



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 11:55 PM UTC

PDB ID : 7A4P / pdb_00007a4p
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:

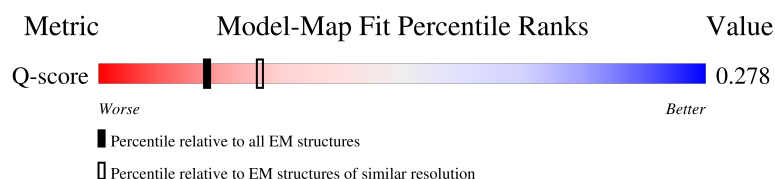
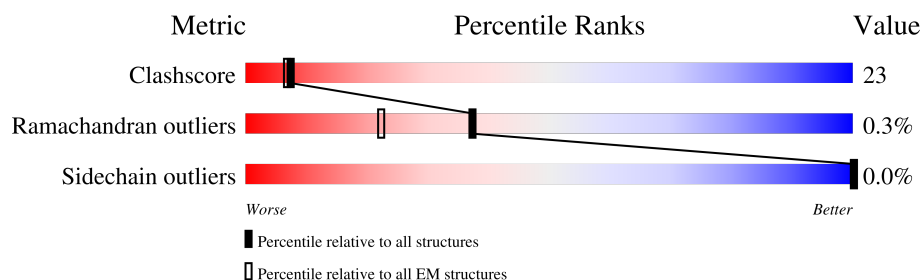
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

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	55% 68% 32%
2	B	731	73% 68% 32%
3	C	80	39% 72% 26% .
4	D	143	83% 69% 31%

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Mol	Chain	Length	Quality of chain
5	E	64	
6	F	165	
7	G	99	
8	J	41	
9	K	86	
10	M	31	
11	I	35	
12	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
20	CL0	A	1011	X	-	-	-
21	CLA	1	601	X	-	-	-
21	CLA	1	602	X	-	-	-
21	CLA	1	603	X	-	-	-
21	CLA	1	604	X	-	-	-
21	CLA	1	605	X	-	-	-
21	CLA	1	606	X	-	-	-
21	CLA	1	607	X	-	-	-
21	CLA	1	608	X	-	-	-
21	CLA	1	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	1	611	X	-	-	-
21	CLA	1	612	X	-	-	-
21	CLA	1	615	X	-	-	-
21	CLA	3	601	X	-	-	-
21	CLA	3	602	X	-	-	-
21	CLA	3	603	X	-	-	-
21	CLA	3	604	X	-	-	-
21	CLA	3	605	X	-	-	-
21	CLA	3	606	X	-	-	-
21	CLA	3	607	X	-	-	-
21	CLA	3	610	X	-	-	-
21	CLA	3	612	X	-	-	-
21	CLA	3	613	X	-	-	-
21	CLA	3	616	X	-	-	-
21	CLA	3	618	X	-	-	-
21	CLA	4	601	X	-	-	-
21	CLA	4	602	X	-	-	-
21	CLA	4	603	X	-	-	-
21	CLA	4	604	X	-	-	-
21	CLA	4	605	X	-	-	-
21	CLA	4	606	X	-	-	-
21	CLA	4	607	X	-	-	-
21	CLA	4	608	X	-	-	-
21	CLA	4	610	X	-	-	-
21	CLA	4	611	X	-	-	-
21	CLA	4	612	X	-	-	-
21	CLA	4	615	X	-	-	-
21	CLA	4	616	X	-	-	-
21	CLA	4	617	X	-	-	-
21	CLA	5	601	X	-	-	-
21	CLA	5	602	X	-	-	-
21	CLA	5	603	X	-	-	-
21	CLA	5	604	X	-	-	-
21	CLA	5	605	X	-	-	-
21	CLA	5	606	X	-	-	-
21	CLA	5	607	X	-	-	-
21	CLA	5	608	X	-	-	-
21	CLA	5	609	X	-	-	-
21	CLA	5	612	X	-	-	-
21	CLA	5	614	X	-	-	-
21	CLA	5	616	X	-	-	-
21	CLA	5	617	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	5	618	X	-	-	-
21	CLA	6	601	X	-	X	-
21	CLA	6	602	X	-	-	-
21	CLA	6	603	X	-	-	-
21	CLA	6	604	X	-	-	-
21	CLA	6	605	X	-	-	-
21	CLA	6	606	X	-	-	-
21	CLA	6	607	X	-	-	-
21	CLA	6	608	X	-	-	-
21	CLA	6	609	X	-	X	-
21	CLA	6	612	X	-	-	-
21	CLA	6	615	X	-	-	-
21	CLA	6	617	X	-	-	-
21	CLA	6	618	X	-	-	-
21	CLA	7	601	X	-	-	-
21	CLA	7	602	X	-	-	-
21	CLA	7	603	X	-	-	-
21	CLA	7	604	X	-	-	-
21	CLA	7	605	X	-	-	-
21	CLA	7	606	X	-	-	-
21	CLA	7	607	X	-	-	-
21	CLA	7	608	X	-	-	-
21	CLA	7	609	X	-	-	-
21	CLA	7	610	X	-	-	-
21	CLA	7	611	X	-	-	-
21	CLA	7	612	X	-	-	-
21	CLA	7	615	X	-	-	-
21	CLA	7	617	X	-	-	-
21	CLA	8	602	X	-	-	-
21	CLA	8	603	X	-	-	-
21	CLA	8	605	X	-	-	-
21	CLA	8	606	X	-	-	-
21	CLA	8	607	X	-	-	-
21	CLA	8	608	X	-	-	-
21	CLA	8	609	X	-	-	-
21	CLA	8	610	X	-	-	-
21	CLA	8	611	X	-	-	-
21	CLA	8	612	X	-	-	-
21	CLA	8	615	X	-	-	-
21	CLA	8	618	X	-	-	-
21	CLA	8	620	X	-	-	-
21	CLA	A	1012	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	A	1013	X	-	-	-
21	CLA	A	1101	X	-	-	-
21	CLA	A	1102	X	-	-	-
21	CLA	A	1103	X	-	-	-
21	CLA	A	1104	X	-	-	-
21	CLA	A	1105	X	-	-	-
21	CLA	A	1106	X	-	-	-
21	CLA	A	1107	X	-	-	-
21	CLA	A	1108	X	-	-	-
21	CLA	A	1109	X	-	-	-
21	CLA	A	1110	X	-	-	-
21	CLA	A	1111	X	-	-	-
21	CLA	A	1112	X	-	-	-
21	CLA	A	1113	X	-	-	-
21	CLA	A	1114	X	-	-	-
21	CLA	A	1115	X	-	-	-
21	CLA	A	1116	X	-	-	-
21	CLA	A	1117	X	-	-	-
21	CLA	A	1118	X	-	-	-
21	CLA	A	1119	X	-	-	-
21	CLA	A	1120	X	-	-	-
21	CLA	A	1121	X	-	-	-
21	CLA	A	1122	X	-	-	-
21	CLA	A	1123	X	-	-	-
21	CLA	A	1124	X	-	-	-
21	CLA	A	1125	X	-	-	-
21	CLA	A	1126	X	-	-	-
21	CLA	A	1127	X	-	-	-
21	CLA	A	1128	X	-	-	-
21	CLA	A	1129	X	-	-	-
21	CLA	A	1130	X	-	-	-
21	CLA	A	1131	X	-	-	-
21	CLA	A	1132	X	-	-	-
21	CLA	A	1133	X	-	-	-
21	CLA	A	1134	X	-	-	-
21	CLA	A	1135	X	-	-	-
21	CLA	A	1136	X	-	-	-
21	CLA	A	1137	X	-	-	-
21	CLA	A	1138	X	-	-	-
21	CLA	A	1139	X	-	-	-
21	CLA	A	1140	X	-	-	-
21	CLA	A	1141	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	B	1021	X	-	-	-
21	CLA	B	1022	X	-	-	-
21	CLA	B	1023	X	-	-	-
21	CLA	B	1201	X	-	-	-
21	CLA	B	1202	X	-	-	-
21	CLA	B	1203	X	-	-	-
21	CLA	B	1204	X	-	-	-
21	CLA	B	1205	X	-	-	-
21	CLA	B	1206	X	-	-	-
21	CLA	B	1207	X	-	-	-
21	CLA	B	1208	X	-	-	-
21	CLA	B	1209	X	-	-	-
21	CLA	B	1210	X	-	-	-
21	CLA	B	1211	X	-	-	-
21	CLA	B	1212	X	-	-	-
21	CLA	B	1213	X	-	-	-
21	CLA	B	1214	X	-	-	-
21	CLA	B	1215	X	-	-	-
21	CLA	B	1216	X	-	-	-
21	CLA	B	1217	X	-	-	-
21	CLA	B	1218	X	-	-	-
21	CLA	B	1219	X	-	-	-
21	CLA	B	1220	X	-	-	-
21	CLA	B	1221	X	-	-	-
21	CLA	B	1222	X	-	-	-
21	CLA	B	1223	X	-	-	-
21	CLA	B	1224	X	-	-	-
21	CLA	B	1225	X	-	-	-
21	CLA	B	1226	X	-	-	-
21	CLA	B	1227	X	-	-	-
21	CLA	B	1228	X	-	-	-
21	CLA	B	1229	X	-	-	-
21	CLA	B	1230	X	-	-	-
21	CLA	B	1231	X	-	-	-
21	CLA	B	1232	X	-	-	-
21	CLA	B	1234	X	-	-	-
21	CLA	B	1235	X	-	-	-
21	CLA	B	1236	X	-	-	-
21	CLA	B	1237	X	-	-	-
21	CLA	B	1238	X	-	-	-
21	CLA	B	1239	X	-	-	-
21	CLA	B	1240	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	F	1301	X	-	-	-
21	CLA	F	1302	X	-	-	-
21	CLA	G	1601	X	-	-	-
21	CLA	G	1602	X	-	-	-
21	CLA	G	1603	X	-	-	-
21	CLA	J	1901	X	-	-	-
21	CLA	K	1401	X	-	-	-
21	CLA	K	1402	X	-	-	-
21	CLA	K	1403	X	-	X	-
21	CLA	K	1404	X	-	-	-
21	CLA	L	1501	X	-	-	-
21	CLA	L	1502	X	-	-	-
21	CLA	L	1503	X	-	-	-
21	CLA	a	601	X	-	-	-
21	CLA	a	602	X	-	-	-
21	CLA	a	603	X	-	-	-
21	CLA	a	604	X	-	-	-
21	CLA	a	605	X	-	-	-
21	CLA	a	607	X	-	-	-
21	CLA	a	608	X	-	-	-
21	CLA	a	611	X	-	-	-
21	CLA	a	612	X	-	-	-
21	CLA	a	615	X	-	-	-
33	ERG	G	5002	X	-	-	-
34	RRX	J	4002	X	-	-	-
37	LUT	1	503	X	-	-	-
37	LUT	5	505	X	-	-	-
37	LUT	6	501	X	-	-	-
37	LUT	6	502	X	-	-	-
37	LUT	7	501	X	-	-	-
37	LUT	a	502	X	-	-	-
38	CHL	1	609	X	-	-	-
38	CHL	1	613	X	-	-	-
38	CHL	3	608	X	-	-	-
38	CHL	3	611	X	-	-	-
38	CHL	4	609	X	-	-	-
38	CHL	4	613	X	-	-	-
38	CHL	4	618	X	-	-	-
38	CHL	5	610	X	-	-	-
38	CHL	5	611	X	-	-	-
38	CHL	5	613	X	-	-	-
38	CHL	6	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
38	CHL	6	611	X	-	-	-
38	CHL	6	613	X	-	-	-
38	CHL	6	619	X	-	-	-
38	CHL	7	613	X	-	-	-
38	CHL	8	601	X	-	-	-
38	CHL	8	604	X	-	-	-
38	CHL	8	613	X	-	-	-
38	CHL	a	606	X	-	-	-
38	CHL	a	609	X	-	-	-
38	CHL	a	610	X	-	-	-
38	CHL	a	613	X	-	-	-
40	QTB	3	506	X	-	-	-
45	XAT	7	502	X	-	-	-
47	C7Z	7	504	X	-	-	-

2 Entry composition [i](#)

There are 48 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	S	0	0
			509	323	91	95			

There are 5 discrepancies between the modelled and reference sequences:

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

- Molecule 6 is a protein called PSI-F.

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

There are 11 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 8 discrepancies between the modelled and reference sequences:

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

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

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

- Molecule 9 is a protein called PSI-K.

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

There are 7 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

- Molecule 12 is a protein called 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		

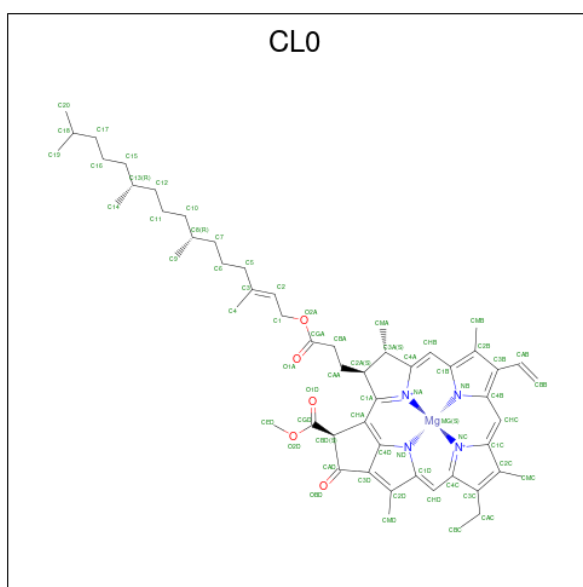
There are 10 discrepancies between the modelled and reference sequences:

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.

