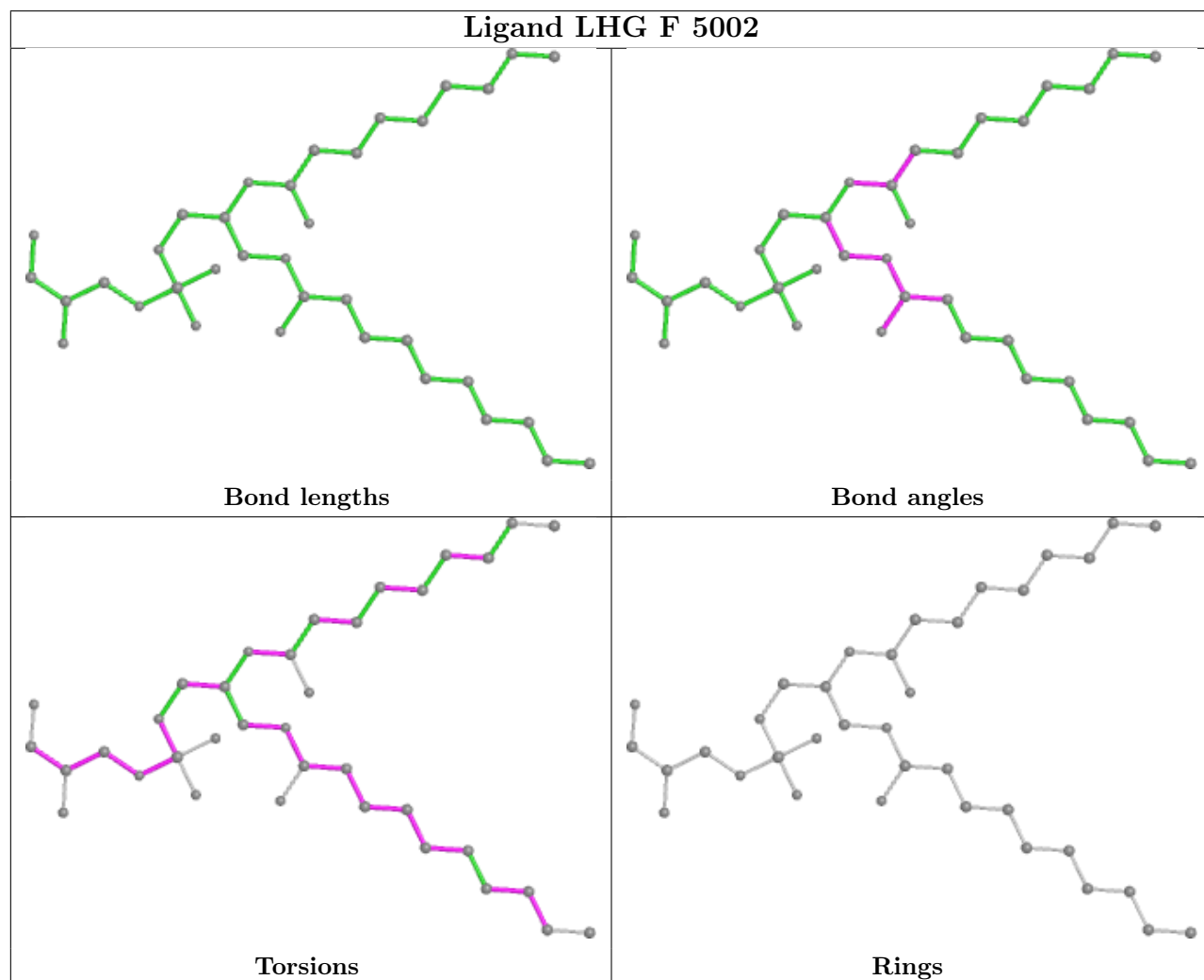


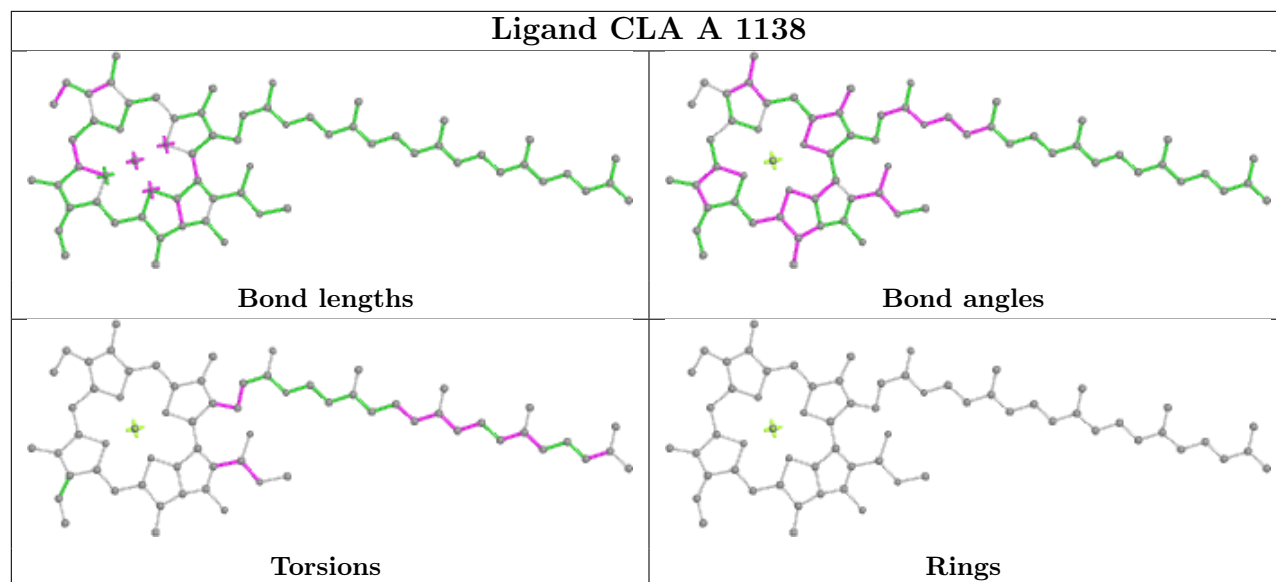
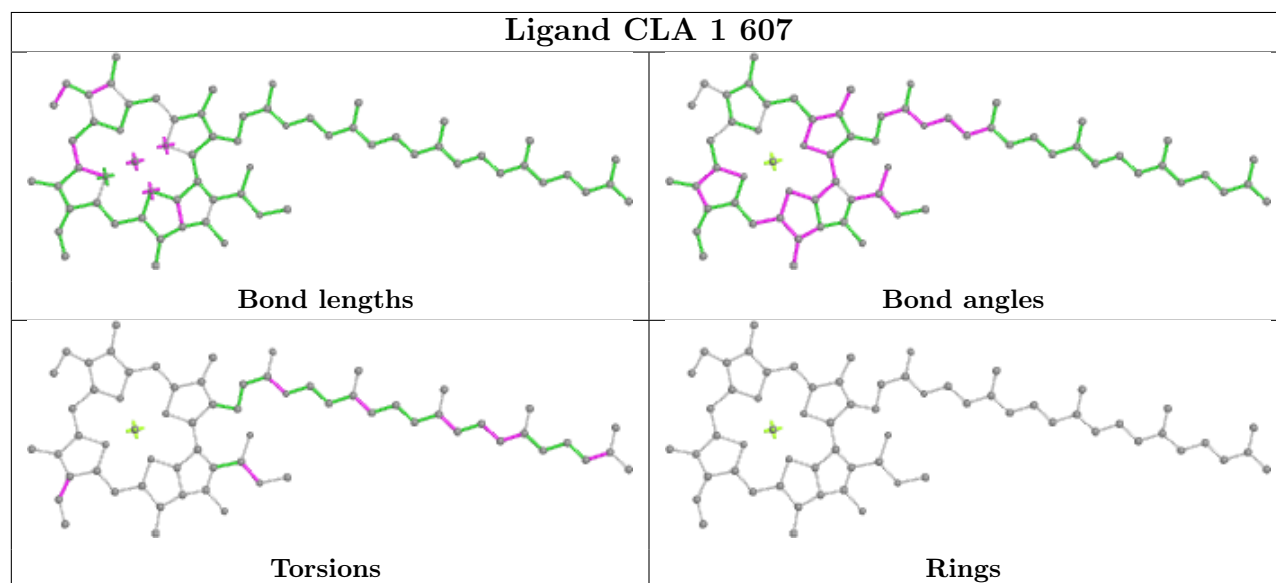


Ligand CLA 6 607

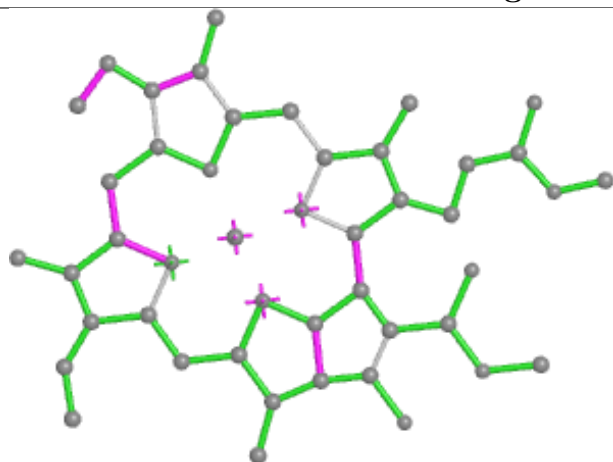


Ligand LHG F 5002

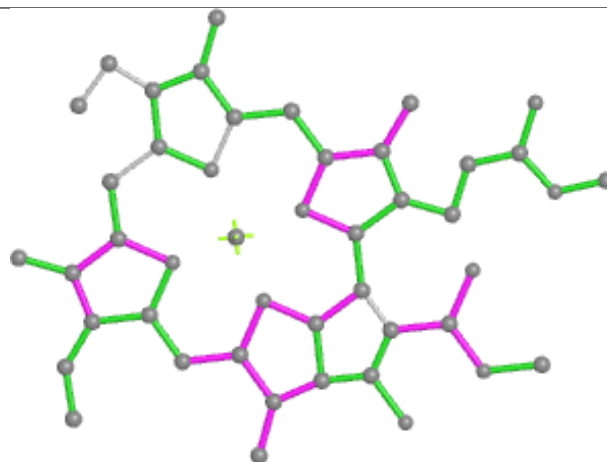


Ligand CLA A 1138**Ligand CLA 1 607**

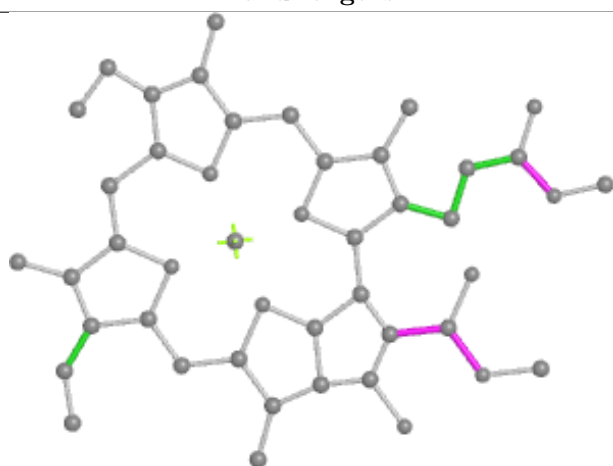
Ligand CLA K 1403



Bond lengths



Bond angles

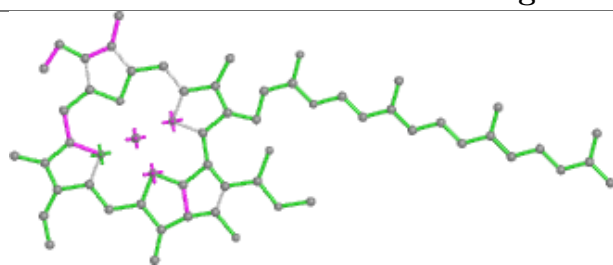


Torsions

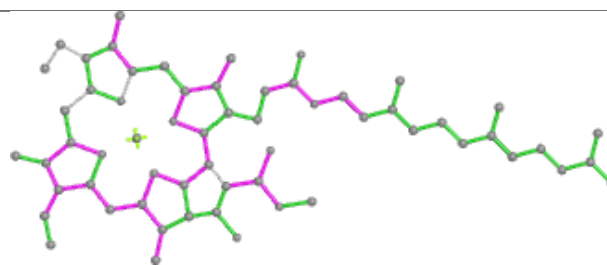


Rings

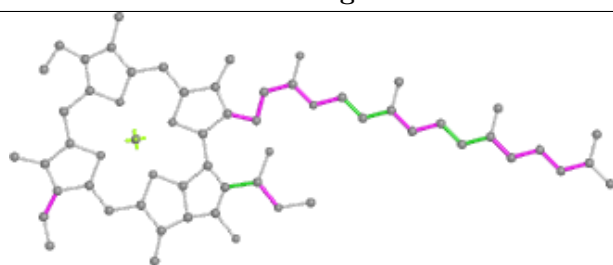
Ligand CLA 7 612



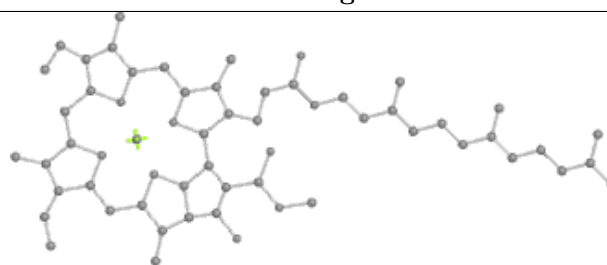
Bond lengths



Bond angles

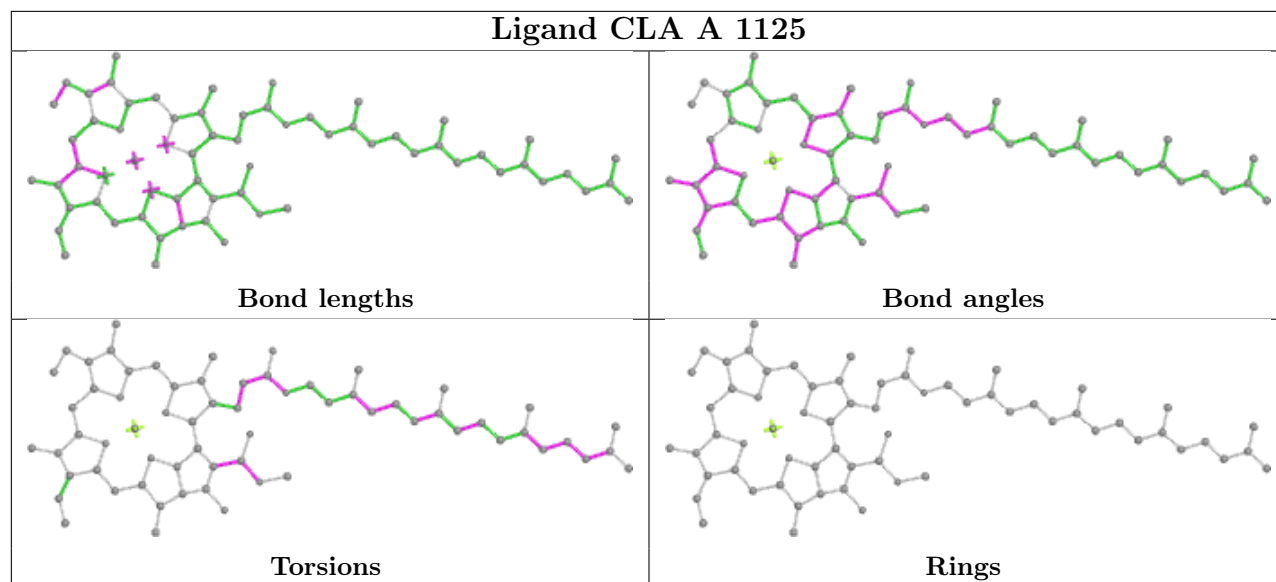


Torsions

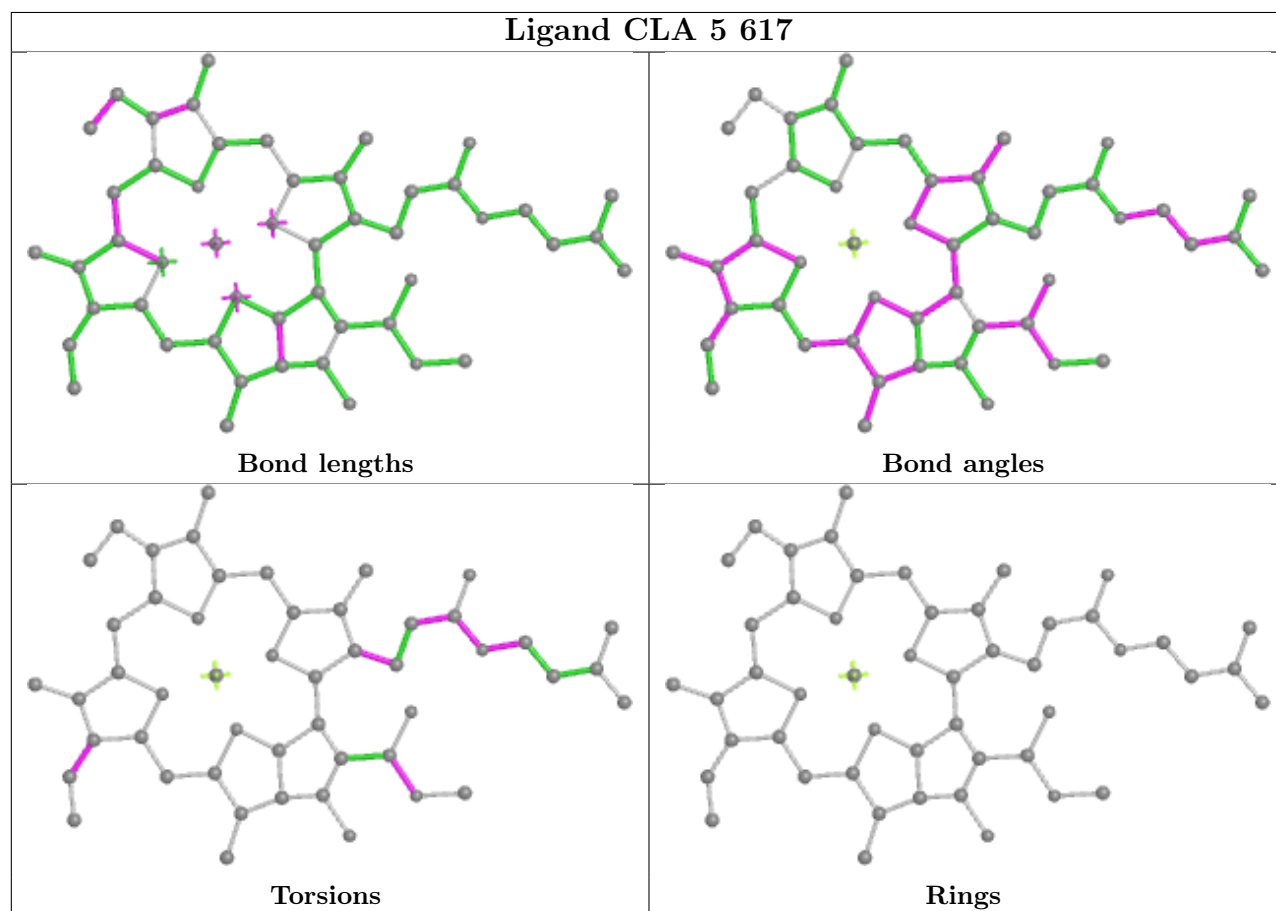


Rings

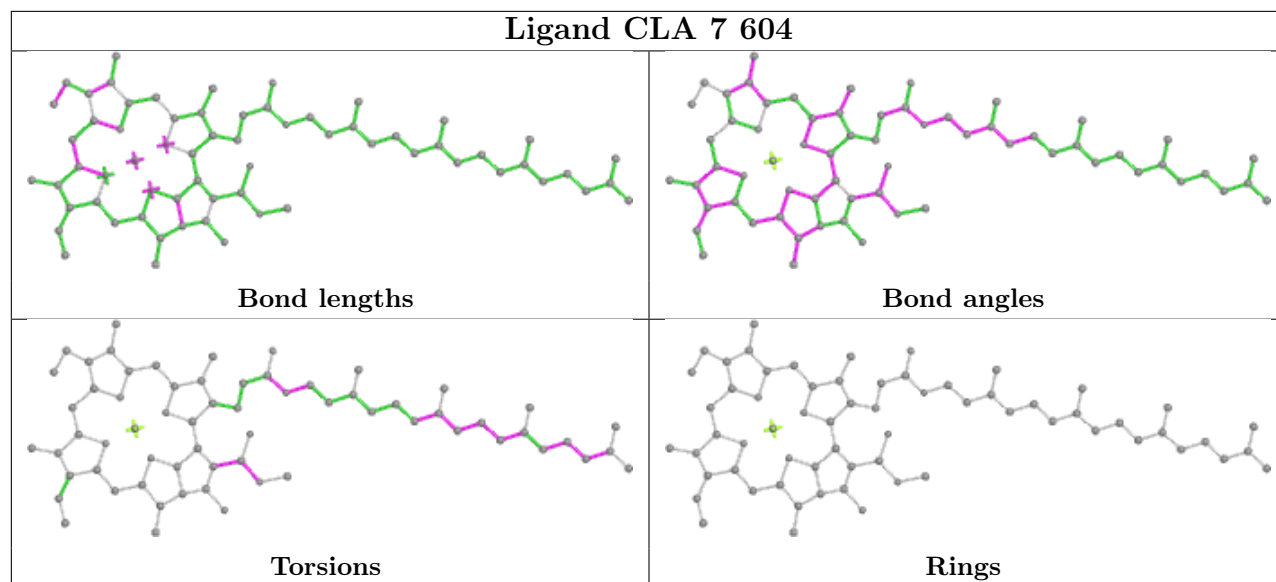
Ligand CLA A 1125



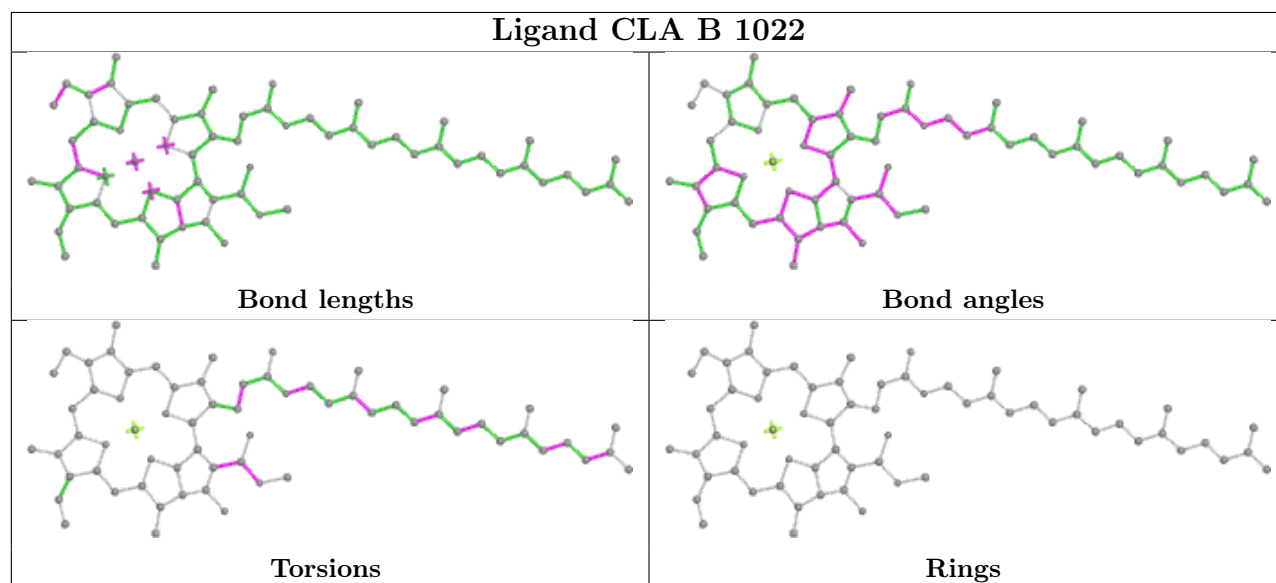
Ligand CLA 5 617



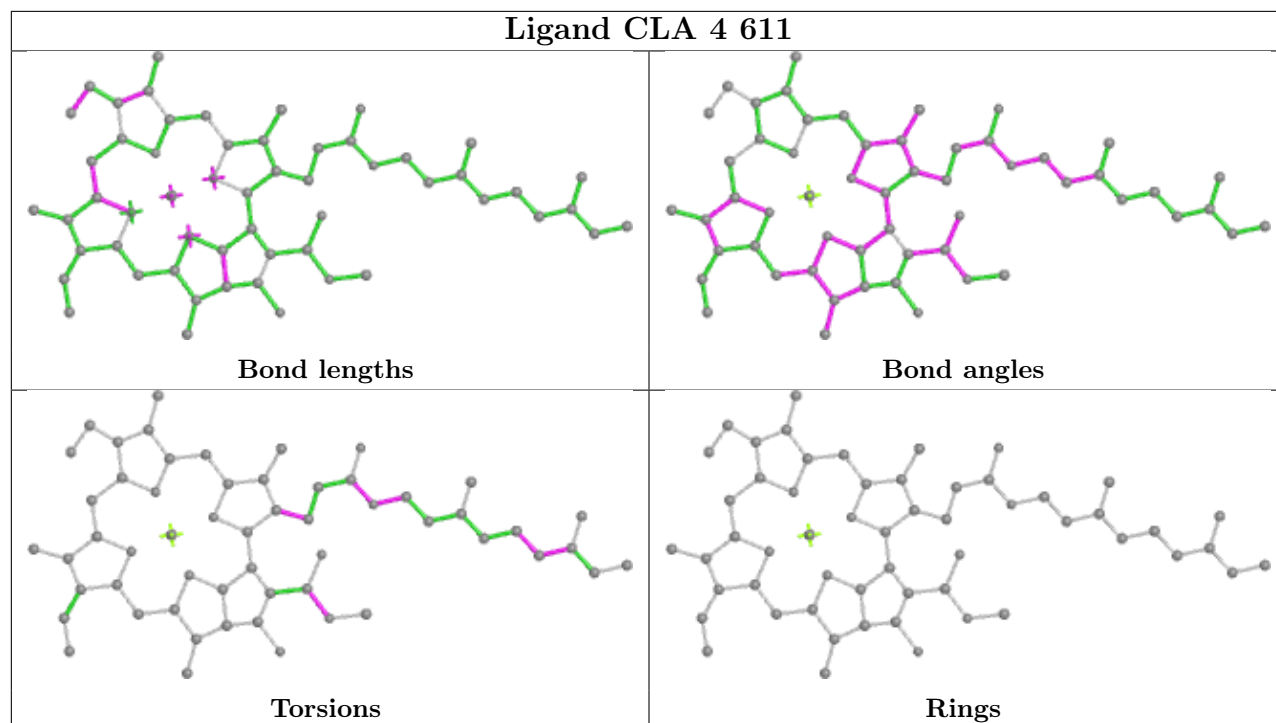
Ligand CLA 7 604



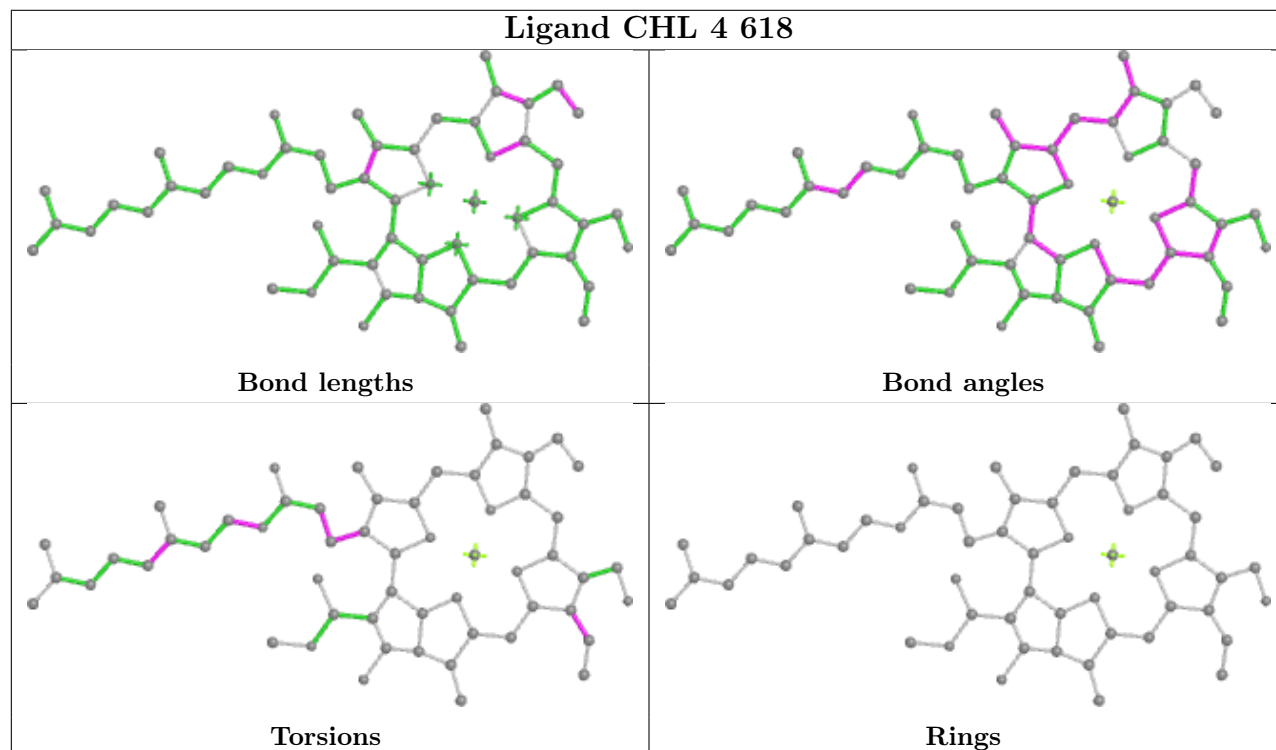
Ligand CLA B 1022



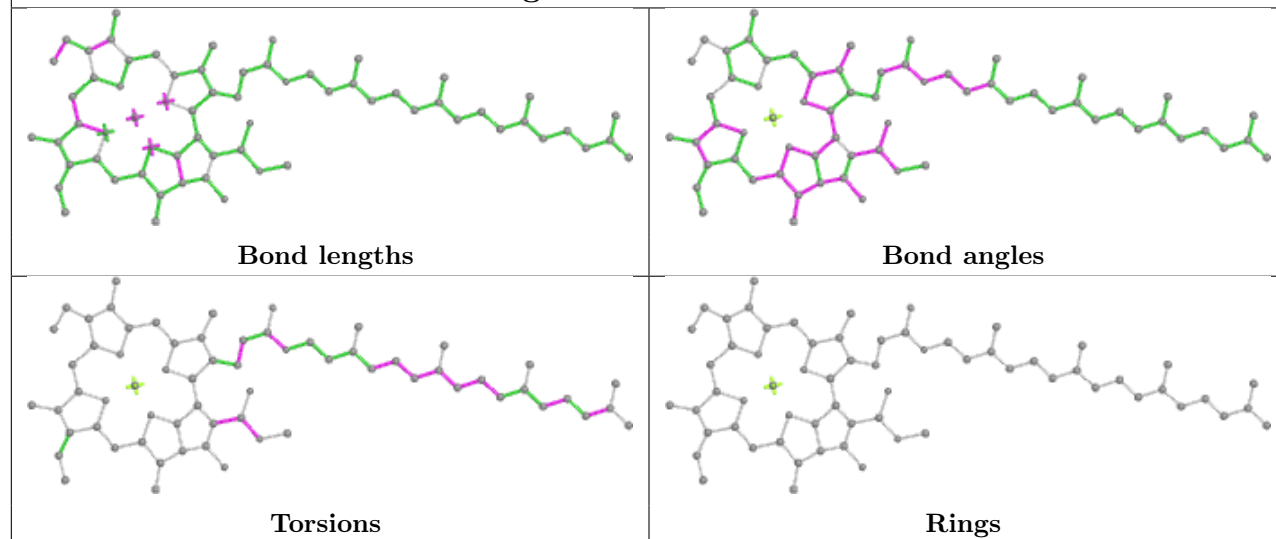
Ligand CLA 4 611



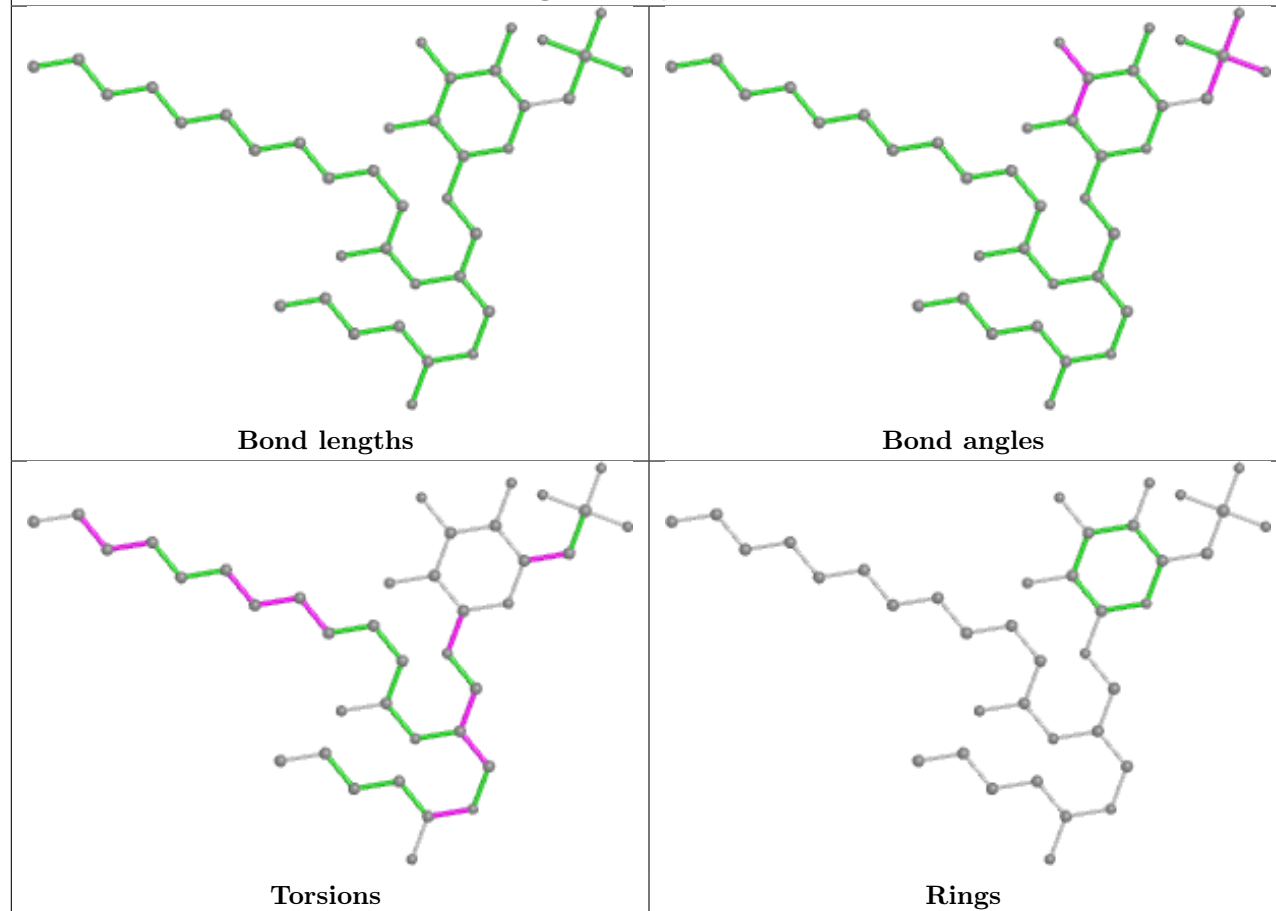
Ligand CHL 4 618

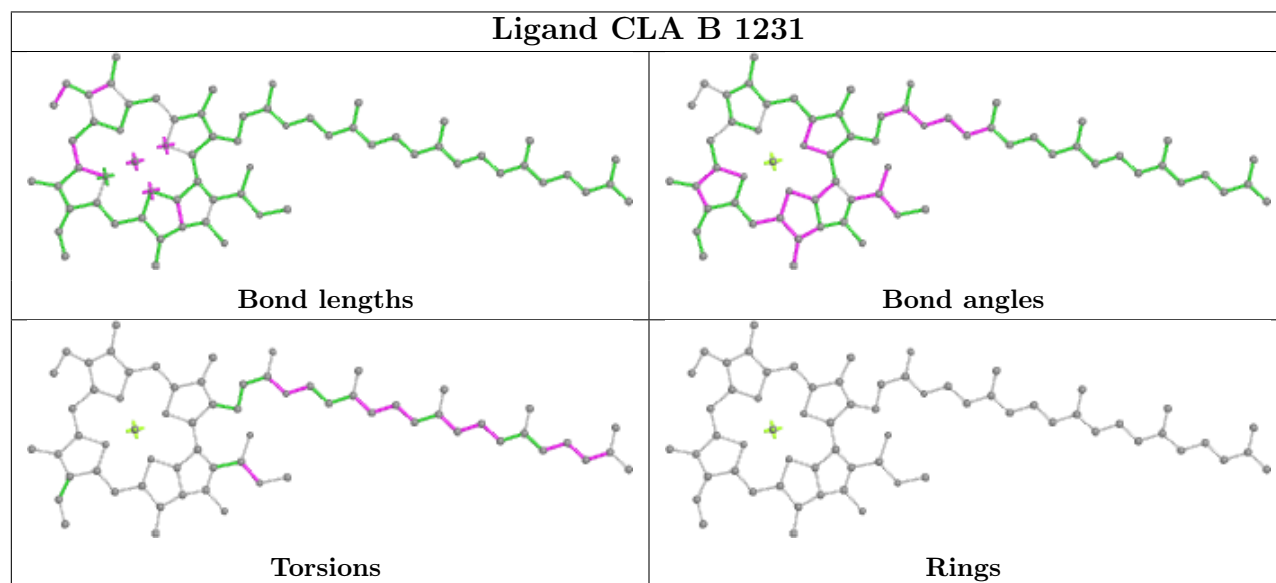
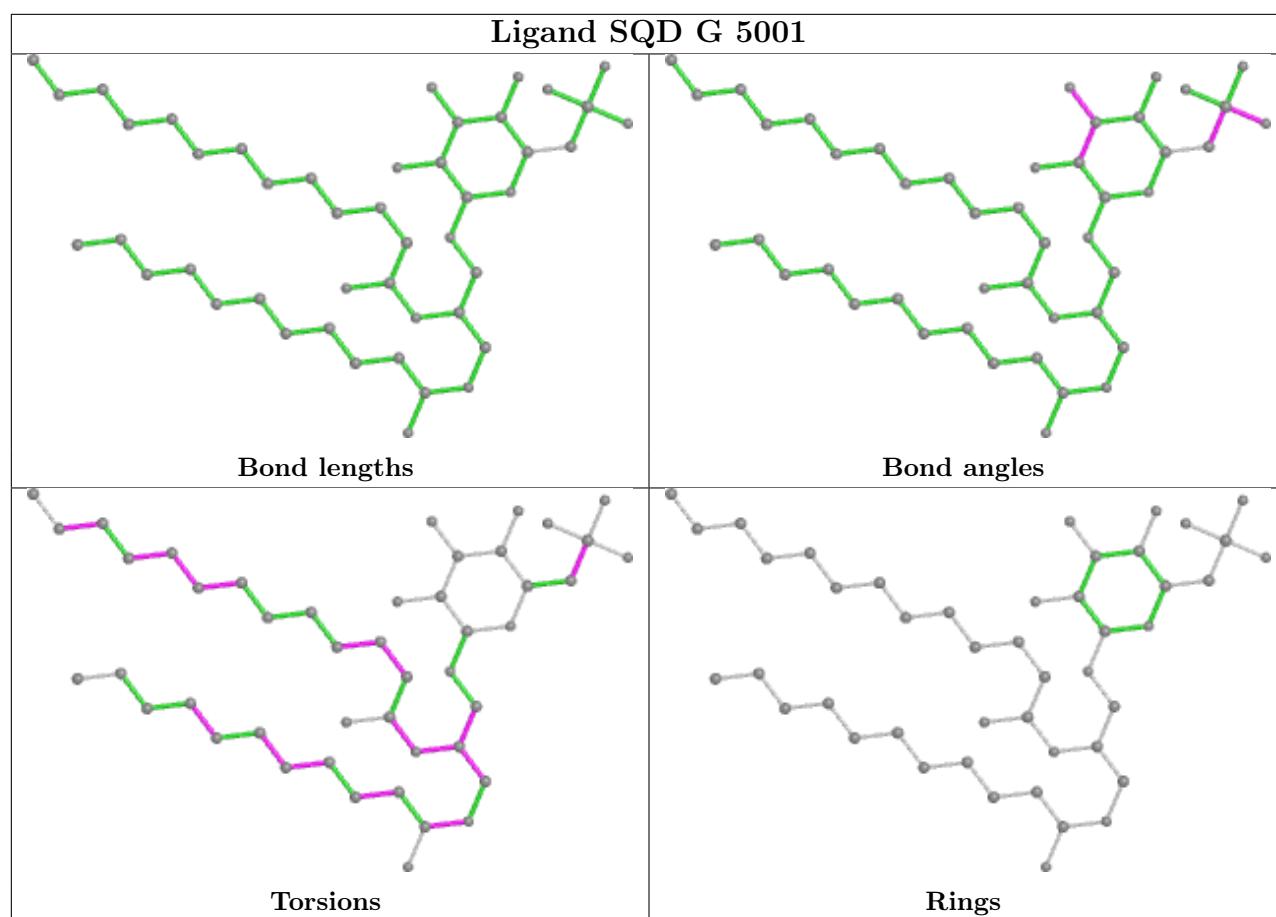


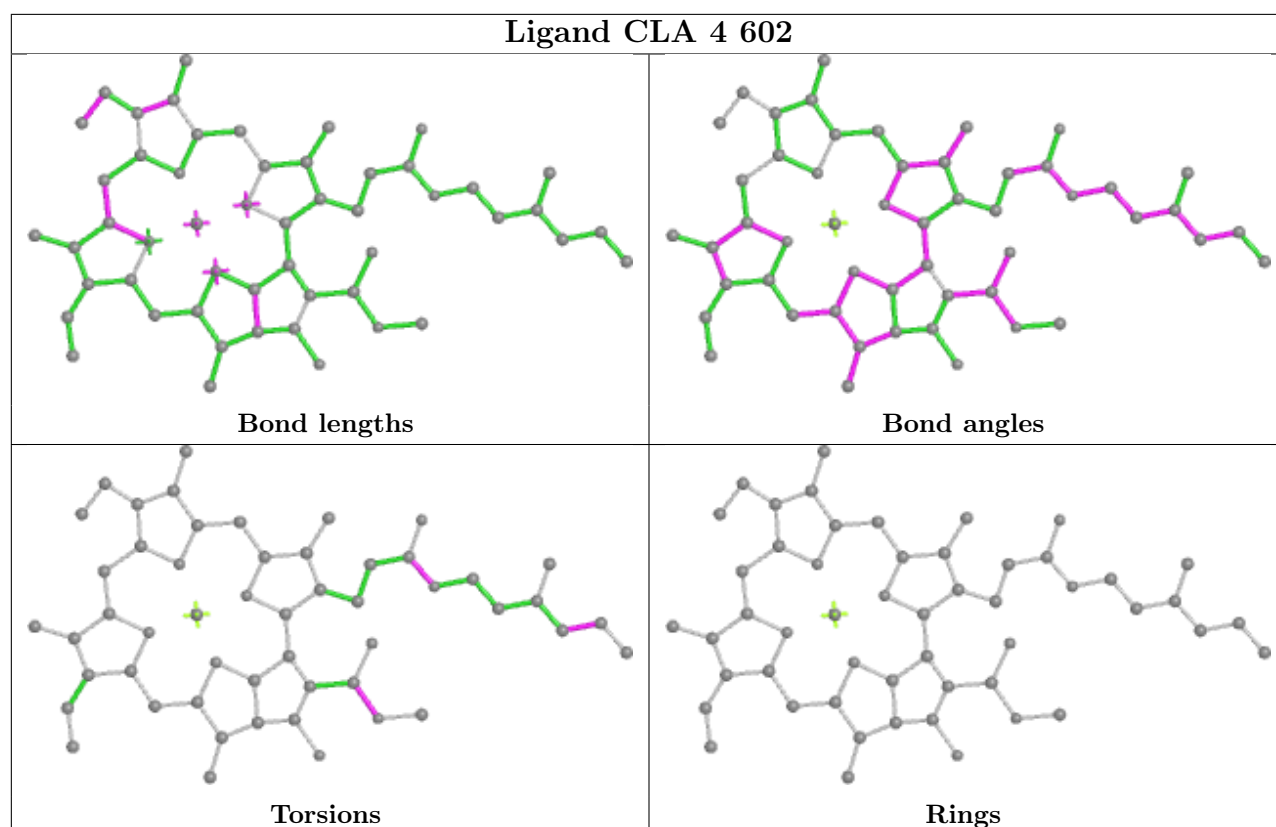
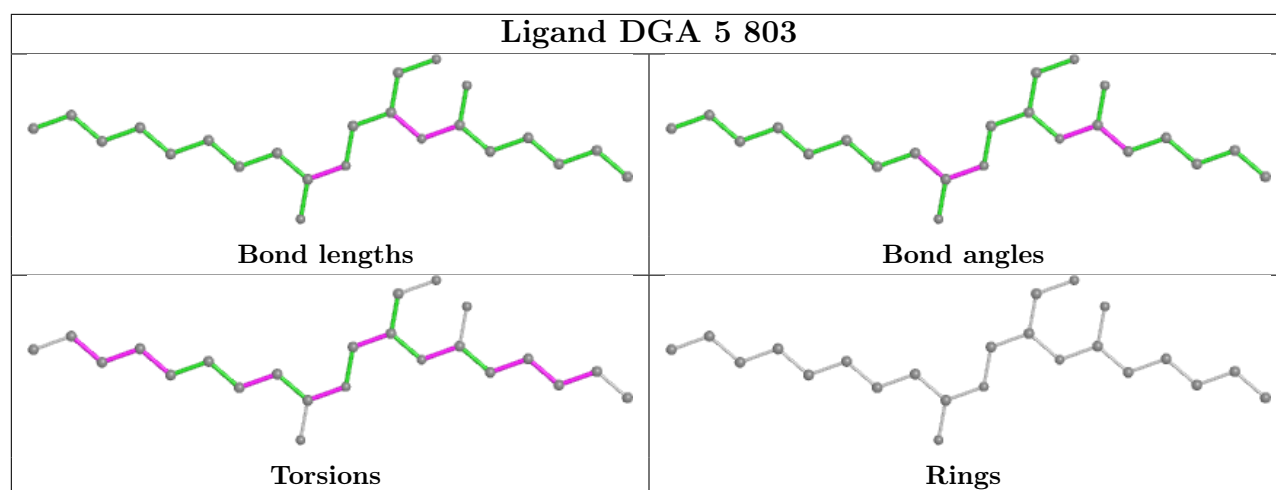
Ligand CLA A 1114

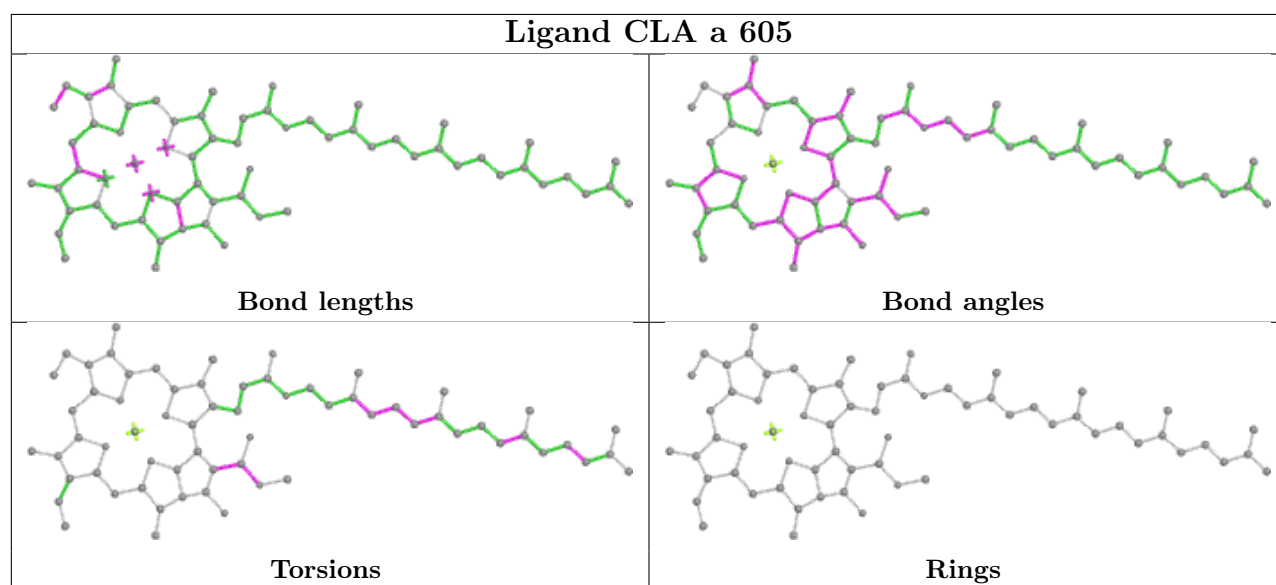
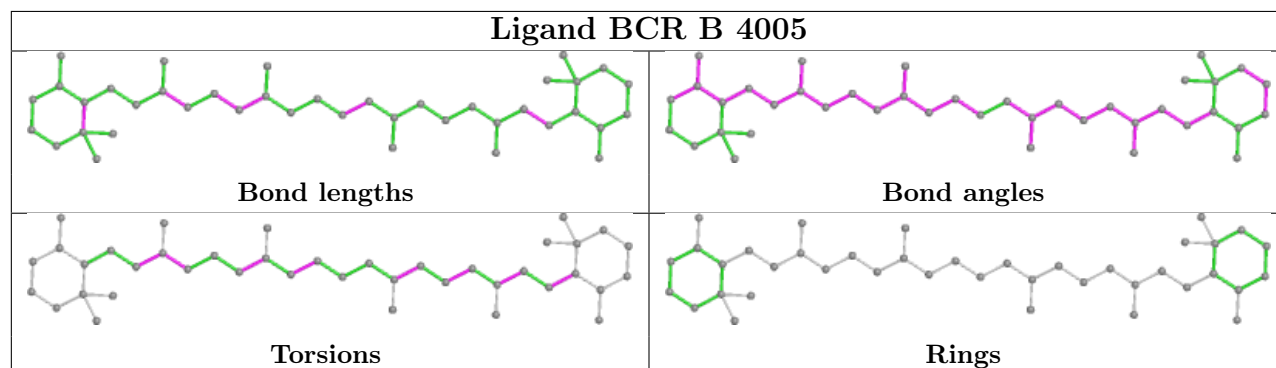
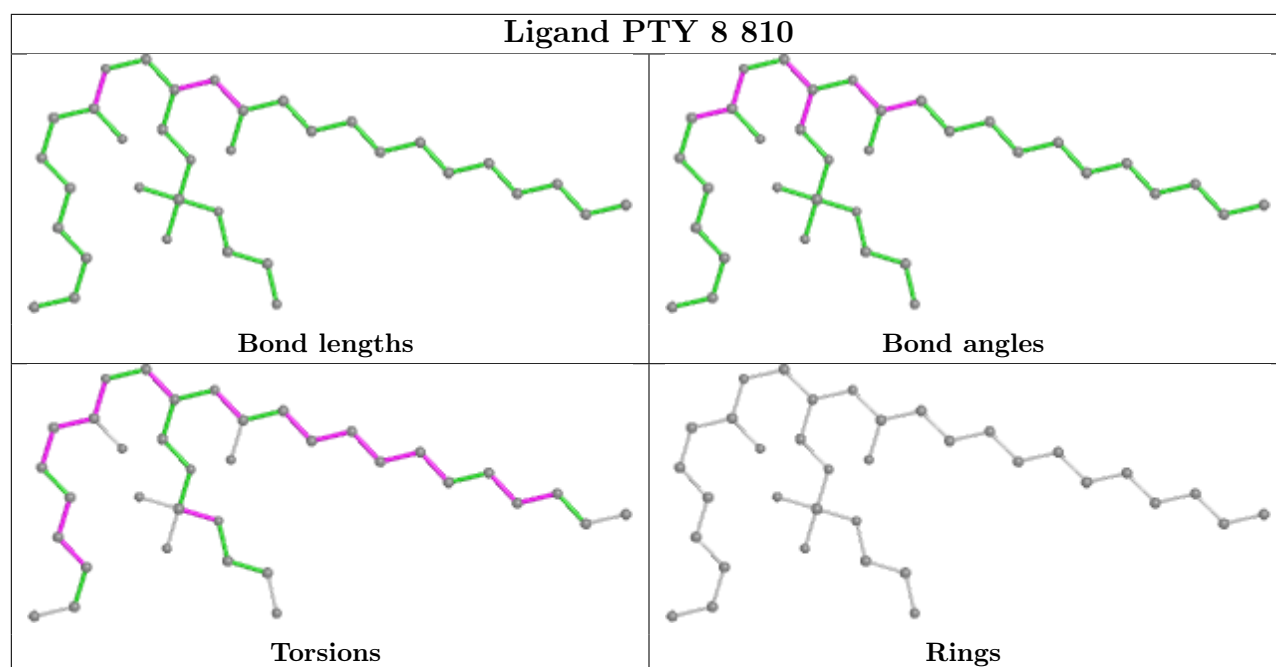


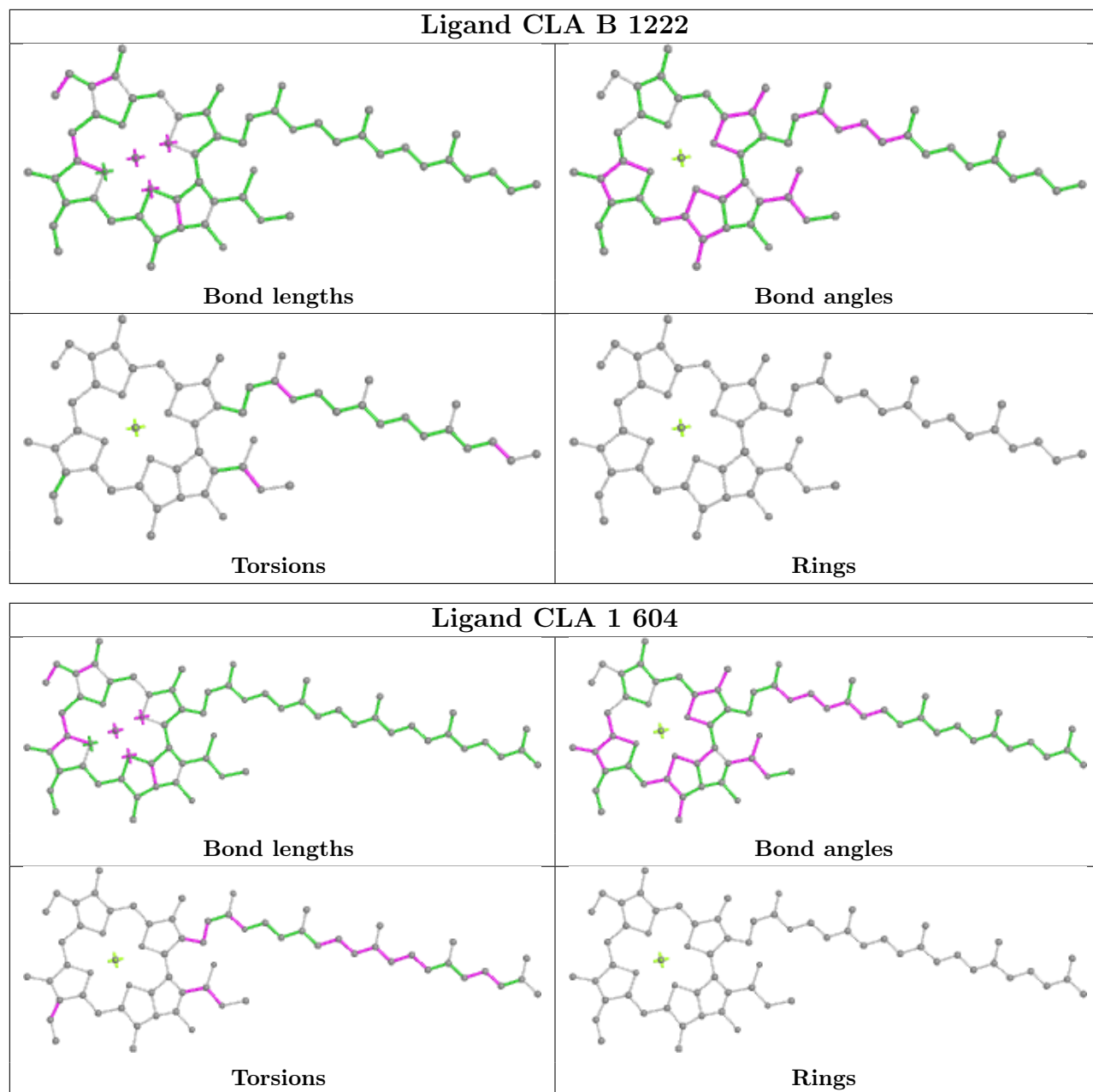
Ligand SQD 7 805

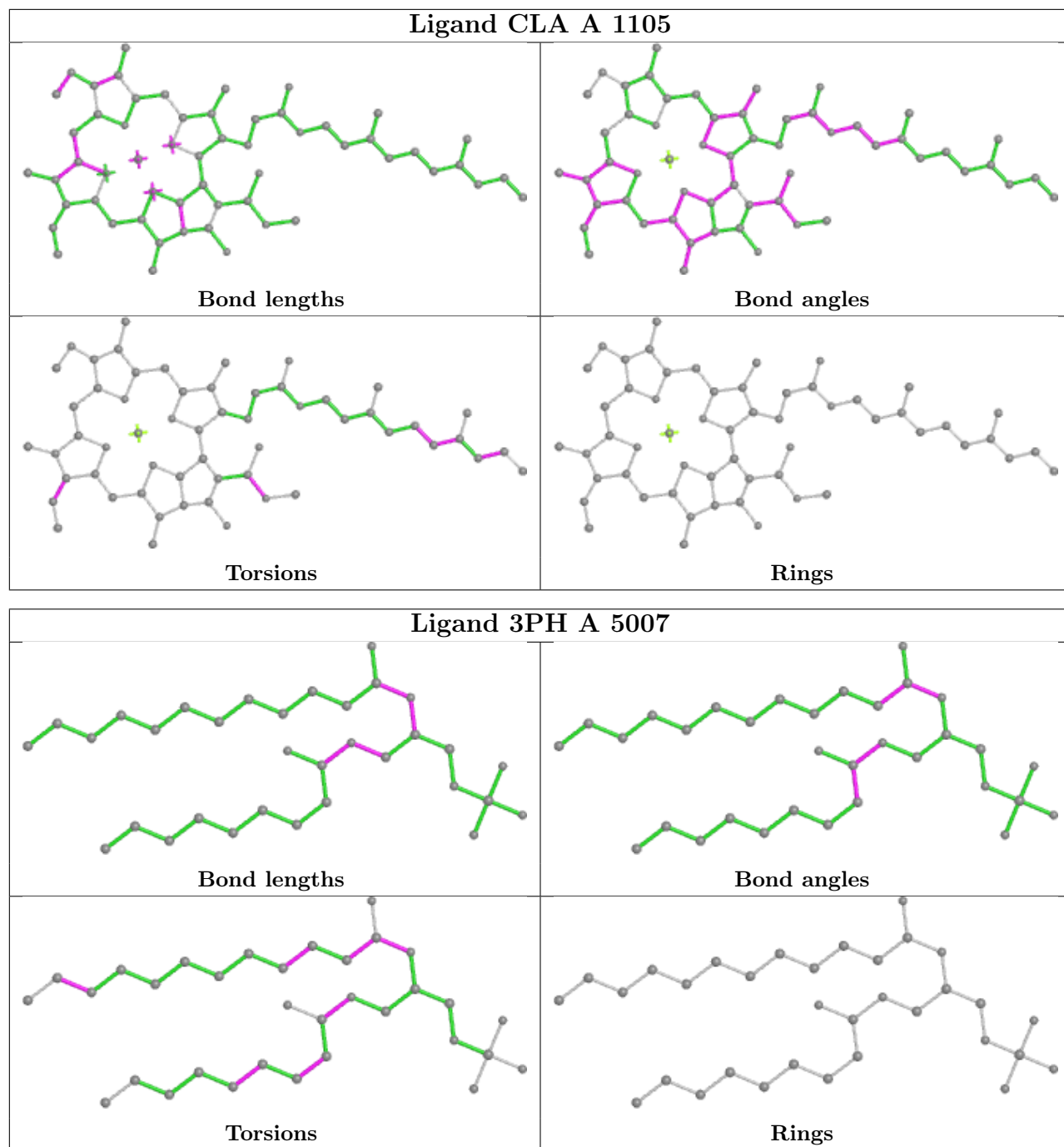




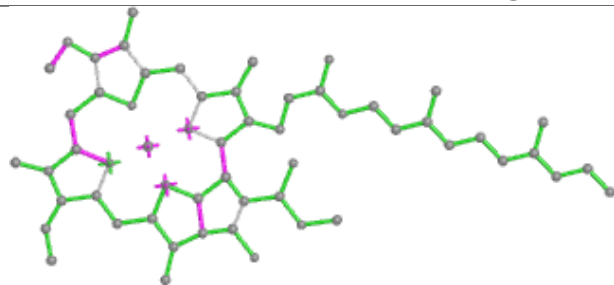




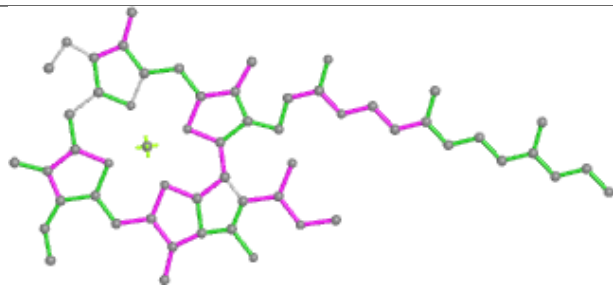




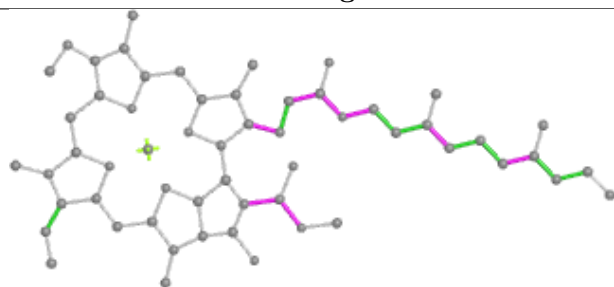
Ligand CLA A 1121



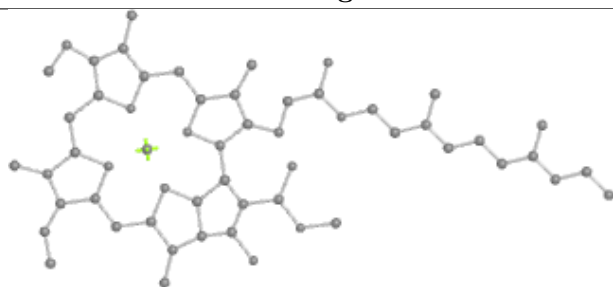
Bond lengths



Bond angles

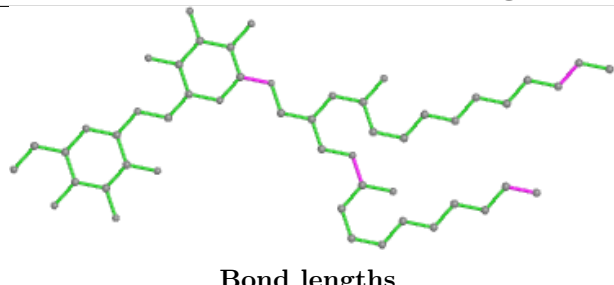


Torsions

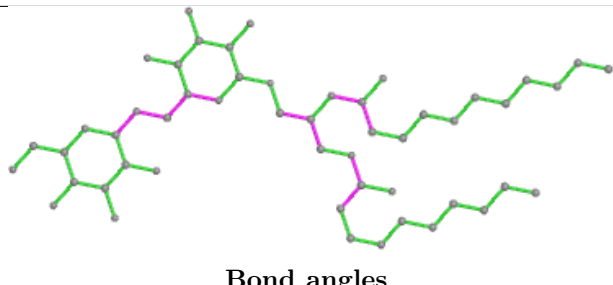


Rings

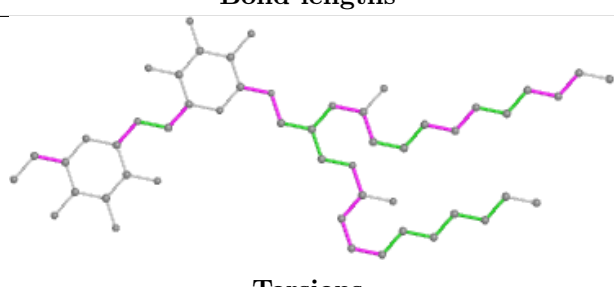
Ligand DGD A 5005



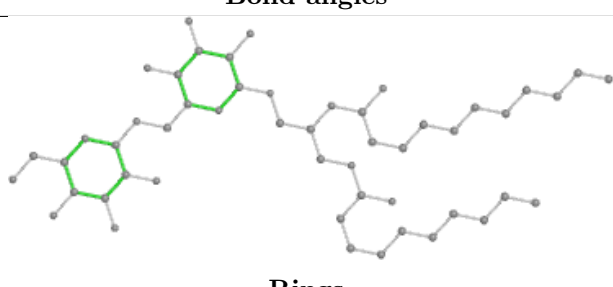
Bond lengths



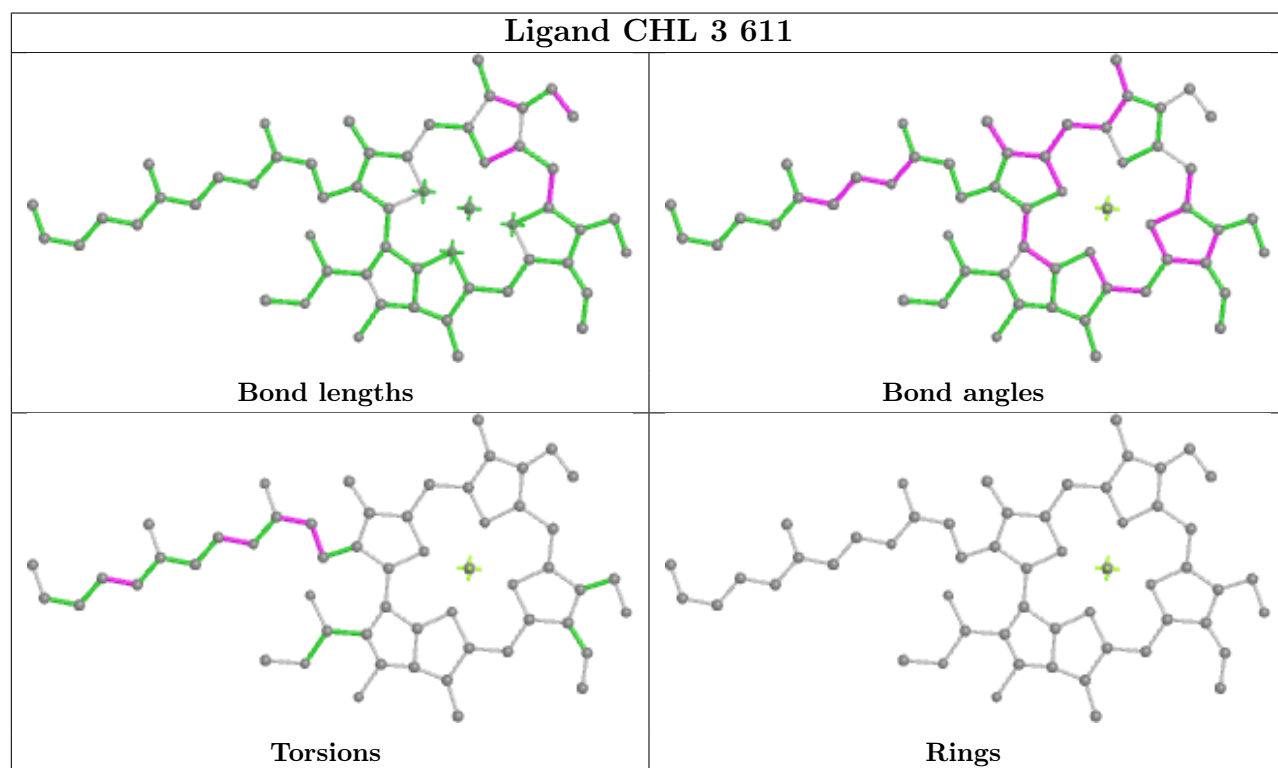
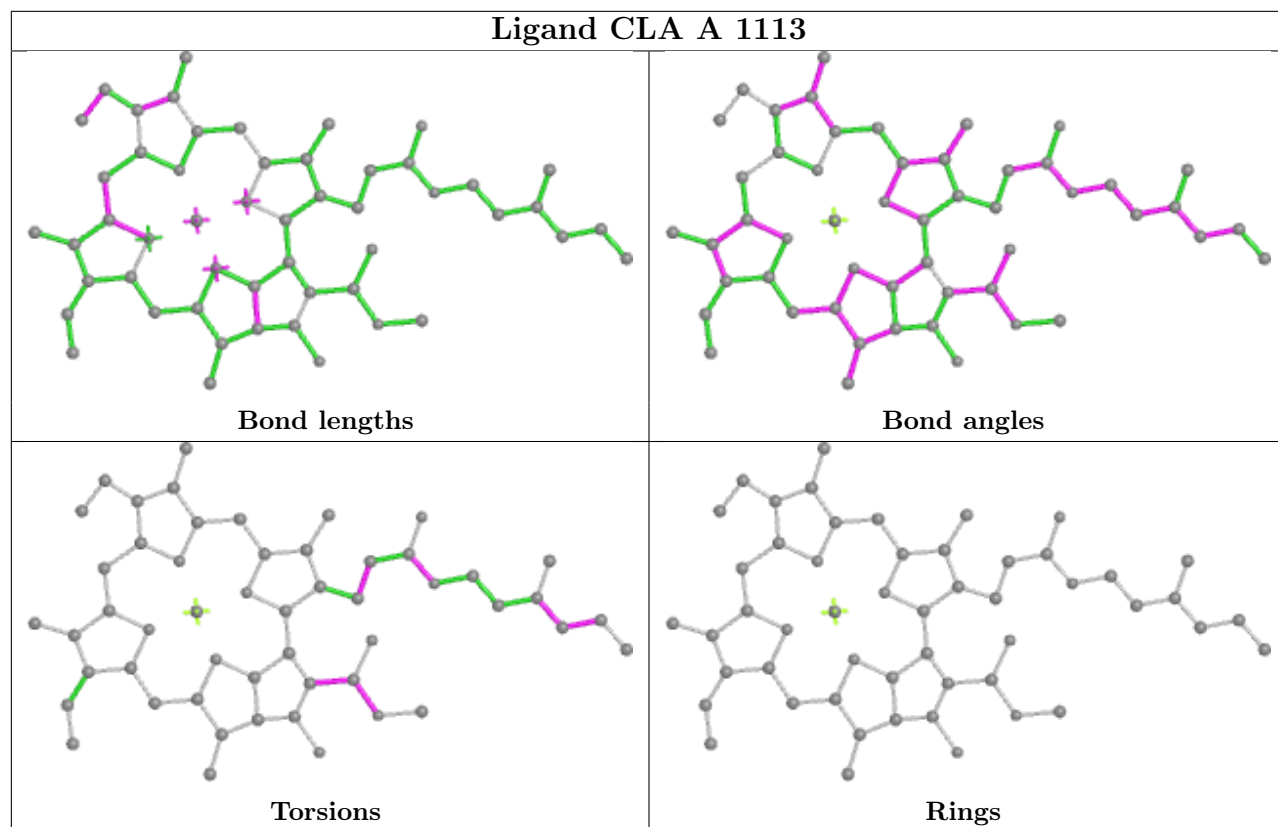
Bond angles

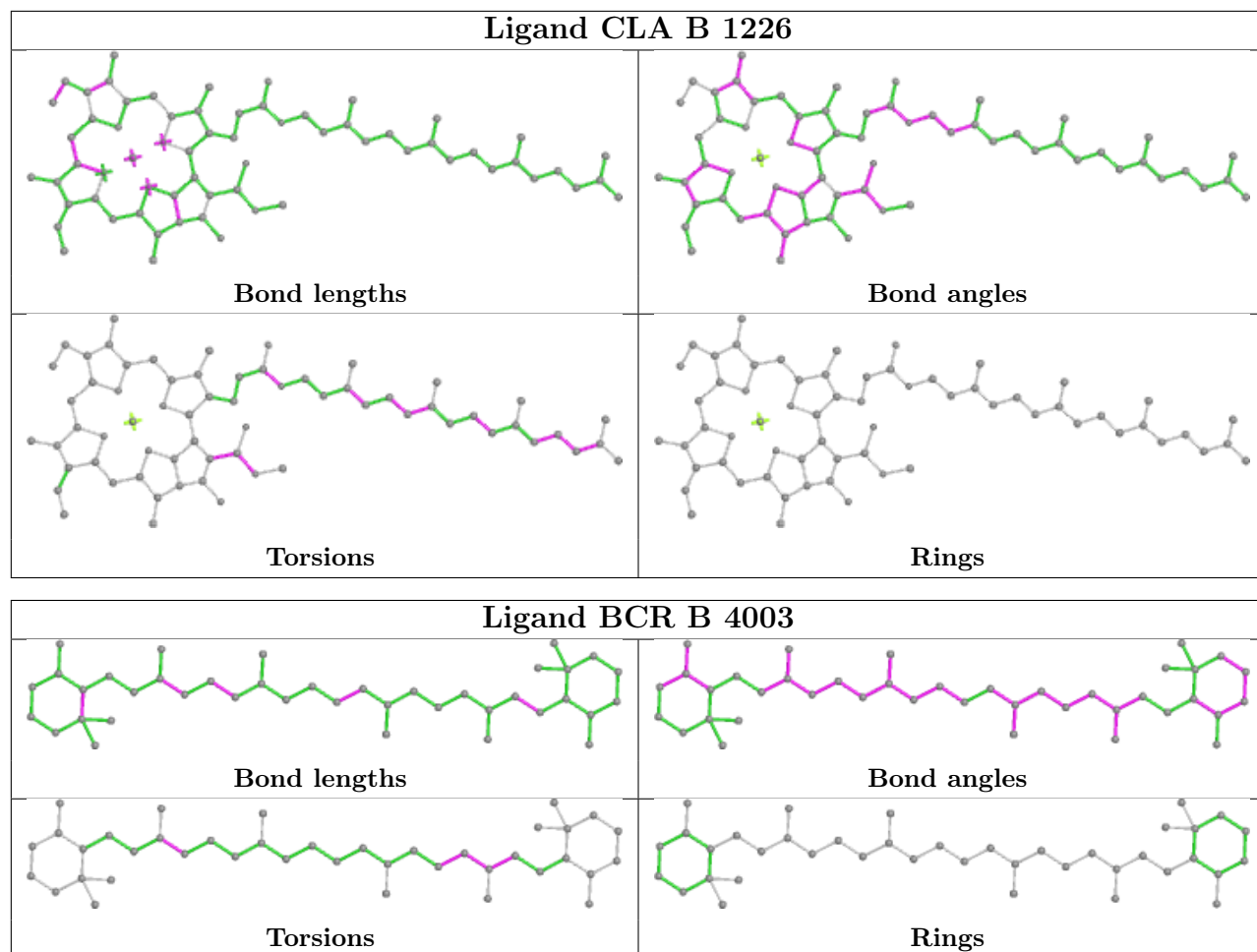


Torsions

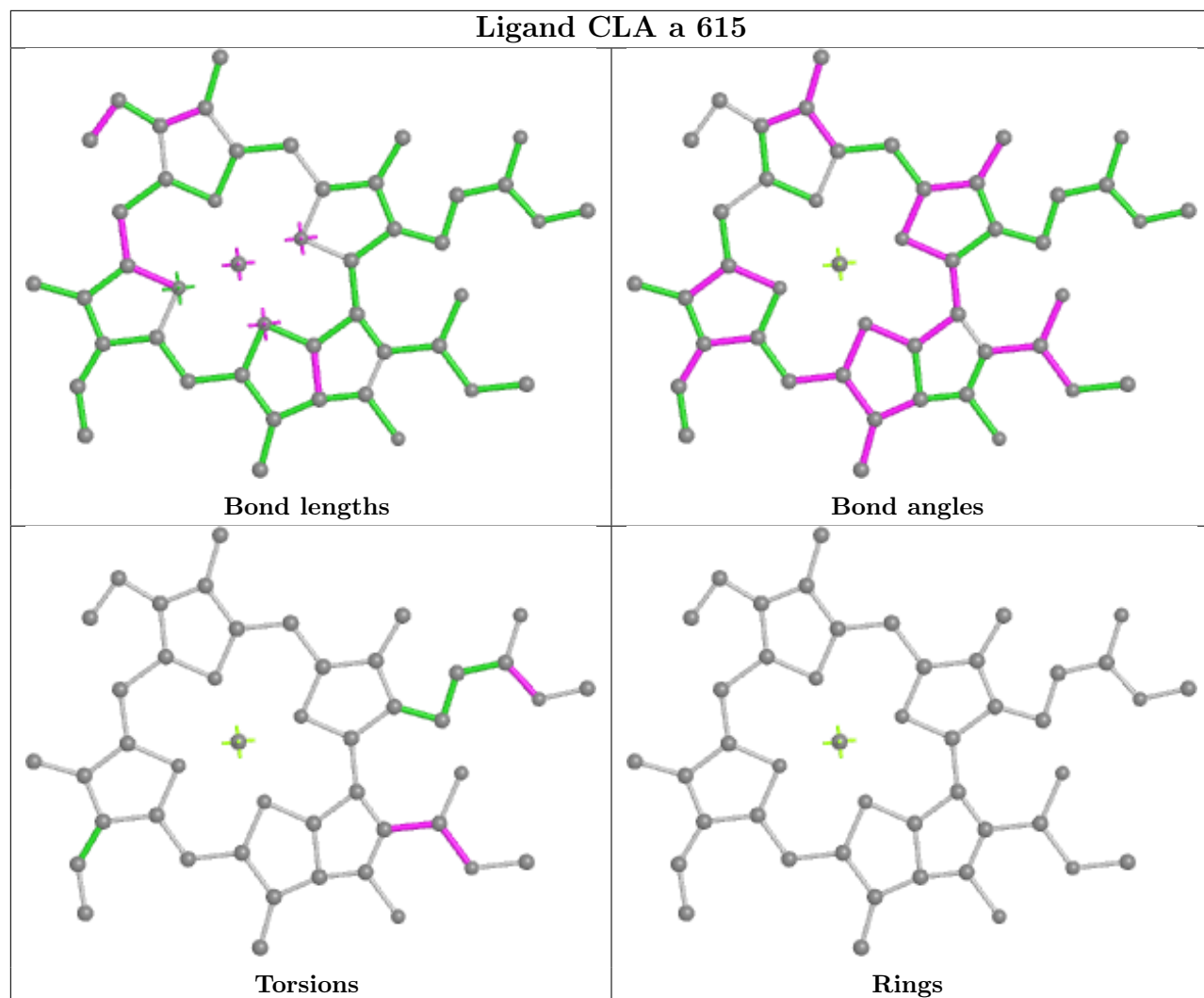


Rings

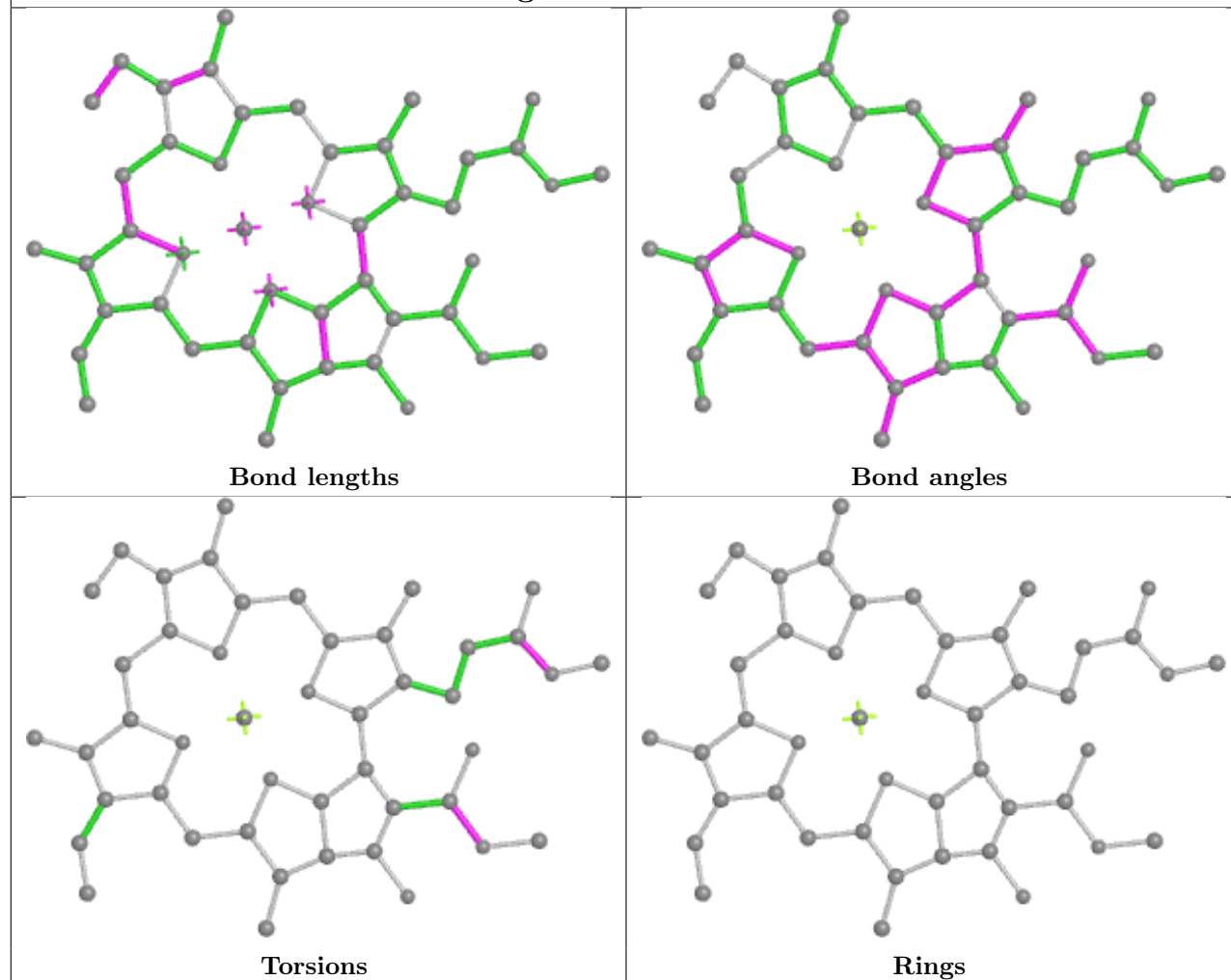




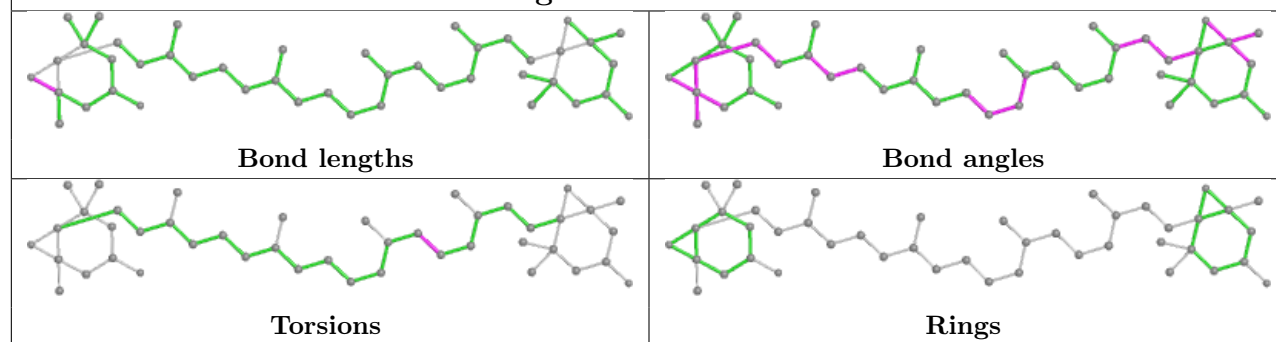
Ligand CLA a 615



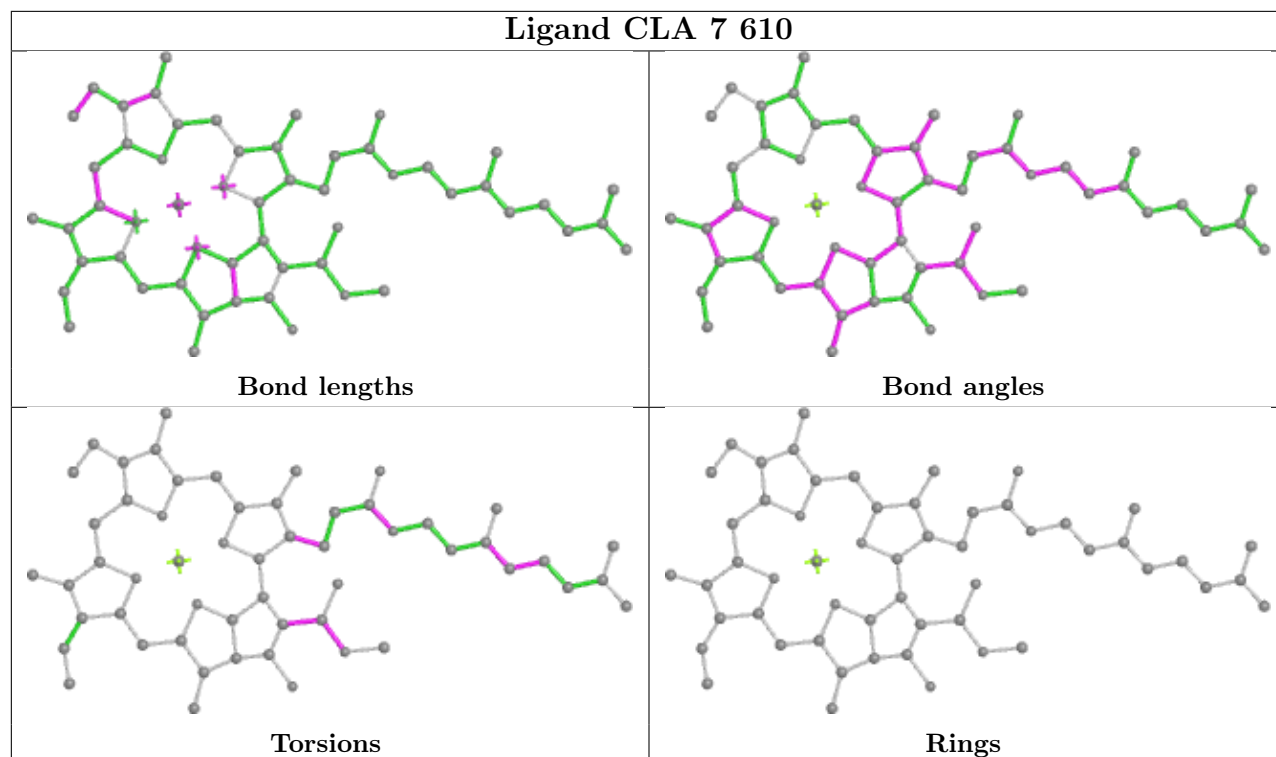
Ligand CLA 5 614



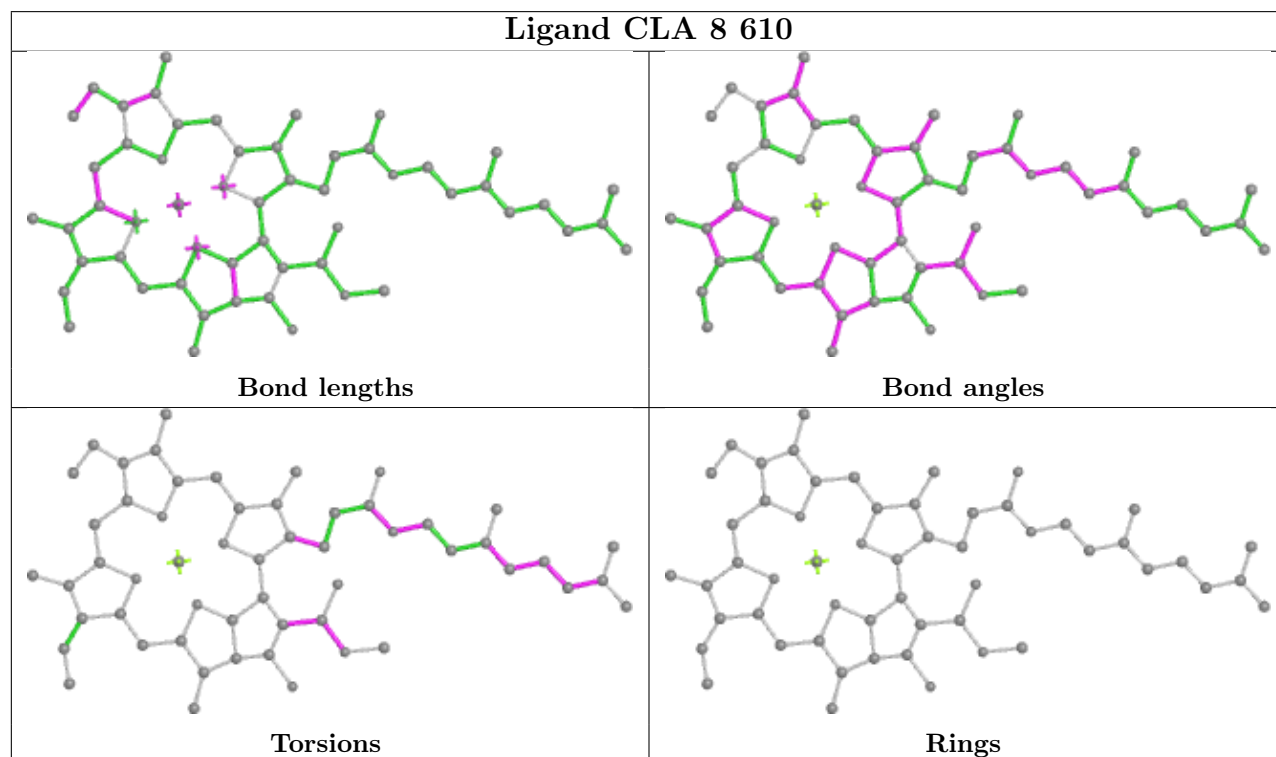
Ligand XAT 7 502

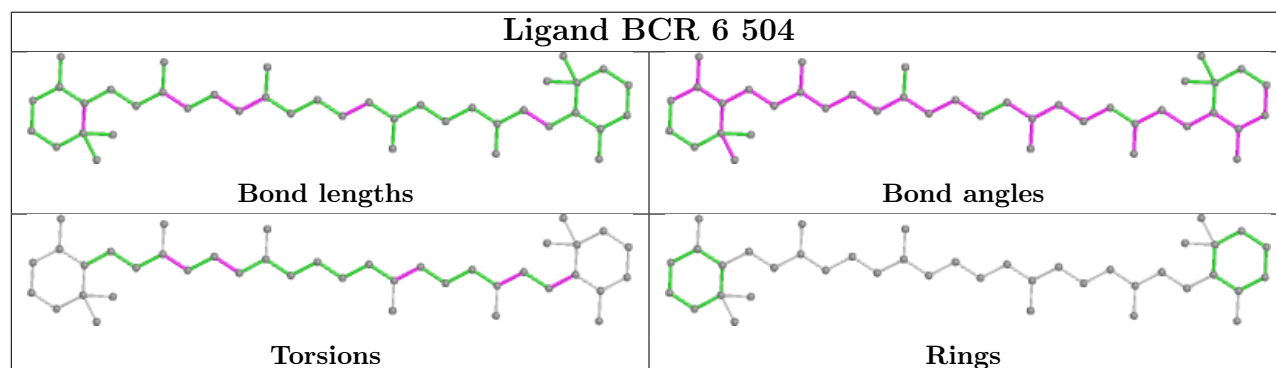
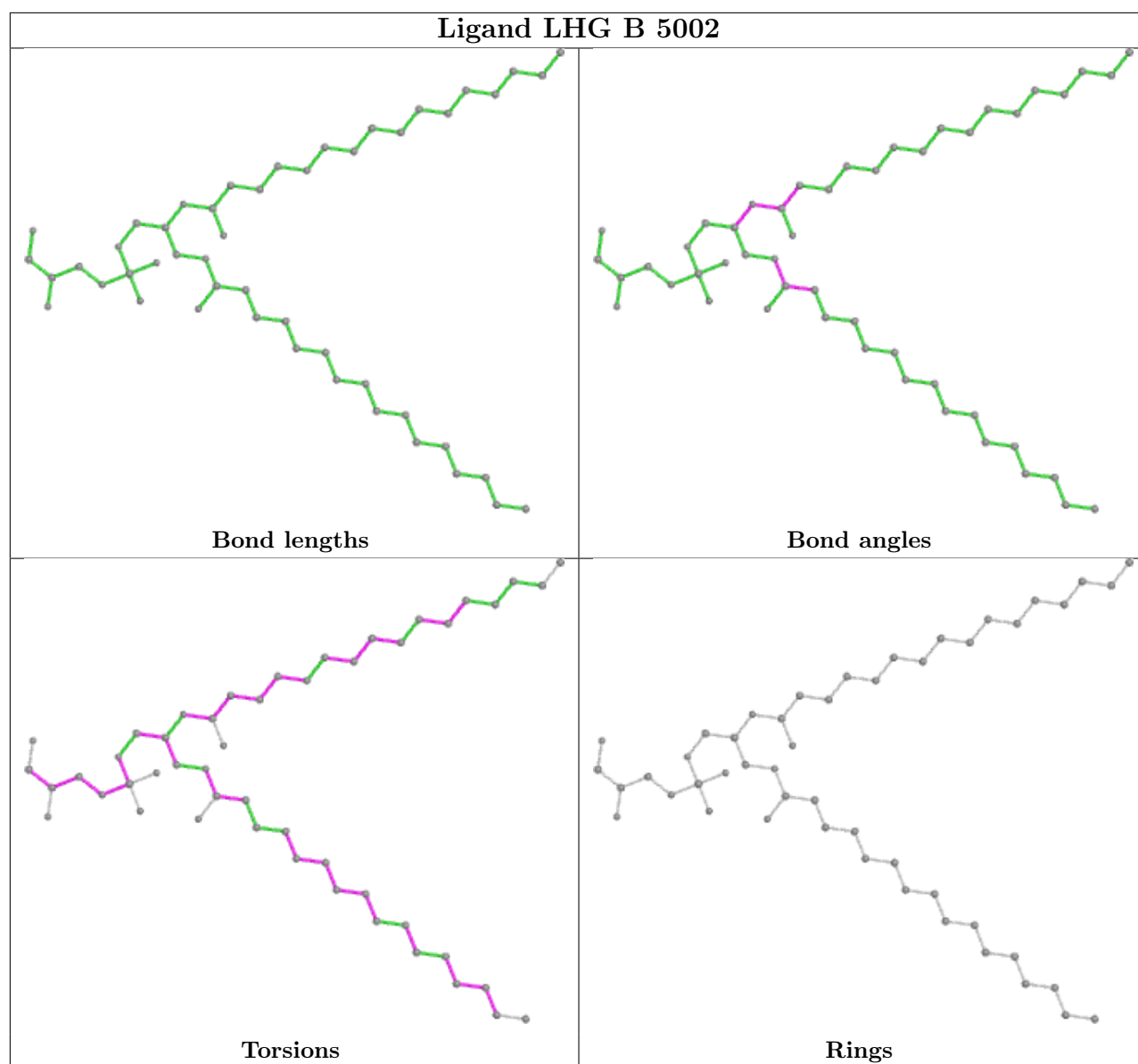