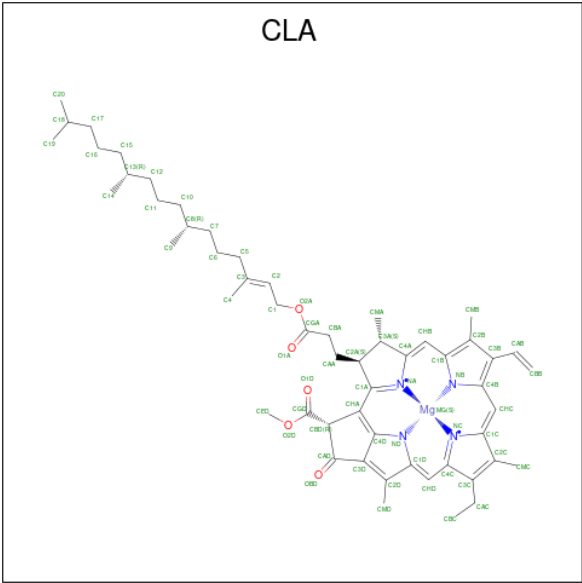
Mol	Chain	Residues	Atoms					AltConf	Trace
19	8	219	Total	C	N	O	S	0	0
			1669	1073	285	305	6		

- Molecule 20 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



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

- Molecule 21 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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

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

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Mol	Chain	Residues	Atoms					AltConf
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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

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Mol	Chain	Residues	Atoms					AltConf
21	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	1	1	Total 57	C 47	Mg 1	N 4	O 5	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	a	1	Total 58	C 48	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	a	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
21	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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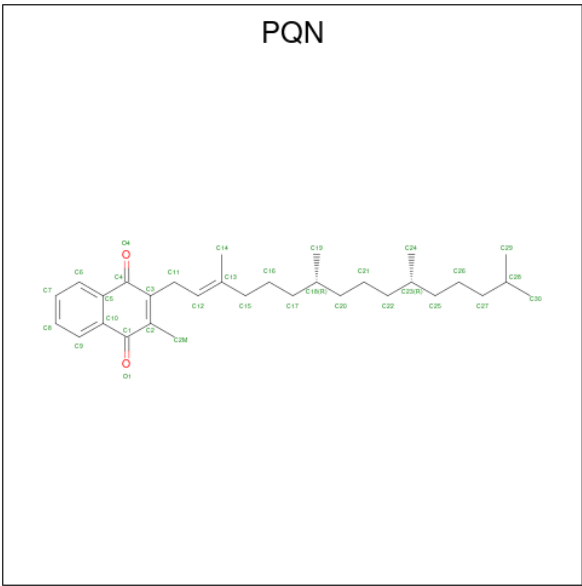
Mol	Chain	Residues	Atoms					AltConf
21	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	7	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
21	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	7	1	Total	C	Mg	N	O	0
			44	34	1	4	5	

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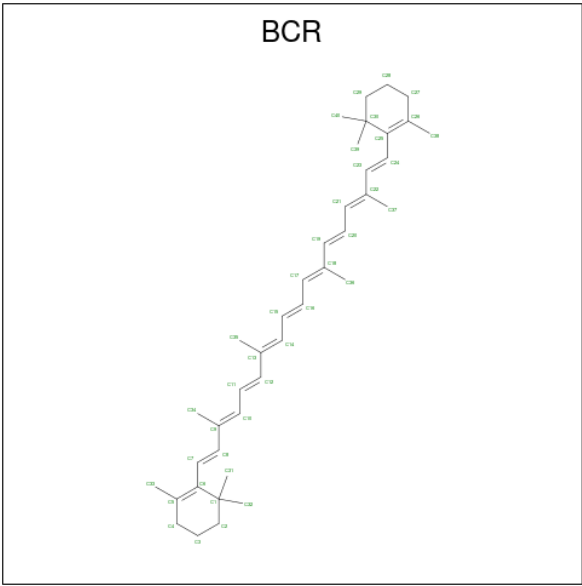
Mol	Chain	Residues	Atoms					AltConf
21	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	7	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
21	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
21	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	7	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
21	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	8	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	8	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
21	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	8	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 22 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



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

- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



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

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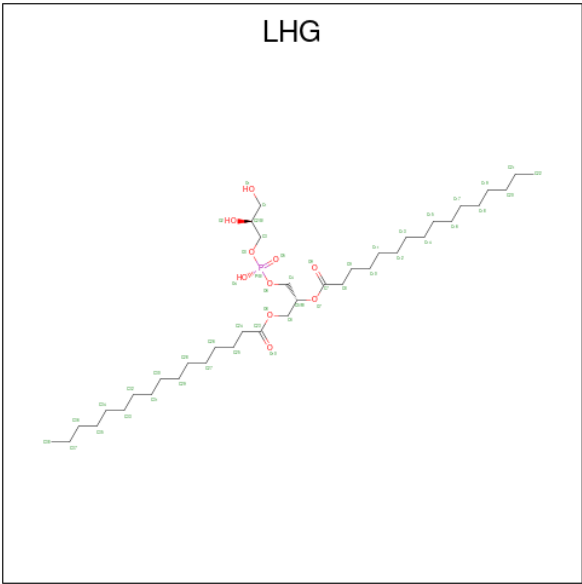
Mol	Chain	Residues	Atoms	AltConf
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C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

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

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



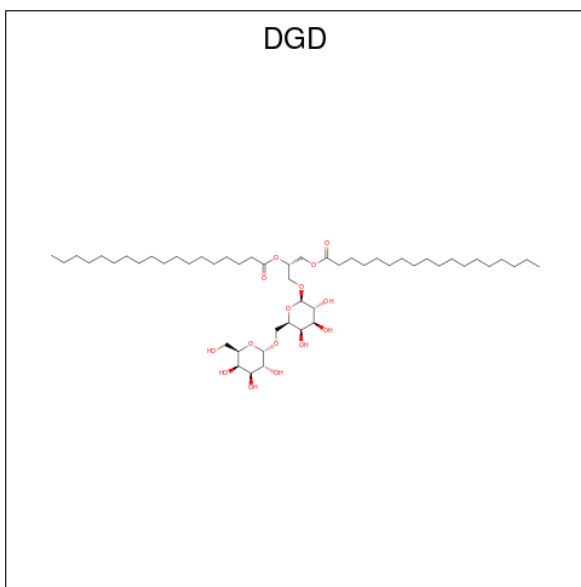
Mol	Chain	Residues	Atoms	AltConf
24	A	1	Total C O P 29 18 10 1	0
24	A	1	Total C O P 49 38 10 1	0

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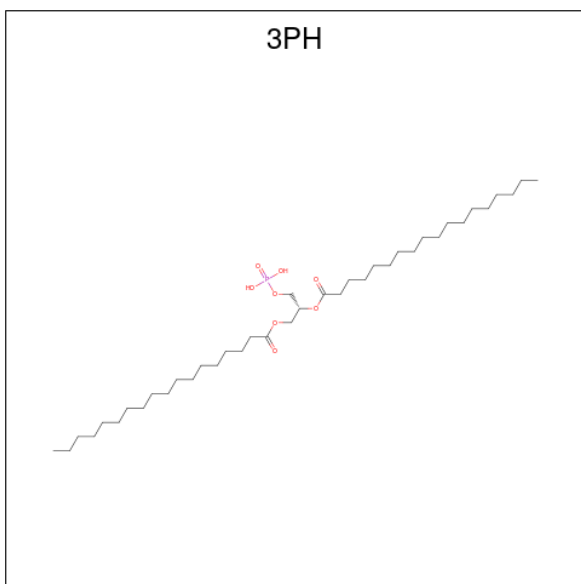
Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O	P	0
			42	31	10	1	
24	B	1	Total	C	O	P	0
			49	38	10	1	
24	B	1	Total	C	O	P	0
			46	35	10	1	
24	F	1	Total	C	O	P	0
			36	25	10	1	
24	F	1	Total	C	O	P	0
			43	32	10	1	
24	1	1	Total	C	O	P	0
			35	24	10	1	
24	1	1	Total	C	O	P	0
			42	31	10	1	
24	a	1	Total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

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



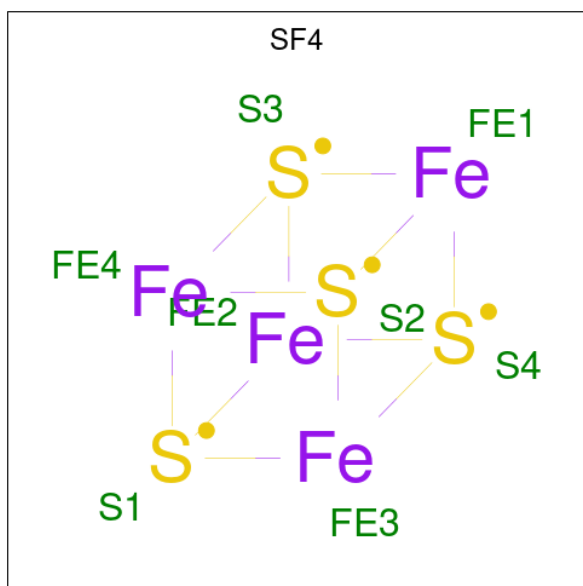
Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	C	O	0
			51	36	15	
25	B	1	Total	C	O	0
			66	51	15	
25	8	1	Total	C	O	0
			66	51	15	

- Molecule 26 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$).



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

- Molecule 27 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 28 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $\text{C}_{24}\text{H}_{46}\text{O}_{11}$).



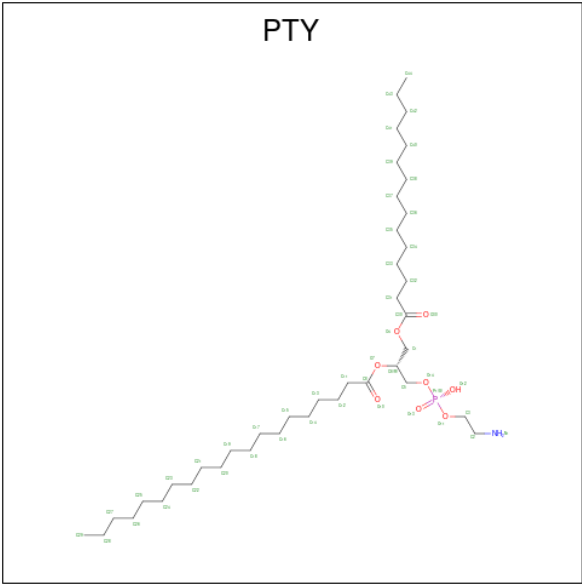
Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total 35	C 24	O 11	0
28	B	1	Total 35	C 24	O 11	0
28	1	1	Total 35	C 24	O 11	0

- Molecule 29 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: $C_{44}H_{85}NO_8P$).



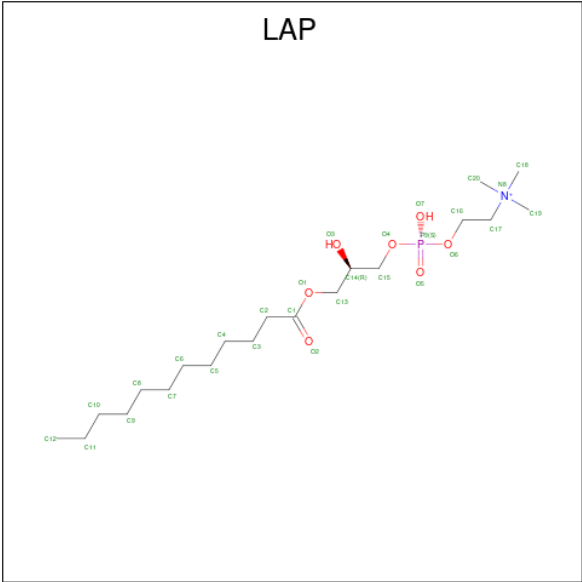
Mol	Chain	Residues	Atoms					AltConf
29	B	1	Total	C	N	O	P	0
			30	20	1	8	1	
29	6	1	Total	C	N	O	P	0
			36	26	1	8	1	

- Molecule 30 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



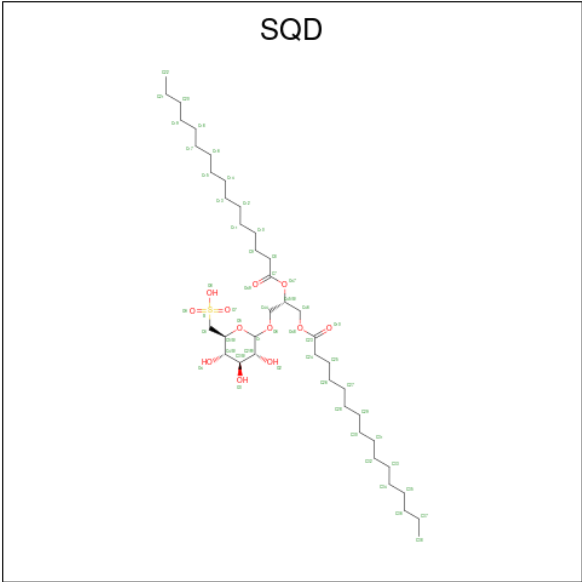
Mol	Chain	Residues	Atoms					AltConf
30	B	1	Total	C	N	O	P	0
			41	31	1	8	1	
30	3	1	Total	C	N	O	P	0
			38	28	1	8	1	
30	5	1	Total	C	N	O	P	0
			38	28	1	8	1	
30	7	1	Total	C	N	O	P	0
			33	23	1	8	1	
30	8	1	Total	C	N	O	P	0
			35	25	1	8	1	

- Molecule 31 is [2-((1-OXODODECANOXY-(2-HYDROXY-3-PROPANYL))-PHOSPHONATE-OXY)-ETHYL]-TRIMETHYLAMMONIUM (CCD ID: LAP) (formula: C₂₀H₄₃NO₇P).



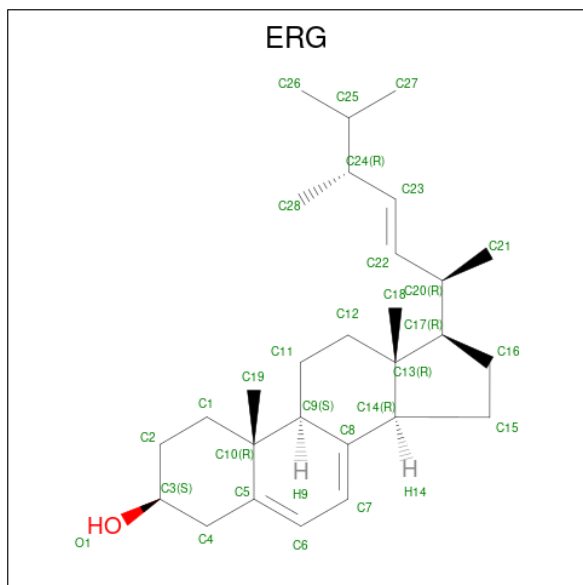
Mol	Chain	Residues	Atoms					AltConf
31	B	1	Total	C	N	O	P	0
			29	20	1	7	1	
31	F	1	Total	C	N	O	P	0
			29	20	1	7	1	
31	K	1	Total	C	N	O	P	0
			29	20	1	7	1	

- Molecule 32 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



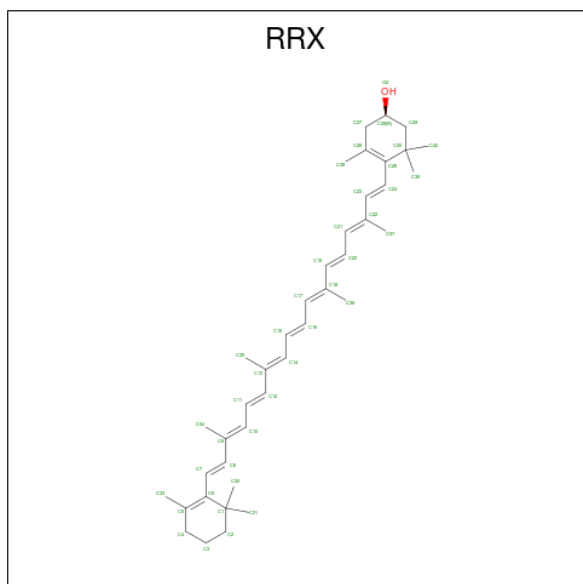
Mol	Chain	Residues	Atoms				AltConf
32	G	1	Total	C	O	S	0
			46	33	12	1	
32	7	1	Total	C	O	S	0
			39	26	12	1	

- Molecule 33 is ERGOSTEROL (CCD ID: ERG) (formula: $C_{28}H_{44}O$).



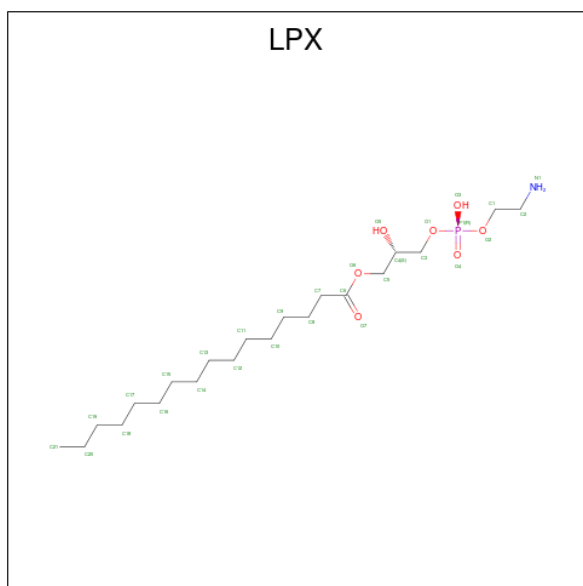
Mol	Chain	Residues	Atoms				AltConf
33	G	1	Total	C	O		0
			29	28	1		

- Molecule 34 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: $C_{40}H_{56}O$).



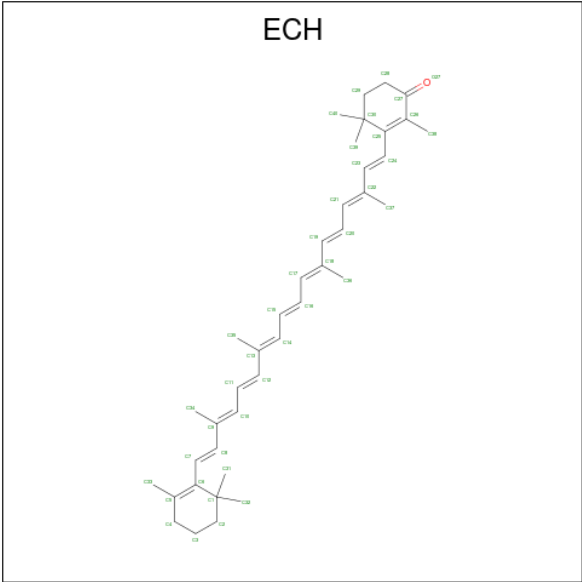
Mol	Chain	Residues	Atoms			AltConf
34	J	1	Total	C	O	0
			41	40	1	

- Molecule 35 is (2S)-3-[[[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (CCD ID: LPX) (formula: C₂₁H₄₄NO₇P).



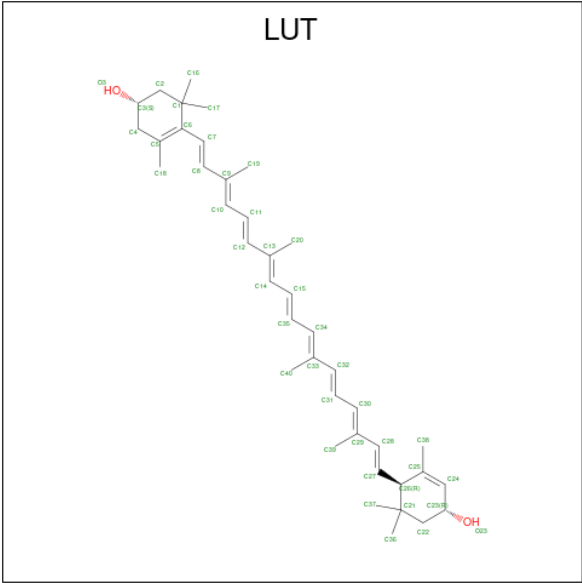
Mol	Chain	Residues	Atoms					AltConf
35	J	1	Total	C	N	O	P	0
			17	8	1	7	1	
35	a	1	Total	C	N	O	P	0
			30	21	1	7	1	

- Molecule 36 is beta,beta-caroten-4-one (CCD ID: ECH) (formula: C₄₀H₅₄O).



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

- Molecule 37 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



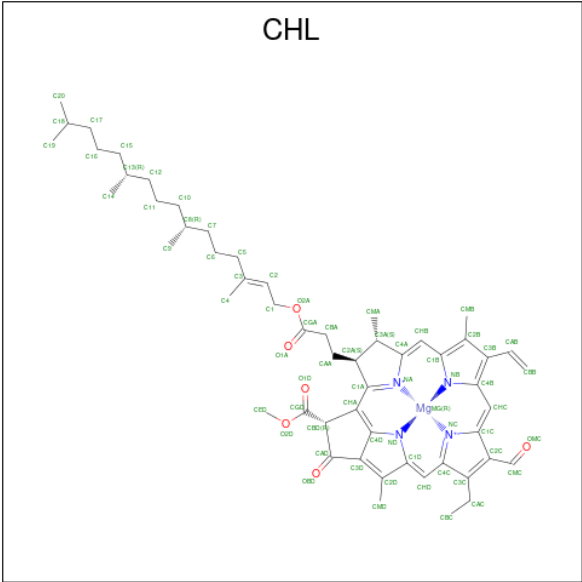
Mol	Chain	Residues	Atoms			AltConf
37	1	1	Total	C	O	0
			42	40	2	
37	1	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
37	1	1	Total	C	O	0
			42	40	2	
37	a	1	Total	C	O	0
			42	40	2	
37	a	1	Total	C	O	0
			42	40	2	
37	a	1	Total	C	O	0
			42	40	2	
37	3	1	Total	C	O	0
			42	40	2	
37	3	1	Total	C	O	0
			42	40	2	
37	4	1	Total	C	O	0
			42	40	2	
37	4	1	Total	C	O	0
			42	40	2	
37	5	1	Total	C	O	0
			42	40	2	
37	5	1	Total	C	O	0
			42	40	2	
37	5	1	Total	C	O	0
			42	40	2	
37	6	1	Total	C	O	0
			42	40	2	
37	6	1	Total	C	O	0
			42	40	2	
37	7	1	Total	C	O	0
			42	40	2	
37	8	1	Total	C	O	0
			42	40	2	
37	8	1	Total	C	O	0
			42	40	2	

- Molecule 38 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



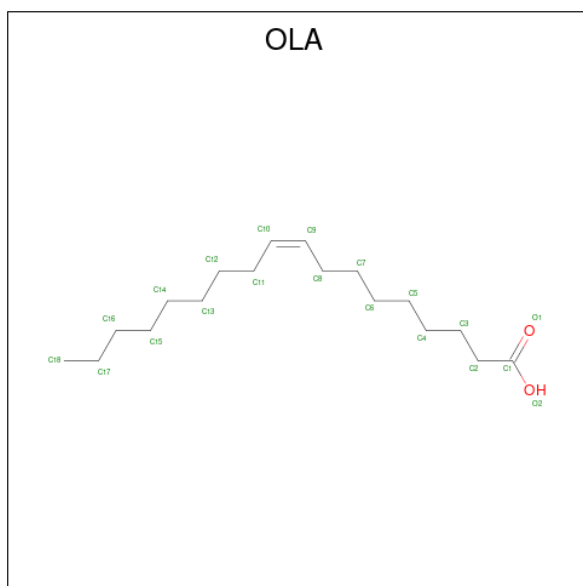
Mol	Chain	Residues	Atoms					AltConf
38	1	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
38	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	a	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
38	a	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
38	a	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
38	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
38	3	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
38	3	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
38	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	4	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
38	4	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
38	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	5	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
38	5	1	Total	C	Mg	N	O	0
			56	45	1	4	6	

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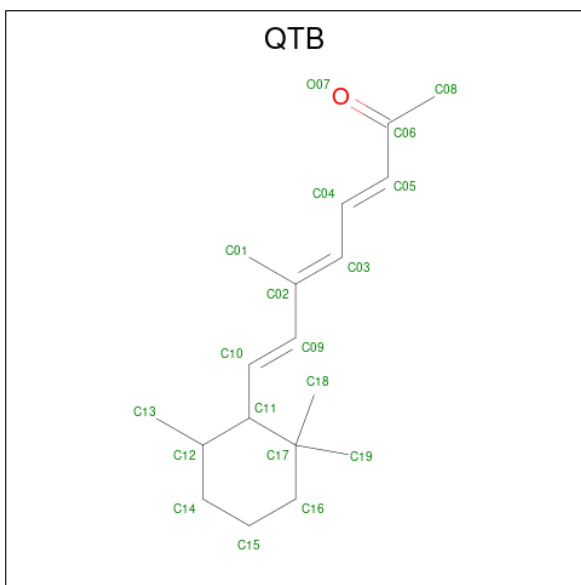
Mol	Chain	Residues	Atoms					AltConf
38	6	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
38	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
38	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
38	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	8	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
38	8	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
38	8	1	Total	C	Mg	N	O	0
			51	40	1	4	6	

- Molecule 39 is OLEIC ACID (CCD ID: OLA) (formula: $C_{18}H_{34}O_2$).



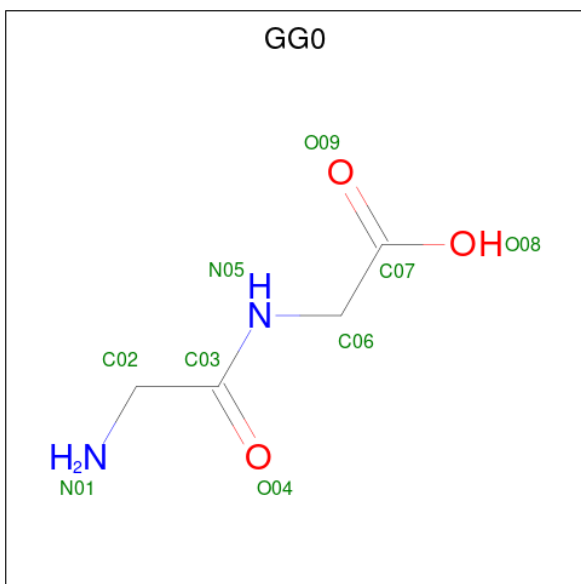
Mol	Chain	Residues	Atoms			AltConf
39	1	1	Total	C	O	0
			20	18	2	
39	8	1	Total	C	O	0
			20	18	2	

- Molecule 40 is (3 {E},5 {E},7 {E})-6-methyl-8-[(6 {R})-2,2,6-trimethylcyclohexyl]octa-3,5,7-trien-2-one (CCD ID: QTB) (formula: $C_{18}H_{28}O$).



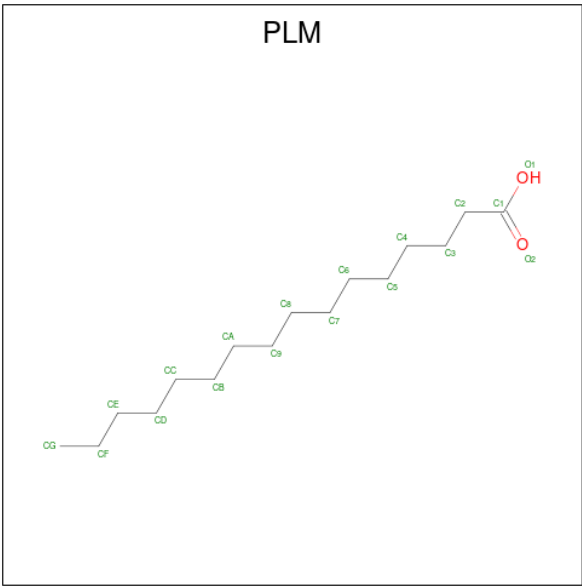
Mol	Chain	Residues	Atoms			AltConf
40	a	1	Total	C	O	0
			19	18	1	
40	3	1	Total	C	O	0
			19	18	1	

- Molecule 41 is 2-(2-azanylethanoylamino)ethanoic acid (CCD ID: GG0) (formula: $C_4H_8N_2O_3$).



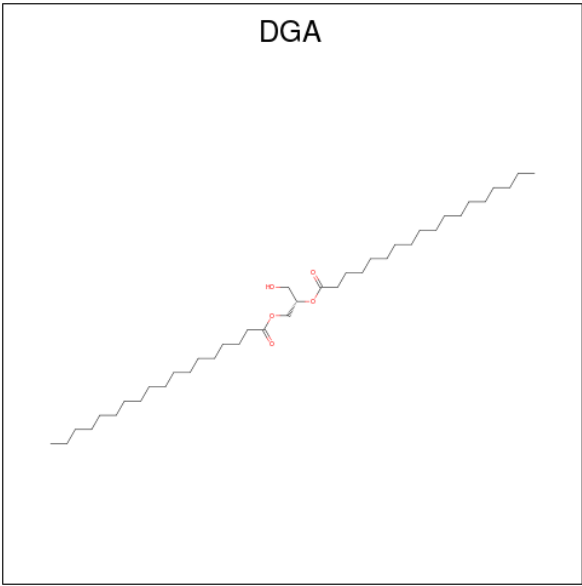
Mol	Chain	Residues	Atoms				AltConf
41	a	1	Total	C	N	O	0
			9	4	2	3	

- Molecule 42 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms			AltConf
42	4	1	Total	C	O	0
			17	16	1	
42	6	1	Total	C	O	0
			18	16	2	

- Molecule 43 is DIACYL GLYCEROL (CCD ID: DGA) (formula: C₃₉H₇₆O₅).



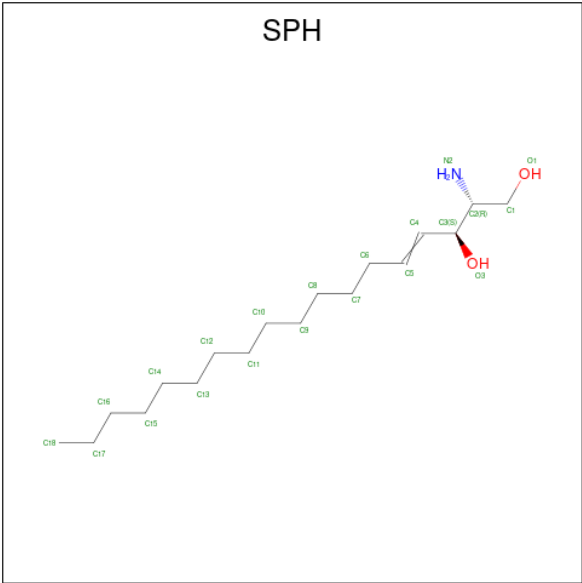
Mol	Chain	Residues	Atoms			AltConf
43	5	1	Total	C	O	0
			23	18	5	

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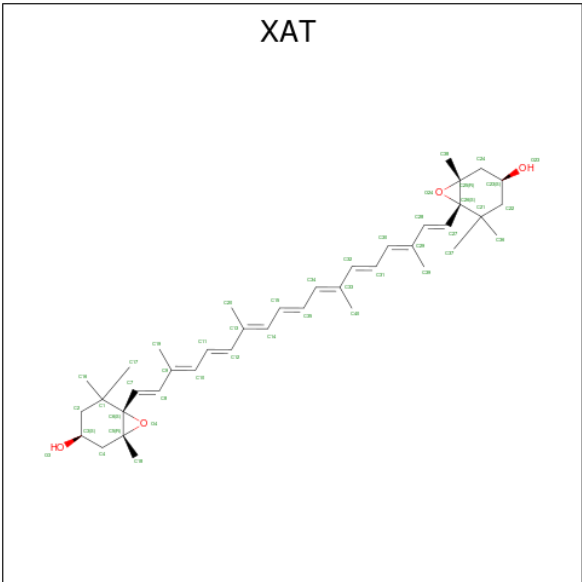
Mol	Chain	Residues	Atoms			AltConf
43	8	1	Total	C	O	0
			30	25	5	

- Molecule 44 is SPHINGOSINE (CCD ID: SPH) (formula: C₁₈H₃₇NO₂).