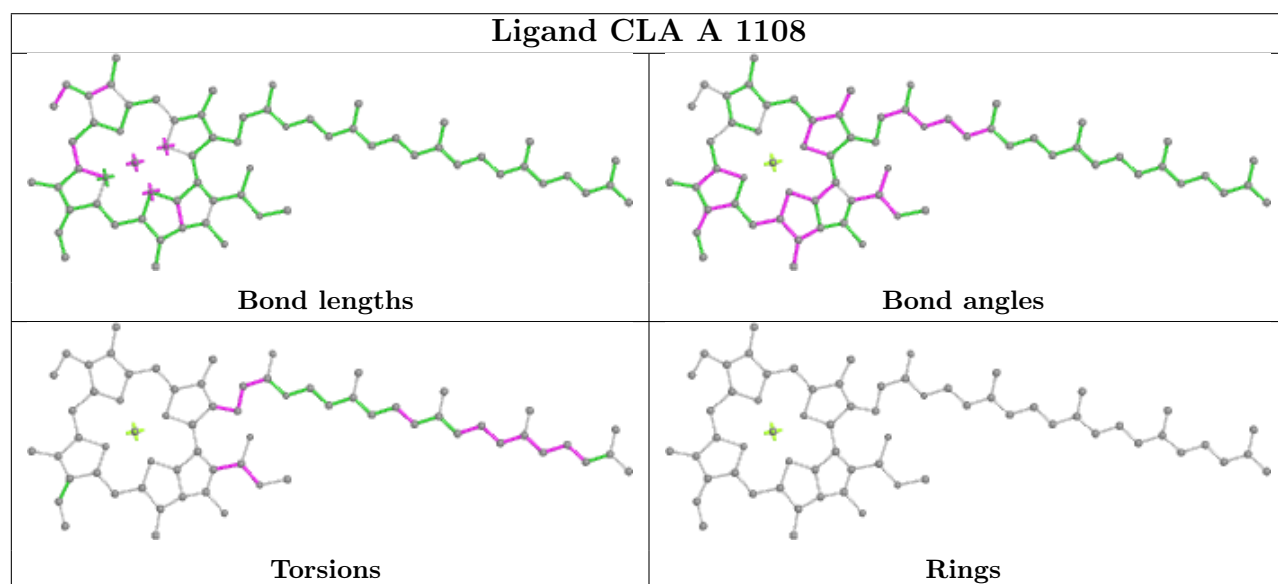
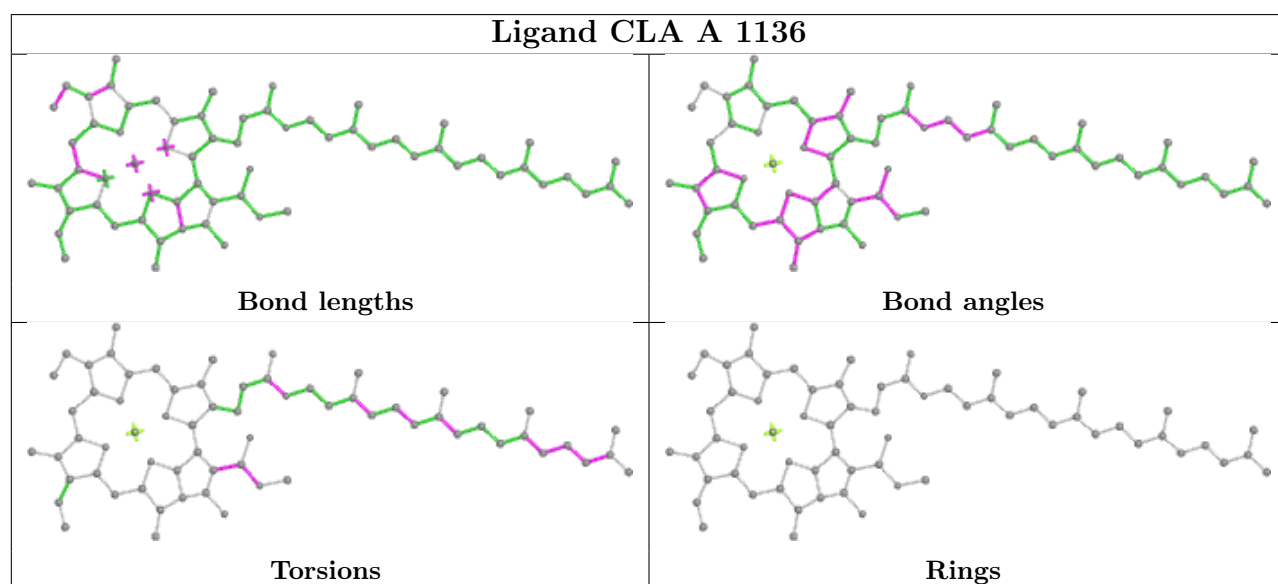
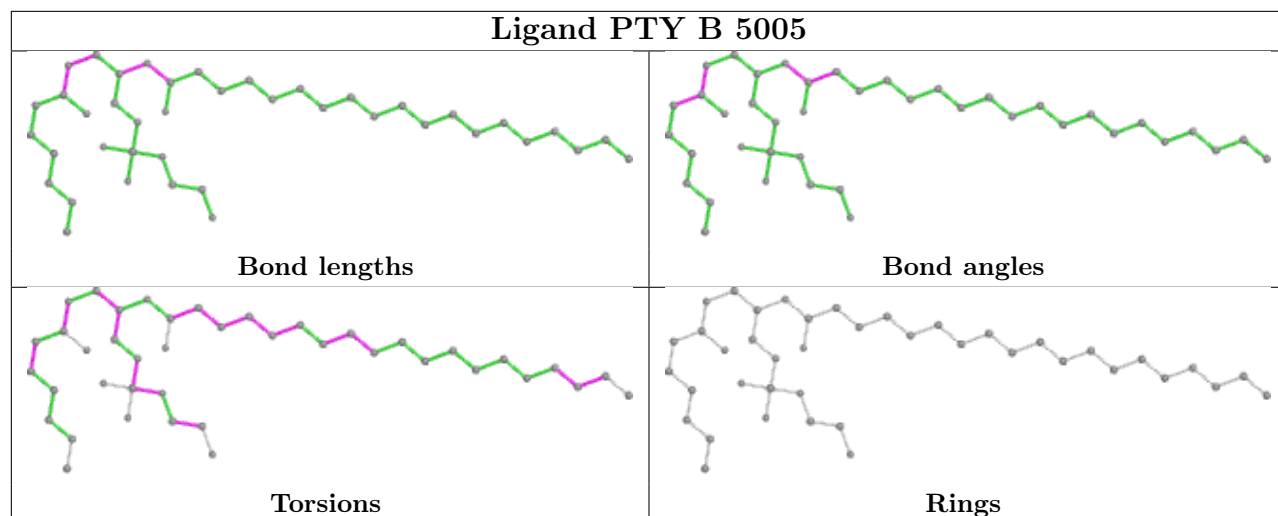
Ligand CLA 7 610



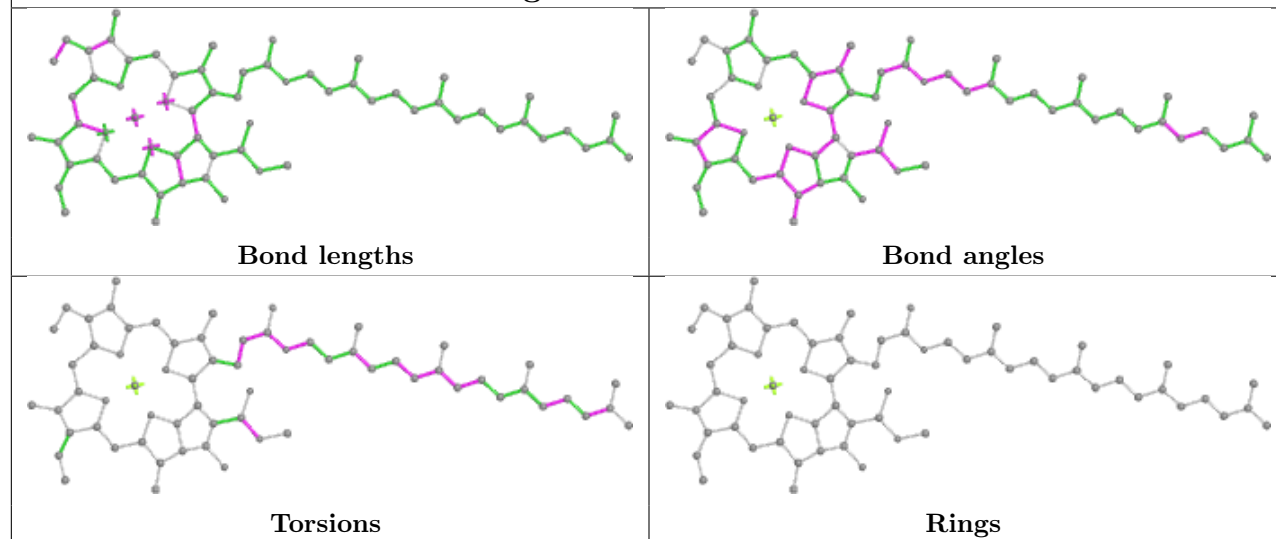
Ligand CLA 8 610



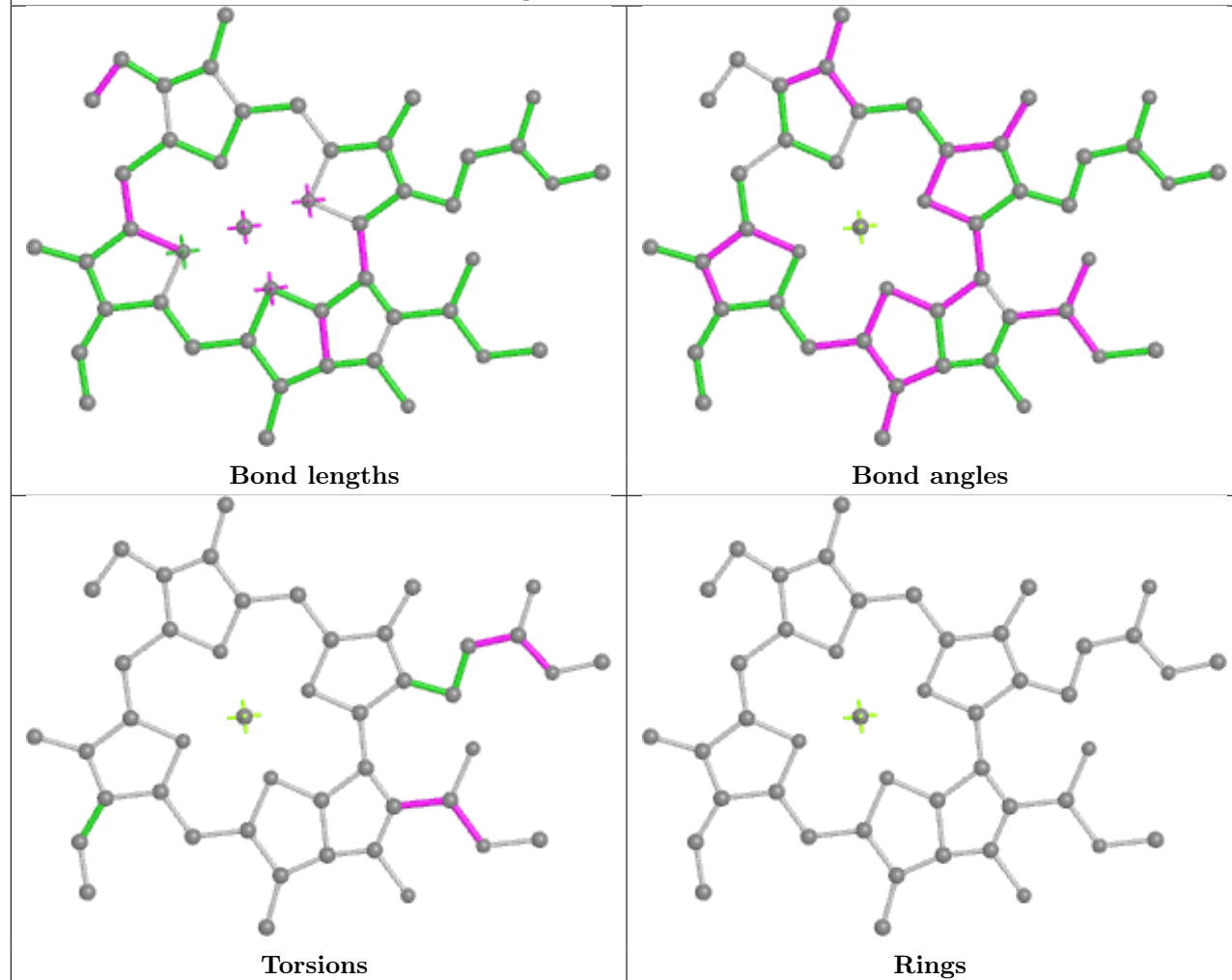




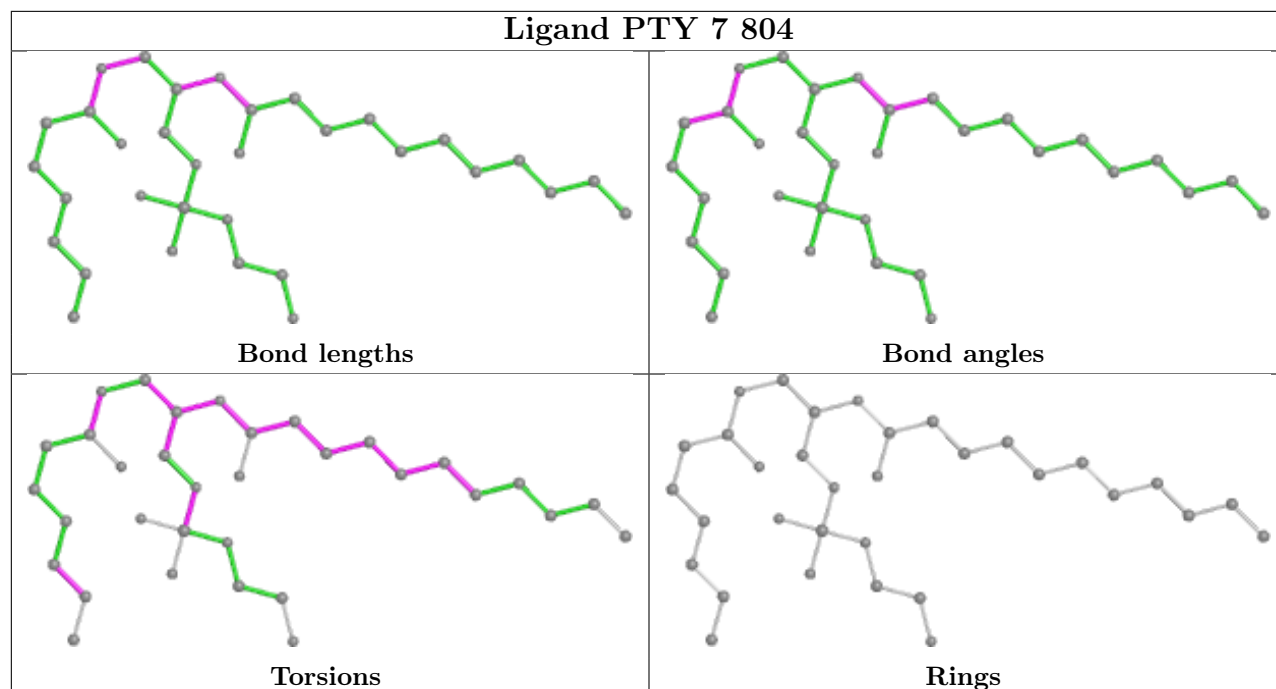
Ligand CLA B 1209



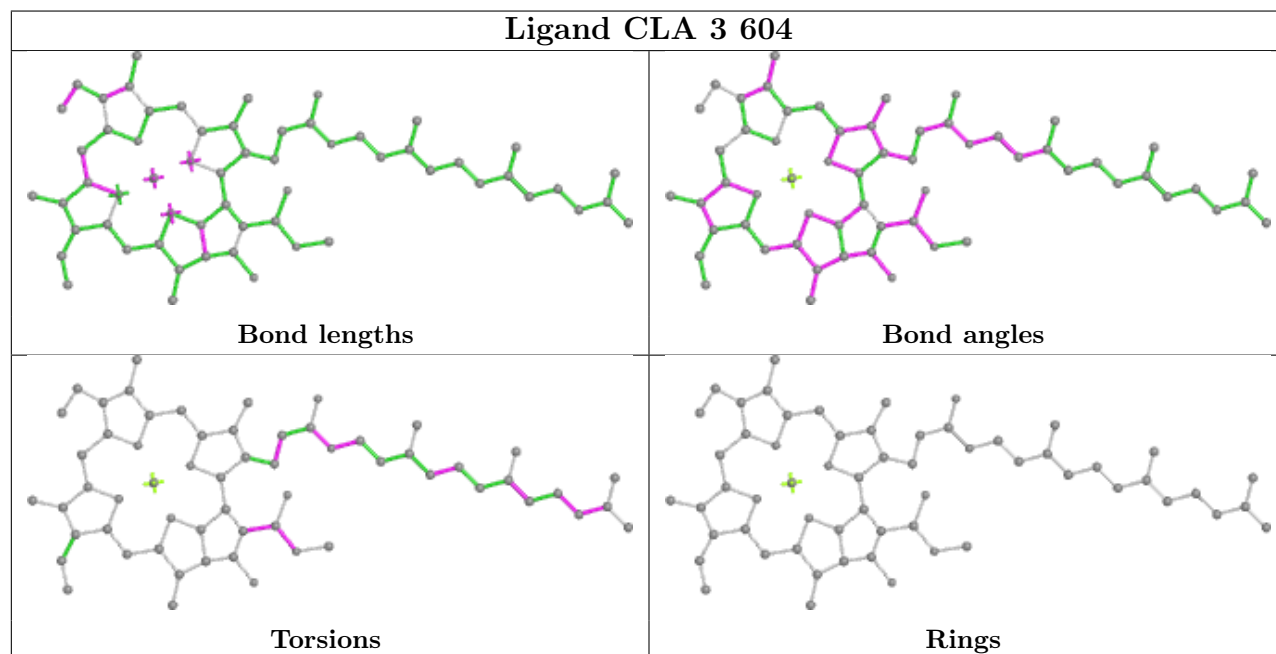
Ligand CLA 3 602



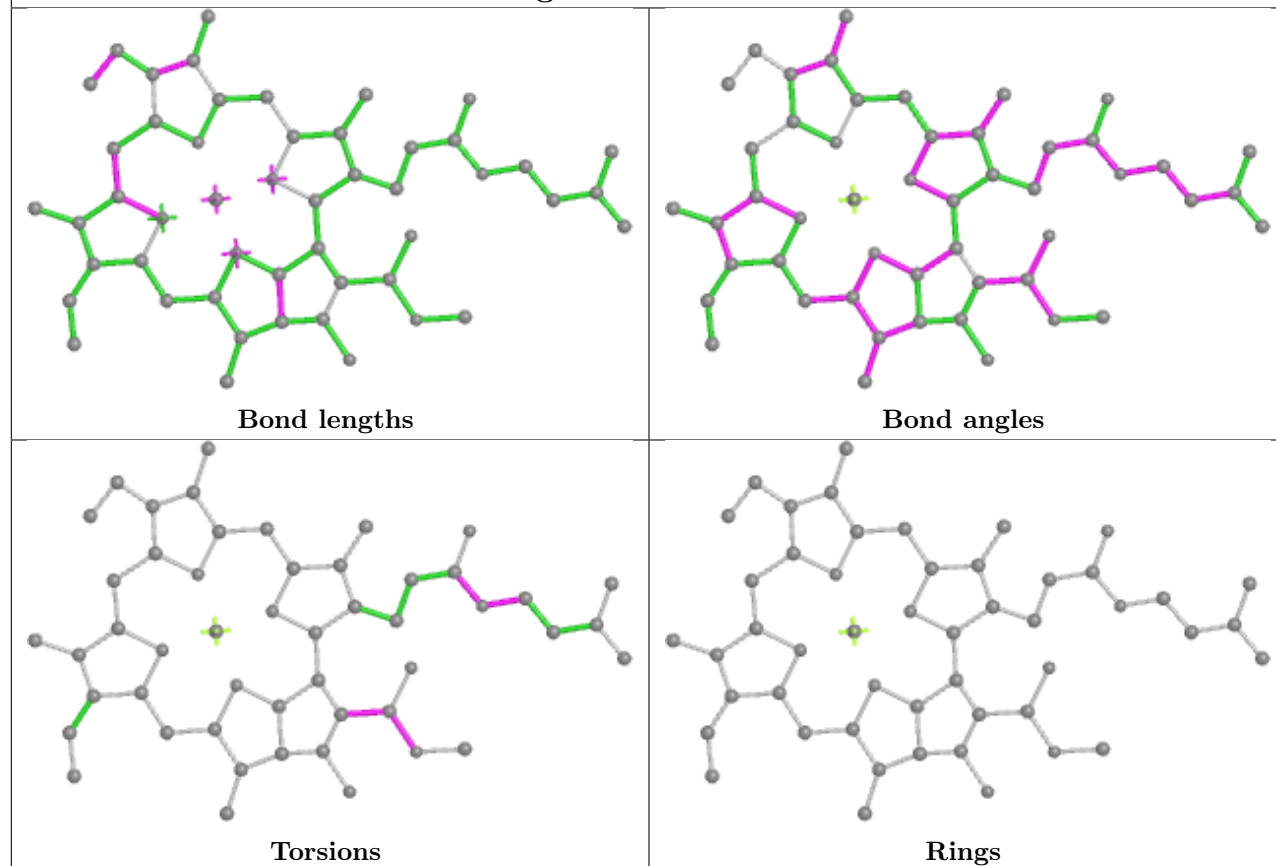
Ligand PTY 7 804



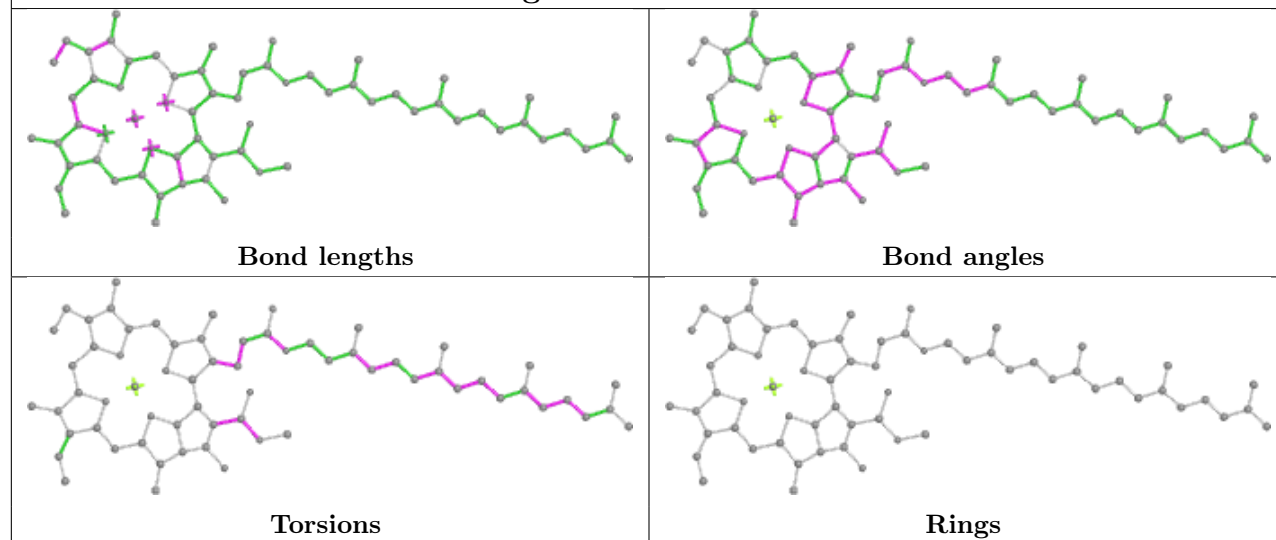
Ligand CLA 3 604

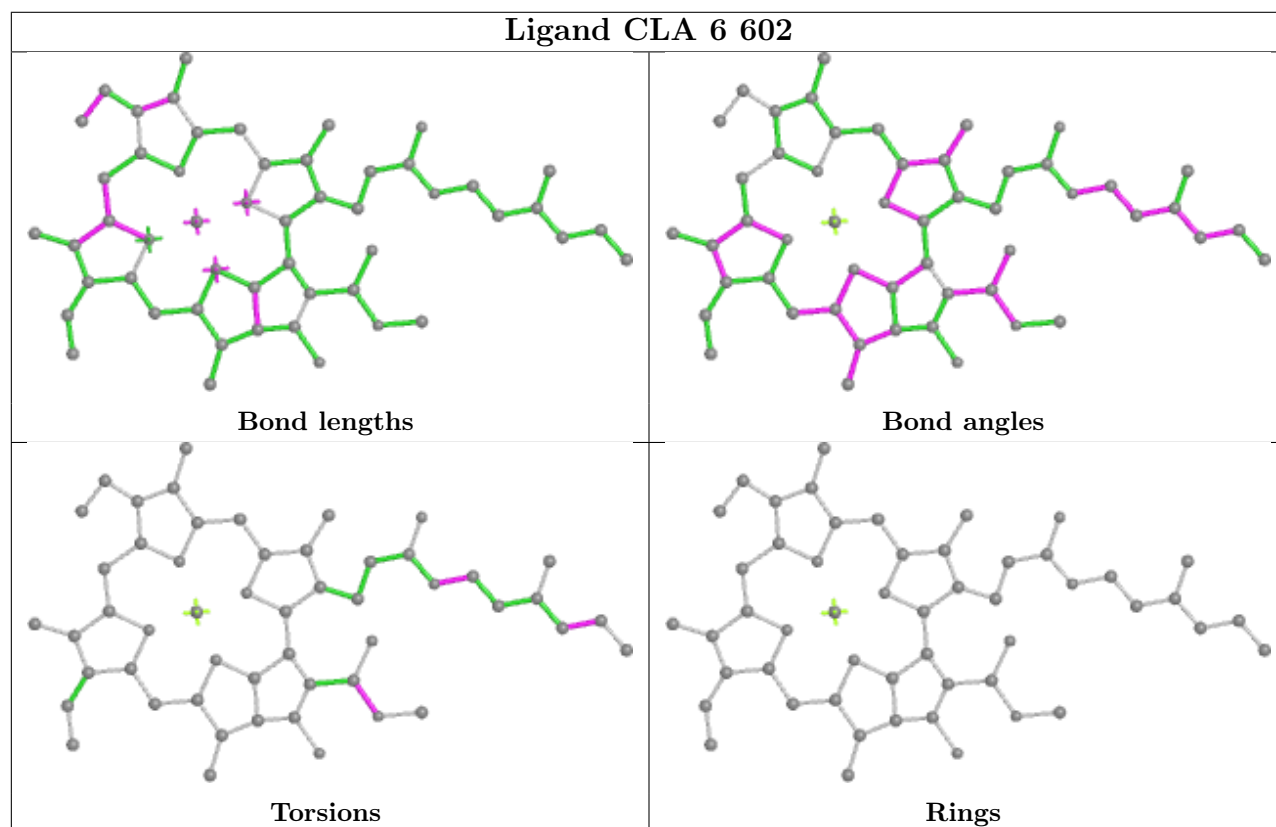
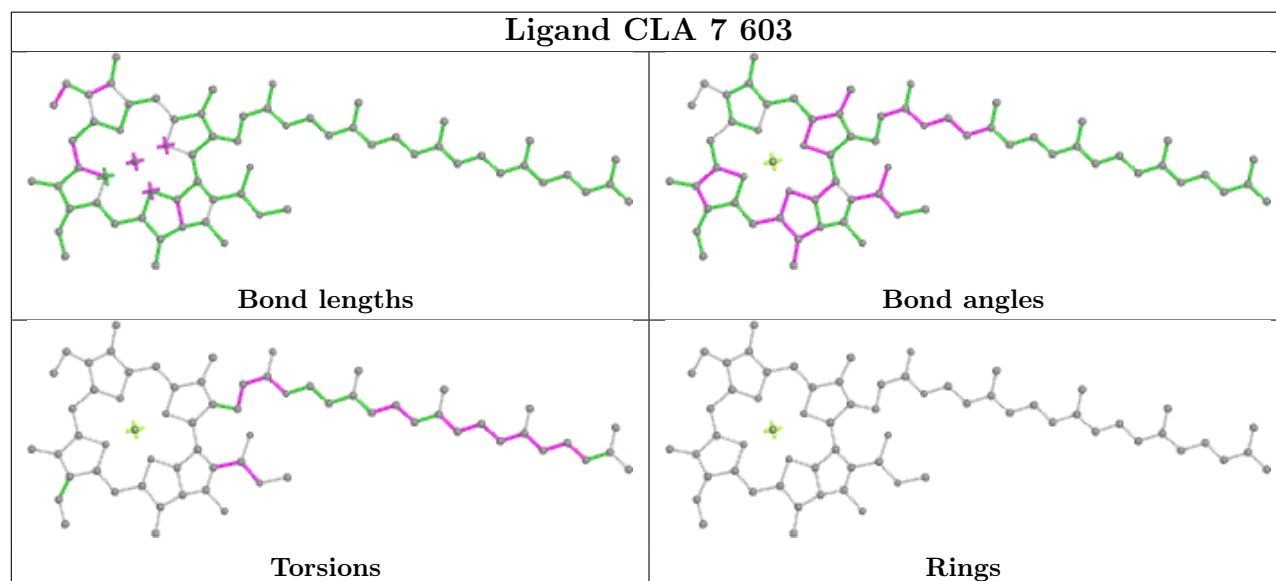
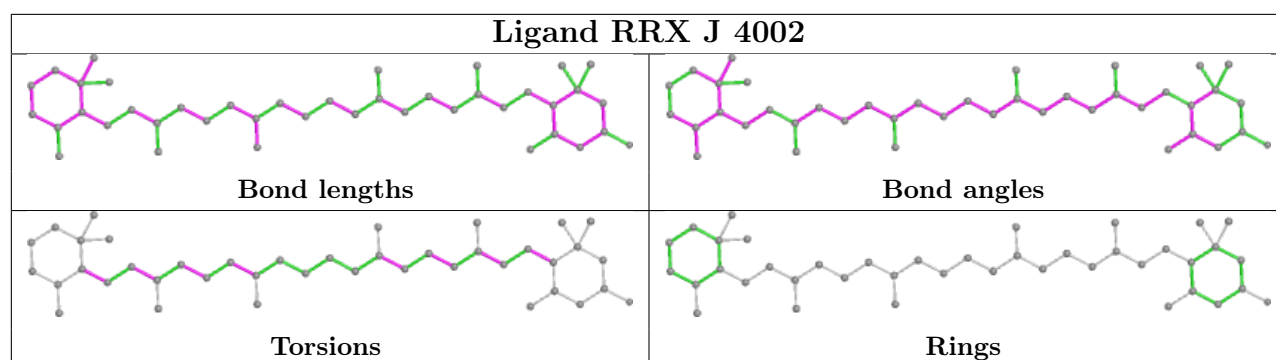


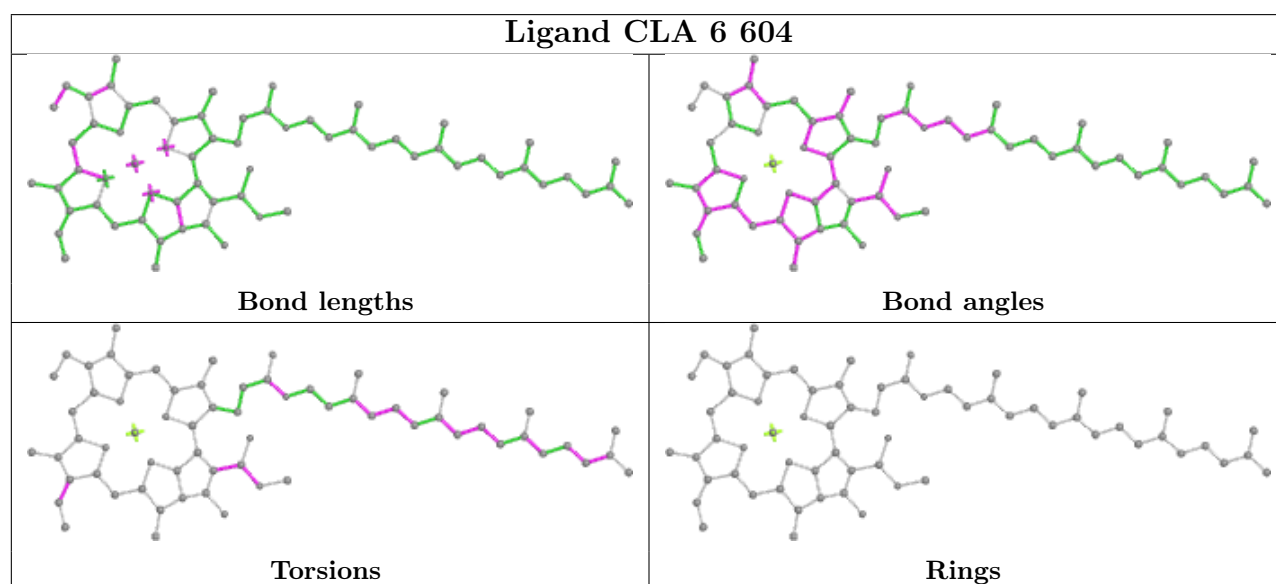
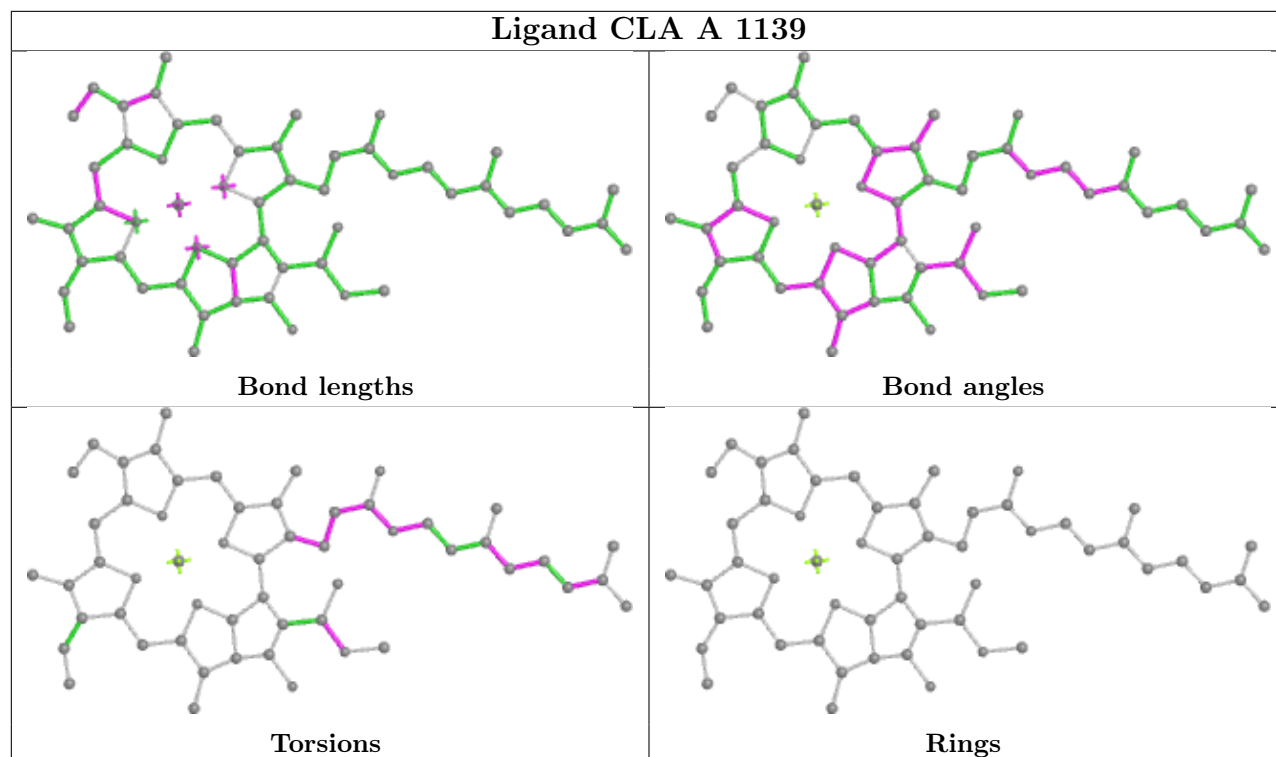
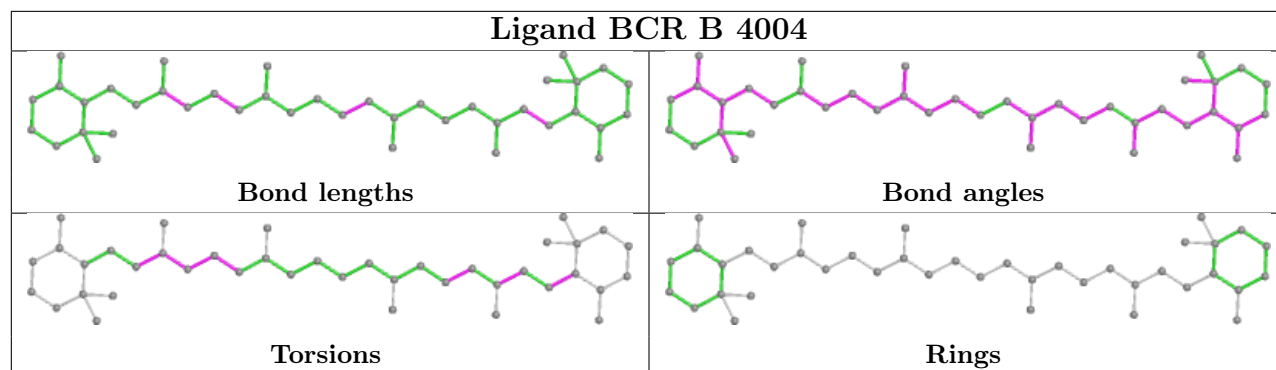
Ligand CLA 8 611



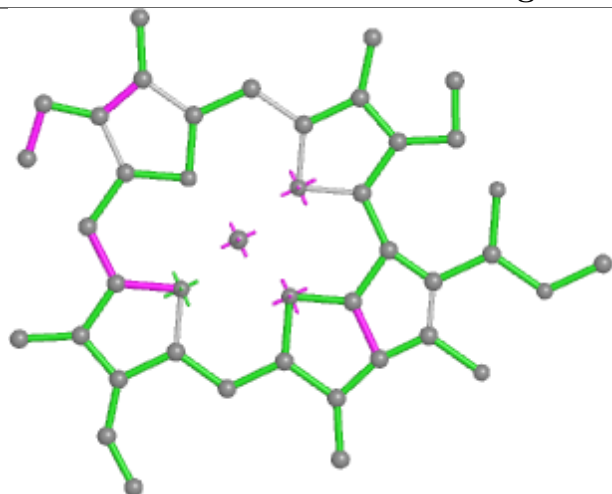
Ligand CLA A 1135



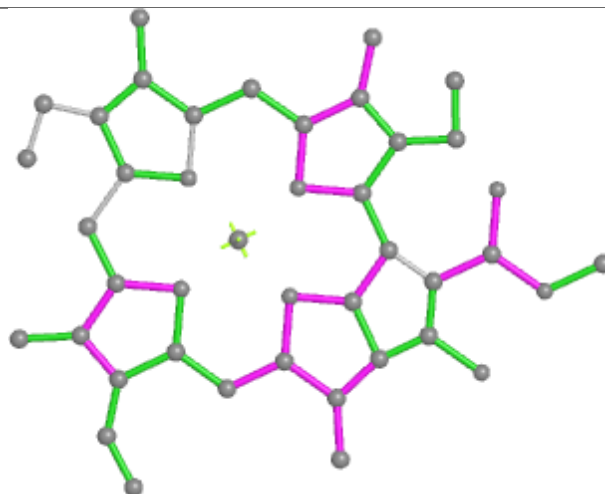




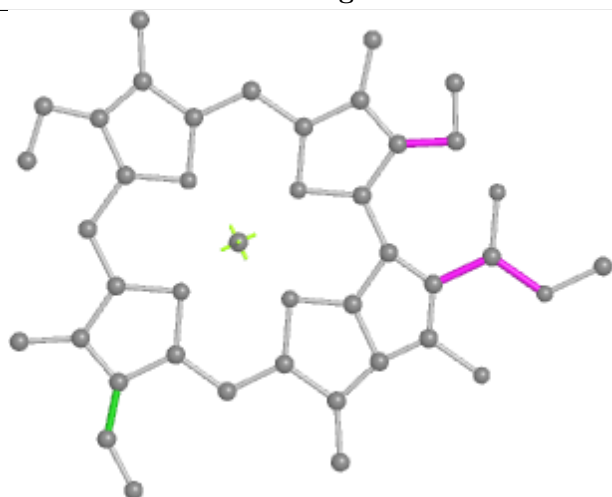
Ligand CLA 7 608



Bond lengths



Bond angles

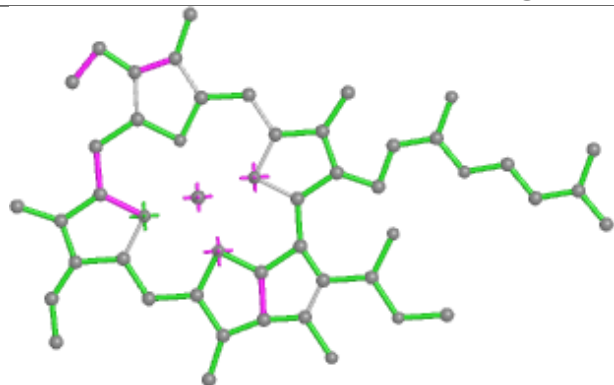


Torsions

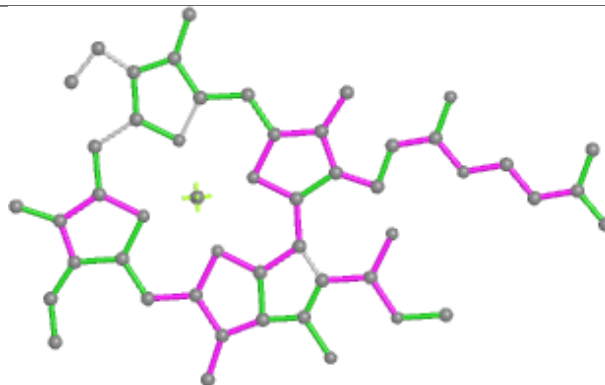


Rings

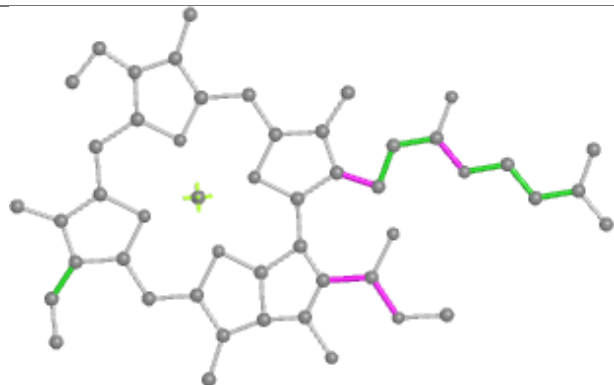
Ligand CLA 5 606



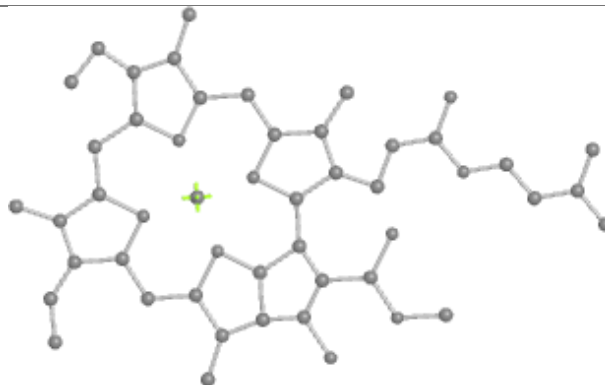
Bond lengths



Bond angles

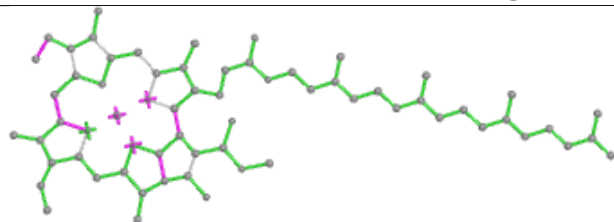


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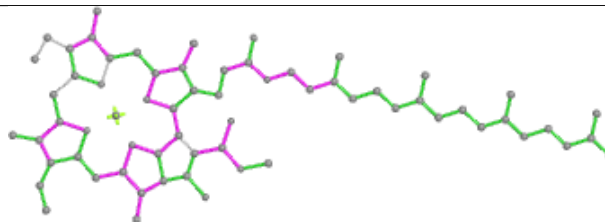


Rings

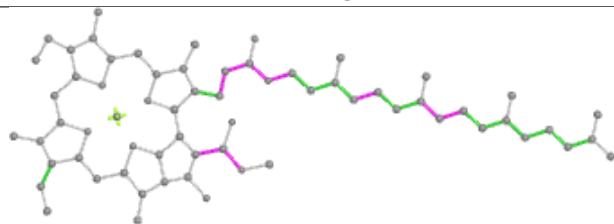
Ligand CLA A 1123



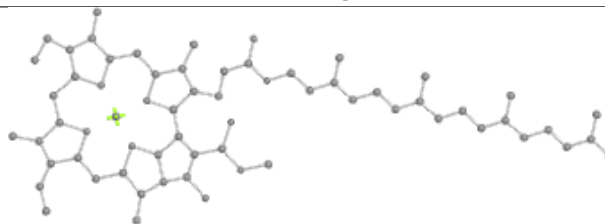
Bond lengths



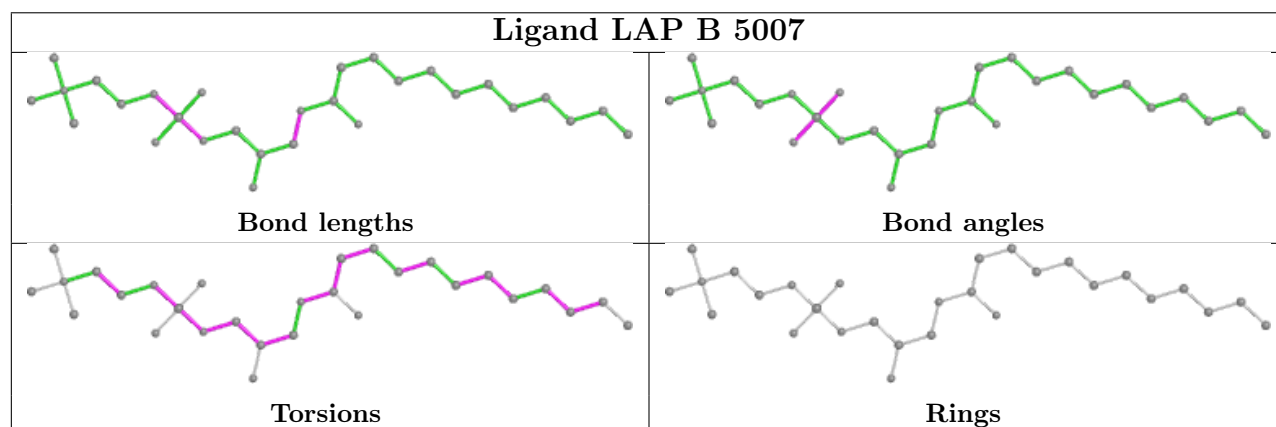
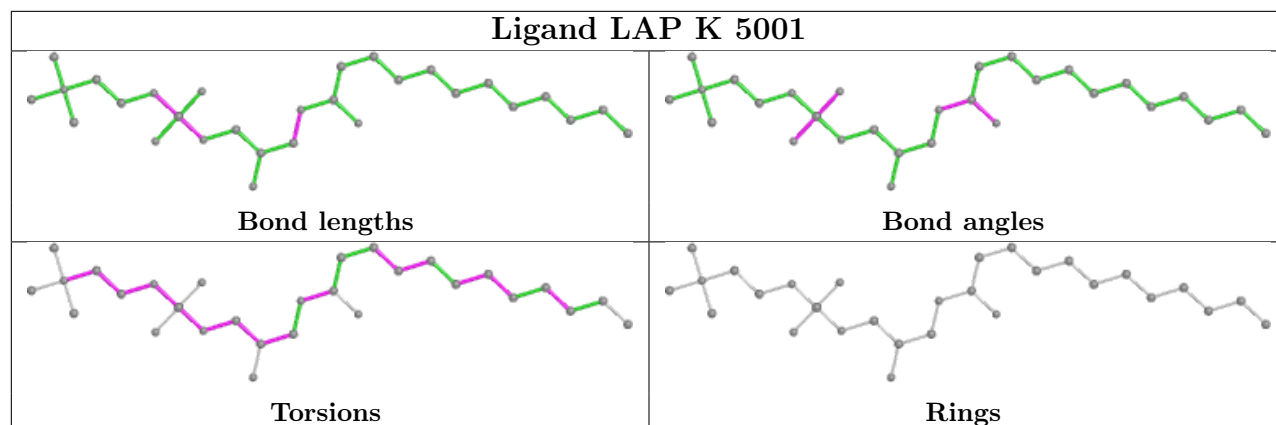
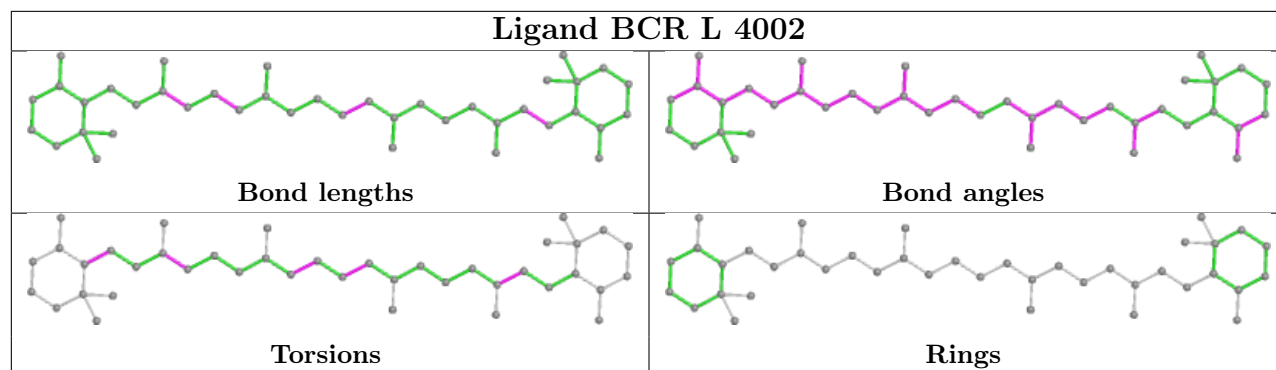
Bond angles

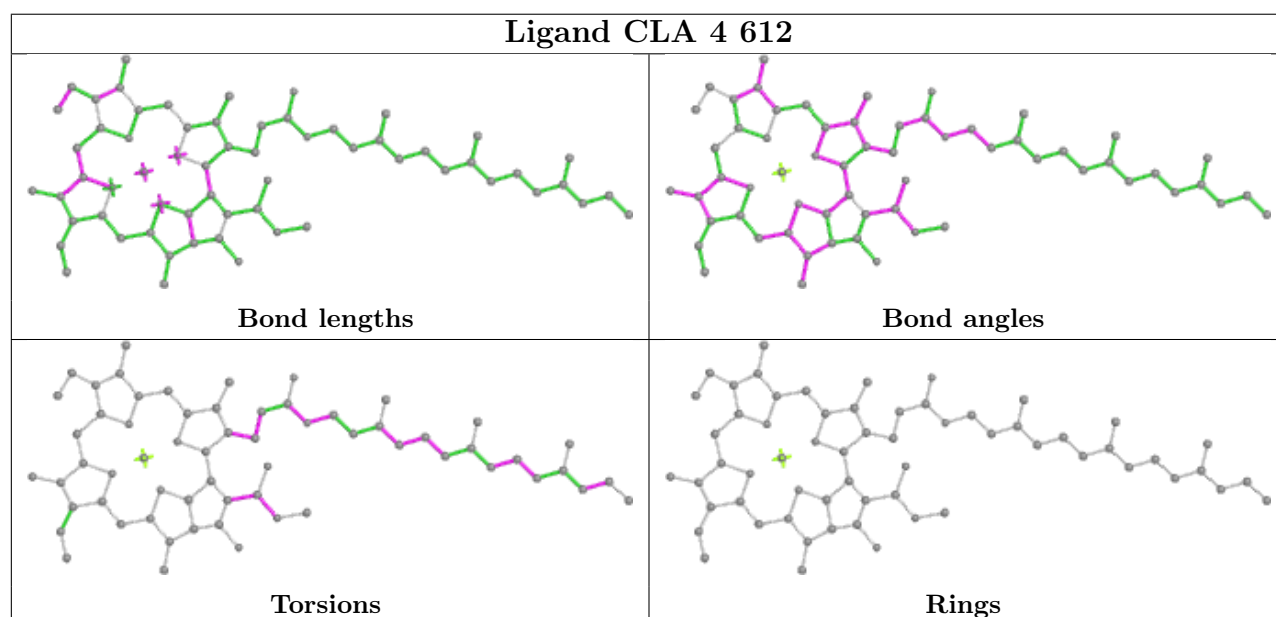
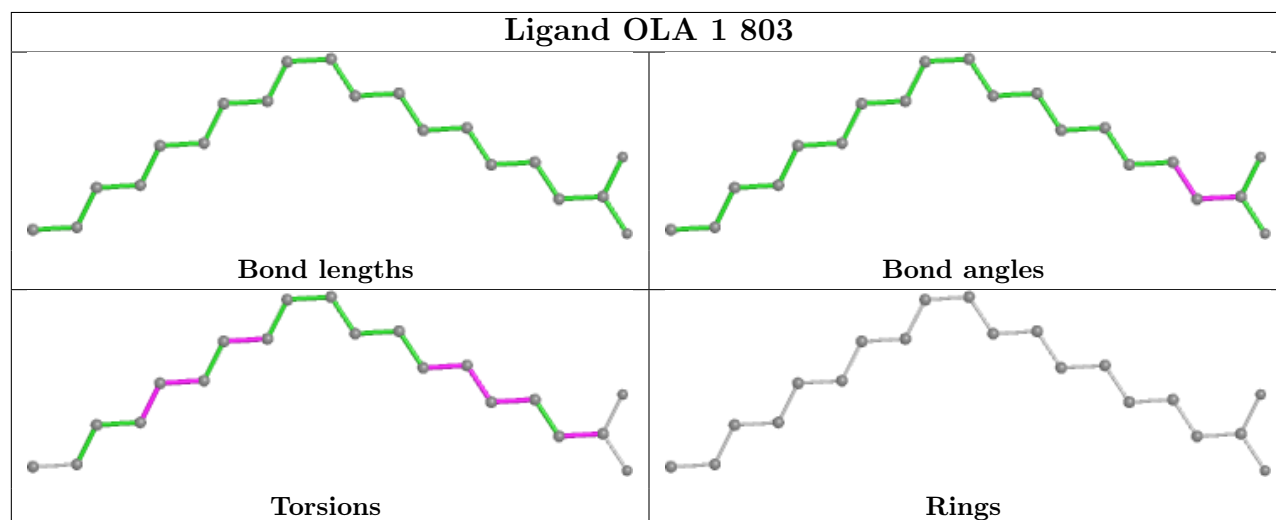
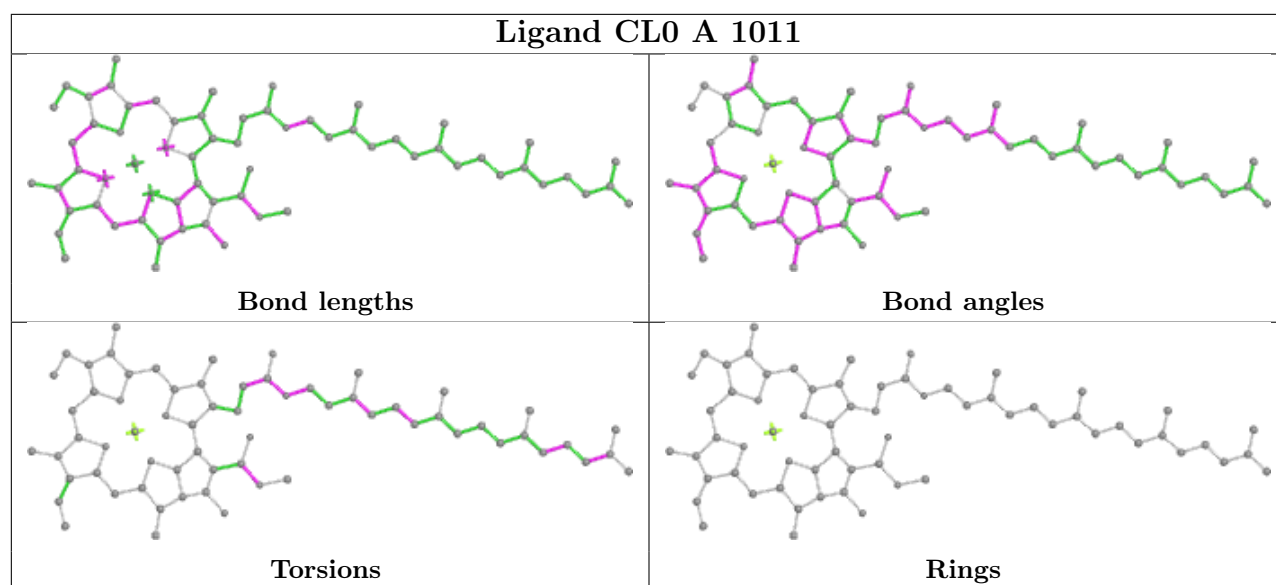


Torsions

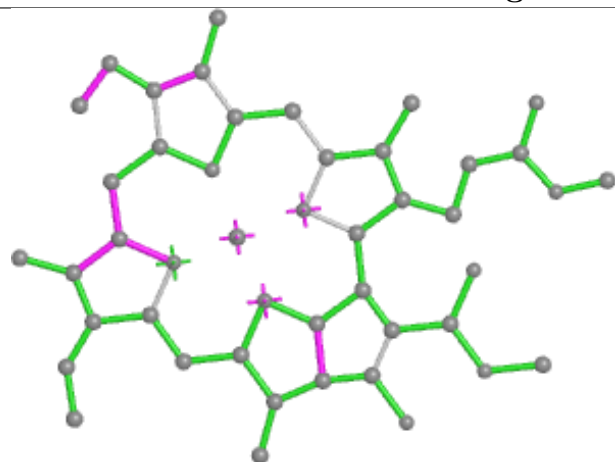


Rings

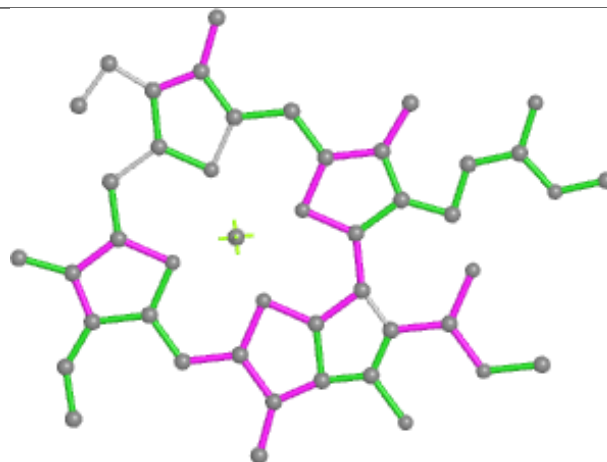




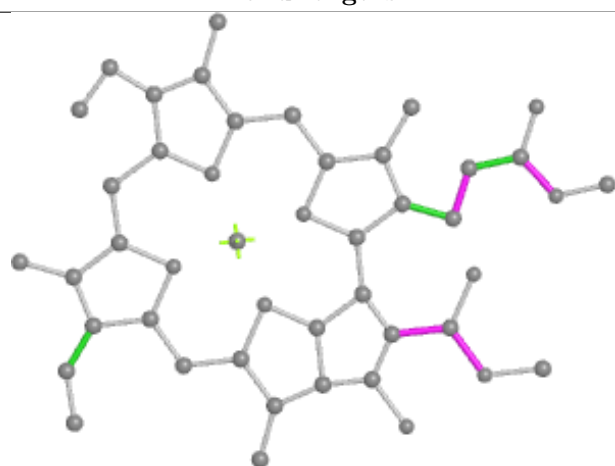
Ligand CLA G 1602



Bond lengths



Bond angles

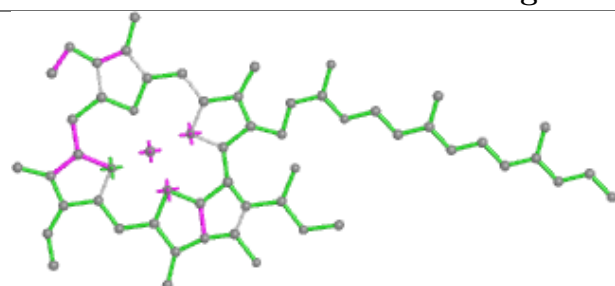


Torsions

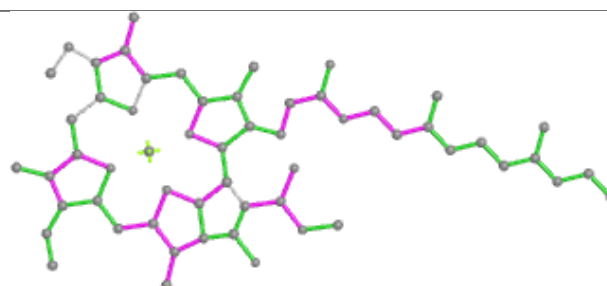


Rings

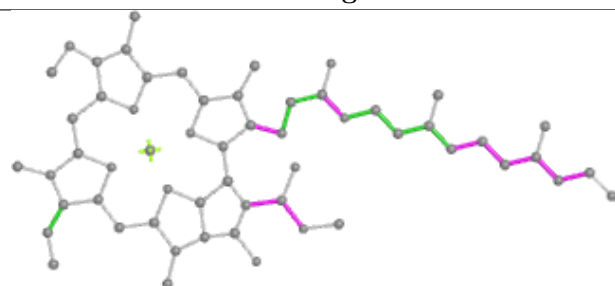
Ligand CLA 1 606



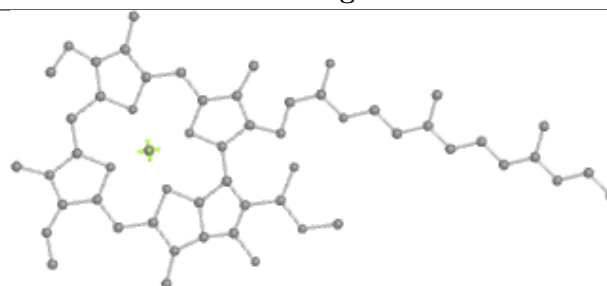
Bond lengths



Bond angles

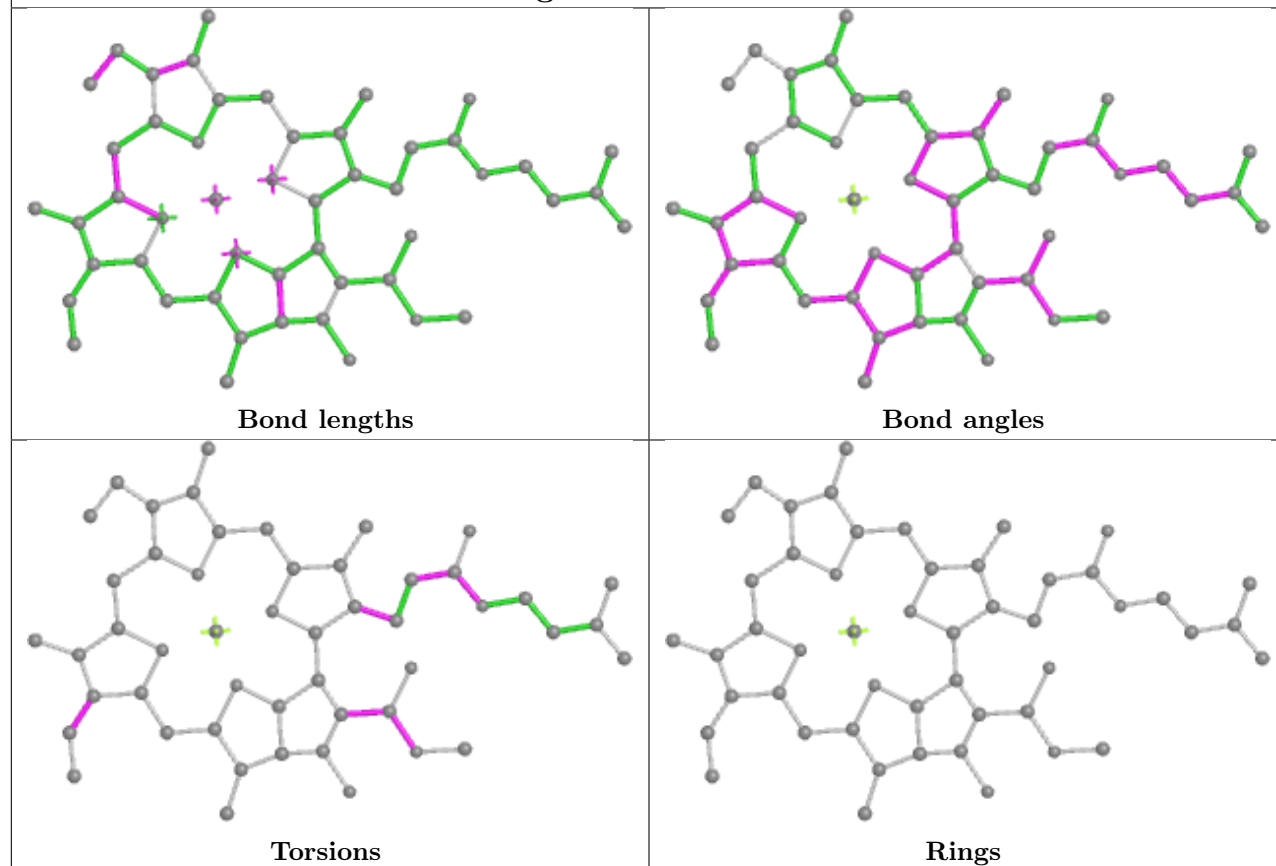


Torsions

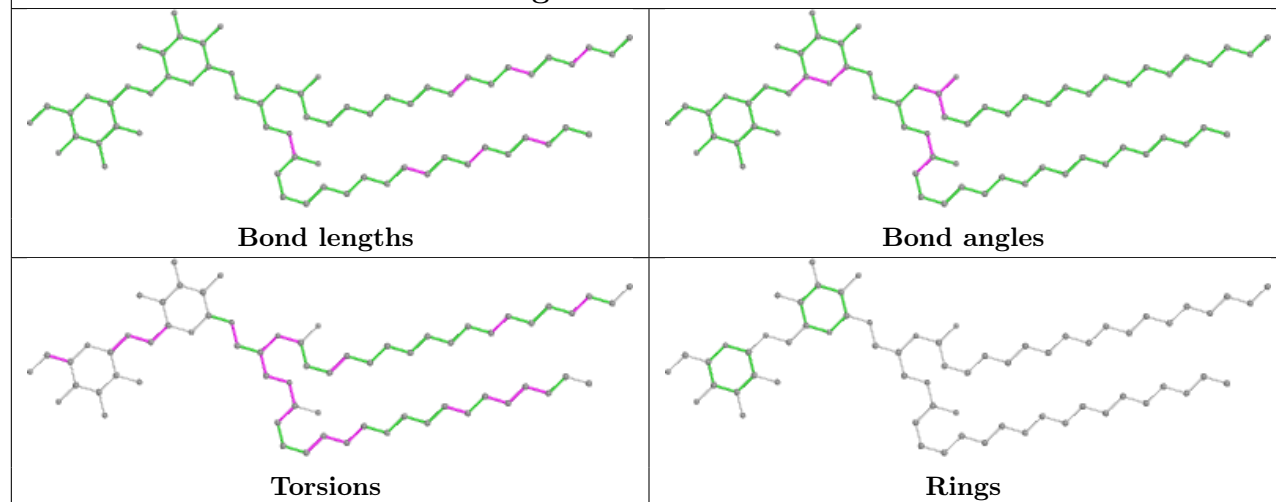


Rings

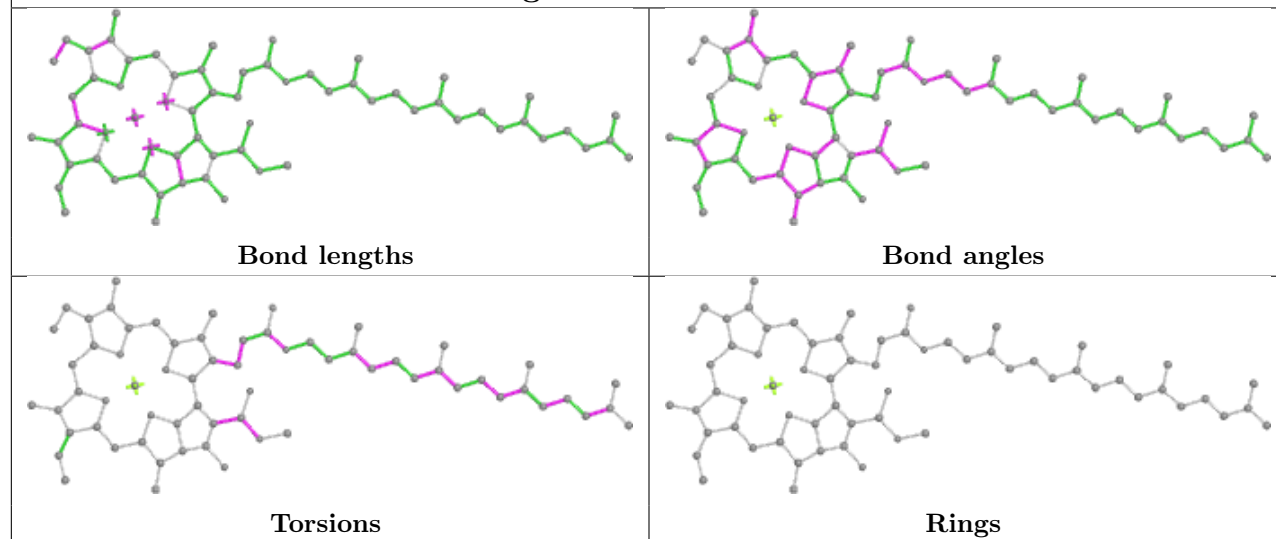
Ligand CLA 6 612



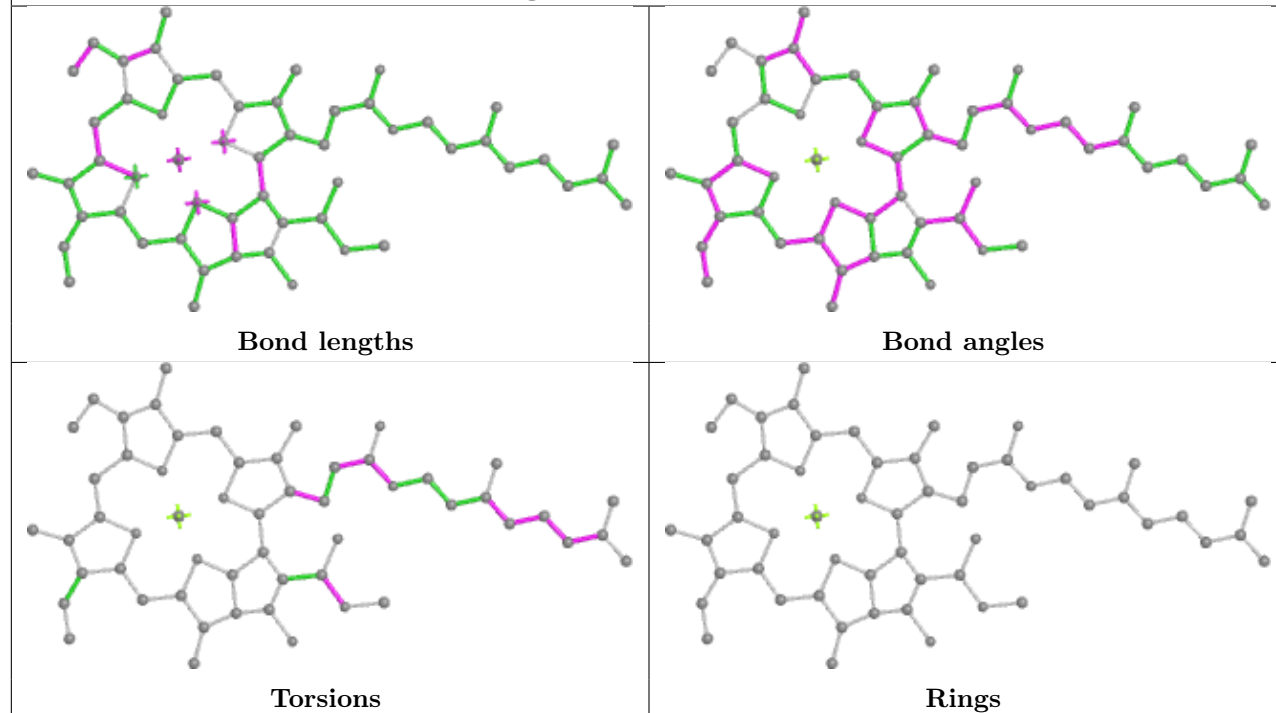
Ligand DGD 8 802

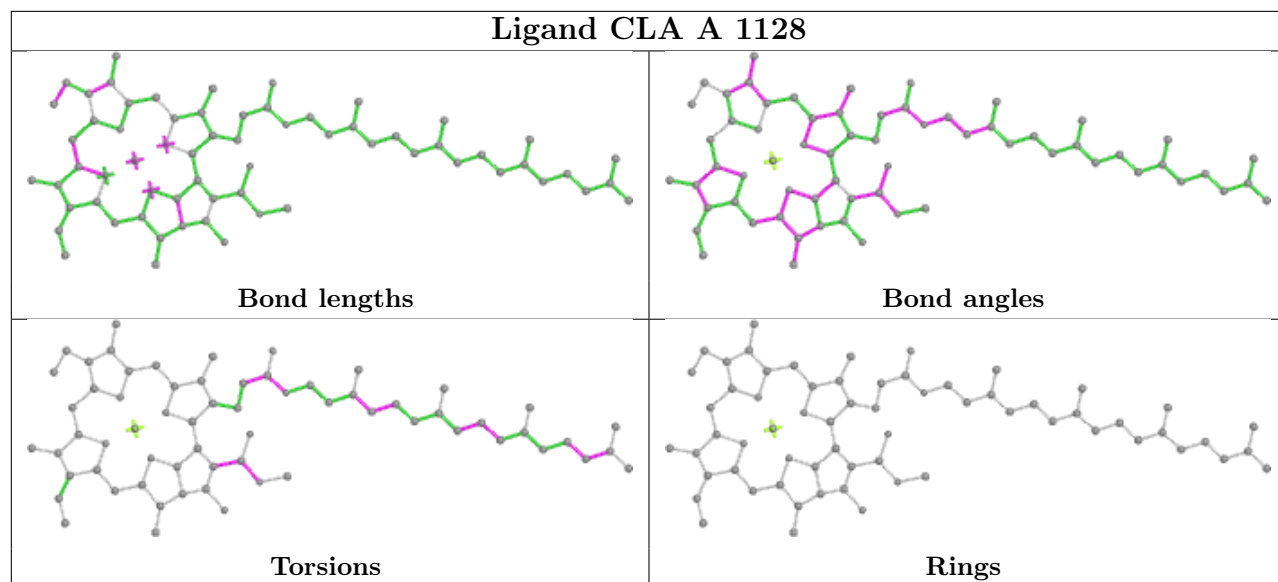
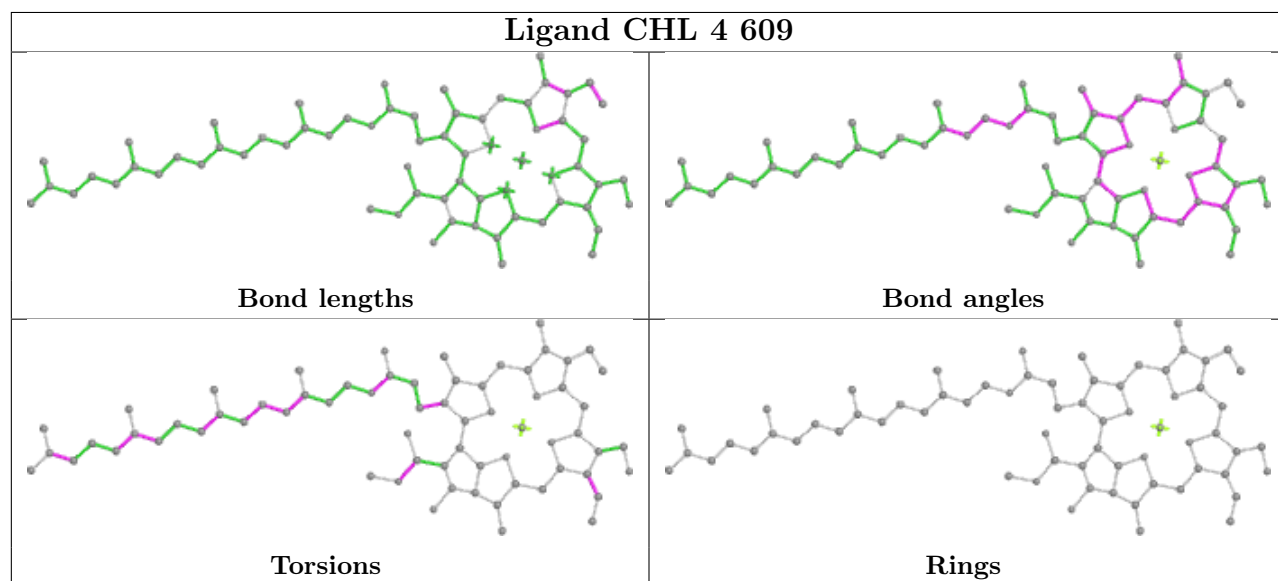


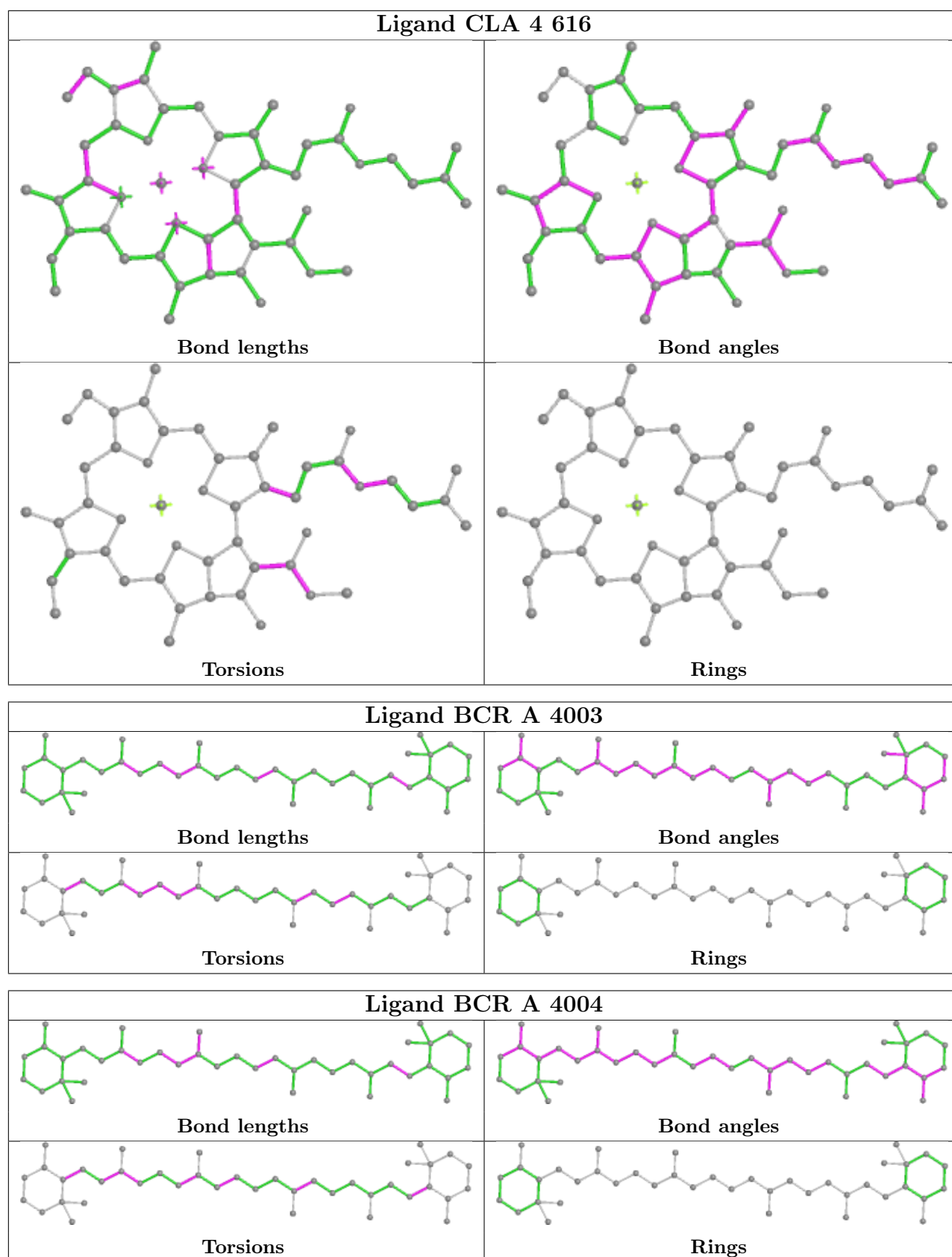
Ligand CLA A 1117

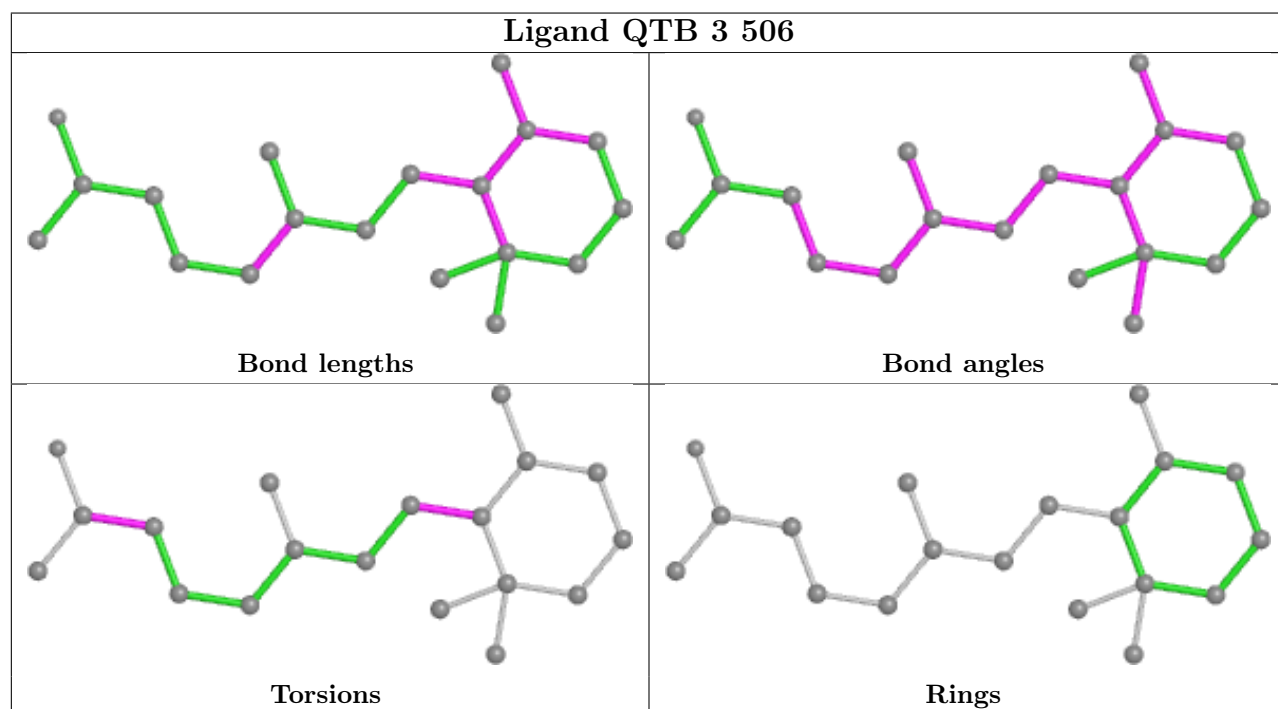
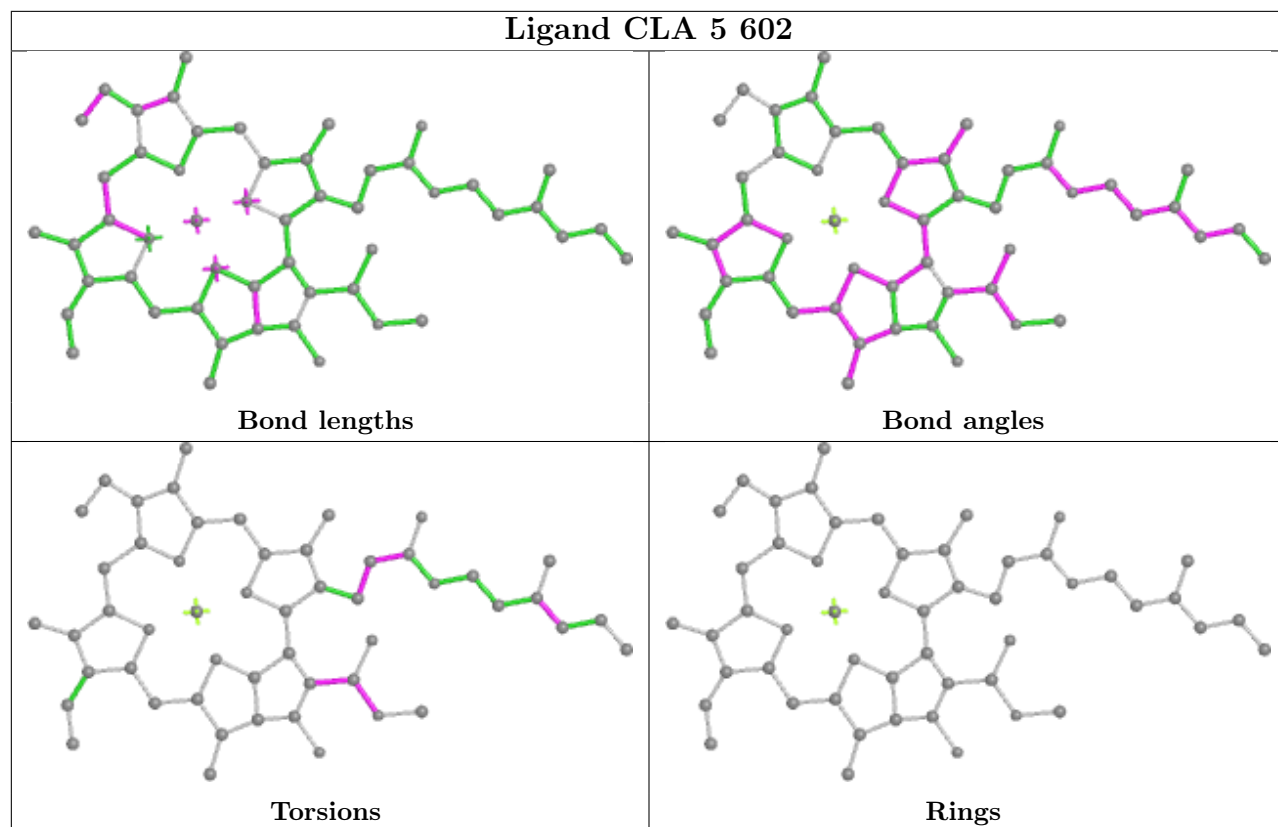


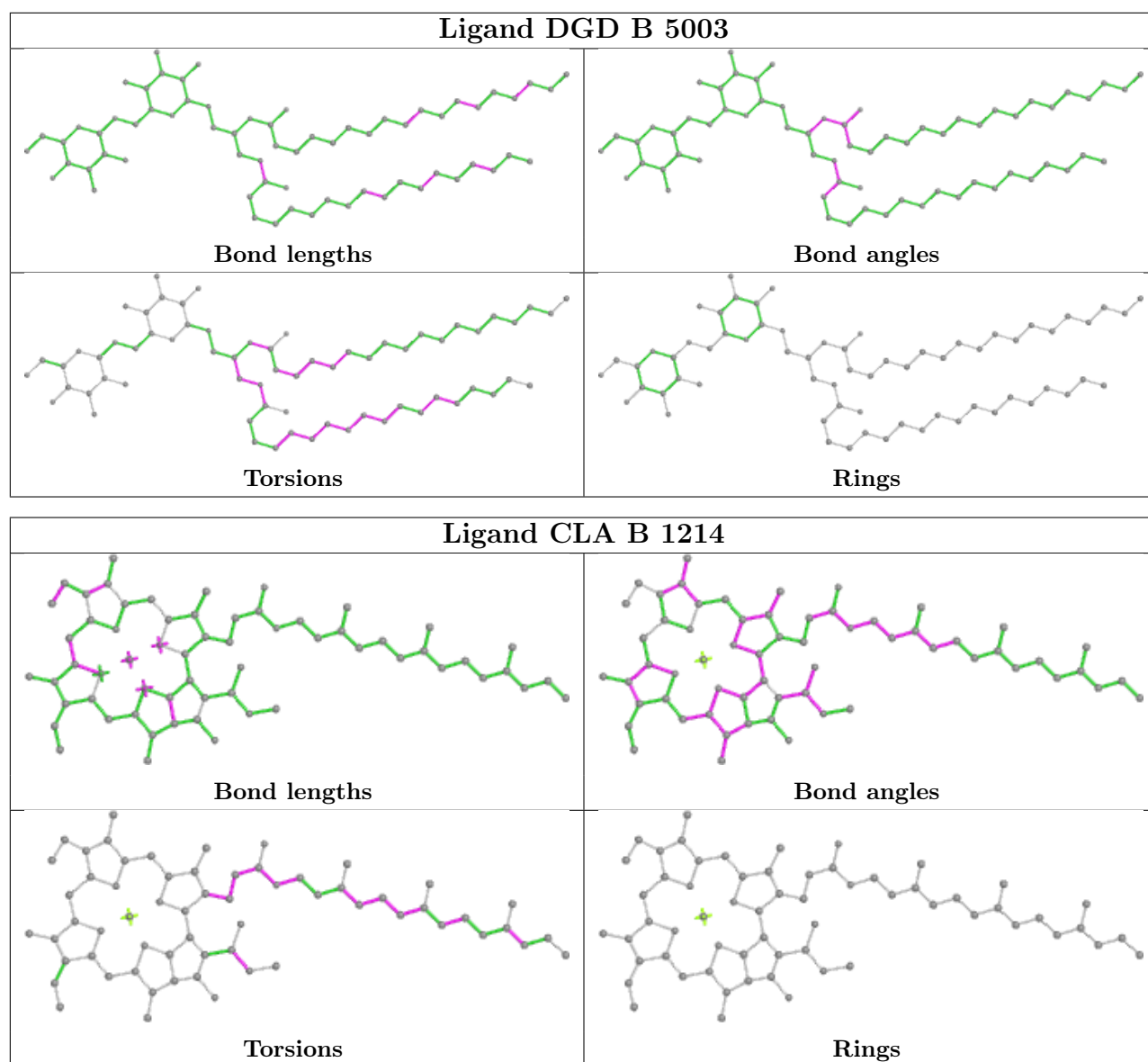
Ligand CLA B 1206

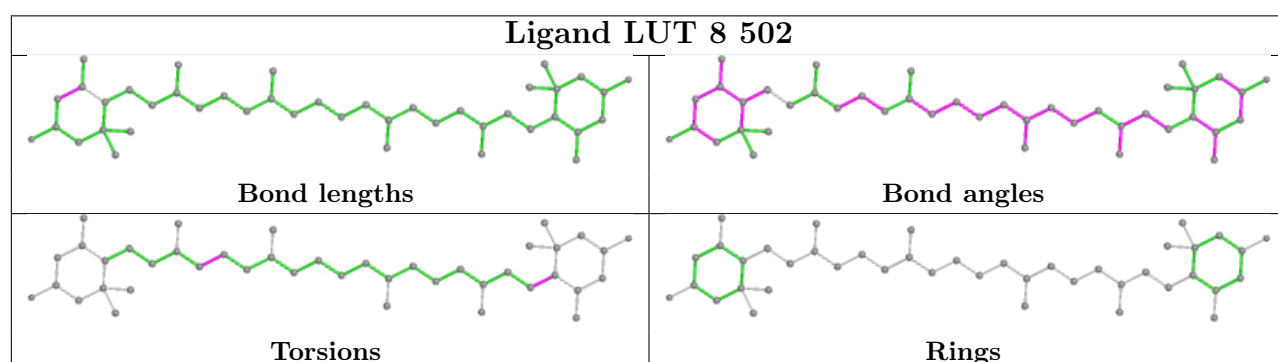
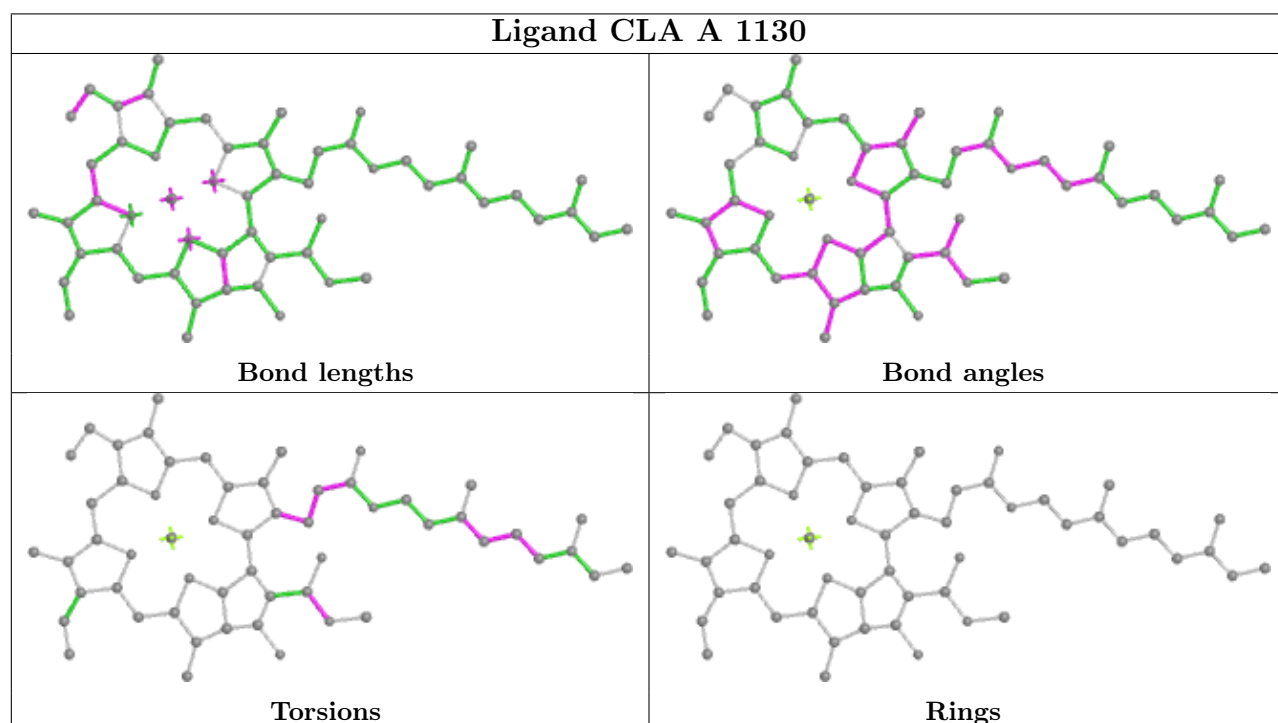
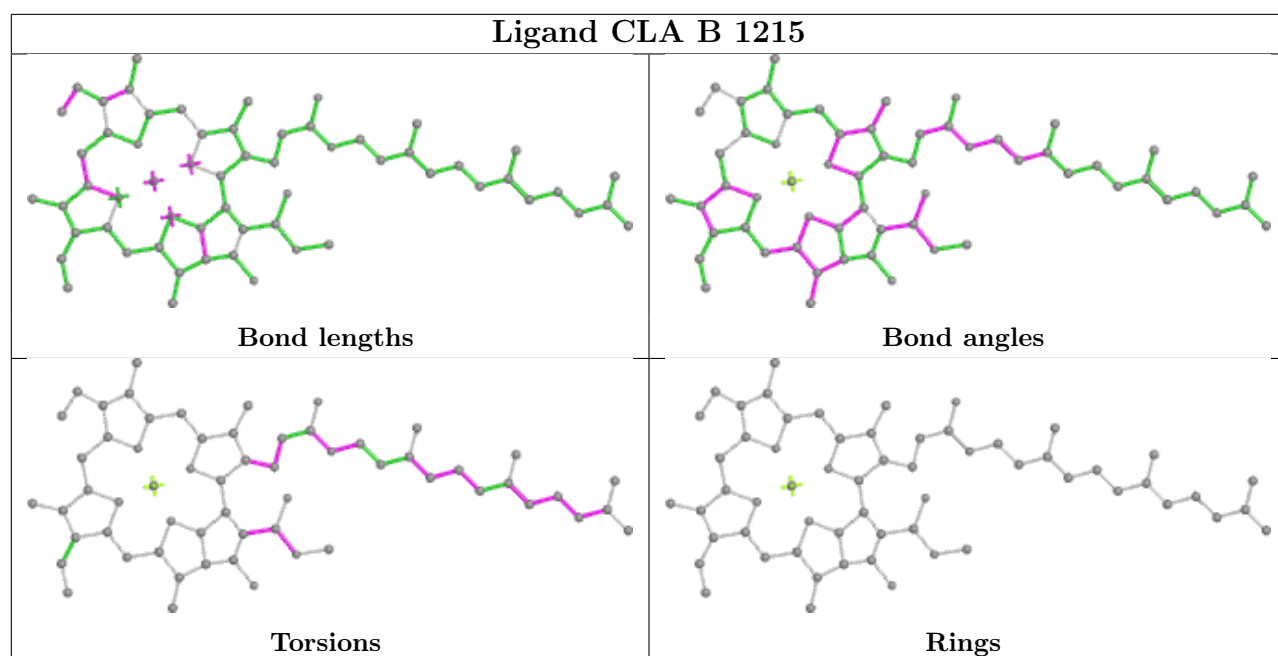


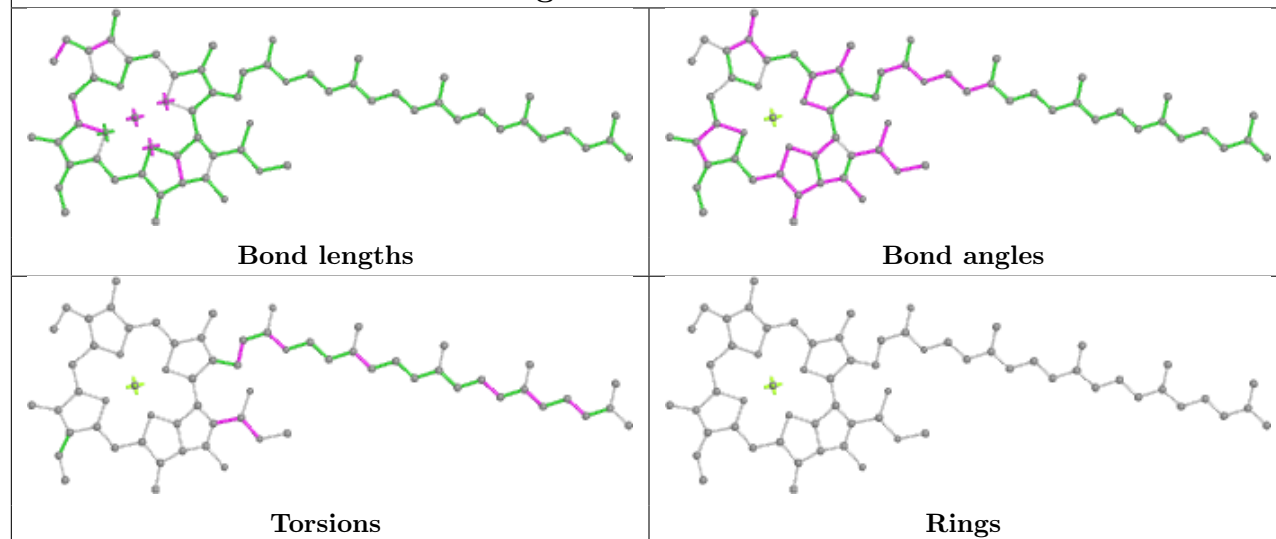
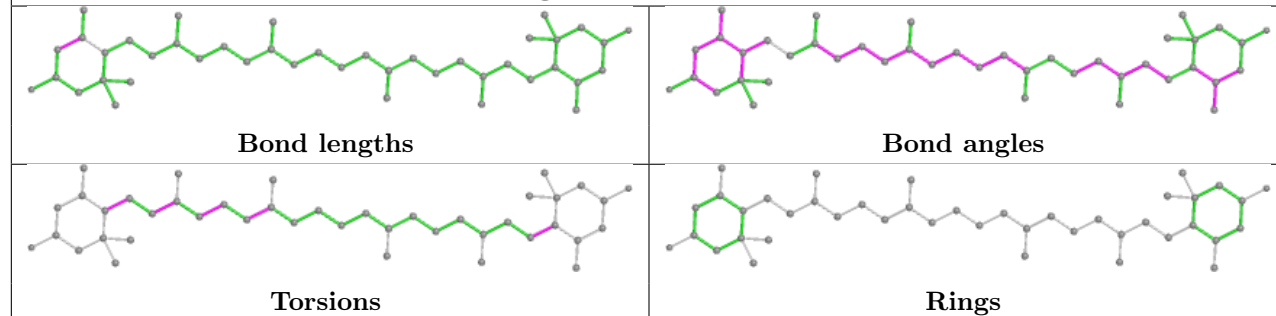
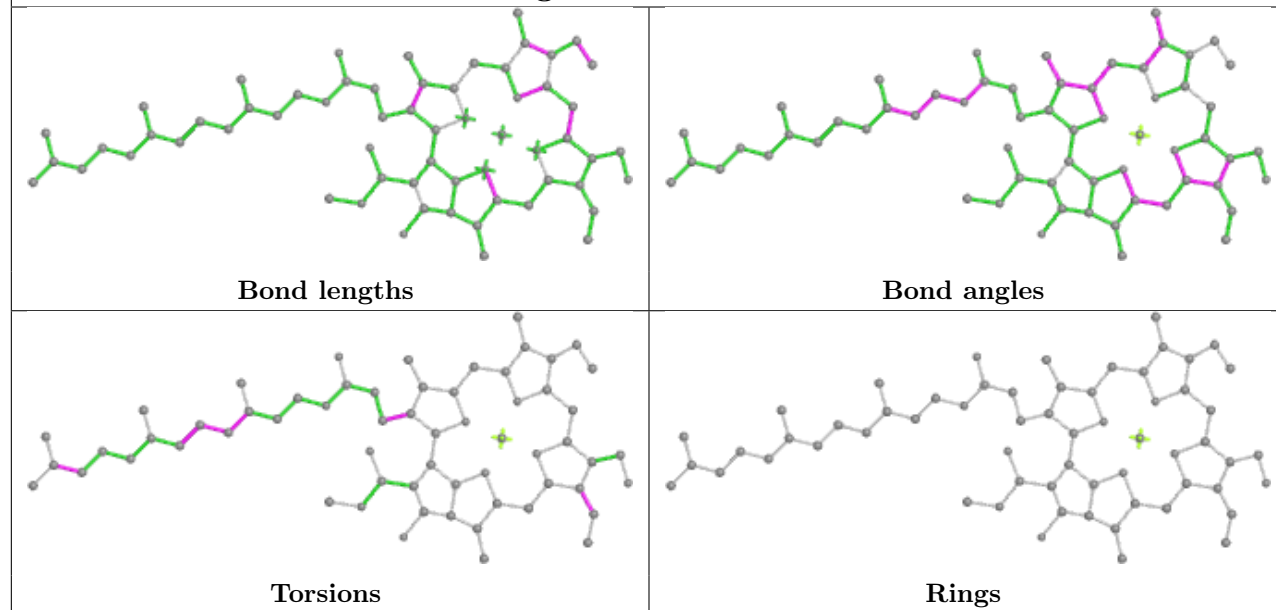
Ligand CLA A 1128**Ligand CHL 4 609**



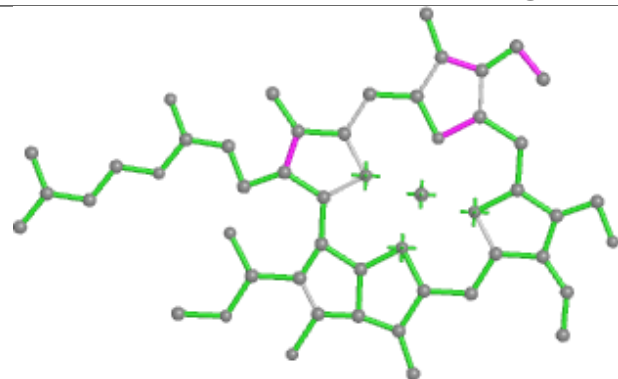




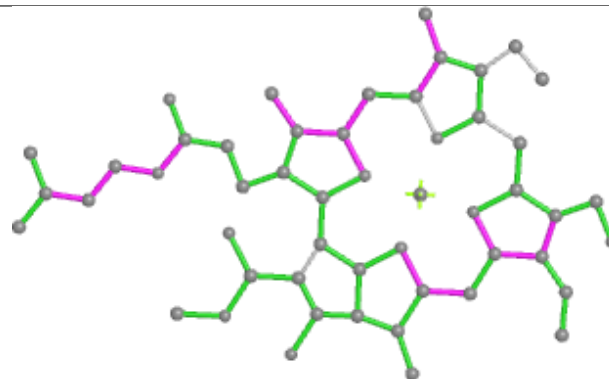


Ligand CLA 5 604**Ligand LUT 1 503****Ligand CHL 8 601**

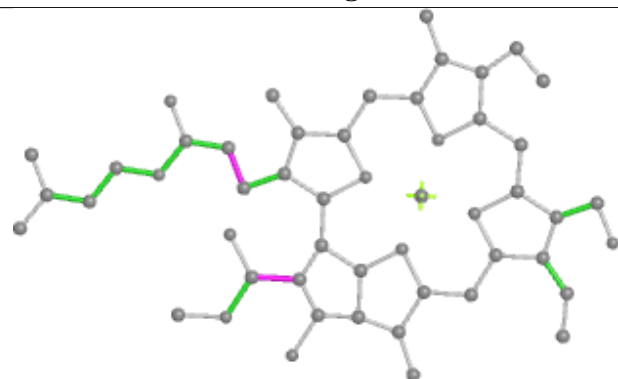
Ligand CHL 8 613



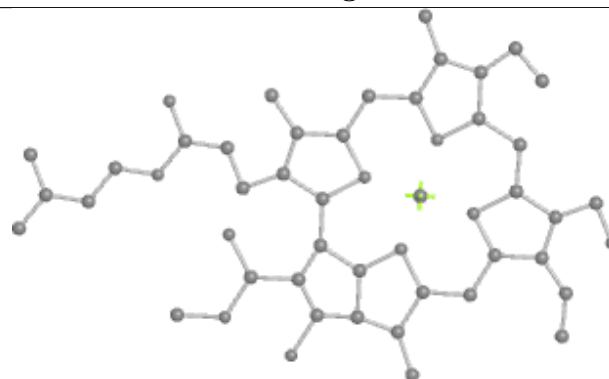
Bond lengths



Bond angles

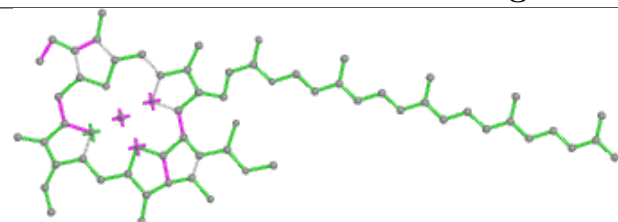


Torsions

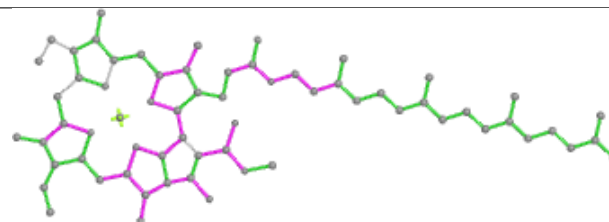


Rings

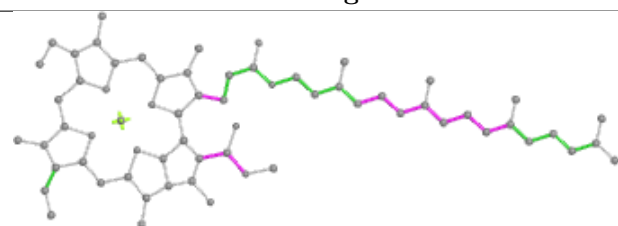
Ligand CLA B 1223



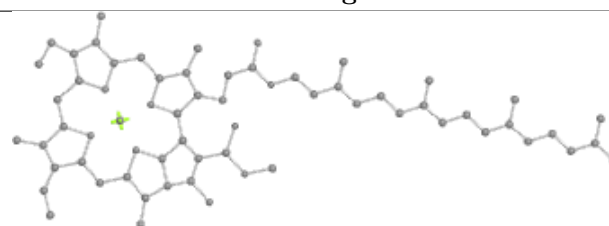
Bond lengths



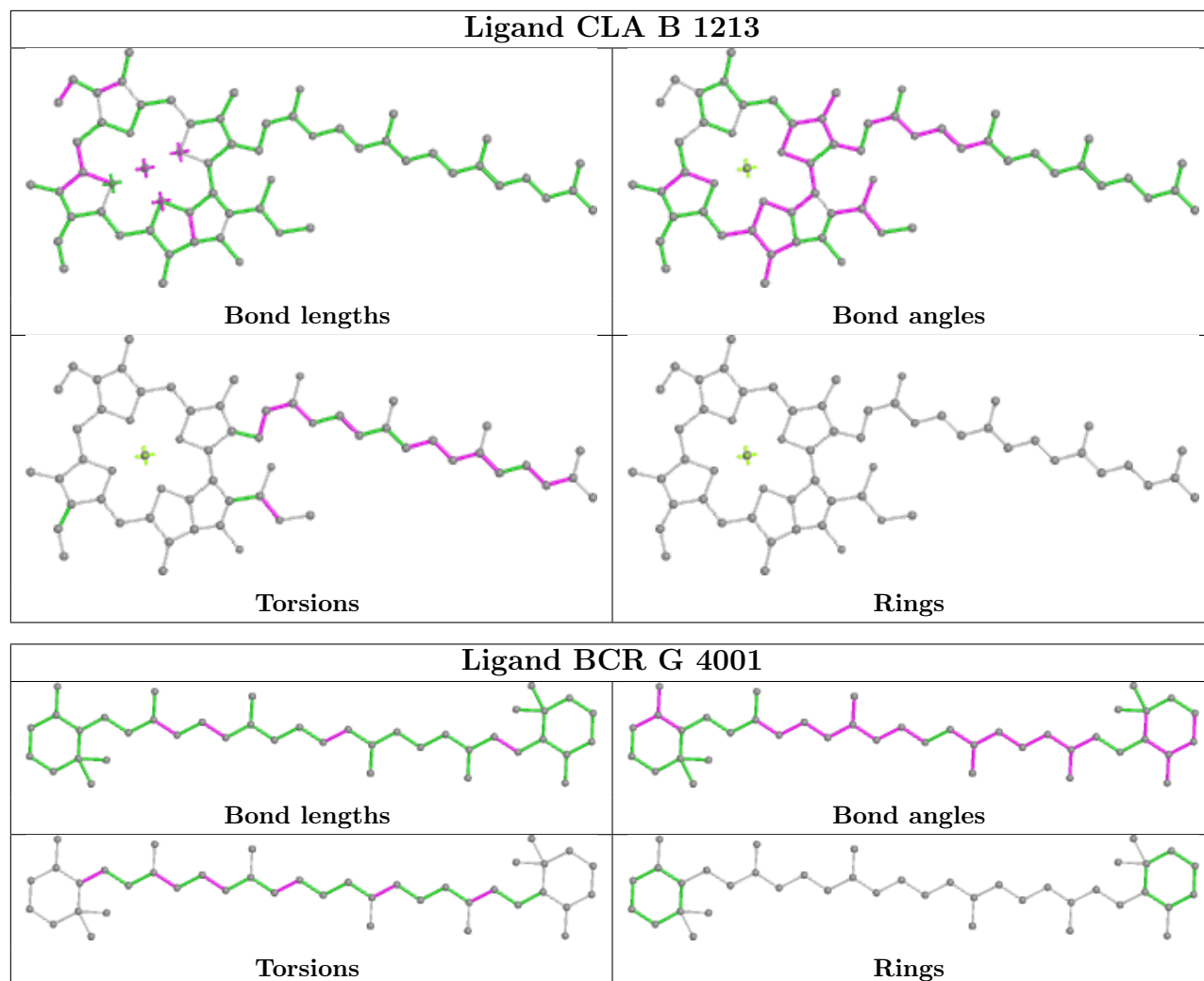
Bond angles

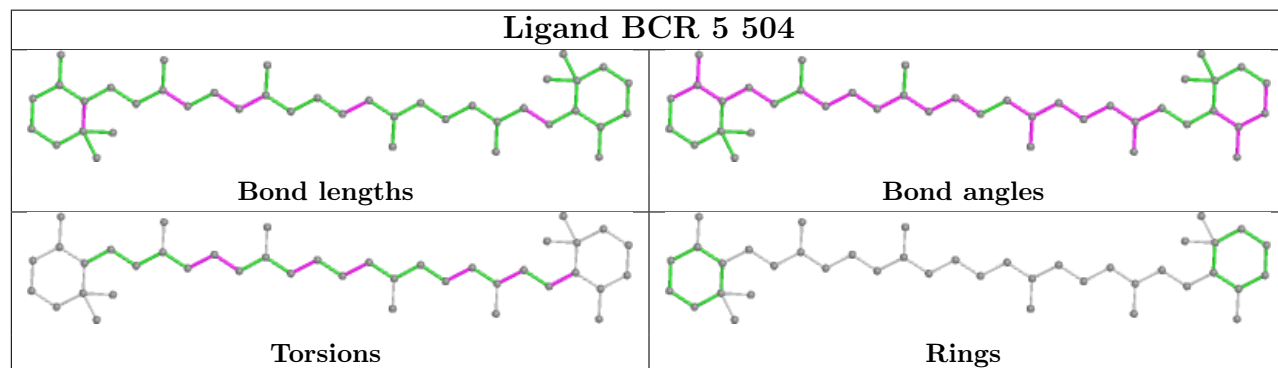
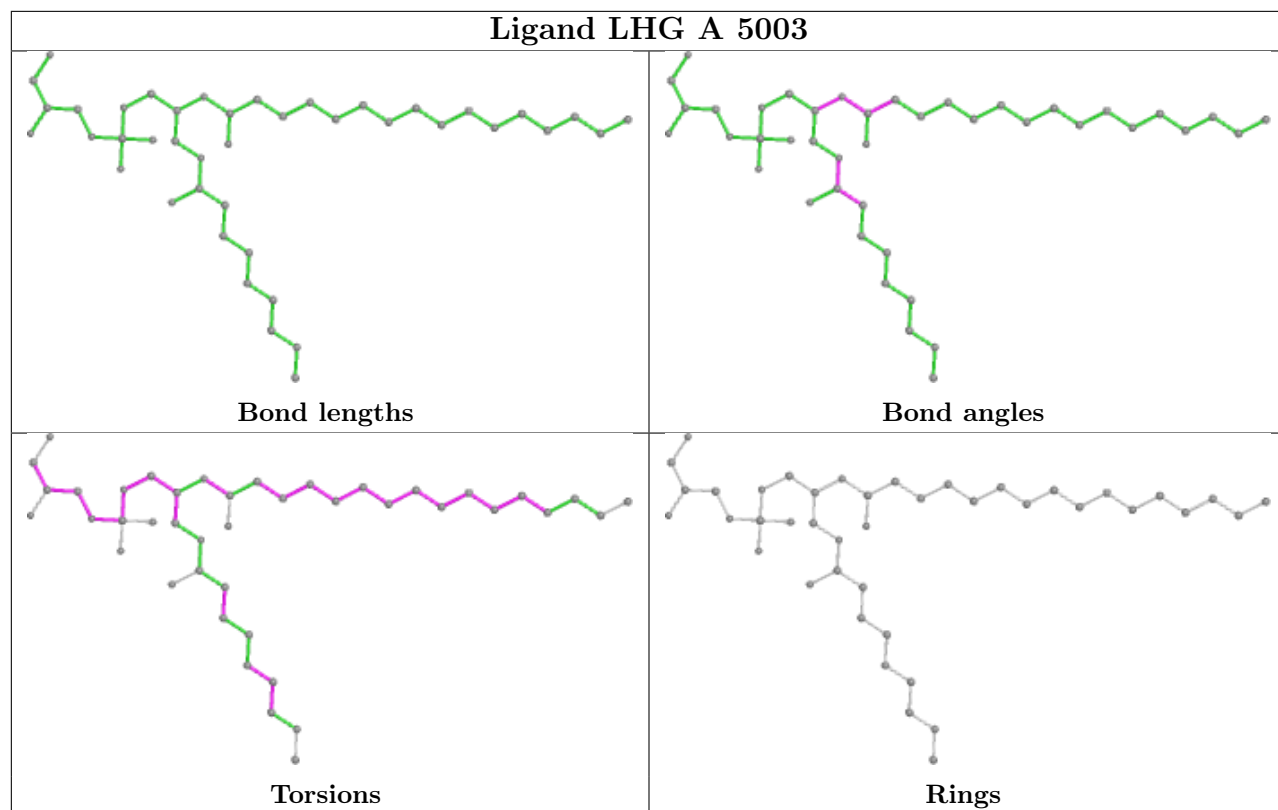


Torsions

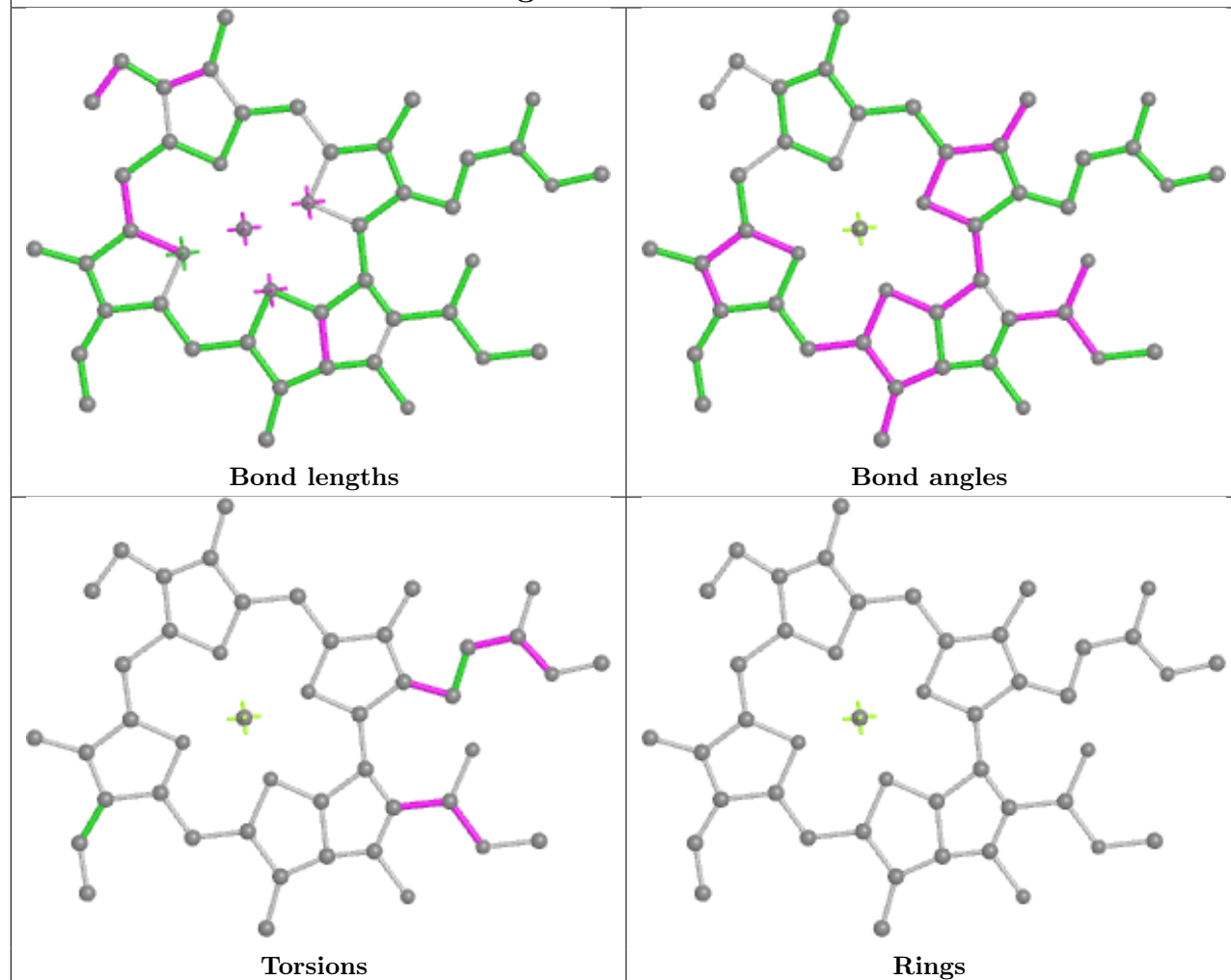


Rings

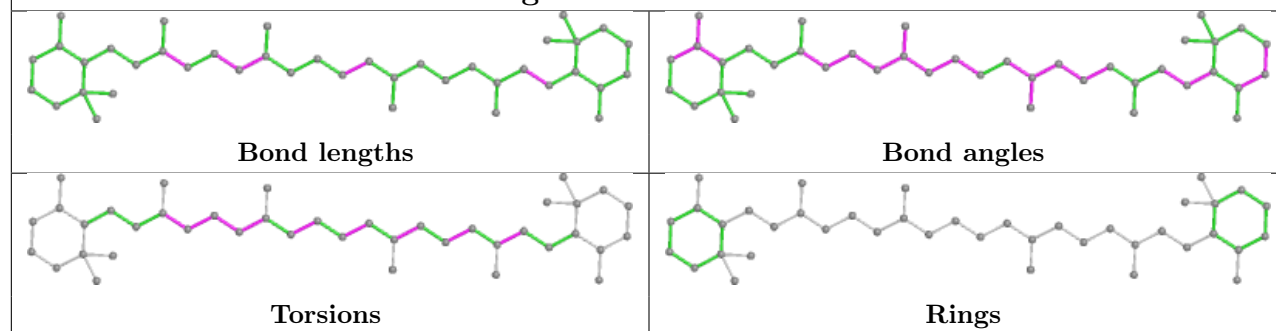




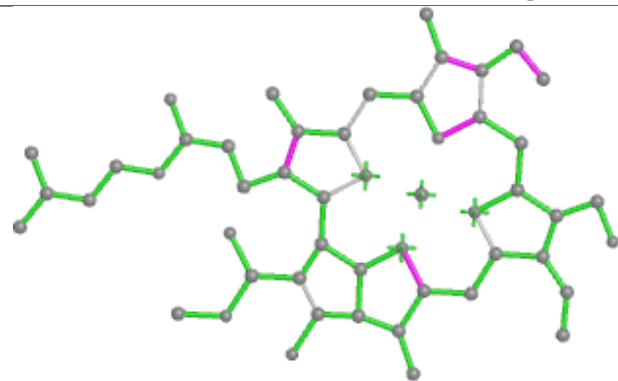
Ligand CLA 6 618



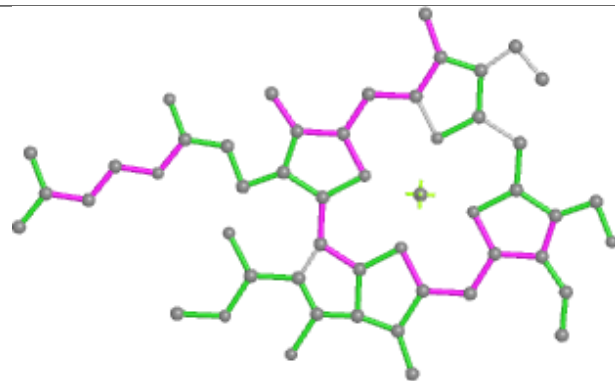
Ligand BCR B 4006



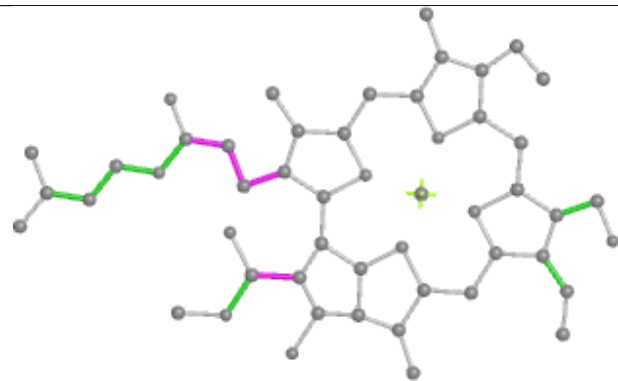
Ligand CHL 5 611



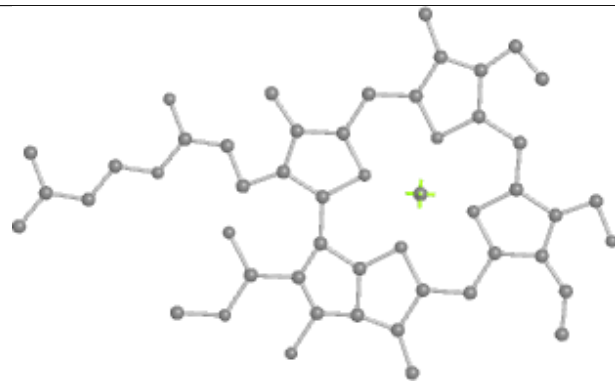
Bond lengths



Bond angles

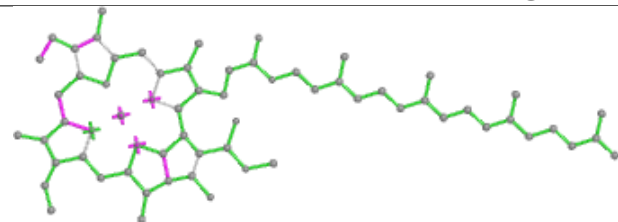


Torsions

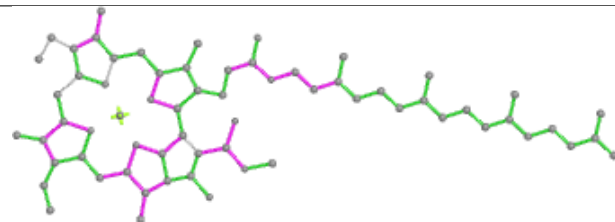


Rings

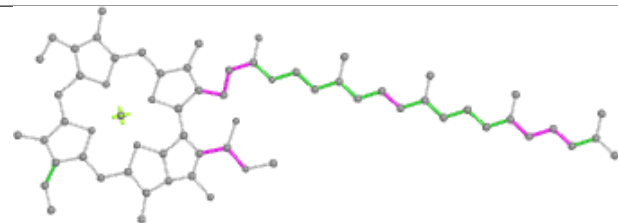
Ligand CLA 3 606



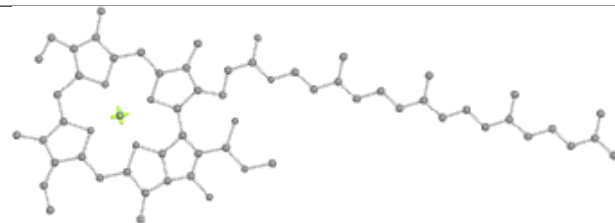
Bond lengths



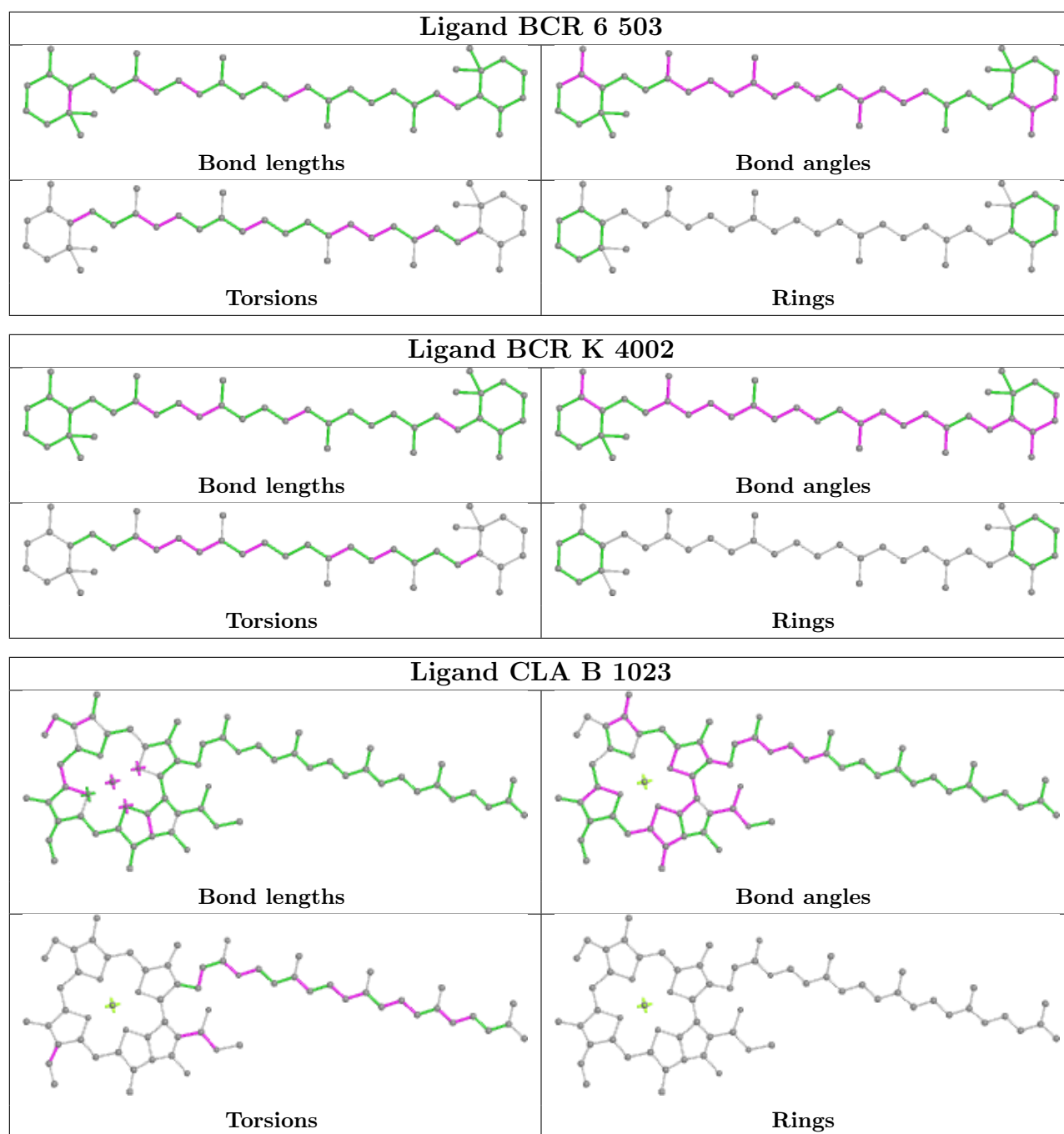
Bond angles

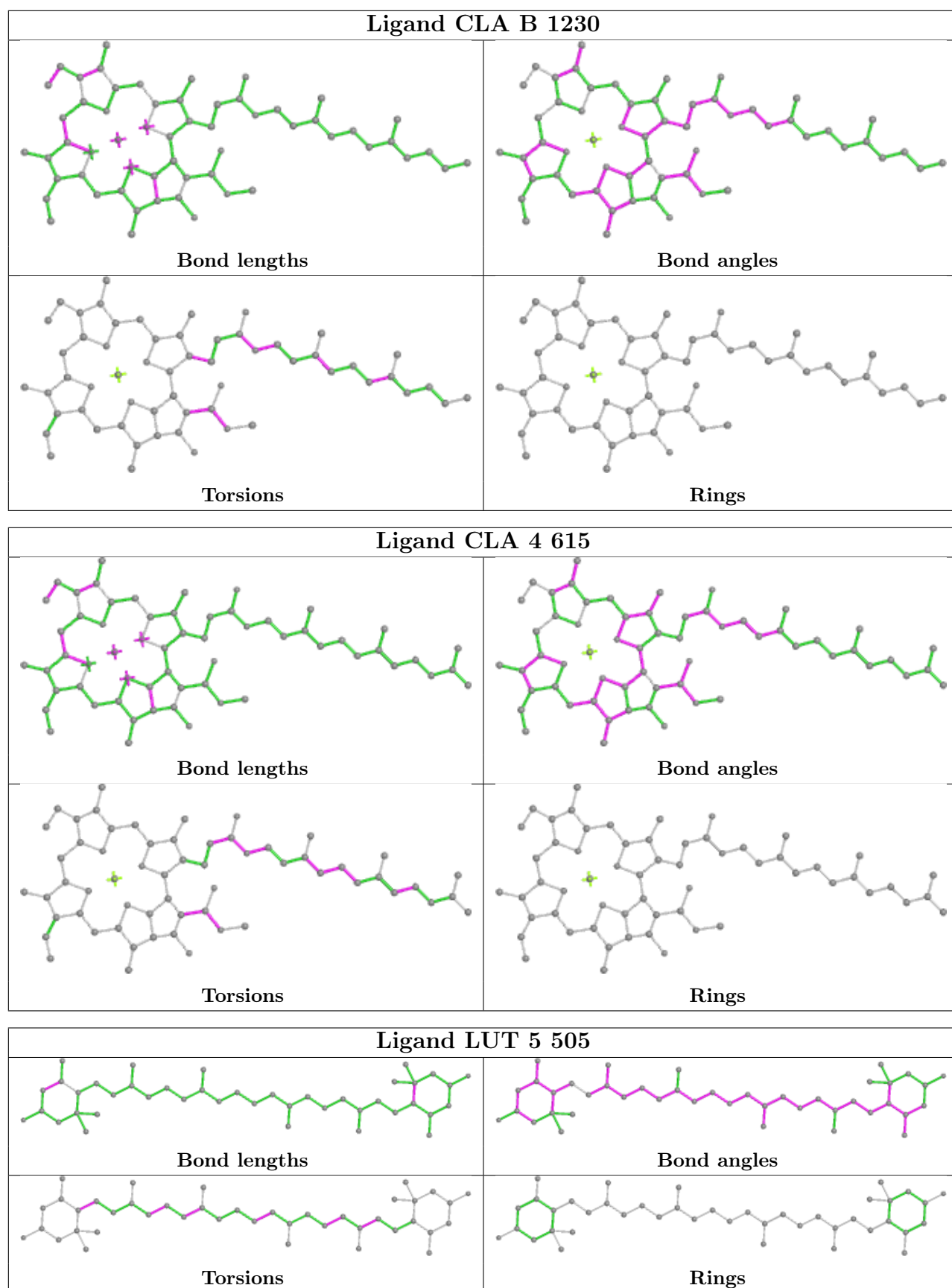


Torsions

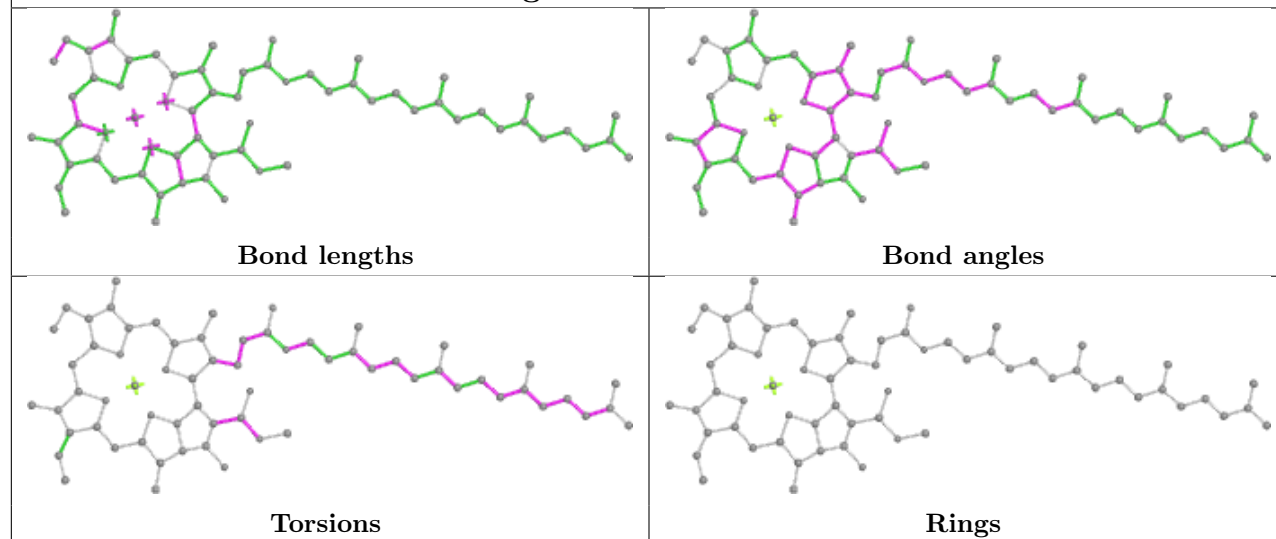


Rings

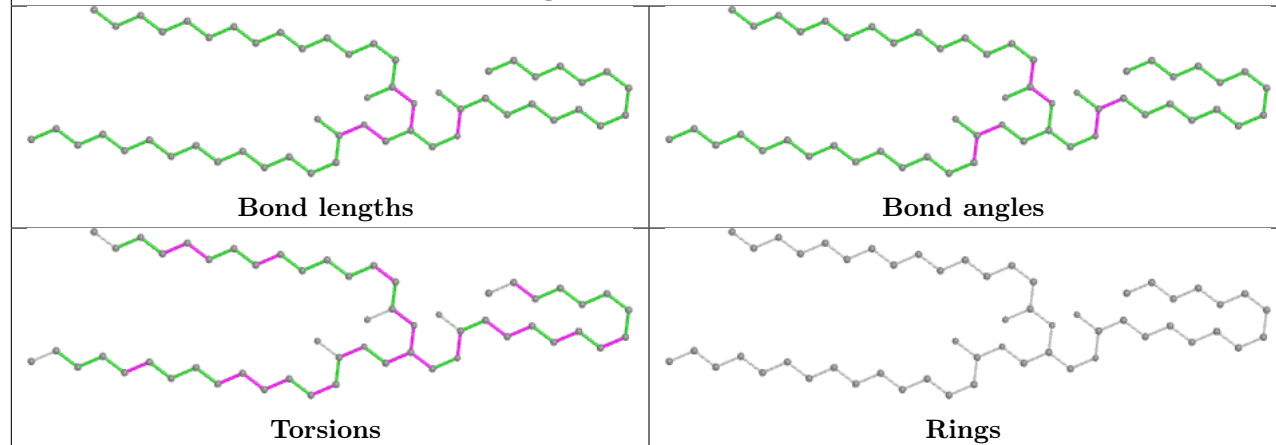




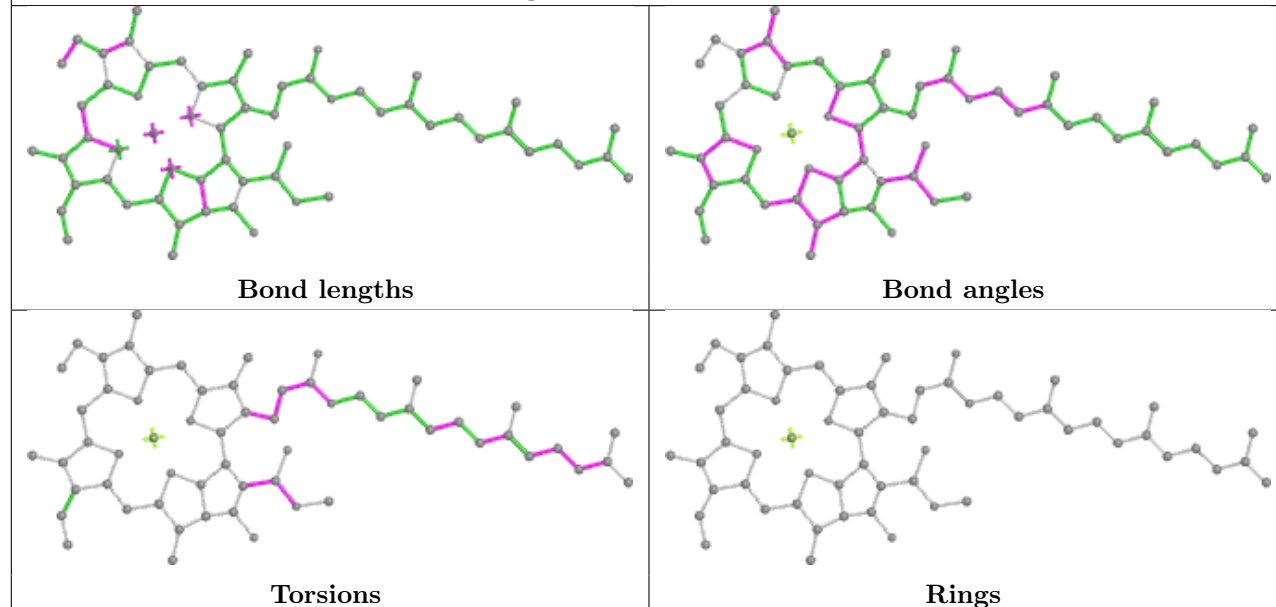
Ligand CLA A 1109



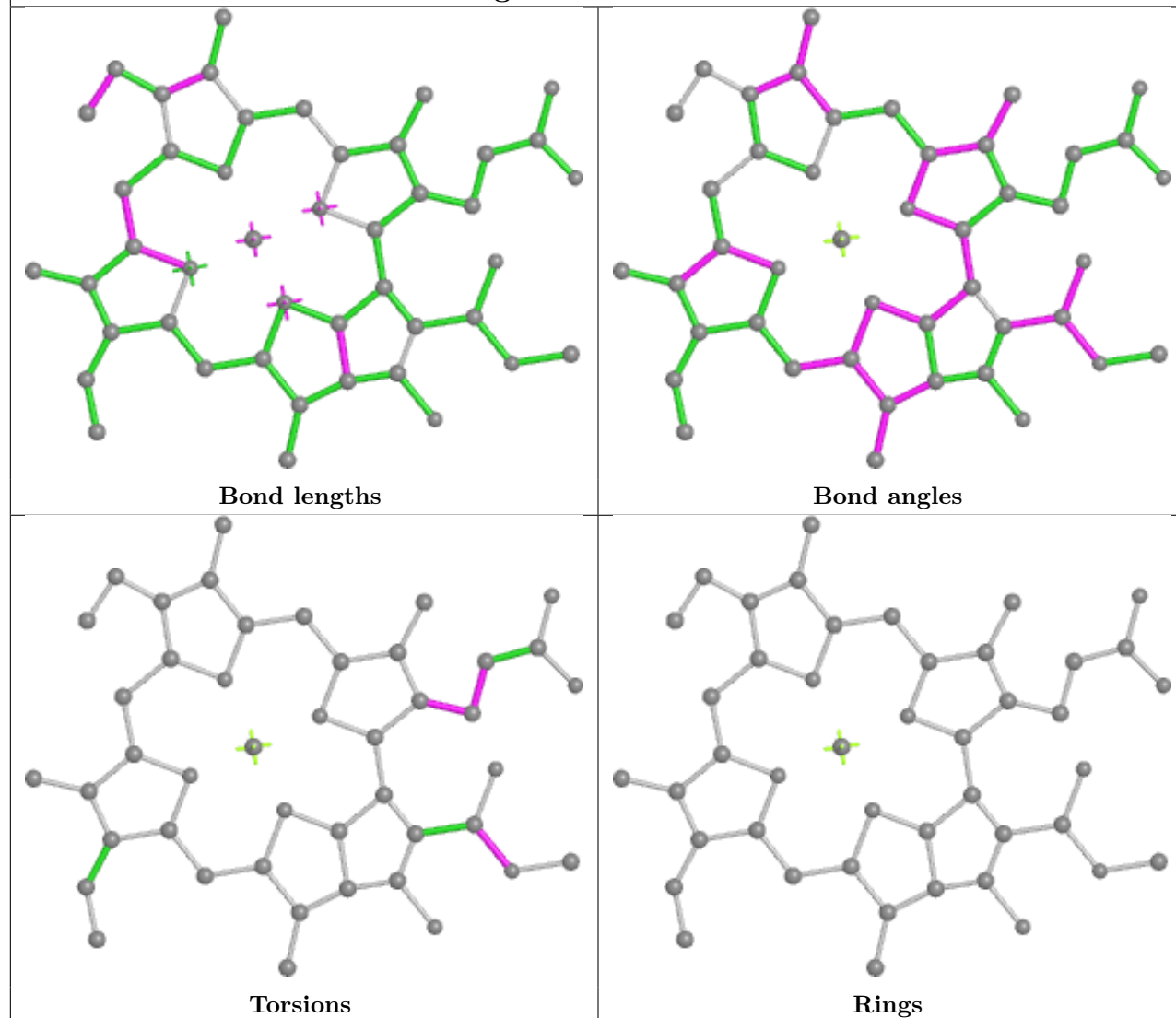
Ligand 4RF 8 808



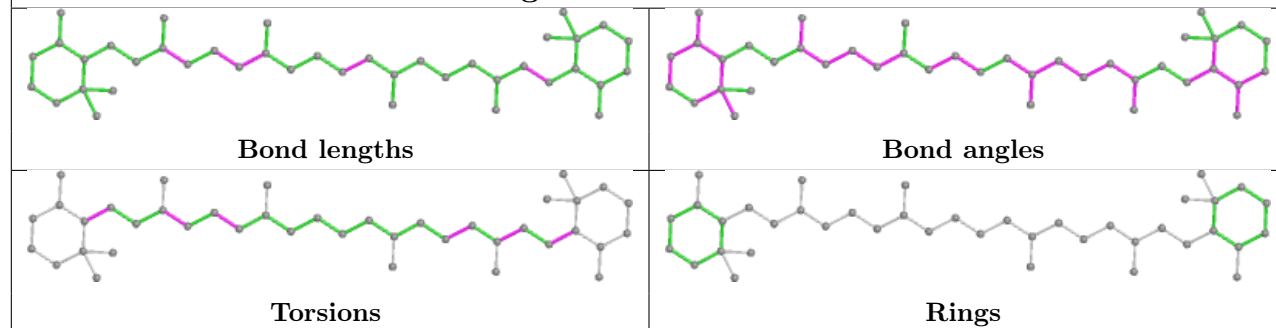
Ligand CLA A 1116

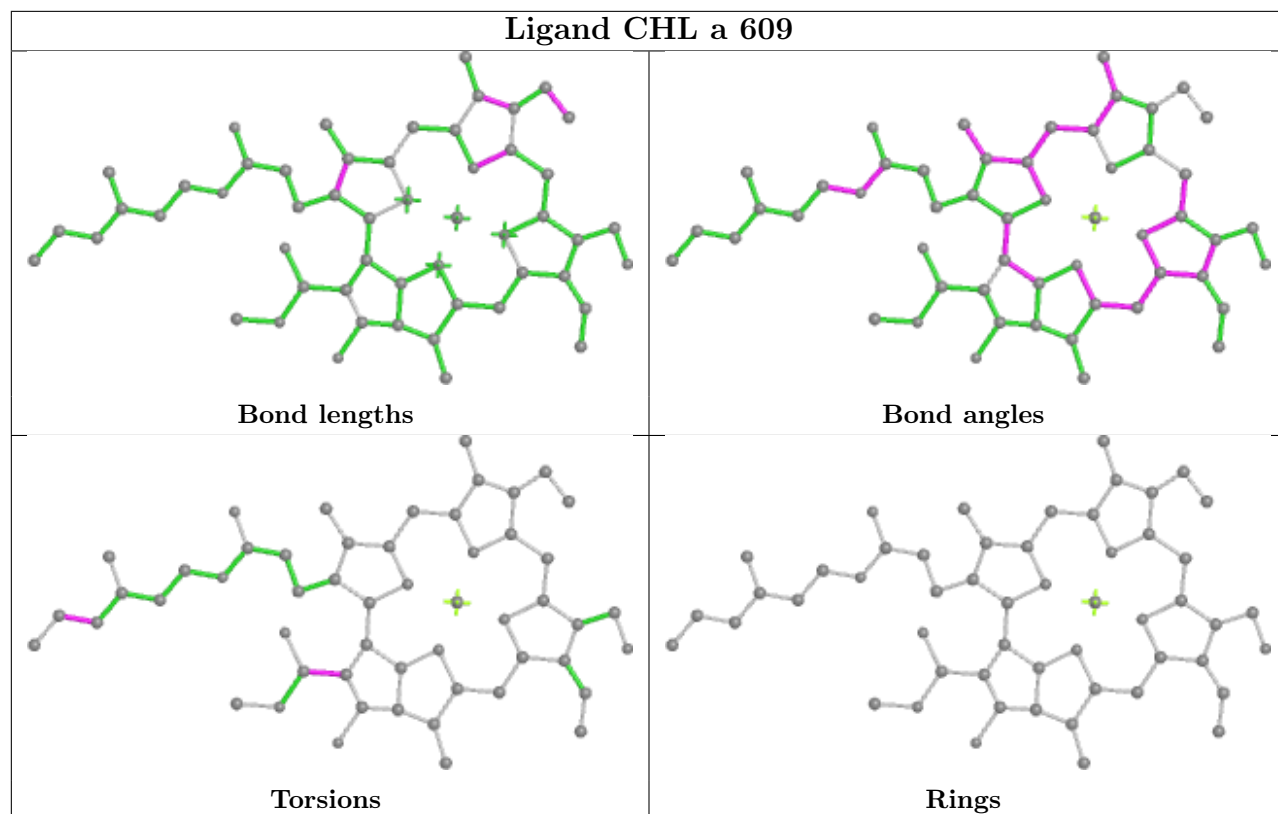


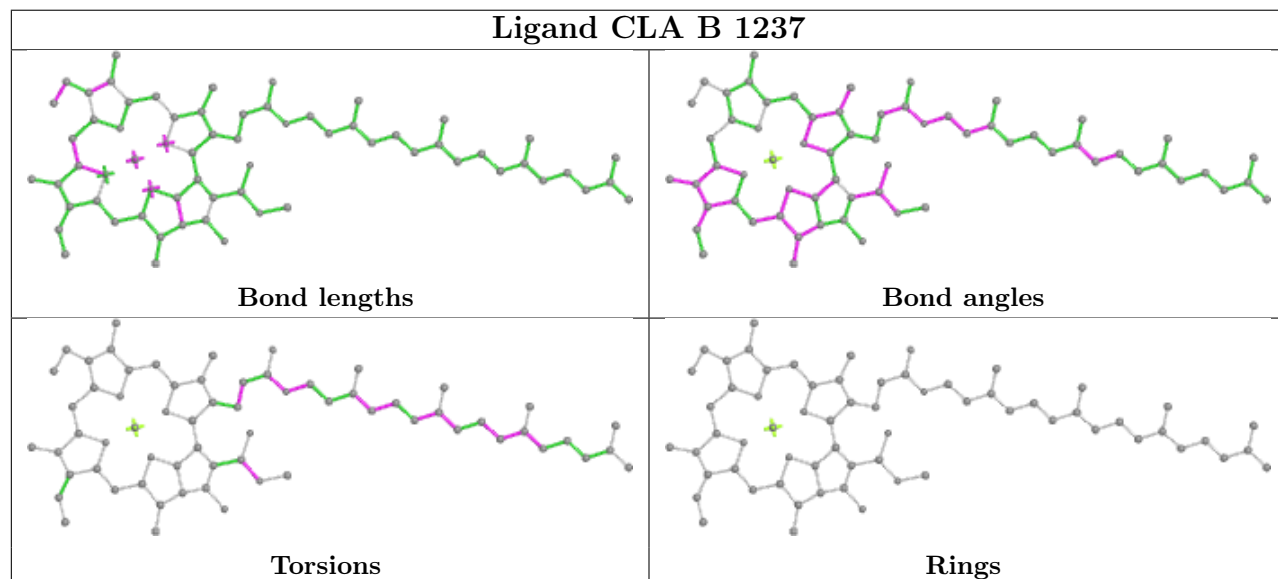
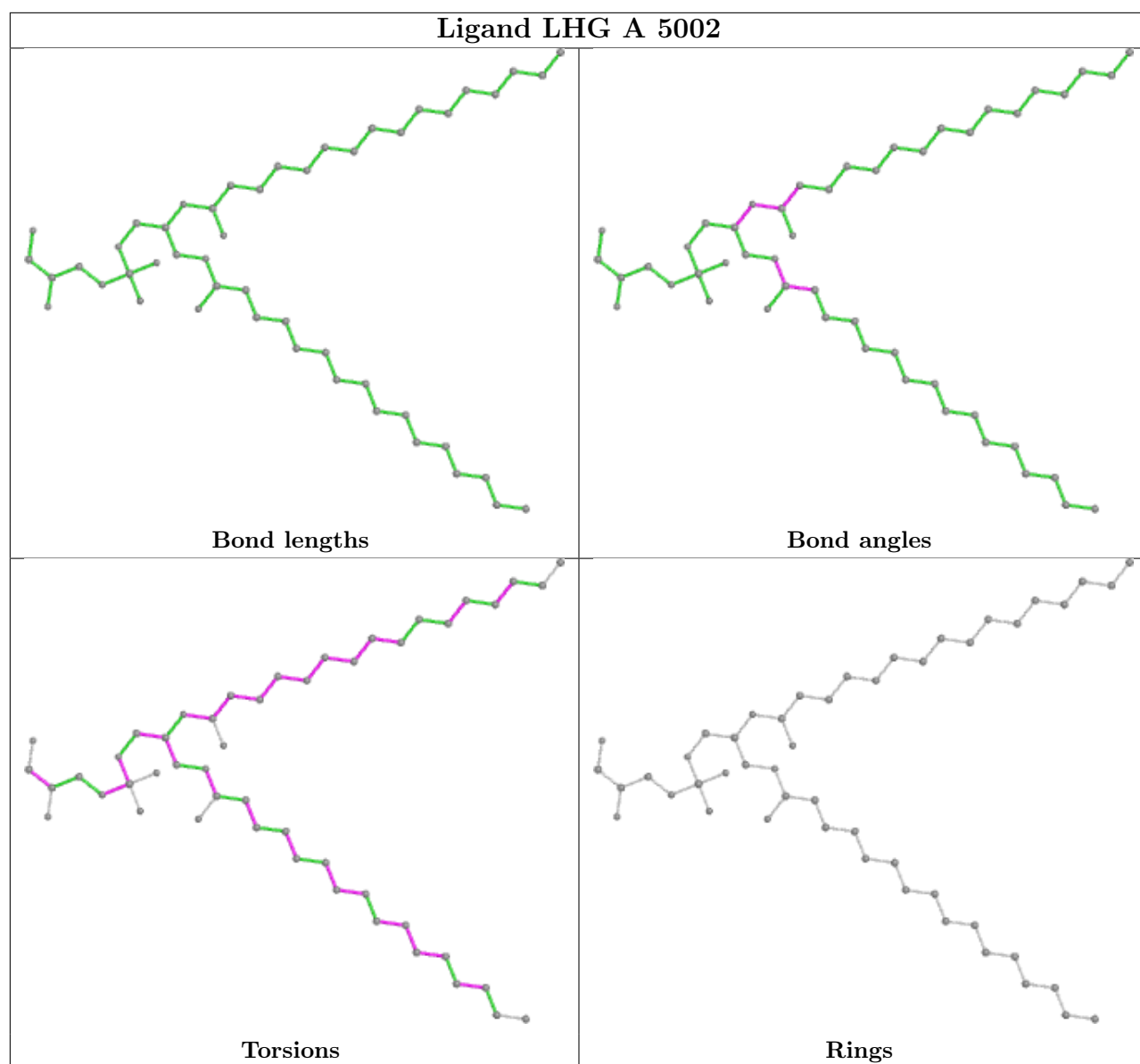
Ligand CLA 1 610



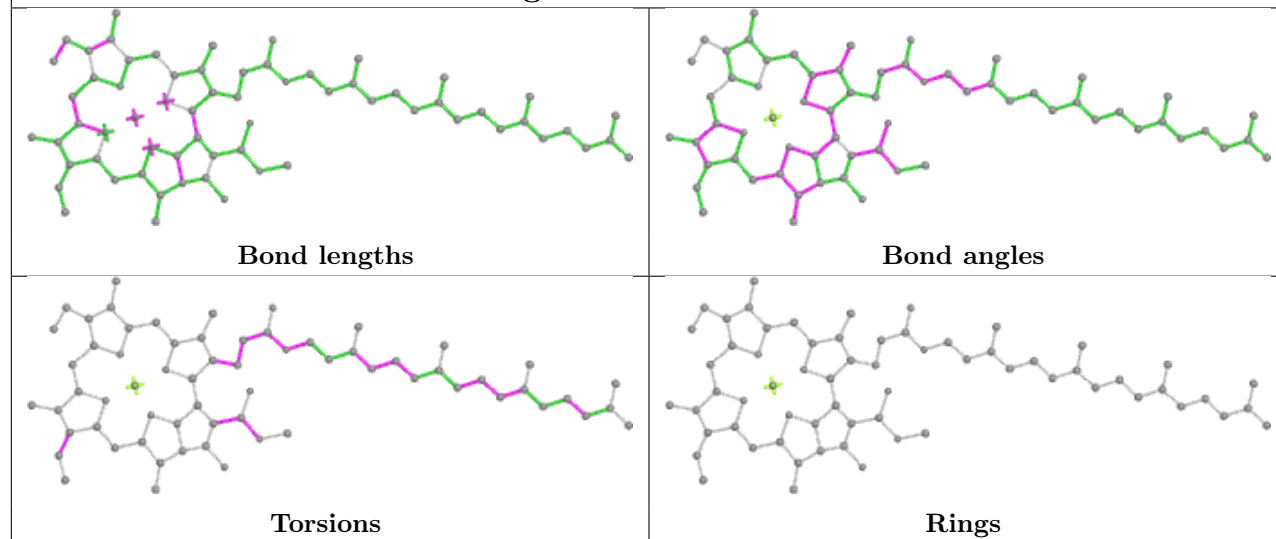
Ligand BCR A 4001



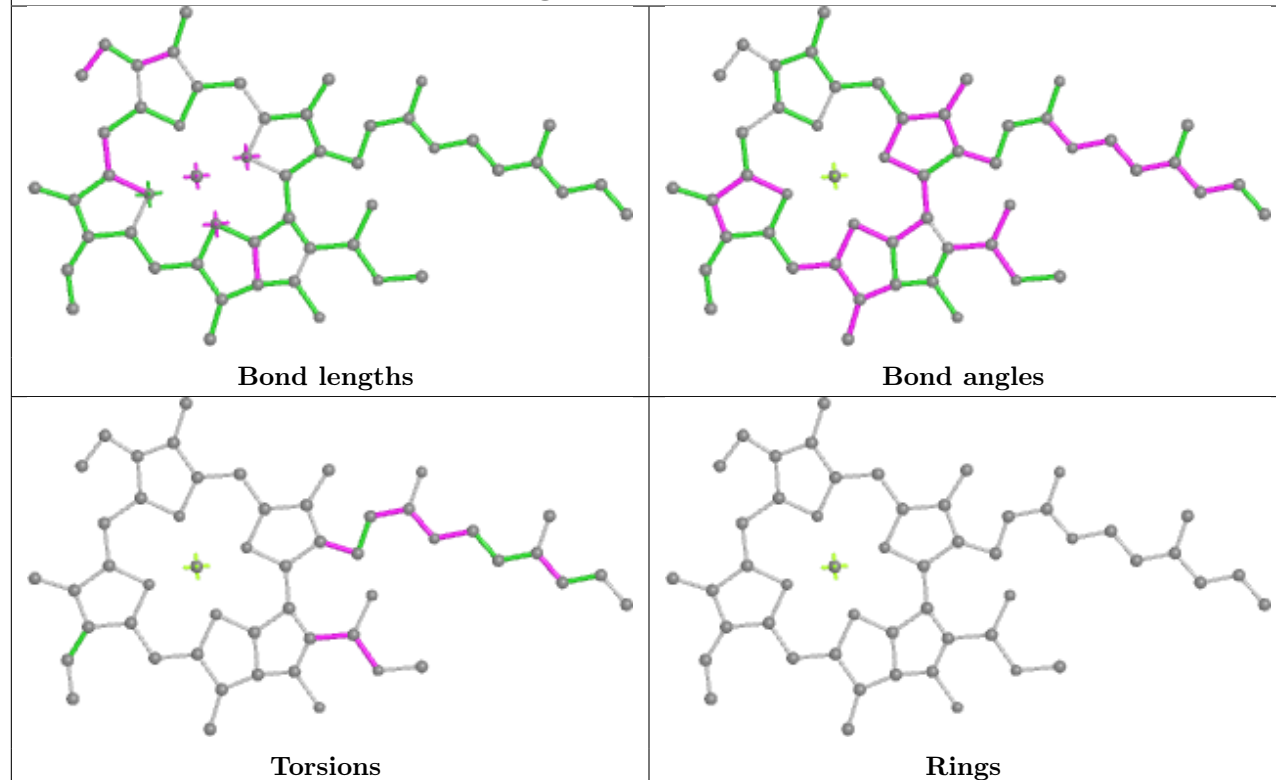




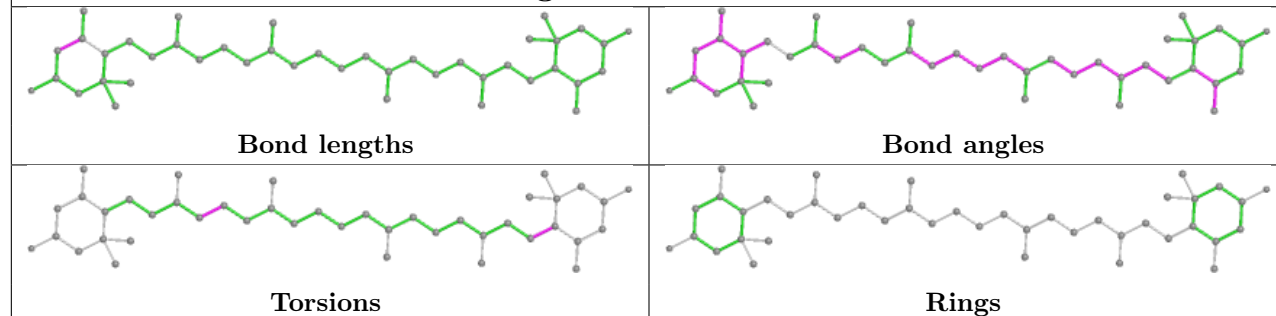
Ligand CLA B 1212

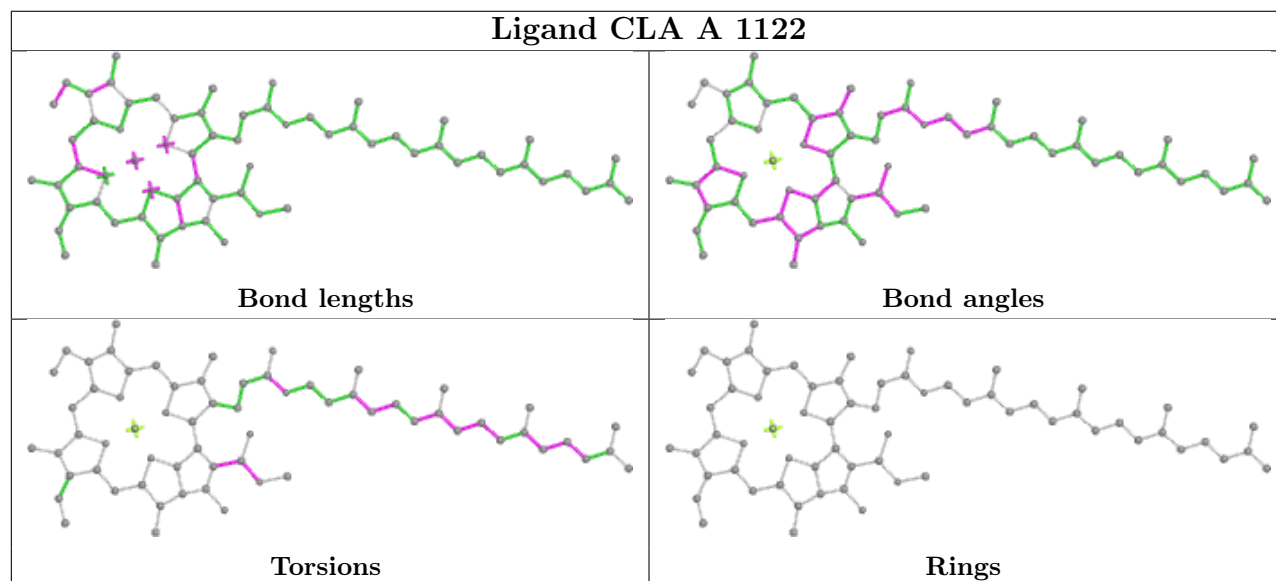
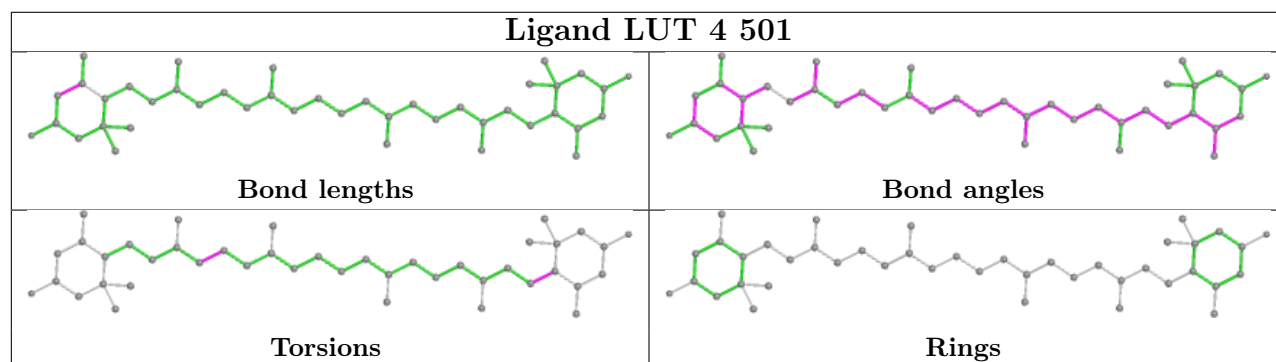
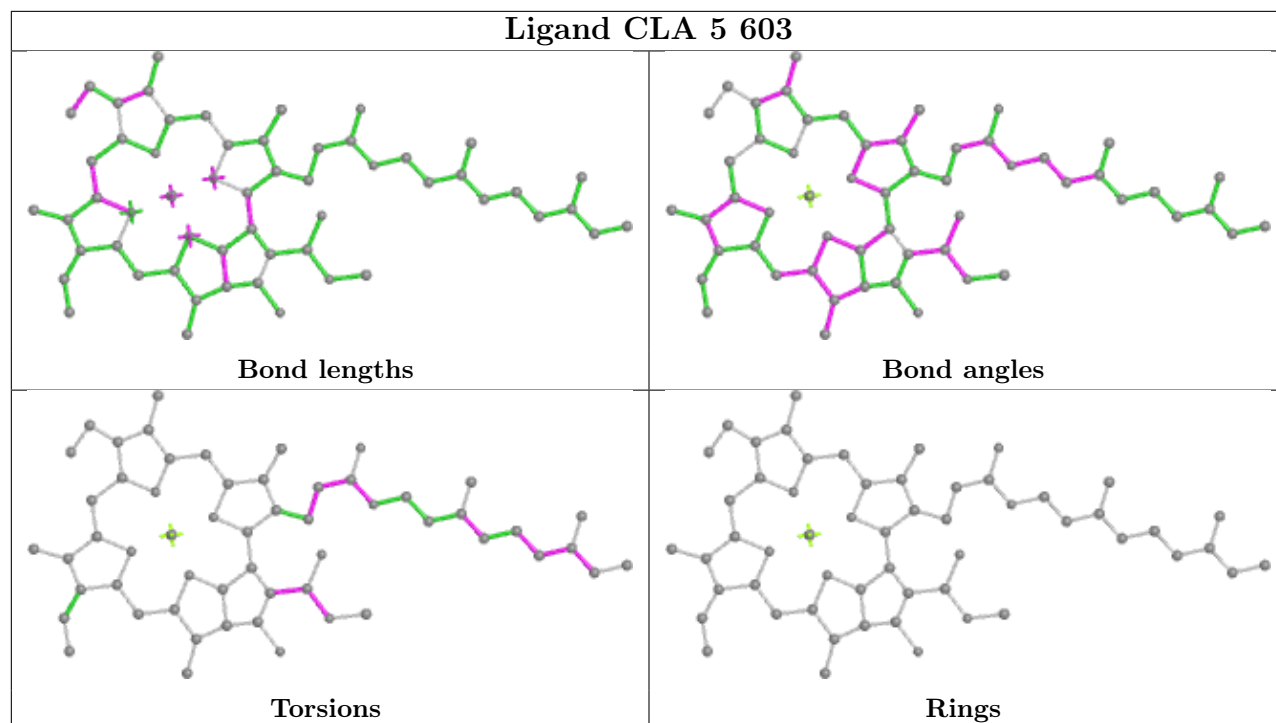