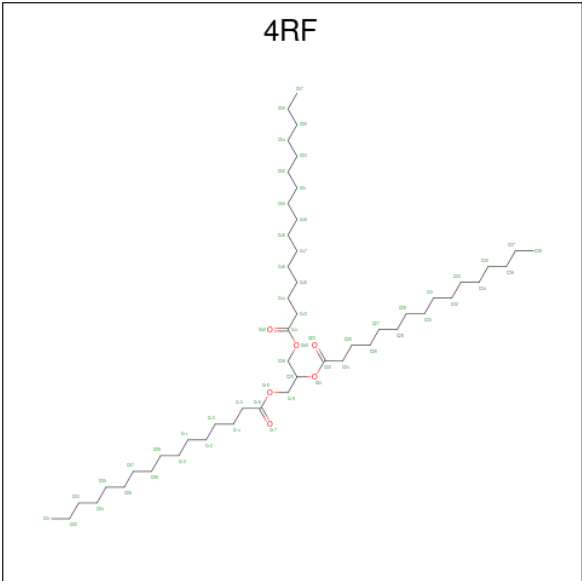
Mol	Chain	Residues	Atoms				AltConf
44	6	1	Total	C	N	O	0
			21	18	1	2	

- Molecule 45 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



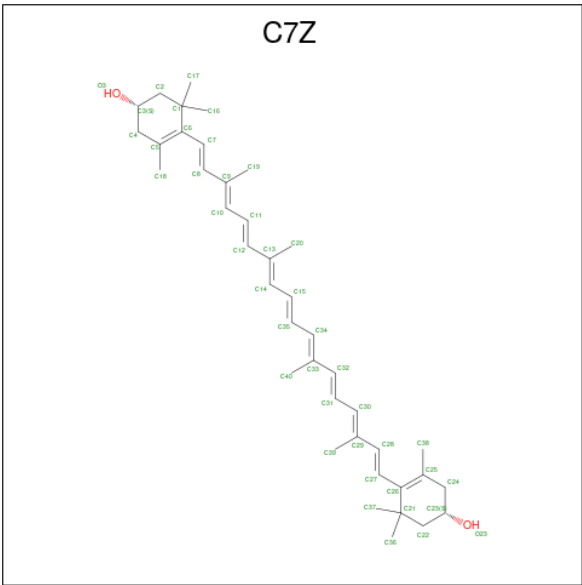
Mol	Chain	Residues	Atoms			AltConf
45	7	1	Total	C	O	0
			44	40	4	

- Molecule 46 is Tripalmitoylglycerol (CCD ID: 4RF) (formula: C₅₁H₉₈O₆).



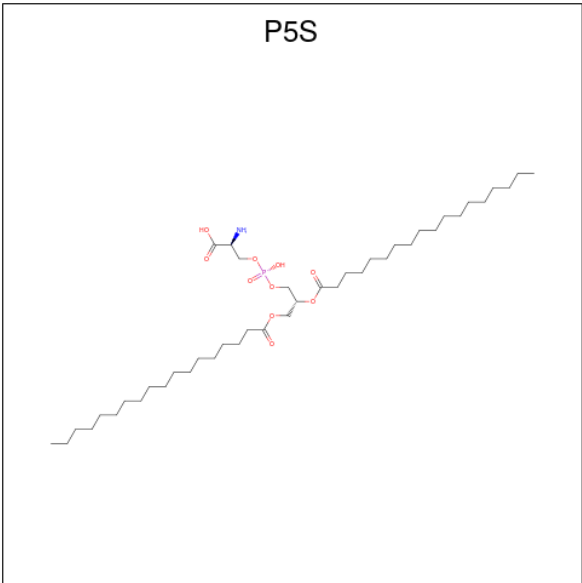
Mol	Chain	Residues	Atoms			AltConf
46	7	1	Total	C	O	0
			32	26	6	
46	8	1	Total	C	O	0
			42	36	6	
46	8	1	Total	C	O	0
			54	48	6	

- Molecule 47 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (CCD ID: C7Z) (formula: C₄₀H₅₆O₂).



Mol	Chain	Residues	Atoms			AltConf
47	7	1	Total	C	O	0
			42	40	2	

- Molecule 48 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (CCD ID: P5S) (formula: C₄₂H₈₂NO₁₀P).



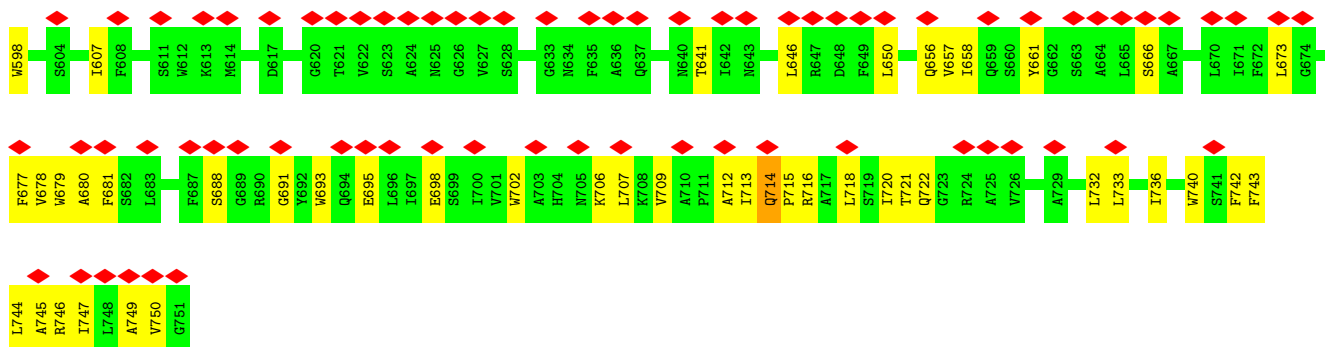
Mol	Chain	Residues	Atoms					AltConf
48	8	1	Total	C	N	O	P	0
			37	25	1	10	1	

3 Residue-property plots

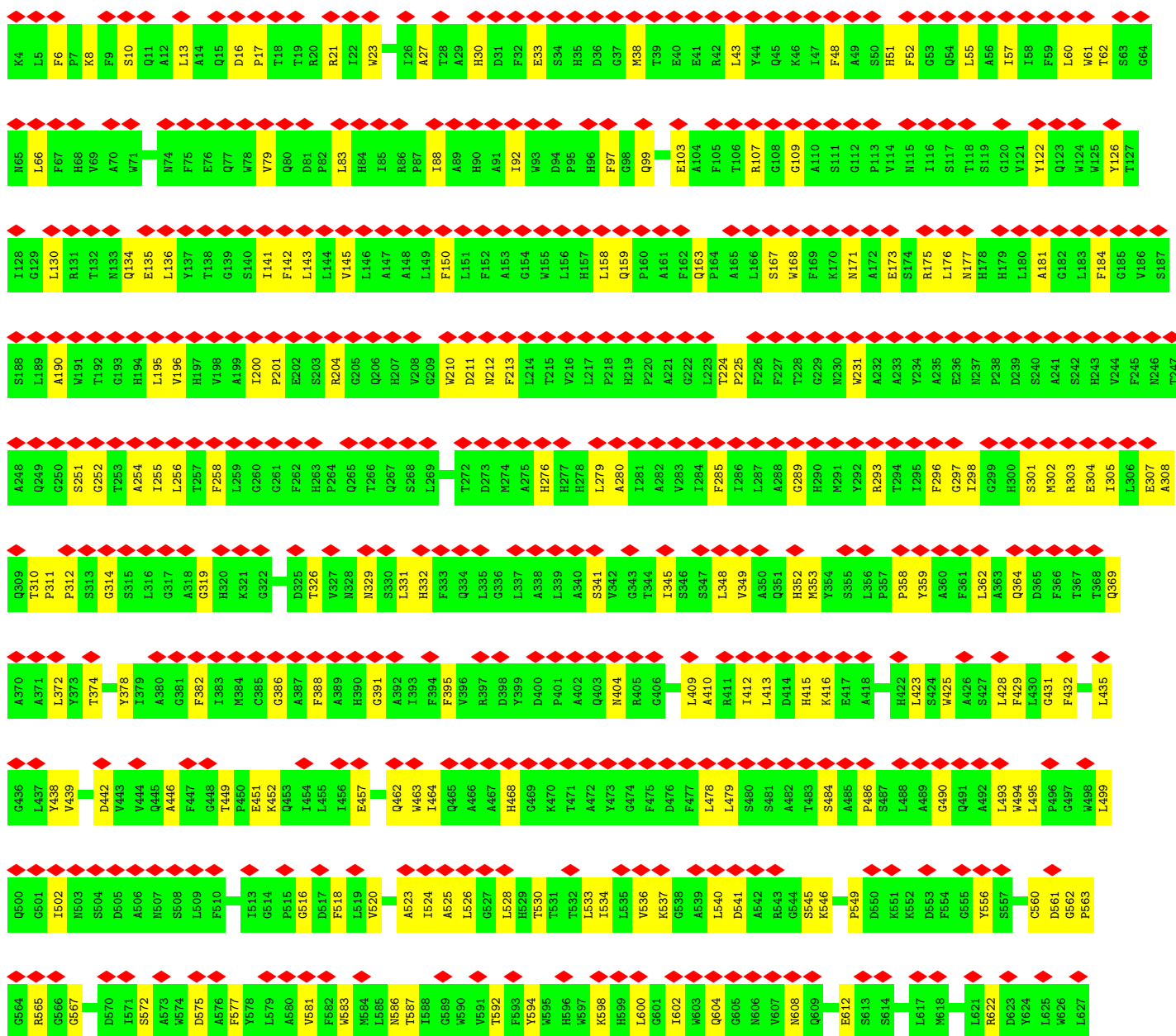
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

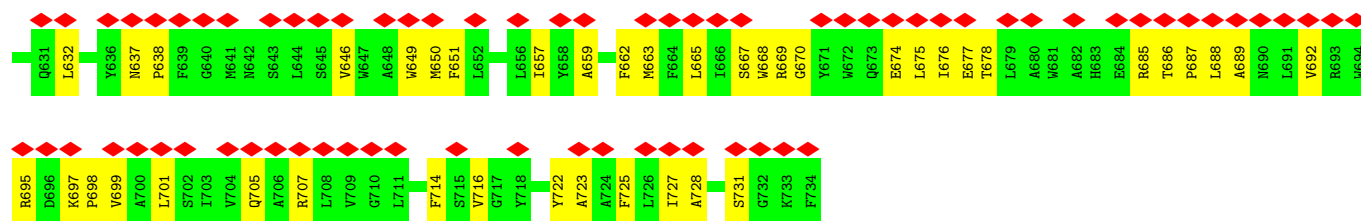
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



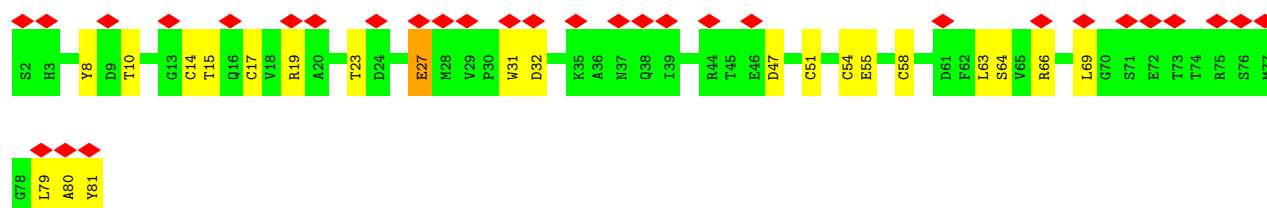
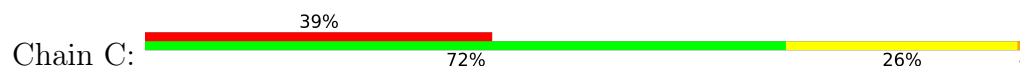


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

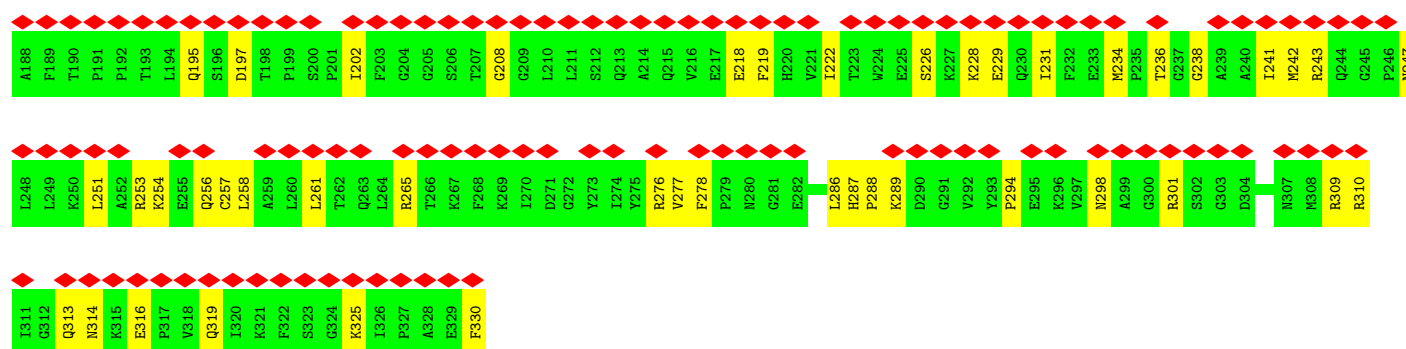
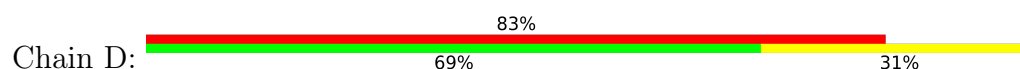




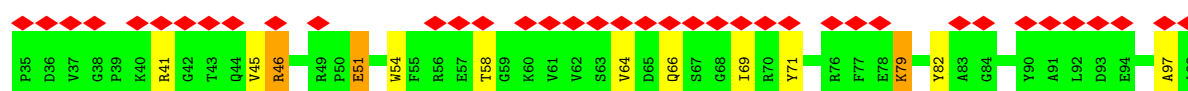
• Molecule 3: Photosystem I iron-sulfur center



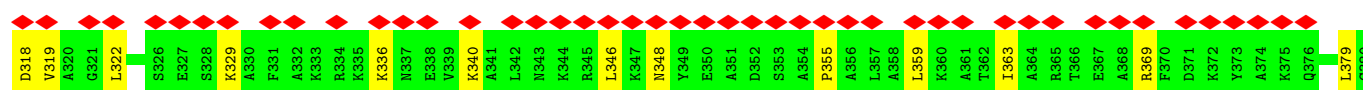
• Molecule 4: Photosystem I reaction center subunit chloroplastic

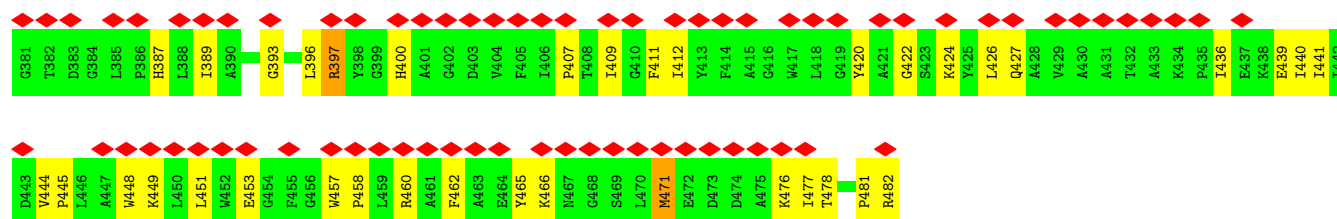


• Molecule 5: Photosystem I reaction center subunit IV

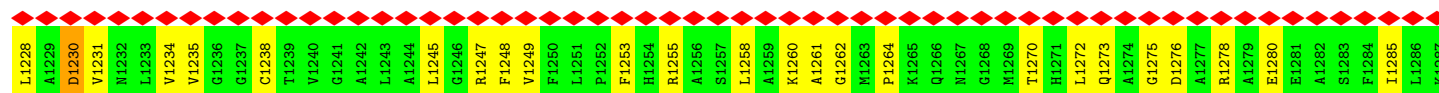


• Molecule 6: PSI-F

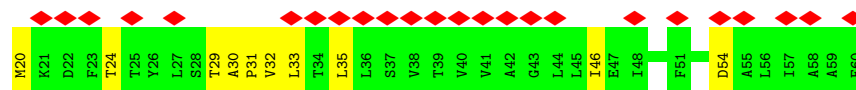
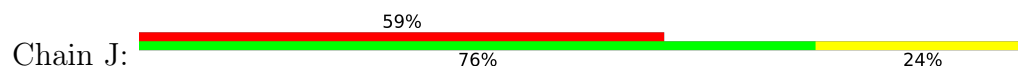