Ligand CLA 8 608

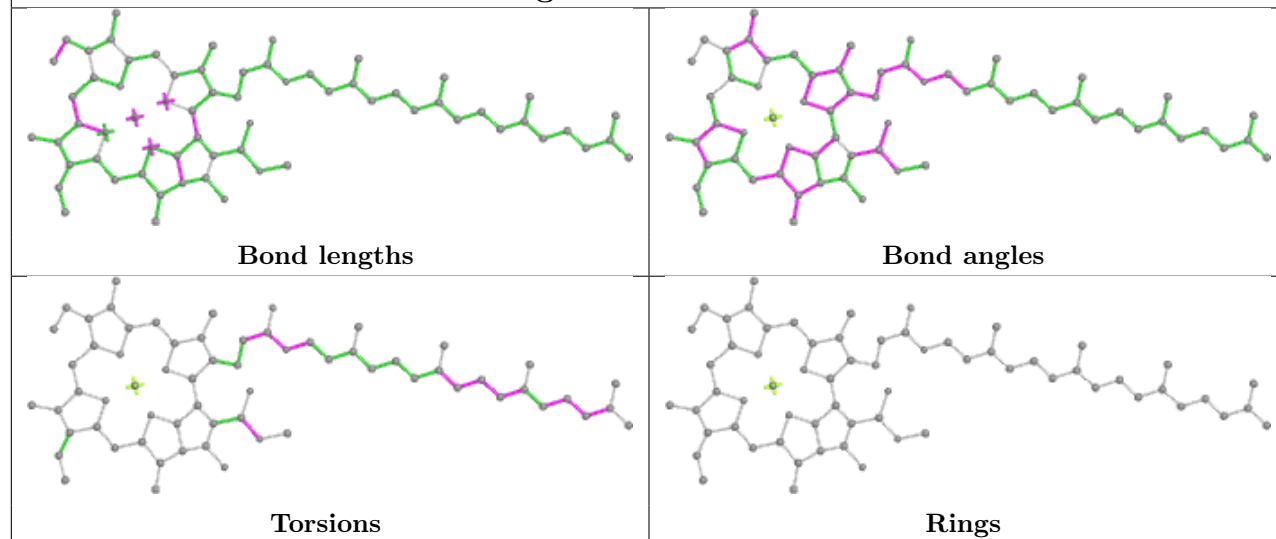


Ligand LUT 4 502

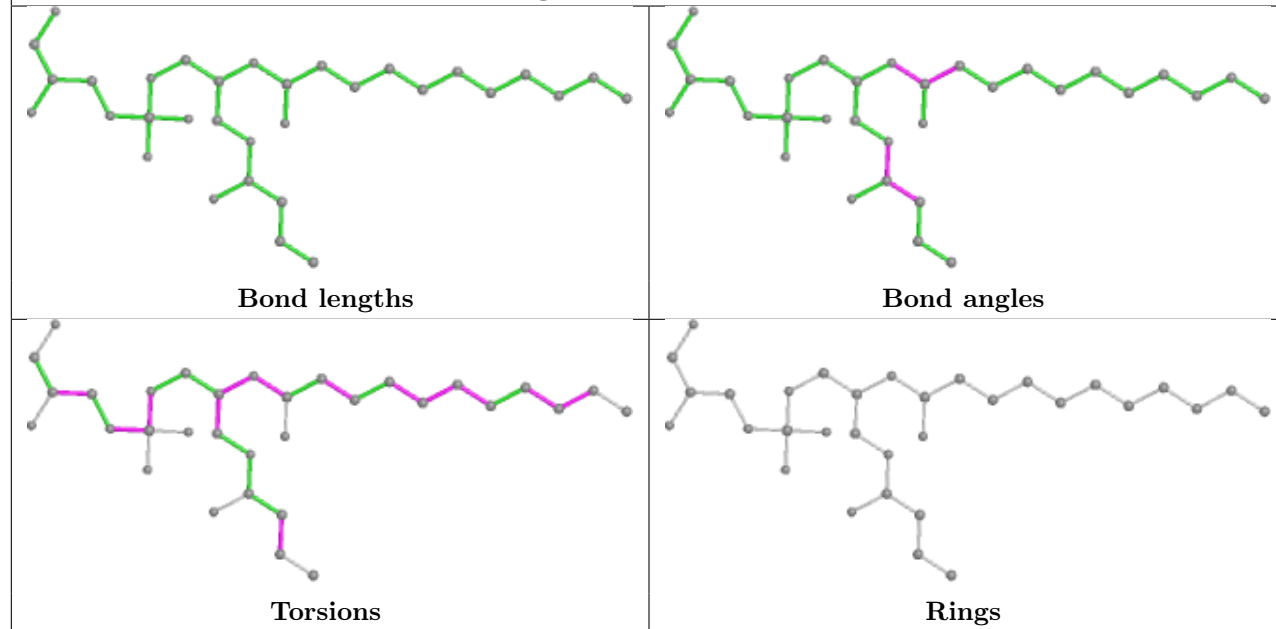


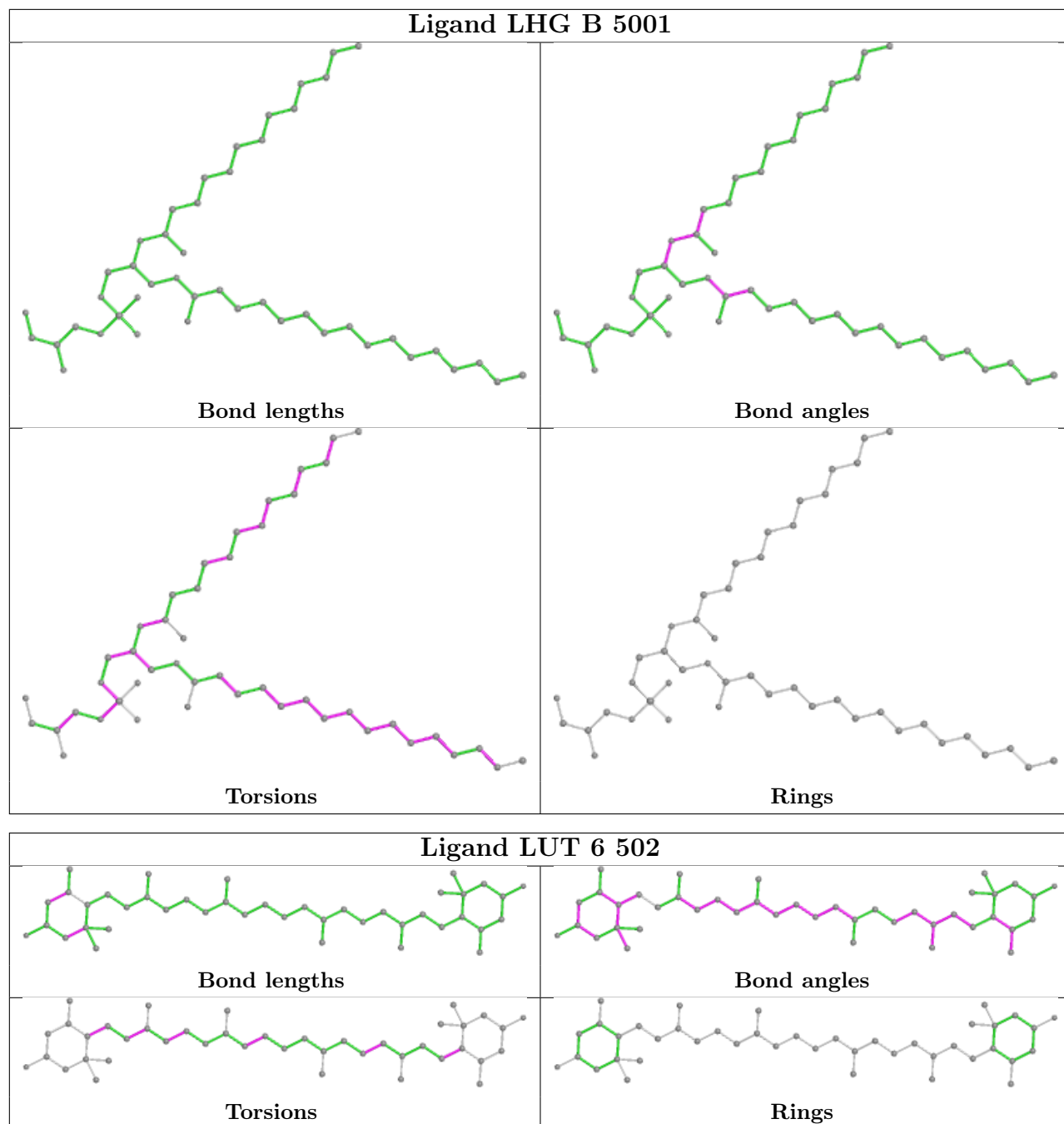


Ligand CLA 8 620

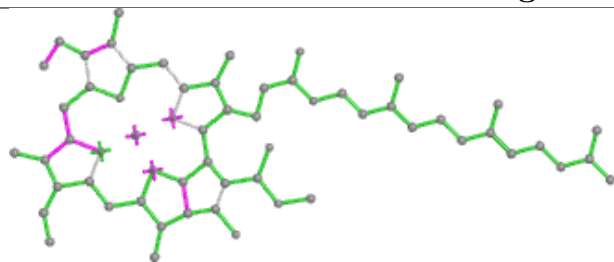


Ligand LHG 4 802

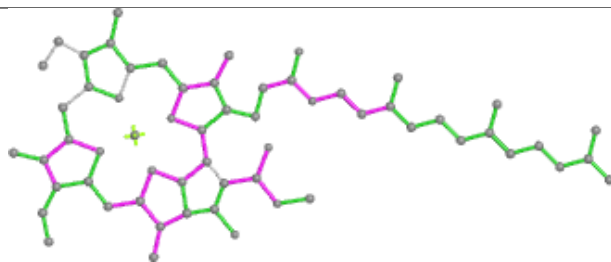




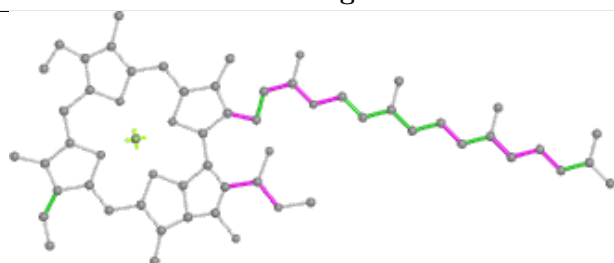
Ligand CLA 1 608



Bond lengths



Bond angles

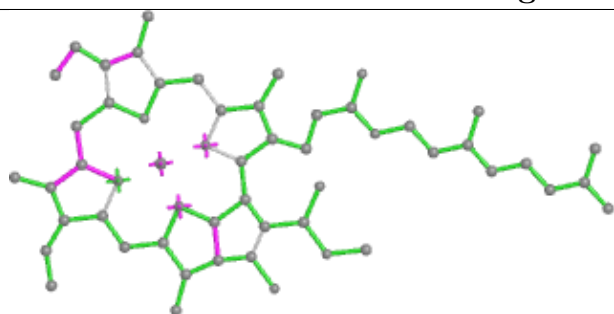


Torsions

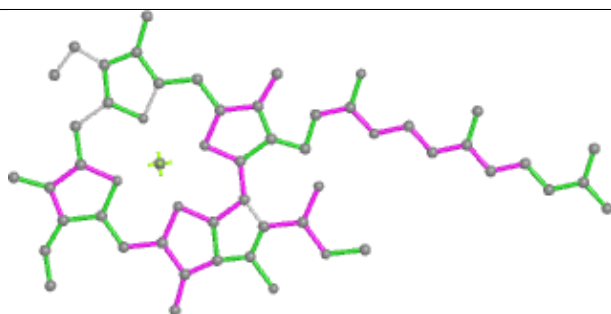


Rings

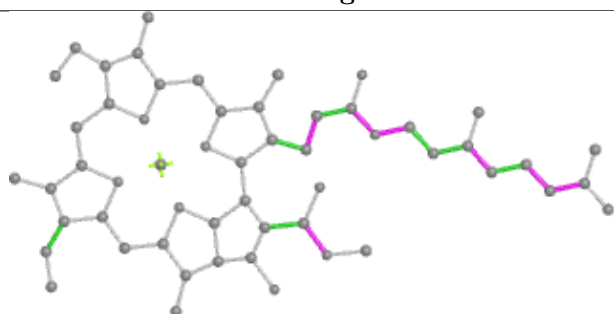
Ligand CLA 1 611



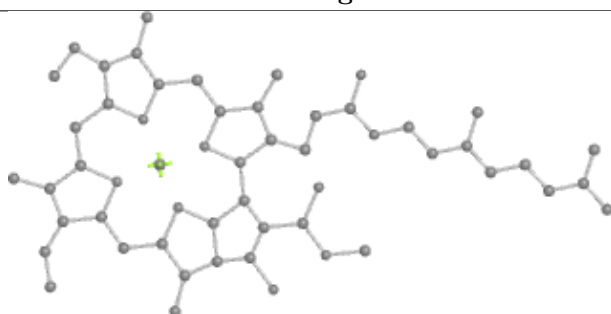
Bond lengths



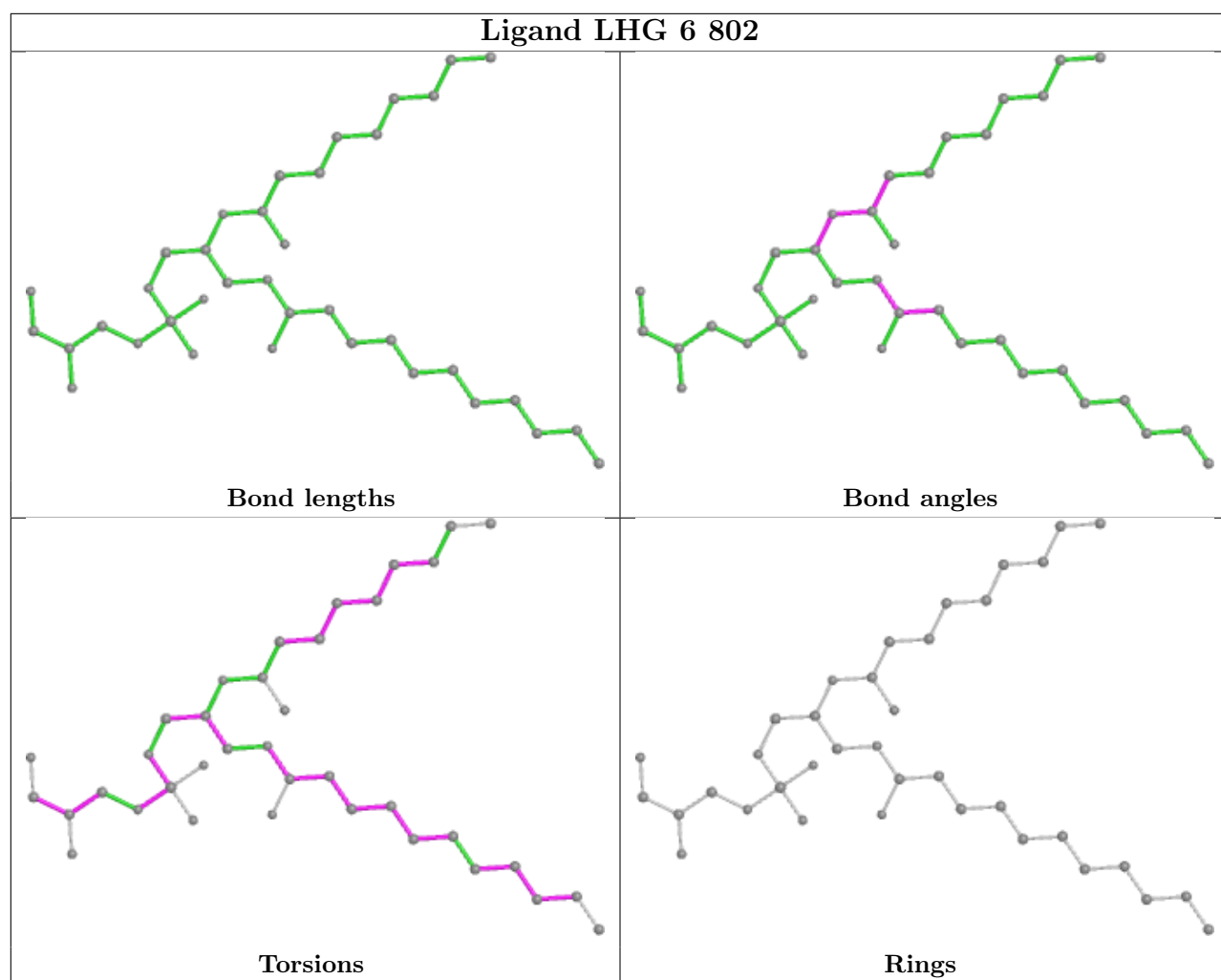
Bond angles



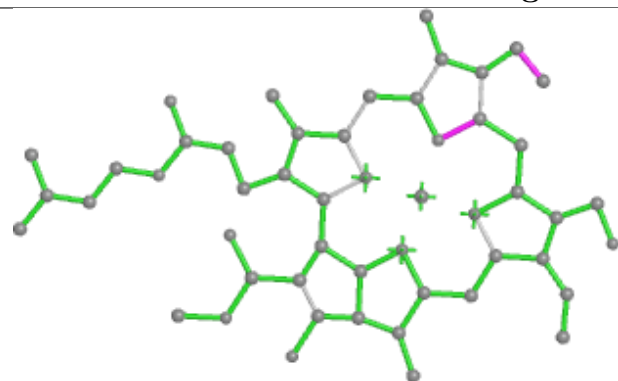
Torsions



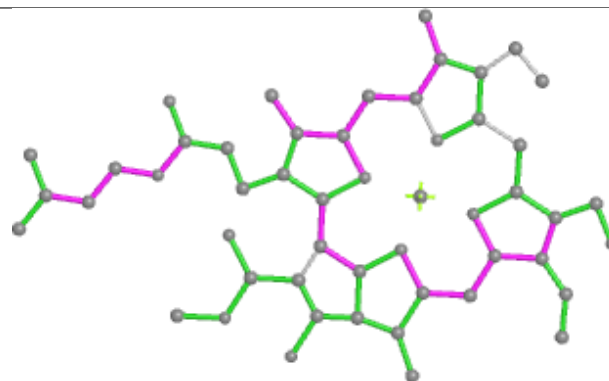
Rings



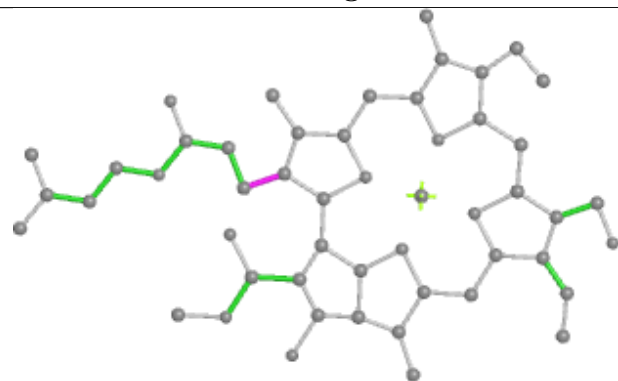
Ligand CHL 6 613



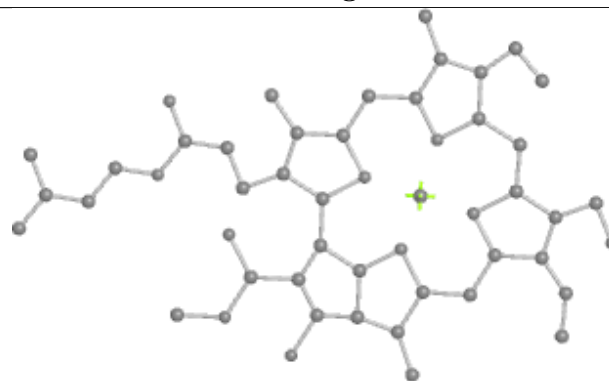
Bond lengths



Bond angles

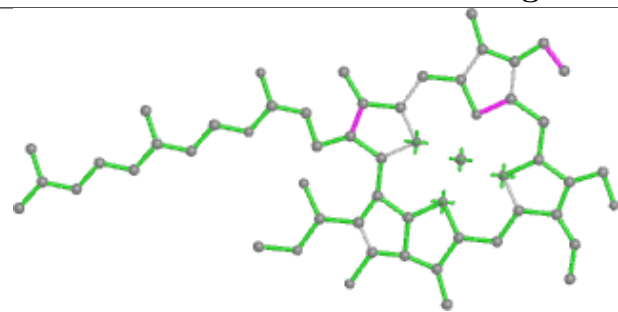


Torsions

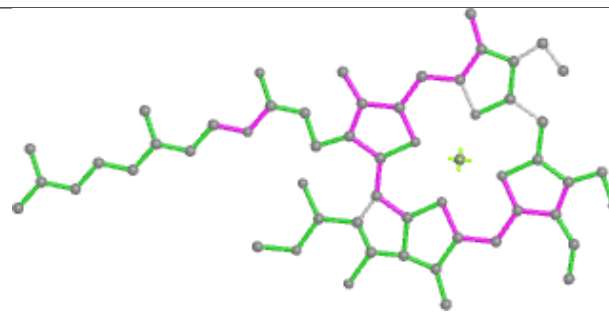


Rings

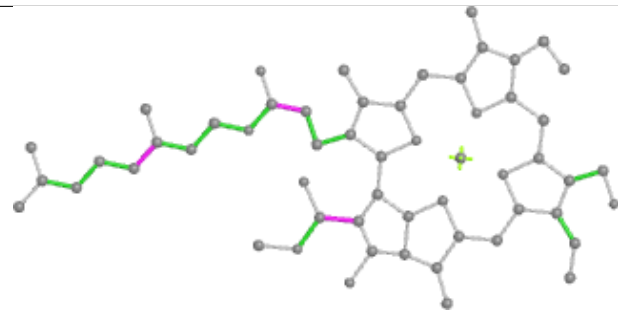
Ligand CHL 6 610



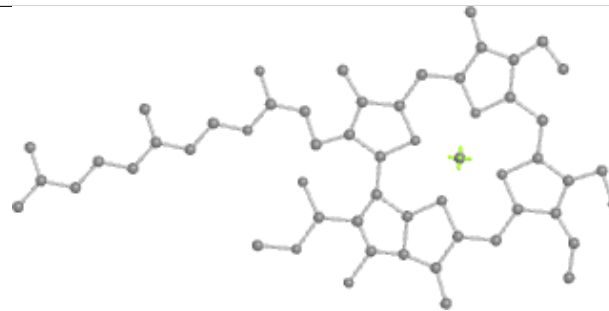
Bond lengths



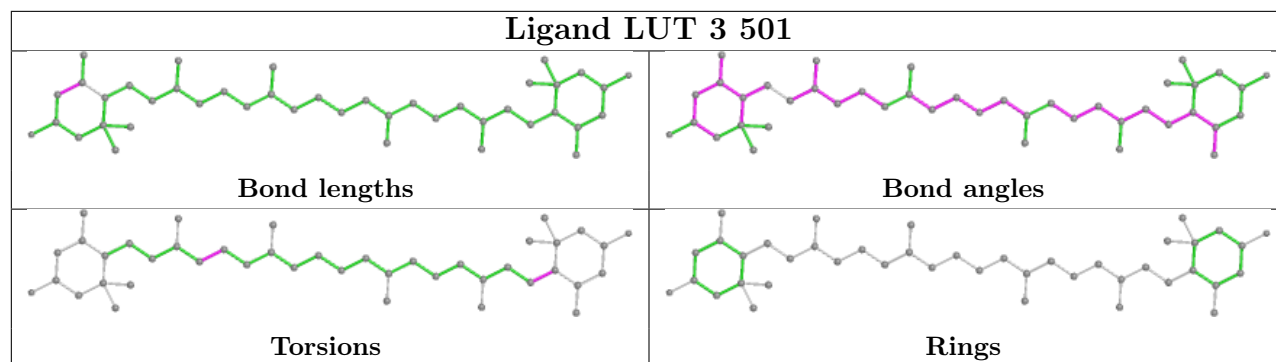
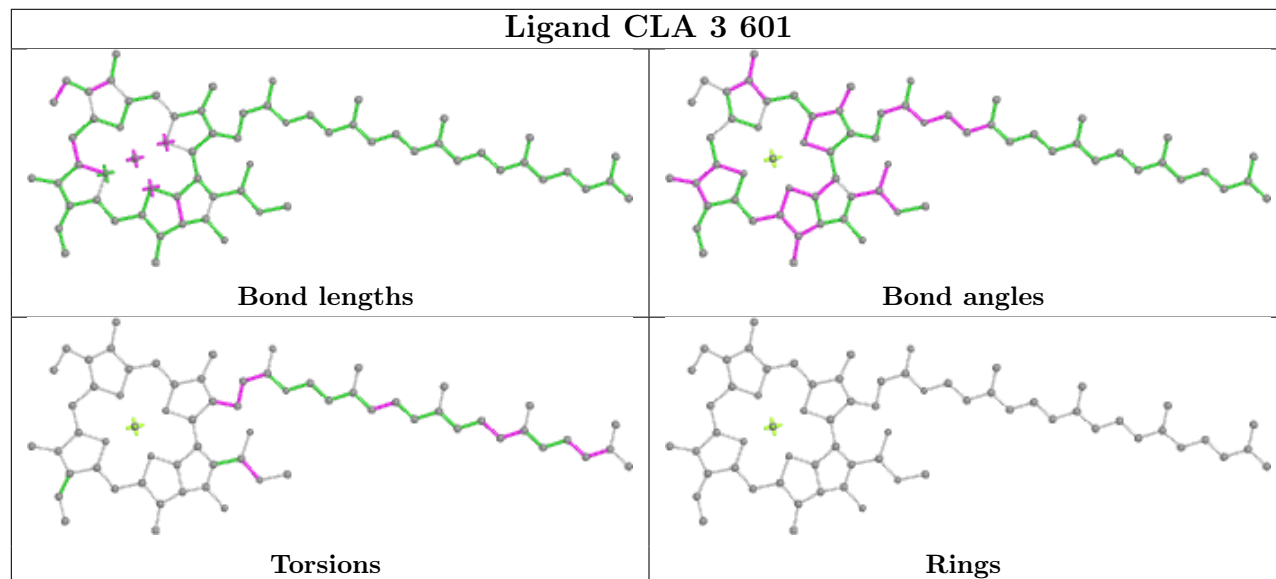
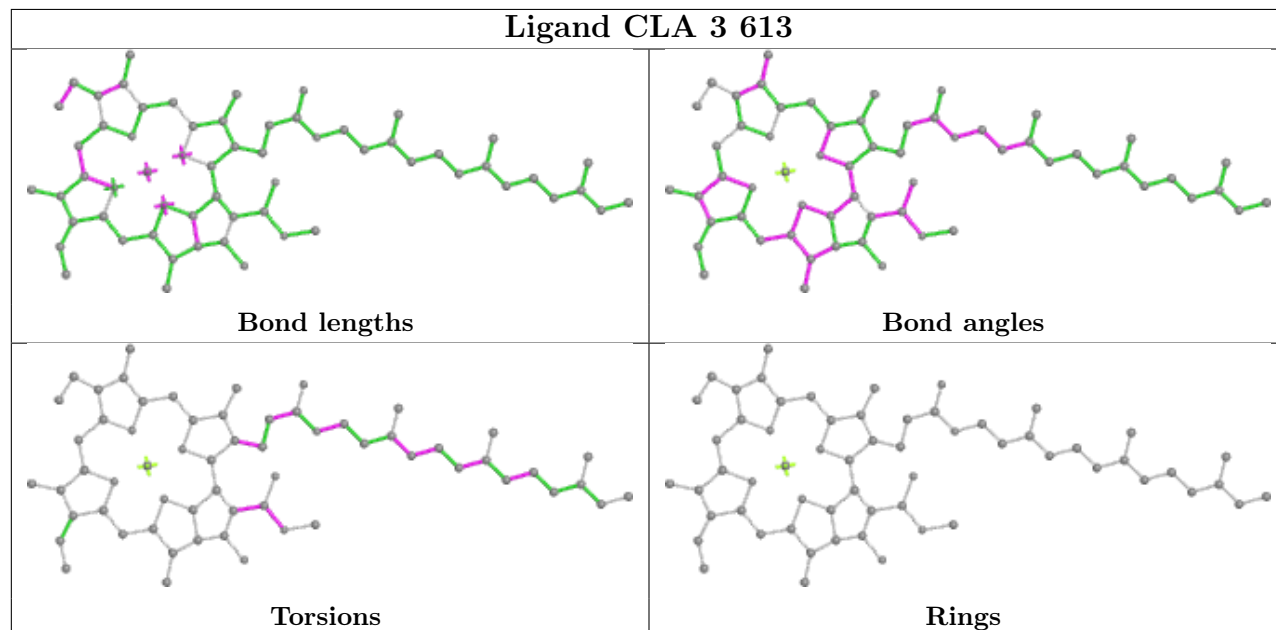
Bond angles

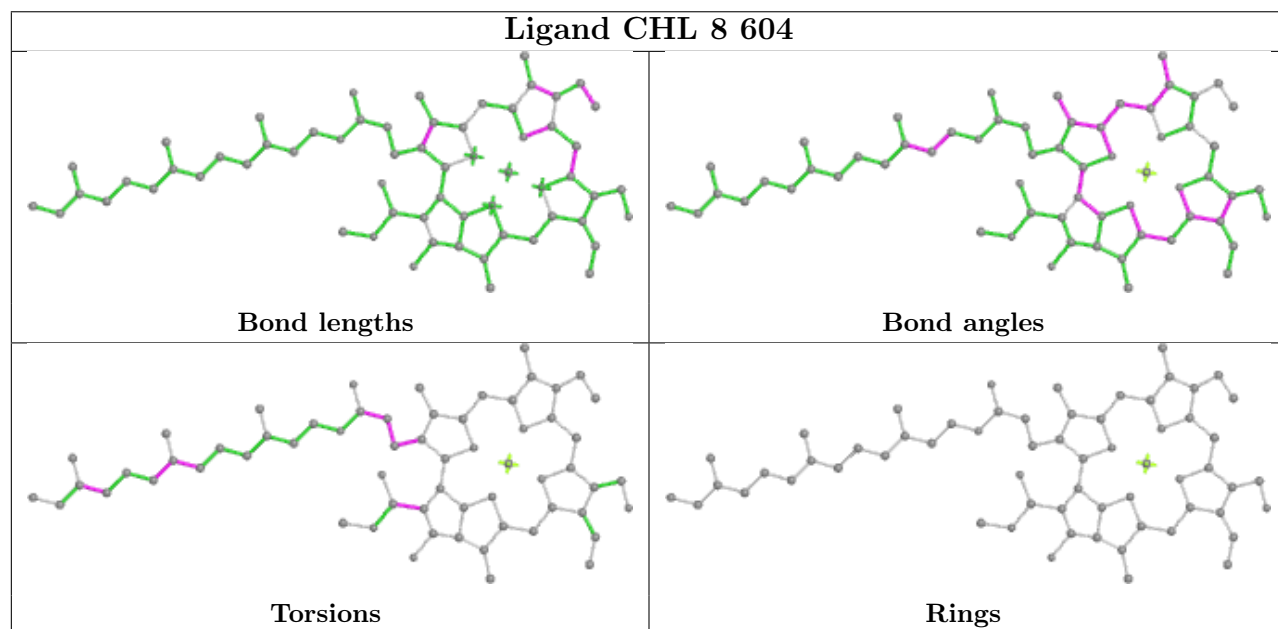
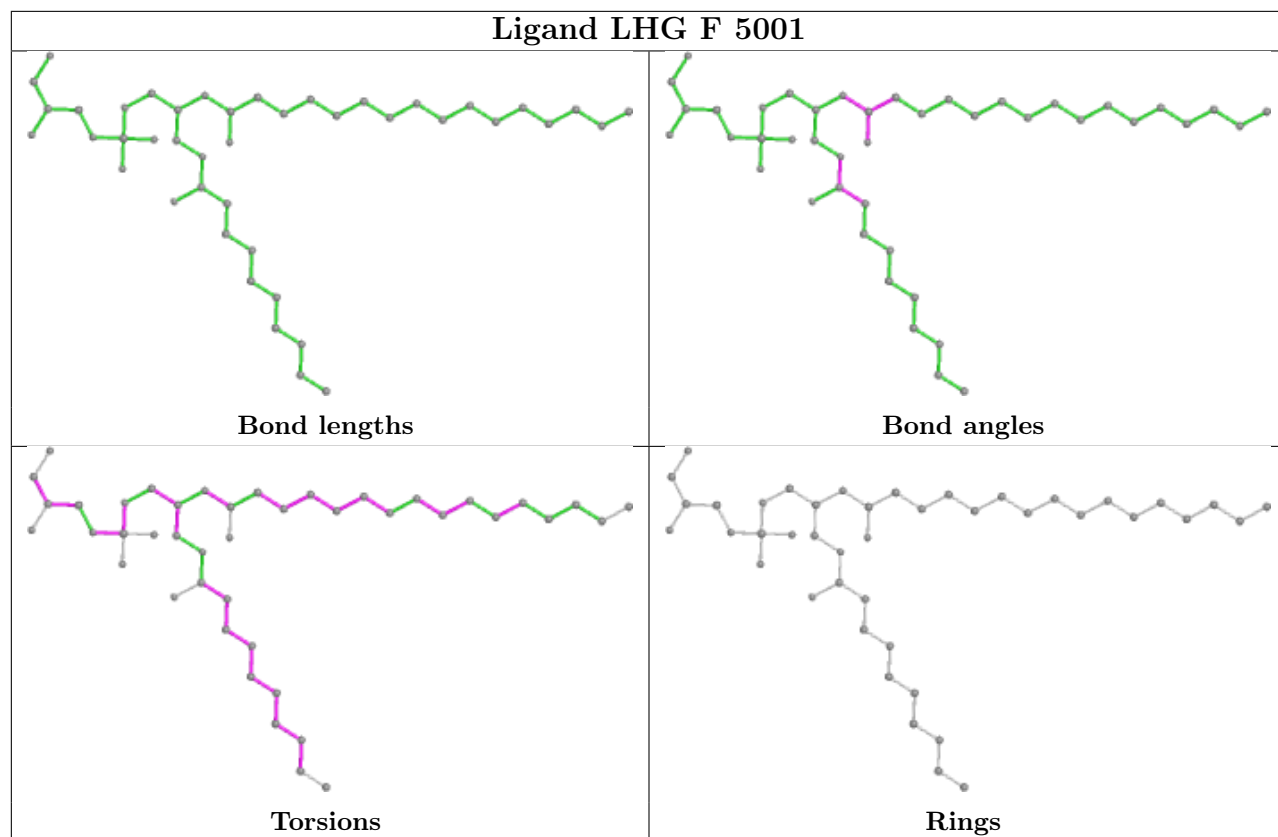


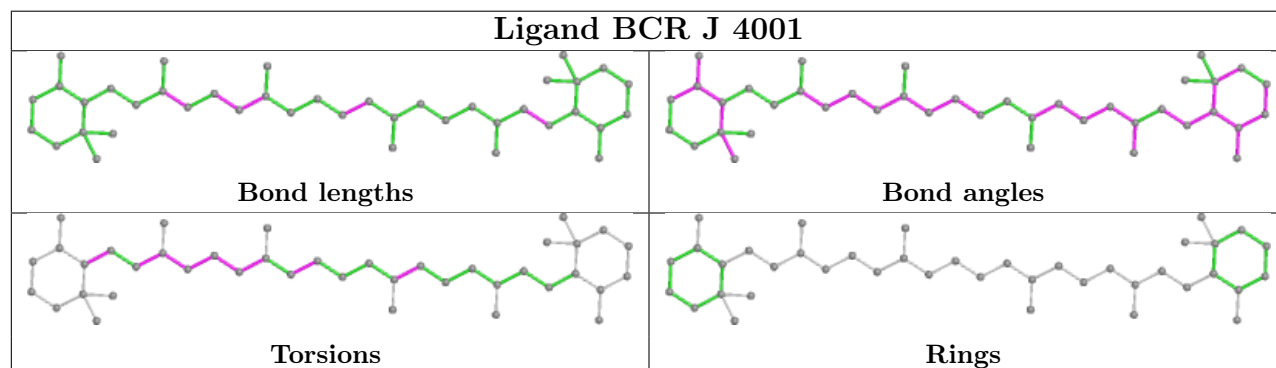
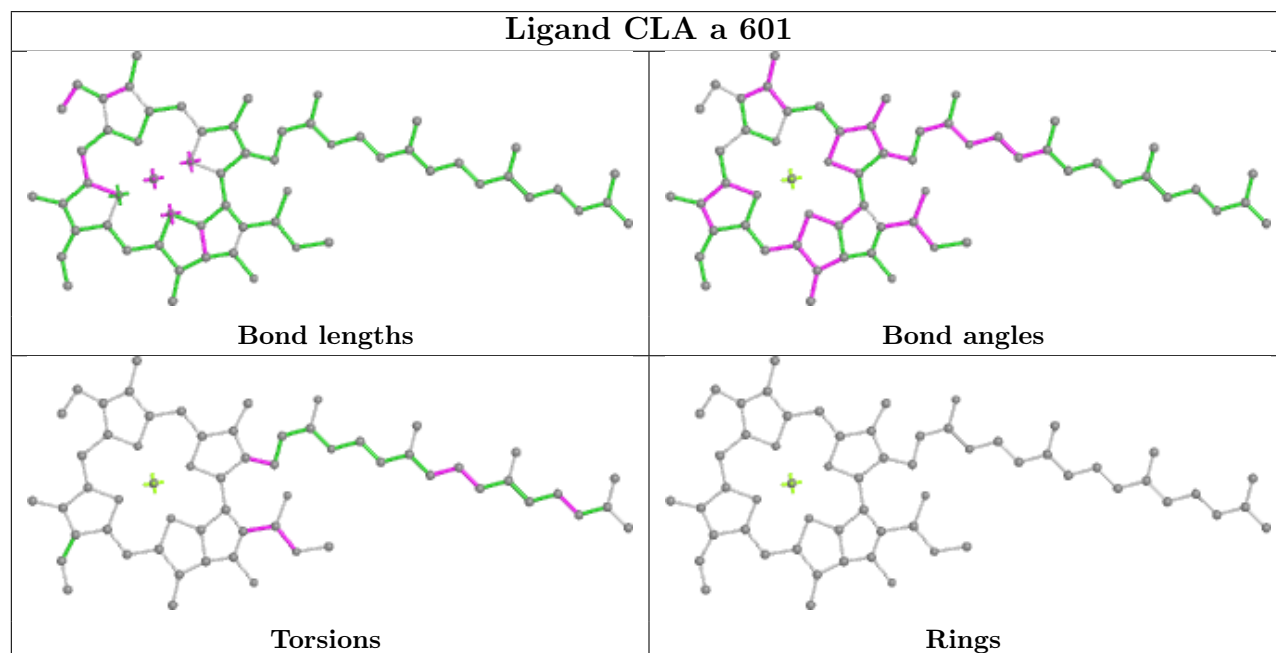
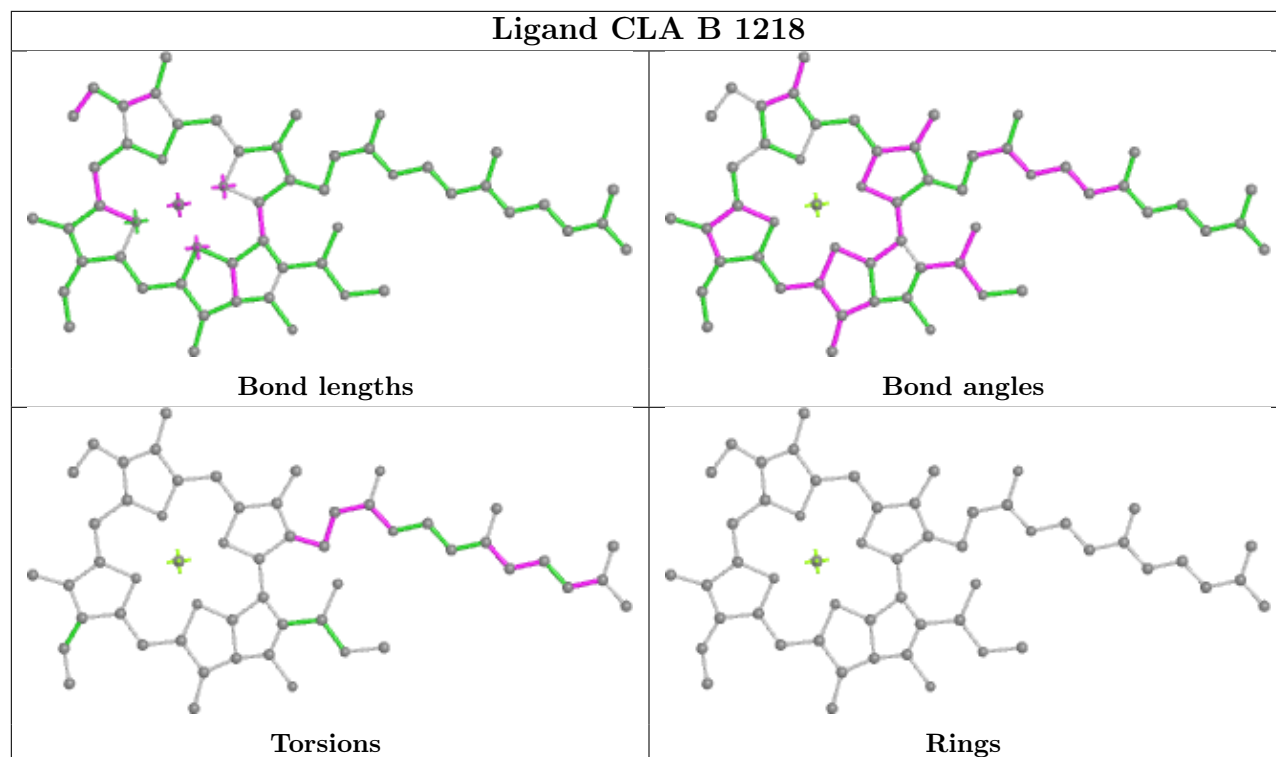
Torsions

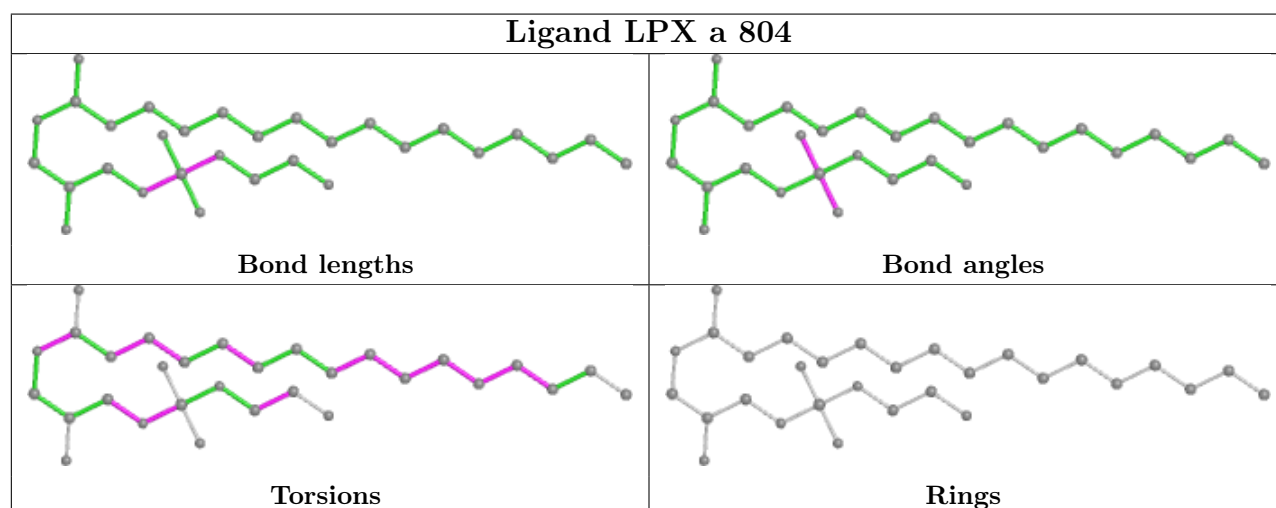
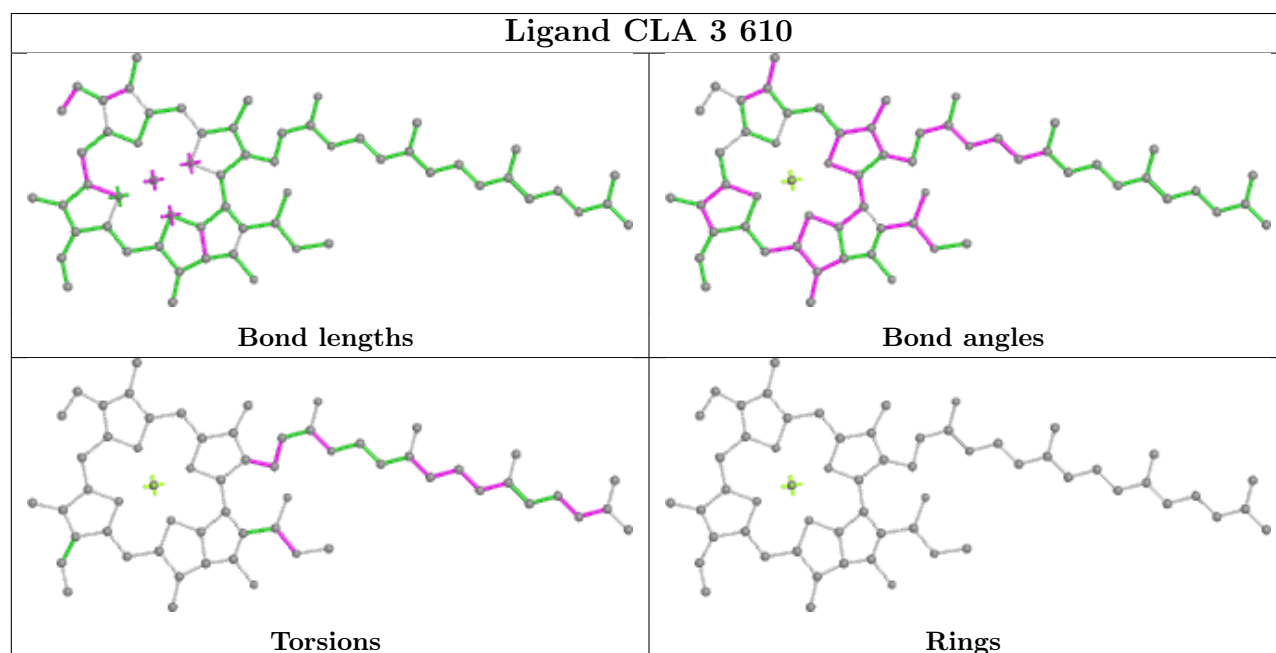
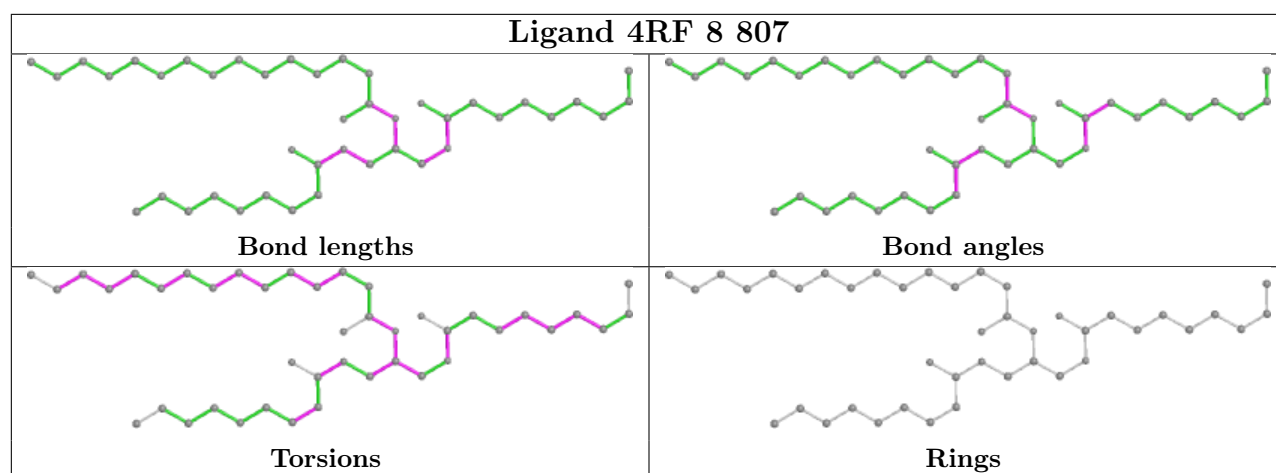


Rings

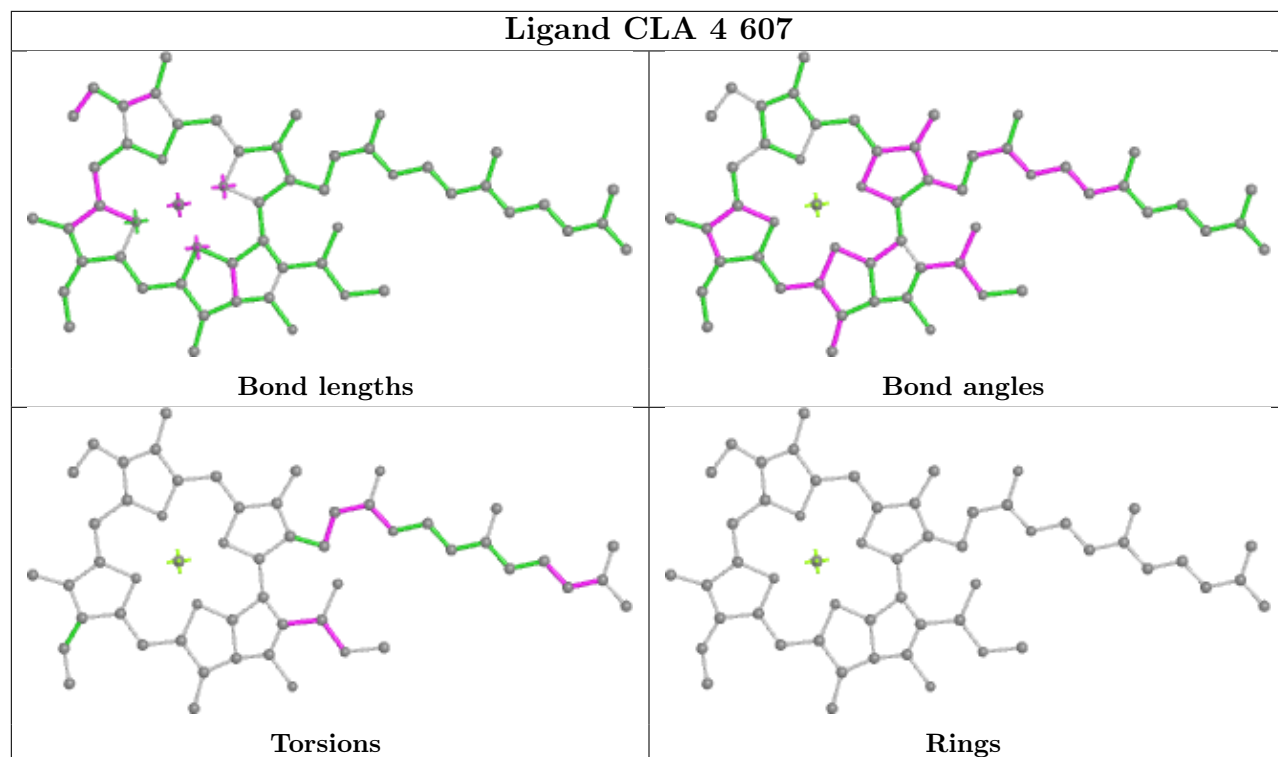
Ligand LUT 3 501**Ligand CLA 3 601****Ligand CLA 3 613**



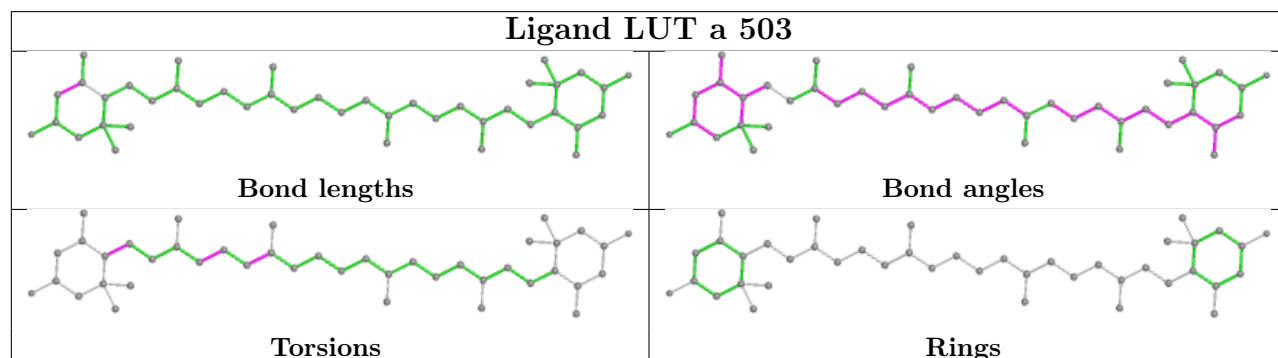




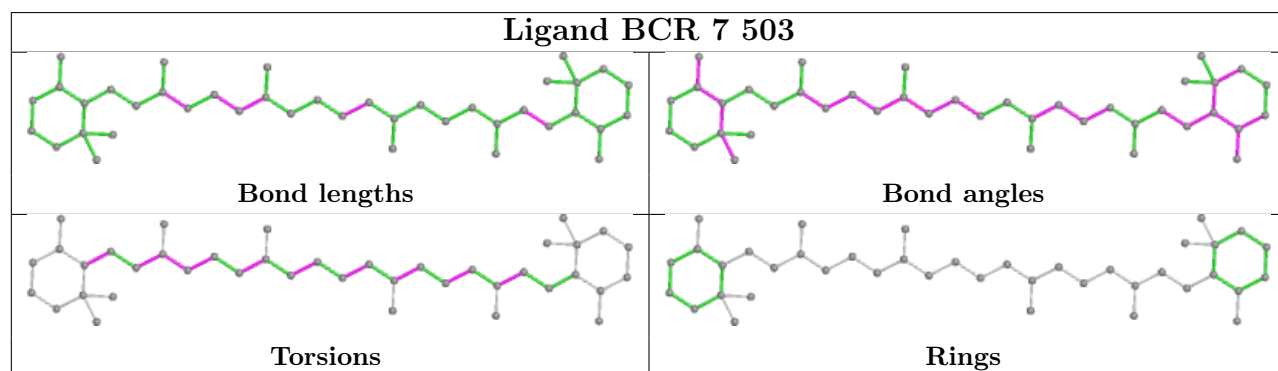
Ligand CLA 4 607

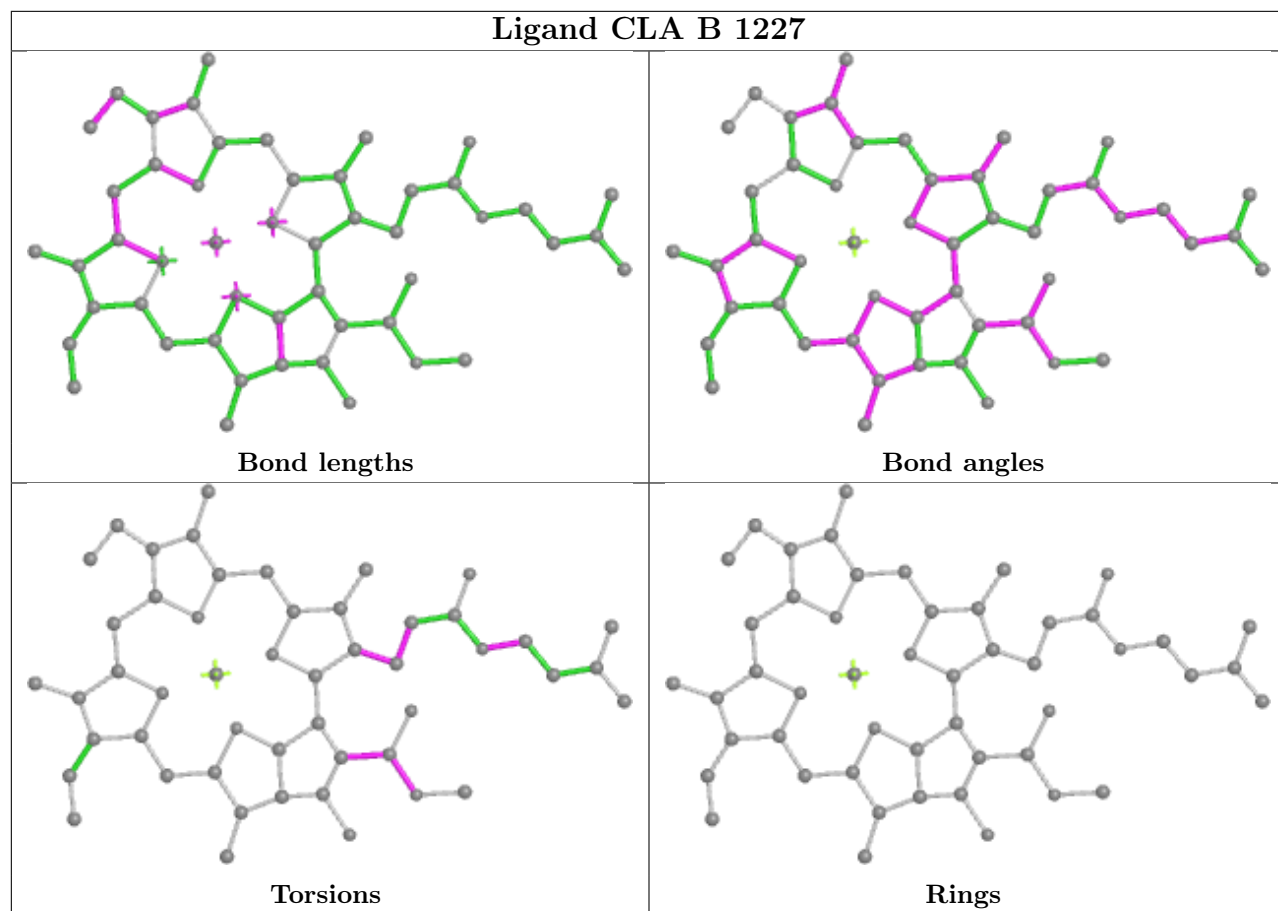
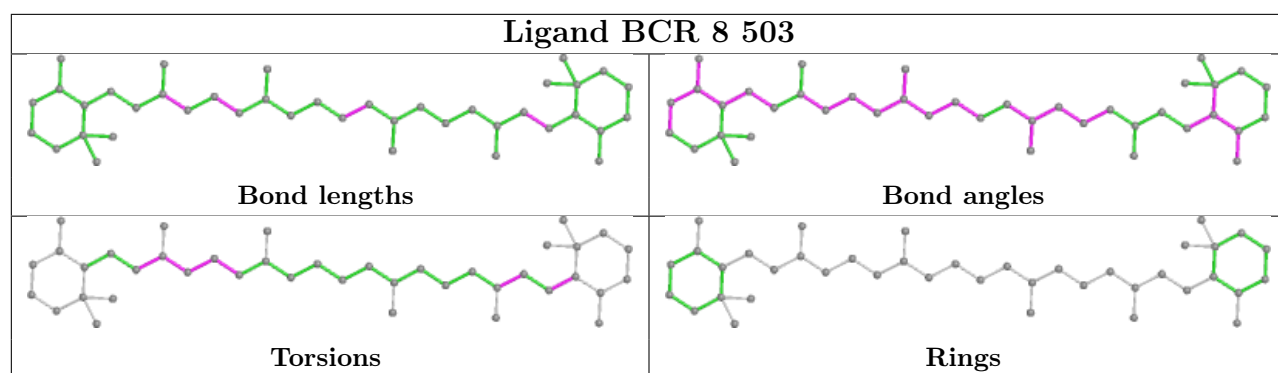


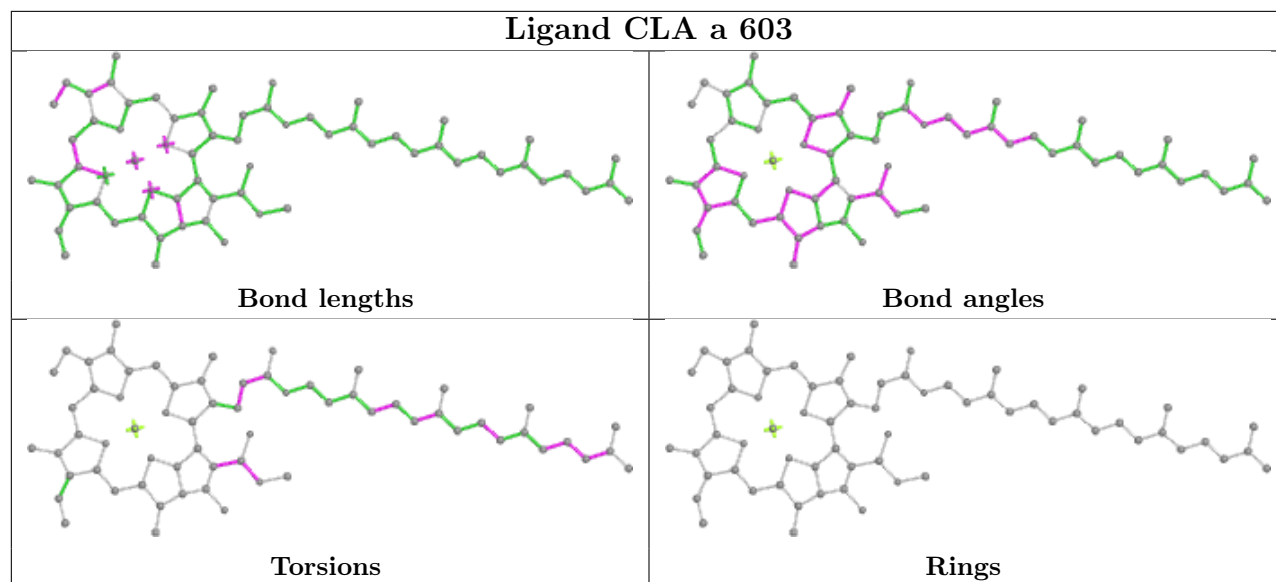
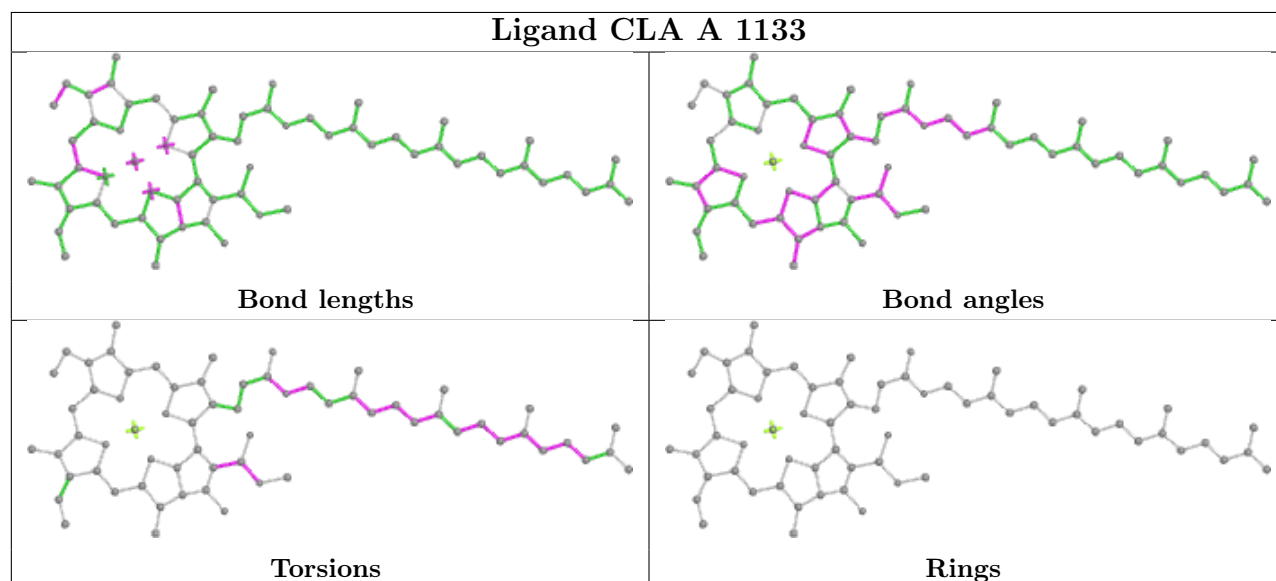
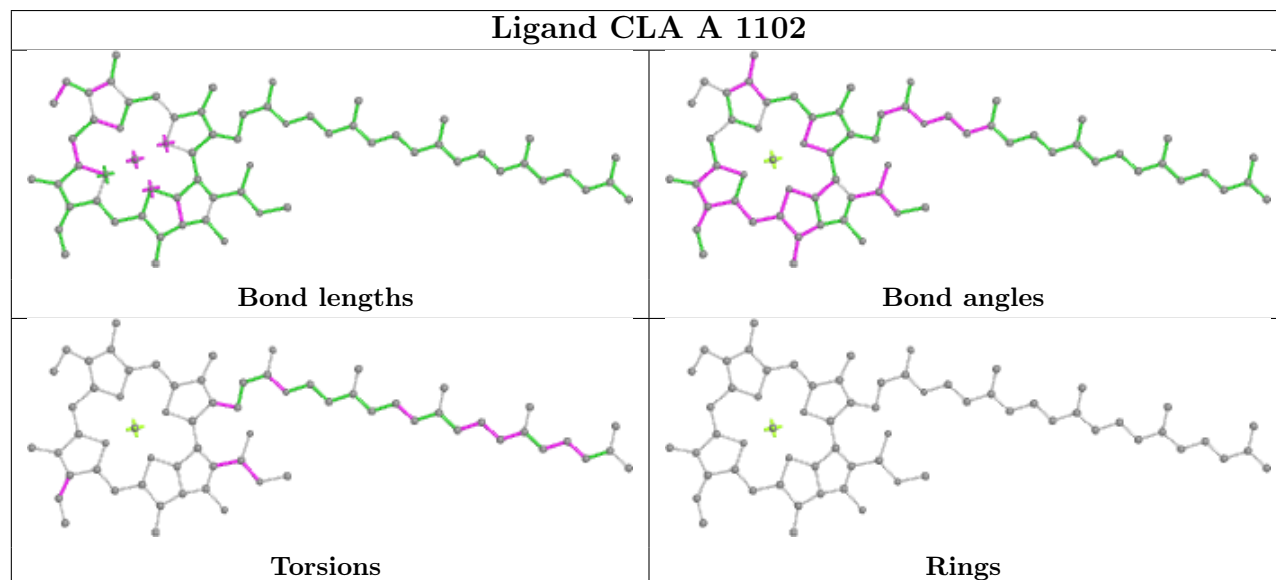
Ligand LUT a 503



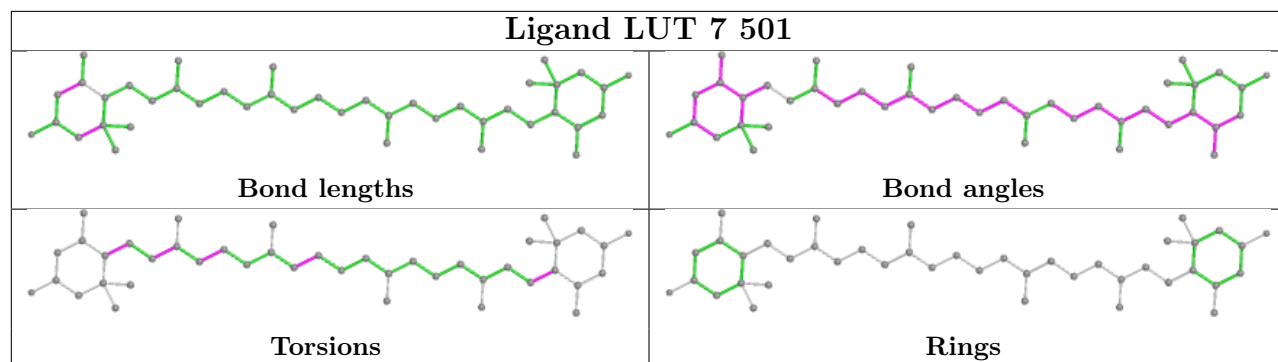
Ligand BCR 7 503



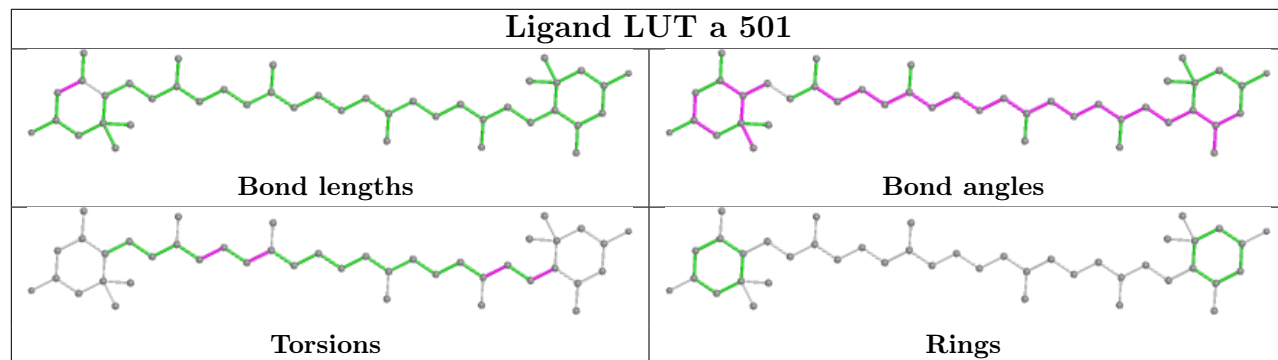


Ligand CLA a 603**Ligand CLA A 1133****Ligand CLA A 1102**

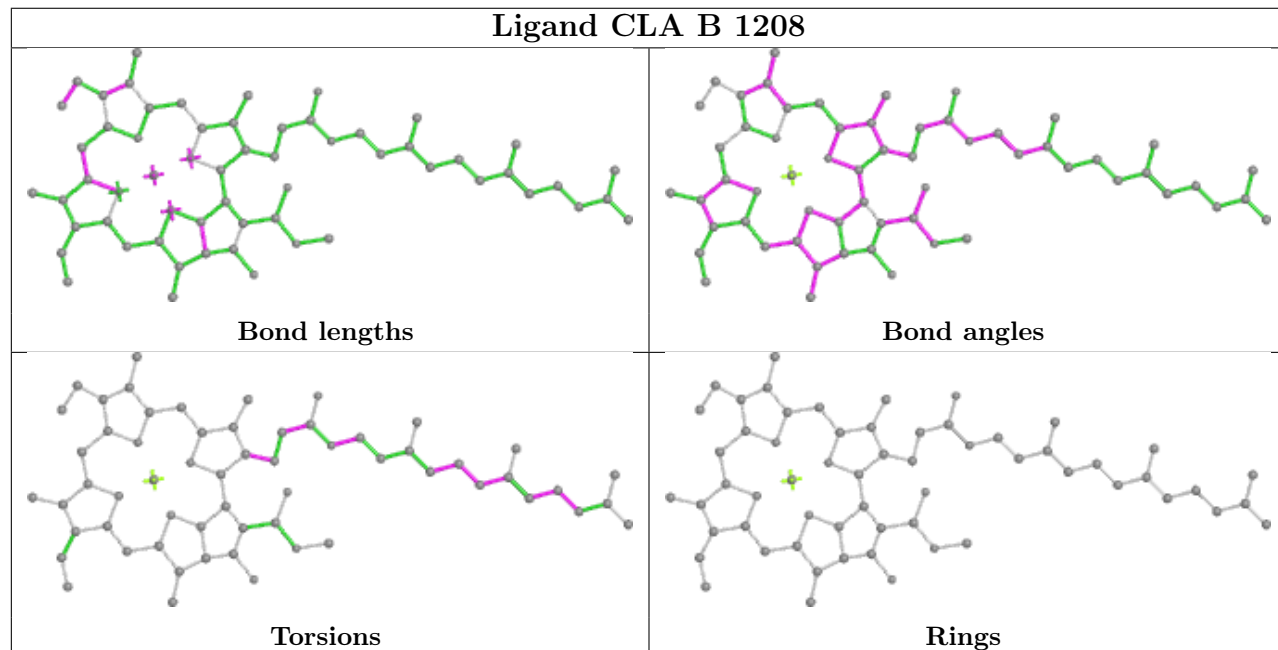
Ligand LUT 7 501



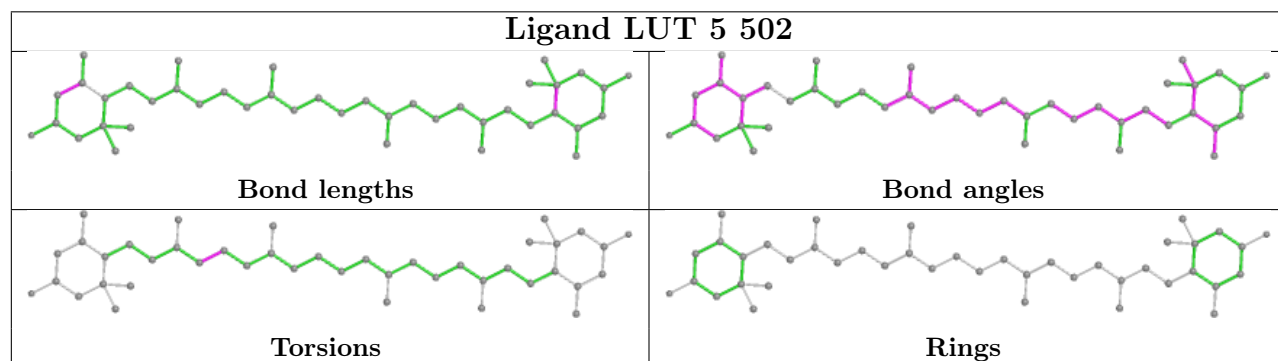
Ligand LUT a 501



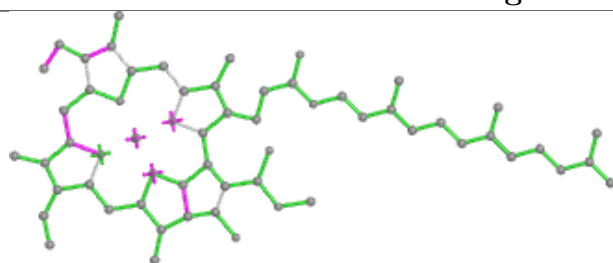
Ligand CLA B 1208



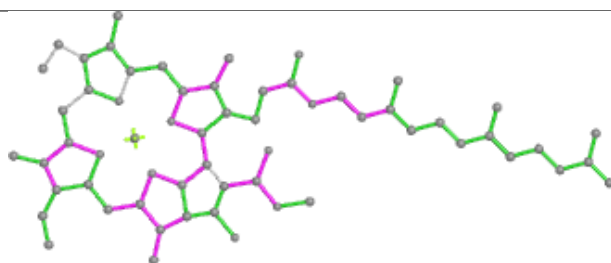
Ligand LUT 5 502



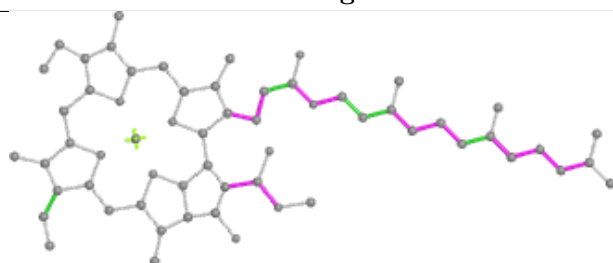
Ligand CLA A 1134



Bond lengths



Bond angles

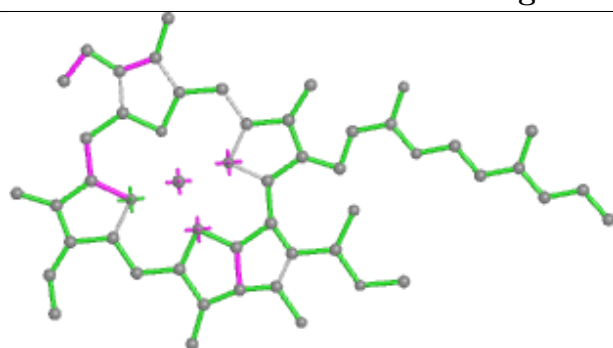


Torsions

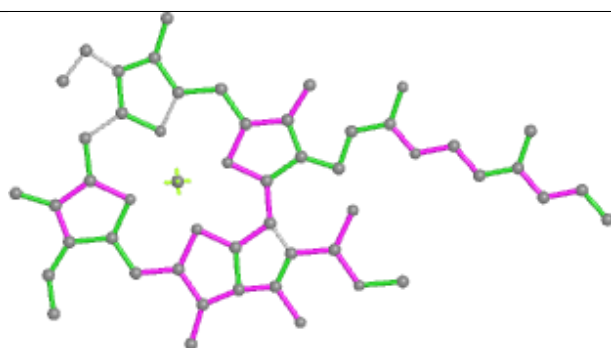


Rings

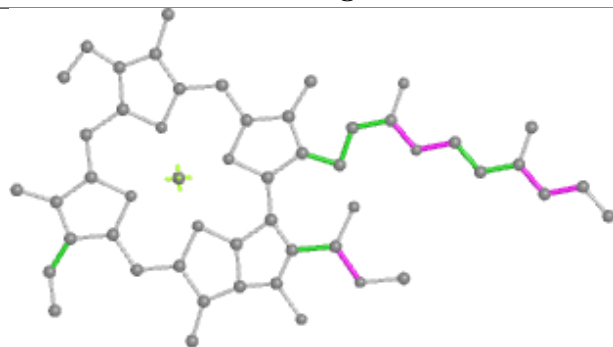
Ligand CLA 8 602



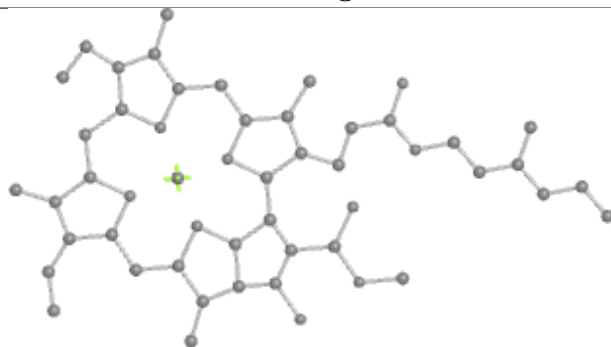
Bond lengths



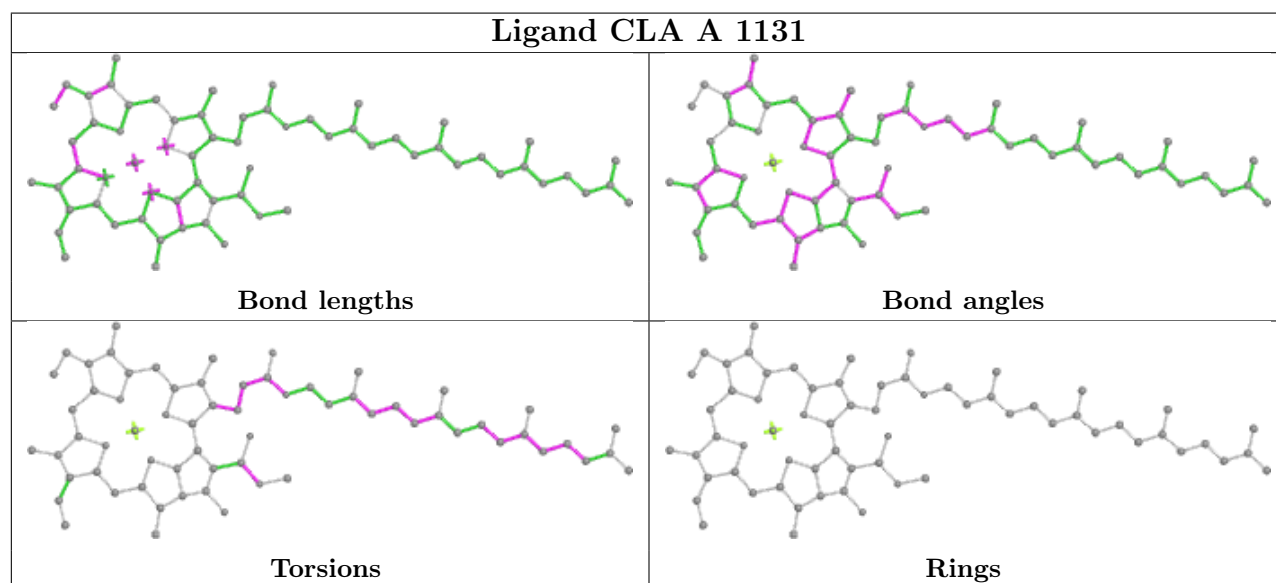
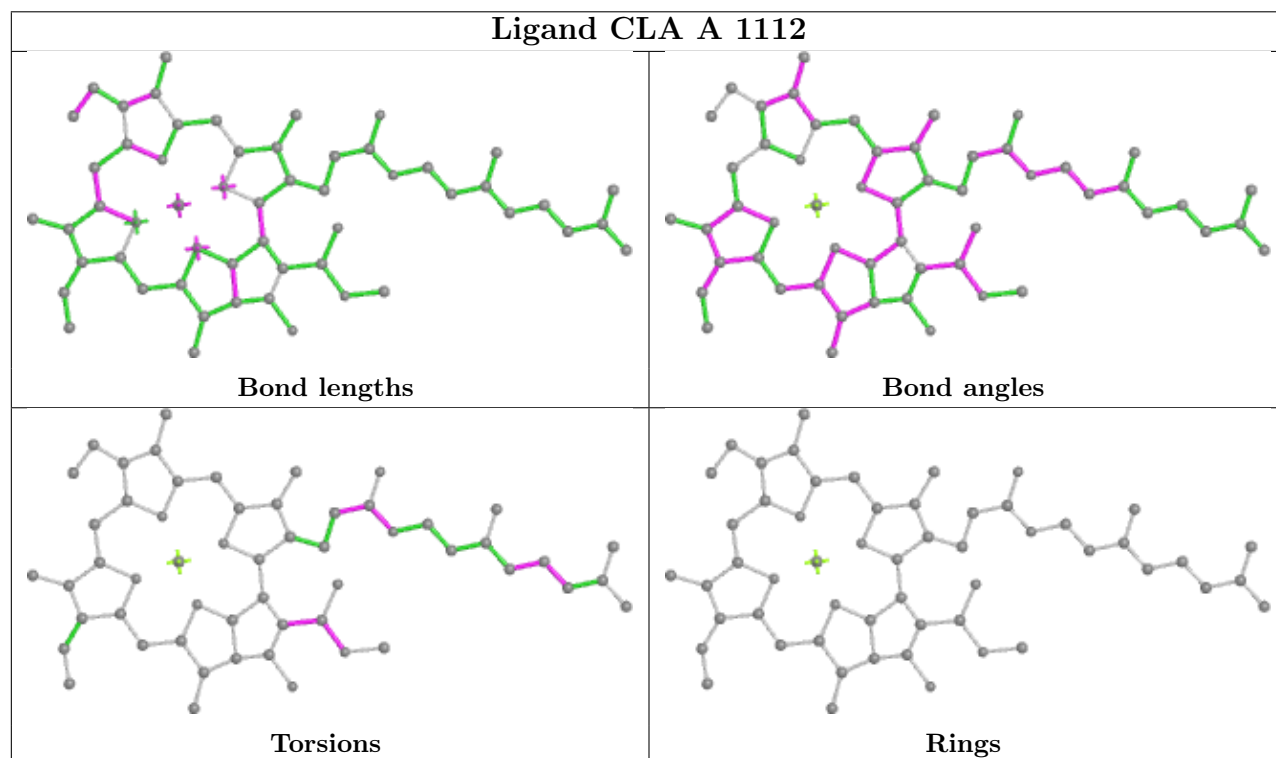
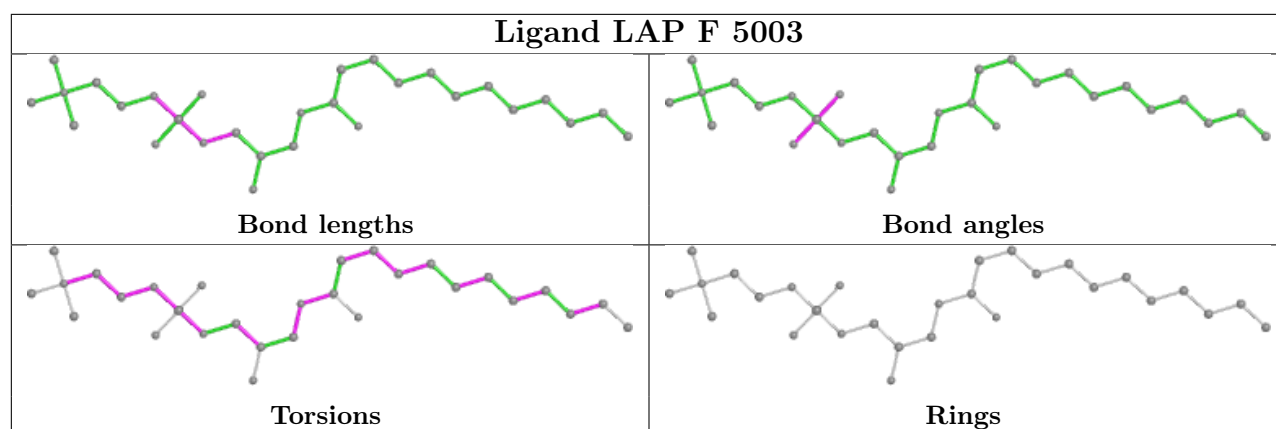
Bond angles



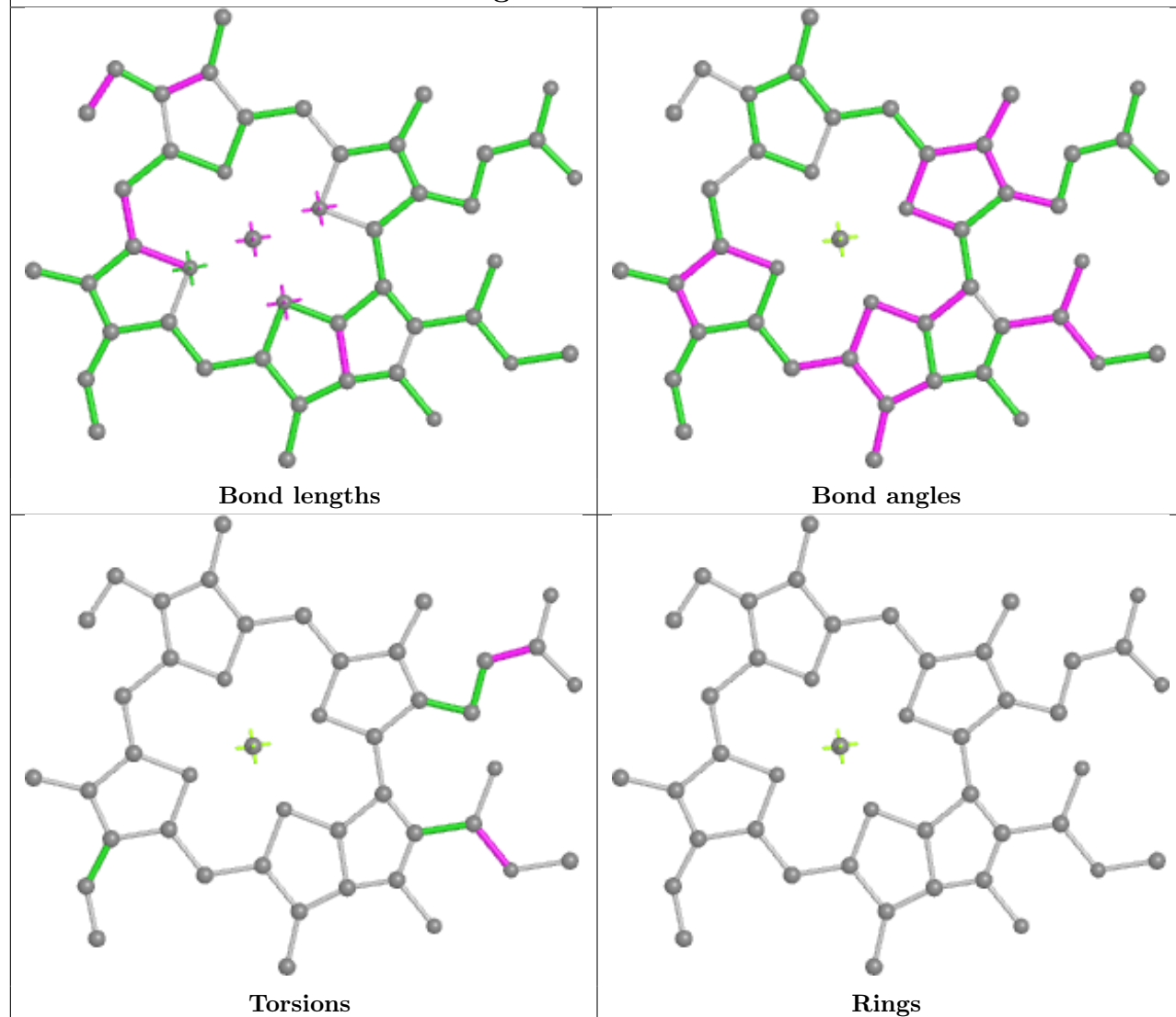
Torsions

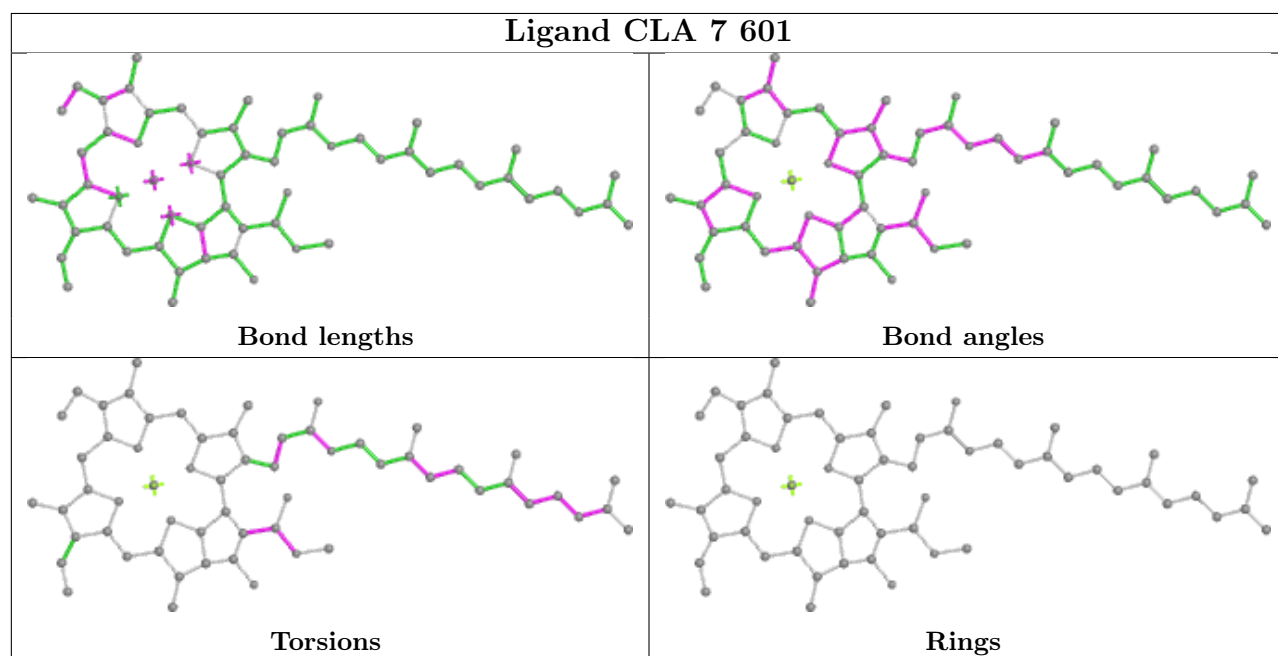
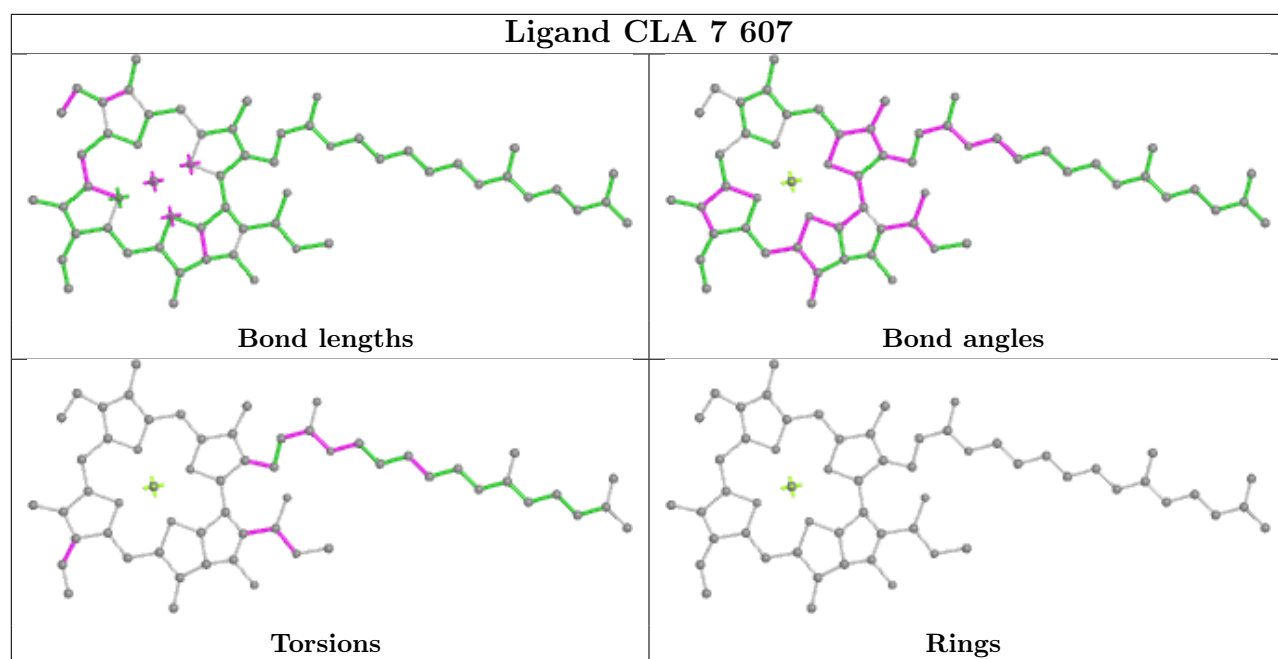