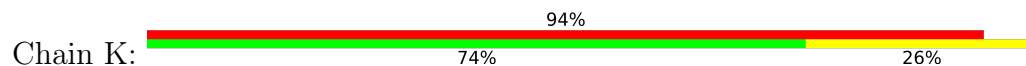
• Molecule 7: Photosystem I reaction center subunit chloroplastic



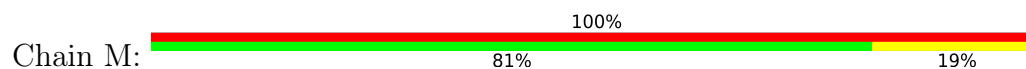
• Molecule 8: Photosystem I reaction center subunit IX



• Molecule 9: PSI-K



• Molecule 10: Photosystem I reaction center subunit XII

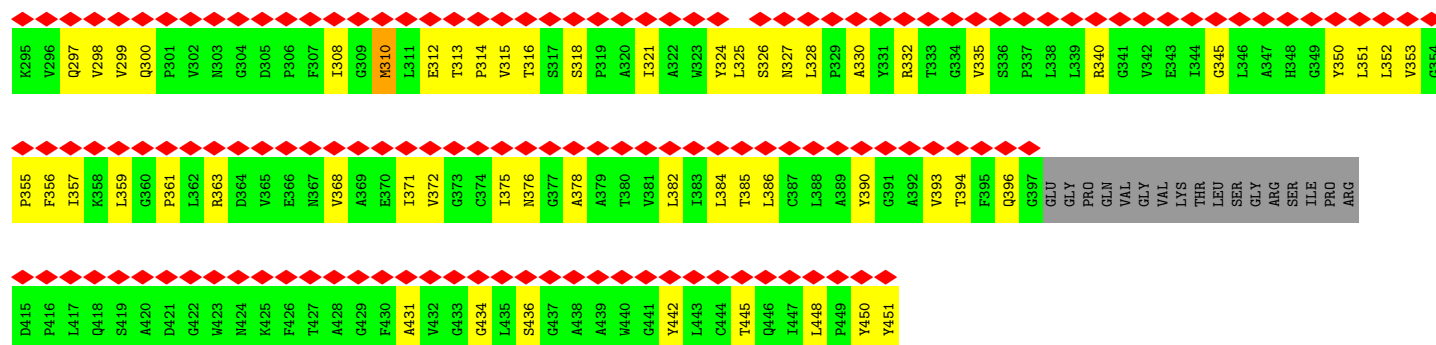
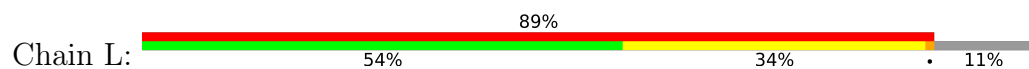


• Molecule 11: Photosystem I reaction center subunit VIII

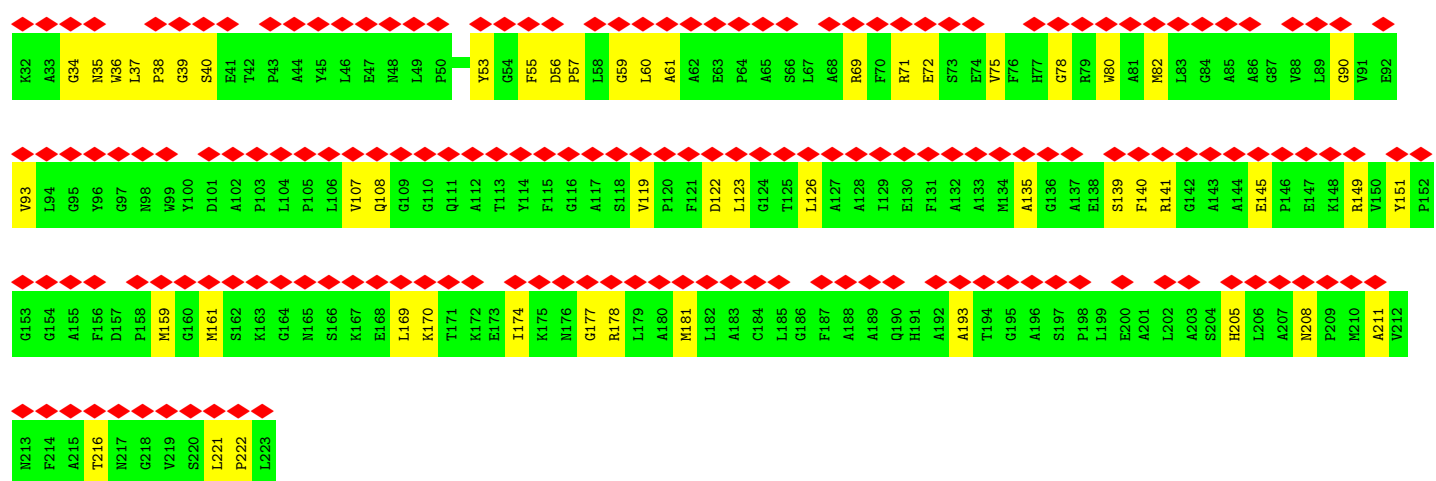
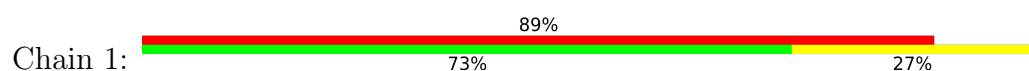




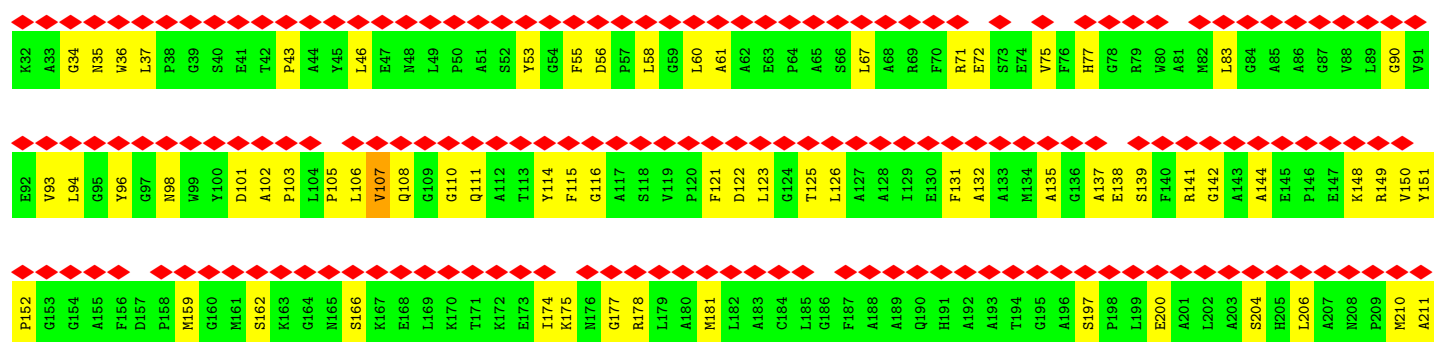
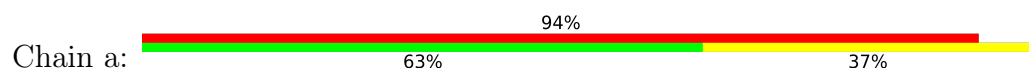
• Molecule 12: PSI subunit V

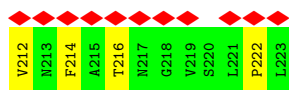


• Molecule 13: Chlorophyll a-b binding protein, chloroplastic

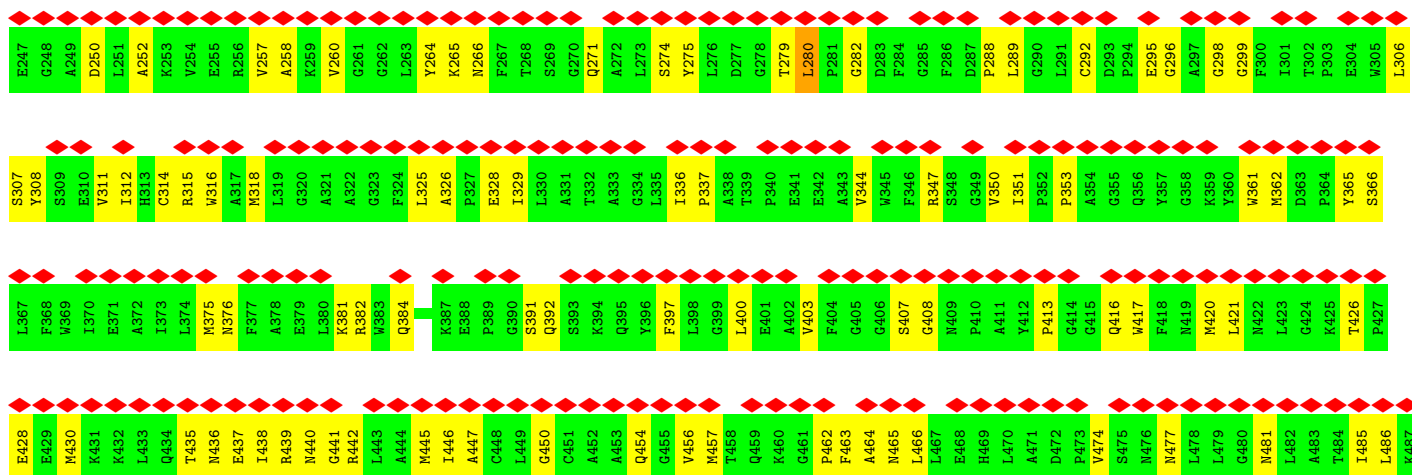
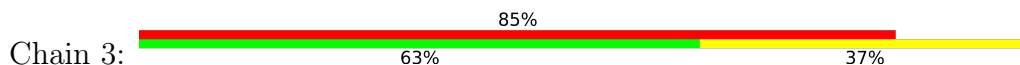


• Molecule 13: Chlorophyll a-b binding protein, chloroplastic

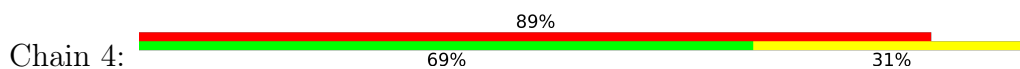




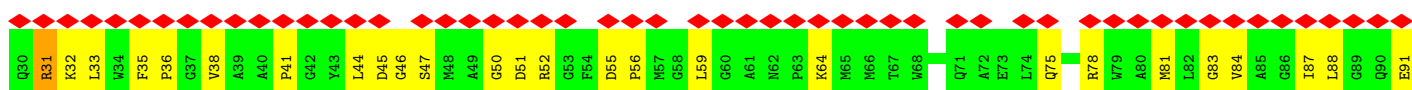
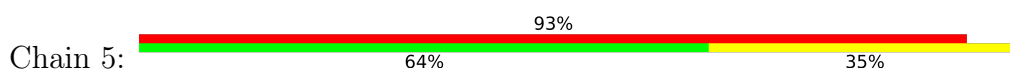
• Molecule 14: Glutathione reductase

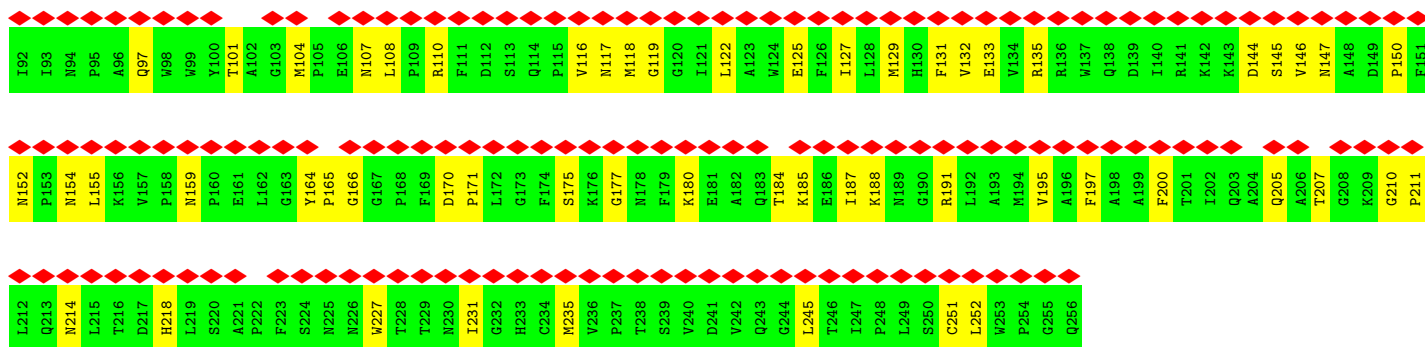


• Molecule 15: Chlorophyll a-b binding protein, chloroplastic



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

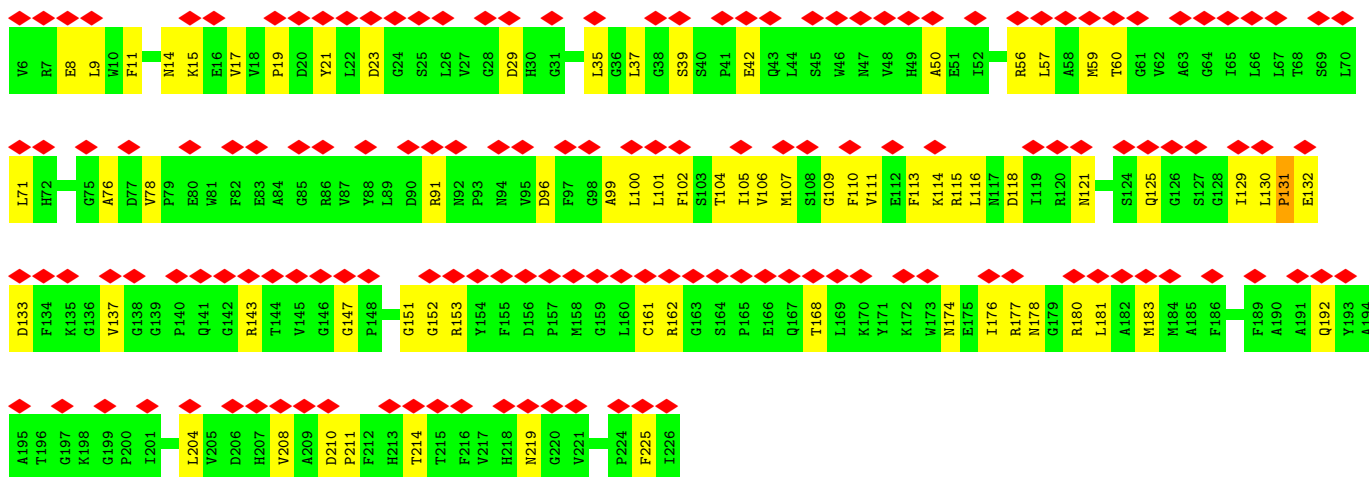




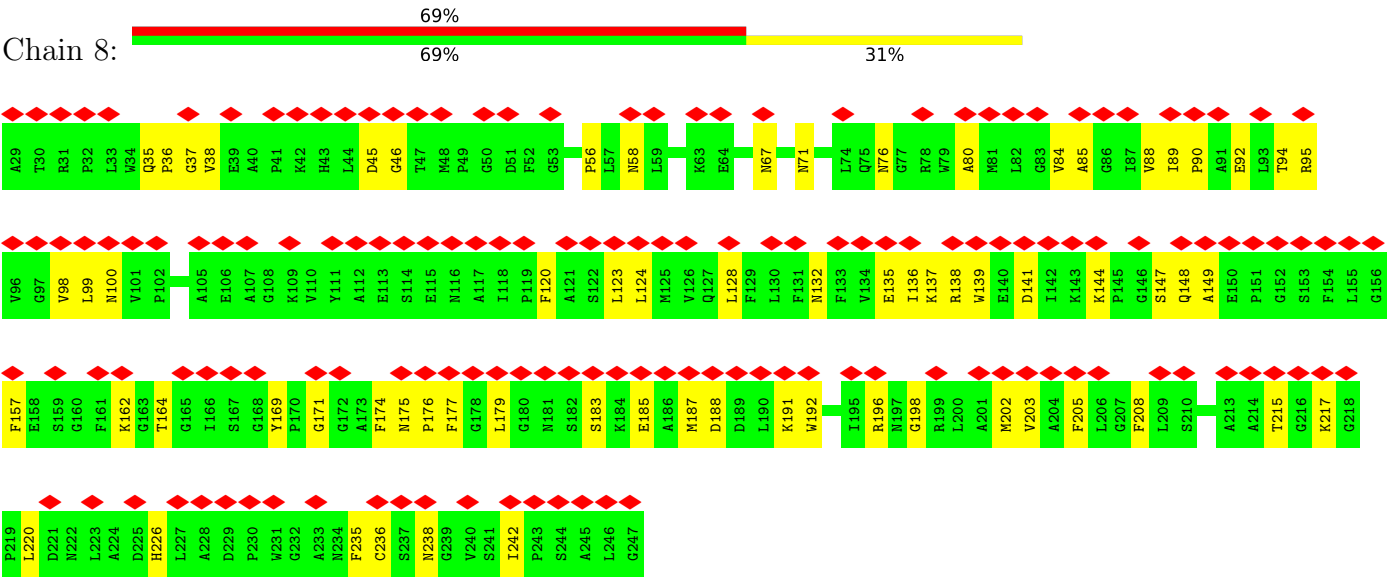
• Molecule 17: Chlorophyll a-b binding protein, chloroplastic



• 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 ($\text{\AA}$)	414.72, 414.72, 414.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.81, 0.81, 0.81	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.35	0/6022	0.44	3/8215 (0.0%)
2	B	0.35	0/6006	0.40	0/8205
3	C	0.36	0/611	0.56	1/828 (0.1%)
4	D	0.35	0/1150	0.50	0/1551
5	E	0.88	3/520 (0.6%)	0.65	4/705 (0.6%)
6	F	0.36	1/1309 (0.1%)	0.71	3/1771 (0.2%)
7	G	0.28	0/743	0.43	0/1007
8	J	0.44	0/322	0.66	0/439
9	K	0.24	0/622	0.39	0/844
10	M	0.24	0/244	0.32	0/330
11	I	0.27	0/276	0.46	0/373
12	L	0.30	0/1068	0.54	1/1462 (0.1%)
13	1	0.29	0/1443	0.45	1/1960 (0.1%)
13	a	0.29	0/1443	0.55	0/1960
14	3	0.29	0/1896	0.45	0/2573
15	4	0.29	0/1681	0.50	0/2285
16	5	0.27	0/1825	0.42	0/2483
17	6	0.31	0/1845	0.49	1/2515 (0.0%)
18	7	0.34	0/1748	0.42	0/2372
19	8	0.33	0/1717	0.45	0/2330
All	All	0.34	4/32491 (0.0%)	0.47	14/44208 (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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	79	LYS	CE-NZ	14.61	1.93	1.49
5	E	79	LYS	CB-CG	-7.54	1.29	1.52
6	F	471	MET	CB-CG	-6.19	1.33	1.52
5	E	51	GLU	CB-CG	-5.87	1.34	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	471	MET	CB-CG-SD	-18.14	58.27	112.70
1	A	714	GLN	CB-CA-C	-9.37	94.36	109.82
12	L	310	MET	CB-CG-SD	-8.75	86.44	112.70
17	6	200	MET	CA-CB-CG	-7.82	98.47	114.10
6	F	471	MET	CG-SD-CE	-7.31	84.81	100.90
1	A	374	MET	CG-SD-CE	-6.86	85.80	100.90
1	A	714	GLN	CA-CB-CG	6.63	127.36	114.10
3	C	27	GLU	CB-CG-CD	-6.18	102.09	112.60
13	1	221	LEU	CB-CG-CD1	-5.78	93.35	110.70
5	E	51	GLU	CG-CD-OE2	-5.37	106.06	118.40
5	E	79	LYS	CG-CD-CE	-5.10	99.57	111.30
5	E	79	LYS	N-CA-CB	-5.03	102.46	110.06
5	E	46	ARG	CB-CG-CD	5.01	122.83	111.30
6	F	397	ARG	N-CA-CB	5.00	117.87	110.56

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	241	0
2	B	5796	0	5576	245	0
3	C	601	0	576	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1124	0	1129	46	0
5	E	509	0	507	11	0
6	F	1277	0	1296	58	0
7	G	727	0	724	53	0
8	J	316	0	332	18	0
9	K	613	0	639	44	0
10	M	239	0	255	11	0
11	I	270	0	287	23	0
12	L	1041	0	1047	52	0
13	1	1405	0	1370	49	0
13	a	1405	0	1370	81	0
14	3	1844	0	1805	94	0
15	4	1631	0	1575	58	0
16	5	1769	0	1719	101	0
17	6	1787	0	1762	189	0
18	7	1698	0	1640	78	0
19	8	1669	0	1619	71	0
20	A	65	0	72	4	0
21	1	693	0	678	73	0
21	3	719	0	726	61	0
21	4	768	0	686	44	0
21	5	739	0	638	57	0
21	6	711	0	649	108	0
21	7	778	0	720	61	0
21	8	699	0	617	55	0
21	A	2621	0	2695	237	0
21	B	2583	0	2678	255	0
21	F	105	0	87	12	0
21	G	141	0	105	7	0
21	J	42	0	31	0	0
21	K	204	0	167	39	0
21	L	155	0	130	22	0
21	a	571	0	540	33	0
22	A	33	0	46	6	0
22	B	33	0	46	5	0
23	3	120	0	159	11	0
23	4	40	0	53	3	0
23	5	80	0	104	9	0
23	6	80	0	105	16	0
23	7	40	0	52	9	0
23	8	40	0	53	5	0
23	A	200	0	264	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	B	280	0	369	32	0
23	F	40	0	53	5	0
23	G	40	0	53	3	0
23	I	40	0	52	8	0
23	J	40	0	53	3	0
23	K	80	0	106	7	0
23	L	120	0	159	24	0
24	1	77	0	97	5	0
24	3	49	0	74	5	0
24	4	81	0	108	20	0
24	5	49	0	74	10	0
24	6	86	0	118	20	0
24	7	128	0	175	12	0
24	8	37	0	44	5	0
24	A	120	0	159	16	0
24	B	95	0	139	9	0
24	F	79	0	101	7	0
24	a	35	0	40	2	0
25	8	66	0	96	13	0
25	A	51	0	60	3	0
25	B	66	0	96	10	0
26	A	33	0	39	1	0
27	A	8	0	0	0	0
27	C	16	0	0	2	0
28	1	35	0	45	9	0
28	A	35	0	46	4	0
28	B	35	0	44	2	0
29	6	36	0	44	3	0
29	B	30	0	34	6	0
30	3	38	0	49	5	0
30	5	38	0	49	2	0
30	7	33	0	39	3	0
30	8	35	0	43	6	0
30	B	41	0	55	4	0
31	B	29	0	42	3	0
31	F	29	0	42	6	0
31	K	29	0	42	3	0
32	7	39	0	41	1	0
32	G	46	0	55	4	0
33	G	29	0	38	16	0
34	J	41	0	56	10	0
35	J	17	0	14	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	a	30	0	43	12	0
36	M	41	0	54	6	0
37	1	126	0	165	16	0
37	3	84	0	110	9	0
37	4	84	0	110	9	0
37	5	126	0	165	20	0
37	6	84	0	110	29	0
37	7	42	0	55	4	0
37	8	84	0	110	17	0
37	a	126	0	165	14	0
38	1	114	0	102	13	0
38	3	98	0	73	8	0
38	4	174	0	154	21	0
38	5	173	0	153	16	0
38	6	224	0	188	52	0
38	7	66	0	70	5	0
38	8	174	0	153	20	0
38	a	203	0	148	26	0
39	1	20	0	33	2	0
39	8	20	0	33	4	0
40	3	19	0	0	0	0
40	a	19	0	0	1	0
41	a	9	0	0	1	0
42	4	17	0	31	1	0
42	6	18	0	31	1	0
43	5	23	0	28	3	0
43	8	30	0	42	5	0
44	6	21	0	37	7	0
45	7	44	0	56	5	0
46	7	32	0	39	6	0
46	8	96	0	142	15	0
47	7	42	0	0	3	0
48	8	37	0	40	1	0
All	All	48636	0	48687	2256	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 23.