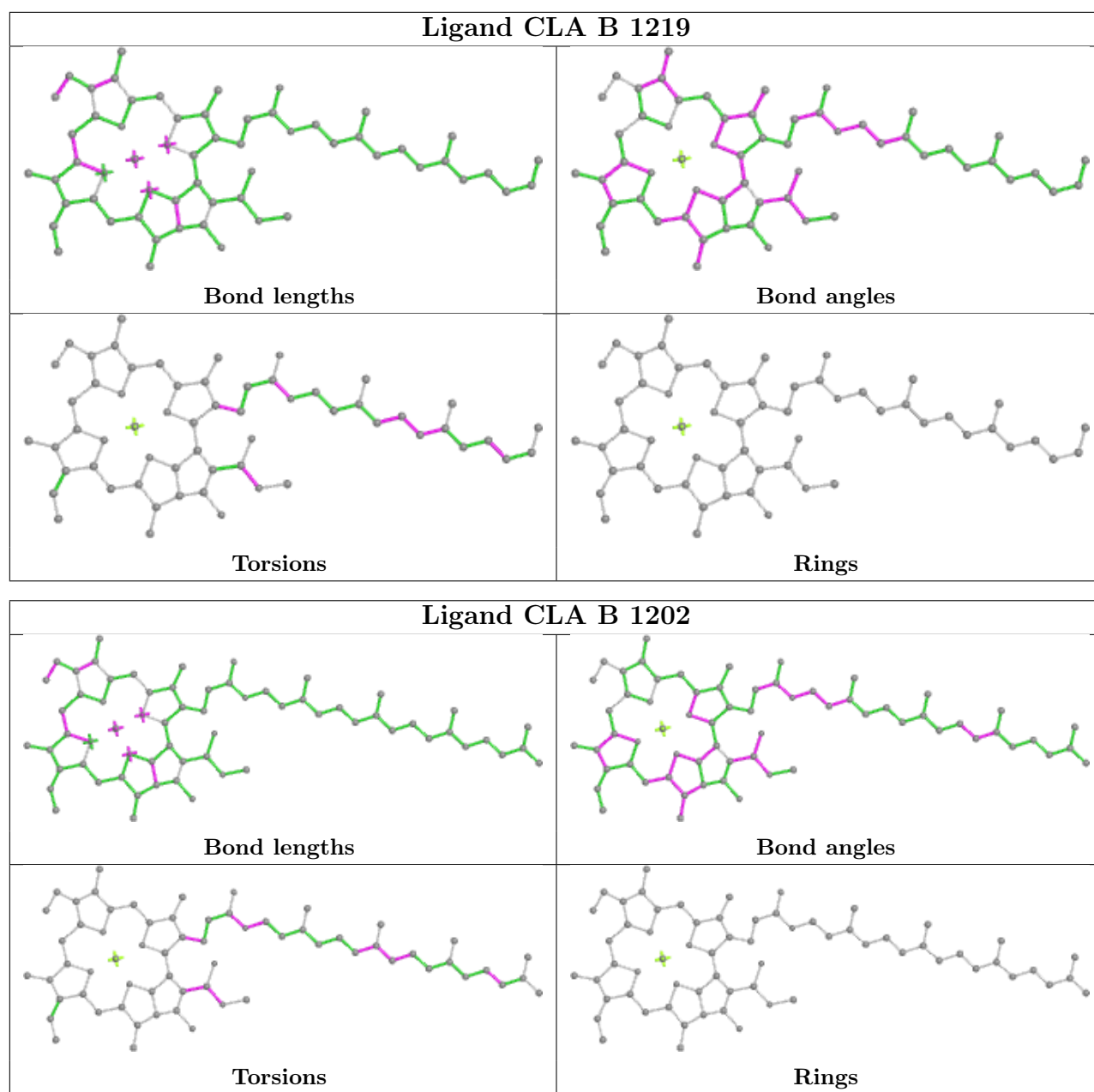
Rings

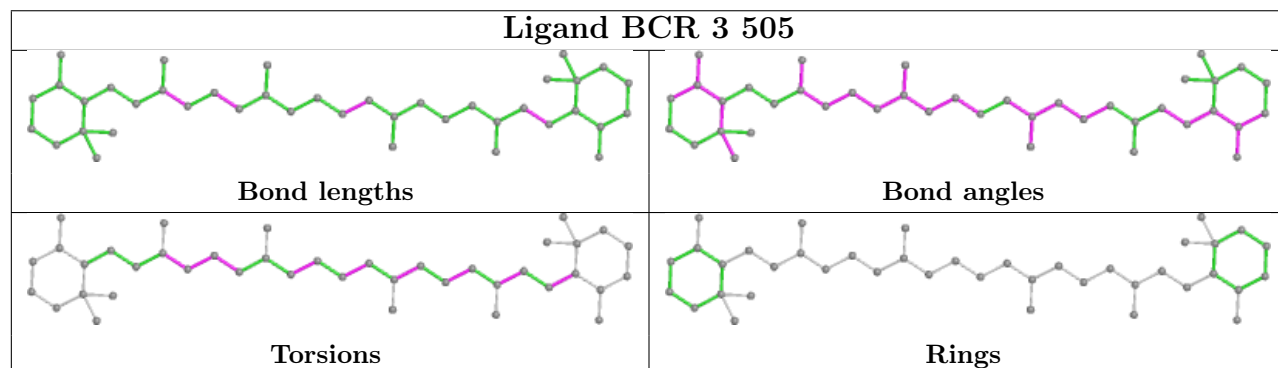
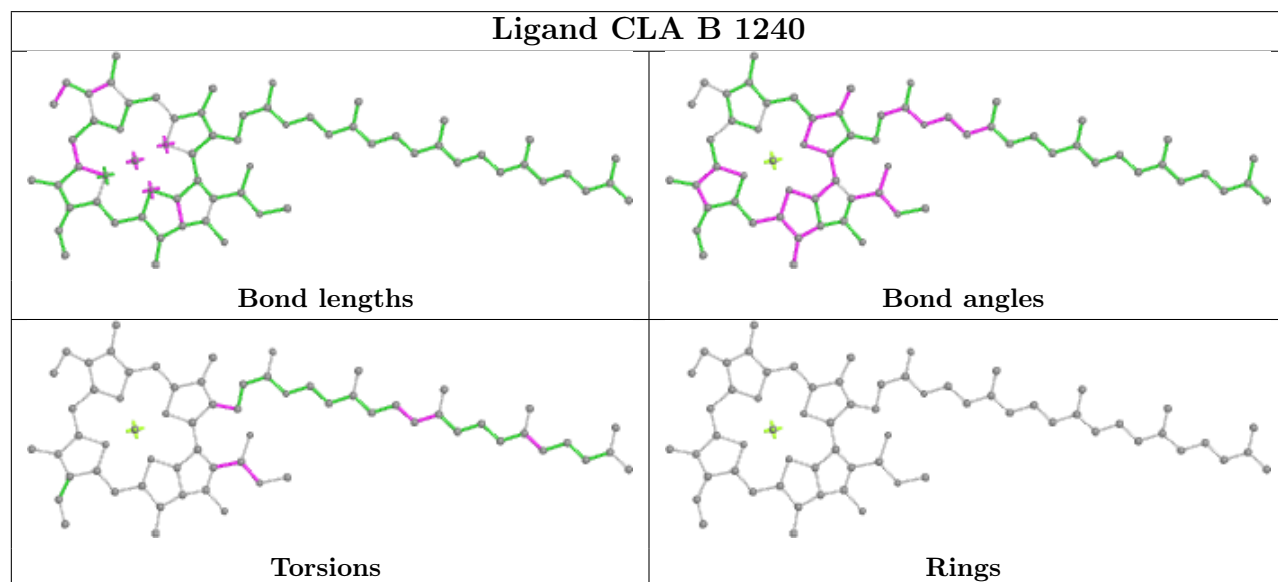
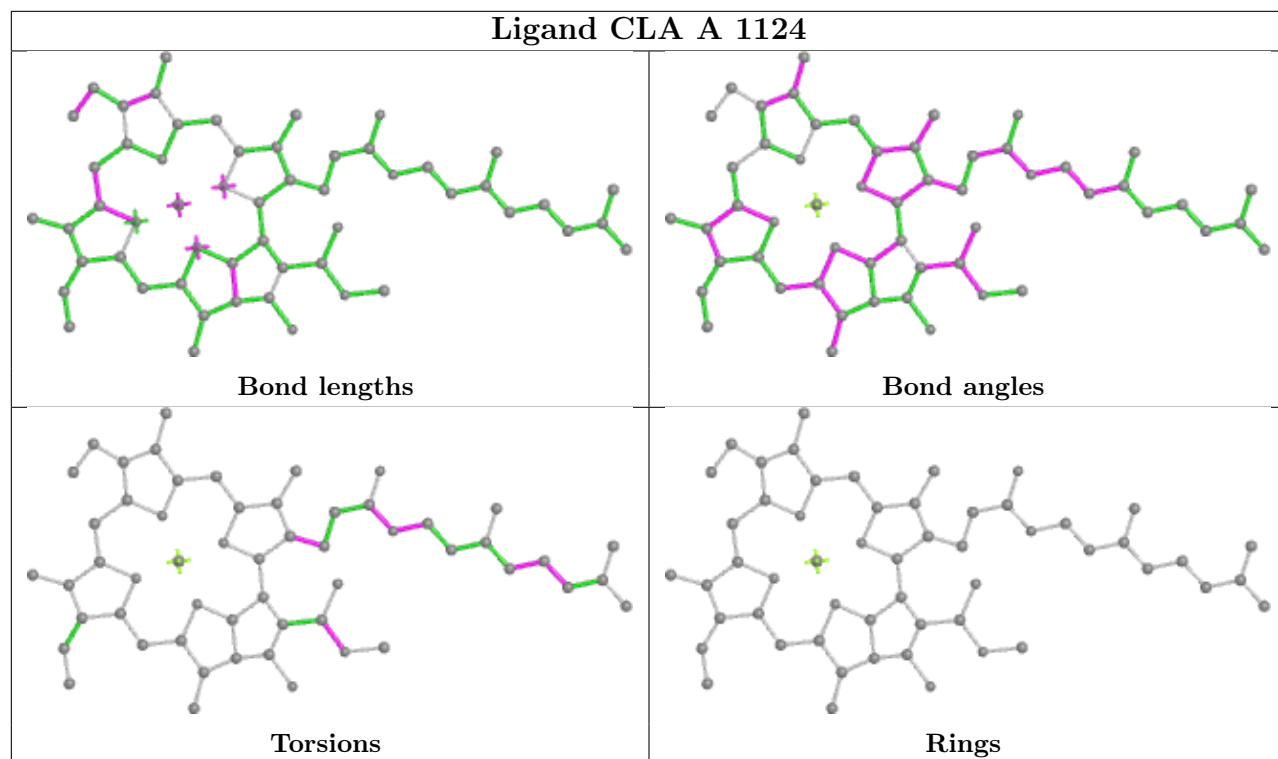


Ligand CLA 6 608

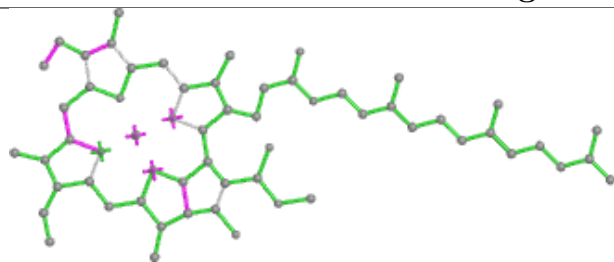




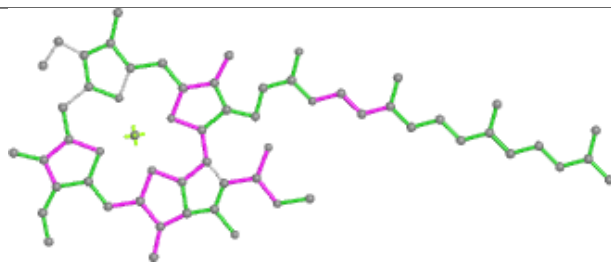




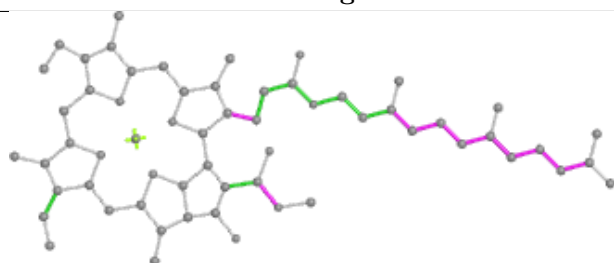
Ligand CLA 6 601



Bond lengths



Bond angles

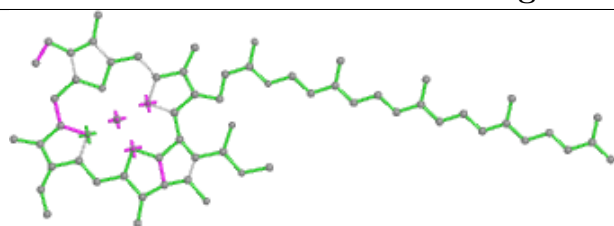


Torsions

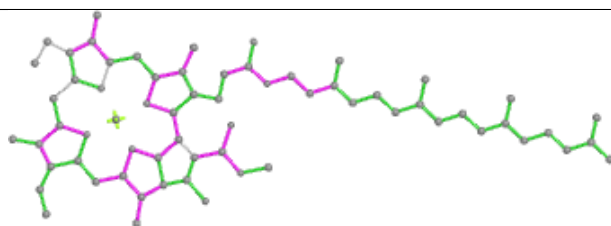


Rings

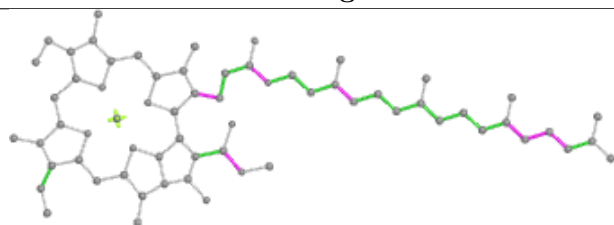
Ligand CLA 3 607



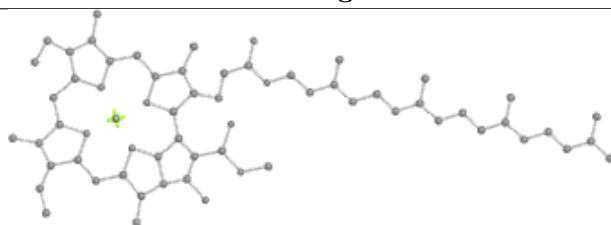
Bond lengths



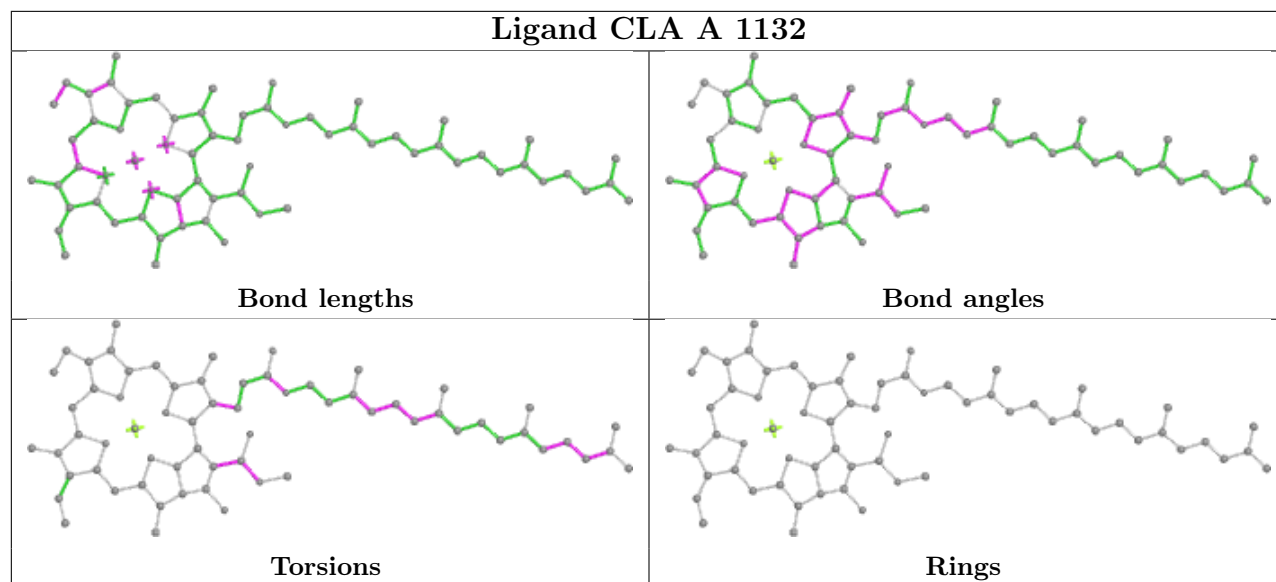
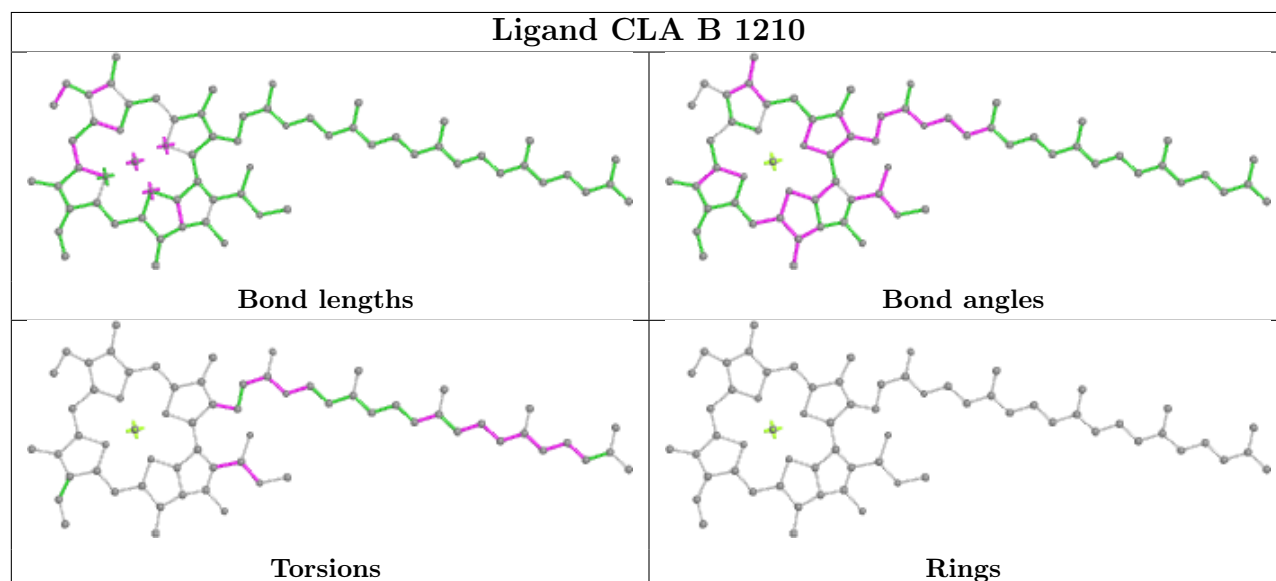
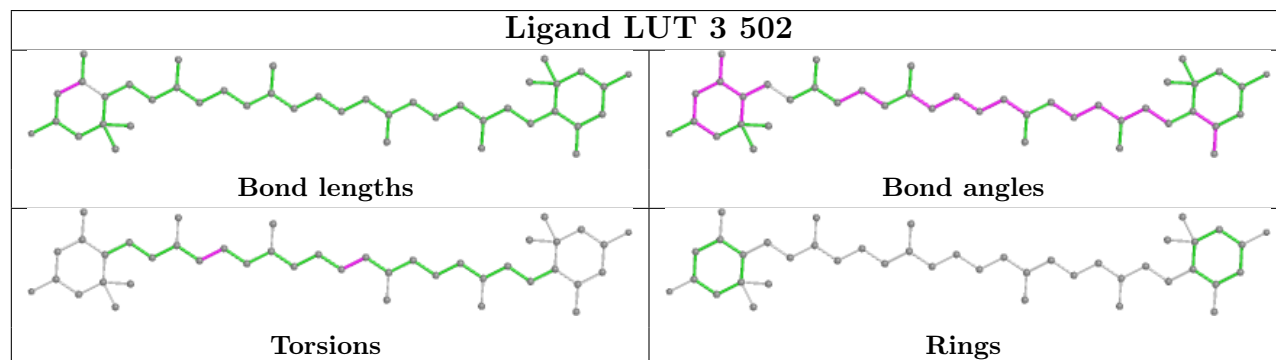
Bond angles

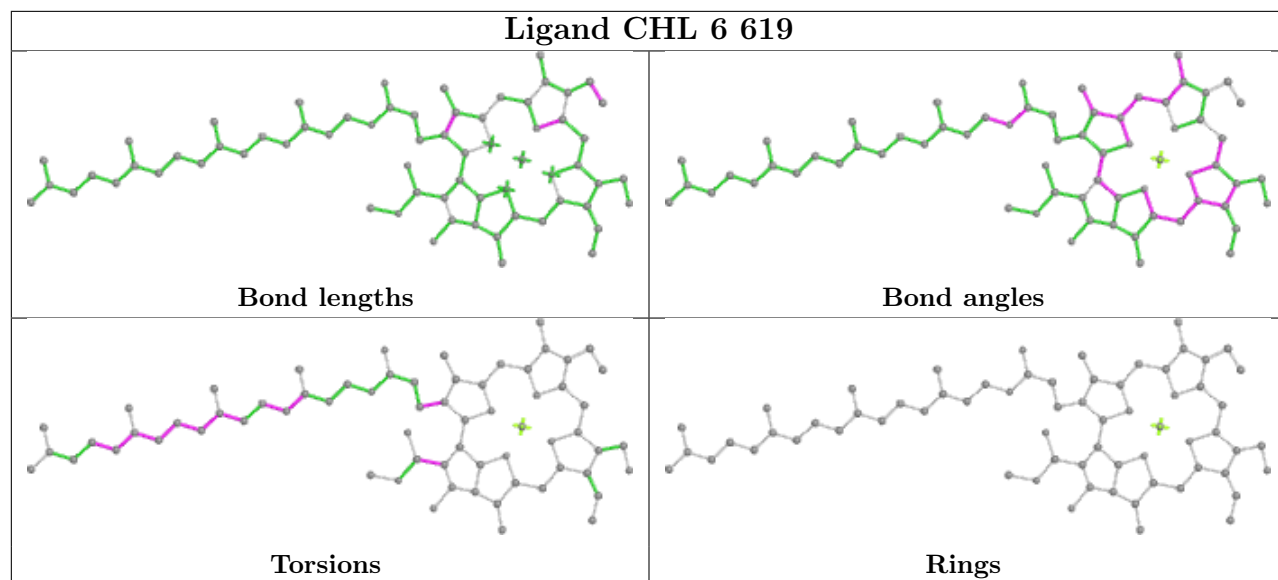
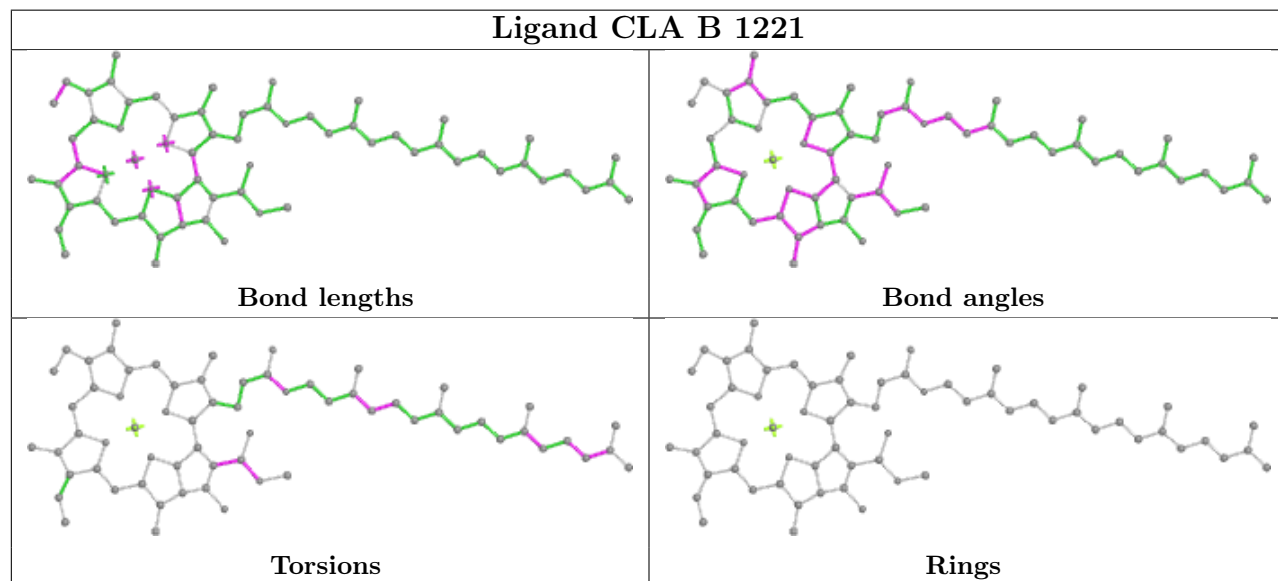


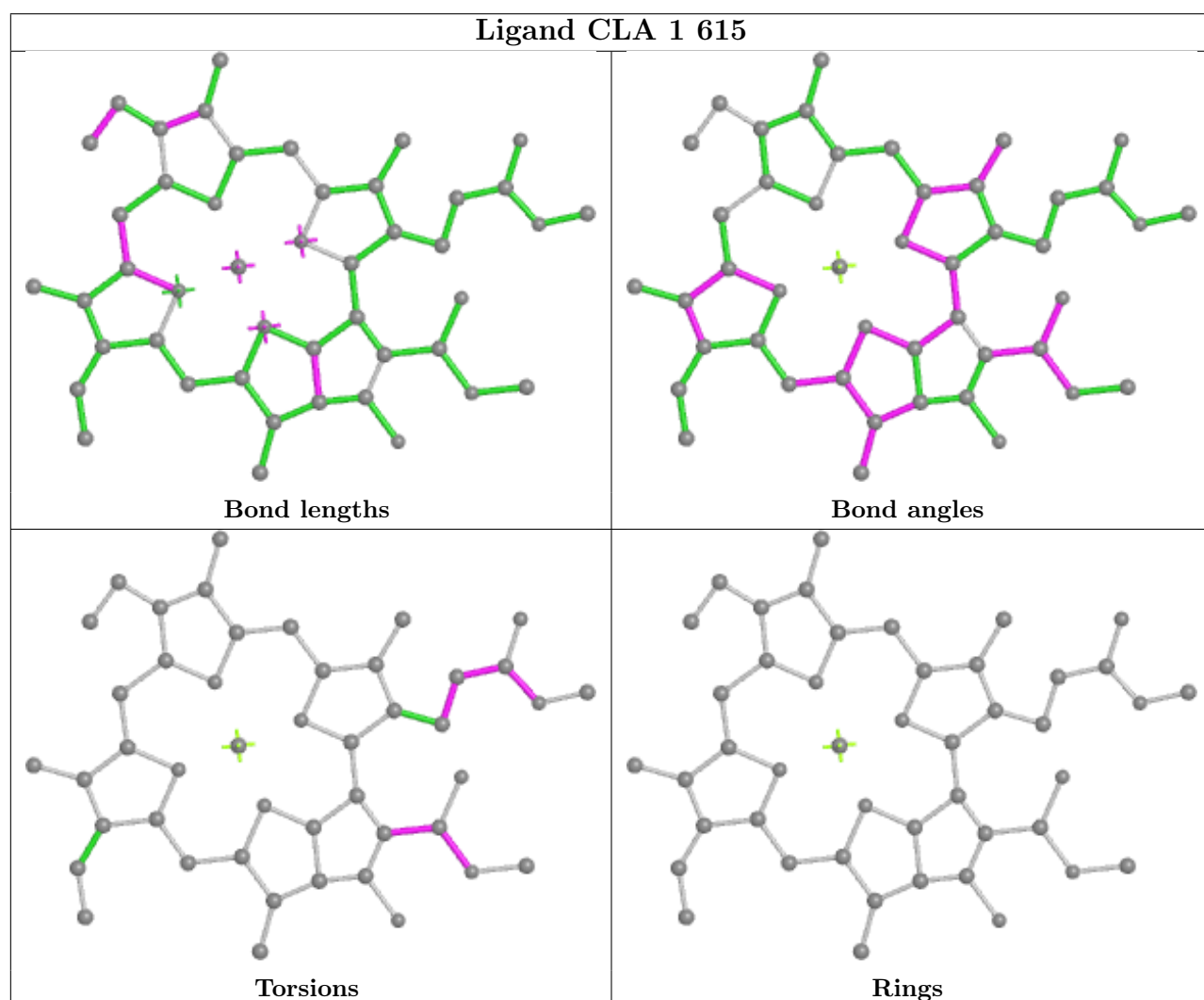
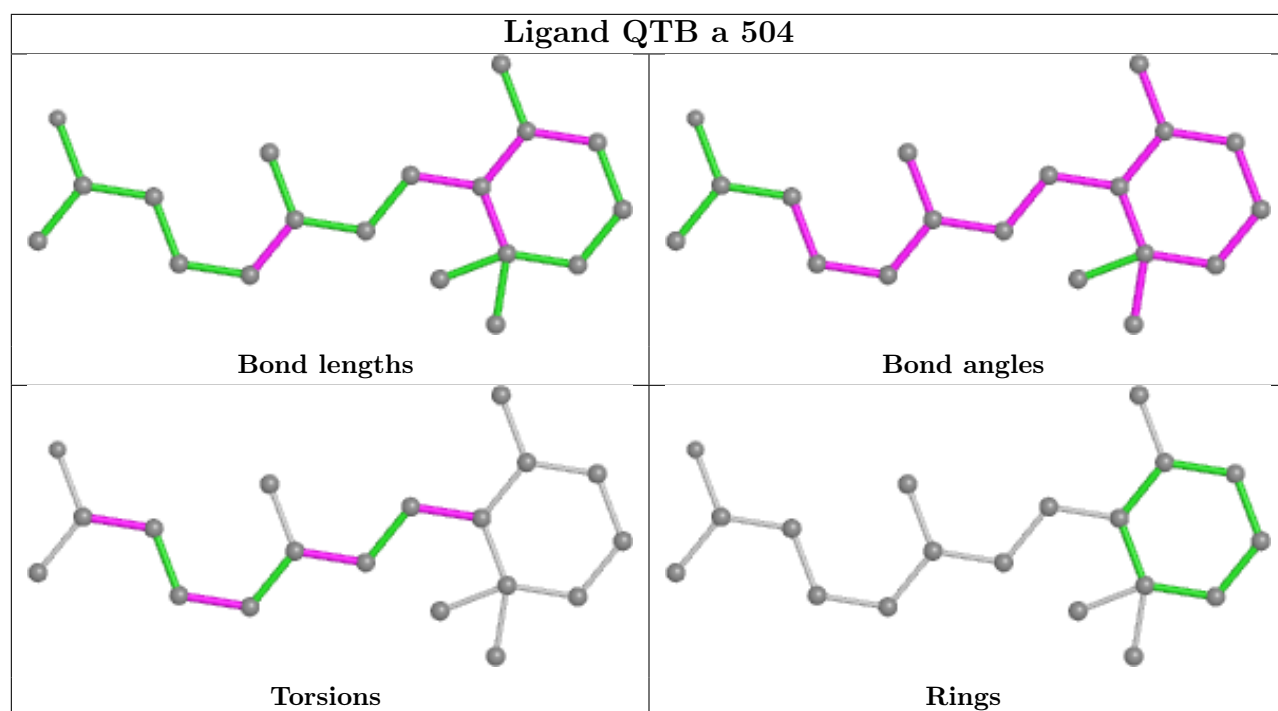
Torsions

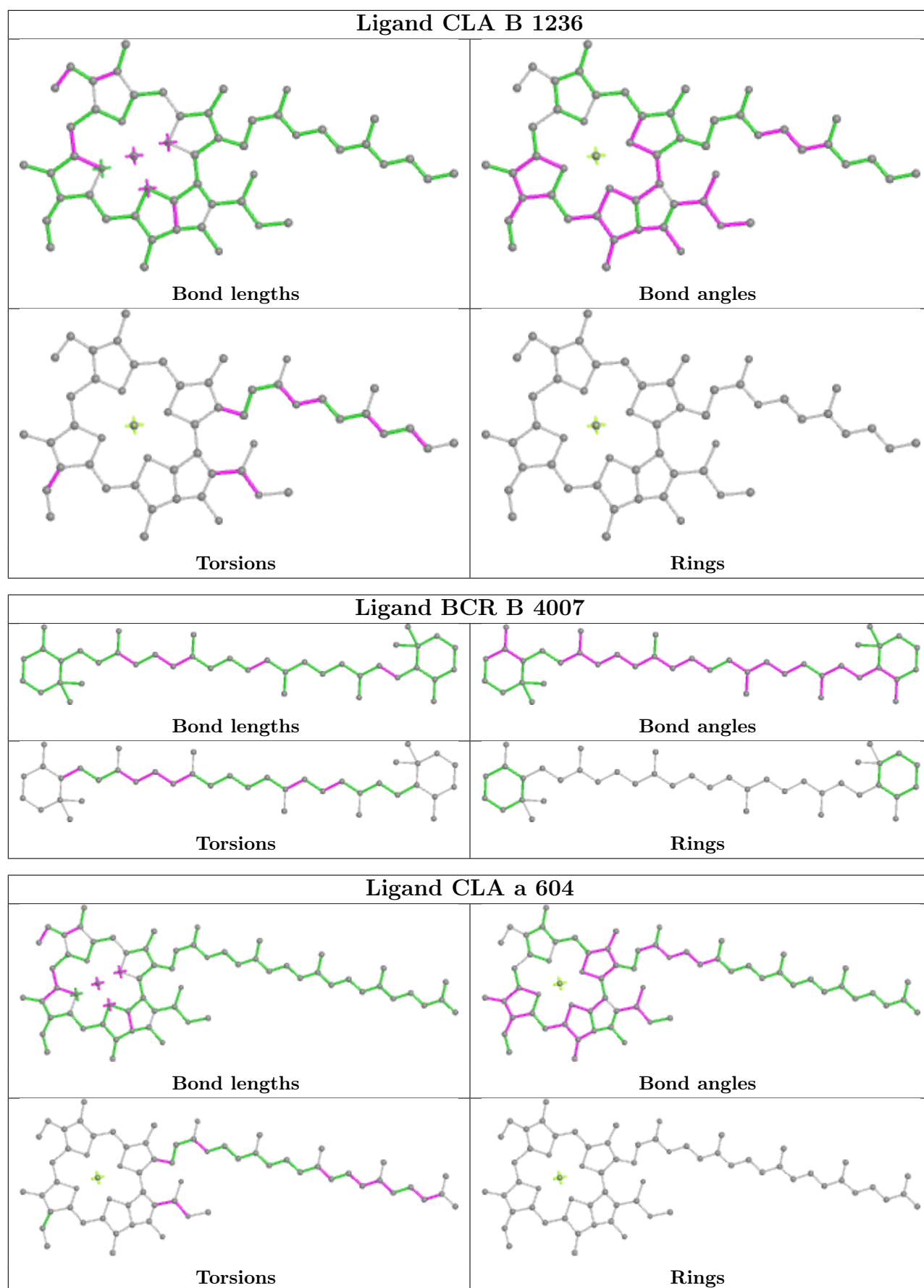


Rings

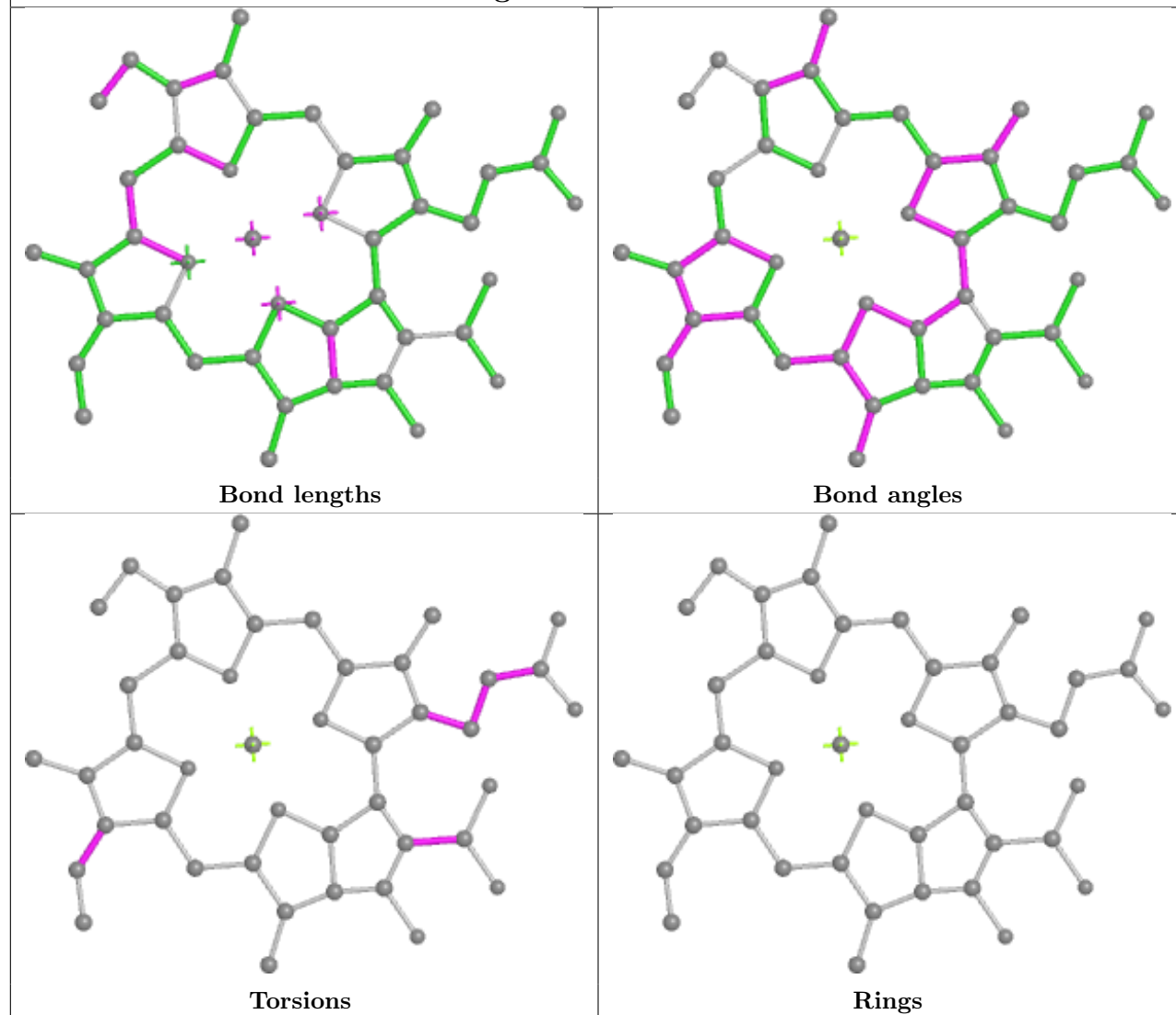
Ligand CLA A 1132**Ligand CLA B 1210****Ligand LUT 3 502**

Ligand CHL 6 619**Ligand CLA B 1221**

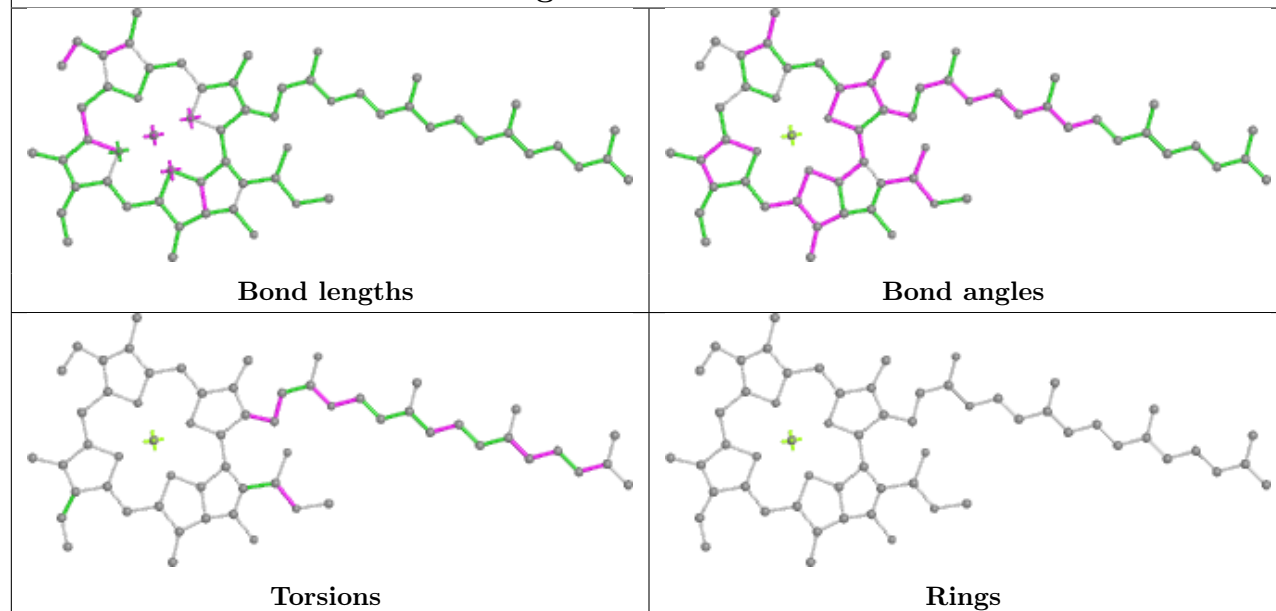


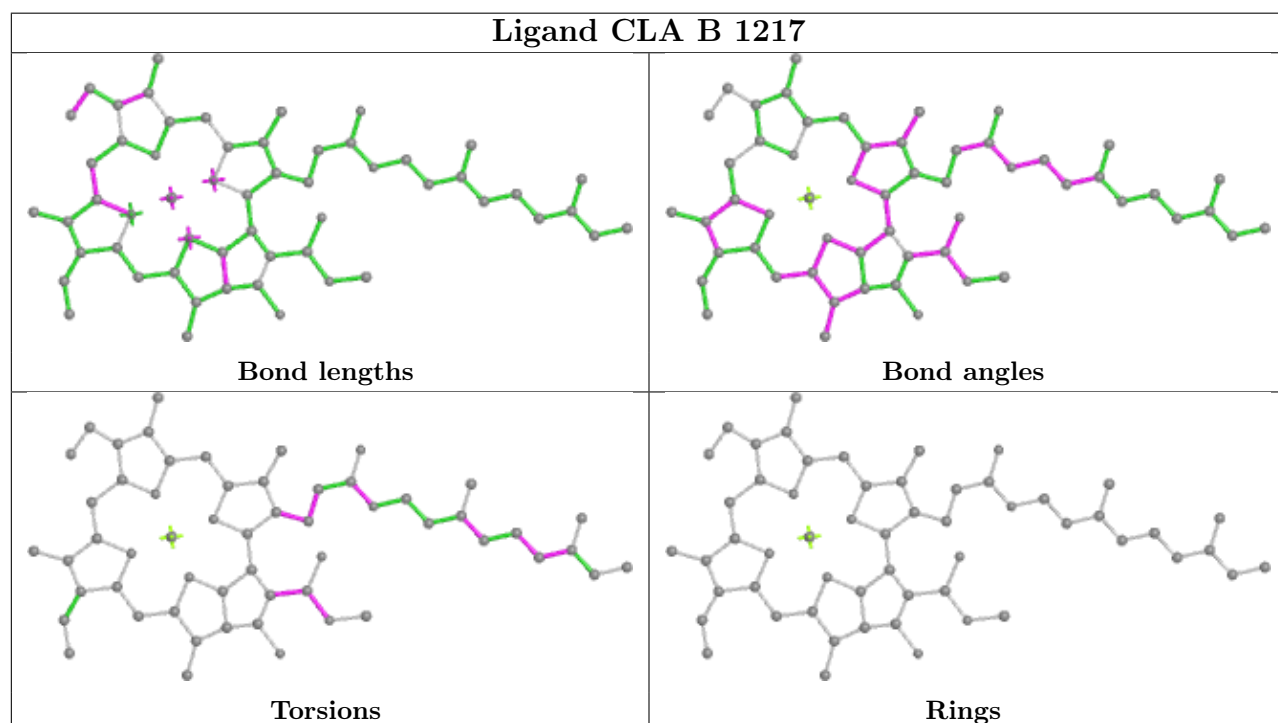
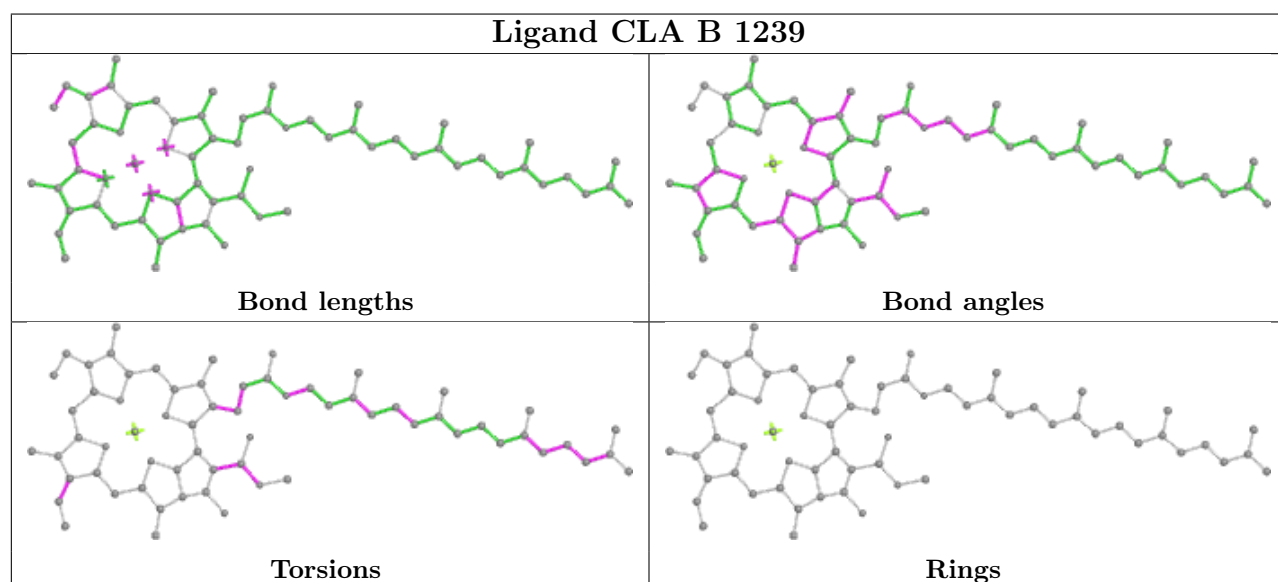
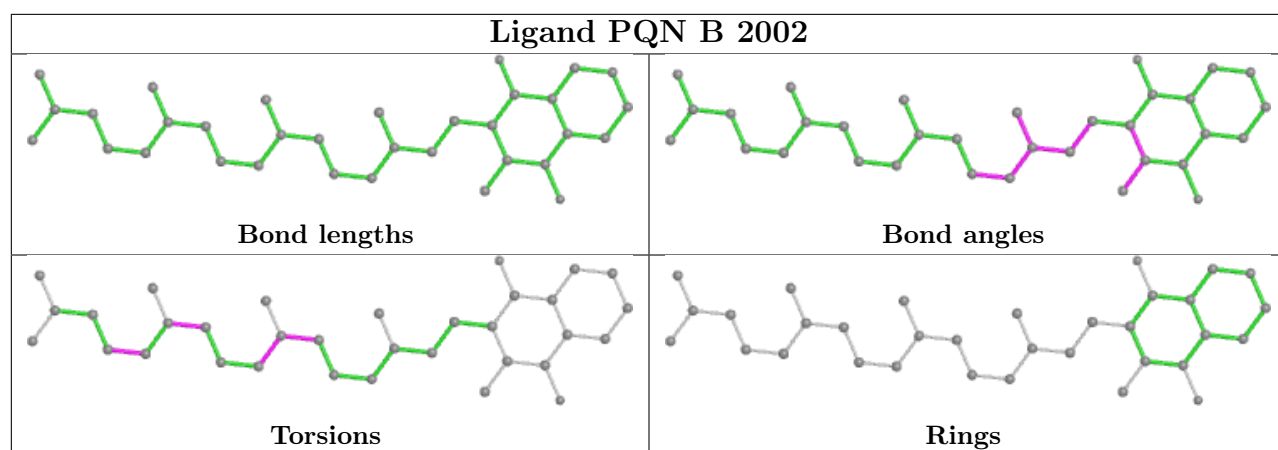


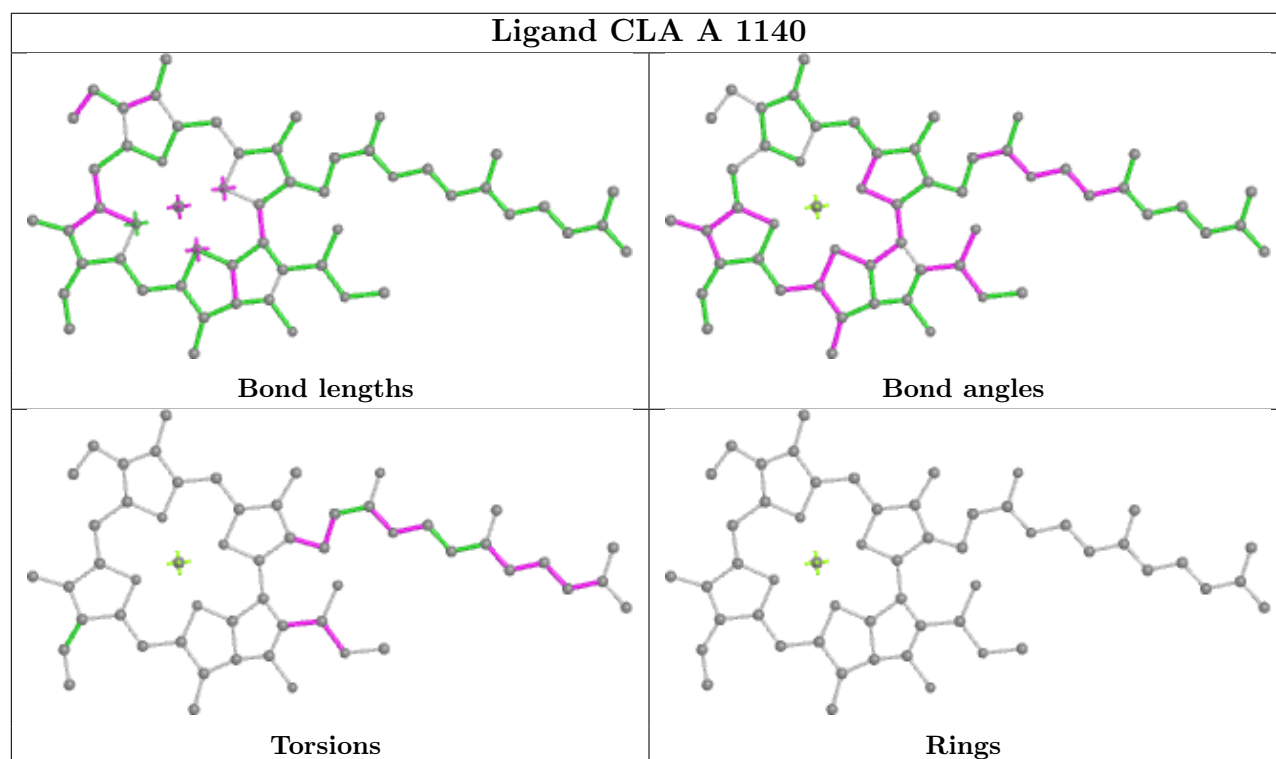
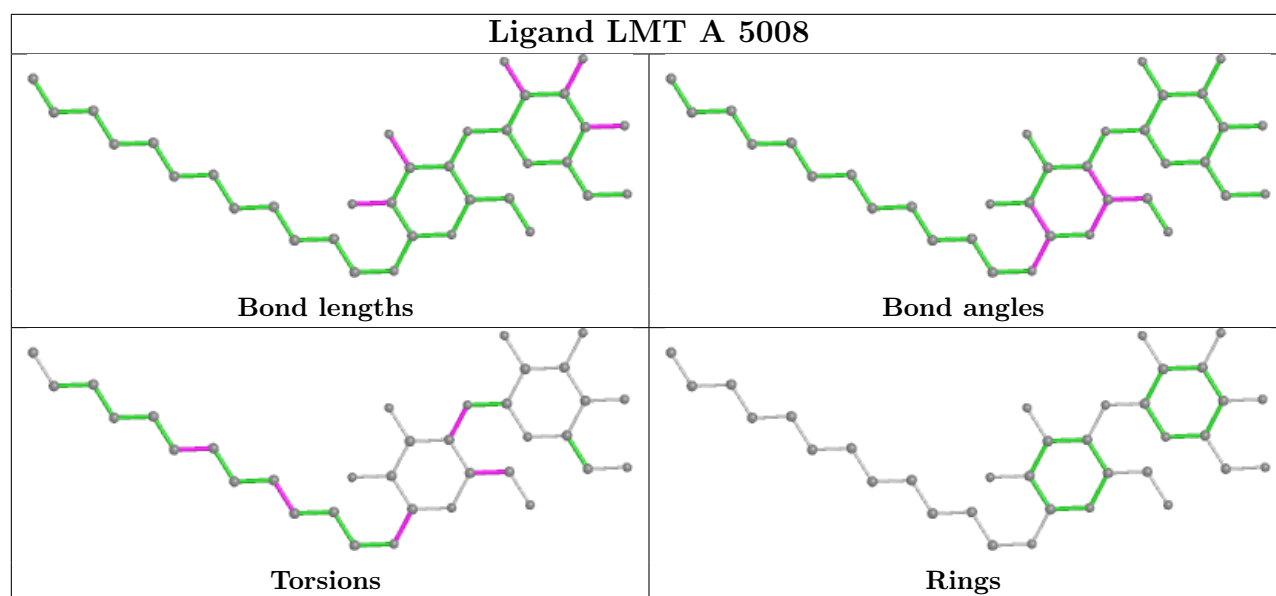
Ligand CLA 7 605



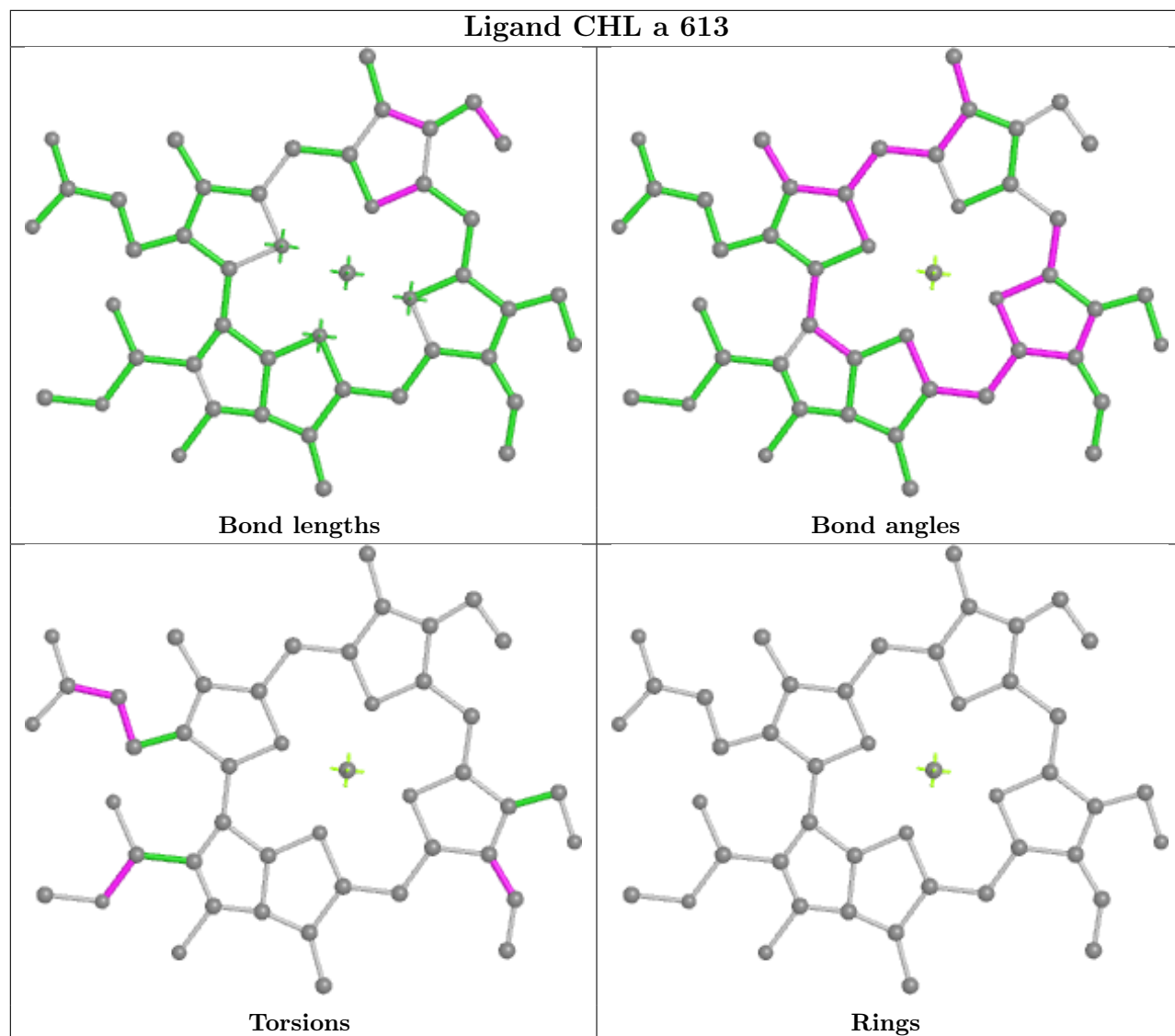
Ligand CLA 5 601



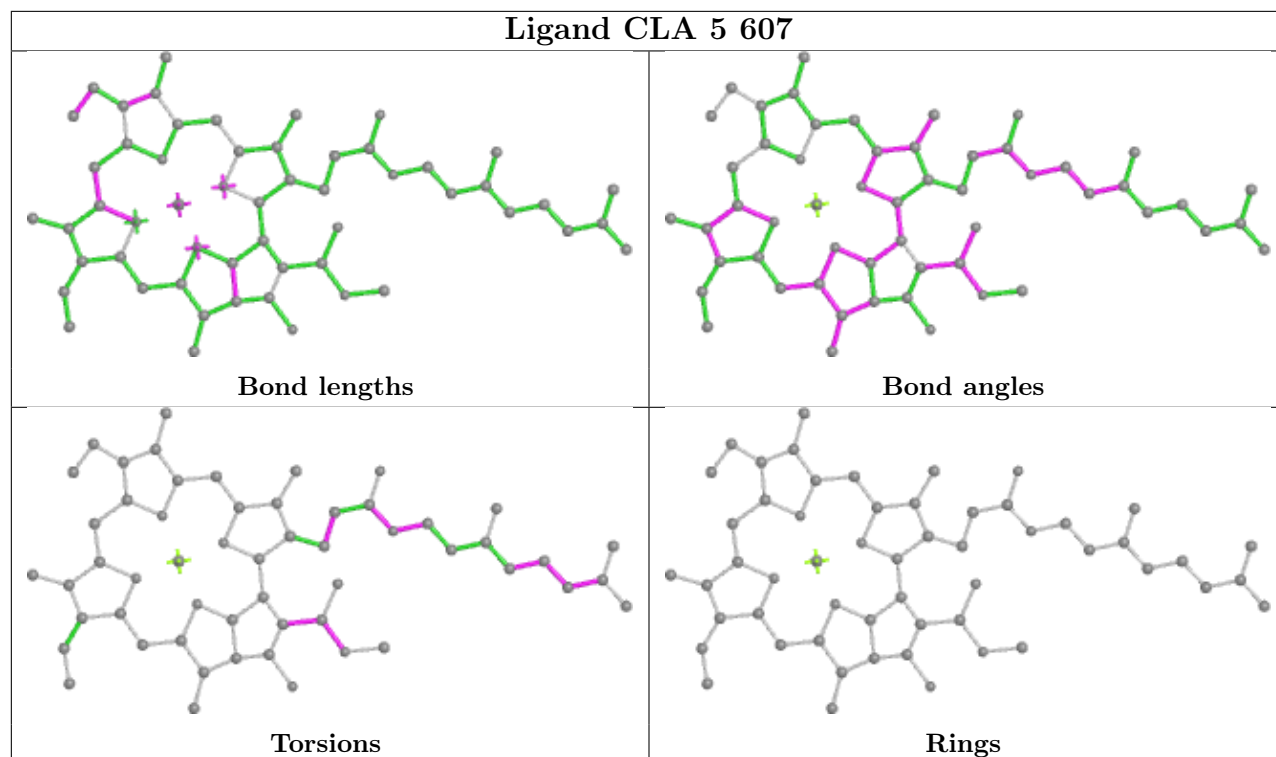




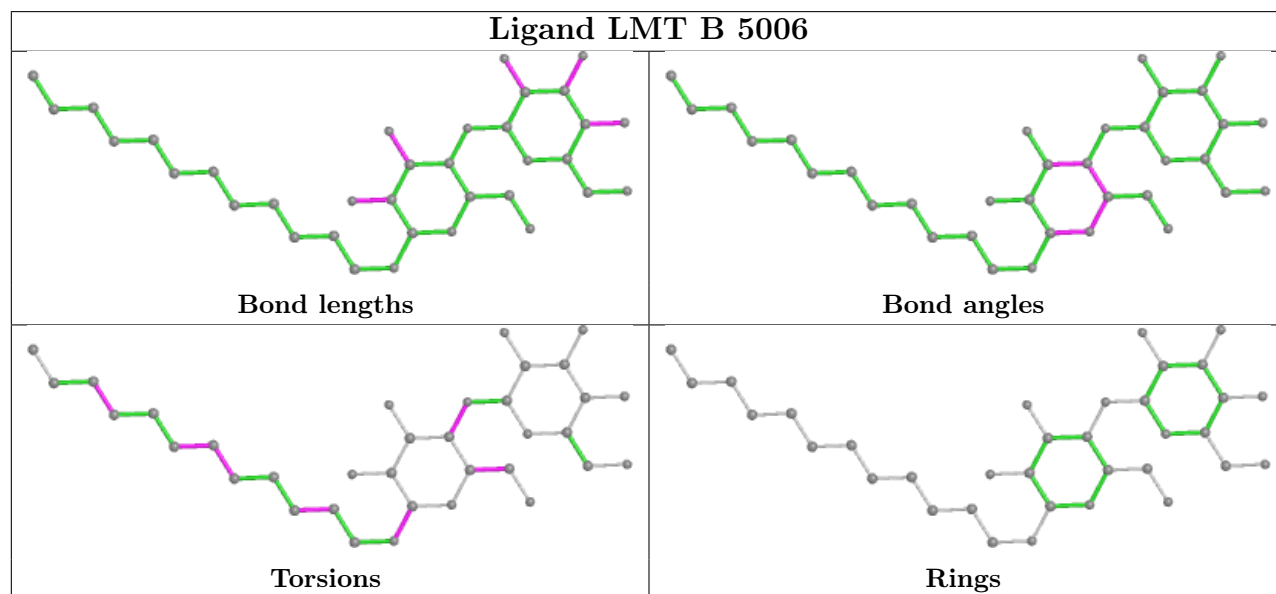
Ligand CHL a 613

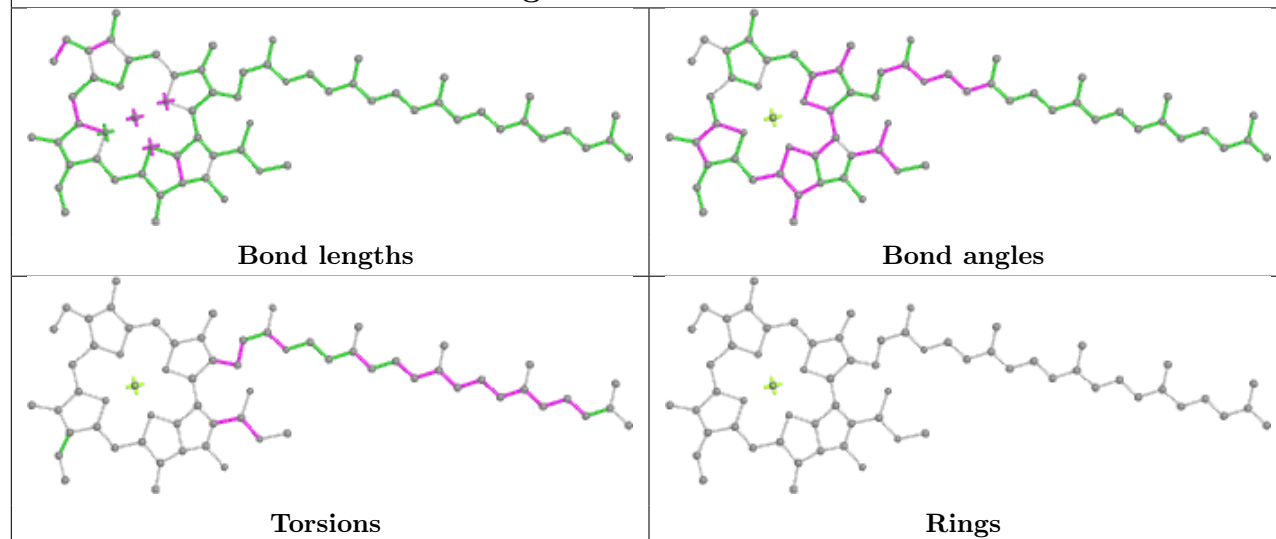
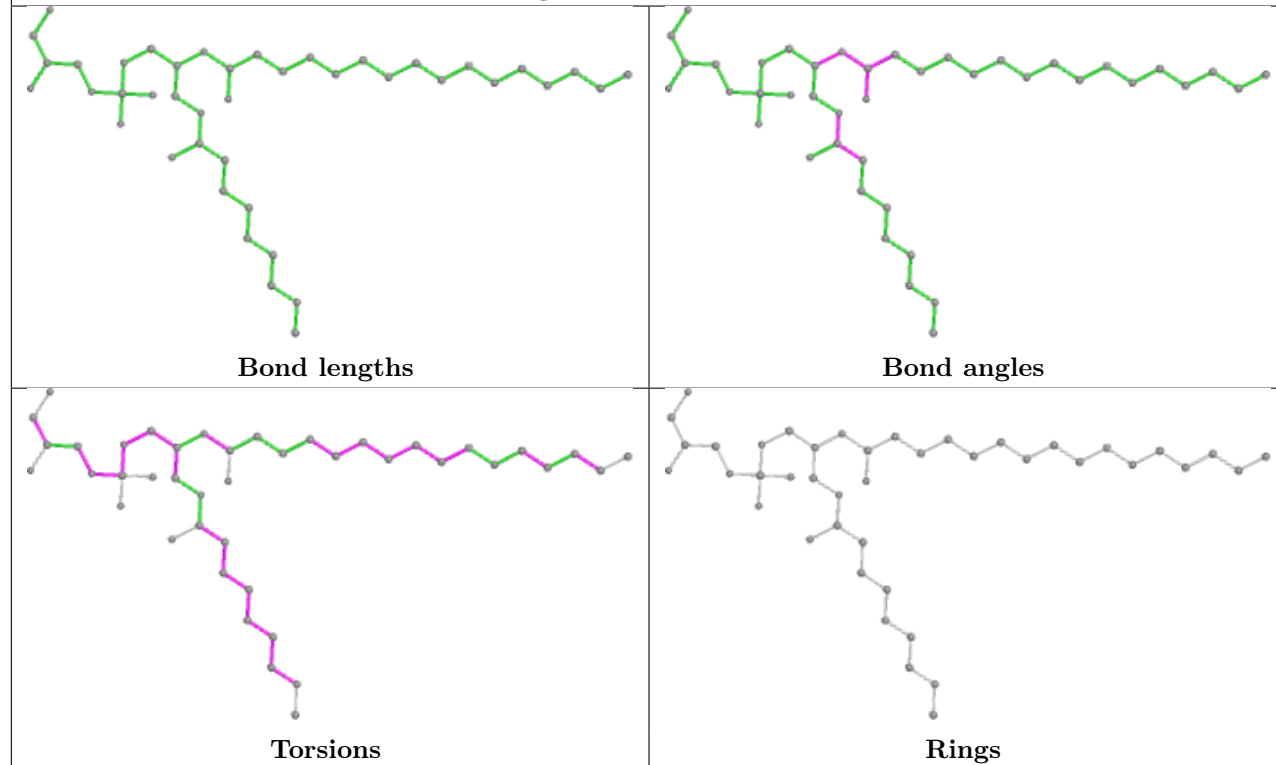


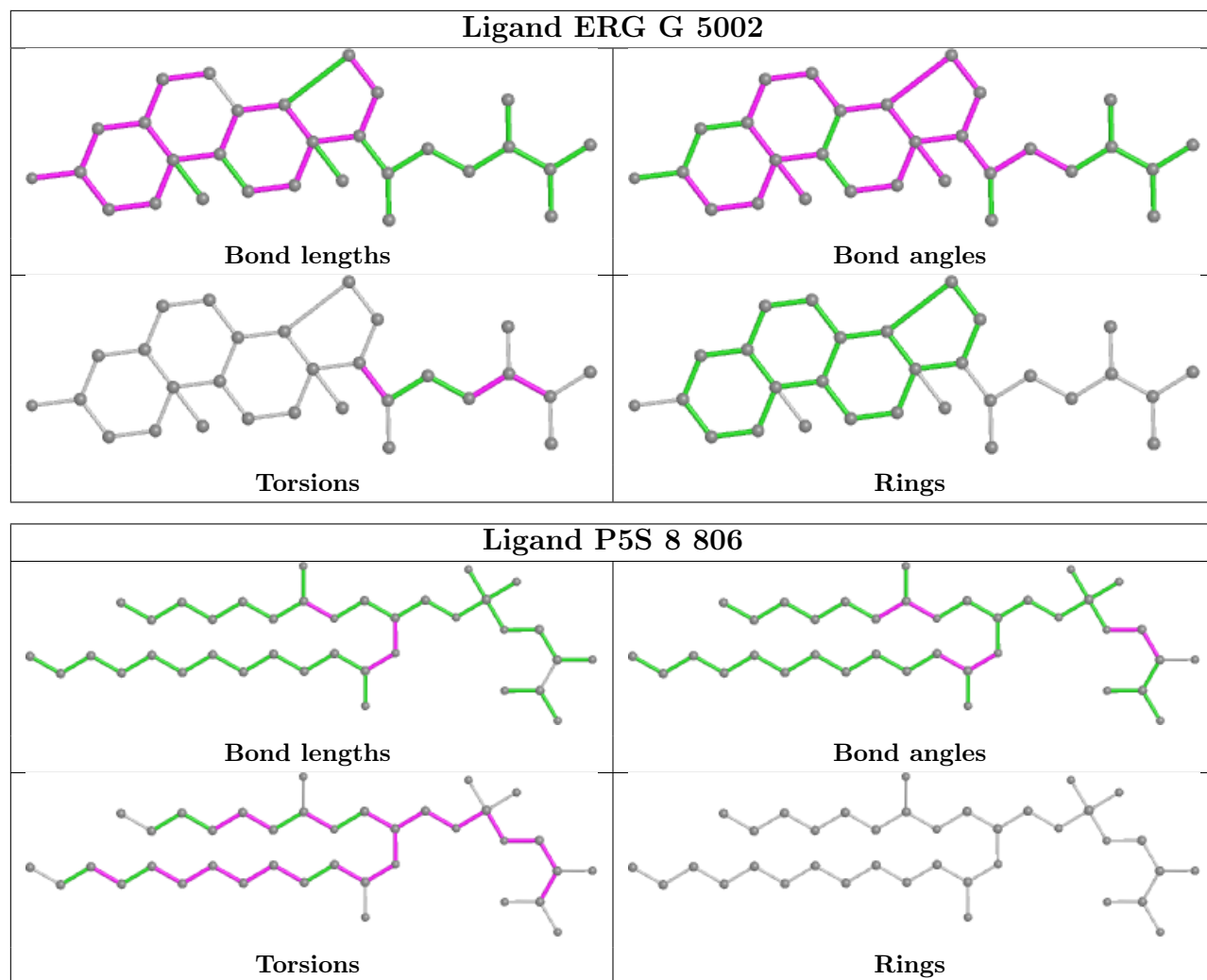
Ligand CLA 5 607



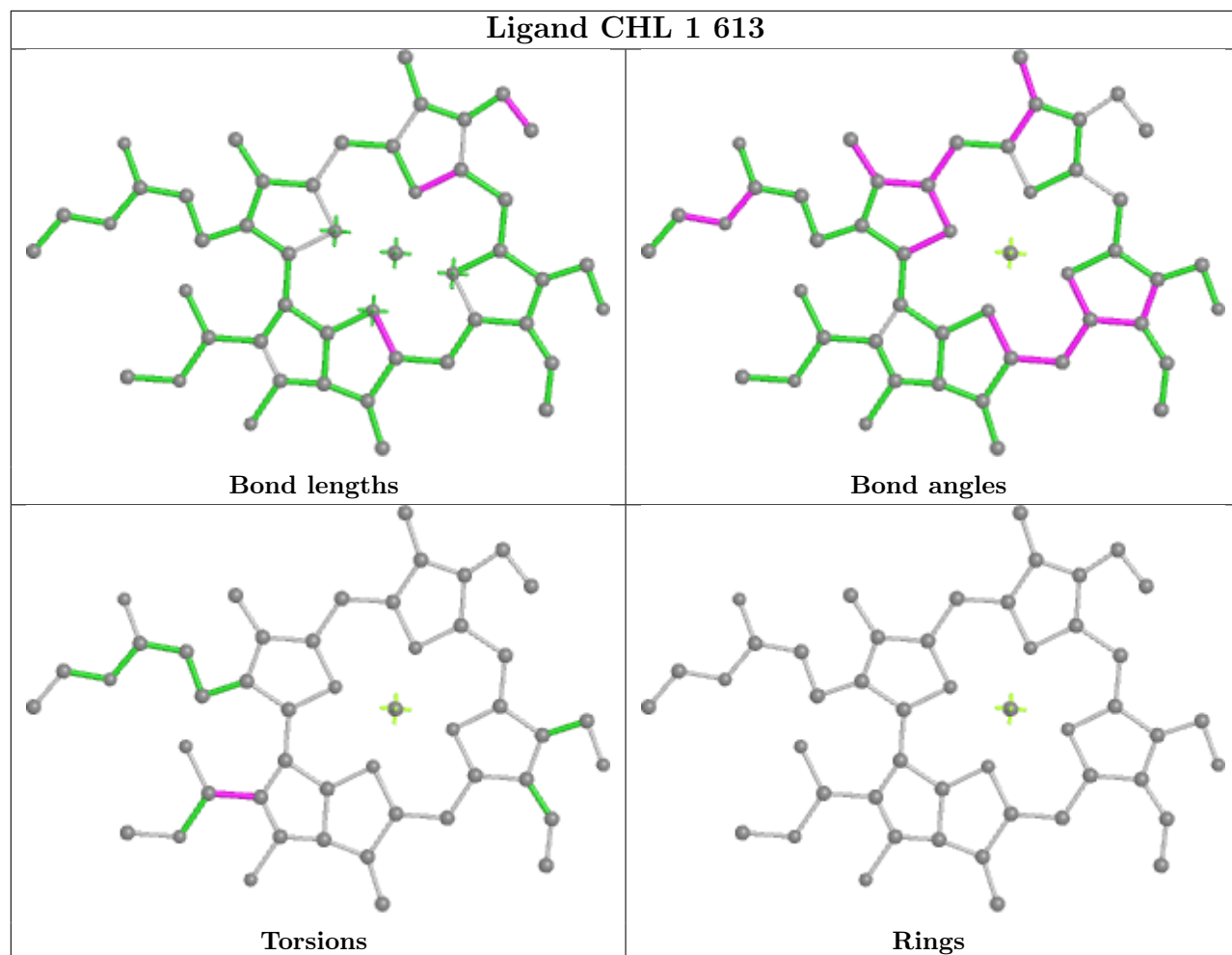
Ligand LMT B 5006



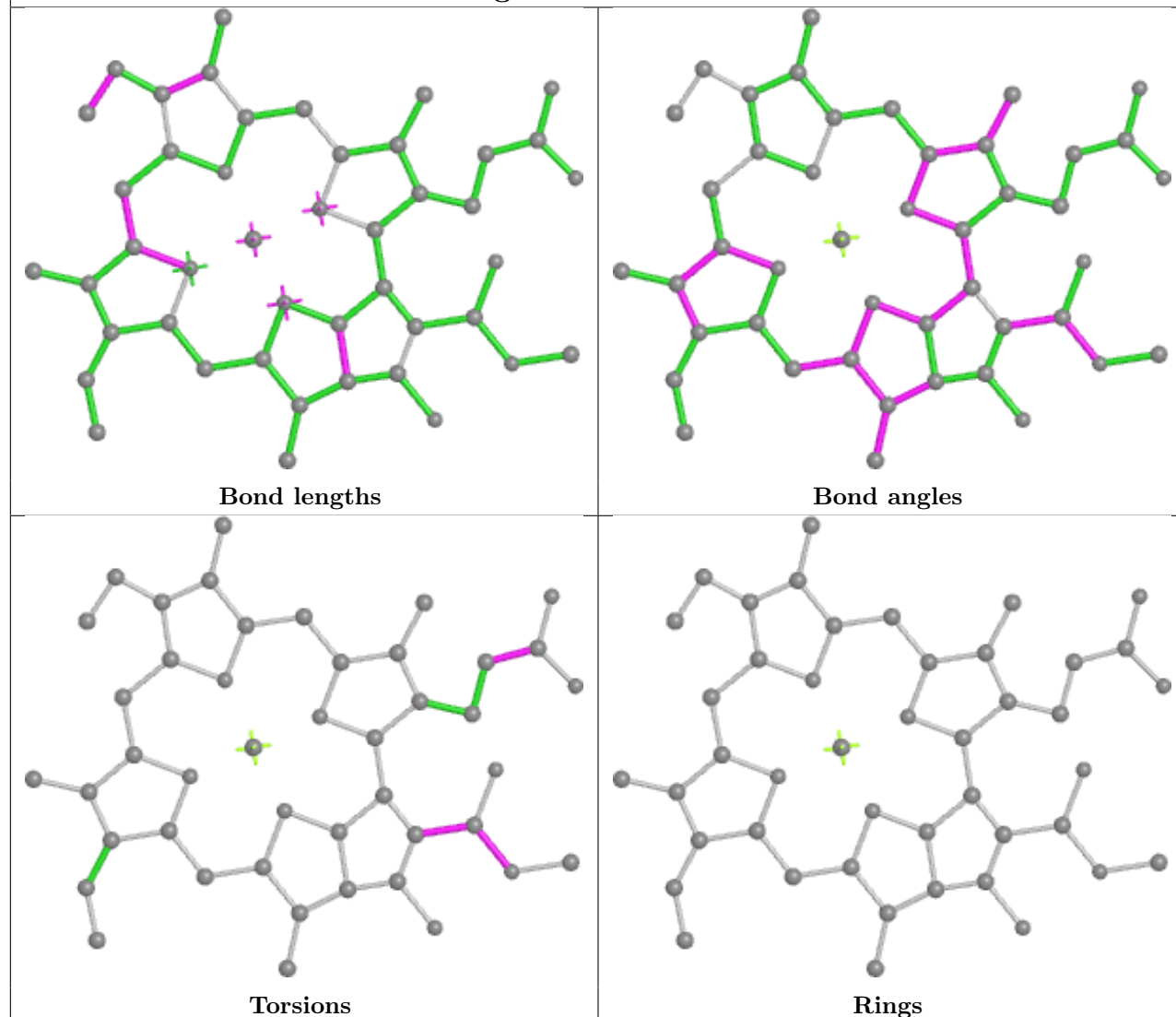
Ligand CLA A 1101**Ligand LHG 1 802**



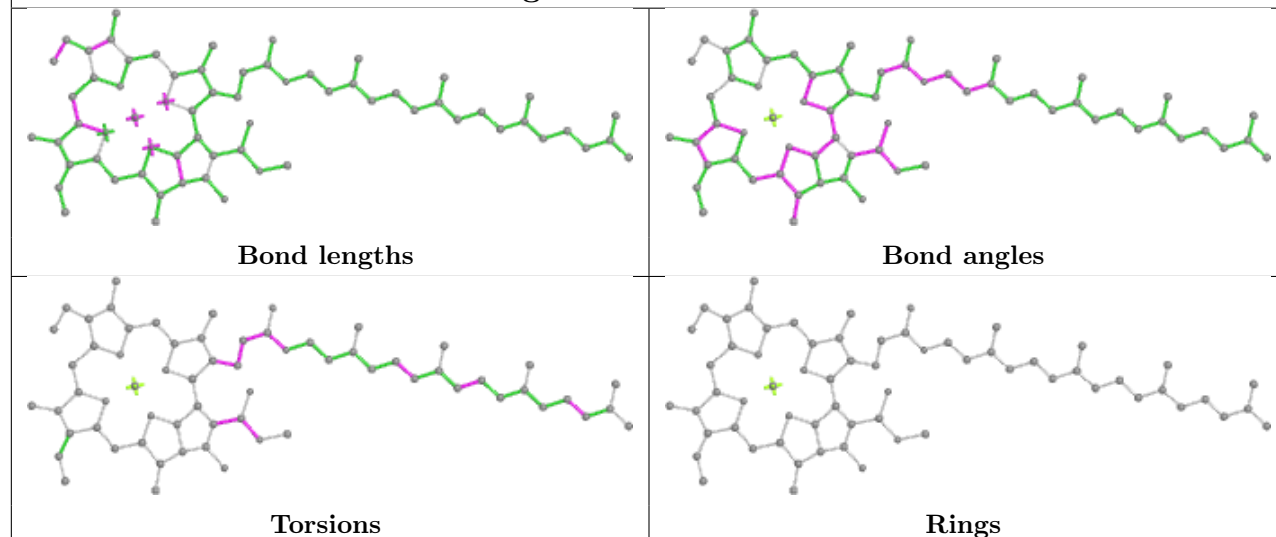
Ligand CHL 1 613

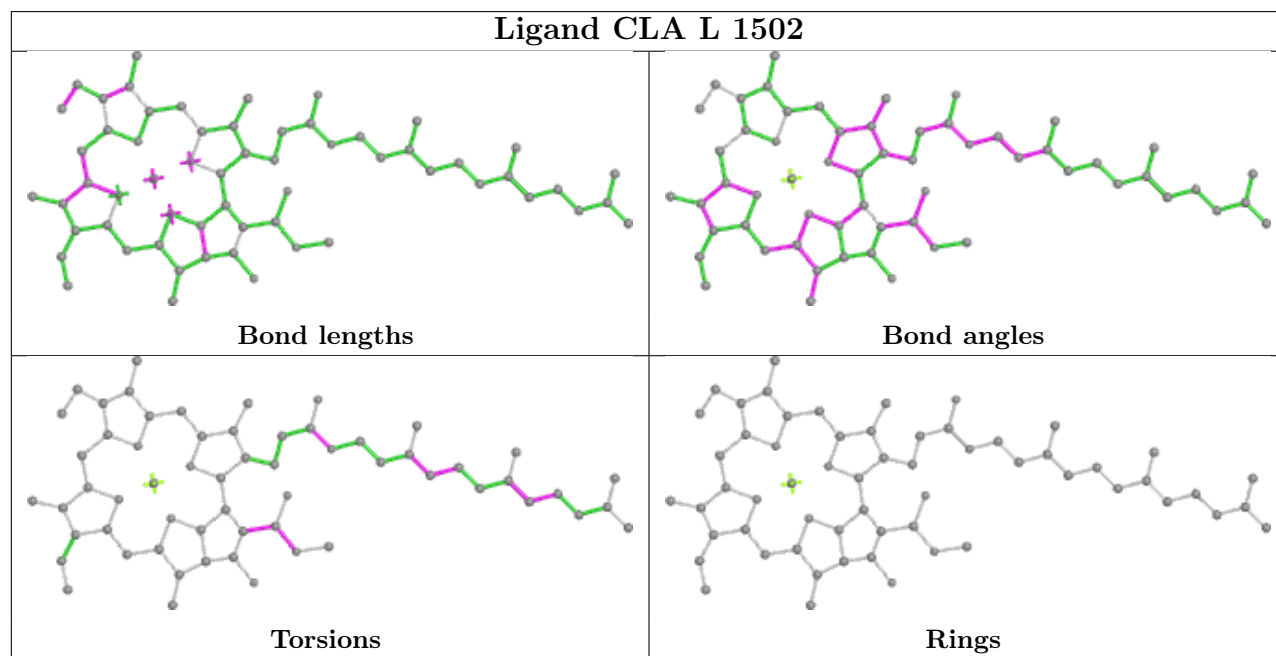
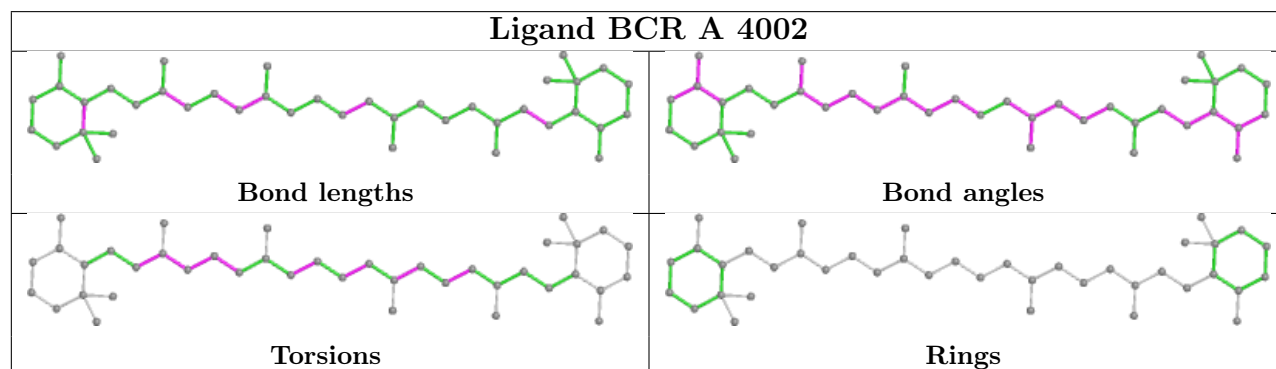
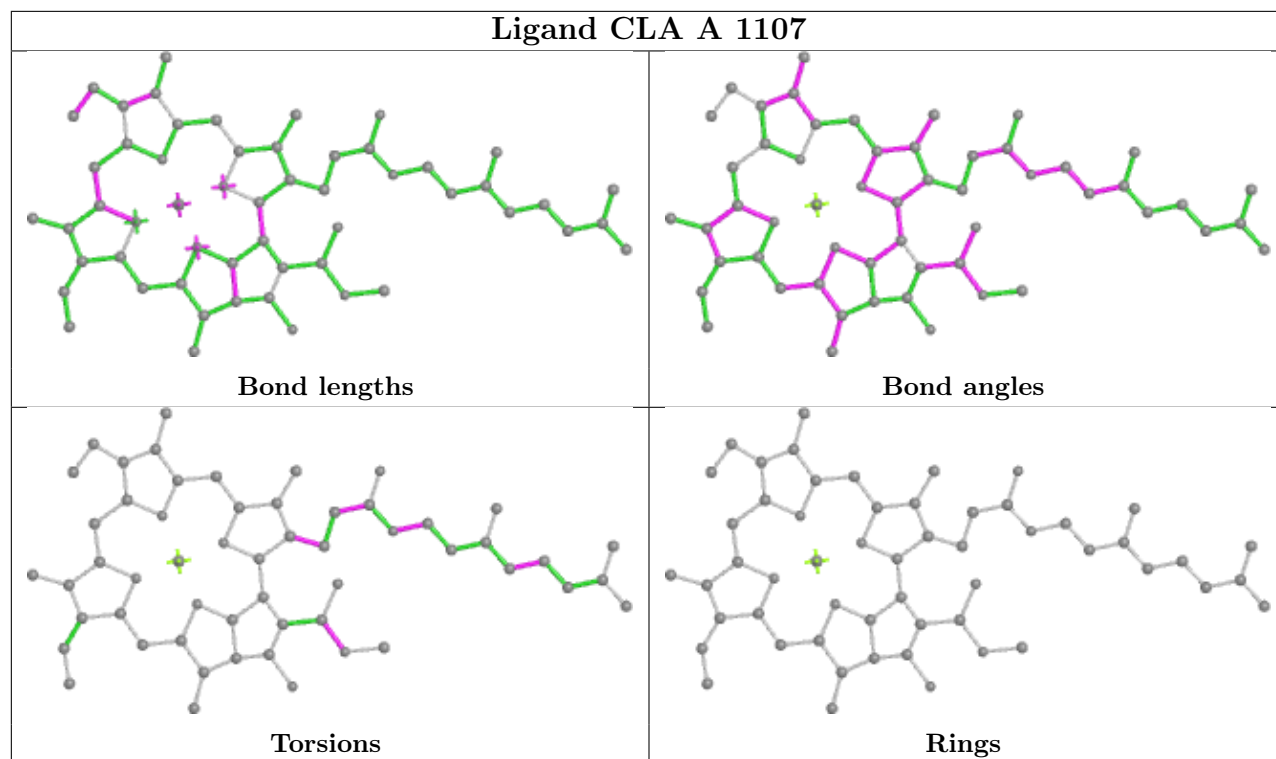