All (2256) 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)
33:G:5002:ERG:O1	33:G:5002:ERG:C3	1.70	1.40
5:E:79:LYS:NZ	5:E:79:LYS:CE	1.93	1.29
21:B:1201:CLA:H72	11:I:29:TYR:CE2	1.77	1.17
17:6:135:ARG:NE	38:6:611:CHL:OMC	1.78	1.14
7:G:1317:SER:HA	33:G:5002:ERG:H7	1.13	1.11
21:B:1204:CLA:H12	11:I:14:VAL:HG21	1.35	1.09
21:B:1204:CLA:H61	23:I:4001:BCR:HC31	1.37	1.06
16:5:32:LYS:HZ2	21:5:609:CLA:H2A	1.18	1.03
29:B:5004:PCW:H322	23:F:4001:BCR:H351	1.41	1.01
17:6:131:TRP:HE1	38:6:611:CHL:CBB	1.73	1.00
2:B:412:ILE:HD13	23:B:4004:BCR:H402	1.41	1.00
1:A:442:ASN:HD22	2:B:675:LEU:HD11	1.26	0.99
11:I:30:ILE:HD13	23:L:4001:BCR:C33	1.95	0.97
21:B:1228:CLA:H2	23:F:4001:BCR:H353	1.48	0.96
7:G:1317:SER:HA	33:G:5002:ERG:C7	1.96	0.94
18:7:11:PHE:CE2	18:7:14:ASN:HB2	2.01	0.94
21:B:1218:CLA:HMD2	23:B:4001:BCR:HC7	1.50	0.93
17:6:152:PHE:CZ	21:6:617: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	21:6:609:CLA:HED2	1.99	0.92
21:B:1201:CLA:H93	11:I:26:MET:HE1	1.51	0.92
17:6:131:TRP:HE1	38:6:611:CHL:HBB2	1.34	0.91
33:G:5002:ERG:H122	13:1:123:LEU:HD23	1.53	0.91
21:8:610:CLA:H12	46:8:808:4RF:H29	1.53	0.91
7:G:1253:PHE:CZ	28:1:804:LMT:H2'	2.06	0.90
7:G:1317:SER:CA	33:G:5002:ERG:H7	2.01	0.90
21:B:1208:CLA:HAA1	7:G:1278:ARG:NH2	1.88	0.89
17:6:169:PHE:HD1	38:6:611: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	21:A:1126:CLA:HAB	2.08	0.88
13:1:35:ASN:O	13:1:37:LEU:N	2.07	0.88
16:5:64:LYS:HE2	43:5:803:DGA:HG2	1.57	0.87
12:L:357:ILE:HG13	12:L:372:VAL:HG11	1.55	0.87
24:4:801:LHG:HC92	23:6:503:BCR:HC22	1.54	0.87
1:A:673:LEU:HB3	21:A:1012:CLA:H2	1.56	0.87
18:7:11:PHE:HE2	18:7:14:ASN:HB2	1.39	0.86
21:A:1131:CLA:HBB1	21:A:1132:CLA:H2	1.55	0.86
17:6:58:TYR:CD1	21:6:609:CLA:HBC2	2.10	0.86
17:6:164:TYR:O	21:6:601:CLA:HED2	1.74	0.86
18:7:113:PHE:HD2	21:8:609:CLA:HAA2	1.40	0.86
11:I:30:ILE:HD13	23:L:4001:BCR:H332	1.55	0.86
1:A:577:GLY:HA2	2:B:563:PRO:HD3	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:3:314:CYS:HB2	14:3:441:GLY:HA3	1.57	0.85
21:B:1240:CLA:H11	24:B:5001:LHG:H242	1.57	0.85
37:4:501:LUT:H32	21:4:601:CLA:HAB	1.57	0.85
1:A:578:PRO:HD3	2:B:562:GLY:HA2	1.57	0.85
21:A:1130:CLA:H102	21:L:1502:CLA:H92	1.57	0.85
17:6:40:LEU:HD12	21:6:609:CLA:HED2	1.58	0.84
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
21:B:1227:CLA:H12	24:B:5001:LHG:H252	1.59	0.83
17:6:128:VAL:CG1	23:6:503:BCR:H17C	2.08	0.83
21:B:1220:CLA:HBA1	23:B:4004:BCR:H16C	1.60	0.83
21:B:1205:CLA:HAB	21:B:1206:CLA:HBA1	1.61	0.83
17:6:165:PRO:HD2	21:6:601:CLA:CAD	2.09	0.83
1:A:45:THR:HG22	1:A:714:GLN:HG2	1.59	0.82
21:4:607:CLA:H11	21:4:607:CLA:H3A	1.59	0.82
21: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
30:7:804:PTY:H351	25:8:802:DGD:HAV2	1.62	0.82
1:A:363:LEU:HD11	21:A:1117:CLA:H72	1.62	0.82
1:A:707:LEU:HD13	23:F:4001:BCR:H321	1.61	0.82
6:F:336:LYS:O	6:F:340:LYS:HG2	1.80	0.82
28:1:804:LMT:H22	21:1:612:CLA:O1A	1.78	0.82
2:B:196:VAL:HG21	21:B:1212:CLA:HBC3	1.59	0.81
16:5:32:LYS:HZ2	21:5:609:CLA:C2A	1.92	0.81
21:B:1218:CLA:HED1	7:G:1258:LEU:HA	1.61	0.81
16:5:64:LYS:NZ	43:5:803:DGA:OA1	2.12	0.81
1:A:657:VAL:HG22	1:A:745:ALA:HB3	1.61	0.81
2:B:57:ILE:HD11	36:M:4001:ECH:H39A	1.60	0.81
21:B:1237:CLA:H151	23:L:4002:BCR:H17C	1.63	0.81
21:B:1204:CLA:H102	23:I:4001:BCR:HC21	1.63	0.81
11:I:26:MET:HG3	23:L:4001:BCR:H312	1.63	0.81
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	21:6:601:CLA:OBD	1.82	0.80
21:B:1238:CLA:O1A	23:L:4001:BCR:H351	1.82	0.79
21:B:1207:CLA:HBA2	12:L:361:PRO:HG3	1.65	0.79
14:3:420:MET:HE3	16:5:56:PRO:CB	2.12	0.79
13:a:75:VAL:HG22	13:a:174:ILE:HD11	1.64	0.79
13:a:58:LEU:HD12	37:a:502:LUT:H222	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:1234:CLA:HBA2	21:B:1235:CLA:HAA2	1.65	0.78
9:K:58:PRO:HD3	21:K:1403:CLA:CHB	2.13	0.78
15:4:234:THR:HG23	23:6:504:BCR:H332	1.66	0.78
15:4:234:THR:CG2	23:6:504:BCR:H332	2.13	0.78
14:3:376:ASN:ND2	21:7:609: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	38:6:611:CHL:C2D	2.13	0.78
13:a:98:ASN:OD1	13:a:197:SER:OG	2.01	0.78
13:1:178:ARG:HB3	21:1:604:CLA:HBC3	1.64	0.78
38:1:609:CHL:HED1	19:8:136:ILE:HG22	1.65	0.78
21:5:617:CLA:HED2	21:5:617:CLA:HAA2	1.65	0.78
1:A:369:HIS:CD2	21:A:1124:CLA:HED2	2.19	0.78
28:B:5006:LMT:O4'	7:G:1260:LYS:HG2	1.84	0.77
16:5:75:GLN:NE2	38:5:611: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	23:6:503:BCR:H17C	1.65	0.77
24:4:802:LHG:H102	21:6:618:CLA:HBA1	1.66	0.77
23:6:503:BCR:H16C	38:6:613:CHL:H43	1.66	0.77
17:6:75:PHE:C	21:6:604:CLA:HMA1	2.10	0.77
15:4:78:ARG:HA	15:4:81:MET:HE2	1.67	0.76
17:6:136:ARG:HG3	38:6:611:CHL:C1D	2.15	0.76
1:A:561:ARG:NH2	4:D:208:GLY:HA2	2.01	0.76
21:A:1130:CLA:H11	21: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	21:B:1236:CLA:HED1	1.65	0.76
14:3:439:ARG:NH1	21:3:607: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	34:J:4002:RRX:H1	1.67	0.76
14:3:420:MET:HE3	16:5:56:PRO:HB2	1.68	0.76
17:6:186:LYS:CB	21:6:607:CLA:HMD1	2.16	0.76
7:G:1323:ARG:NH1	21:G:1603:CLA:OBD	2.19	0.75
17:6:164:TYR:HB3	21:6:601: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
13:a:138:GLU:OE1	13:a:141:ARG:HD3	1.87	0.75
17:6:184:GLU:HB2	21:6:601:CLA:C2B	2.17	0.75
2:B:173:GLU:OE2	7:G:1264:PRO:HB3	1.87	0.75
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	21:L:1502:CLA:O1A	2.04	0.75
37:5:505:LUT:H173	21:7:608:CLA:HAB	1.66	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:1236:CLA:HHC	21:B:1236:CLA:HBB1	1.70	0.74
21:A:1101:CLA:HBB1	21:A:1101:CLA:HHC	1.70	0.74
17:6:87:MET:SD	21:6:601:CLA:HAB	2.27	0.74
25:8:802:DGD:HBN2	21:8:609:CLA:H141	1.68	0.74
9:K:58:PRO:CD	21:K:1403:CLA:CHB	2.65	0.74
1:A:121:ILE:HD13	34:J:4002:RRX:H18	1.70	0.74
21: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
15:4:109:ASP:OD1	15:4:112:ASN:ND2	2.21	0.73
12:L:357:ILE:HA	12:L:372:VAL:HG21	1.71	0.73
16:5:32:LYS:NZ	21:5:609:CLA:H2A	2.02	0.73
16:5:117:ASN:HD22	17:6:222:GLY:HA2	1.52	0.73
21:1:603:CLA:HBB1	21:1:603:CLA:H91	1.70	0.73
9:K:107:ILE:HG12	21:K:1402:CLA:CBB	2.18	0.72
13:1:178:ARG:HA	13:1:181:MET:HE2	1.71	0.72
13:a:35:ASN:ND2	13:a:35:ASN:O	2.19	0.72
14:3:329:ILE:HG21	23:3:504:BCR:H272	1.71	0.72
21:3:618:CLA:HHC	21:3:618:CLA:HBB1	1.71	0.72
6:F:444:VAL:HG11	35:J:5001:LPX:H7A	1.70	0.72
16:5:145:SER:OG	17:6:42:GLY:O	2.05	0.72
21:1:602:CLA:HMD2	21:1:607:CLA:H43	1.72	0.72
17:6:183:LYS:HD3	21:6:602:CLA:HBD	1.71	0.72
21:B:1201:CLA:H43	21:B:1201:CLA:H121	1.71	0.72
38:a:613:CHL:HBB1	38:a:613:CHL:HHC	1.72	0.72
15:4:125:ILE:HG22	15:4:129:MET:HE2	1.70	0.72
19:8:187:MET:HG3	19:8:191:LYS:HE3	1.72	0.72
21:7:610:CLA:H91	24:7:803: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
21:A:1109:CLA:HBA1	21:A:1109:CLA:CHA	2.21	0.71
13:1:169:LEU:HB3	21:1:601:CLA:HMA2	1.72	0.71
16:5:56:PRO:HD2	37:5:502:LUT:H23	1.72	0.71
17:6:194:ALA:HB1	37:6:501:LUT:H7	1.71	0.71
1:A:575:CYS:SG	2:B:563:PRO:HB3	2.30	0.71
21:A:1103:CLA:H11	21:A:1104:CLA:HBB1	1.71	0.71
38:4:609:CHL:HHB	38:4:609:CHL:HBC3	1.71	0.71
1:A:190:TRP:CZ2	21:A:1108:CLA:HMA1	2.26	0.71
21:A:1107:CLA:H43	23:J:4001:BCR:H10C	1.73	0.71
21:A:1114:CLA:H93	21:3:610:CLA:HMC1	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1138:CLA:HBB2	6:F:422:GLY:HA3	1.73	0.71
7:G:1255:ARG:NH2	7:G:1293:GLY:O	2.24	0.71
2:B:177:ASN:HB3	21:B:1217:CLA:HMD2	1.73	0.70
21:B:1218:CLA:CED	7:G:1258:LEU:HD23	2.21	0.70
2:B:258:PHE:HE2	2:B:494:TRP:CE3	2.07	0.70
37:8:501:LUT:H373	38:8:601:CHL:H51	1.73	0.70
21:A:1109:CLA:H201	34:J:4002:RRX:H43	1.72	0.70
21:3:603:CLA:H172	24:3:801:LHG:H322	1.72	0.70
21:3:616:CLA:HHC	21:3:616:CLA:HBB1	1.73	0.70
21:5:607:CLA:HBB1	21:5:607:CLA:HHC	1.72	0.70
17:6:131:TRP:NE1	38:6:611:CHL:CBB	2.52	0.70
1:A:178:TRP:CZ2	30:3:802: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
21:A:1013:CLA:HBA2	2:B:428:LEU:HD23	1.74	0.70
21:B:1217:CLA:HBB1	21: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	21:A:1103:CLA:OBD	2.20	0.70
24:4:801:LHG:H222	21:6:618:CLA:HMC3	1.72	0.70
21:A:1012:CLA:H43	2:B:439:VAL:HG22	1.74	0.69
28:1:804:LMT:H82	21:1:605:CLA:HMD2	1.74	0.69
14:3:381:LYS:HD2	38:3:611:CHL:HBB1	1.73	0.69
16:5:97:GLN:HE22	16:5:107:ASN:HD22	1.38	0.69
17:6:186:LYS:HB2	21:6:607:CLA:HMD1	1.74	0.69
2:B:378:TYR:CD2	21:B:1224:CLA:HAB	2.28	0.69
2:B:688:LEU:HB3	23:L:4002:BCR:HC31	1.73	0.69
17:6:265:PRO:HD2	21:6:615:CLA:HED2	1.74	0.69
21:B:1213:CLA:H92	23: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	37:3:502:LUT:H222	1.74	0.69
23:3:504:BCR:C10	38:3:611:CHL:HBA1	2.23	0.69
24:4:801:LHG:C9	23:6:503:BCR:HC22	2.22	0.69
16:5:78:ARG:NH1	38:5:611:CHL:OBD	2.25	0.69
1:A:265:PHE:HD2	31: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	24:6:801:LHG:H302	1.72	0.69
21:1:602:CLA:HBB1	21:1:602:CLA:HHC	1.74	0.69
18:7:11:PHE:CD2	18:7:14:ASN:HB2	2.27	0.69
21:7:617:CLA:HHC	21:7:617:CLA:HBB1	1.74	0.69
11:I:26:MET:HE2	23:L:4001:BCR:HC32	1.75	0.68
16:5:146:VAL:HG13	17:6:42:GLY:HA3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:6:801:LHG:H121	24:6:801:LHG:H312	1.76	0.68
2:B:598:LYS:O	2:B:602:ILE:HG12	1.94	0.68
13:a:36:TRP:HE1	38:a:609:CHL:C2B	2.07	0.68
37:5:502:LUT:H31	21:5:604:CLA:H161	1.75	0.68
23:7:503:BCR:HC31	24:8:801:LHG:HC81	1.75	0.68
21:B:1209:CLA:HBB2	21: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
30:8:810:PTY:HN11	30:8:810:PTY:HC51	1.57	0.68
2:B:258:PHE:CE2	2:B:494:TRP:CE3	2.81	0.68
21:B:1207:CLA:H112	12:L:378:ALA:HB2	1.75	0.68
38:a:606:CHL:H43	38:a:613:CHL:HBD	1.76	0.68
23:3:504:BCR:H10C	38:3:611:CHL:HBA1	1.74	0.68
17:6:186:LYS:NZ	21:6:607:CLA:O1D	2.22	0.68
19:8:128:LEU:HD13	21:8:618:CLA:HAB	1.74	0.68
12:L:326:SER:O	12:L:332:ARG:NH1	2.27	0.68
13:a:139:SER:O	35:a:804:LPX:H3	1.94	0.68
17:6:164:TYR:HB3	21:6:601:CLA:O1D	1.94	0.68
17:6:186:LYS:NZ	24:6:801:LHG:O5	2.26	0.68
17:6:186:LYS:HG3	21:6:607:CLA:O1D	1.94	0.68
1:A:439:SER:OG	2:B:678:THR:HG22	1.94	0.67
21:1:607:CLA:H51	21:1:607:CLA:H92	1.76	0.67
15:4:192:LEU:HD11	24:4:801:LHG:H282	1.75	0.67
21:B:1201:CLA:HBA2	10:M:30:TYR:HD1	1.58	0.67
17:6:135:ARG:HB3	38:6:611:CHL:CMC	2.23	0.67
17:6:184:GLU:HB2	21:6:601:CLA:CMB	2.24	0.67
38:7:613:CHL:HHC	38:7:613:CHL:HBB1	1.76	0.67
13:1:222:PRO:HG2	21:1:615:CLA:HBB1	1.76	0.67
21:a:605:CLA:H51	23:8:503:BCR:H341	1.75	0.67
17:6:229:ALA:HB2	17:6:239:PRO:HD3	1.77	0.67
1:A:318:ILE:HG13	21:A:1118:CLA:HED1	1.77	0.67
21:A:1106:CLA:HBB2	21:A:1126:CLA:H171	1.75	0.67
1:A:245:LEU:HD11	21:A:1114:CLA:HAC2	1.76	0.67
34:J:4002:RRX:H46	34:J:4002:RRX:H51	1.76	0.67
15:4:45:ARG:HG3	15:4:48:LEU:HD13	1.77	0.67
21:5:618:CLA:HBB1	21:5:618:CLA:HHC	1.77	0.67
2:B:258:PHE:CE2	2:B:494:TRP:HB3	2.30	0.67
21:B:1204:CLA:C1	11:I:14:VAL:HG21	2.21	0.67
14:3:457:MET:HE1	14:3:485:ILE:HG22	1.75	0.67
14:3:481:ASN:HD21	21:3:603:CLA:HED2	1.58	0.67
12:L:335:VAL:HB	12:L:340:ARG:HD2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:181:MET:SD	21:a:604:CLA:HBB1	2.35	0.67
16:5:227:TRP:NE1	21:5:608:CLA:O1D	2.26	0.67
45:7:502:XAT:C33	21:7:605:CLA:HAB	2.25	0.67
19:8:124:LEU:HD21	39:8:809:OLA:H141	1.77	0.67
21:A:1116:CLA:H111	21:A:1134:CLA:HBA1	1.75	0.66
19:8:120:PHE:CZ	46:8:808:4RF:H41	2.30	0.66
46:8:808:4RF:H42	46:8:808:4RF:H69	1.76	0.66
17:6:125:GLU:OE1	38:6:613:CHL:CHB	2.43	0.66
24:5:801:LHG:H121	24:5:801:LHG:H241	1.75	0.66
14:3:417:TRP:O	14:3:420:MET:HG3	1.94	0.66
23:7:503:BCR:H333	21:8:607:CLA:HAB	1.78	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
37:5:501:LUT:H371	21:5:601:CLA:H92	1.78	0.66
1:A:587:SER:OG	1:A:590:ASP:OD2	2.12	0.66
21:A:1136:CLA:H102	21:A:1136:CLA:HBB1	1.78	0.66
2:B:175:ARG:HB2	21: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