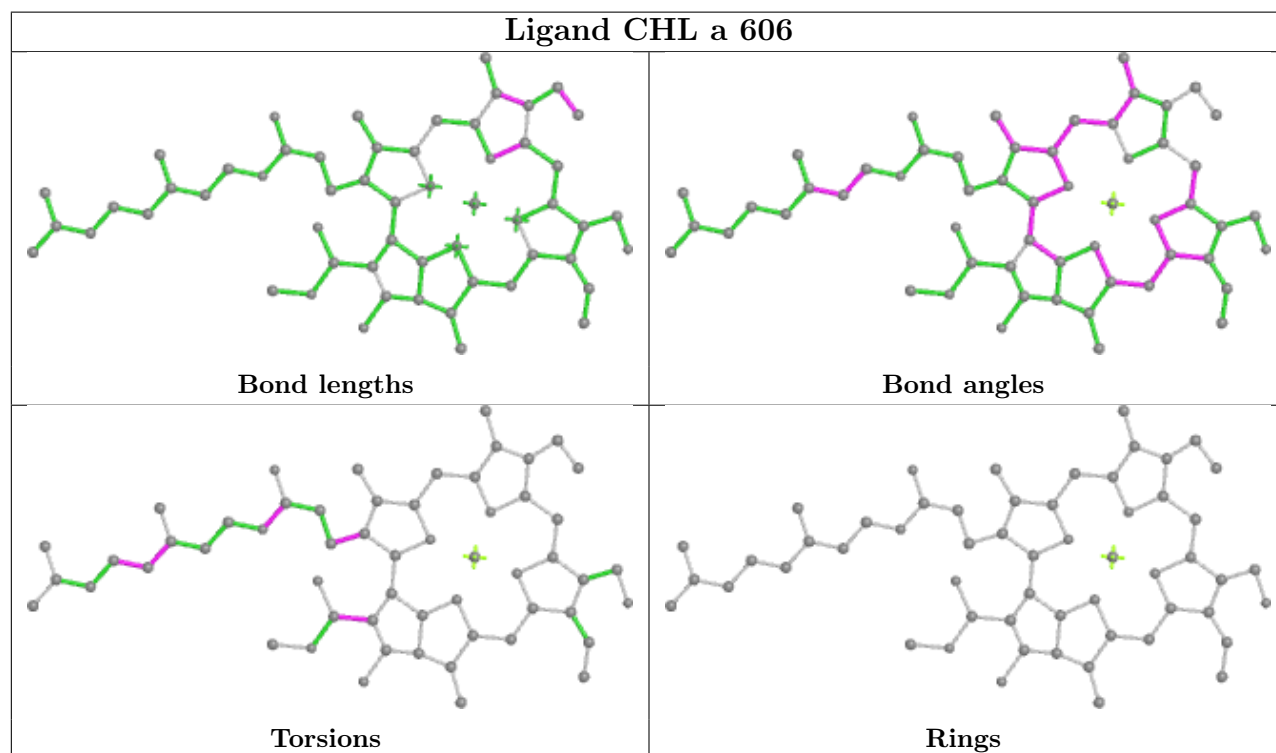
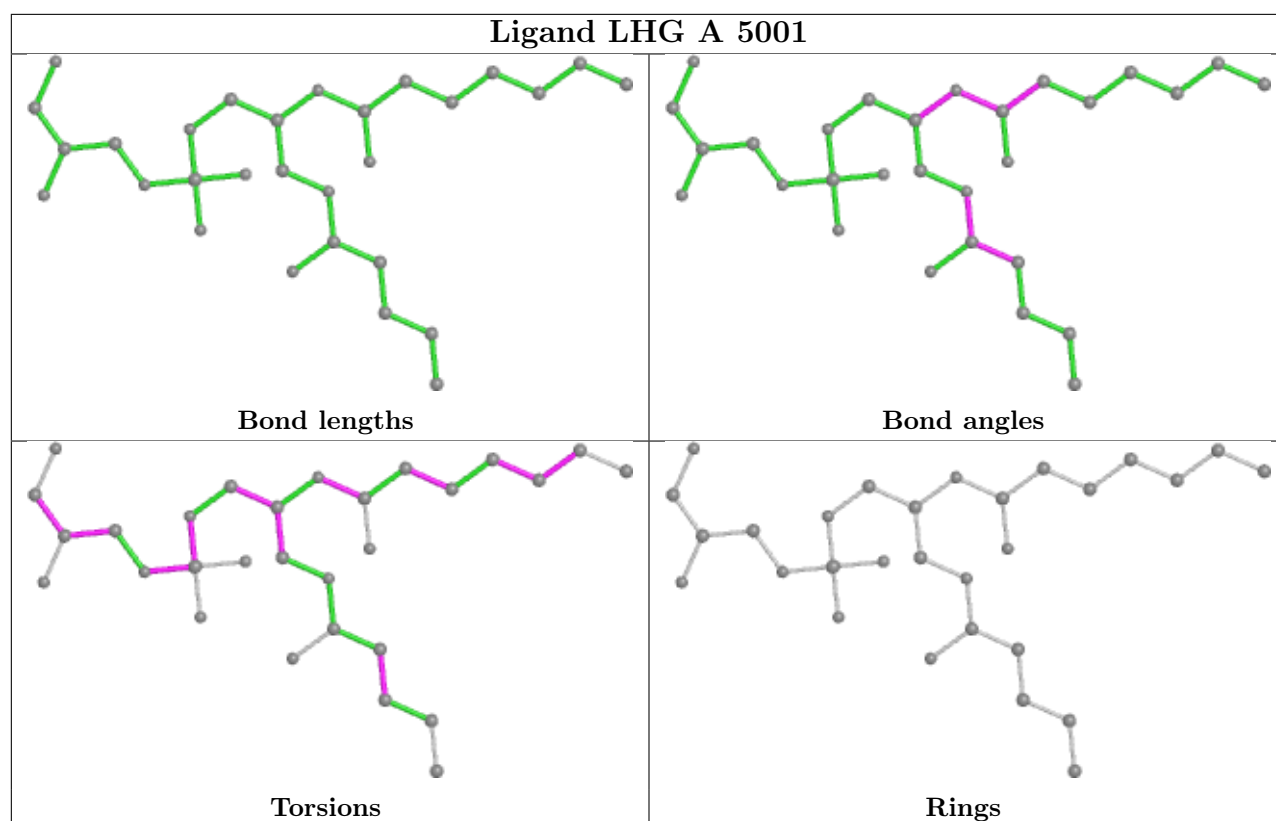
Ligand CLA 8 605

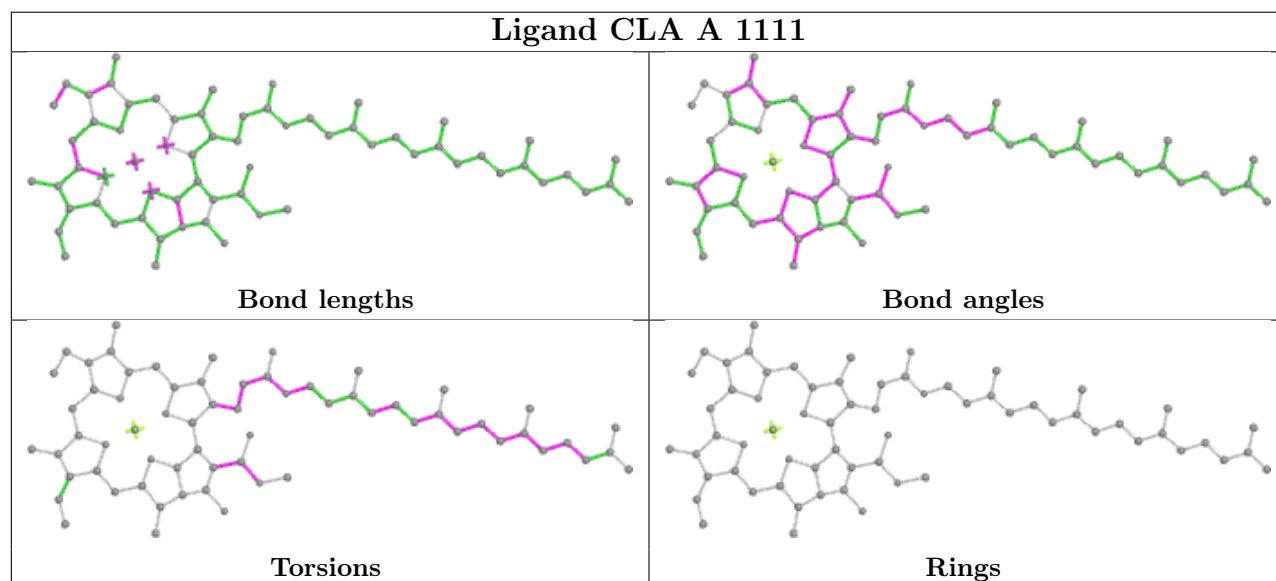
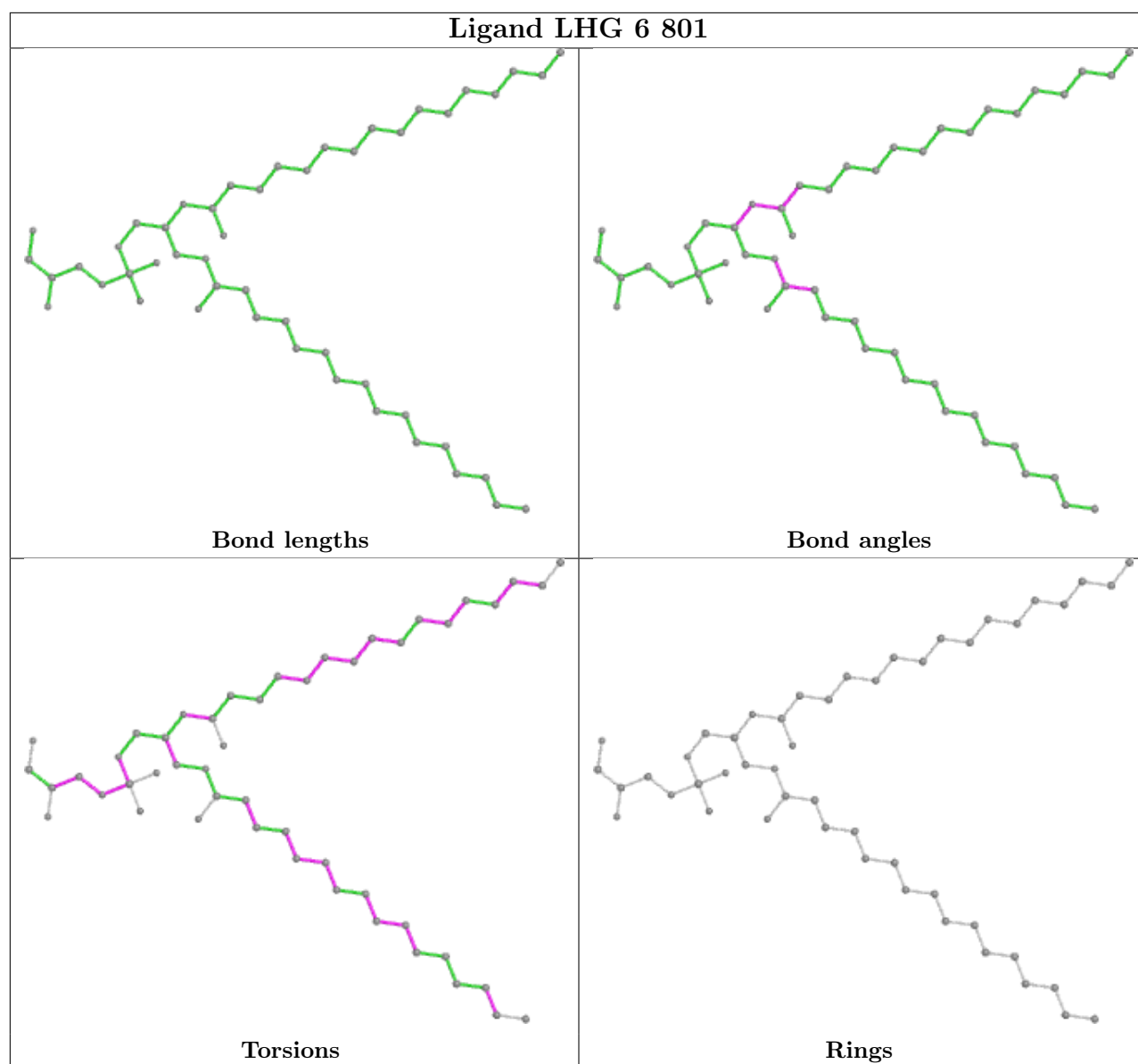


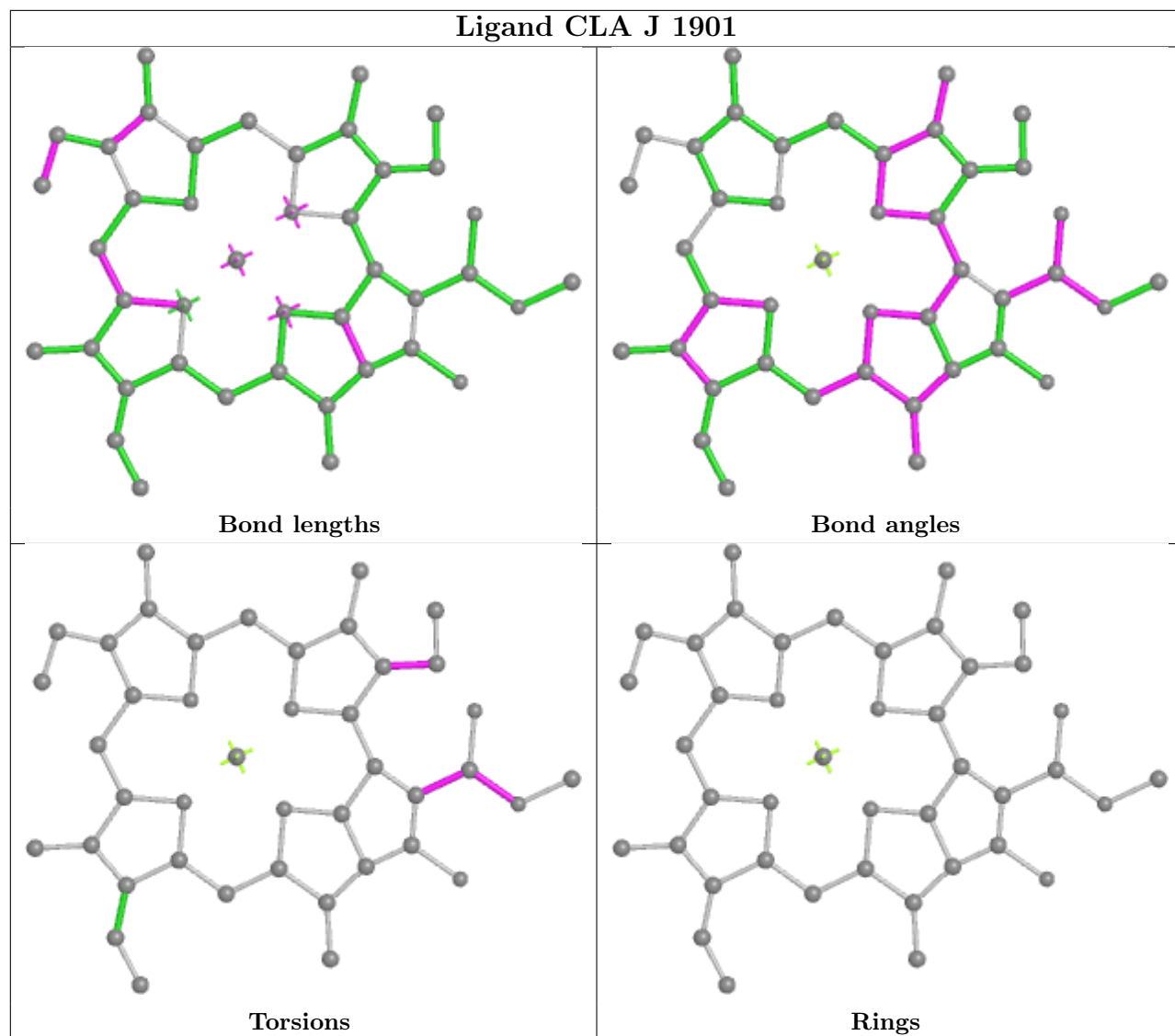
Ligand CLA A 1127



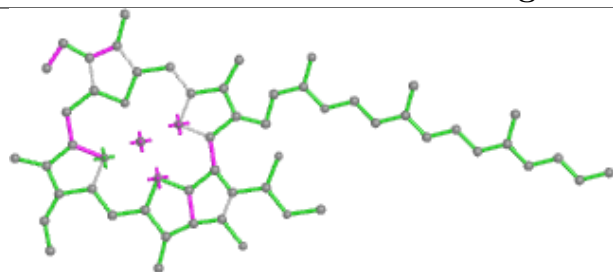




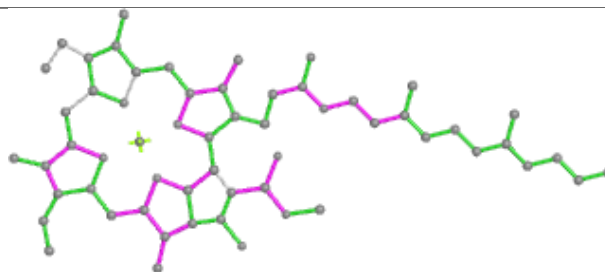




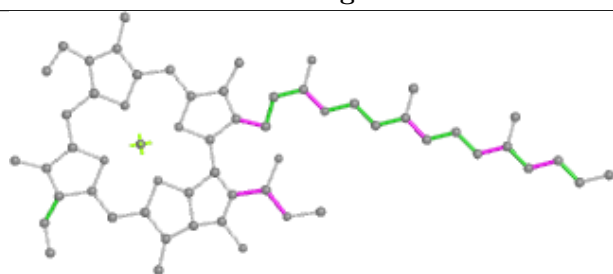
Ligand CLA a 607



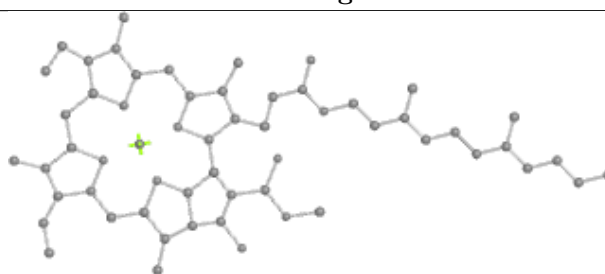
Bond lengths



Bond angles

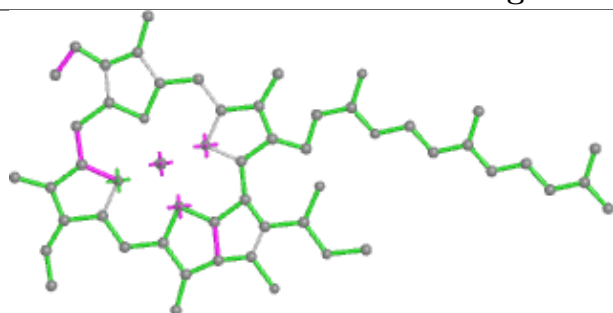


Torsions

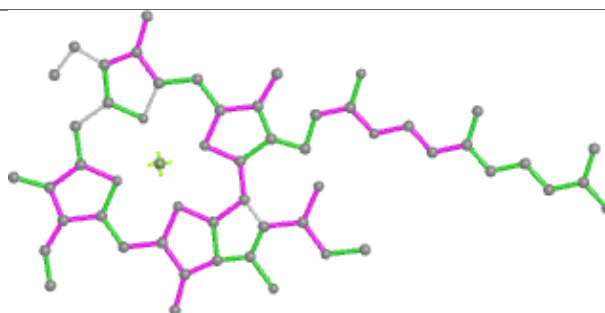


Rings

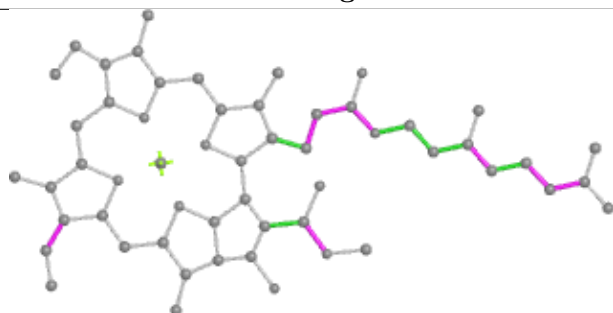
Ligand CLA F 1302



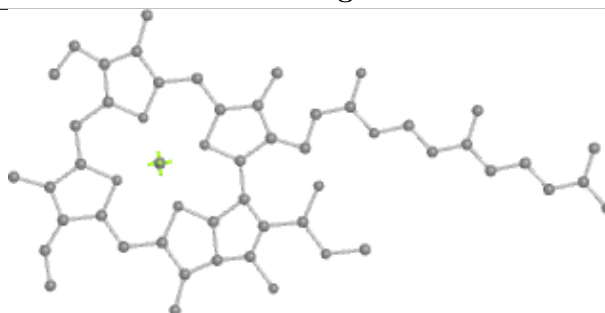
Bond lengths



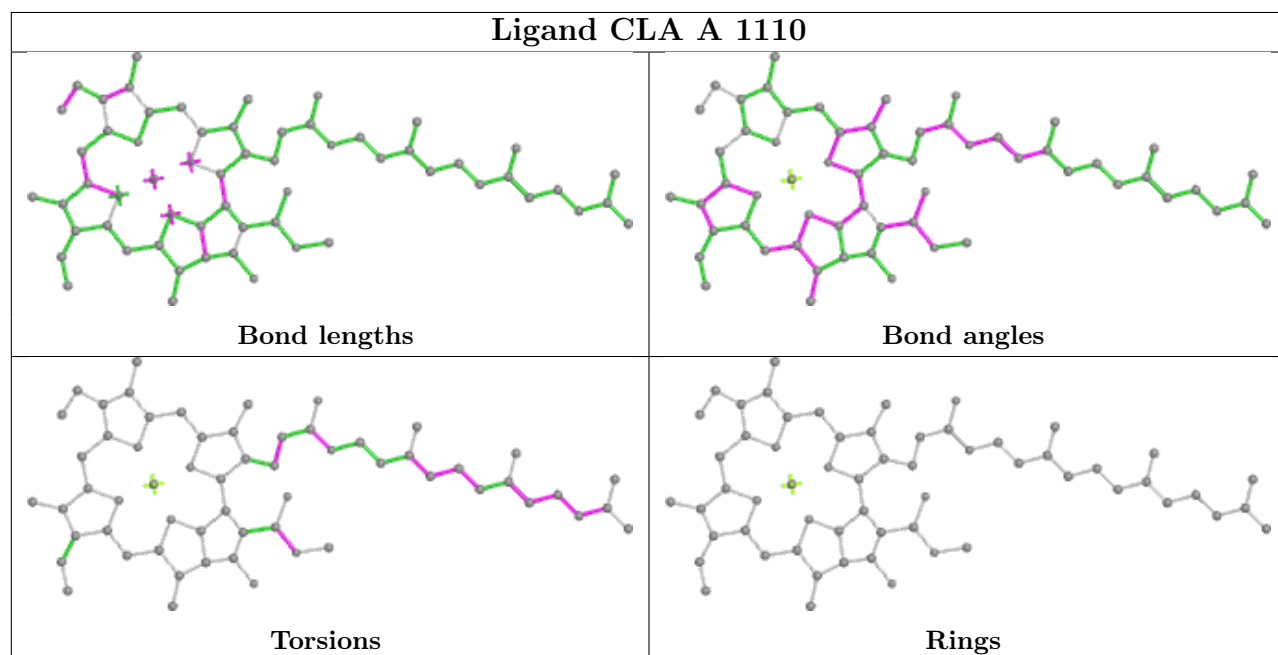
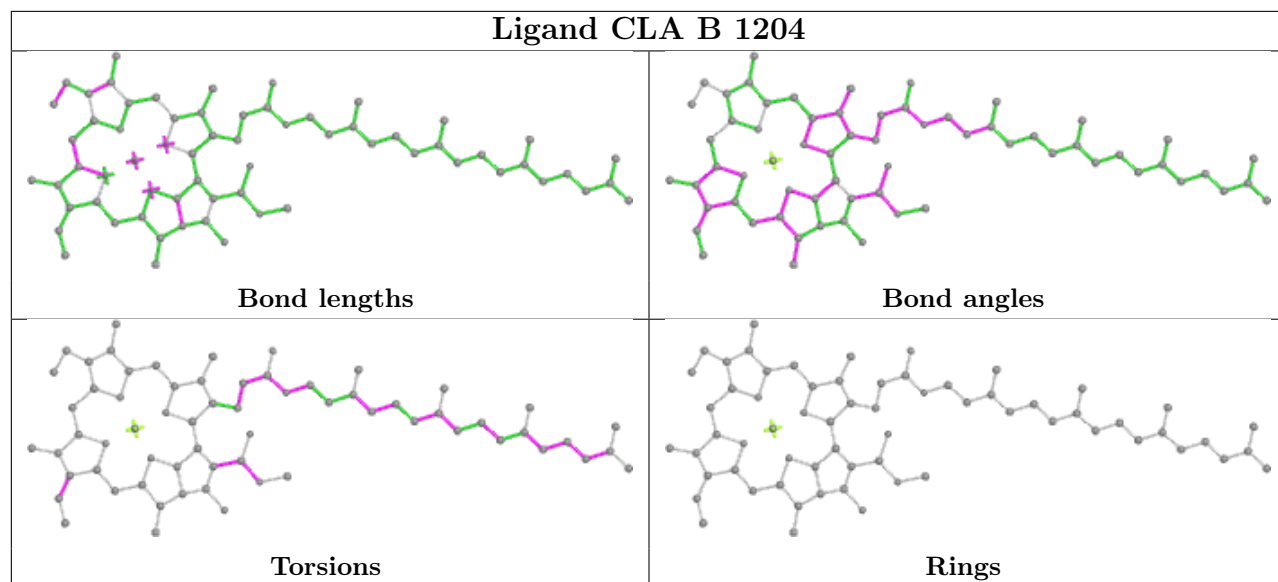
Bond angles



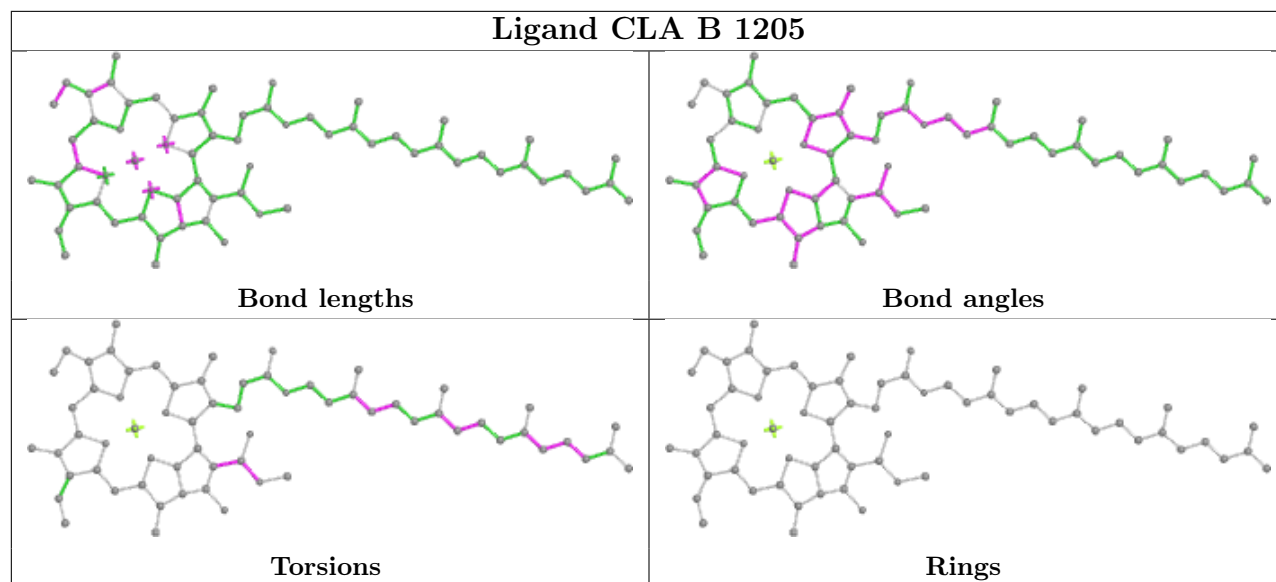
Torsions



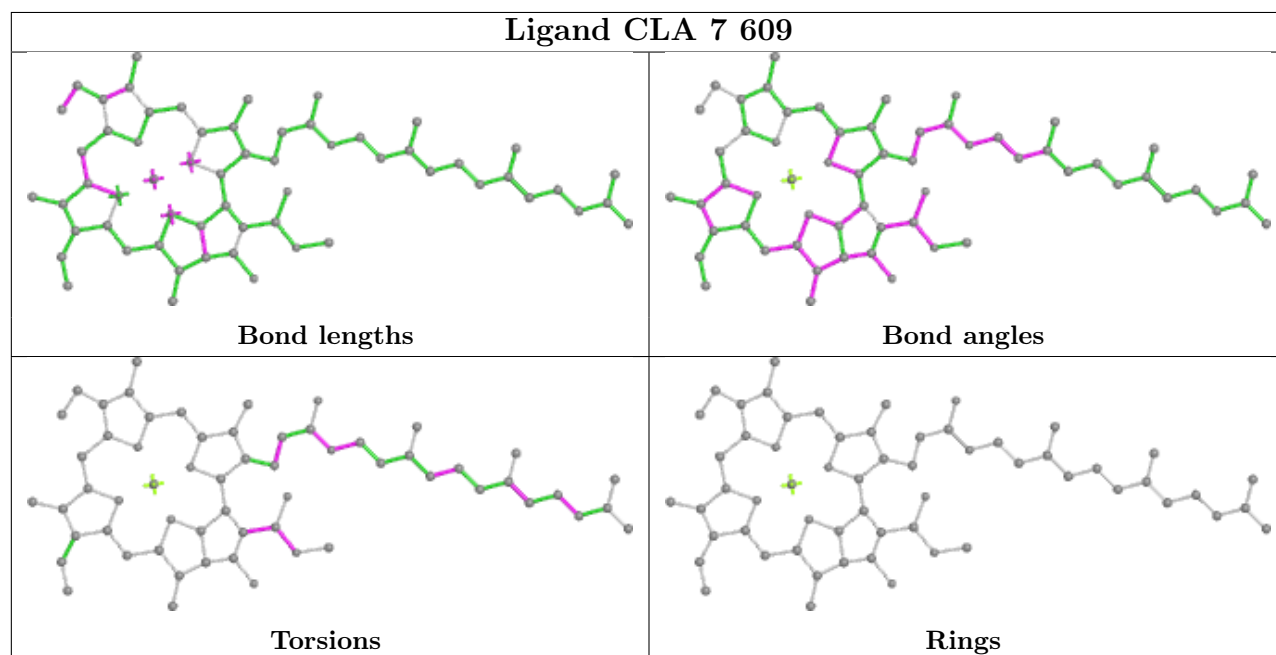
Rings

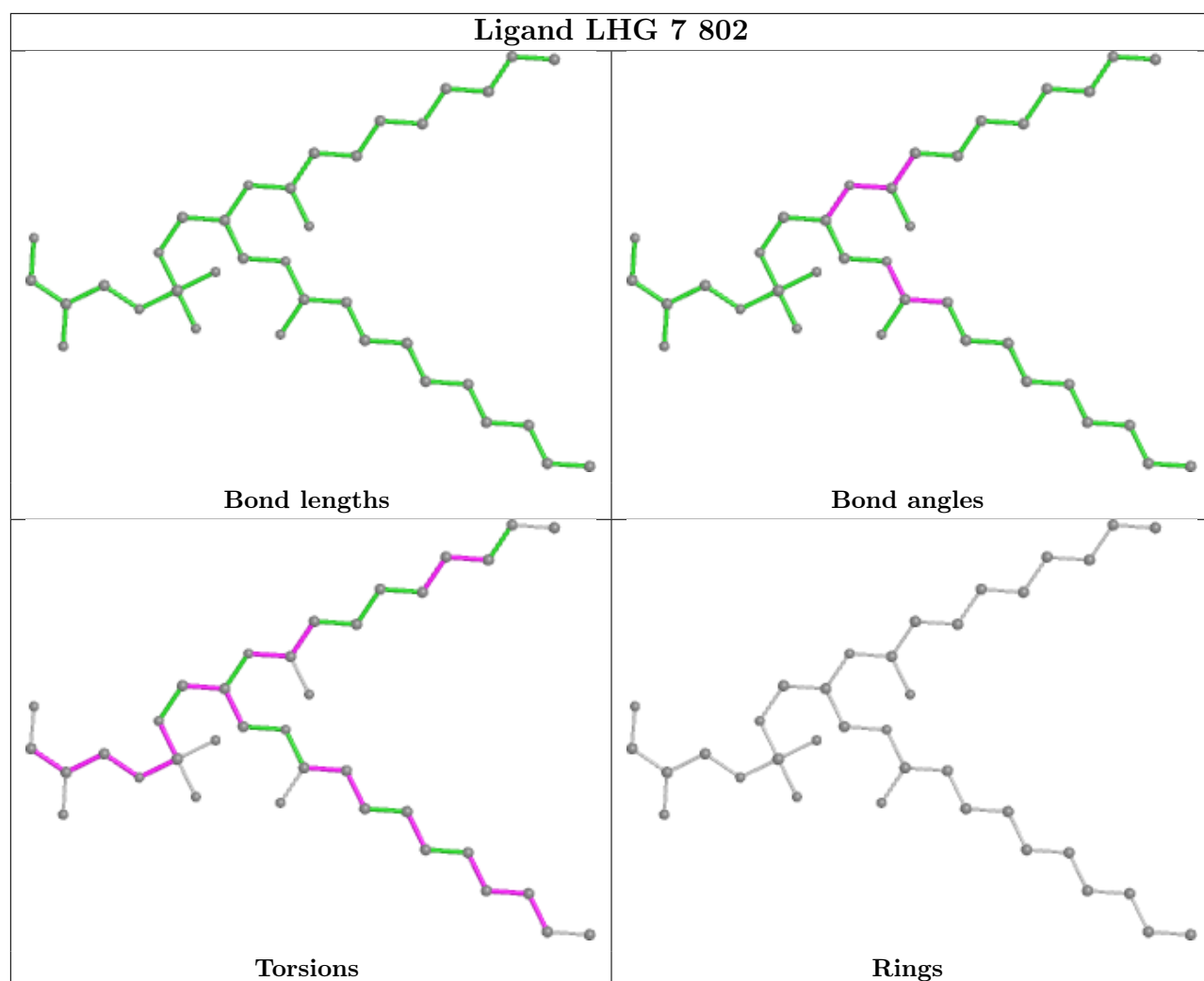


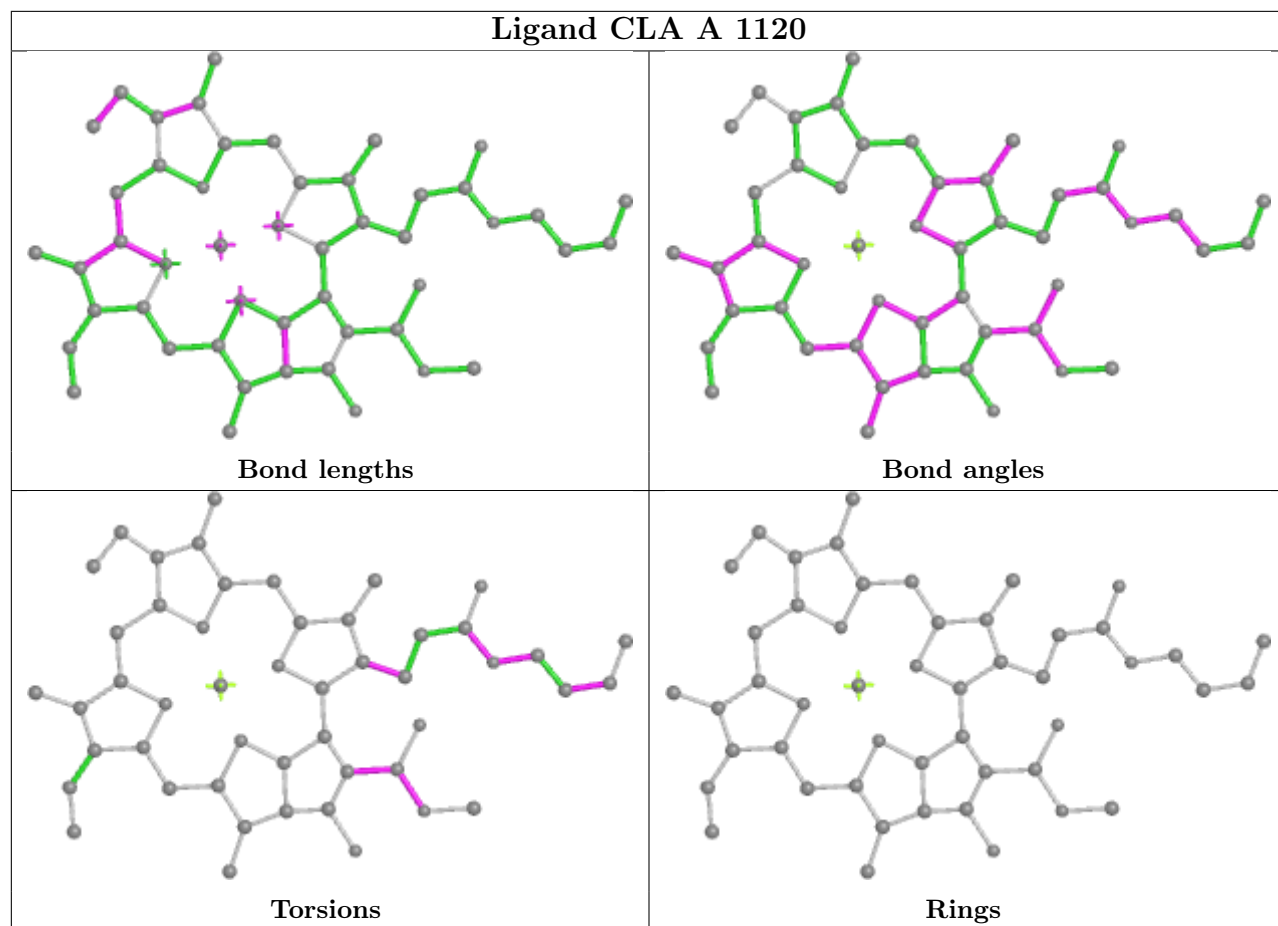
Ligand CLA B 1205



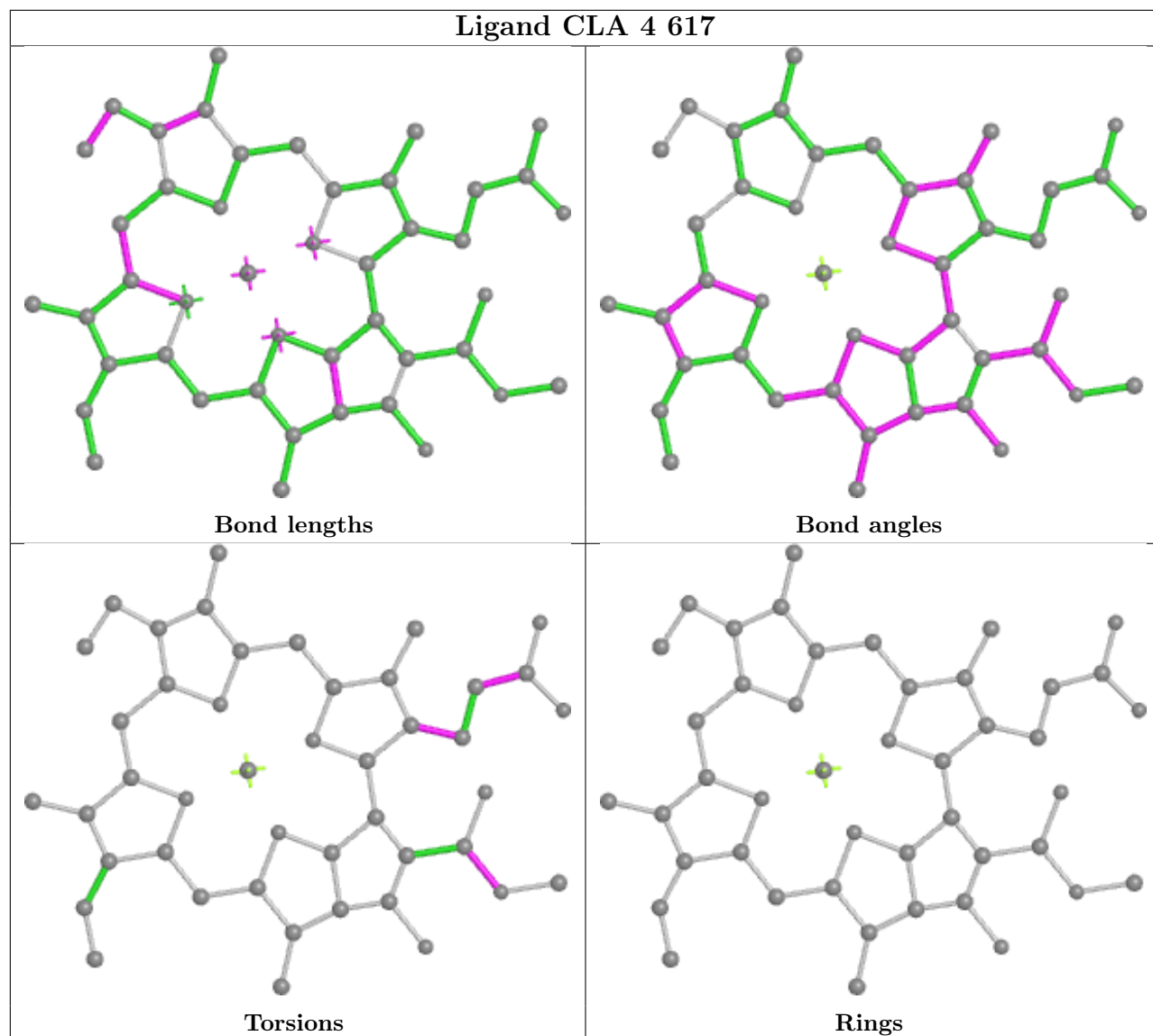
Ligand CLA 7 609

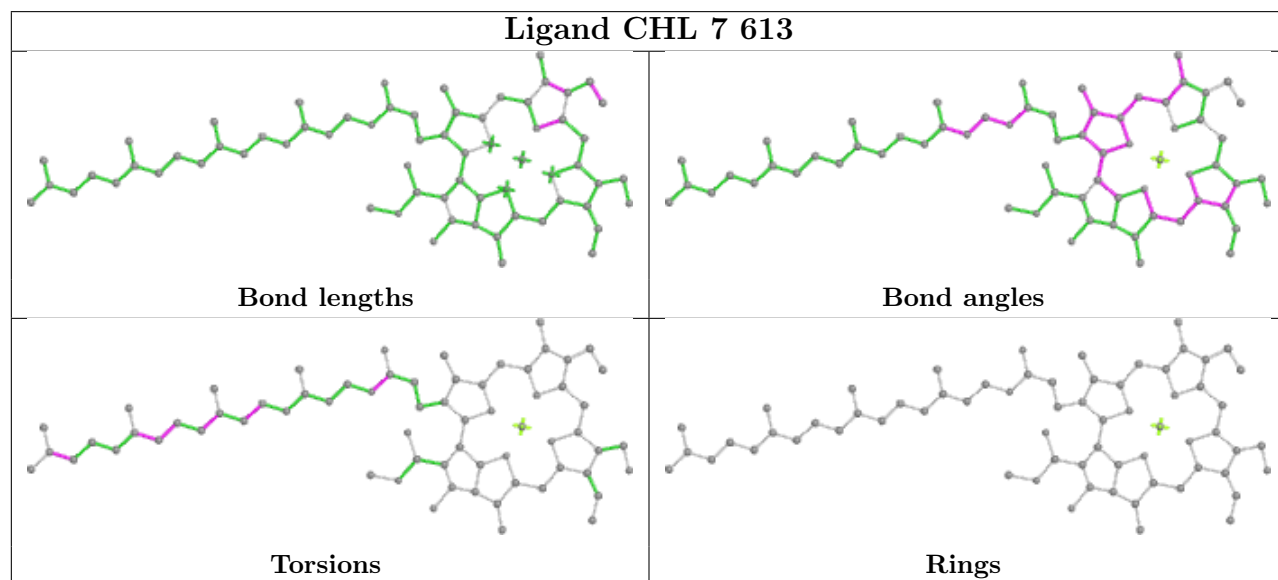
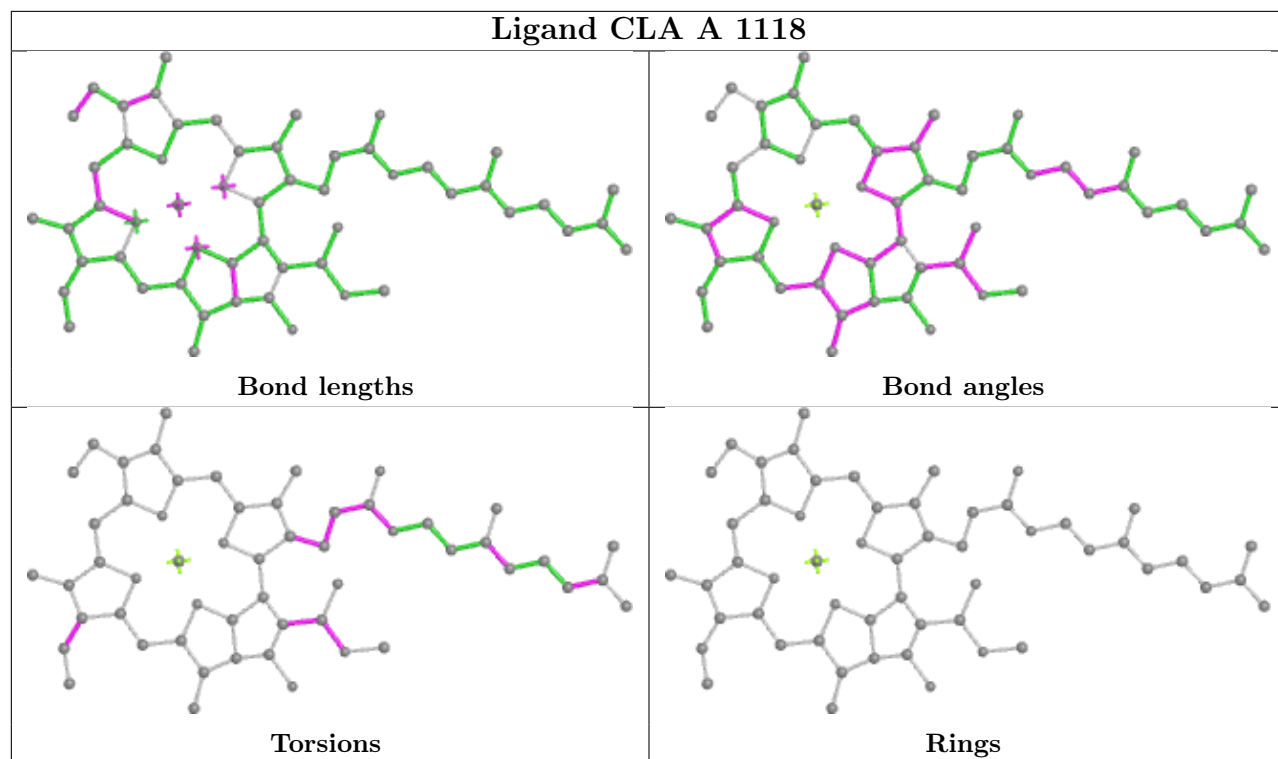




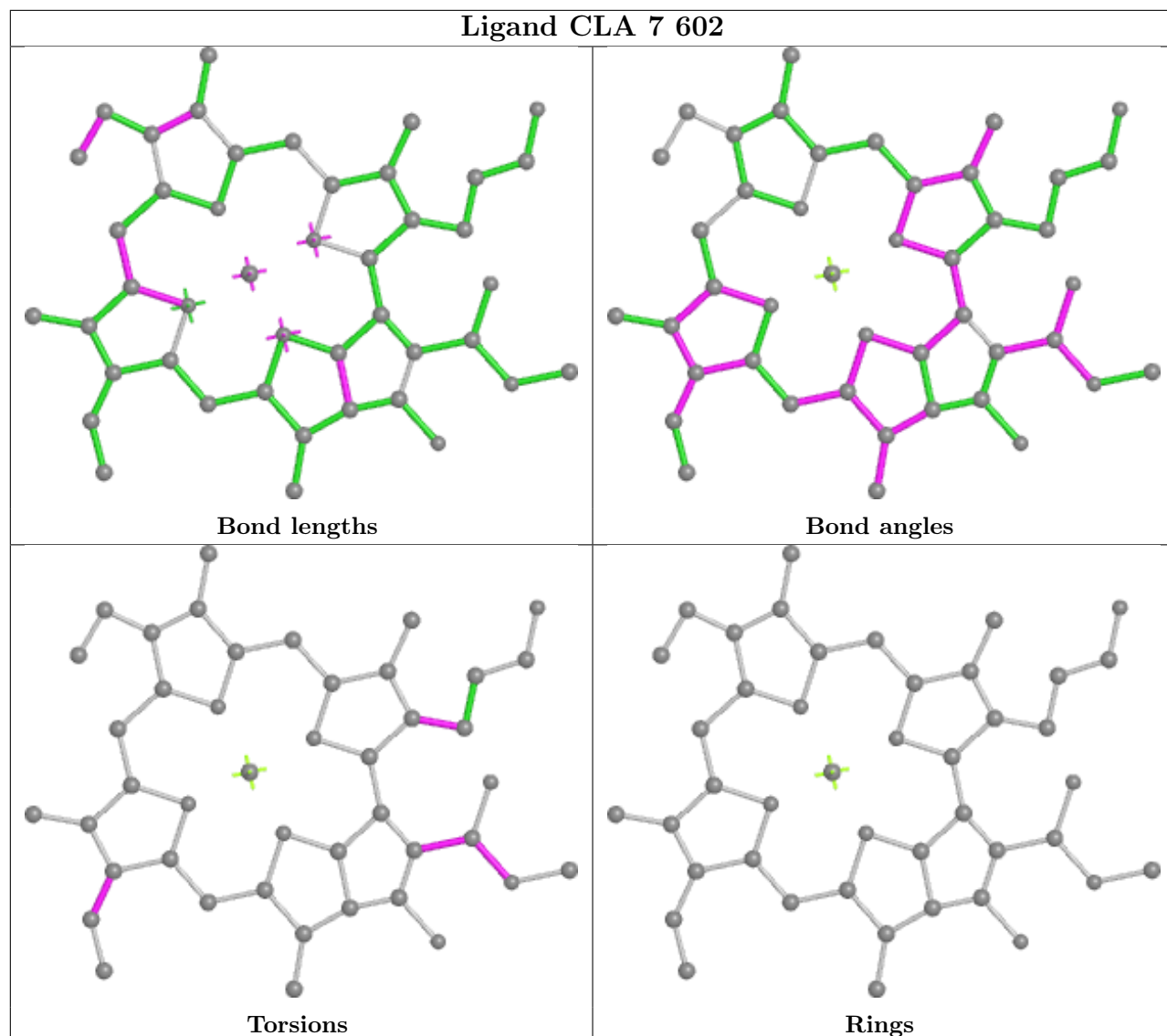


Ligand CLA 4 617

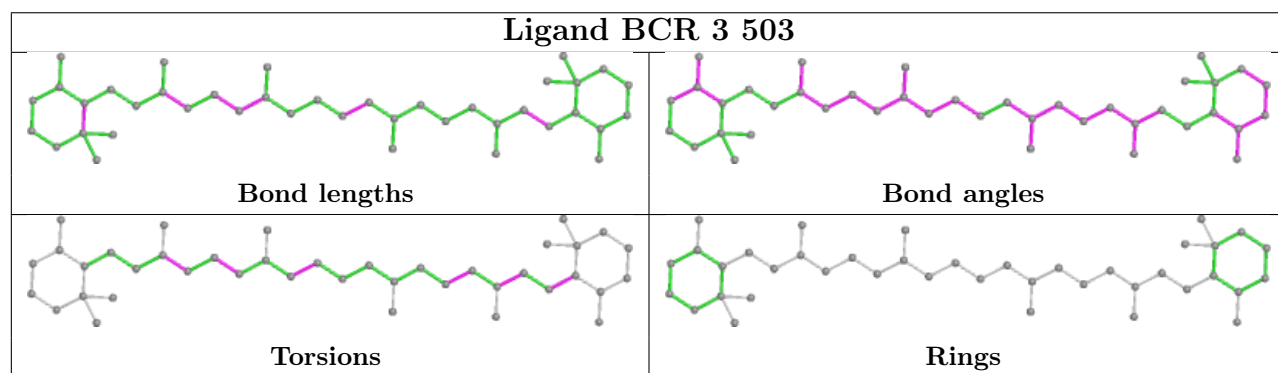


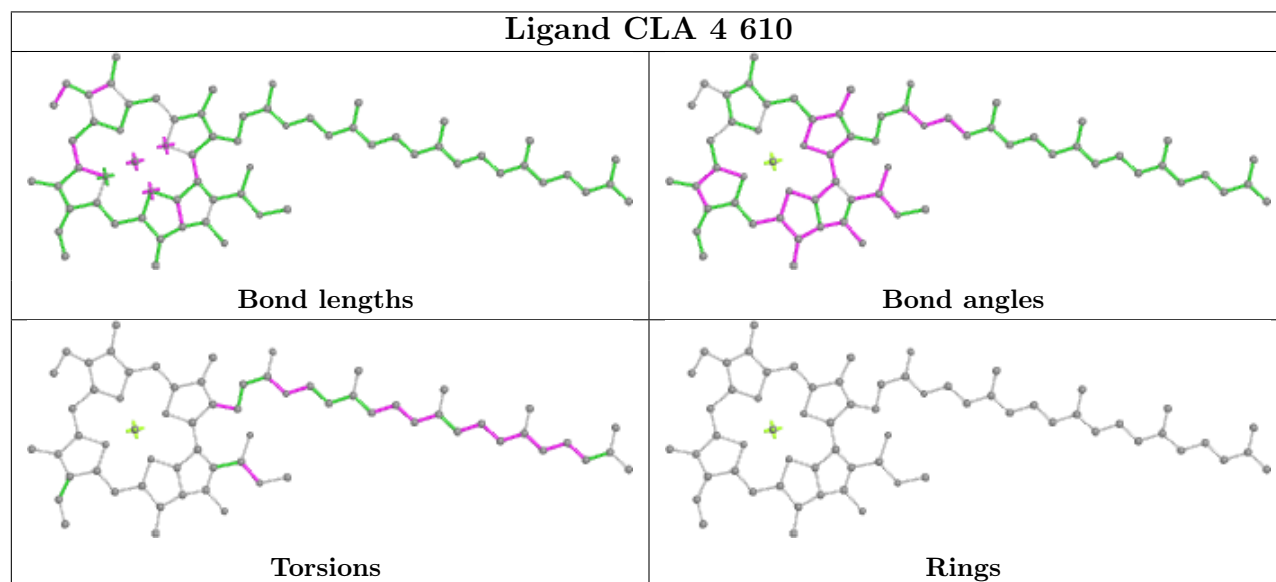
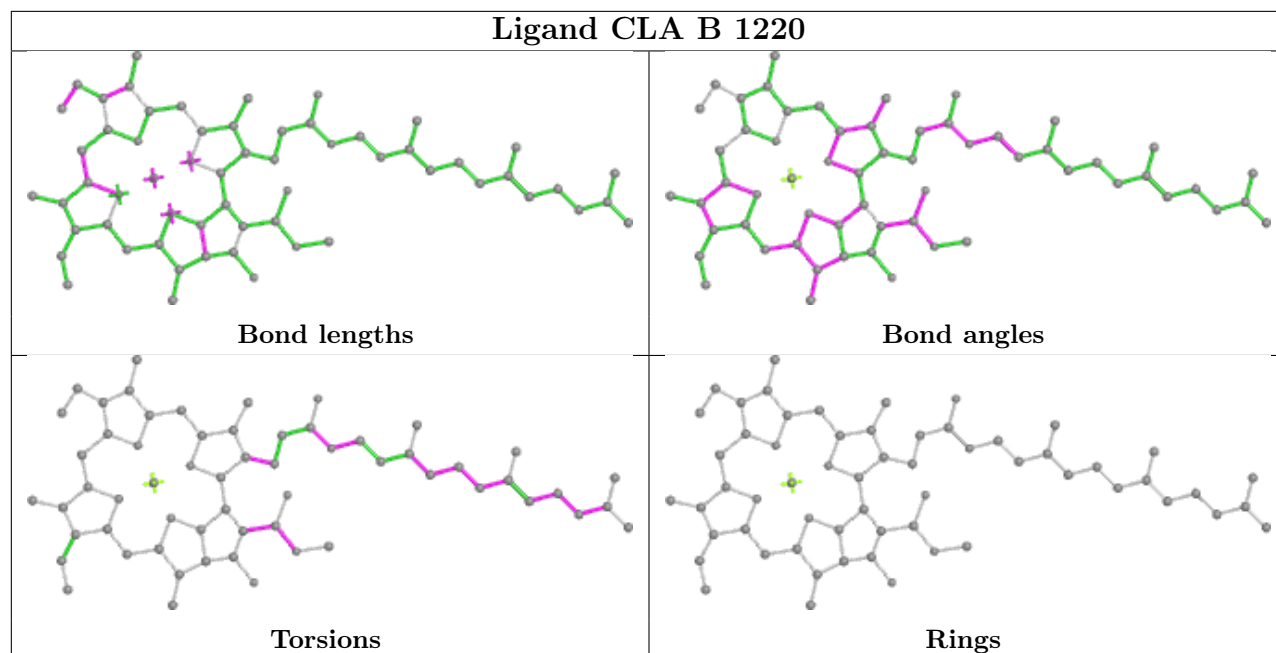


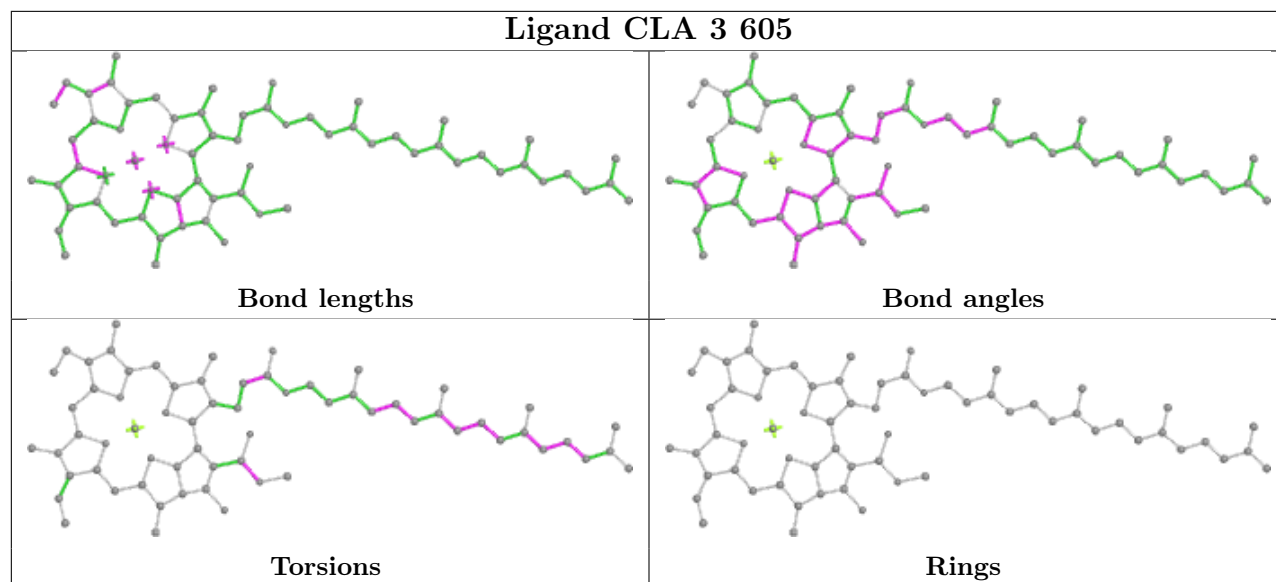
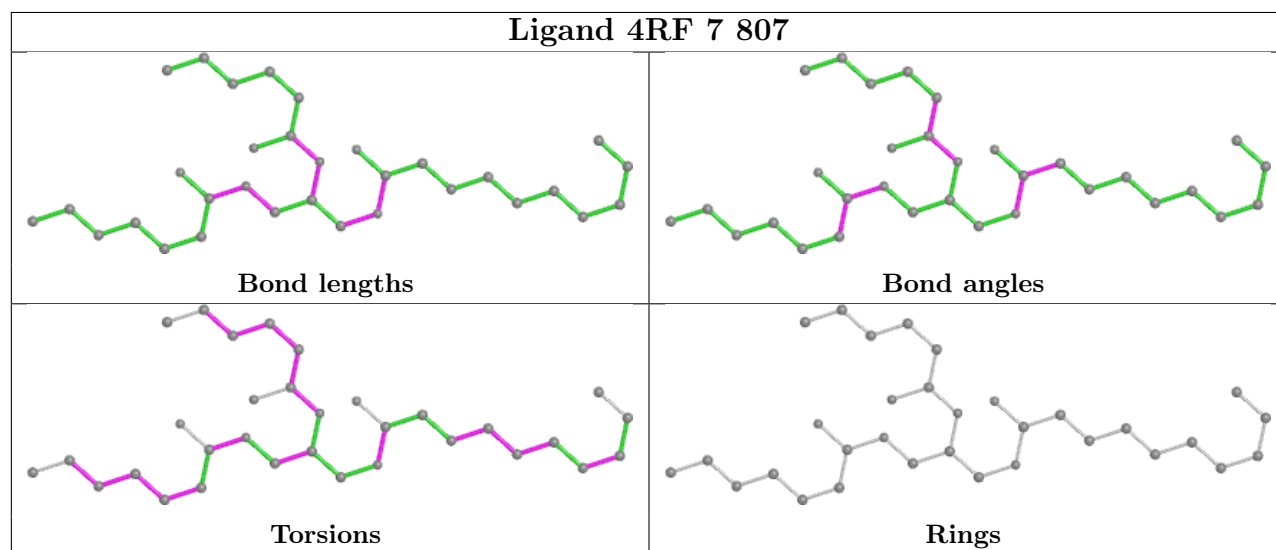
Ligand CLA 7 602

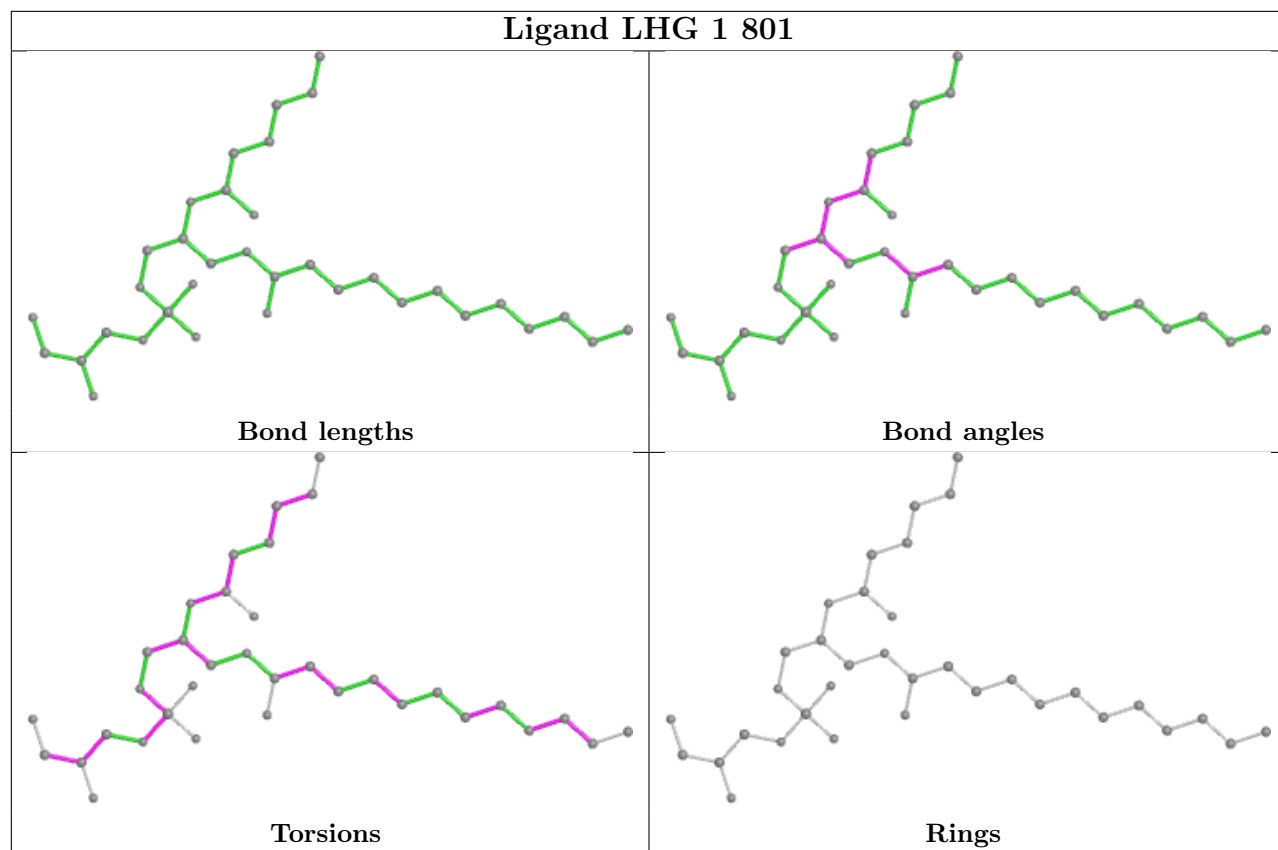


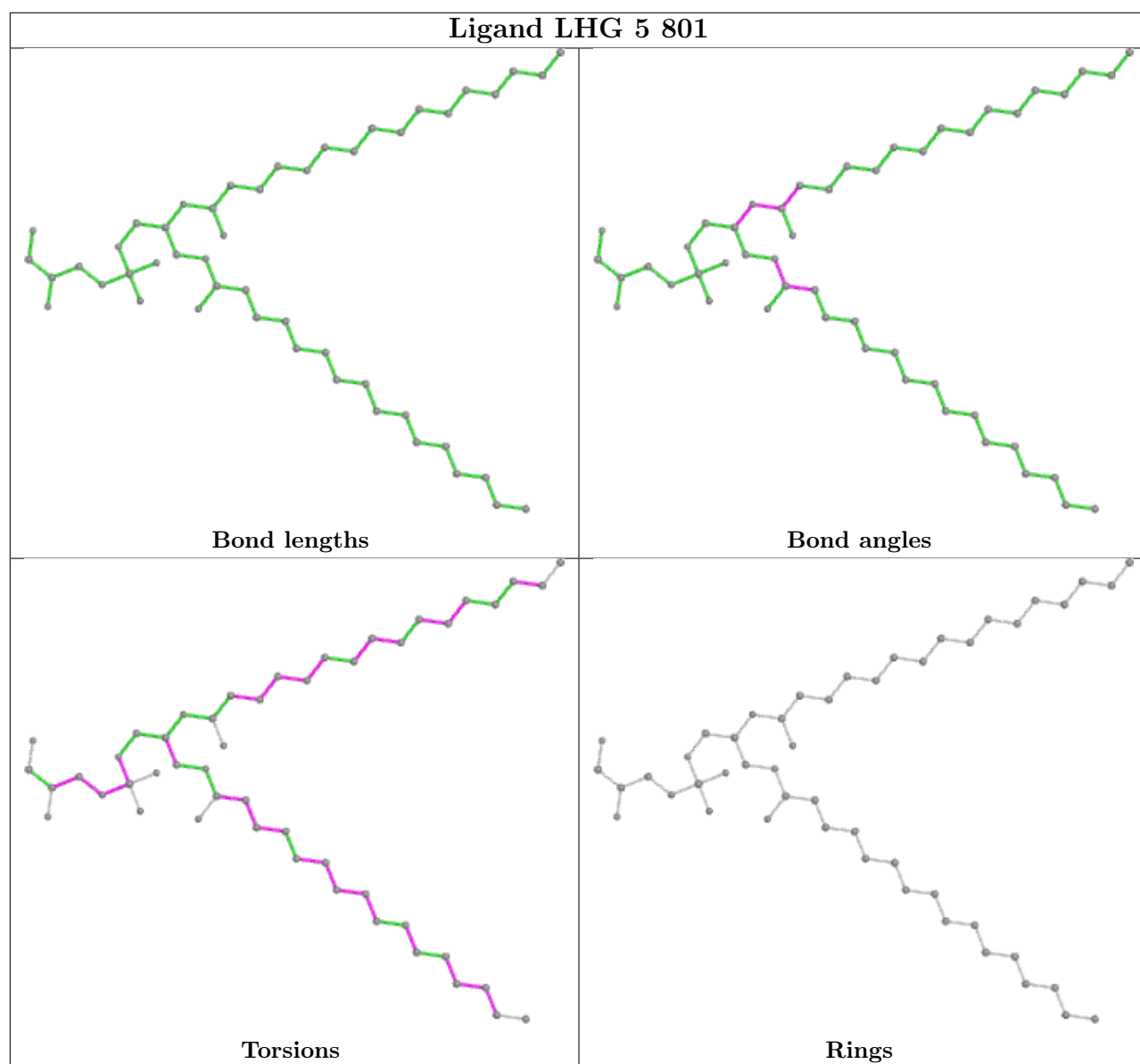
Ligand BCR 3 503



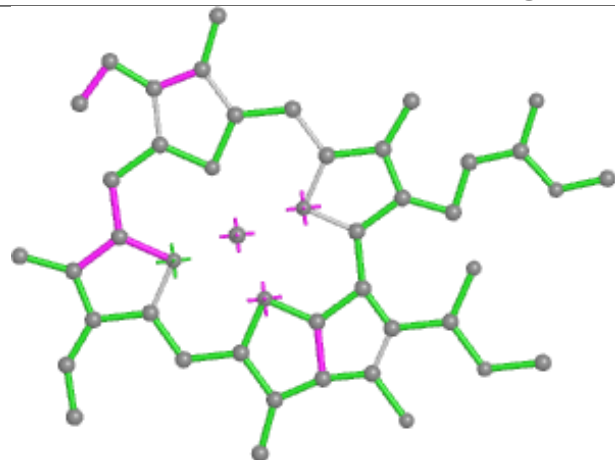


Ligand CLA 3 605**Ligand 4RF 7 807**

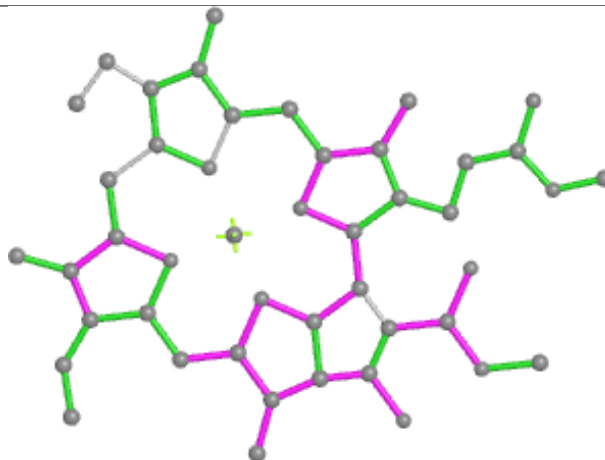




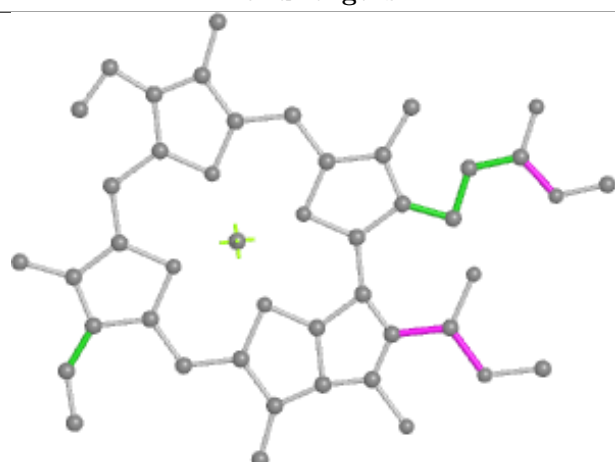
Ligand CLA 6 605



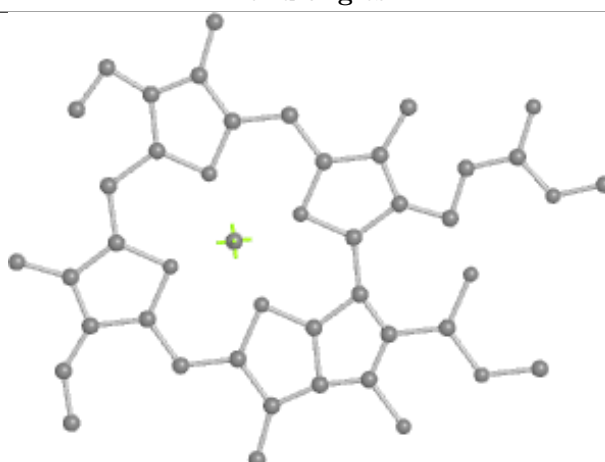
Bond lengths



Bond angles

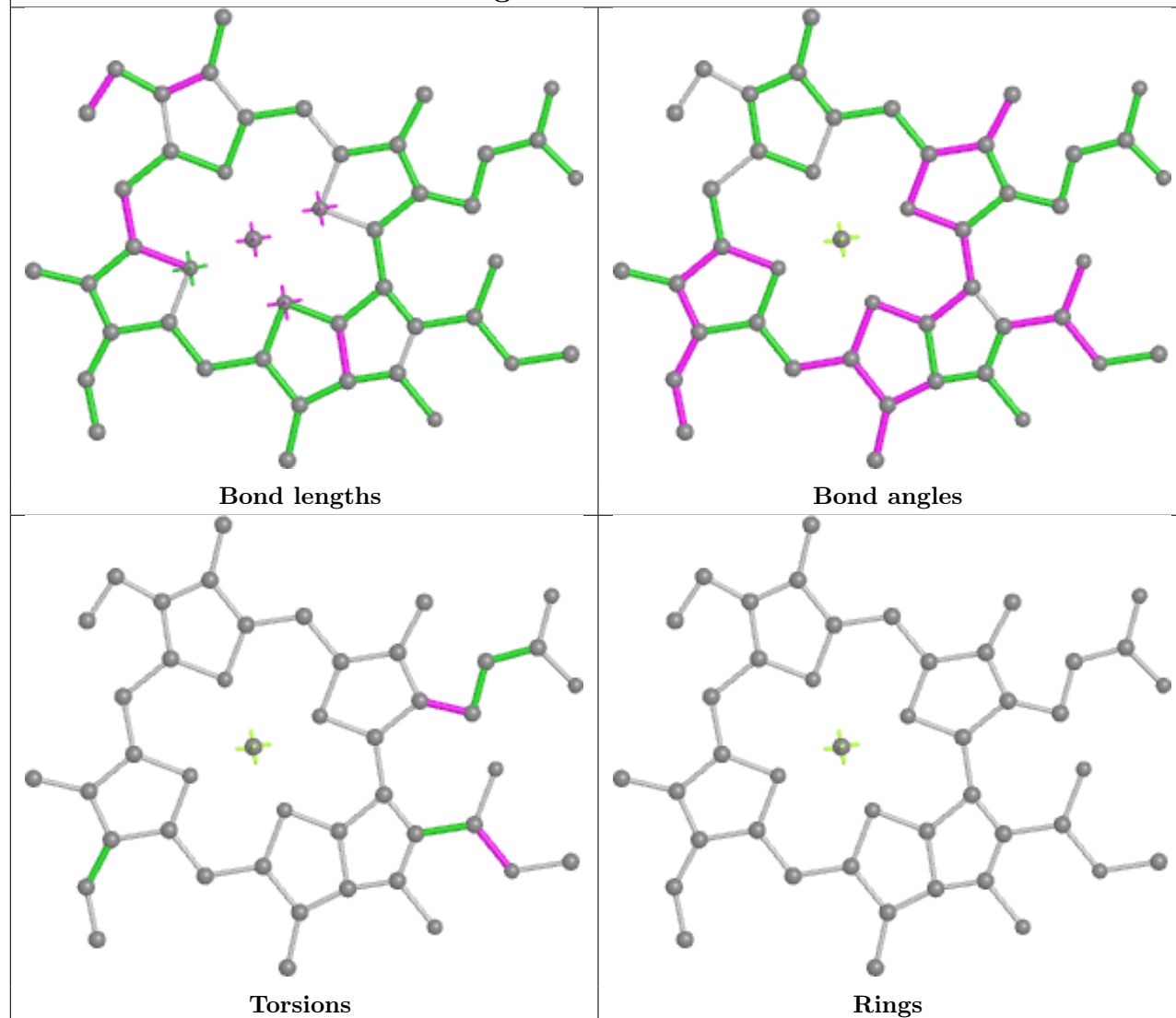


Torsions

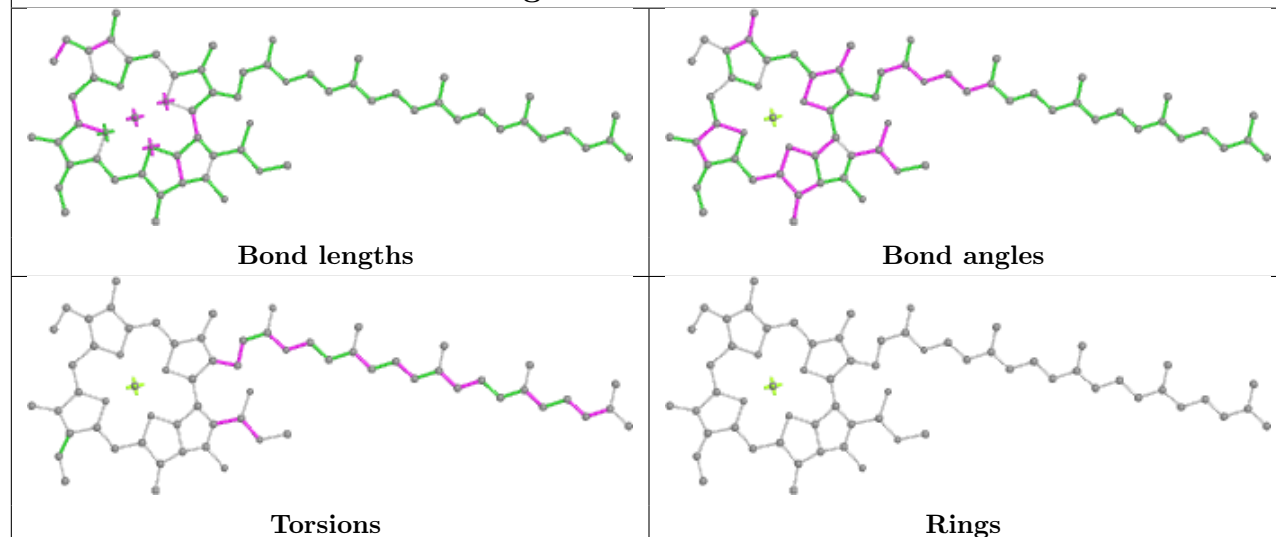


Rings

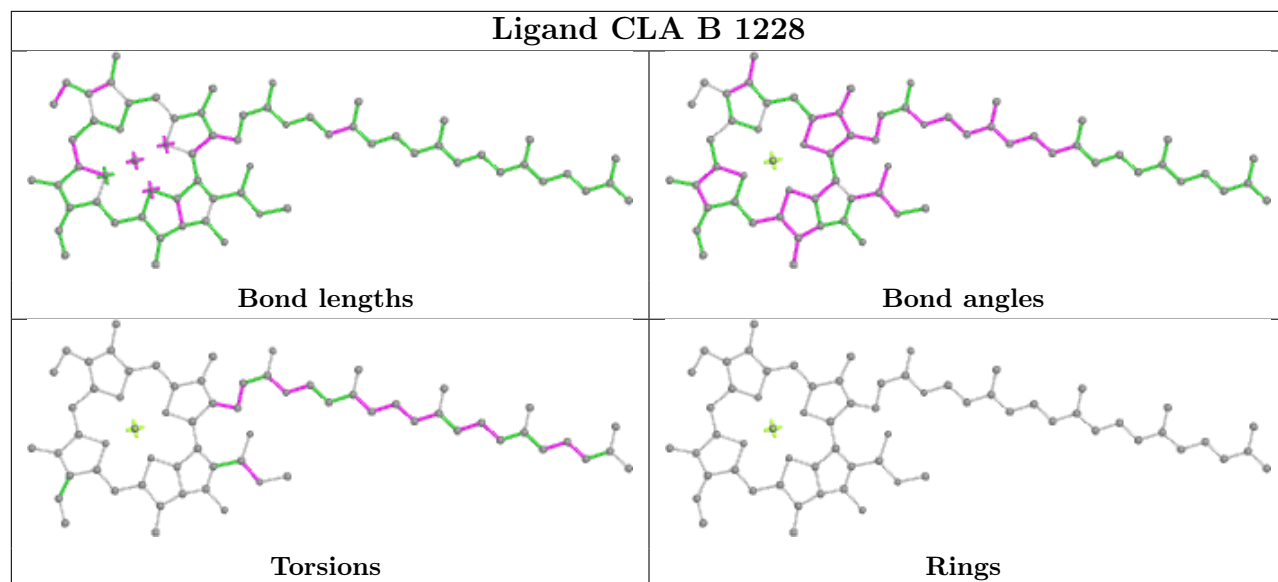
Ligand CLA 6 617



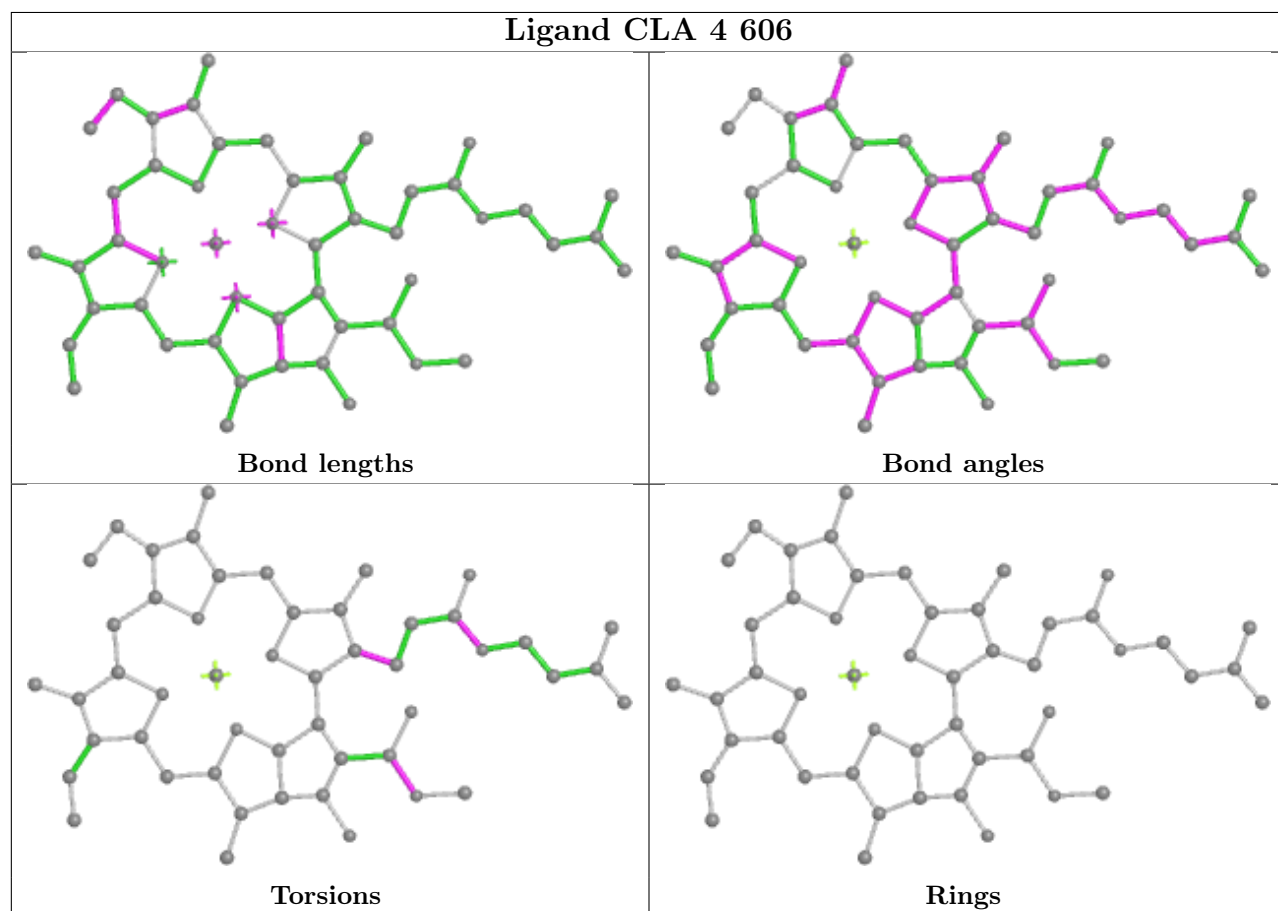
Ligand CLA B 1235

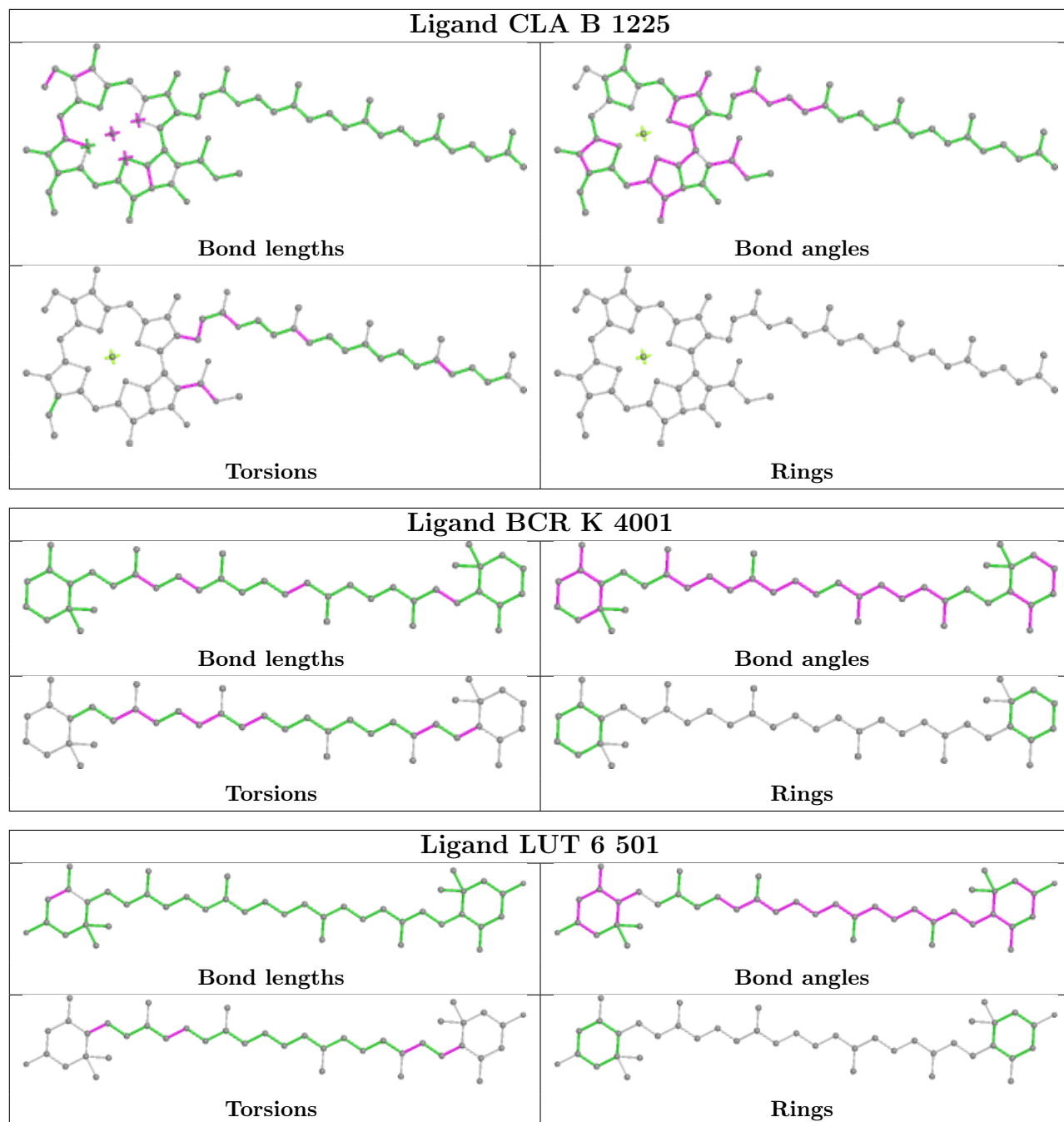


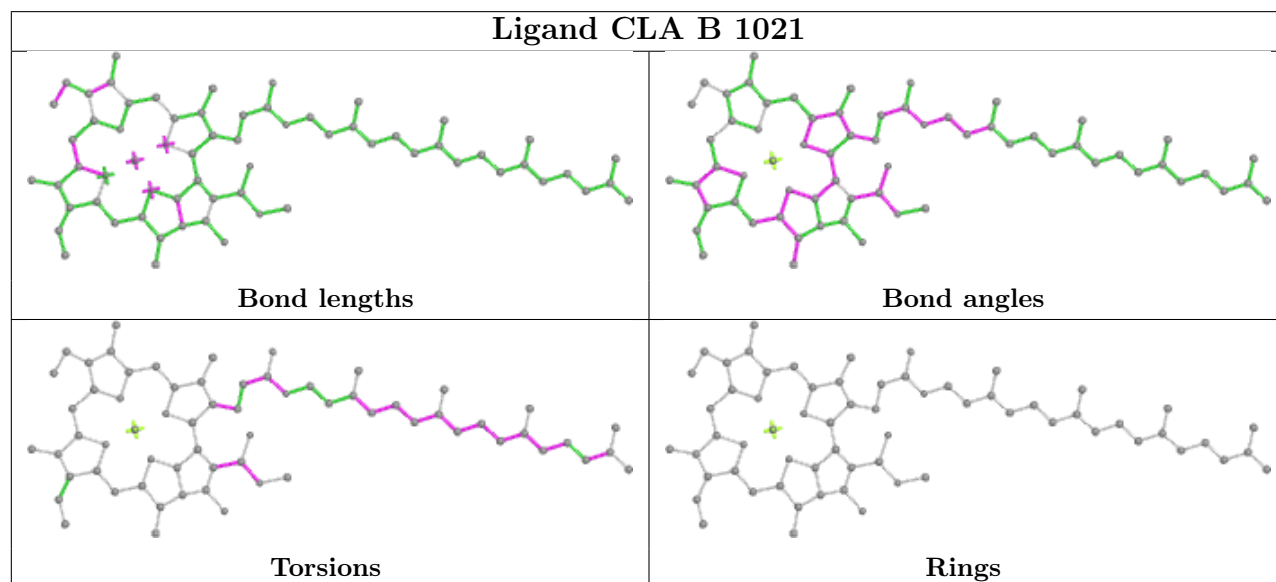
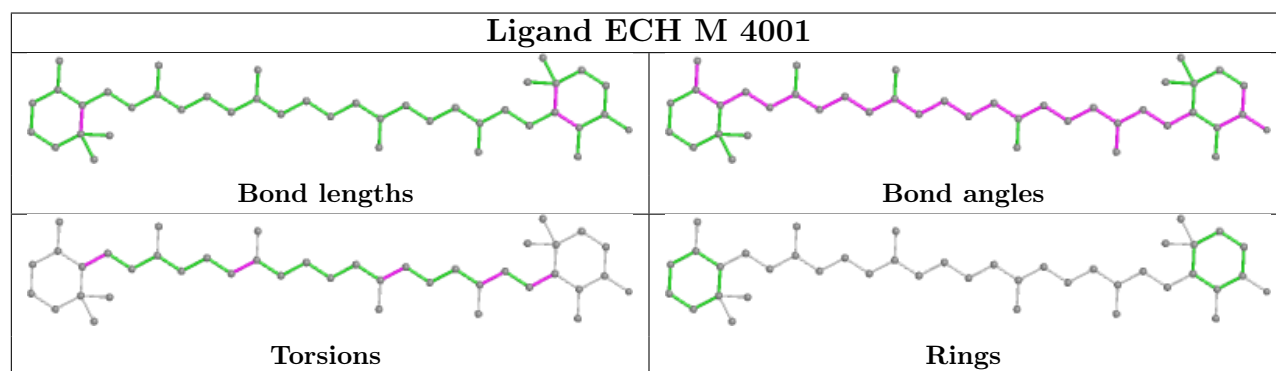
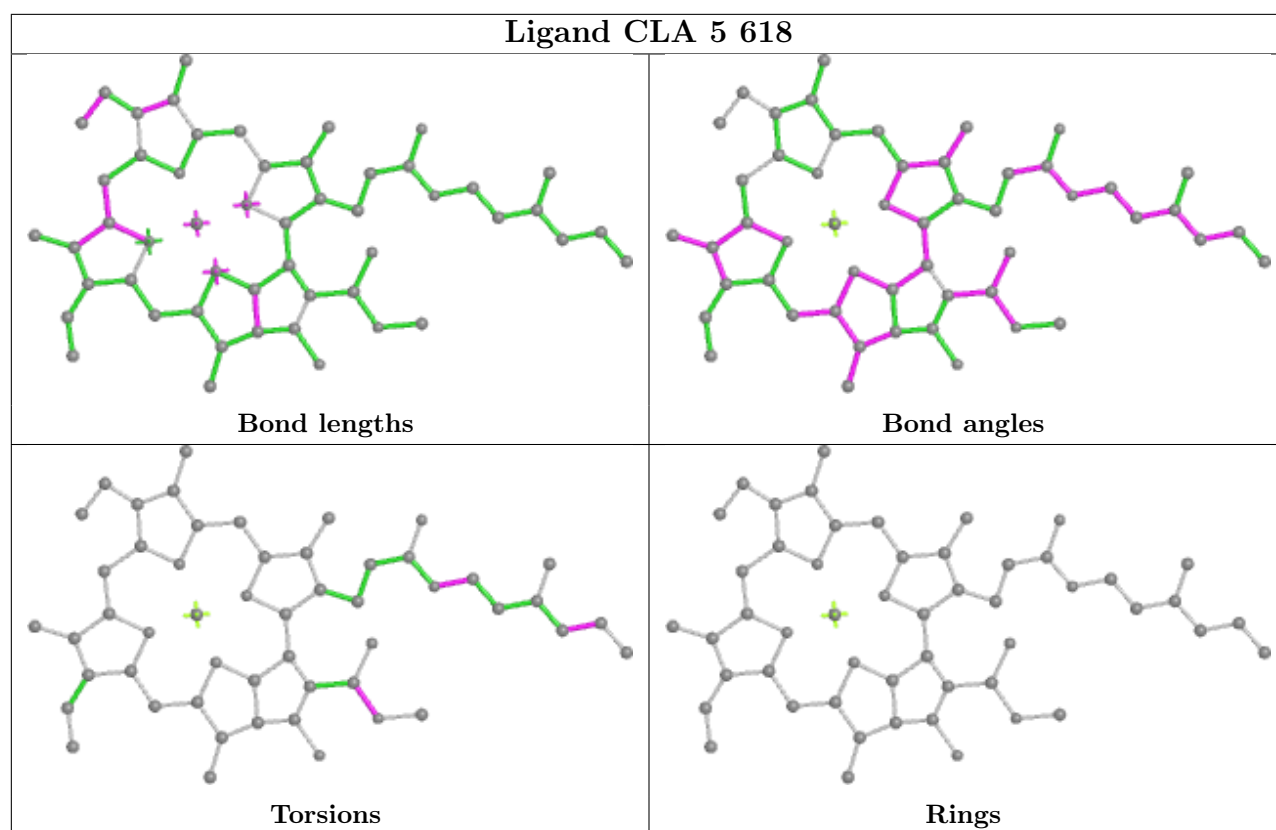
Ligand CLA B 1228



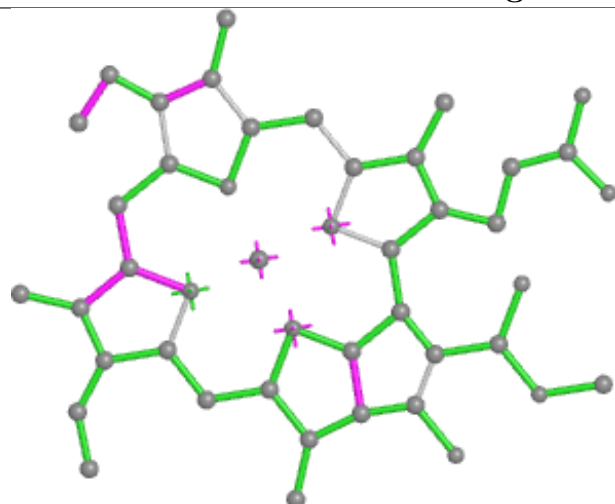
Ligand CLA 4 606



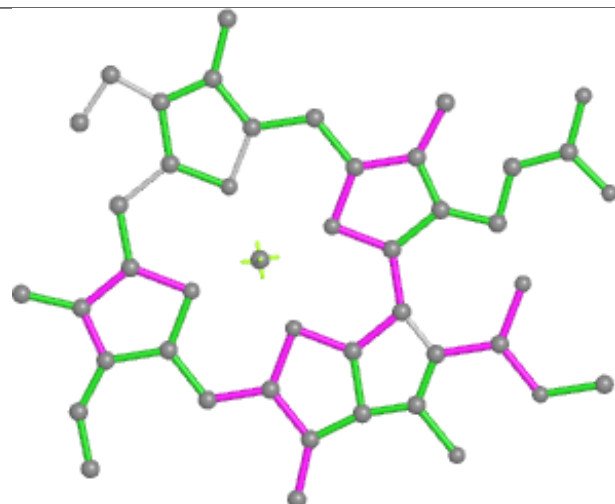




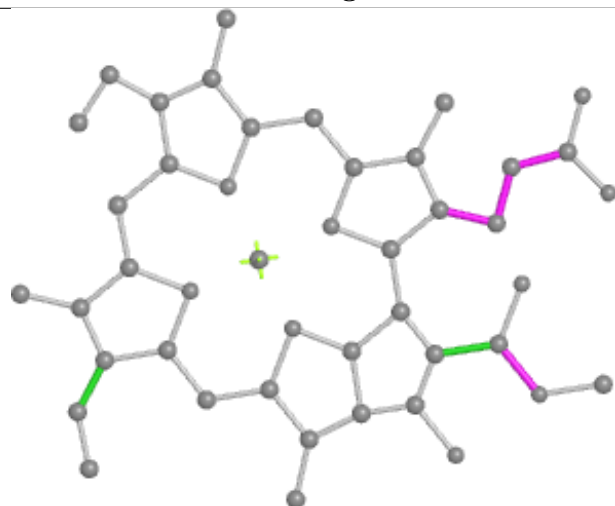
Ligand CLA G 1603



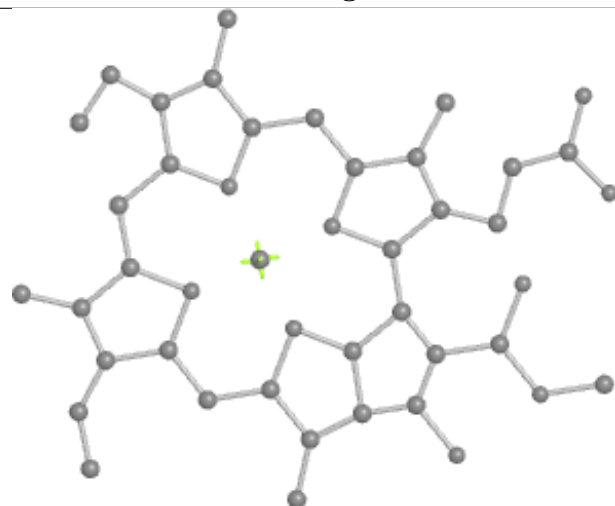
Bond lengths



Bond angles

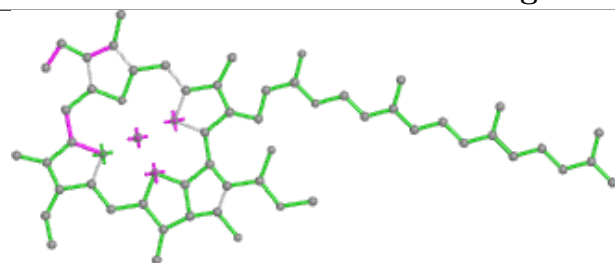


Torsions

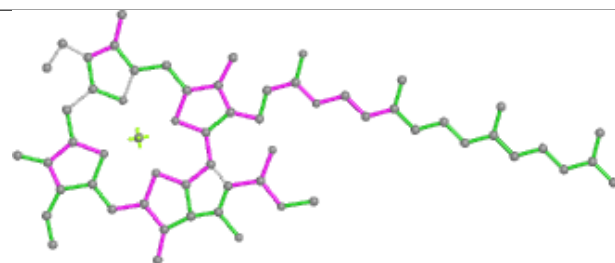


Rings

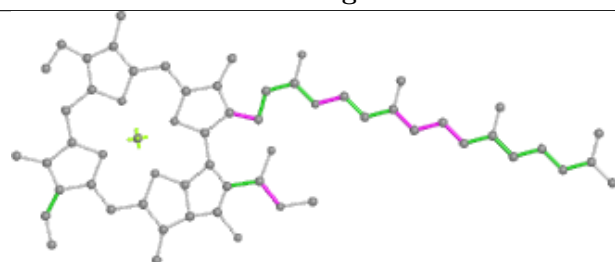
Ligand CLA 4 601



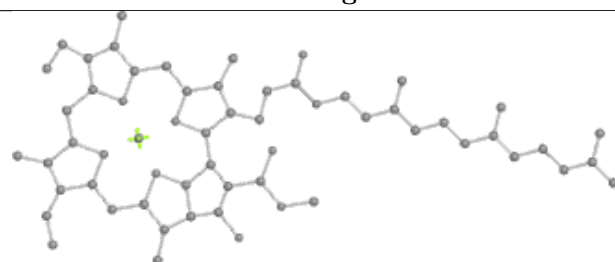
Bond lengths



Bond angles

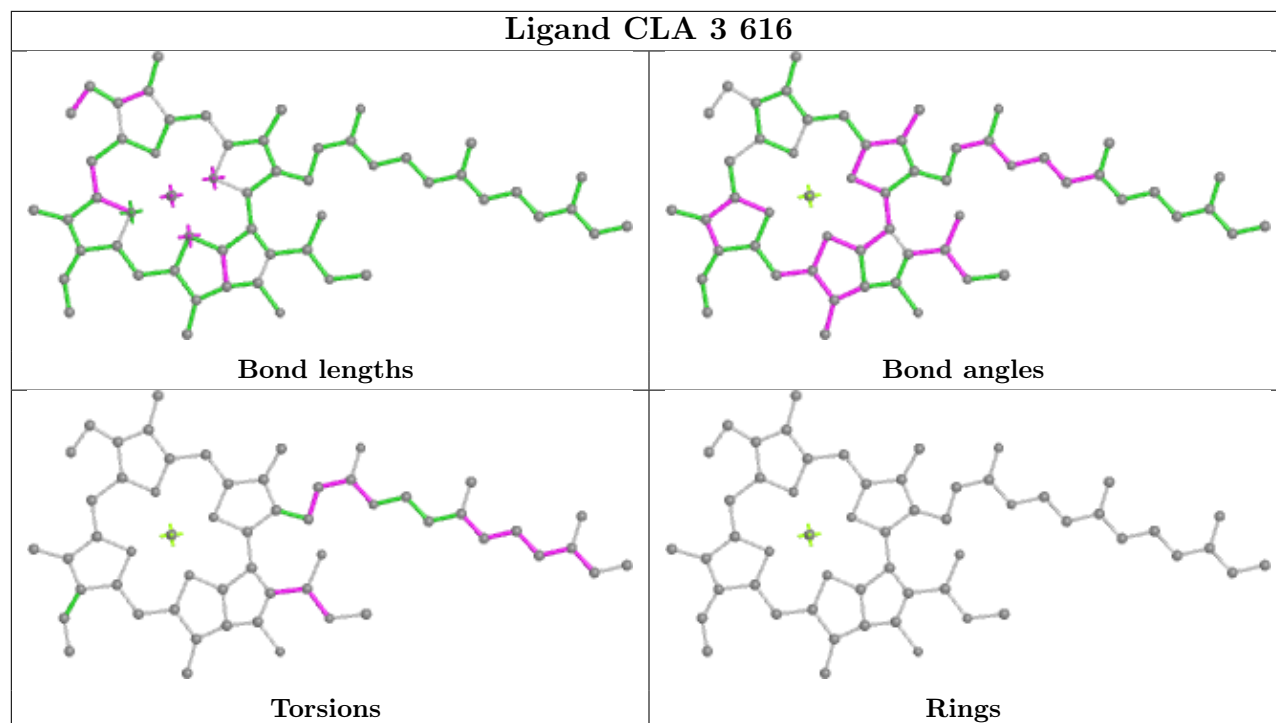


Torsions

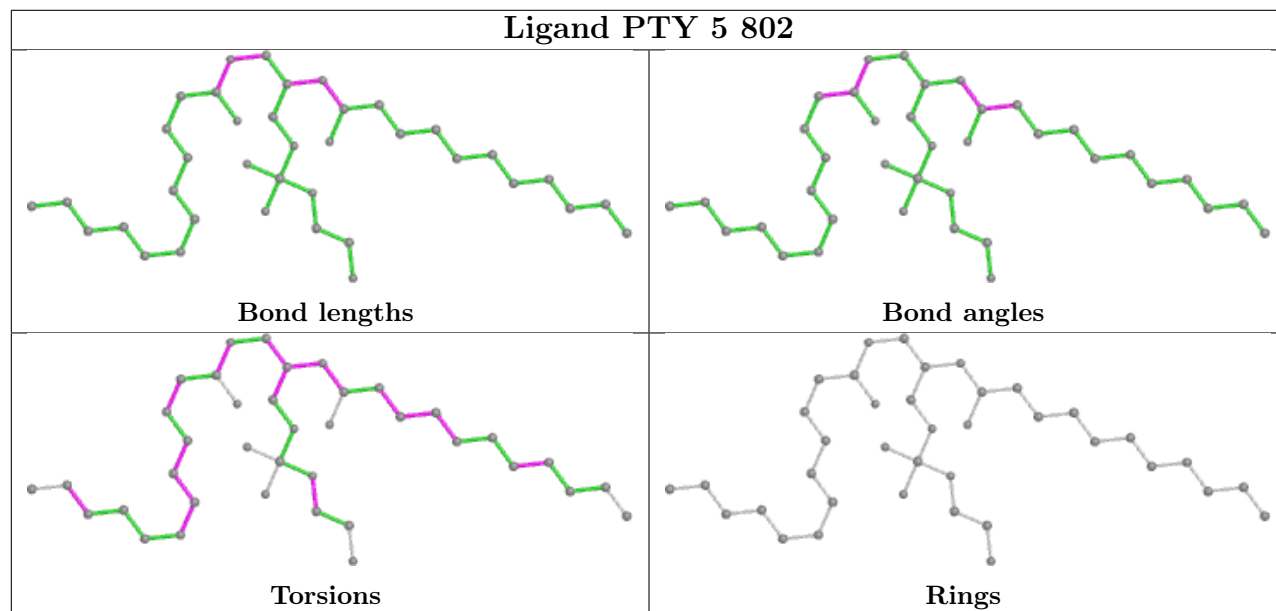


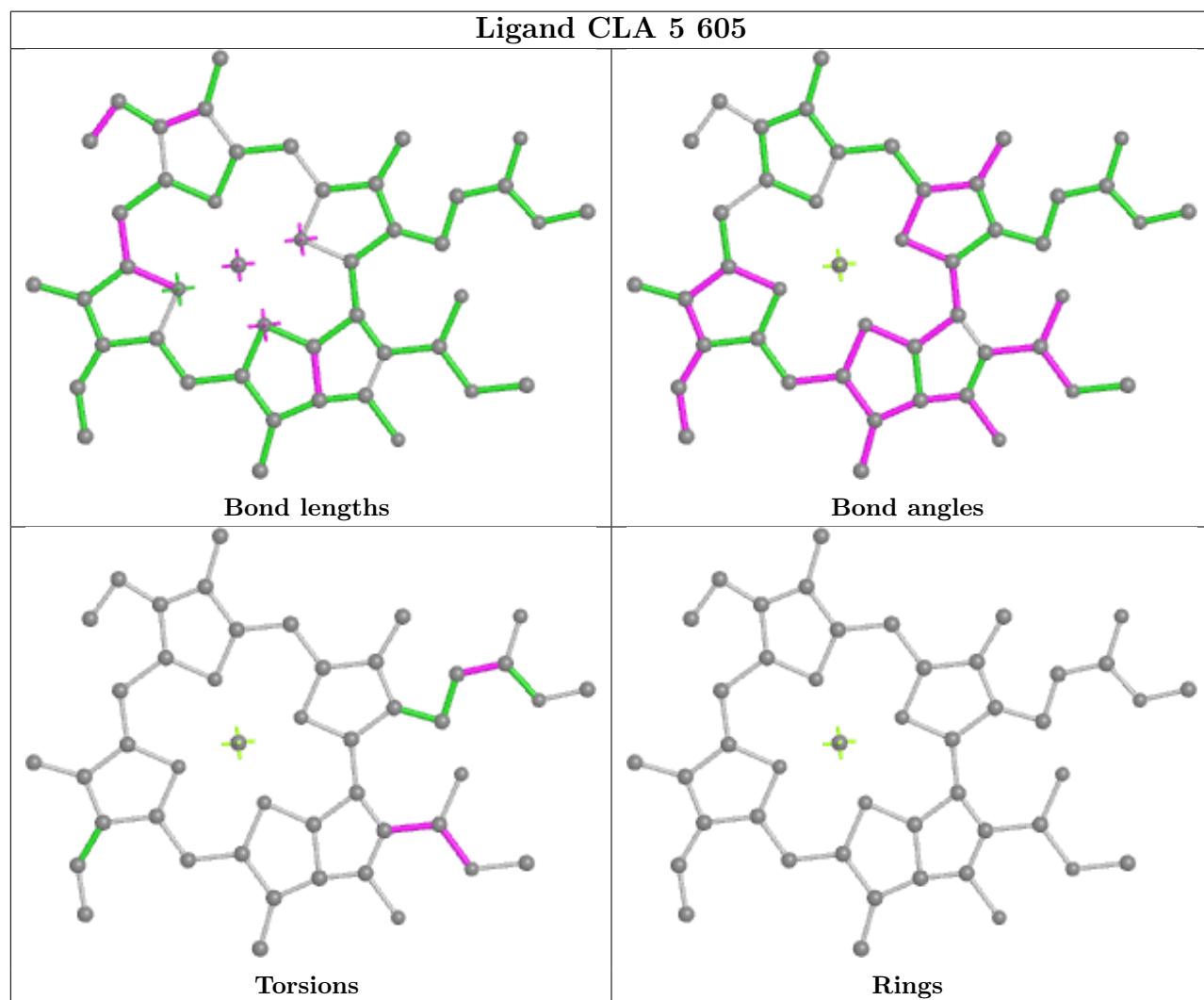
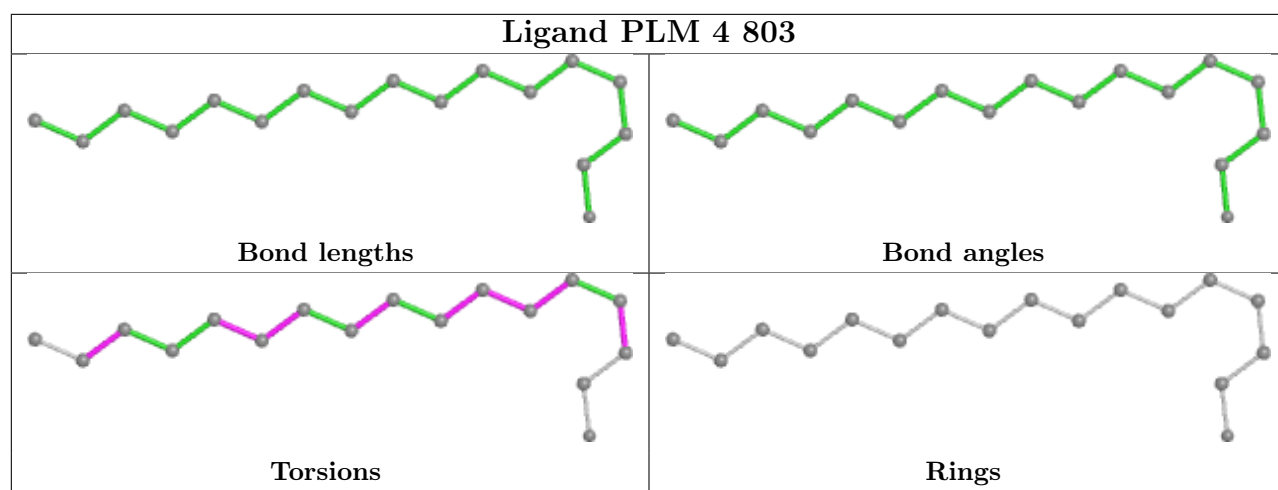
Rings

Ligand CLA 3 616

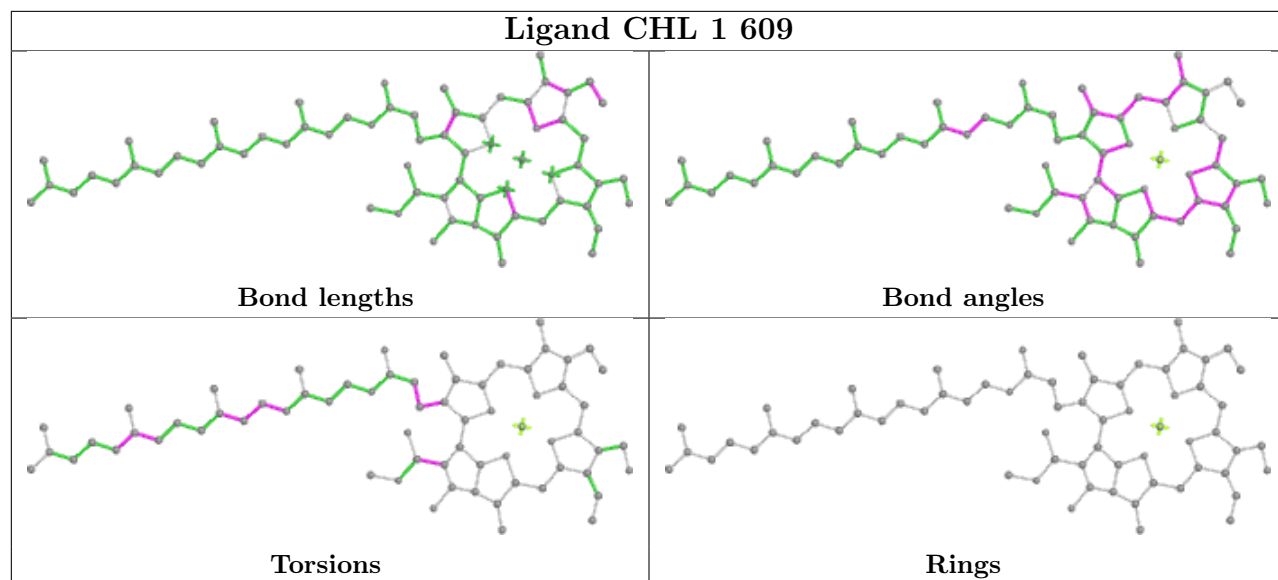


Ligand PTY 5 802

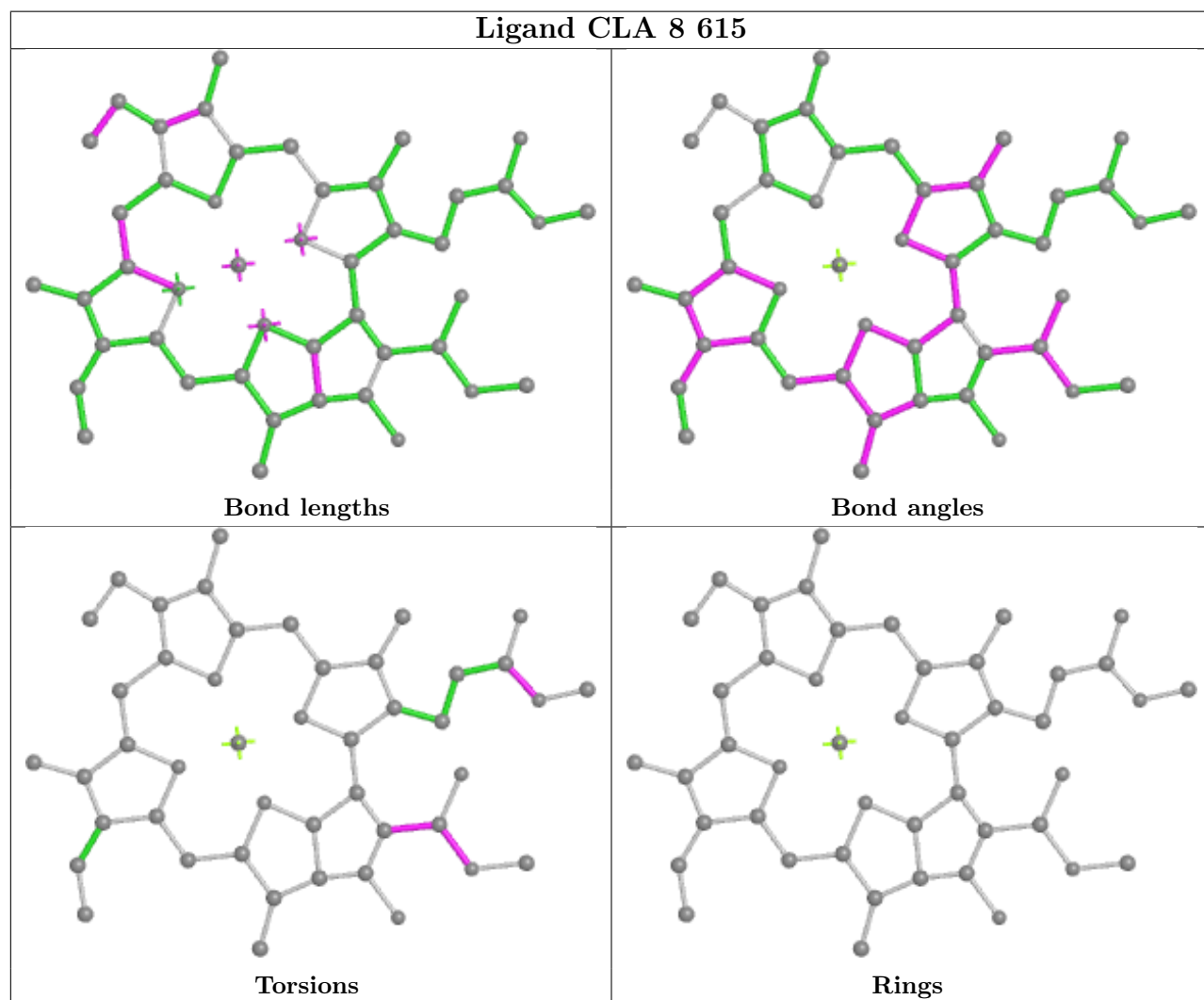




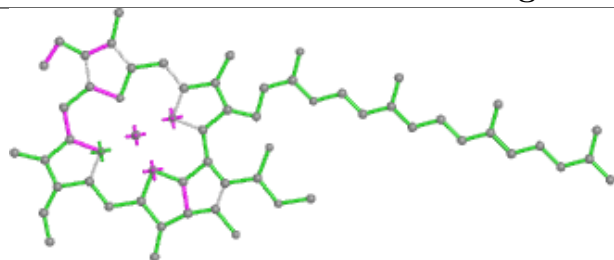
Ligand CHL 1 609



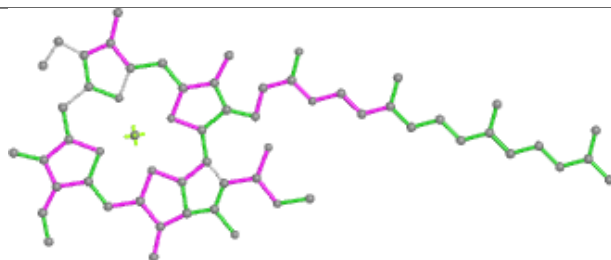
Ligand CLA 8 615



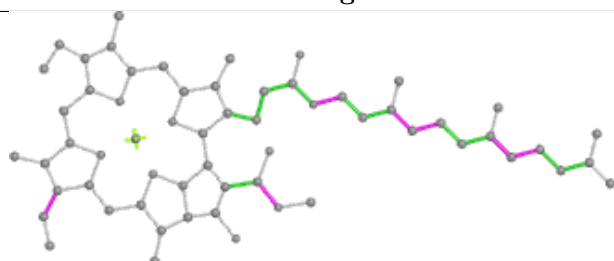
Ligand CLA 7 611



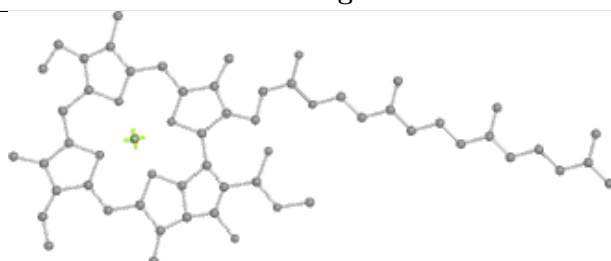
Bond lengths



Bond angles

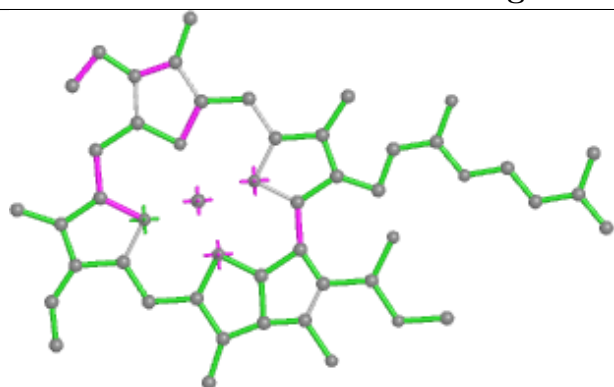


Torsions

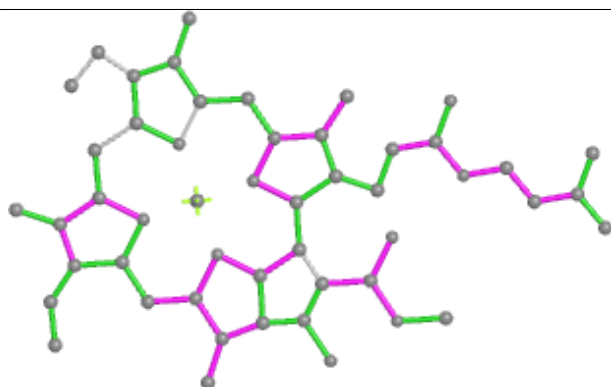


Rings

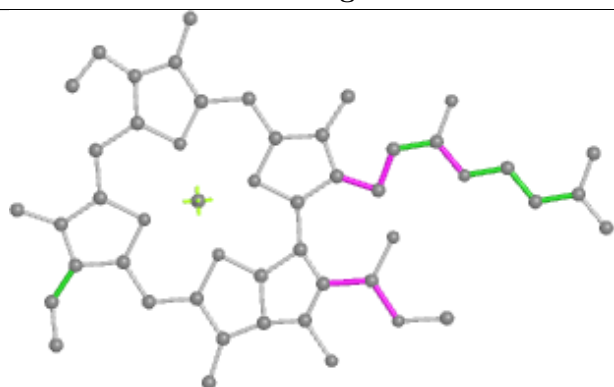
Ligand CLA L 1501



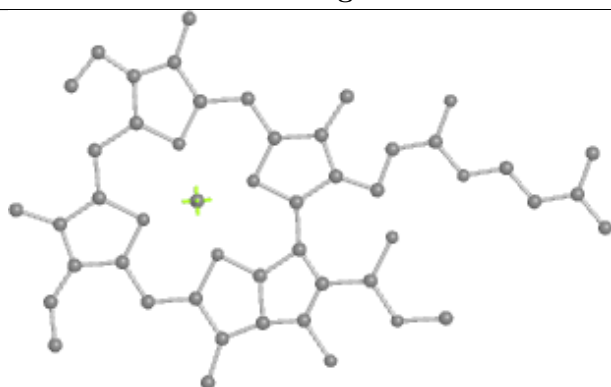
Bond lengths



Bond angles

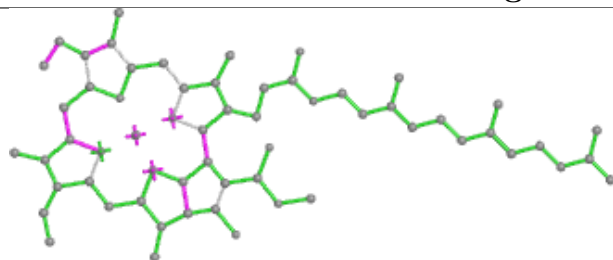


Torsions

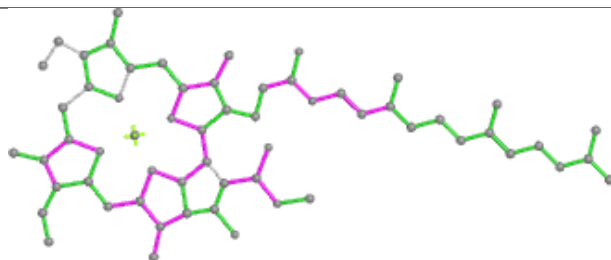


Rings

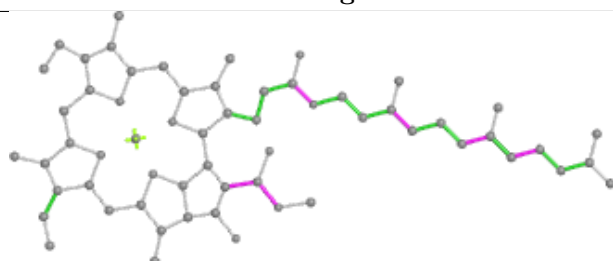
Ligand CLA A 1115



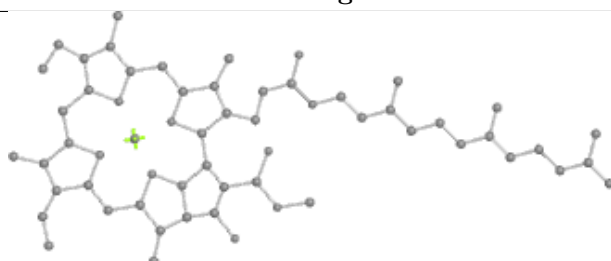
Bond lengths



Bond angles

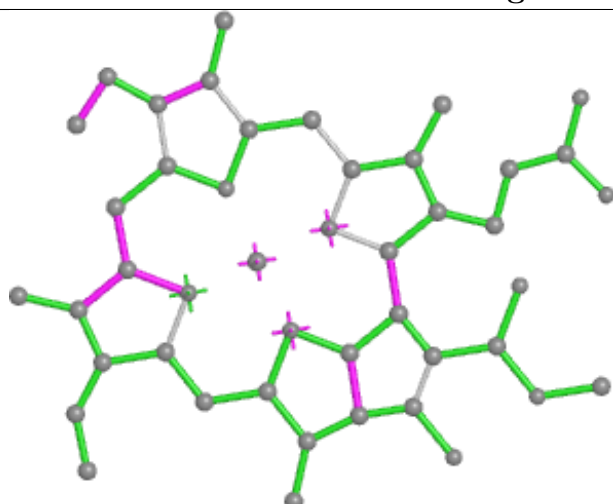


Torsions

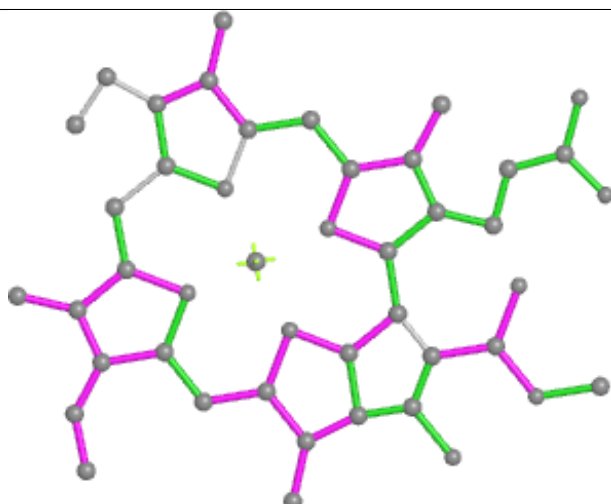


Rings

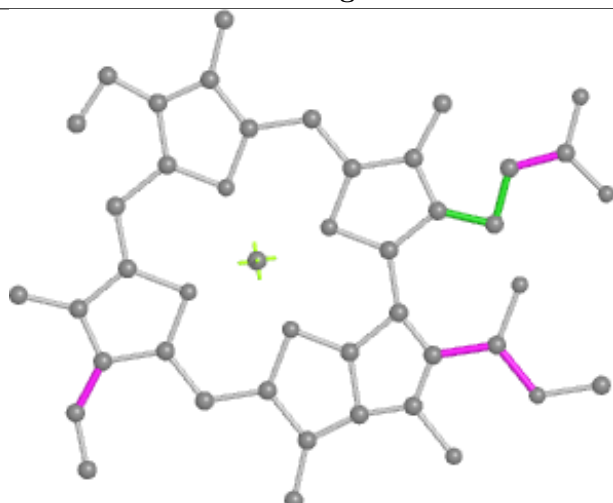
Ligand CLA L 1503



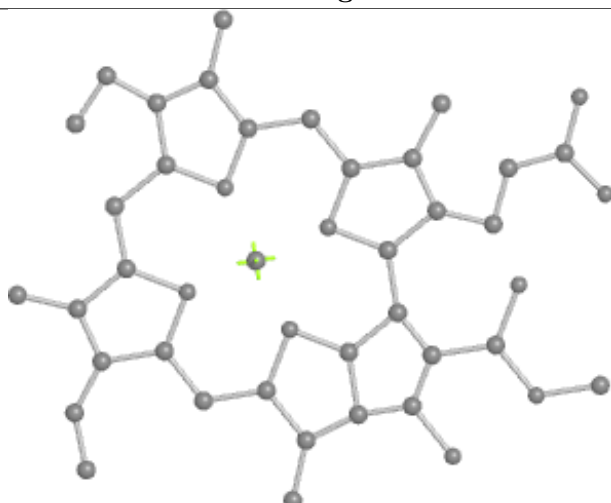
Bond lengths



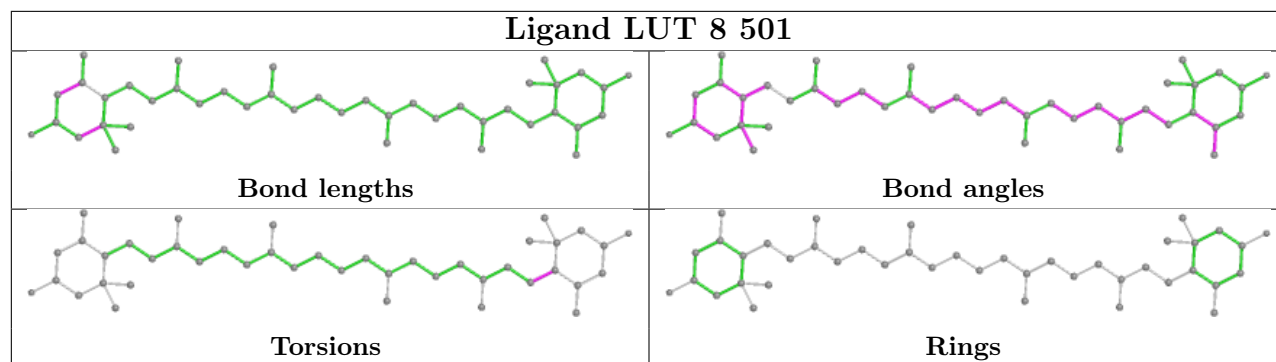
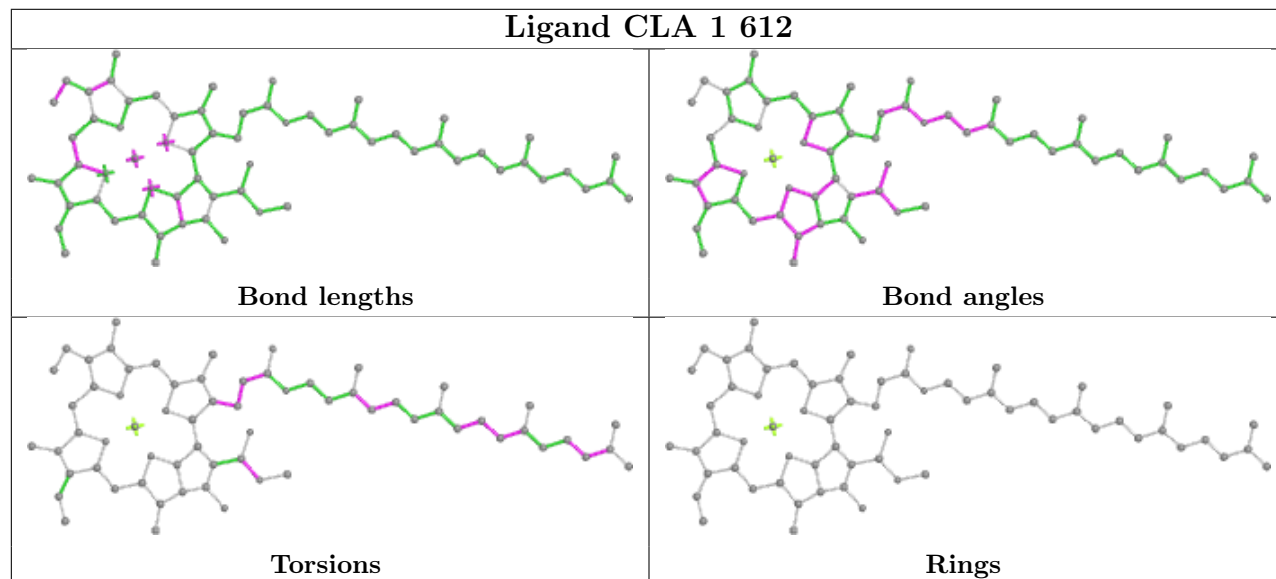
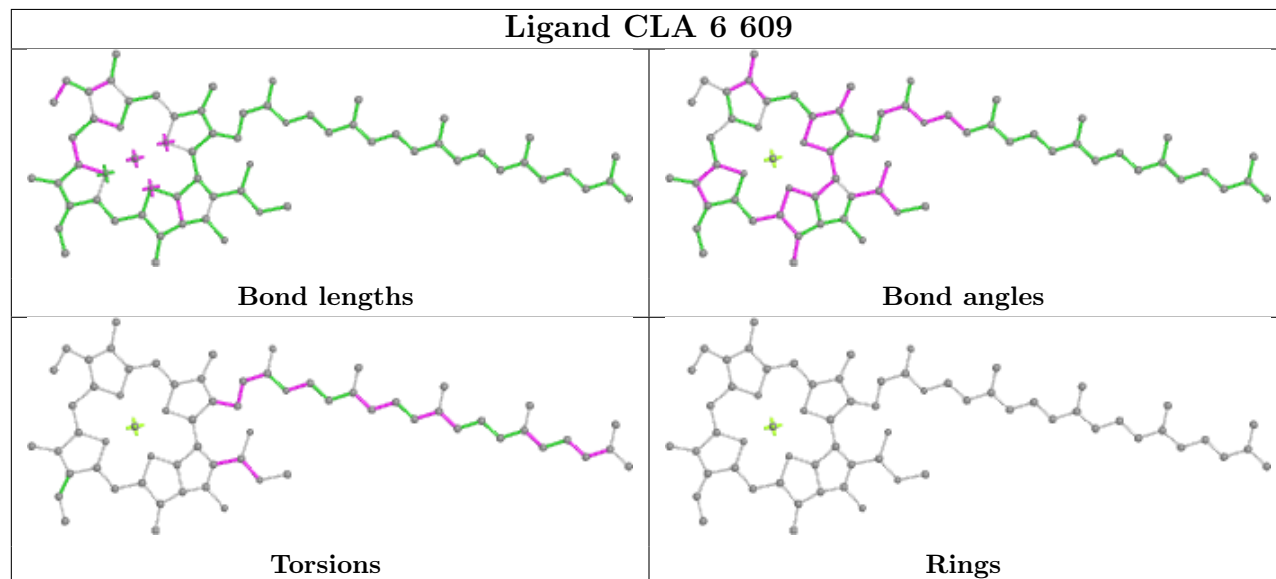
Bond angles

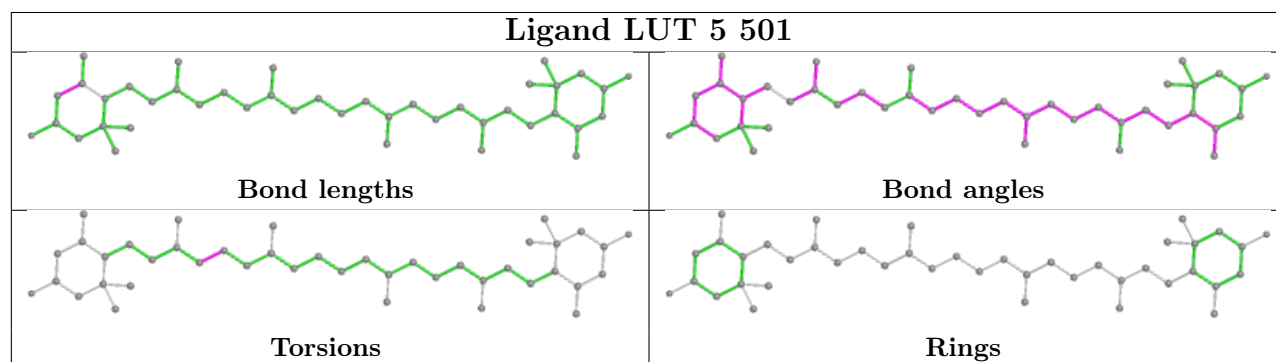
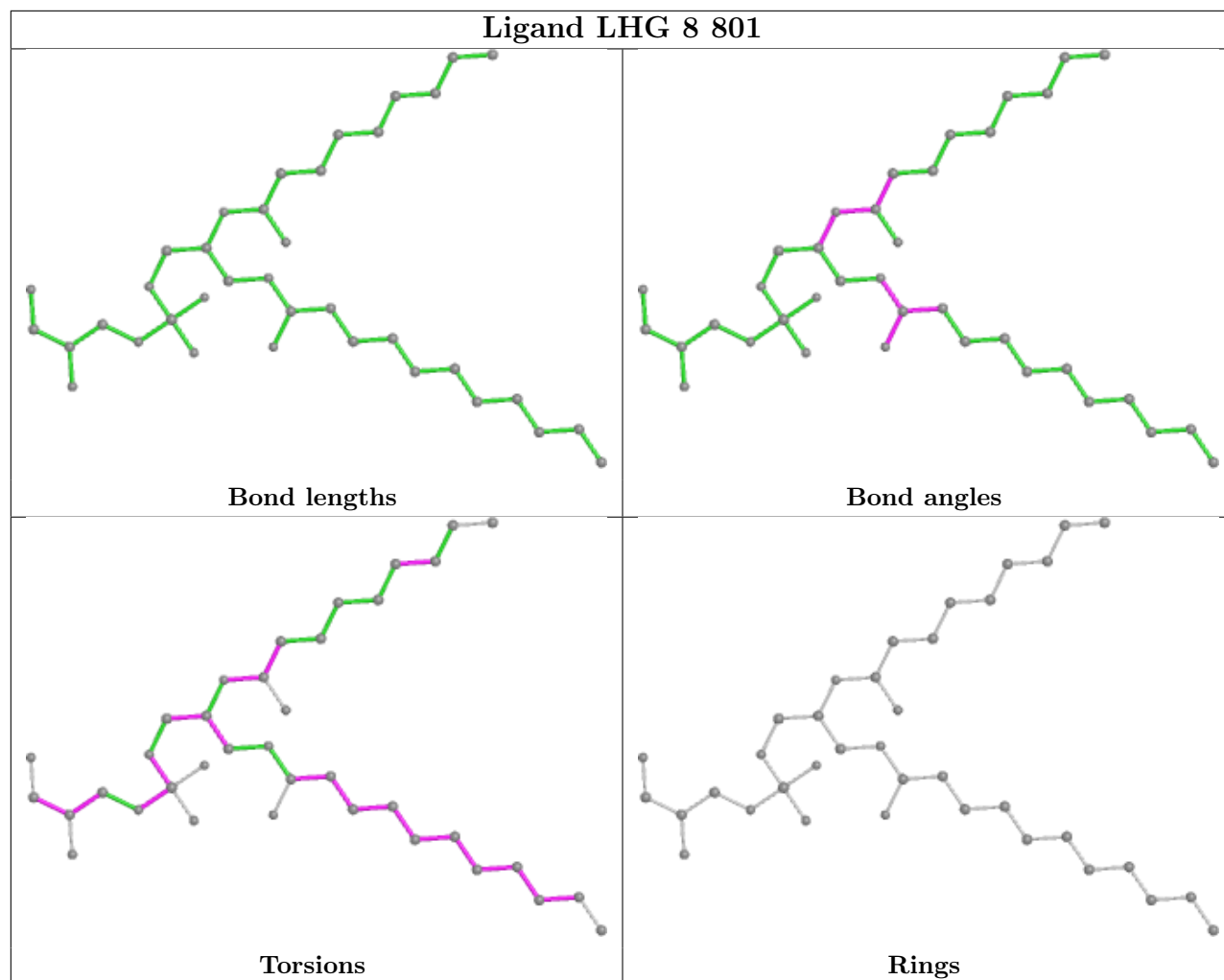
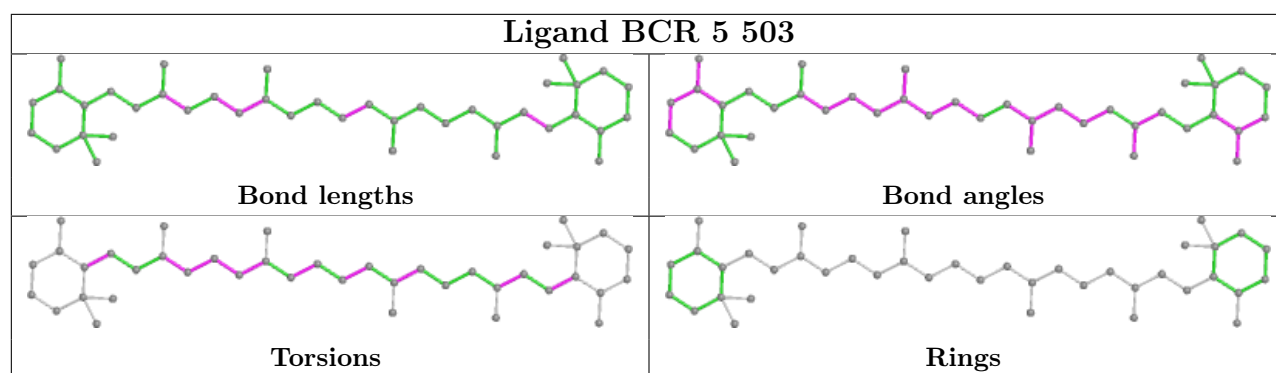


Torsions

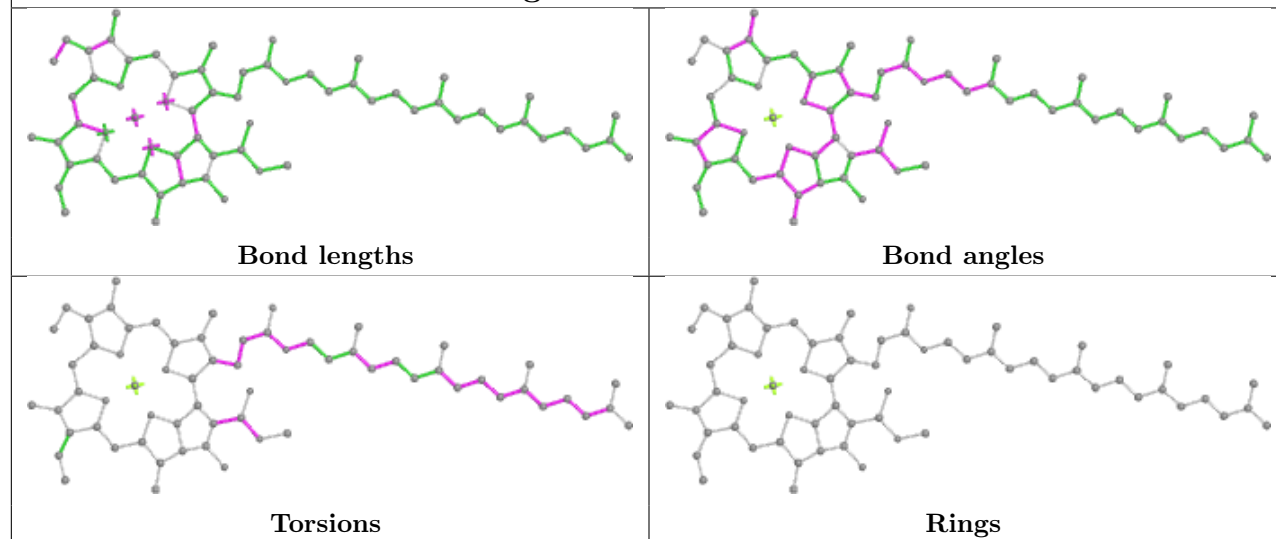


Rings

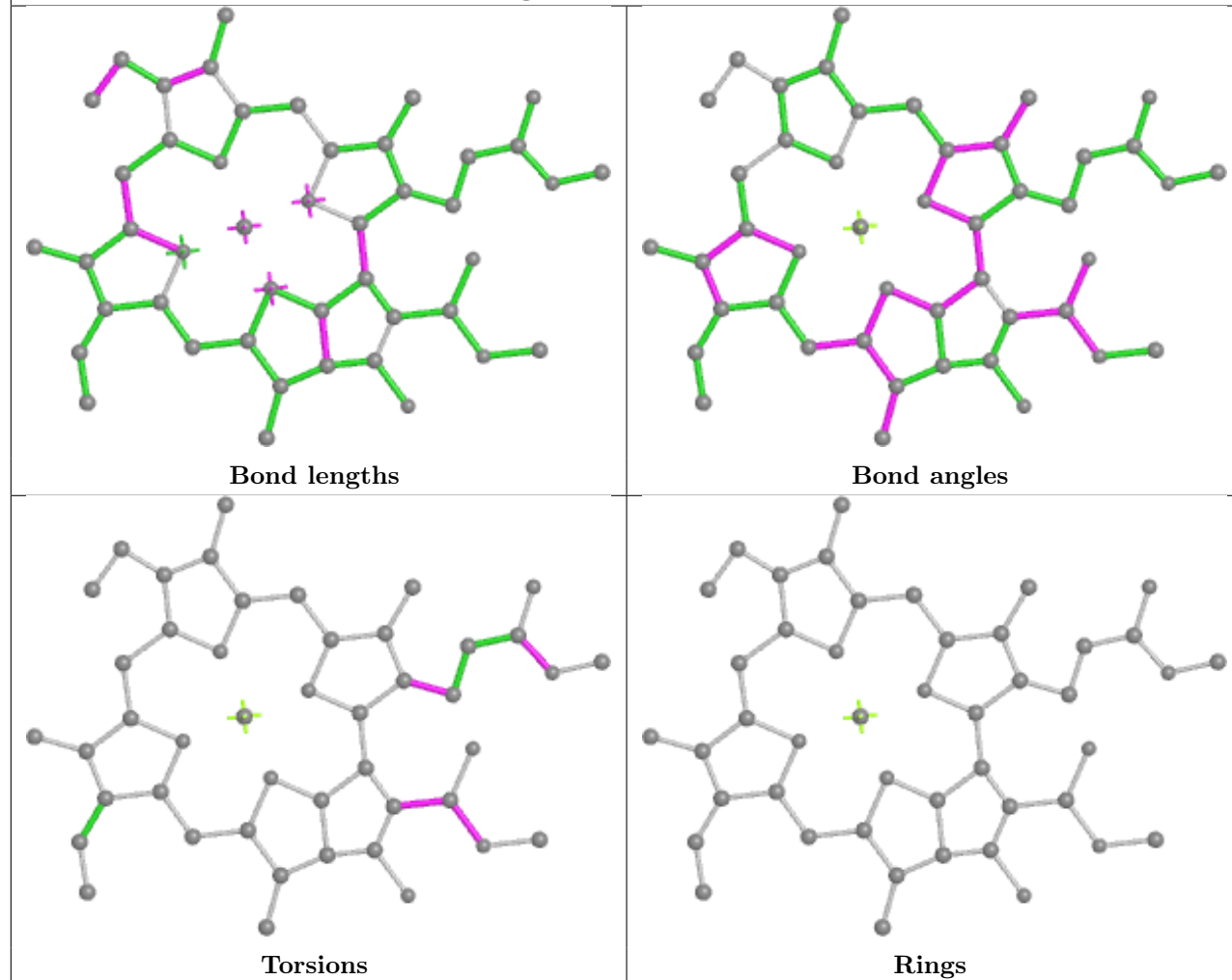
Ligand LUT 8 501**Ligand CLA 1 612****Ligand CLA 6 609**

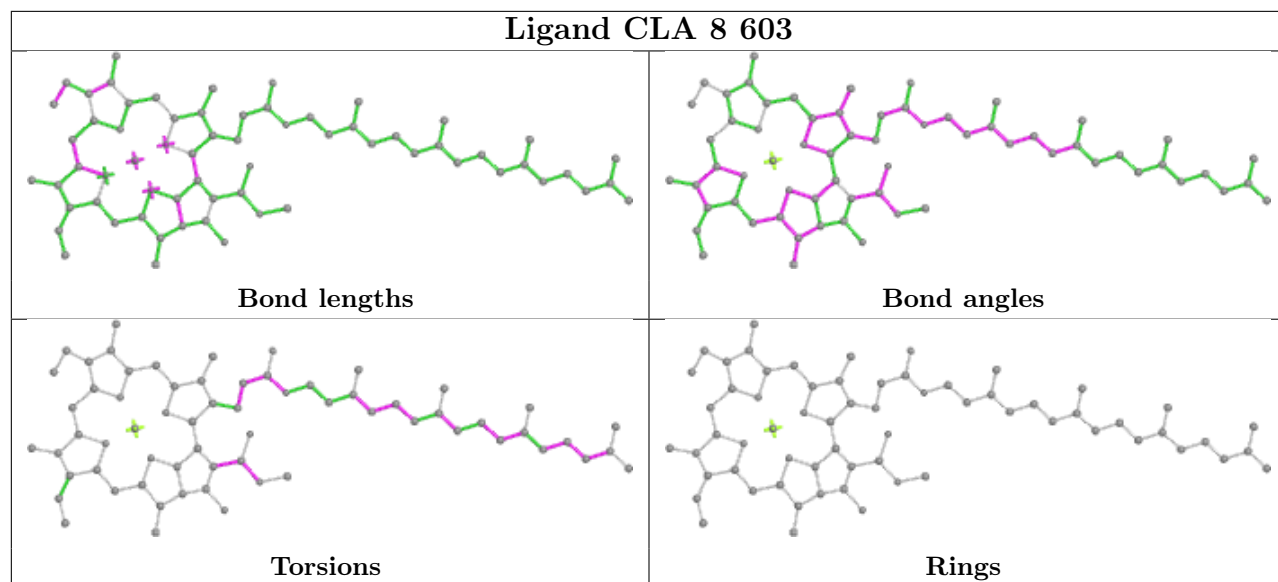
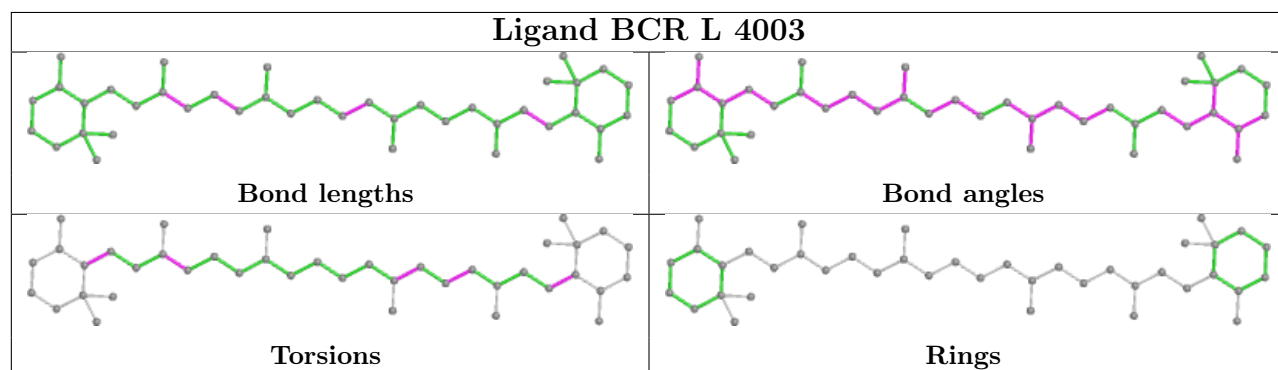


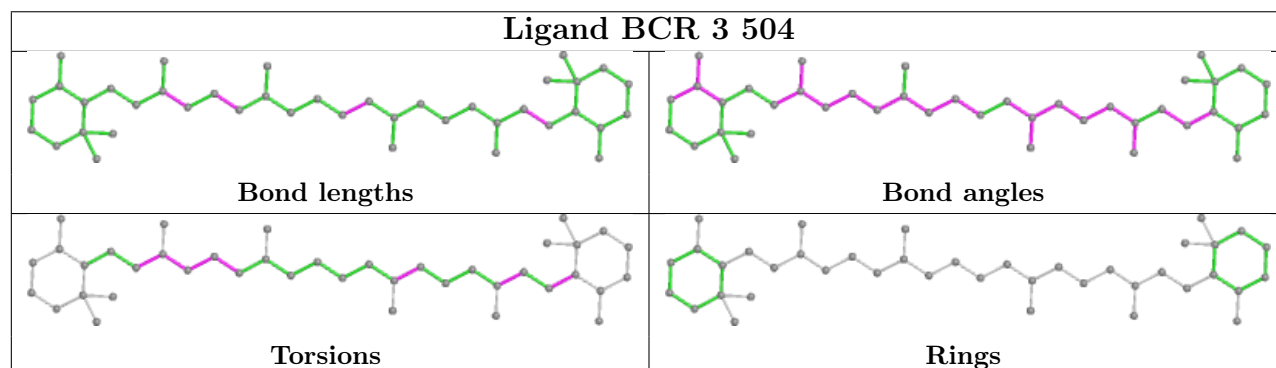
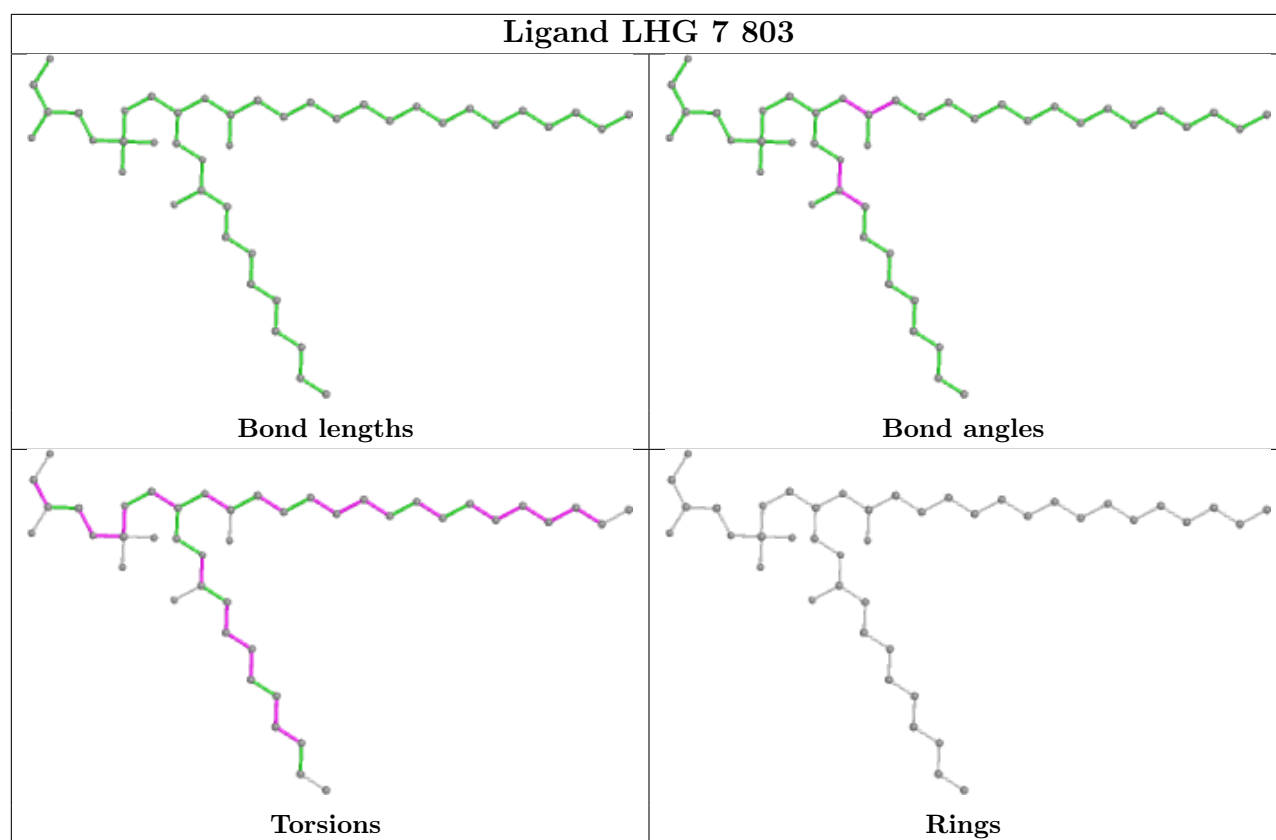
Ligand CLA B 1224



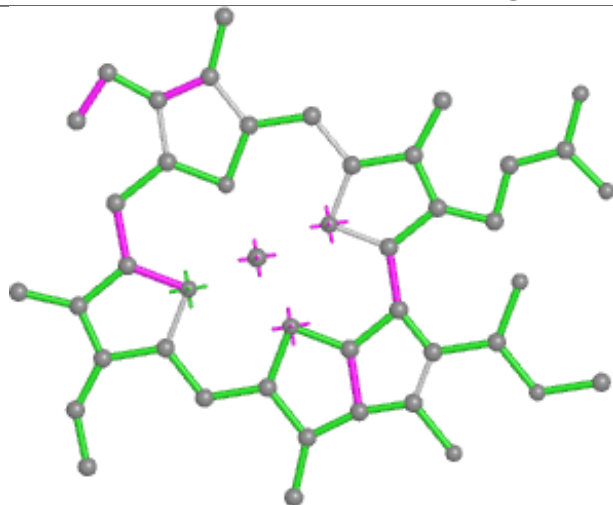
Ligand CLA 3 618



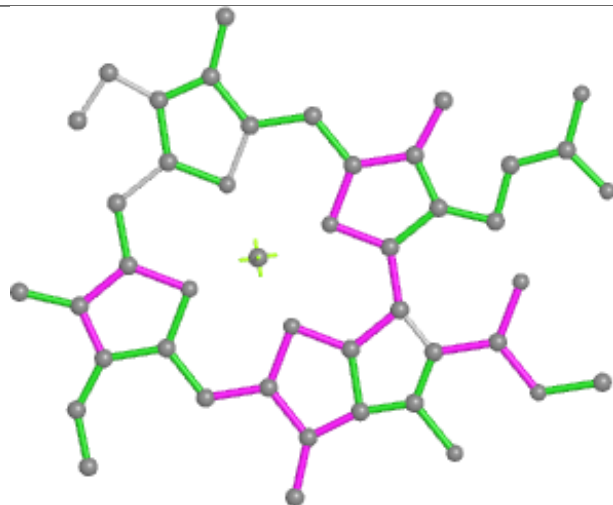
Ligand CLA 8 603**Ligand BCR L 4003**



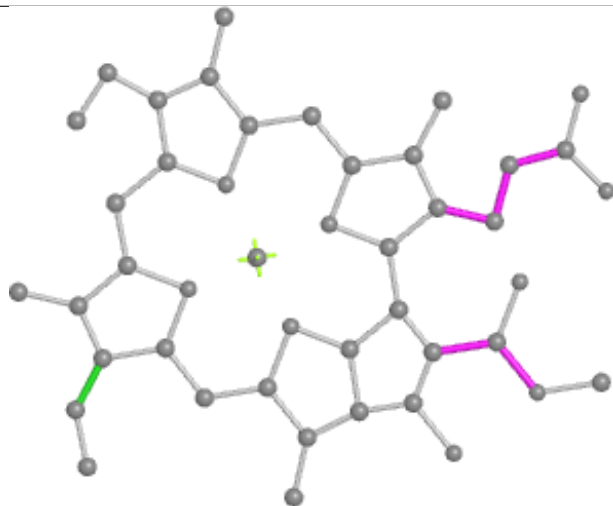
Ligand CLA A 1141



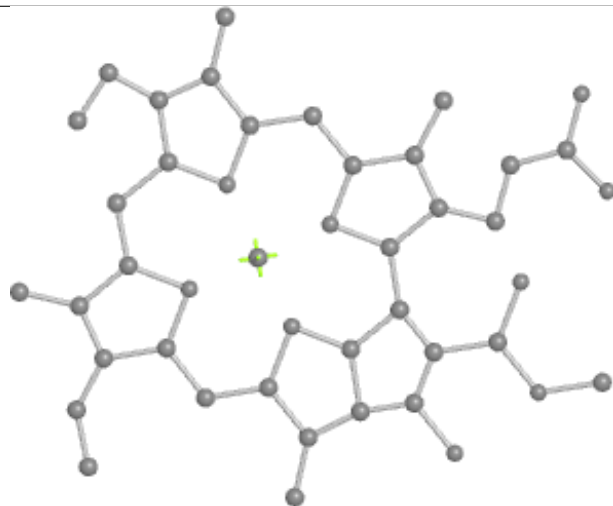
Bond lengths



Bond angles

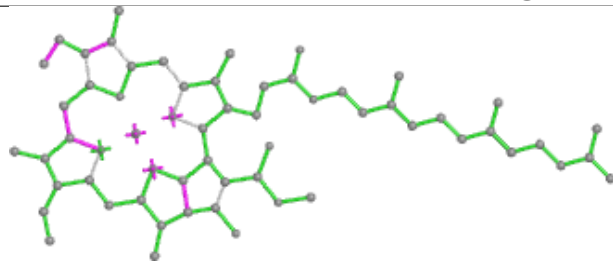


Torsions

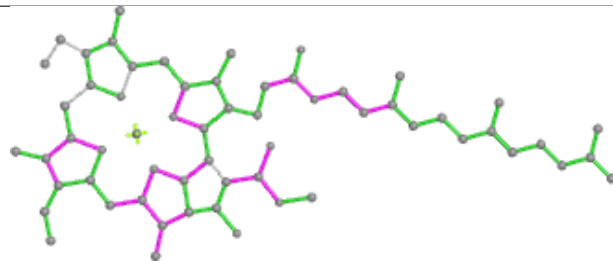


Rings

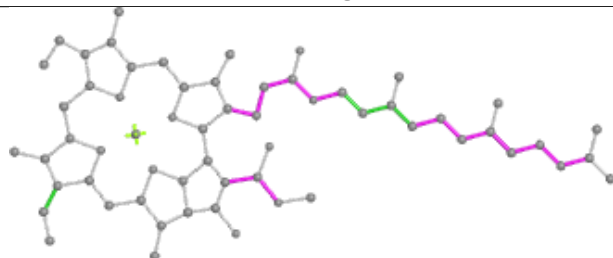
Ligand CLA 8 609



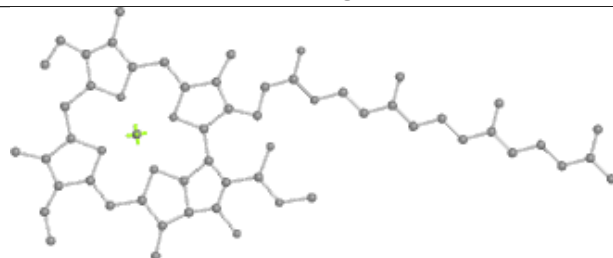
Bond lengths



Bond angles

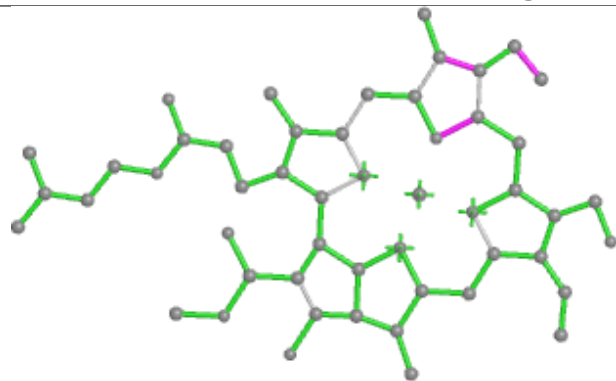


Torsions

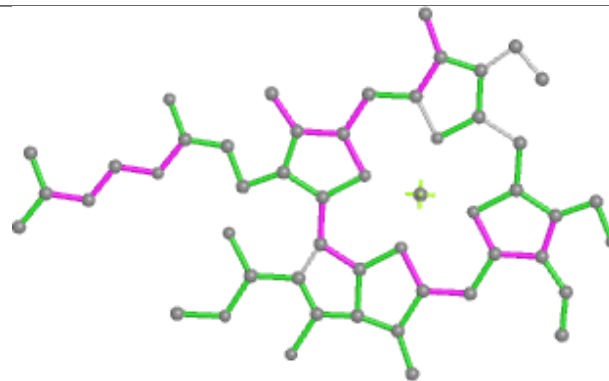


Rings

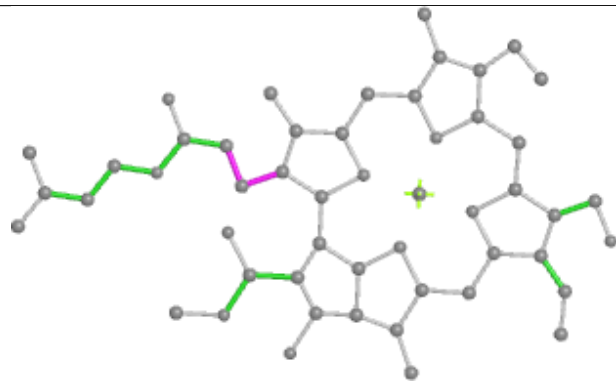
Ligand CHL 6 611



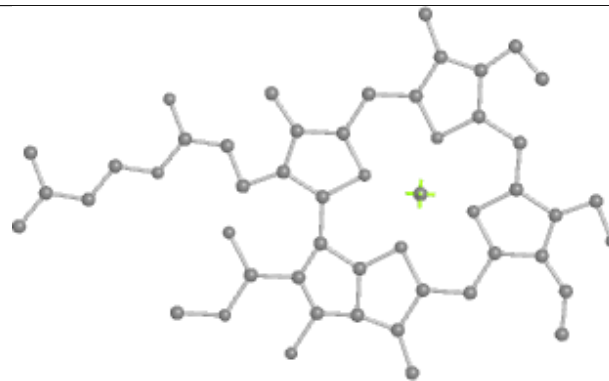
Bond lengths



Bond angles

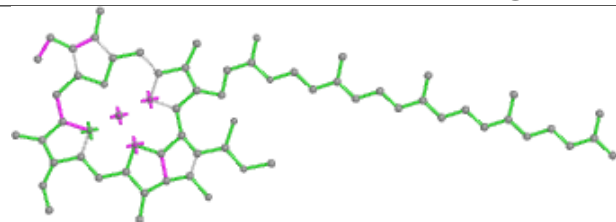


Torsions

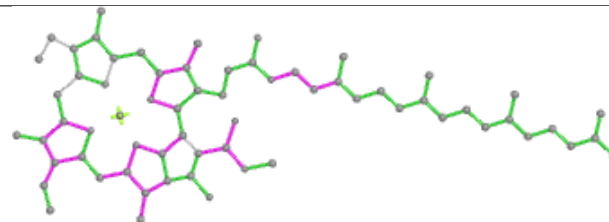


Rings

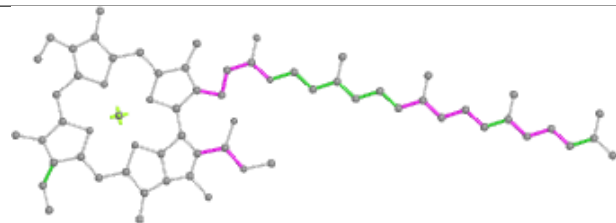
Ligand CLA A 1106



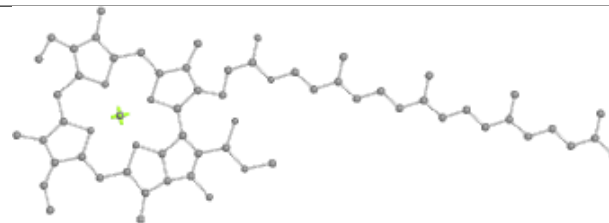
Bond lengths



Bond angles

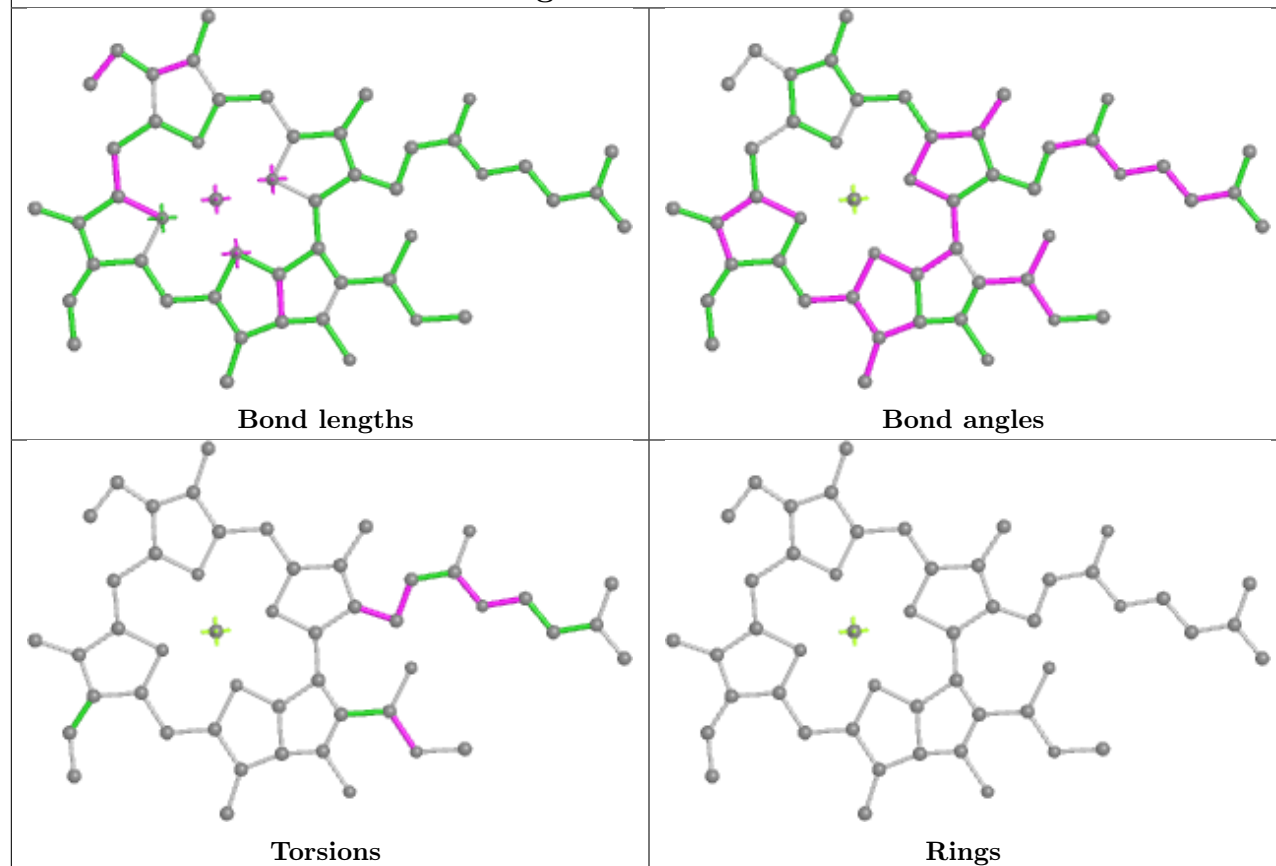


Torsions

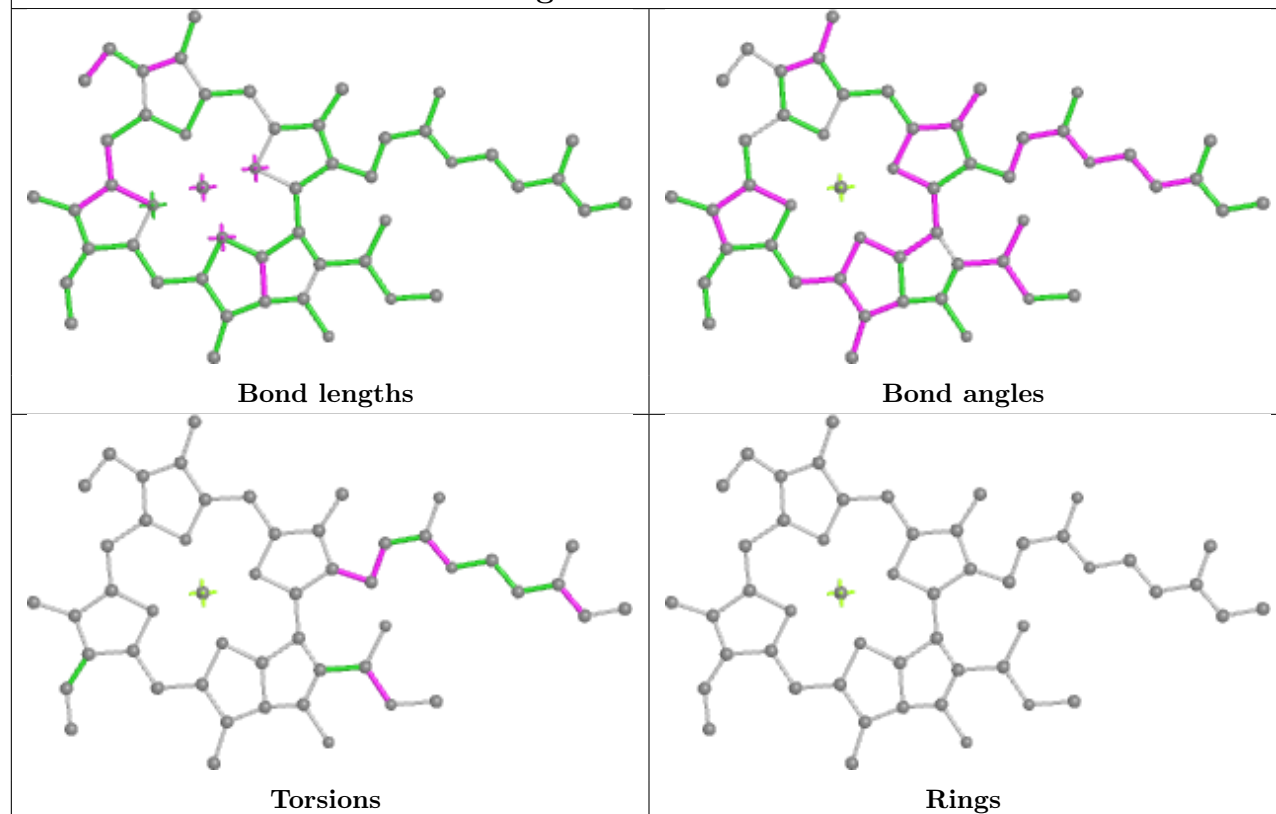


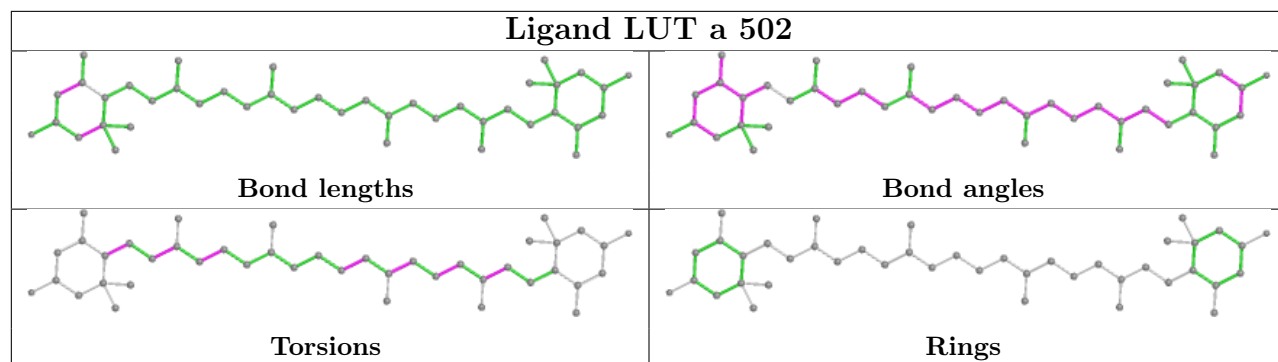
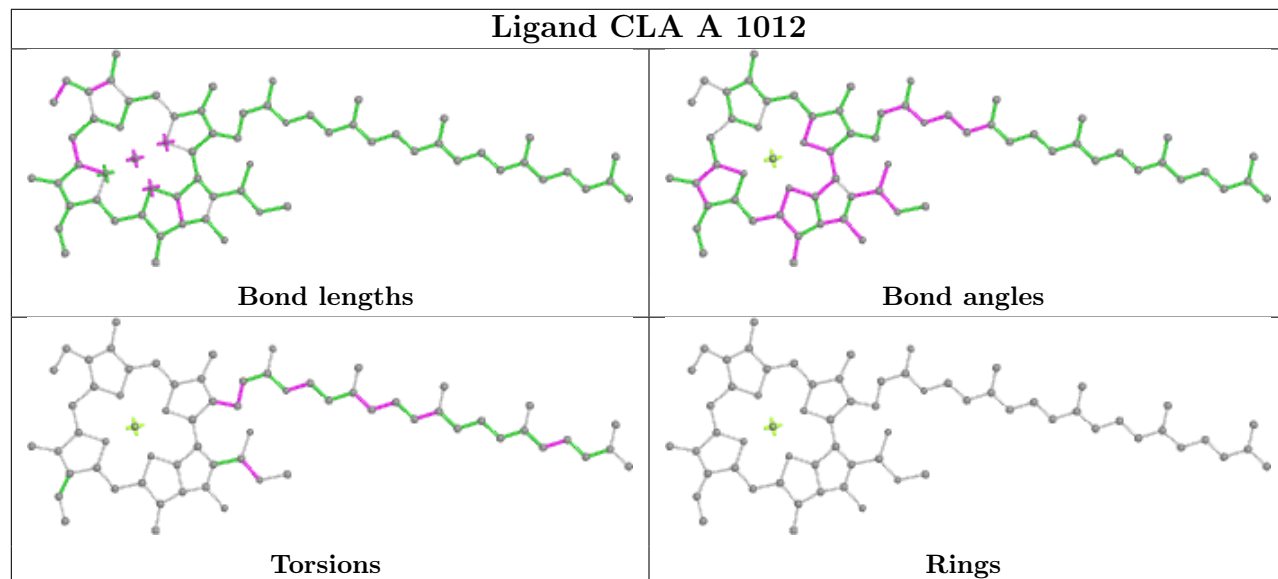
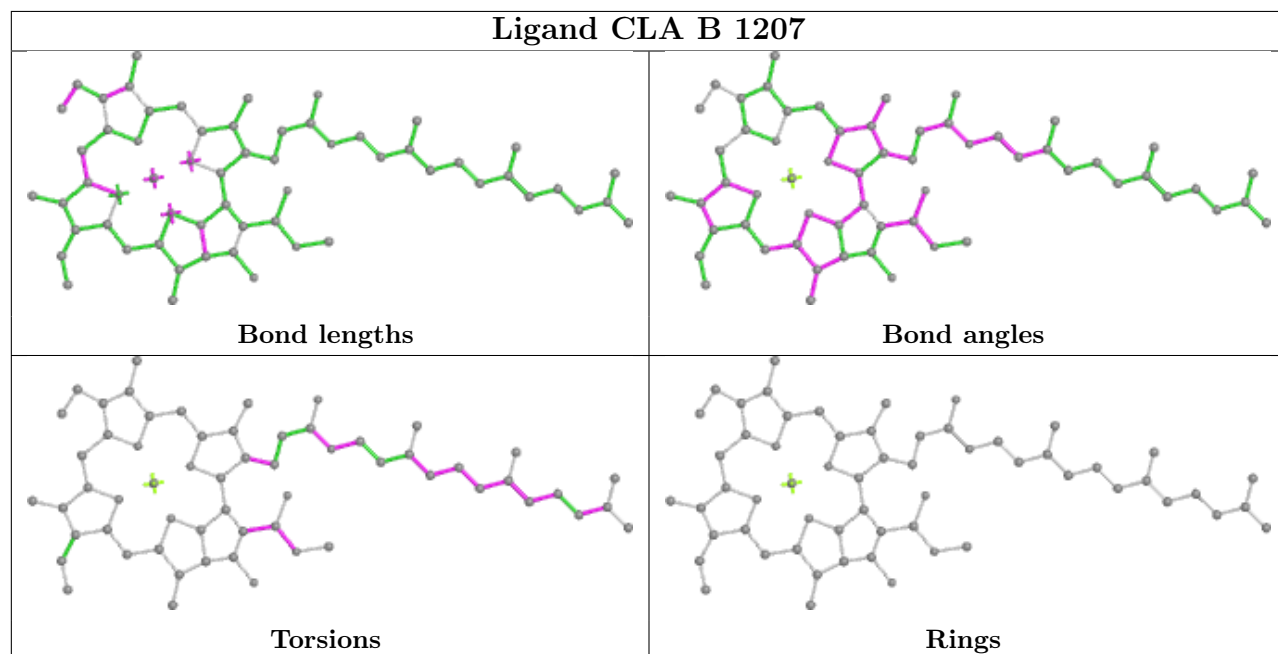
Rings

Ligand CLA a 611

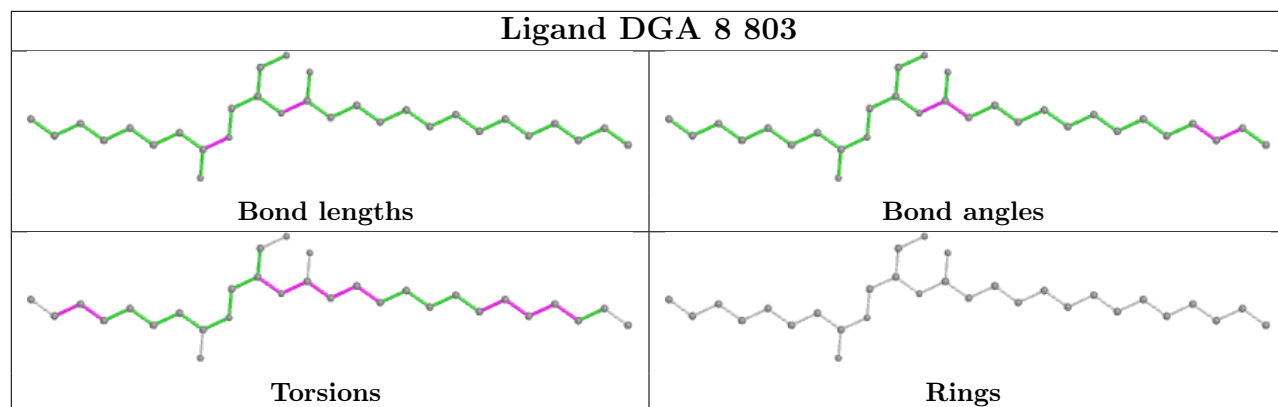


Ligand CLA 5 609

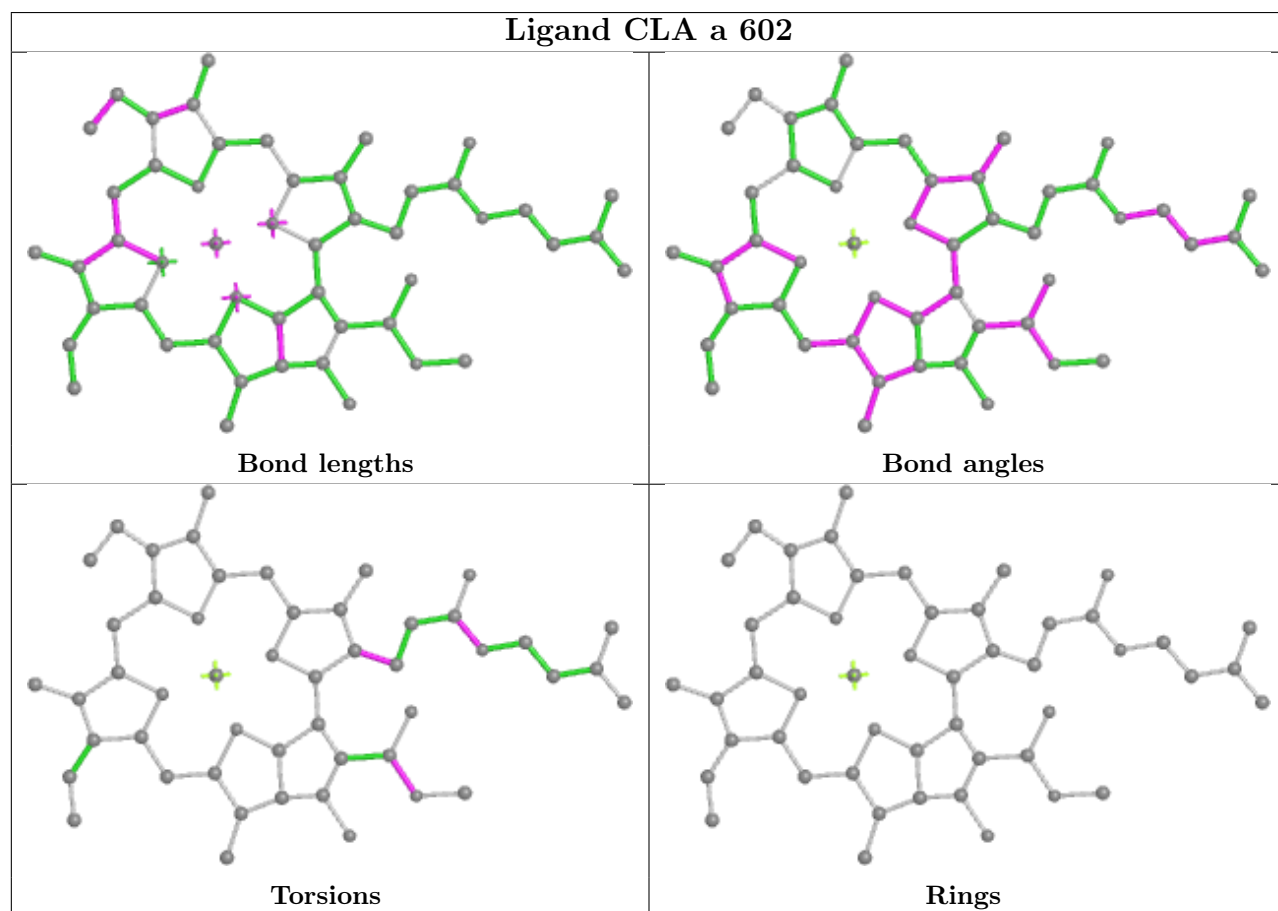


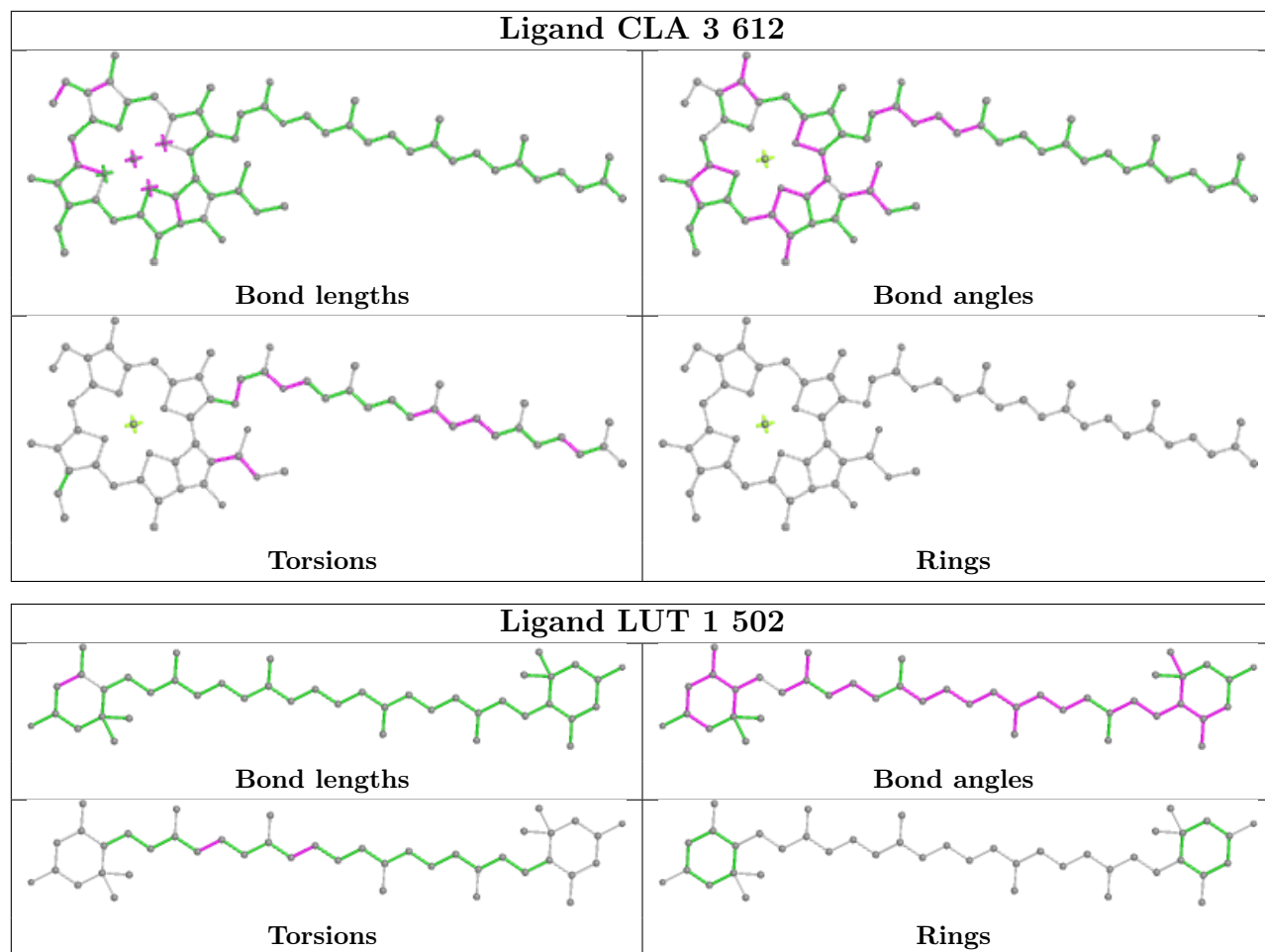
Ligand LUT a 502**Ligand CLA A 1012****Ligand CLA B 1207**

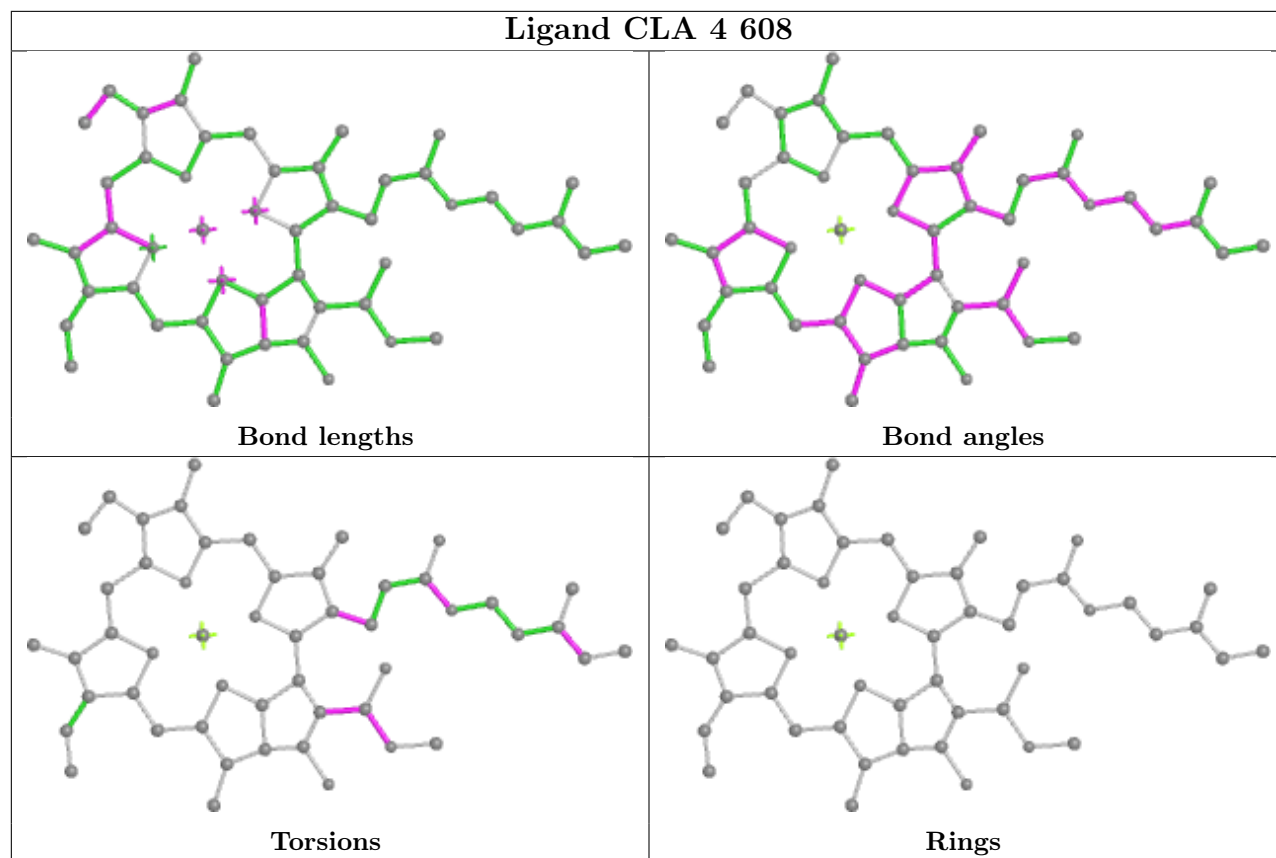
Ligand DGA 8 803



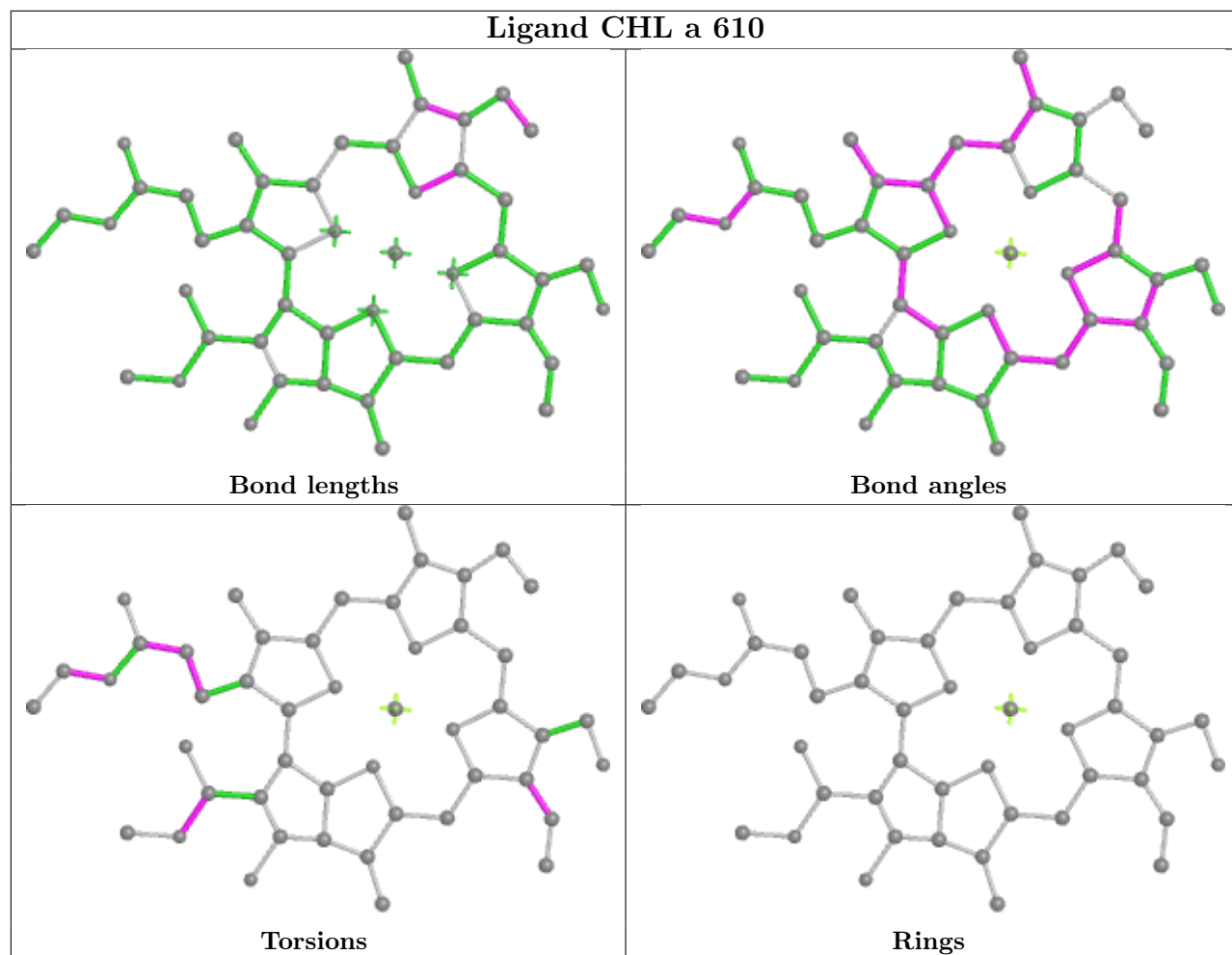
Ligand CLA a 602



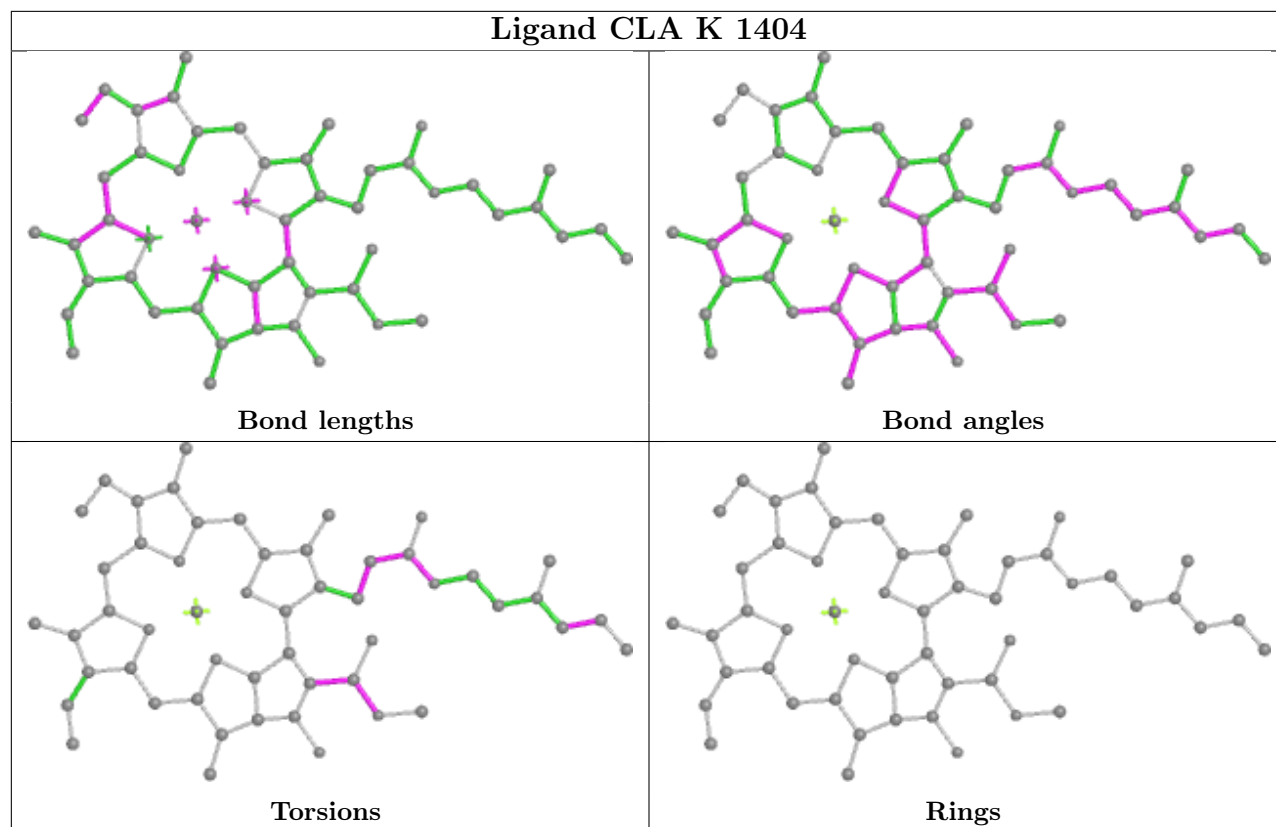




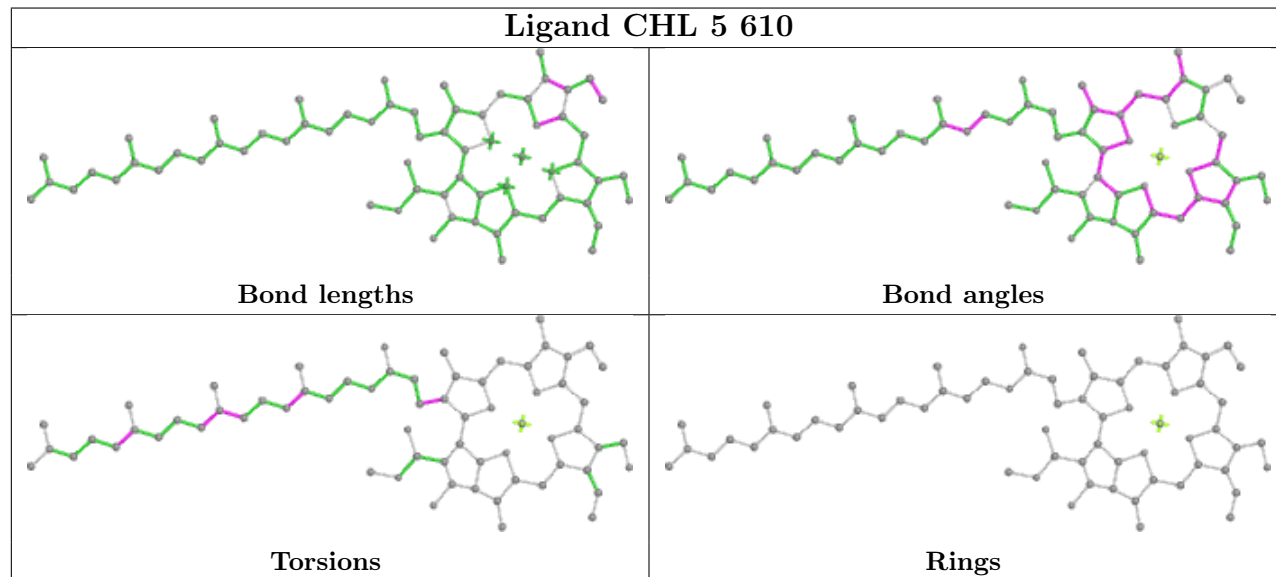
Ligand CHL a 610



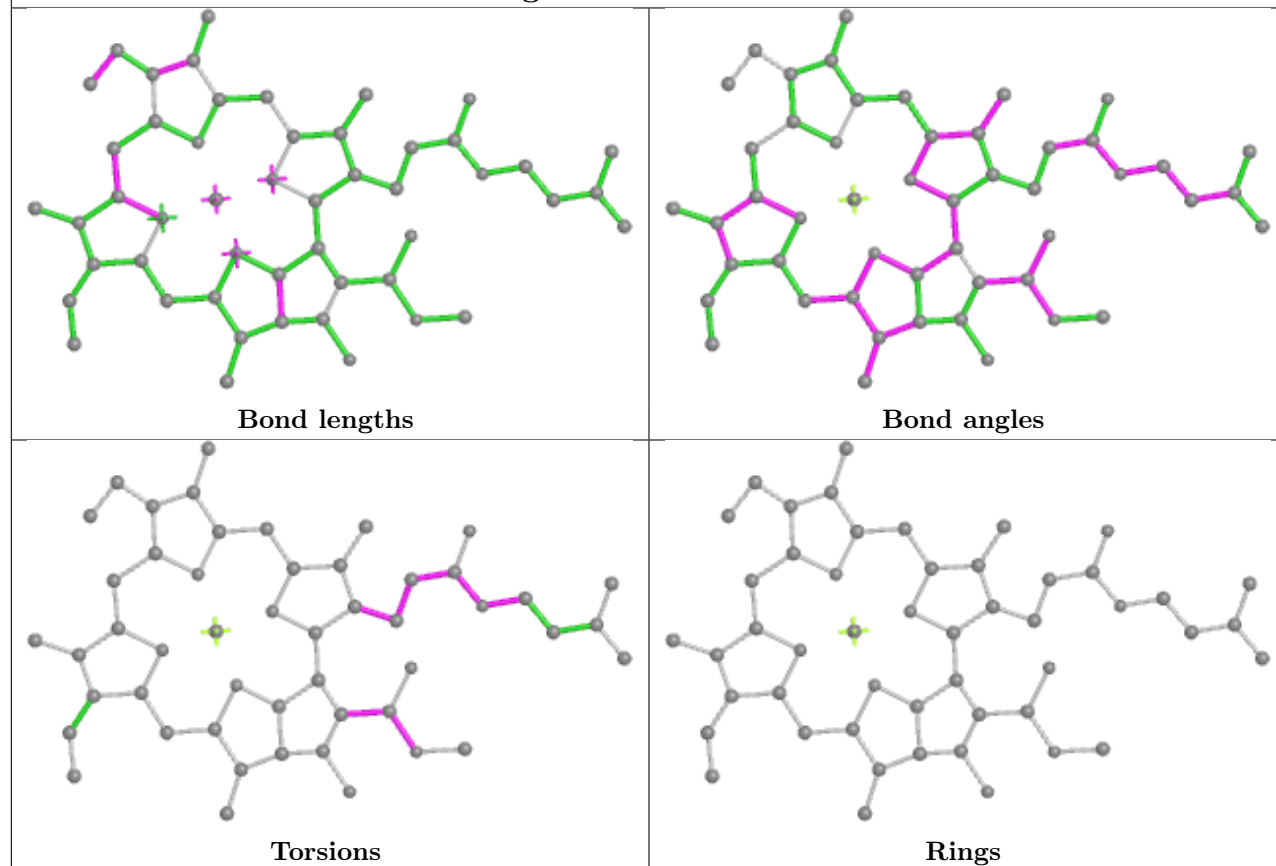
Ligand CLA K 1404



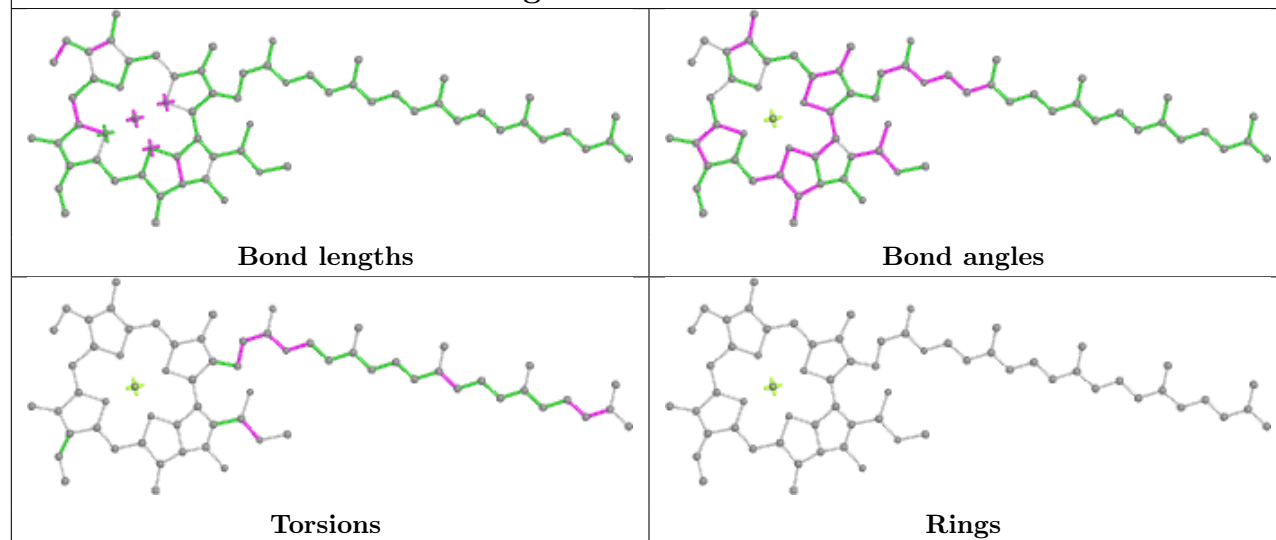
Ligand CHL 5 610

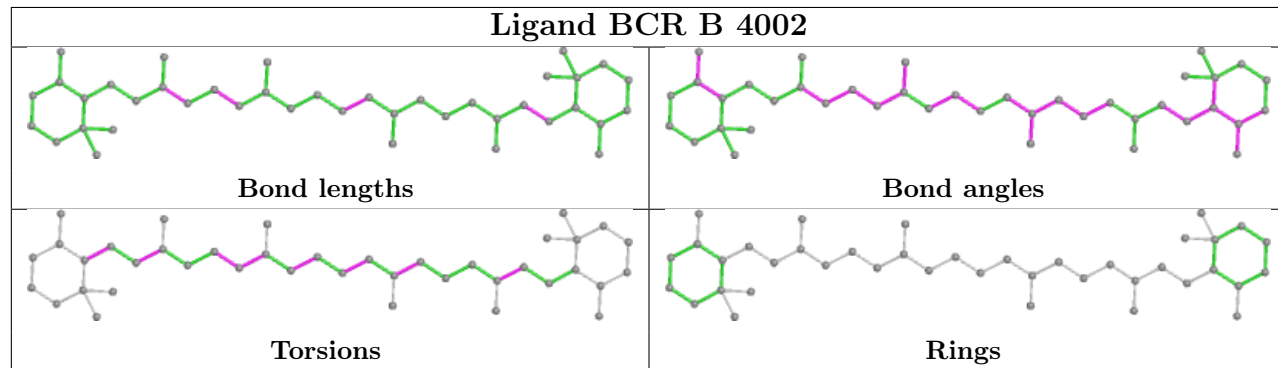
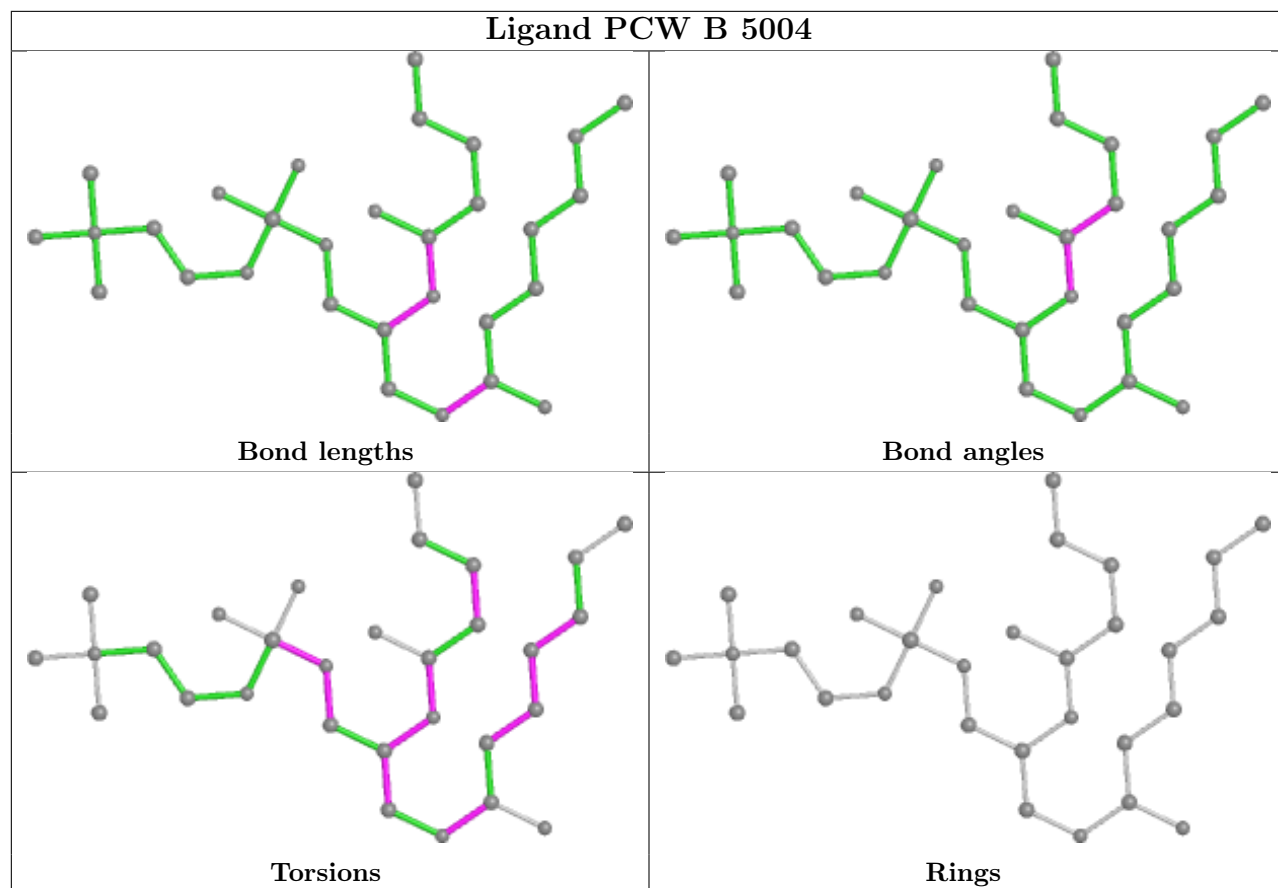


Ligand CLA G 1601

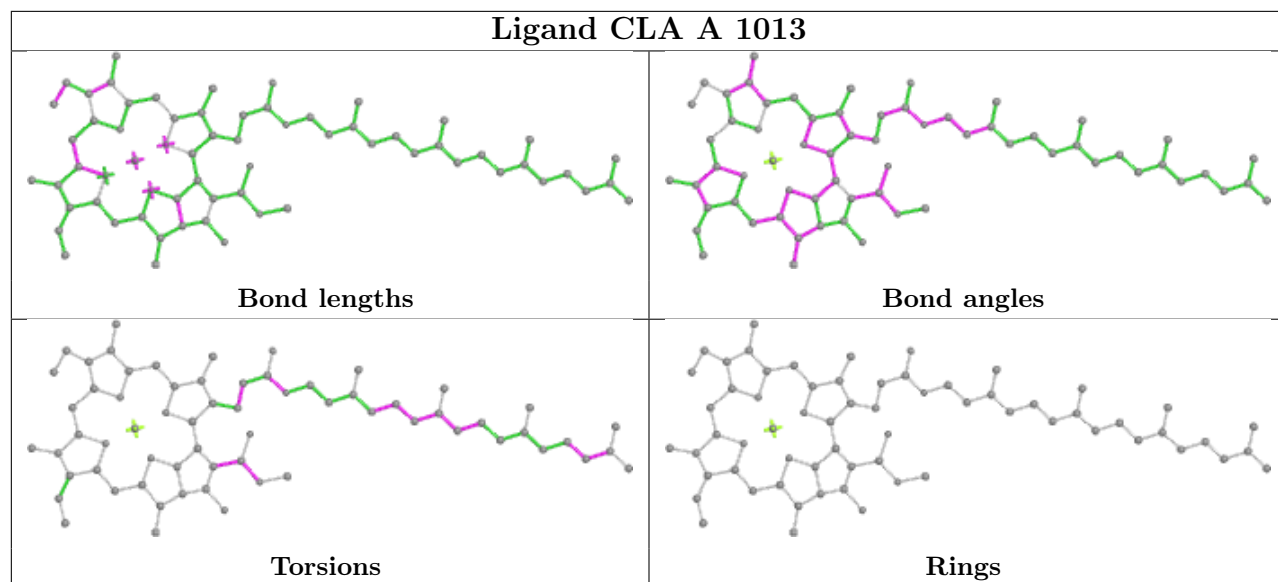


Ligand CLA B 1238

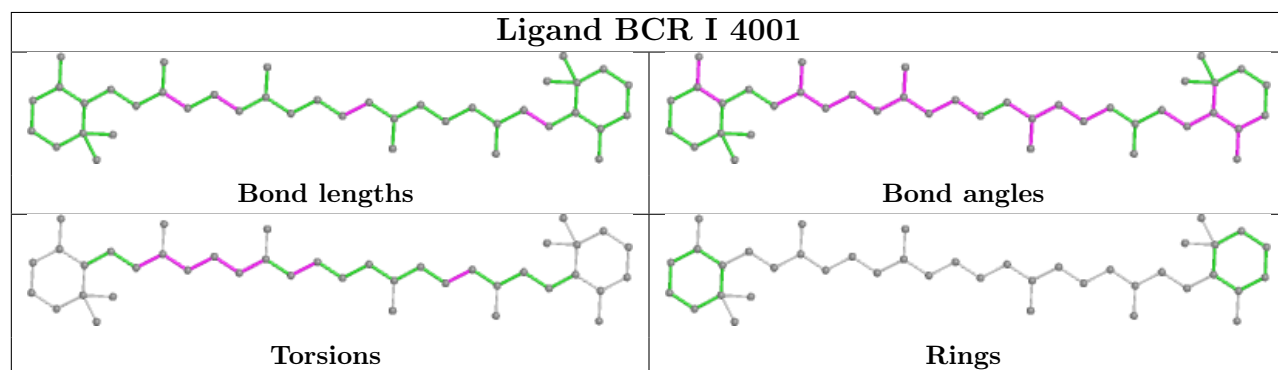




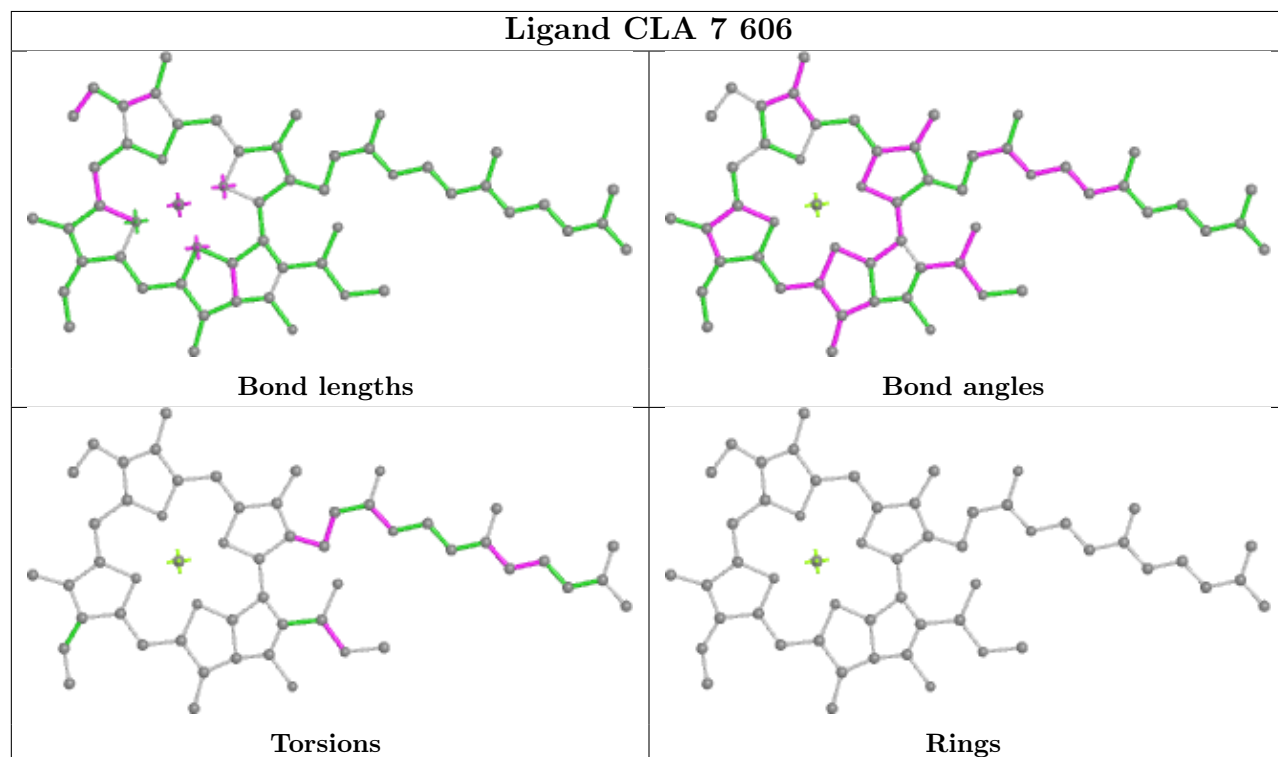
Ligand CLA A 1013



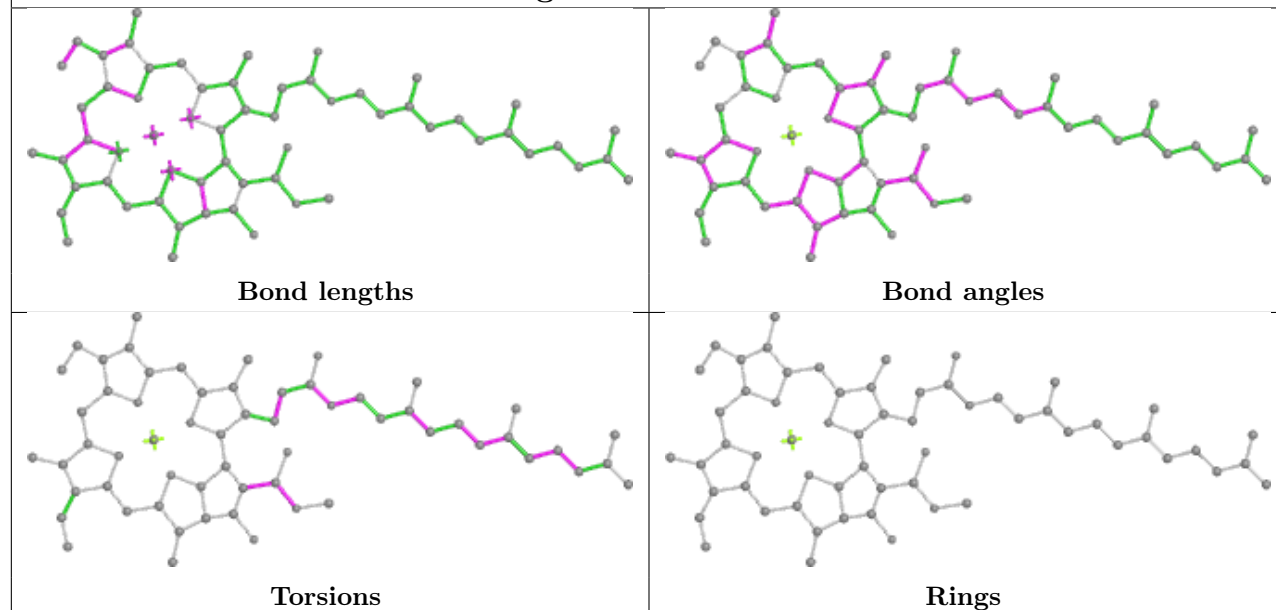
Ligand BCR I 4001



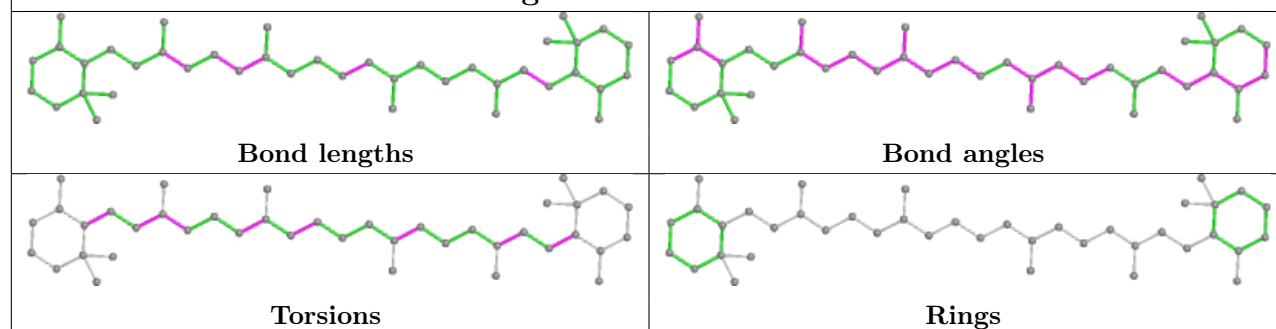
Ligand CLA 7 606



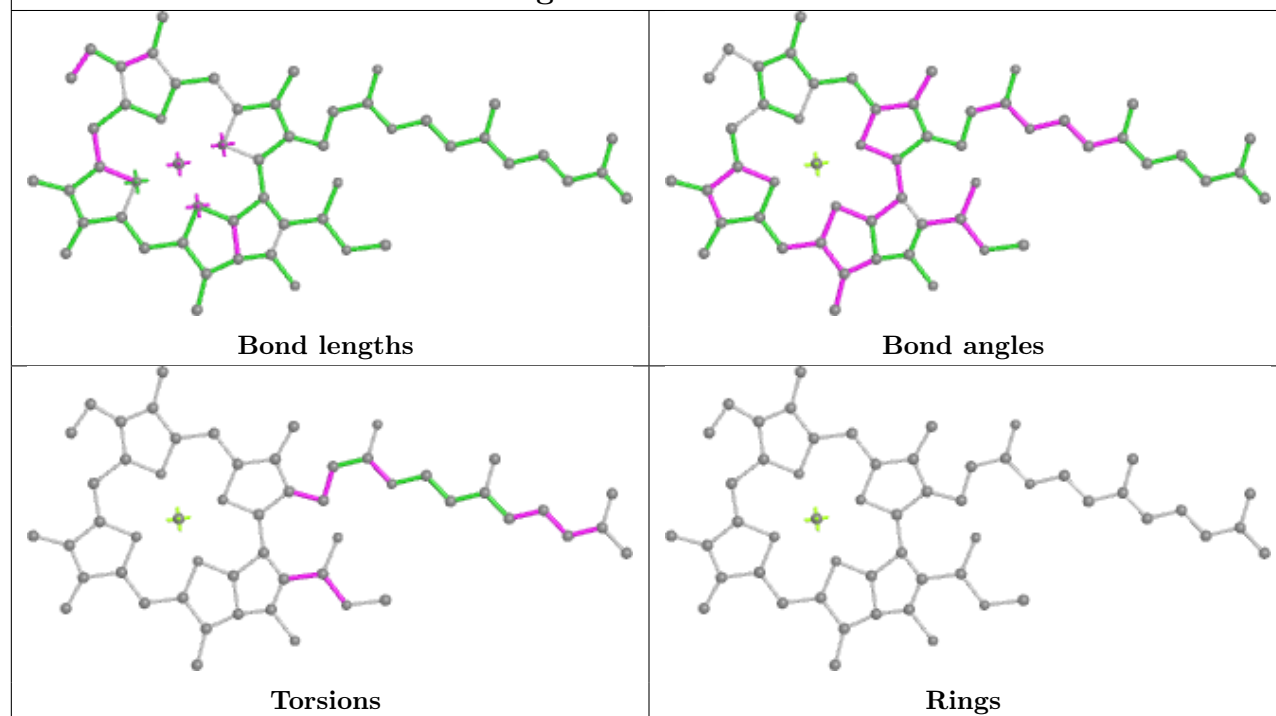
Ligand CLA 4 604

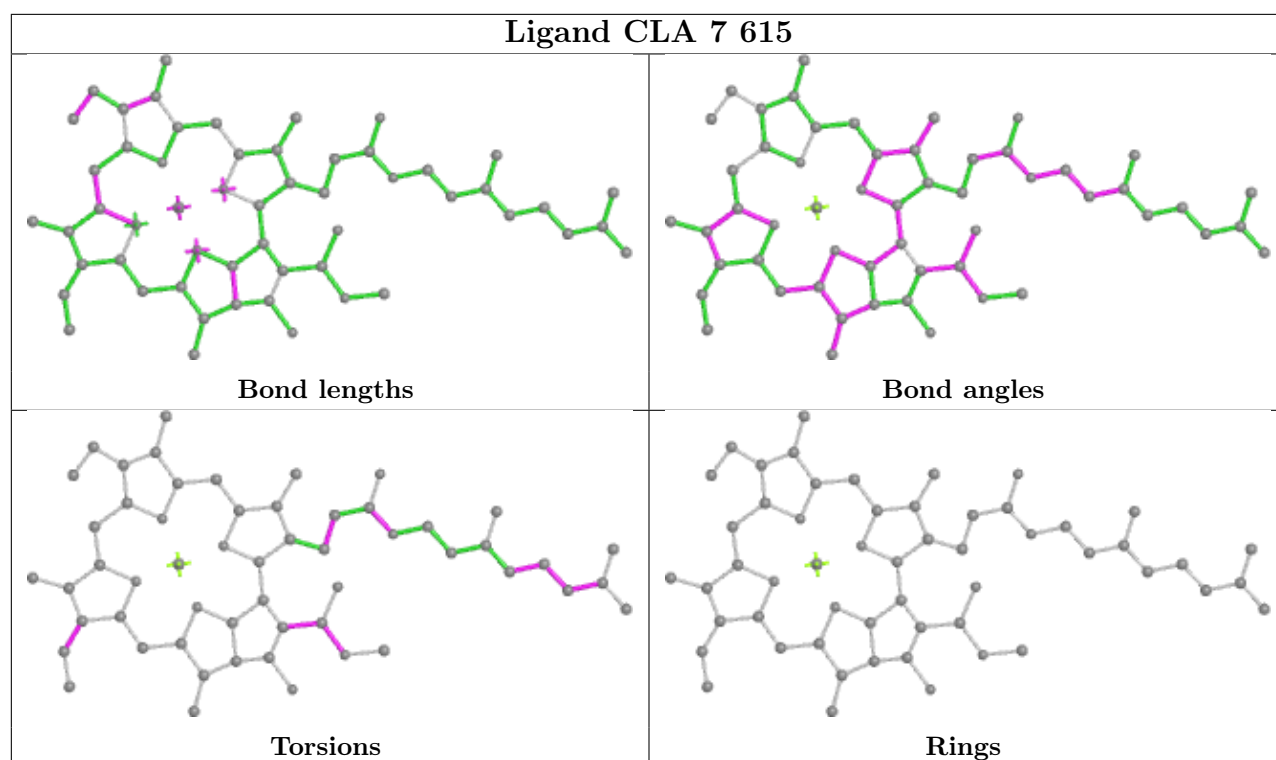


Ligand BCR B 4001



Ligand CLA 7 617





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.

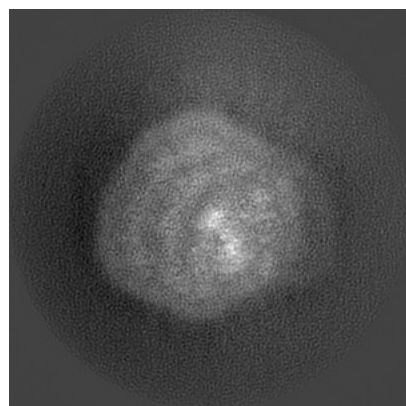
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11640. These allow visual inspection of the internal detail of the map and identification of artifacts.

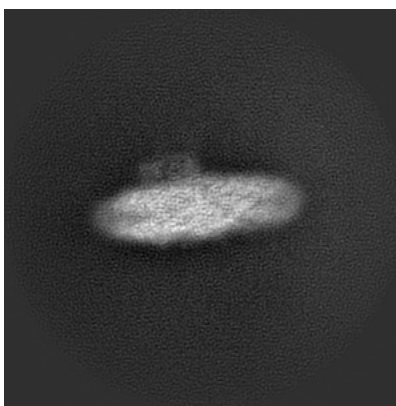
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

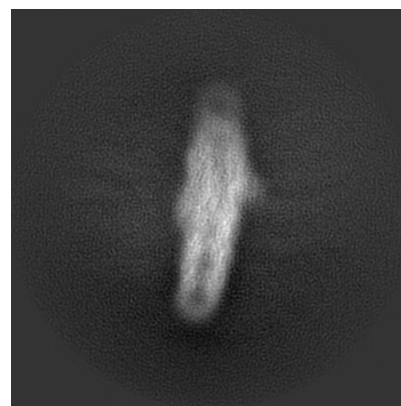
6.1.1 Primary map



X

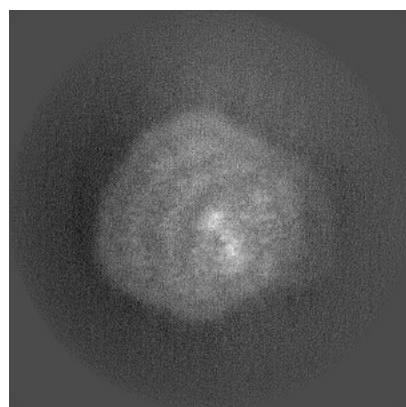


Y

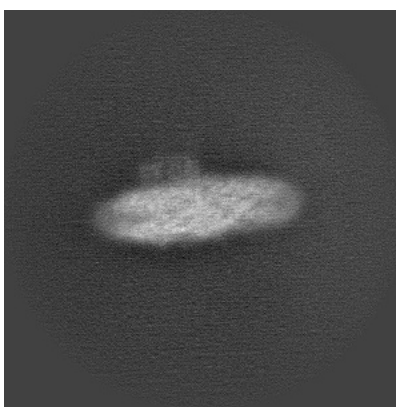


Z

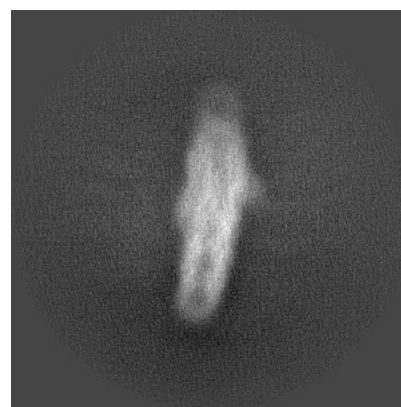
6.1.2 Raw map



X



Y

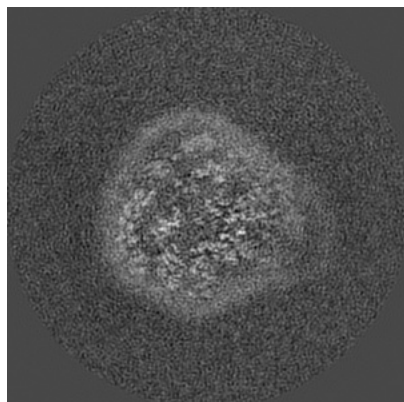


Z

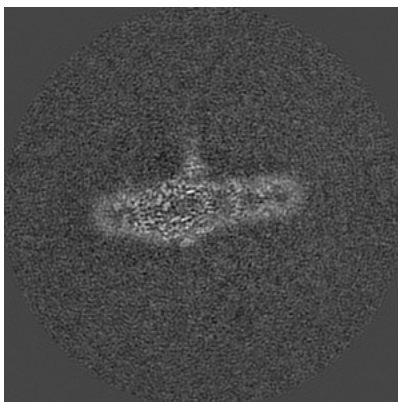
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

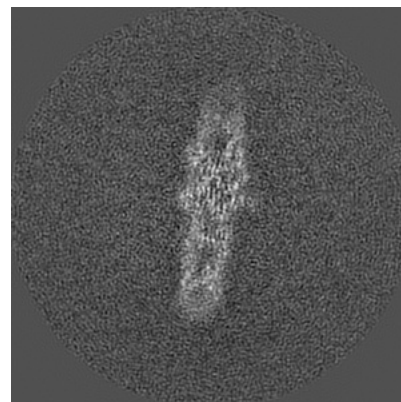
6.2.1 Primary map



X Index: 256

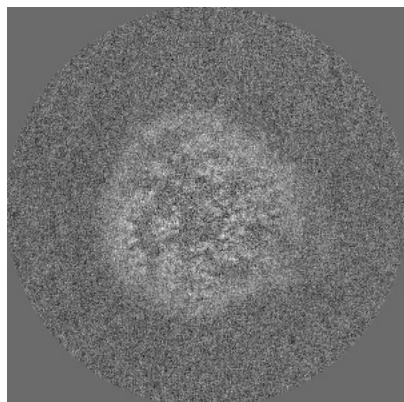


Y Index: 256

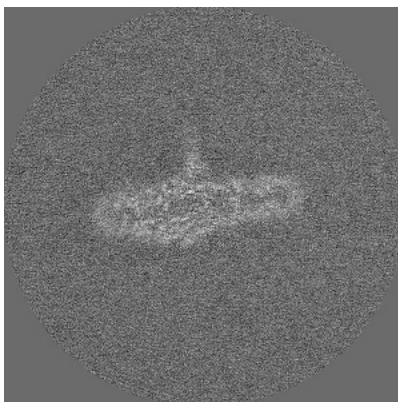


Z Index: 256

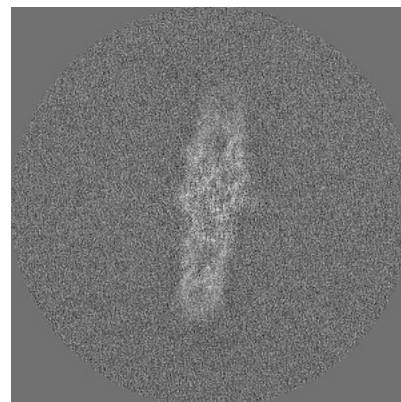
6.2.2 Raw map



X Index: 256



Y Index: 256

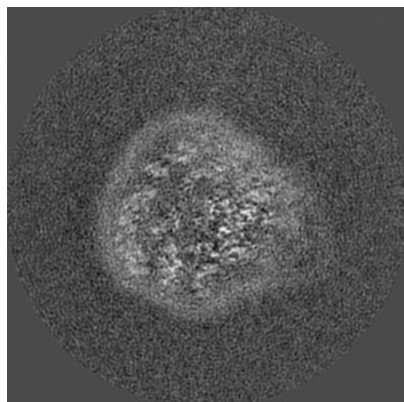


Z Index: 256

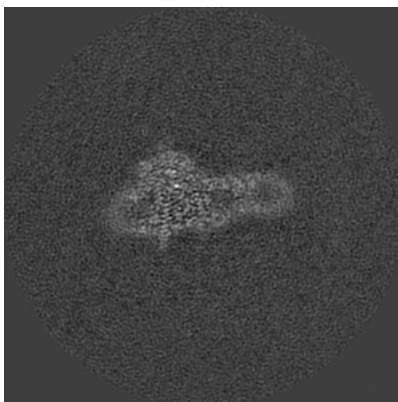
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

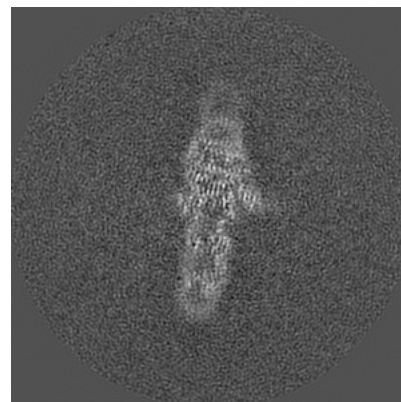
6.3.1 Primary map



X Index: 254

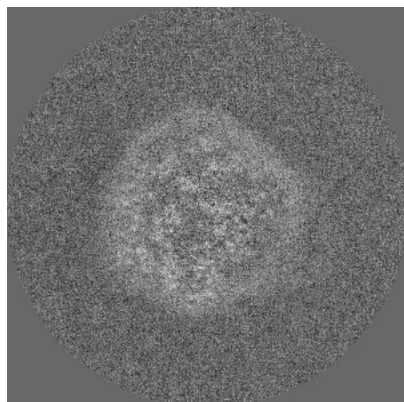


Y Index: 284

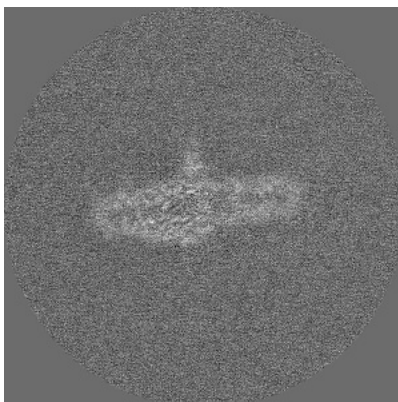


Z Index: 247

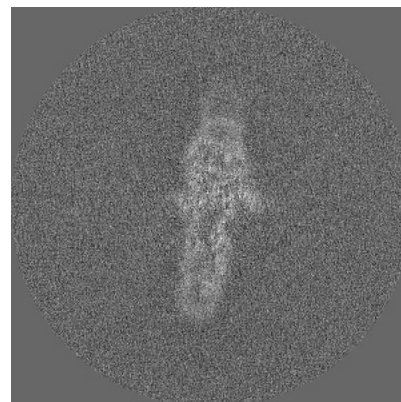
6.3.2 Raw map



X Index: 259



Y Index: 257

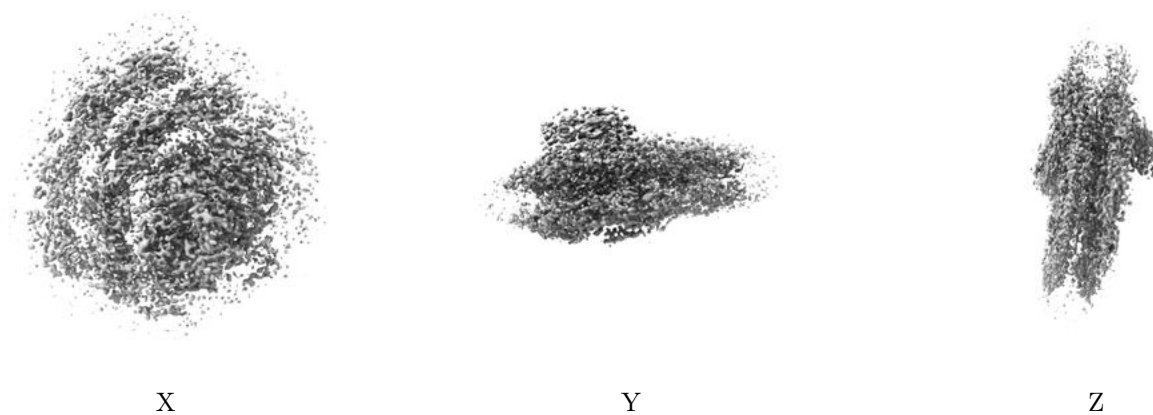


Z Index: 248

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

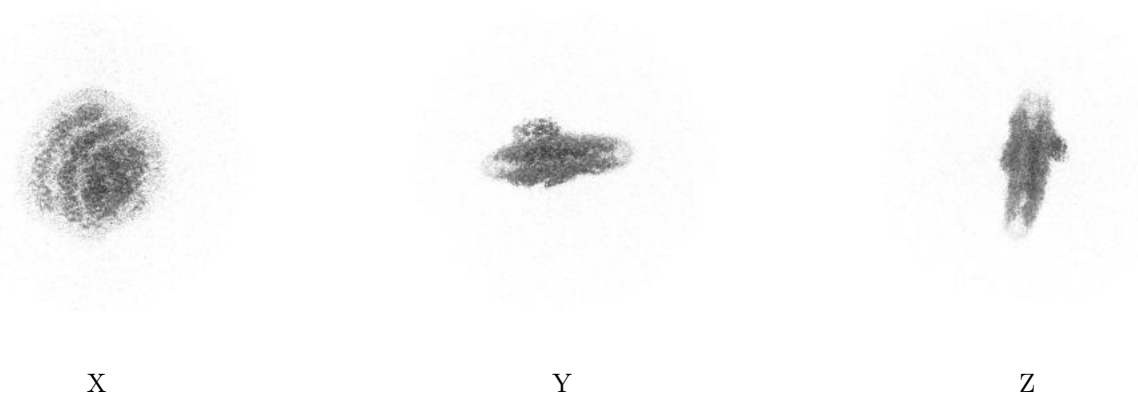
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



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

6.4.2 Raw map



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

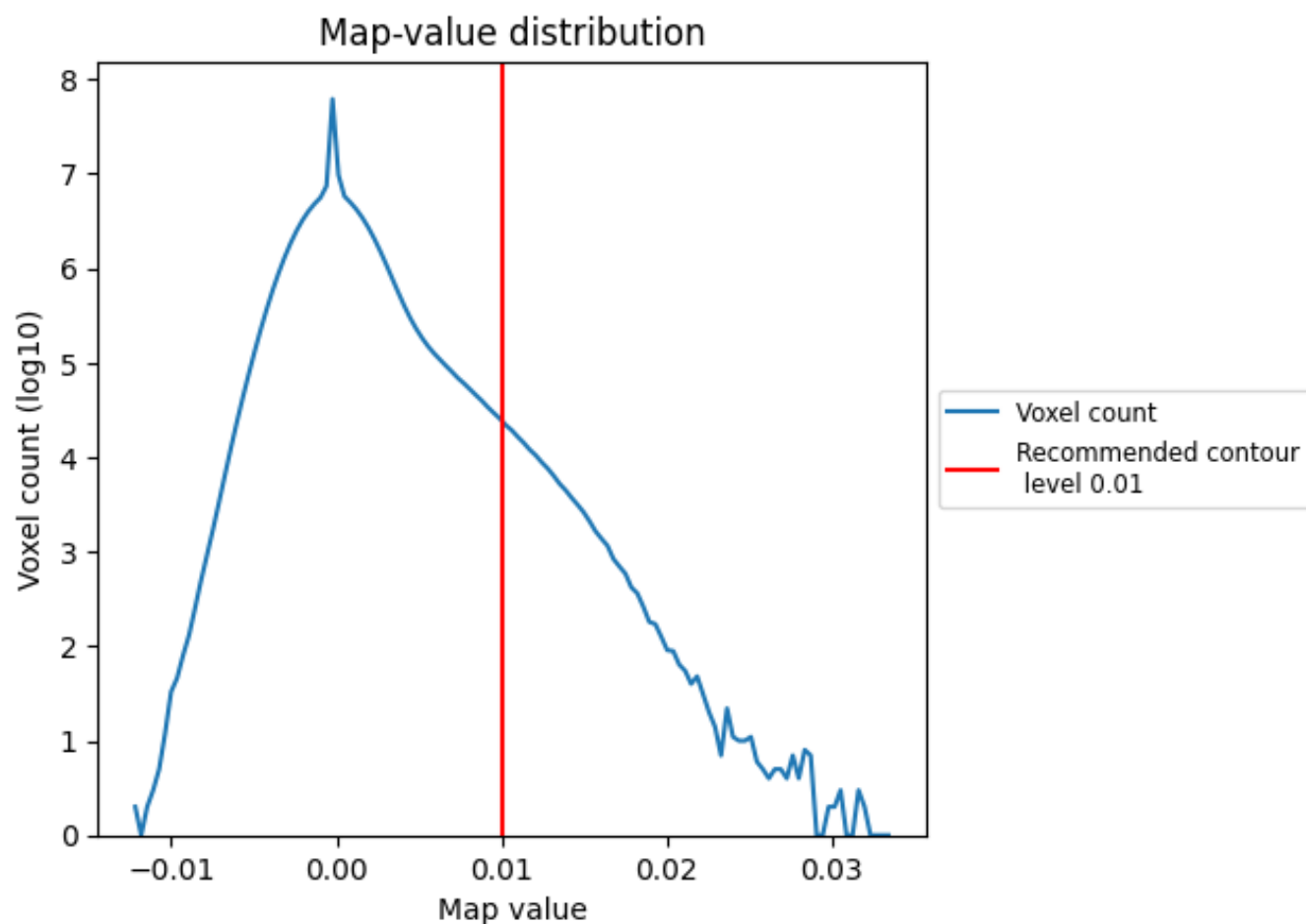
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

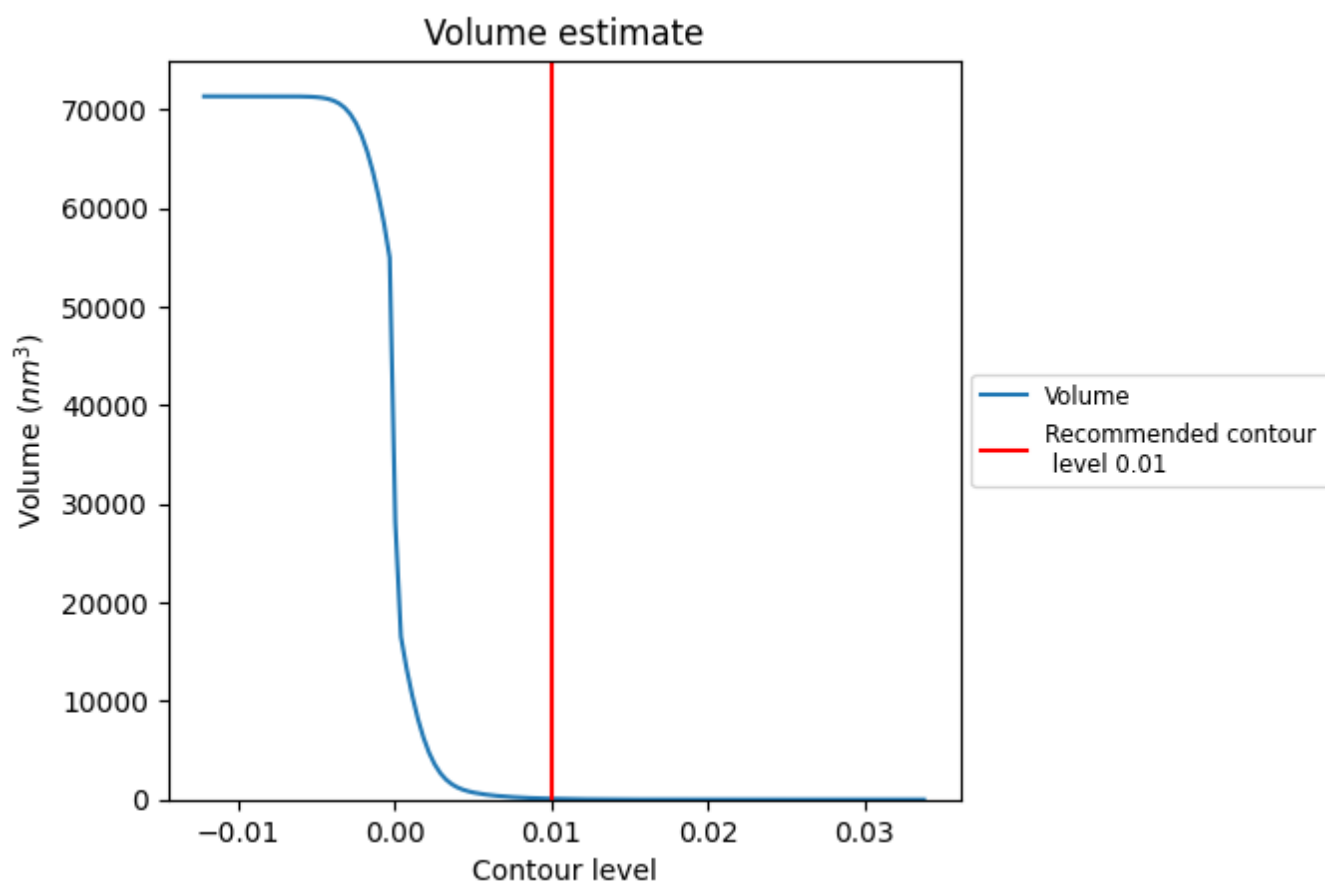
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

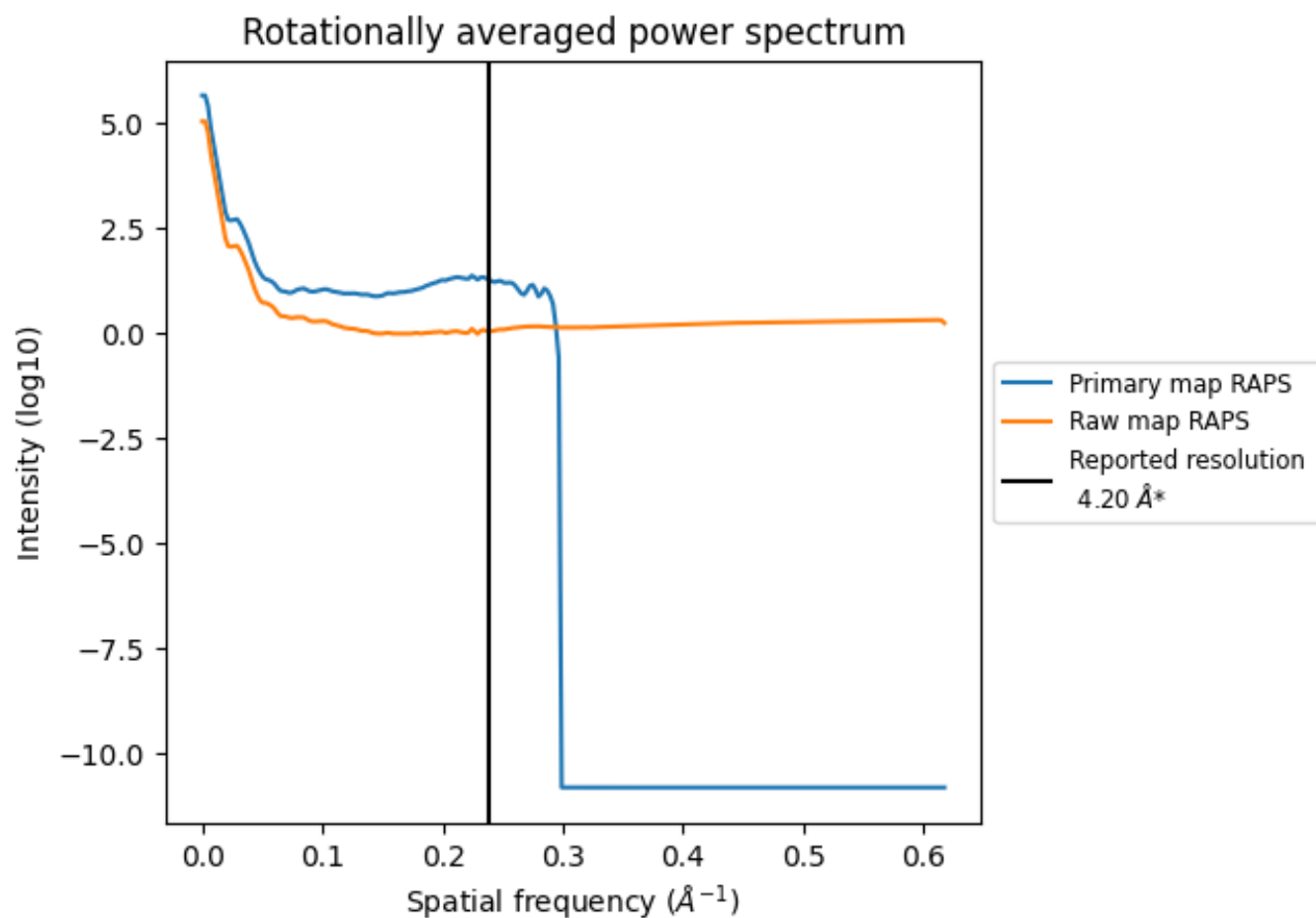
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 88 nm³; this corresponds to an approximate mass of 79 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 ⓘ

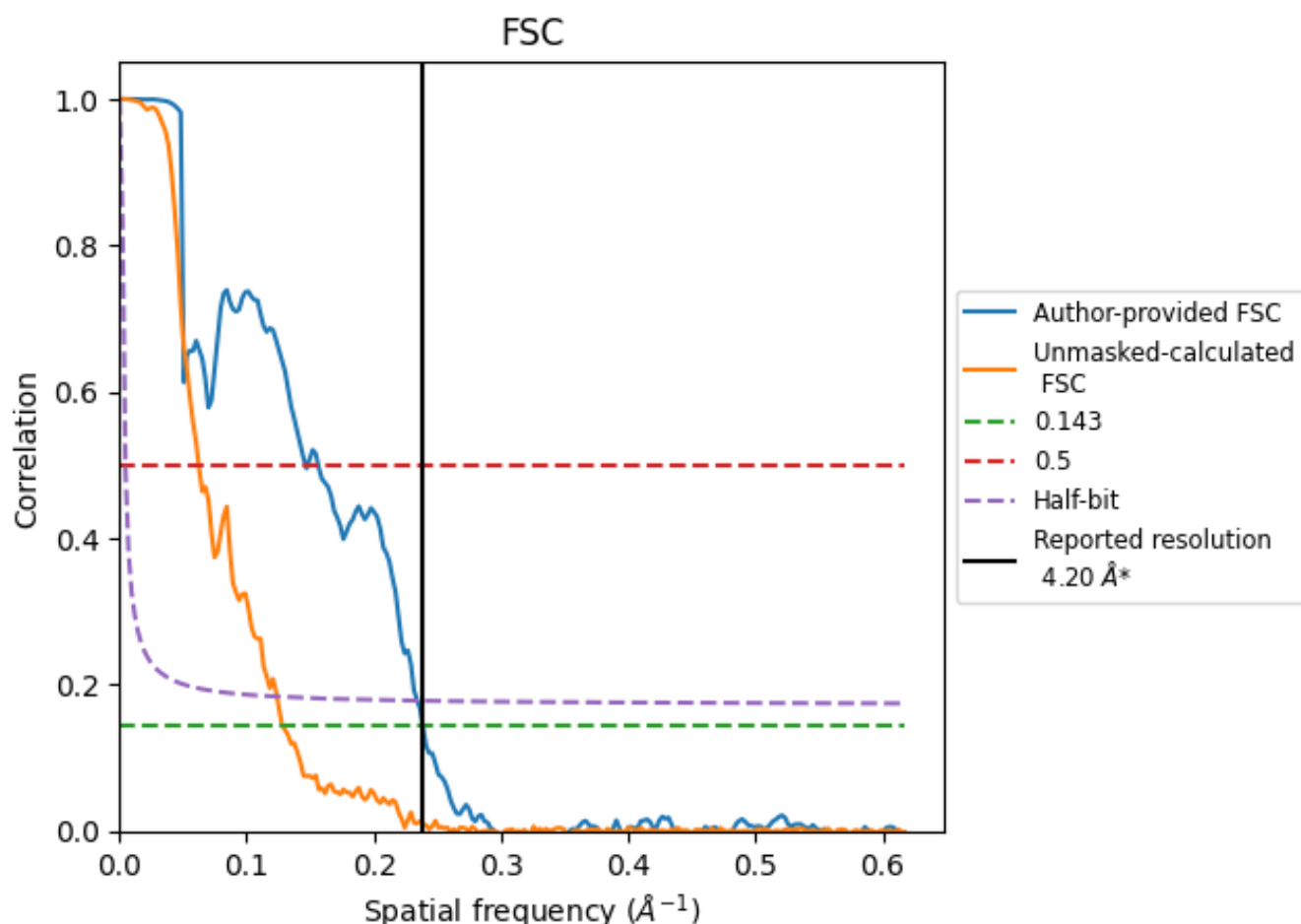


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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 0.238 Å⁻¹

8.2 Resolution estimates [i](#)

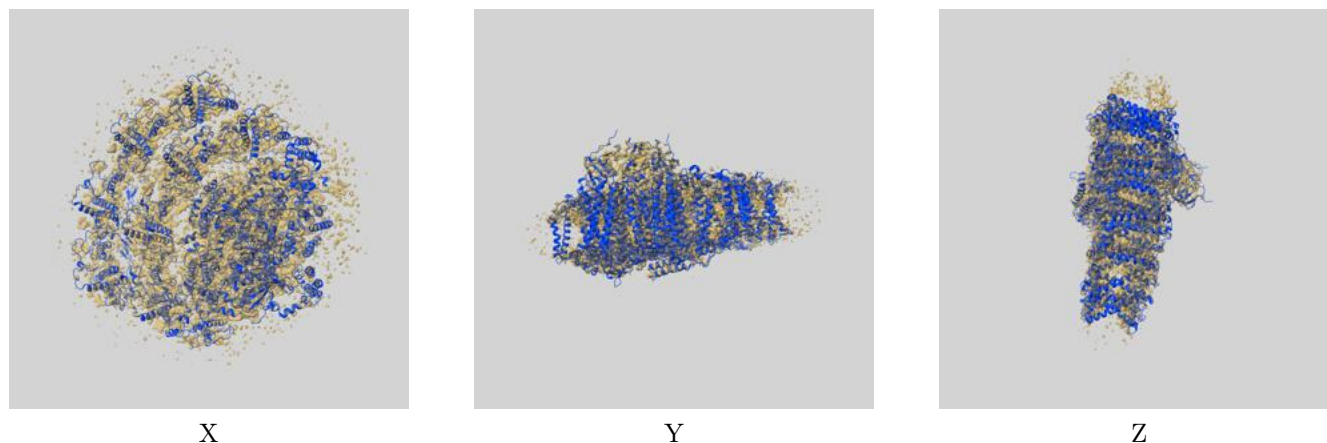
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.19	6.84	4.27
Unmasked-calculated*	7.81	16.08	8.08

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.81 differs from the reported value 4.2 by more than 10 %

9 Map-model fit [i](#)

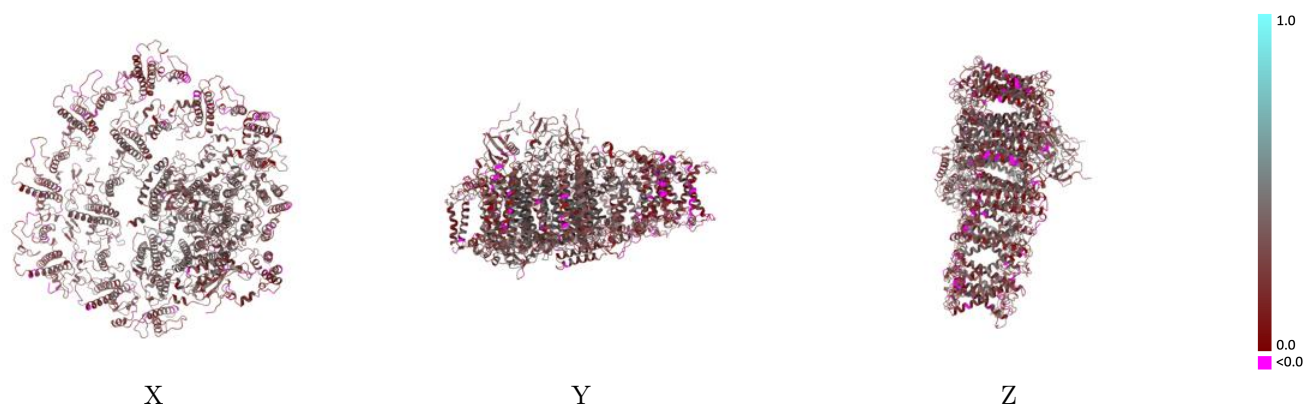
This section contains information regarding the fit between EMDB map EMD-11640 and PDB model 7A4P. Per-residue inclusion information can be found in section [3](#) on page [47](#).

9.1 Map-model overlay [i](#)



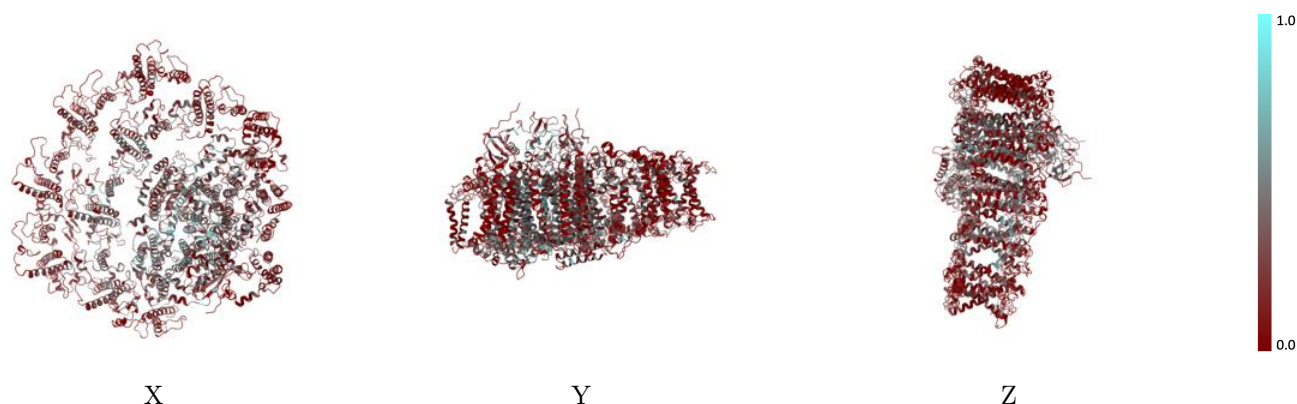
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



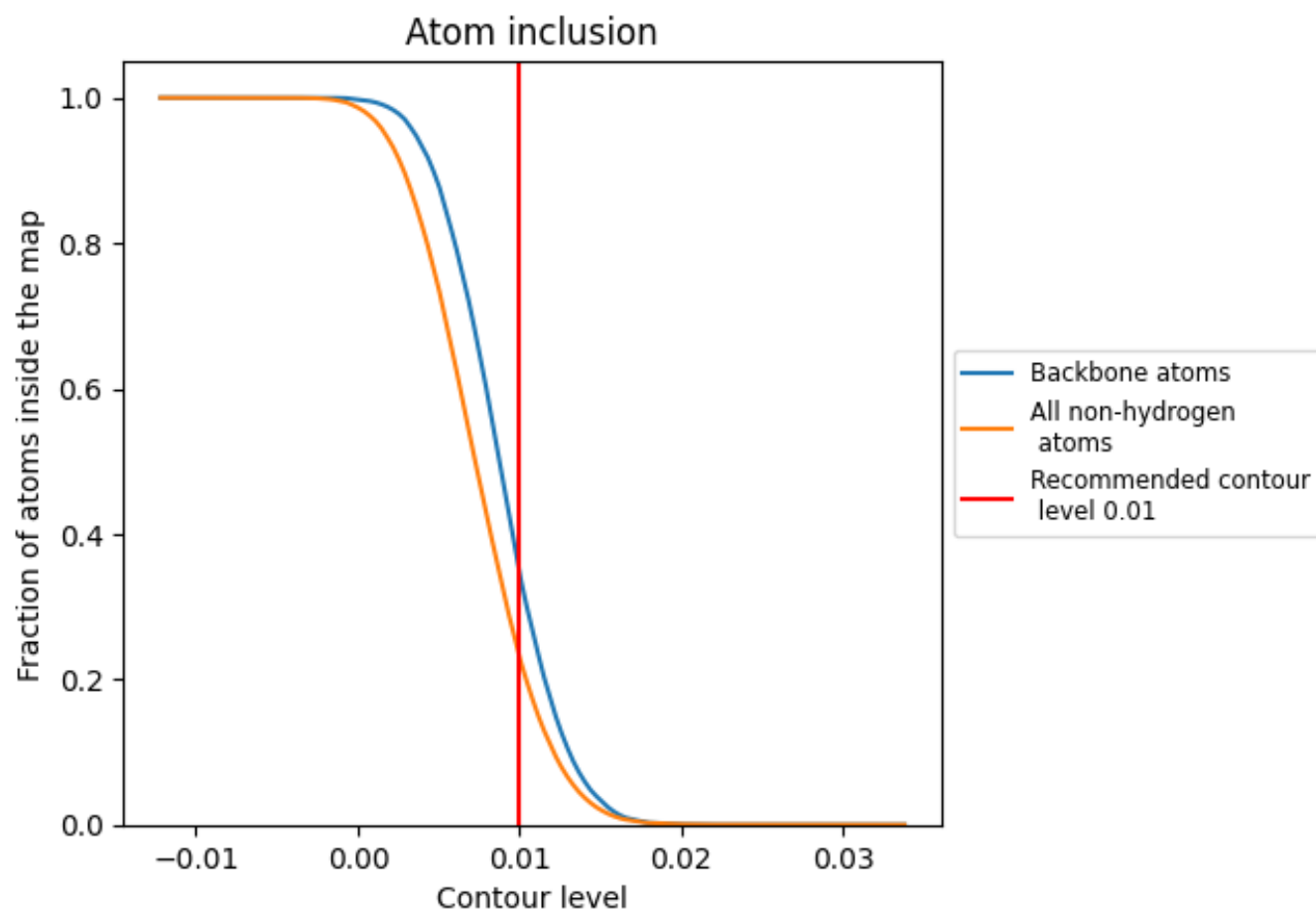
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 35% of all backbone atoms, 23% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.2307	<div></div> 0.2780
1	<div></div> 0.1747	<div></div> 0.2150
3	<div></div> 0.2005	<div></div> 0.2770
4	<div></div> 0.1774	<div></div> 0.2250
5	<div></div> 0.1115	<div></div> 0.2330
6	<div></div> 0.1124	<div></div> 0.2290
7	<div></div> 0.2874	<div></div> 0.2990
8	<div></div> 0.2743	<div></div> 0.2880
A	<div></div> 0.3560	<div></div> 0.3500
B	<div></div> 0.2601	<div></div> 0.3140
C	<div></div> 0.4478	<div></div> 0.3400
D	<div></div> 0.2226	<div></div> 0.2740
E	<div></div> 0.3191	<div></div> 0.2800
F	<div></div> 0.2752	<div></div> 0.2970
G	<div></div> 0.0354	<div></div> 0.1850
I	<div></div> 0.0874	<div></div> 0.2110
J	<div></div> 0.2984	<div></div> 0.3560
K	<div></div> 0.0939	<div></div> 0.2190
L	<div></div> 0.0512	<div></div> 0.1760
M	<div></div> 0.0290	<div></div> 0.1970
a	<div></div> 0.1456	<div></div> 0.1790

1.0

0.0

<0.0