21:A:1104:CLA:H92	24:A:5002:LHG:H352	1.78	0.66
21:F:1301:CLA:HBB1	21: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	33:G:5002:ERG:H181	1.78	0.66
22:A:2001:PQN:H162	23:B:4006:BCR:H382	1.77	0.65
16:5:131:PHE:HB2	21:6:609:CLA:H42	1.78	0.65
9:K:102:ILE:HG22	21:K:1402:CLA:HBC1	1.77	0.65
2:B:143:LEU:HD21	23:B:4003:BCR:H23C	1.77	0.65
21:B:1231:CLA:HBC1	24:1:802:LHG:H211	1.78	0.65
43:8:803:DGA:HB81	43:8:803:DGA:HA32	1.78	0.65
21:A:1012:CLA:H201	21:A:1106:CLA:H122	1.78	0.65
23:3:504:BCR:H363	21:3:601:CLA:H121	1.78	0.65
18:7:125:GLN:NE2	19:8:36:PRO:O	2.27	0.65
28:1:804:LMT:H5'	21:1:612:CLA:HMA3	1.79	0.65
1:A:712:ALA:N	6:F:439:GLU:OE2	2.29	0.65
18:7:100:LEU:HG	21:7:610: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	21: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
21:1:607:CLA:HBA1	40:a:504:QTB:C09	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:4:609:CHL:H161	21:4:608:CLA:H2	1.78	0.64
38:5:610:CHL:HBB1	38:5:610:CHL:HHC	1.78	0.64
4:D:234:MET:HE2	4:D:236:THR:OG1	1.97	0.64
33:G:5002:ERG:O1	33:G:5002:ERG:C2	2.41	0.64
11:I:23:MET:HG2	23:L:4001:BCR:H10C	1.80	0.64
34:J:4002:RRX:H17	34:J:4002:RRX:H21	1.80	0.64
9:K:56:LEU:HD23	21:K:1403:CLA:HHD	1.80	0.64
17:6:80:ARG:HH11	17:6:163:GLY:HA3	1.61	0.64
1:A:199:ASN:HB3	21:A:1118:CLA:HMD1	1.80	0.64
7:G:1234:VAL:HG21	7:G:1314:LEU:HD21	1.79	0.64
17:6:164:TYR:C	21:6:601:CLA:HED2	2.22	0.64
46:8:808:4RF:H50	39:8:809:OLA:H152	1.79	0.64
21:A:1125:CLA:HBB1	21: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	21:6:601:CLA:O1D	1.96	0.64
18:7:111:VAL:CG1	23:7:503:BCR:H16C	2.28	0.64
21:B:1220:CLA:HAB	21:B:1227:CLA:HMD1	1.77	0.64
1:A:369:HIS:NE2	21:A:1124:CLA:OBD	2.30	0.64
2:B:464:ILE:HD12	21:B:1234:CLA:O1A	1.97	0.64
2:B:646:VAL:HG21	21:B:1205:CLA:HAC1	1.79	0.64
37:1:501:LUT:H27	21:1:611:CLA:H42	1.80	0.64
16:5:135:ARG:NH1	21:6:609:CLA:OBD	2.31	0.64
6:F:336:LYS:HG3	6:F:340:LYS:HE3	1.79	0.64
17:6:39:TRP:CE3	17:6:40:LEU:HB2	2.33	0.64
16:5:150:PRO:HD3	21:5:618:CLA:HMC2	1.80	0.64
2:B:296:PHE:C	7:G:1285:ILE:HD13	2.23	0.63
1:A:72:LYS:HD3	21:A:1109:CLA:OBD	1.99	0.63
2:B:518:PHE:HA	21:B:1235:CLA:HED1	1.79	0.63
13:a:108:GLN:NE2	13:a:110:GLY:O	2.31	0.63
21:4:616:CLA:HBD	21:4:616:CLA:H2	1.79	0.63
14:3:420:MET:O	16:5:38:VAL:HG23	1.98	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	36:M:4001:ECH:H37A	2.28	0.63
16:5:32:LYS:NZ	21:5:609:CLA:C2A	2.61	0.63
16:5:59:LEU:HD13	21:5:604:CLA:H42	1.79	0.63
18:7:29:ASP:HA	21:7:604:CLA:O1D	1.98	0.63
38:4:618:CHL:HBB1	38:4:618:CHL:HHC	1.81	0.63
17:6:190:LEU:HG	37:6:501:LUT:H191	1.81	0.63
21:A:1102:CLA:HBA2	21:A:1109:CLA:H61	1.80	0.63
28:1:804:LMT:H82	21:1:605:CLA:CMD	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:139:SER:OG	35:a:804:LPX:H5	1.98	0.63
16:5:47:SER:O	16:5:180:LYS:NZ	2.31	0.63
21:A:1137:CLA:H43	23:A:4004:BCR:H19C	1.80	0.63
2:B:33:GLU:OE1	2:B:332:HIS:NE2	2.21	0.63
46:8:808:4RF:H77	46:8:808:4RF:H12	1.81	0.63
37:5:505:LUT:H371	37:5:505:LUT:H28	1.81	0.63
2:B:99:GLN:O	2:B:103:GLU:HG3	1.99	0.62
21: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
28:1:804:LMT:H61	21:1:612: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	43:8:803:DGA:HB72	2.34	0.62
21:4:610:CLA:HBA1	21:4:612:CLA:HBC3	1.81	0.62
21:A:1013:CLA:H101	23:A:4005:BCR:H23C	1.81	0.62
14:3:306:LEU:HB3	21:3:604:CLA:HMA2	1.79	0.62
37:4:502:LUT:H28	21:4:604:CLA:H52	1.80	0.62
17:6:80:ARG:NH1	17:6:163:GLY:HA3	2.14	0.62
21:6:604:CLA:HBC2	21:6:609:CLA:HBB2	1.79	0.62
19:8:135:GLU:OE1	19:8:138:ARG:NH2	2.21	0.62
21:A:1108:CLA:HHC	21:A:1108:CLA:HBB1	1.81	0.62
2:B:659:ALA:C	21:B:1023:CLA:HAB	2.24	0.62
18:7:101:LEU:HD21	24:7:803:LHG:H192	1.81	0.62
9:K:58:PRO:HD2	21:K:1403:CLA:C1B	2.29	0.62
38:a:609:CHL:HHC	38:a:609:CHL:HBB1	1.81	0.62
24:a:801:LHG:H322	42:4:803:PLM:HG1	1.82	0.62
17:6:150:PRO:HD3	21:6:617:CLA:HMC2	1.81	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	21:7:611:CLA:HAC2	1.82	0.62
1:A:45:THR:HG22	1:A:714:GLN:CG	2.30	0.62
5:E:45:VAL:HG12	5:E:97:ALA:HA	1.81	0.62
13:1:61:ALA:HB2	21:1:604:CLA:HBA1	1.82	0.62
17:6:182:VAL:CG1	21:6:607: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
38:3:608:CHL:HHC	38:3:608:CHL:HBB1	1.81	0.62
38:4:609:CHL:HHC	38:4:609:CHL:HBB1	1.80	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
9:K:51:ALA:HB2	21:K:1403:CLA:HBC2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
14:3:457:MET:HG2	21:3:603:CLA:HMD1	1.82	0.61
17:6:164:TYR:CA	21:6:601:CLA:O1D	2.48	0.61
21:8:605:CLA:HHC	21:8:605:CLA:HBB1	1.81	0.61
12:L:351:LEU:HD21	21:L:1502:CLA:HMB2	1.82	0.61
15:4:39:PRO:HG3	15:4:55:ASP:HB3	1.81	0.61
17:6:164:TYR:CB	21:6:601:CLA:O1D	2.48	0.61
1:A:279:GLN:HG2	1:A:503:LEU:HD12	1.82	0.61
21:A:1138:CLA:H2	21: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
21:A:1118:CLA:H51	14:3:288:PRO:HG3	1.82	0.61
21:A:1130:CLA:C3	21:L:1502:CLA:H8	2.30	0.61
12:L:363:ARG:HA	12:L:368:VAL:HG21	1.82	0.61
38:a:606:CHL:HMA1	38:a:613:CHL:HBC3	1.81	0.61
17:6:75:PHE:HB2	21:6:604:CLA:HMA2	1.82	0.61
19:8:238:ASN:ND2	21:8:603:CLA:OBD	2.34	0.61
2:B:688:LEU:HD12	23:L:4002:BCR:HC41	1.82	0.61
21:7:609:CLA:H2	24:7:801:LHG:H282	1.81	0.61
1:A:220:VAL:HG13	1:A:240:PRO:HB3	1.83	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
13:1:82:MET:SD	21:1:601:CLA:HAB	2.40	0.61
17:6:121:LEU:HD21	38:6:613:CHL:C1D	2.31	0.61
2:B:62:THR:HG23	2:B:143:LEU:HD13	1.83	0.61
21:B:1202:CLA:H11	21:B:1203:CLA:HBB1	1.83	0.61
21: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	21:K:1403:CLA:C2C	2.31	0.61
11:I:1:MET:HE2	11:I:4:GLN:OE1	2.01	0.61
38:a:606:CHL:HHC	38:a:606:CHL:HBB1	1.83	0.61
37:6:501:LUT:H373	38:6:611:CHL:H42	1.82	0.61
2:B:646:VAL:HA	21:B:1206:CLA:CBC	2.31	0.60
1:A:438:ILE:HG13	1:A:556:TYR:HE1	1.67	0.60
21:A:1140:CLA:H61	8:J:33:LEU:HD21	1.81	0.60
21:B:1231:CLA:HHC	21:B:1231:CLA:HBB1	1.81	0.60
23:3:504:BCR:H14C	38:3:611:CHL:H72	1.82	0.60
15:4:129:MET:HE3	38:4:613:CHL:HMA2	1.82	0.60
16:5:117:ASN:ND2	17:6:222:GLY:HA2	2.17	0.60
21:A:1130:CLA:HBB1	21:A:1136:CLA:H192	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:7:111:VAL:HG11	23:7:503:BCR:H16C	1.84	0.60
21:A:1012:CLA:C4	2:B:439:VAL:HG13	2.32	0.60
21:B:1240:CLA:HHB	24:B:5001:LHG:HC81	1.82	0.60
14:3:382:ARG:HG3	38:3:611:CHL:CHD	2.31	0.60
16:5:170:ASP:OD1	37:5:501:LUT:O23	2.19	0.60
2:B:659:ALA:HB3	21:B:1023:CLA:HBB2	1.82	0.60
12:L:445:THR:HG22	12:L:451:TYR:CE1	2.36	0.60
21:a:605:CLA:H102	21:8:611:CLA:HBB1	1.84	0.60
24:A:5003:LHG:O3	24:A:5003:LHG:O1	2.14	0.60
2:B:478:LEU:HD22	2:B:486:PRO:HG3	1.82	0.60
2:B:659:ALA:O	21:B:1023:CLA:HAB	2.02	0.60
21:B:1212:CLA:H203	23:B:4002:BCR:H311	1.83	0.60
14:3:325:LEU:HD23	21:3:607: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	21:5:609:CLA:HED2	1.65	0.60
17:6:142:LYS:HG3	17:6:145:SER:HB3	1.84	0.60
7:G:1312:TYR:OH	33:G:5002:ERG:H272	2.02	0.60
24:4:801:LHG:H111	24:4:801:LHG:H271	1.83	0.60
6:F:444:VAL:HG22	8:J:33:LEU:HD11	1.83	0.59
9:K:56:LEU:HD23	21:K:1403:CLA:CHD	2.32	0.59
33:G:5002:ERG:O1	33:G:5002:ERG:C4	2.42	0.59
16:5:166:GLY:N	21:5:601:CLA:OBD	2.30	0.59
17:6:181:LYS:HG3	21:6:601:CLA:CMA	2.31	0.59
17:6:182:VAL:HG12	21:6:607:CLA:HED2	1.84	0.59
21:7:604:CLA:O1A	21:7:604:CLA:H3A	2.02	0.59
1:A:384:TYR:HB3	1:A:747:ILE:HD11	1.83	0.59
14:3:260:VAL:O	24:3:801:LHG:HC11	2.02	0.59
21:B:1219:CLA:HBB1	21:B:1219:CLA:HMB1	1.84	0.59
18:7:42:GLU:HG2	46:7:807:4RF:H41	1.84	0.59
12:L:328:LEU:HD21	21:L:1501:CLA:HAB	1.84	0.59
21:7:617:CLA:HAA1	25:8:802:DGD:HA81	1.83	0.59
1:A:554:VAL:HG21	23:A:4004:BCR:HC31	1.85	0.59
24: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
38:1:609:CHL:HHC	38:1:609:CHL:HBB1	1.83	0.59
17:6:216:HIS:ND1	17:6:223:THR:OG1	2.34	0.59
1:A:39:LEU:O	1:A:48:TRP:NE1	2.26	0.59
2:B:352:HIS:ND1	21: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:6:501:LUT:H23	21:6:601:CLA:H11	1.84	0.59
1:A:15:ILE:HG21	21:A:1108:CLA:HAA2	1.85	0.59
22:A:2001:PQN:H201	21:A:1101:CLA:H42	1.84	0.59
8:J:20:MET:HE1	18:7:37:LEU:HA	1.84	0.59
38:5:611:CHL:HBB1	38:5:611:CHL:HHC	1.84	0.59
19:8:139:TRP:CE3	21:8:612:CLA:HMA3	2.38	0.59
2:B:167:SER:OG	7:G:1275:GLY:C	2.46	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
37:8:502:LUT:H32	38:8:604:CHL:CBB	2.33	0.59
1:A:440:HIS:ND1	21:A:1129:CLA:HMB1	2.18	0.59
2:B:167:SER:OG	7:G:1276:ASP:N	2.36	0.59
13:1:141:ARG:NH2	21:1:612:CLA:O1D	2.34	0.59
38:a:610:CHL:HHC	38:a:610:CHL:HBB1	1.85	0.59
9:K:83:ASN:HB3	21:K:1404:CLA:CAD	2.32	0.58
13:a:139:SER:CB	35:a:804:LPX:H5	2.33	0.58
37:3:501:LUT:H28	21:3:601:CLA:H43	1.84	0.58
21:A:1116:CLA:HHC	21:A:1116:CLA:HBB1	1.84	0.58
21: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
21:B:1023:CLA:H2	21:B:1023:CLA:HMA3	1.84	0.58
21:a:602:CLA:HHC	21:a:602:CLA:HBB1	1.85	0.58
16:5:145:SER:O	17:6:42:GLY:HA2	2.03	0.58
17:6:41:PRO:CD	21:6:609:CLA:C3D	2.80	0.58
2:B:27:ALA:HB2	25:B:5003:DGD:HA51	1.84	0.58
2:B:181:ALA:HB2	2:B:289:GLY:HA3	1.85	0.58
21:B:1228:CLA:C4A	21:B:1228:CLA:HBA2	2.29	0.58
24:F:5001:LHG:H302	24:F:5001:LHG:H251	1.84	0.58
13:a:35:ASN:O	13:a:37:LEU:N	2.37	0.58
21:A:1102:CLA:HBB1	21:A:1102:CLA:HMB1	1.84	0.58
2:B:429:PHE:CE1	21: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	21:4:601: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
2:B:676:ILE:HG23	21:B:1238:CLA:HMC1	1.85	0.58
11:I:26:MET:HG3	23:L:4001:BCR:C31	2.32	0.58
17:6:87:MET:HG2	37:6:501:LUT:C15	2.34	0.58
24:B:5001:LHG:H332	31:B:5007:LAP:H71	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:607:CLA:H93	35:a:804:LPX:H11	1.86	0.58
15:4:224:PHE:HA	15:4:227:ASN:HD21	1.68	0.58
17:6:193:LEU:HD13	21:6:603:CLA:H91	1.86	0.58
21:B:1202:CLA:H93	21:B:1210:CLA:H2	1.86	0.58
21:B:1237:CLA:H203	21:L:1502:CLA:CBB	2.34	0.58
21:F:1302:CLA:HBD	46:7:807:4RF:H5	1.85	0.58
13:a:214:PHE:HB3	21:a:603:CLA:H12	1.85	0.58
17:6:155:PHE:HE2	21:6:617:CLA:HAA1	1.69	0.58
2:B:285:PHE:HE1	21:B:1216:CLA:HAB	1.68	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
24:4:801:LHG:HC81	23:6:503:BCR:HC31	1.86	0.58
16:5:51:ASP:OD2	21:5:604:CLA:HED2	2.04	0.58
21:A:1130:CLA:H42	21:L:1502:CLA:H102	1.84	0.57
21:B:1211:CLA:H3A	23:B:4003:BCR:H383	1.86	0.57
21:B:1232:CLA:HAA2	21:G:1603:CLA:CMA	2.34	0.57
21:1:608:CLA:H11	38:1:609:CHL:H42	1.86	0.57
17:6:155:PHE:CE2	21:6:617:CLA:HAA1	2.38	0.57
21:6:604:CLA:O1A	21:6:604:CLA:H3A	2.03	0.57
21:A:1107:CLA:HBA2	21:A:1107:CLA:CHA	2.34	0.57
2:B:23:TRP:CG	2:B:705:GLN:HE22	2.23	0.57
7:G:1313:ILE:HD12	33:G:5002:ERG:H213	1.86	0.57
21:K:1402:CLA:HHC	21: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
21:A:1012:CLA:HBC2	2:B:586:ASN:HB2	1.87	0.57
24:B:5002:LHG:H112	24:B:5002:LHG:H272	1.86	0.57
38:4:613:CHL:HHC	38:4:613:CHL:HBB1	1.86	0.57
17:6:186:LYS:HB3	21:6:607:CLA:CMD	2.34	0.57
21:A:1122:CLA:H11	21:A:1133:CLA:H202	1.86	0.57
21:B:1201:CLA:HAB	21:B:1203:CLA:CAD	2.34	0.57
3:C:23:THR:HG22	3:C:47:ASP:HB3	1.86	0.57
9:K:64:THR:HG21	21:K:1403:CLA:HMA3	1.87	0.57
37:1:503:LUT:H28	37:1:503:LUT:H361	1.87	0.57
13:a:135:ALA:HB3	35:a:804:LPX:H10	1.85	0.57
18:7:8:GLU:OE2	24:7:801: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	21:L:1501:CLA:HAC1	1.86	0.57
17:6:165:PRO:CD	21:6:601:CLA:OBD	2.53	0.57
21:A:1104:CLA:HAB	21:A:1127:CLA:HBB1	1.85	0.57
21:A:1107:CLA:C4	23:J:4001:BCR:H10C	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:316:GLU:HB3	4:D:319:GLN:HG3	1.87	0.57
13:a:83:LEU:HB3	38:a:606:CHL:HBB2	1.87	0.57
14:3:275:TYR:HE2	14:3:292:CYS:HB3	1.70	0.57
14:3:366:SER:HB3	21:7:608:CLA:HED1	1.87	0.57
21:5:617:CLA:HED3	44:6:806:SPH:H141	1.86	0.57
17:6:62:PRO:HG3	44:6:806:SPH:H122	1.87	0.57
37:7:501:LUT:H30	21:7:601:CLA:H71	1.86	0.57
21:A:1137:CLA:HBB1	21:A:1137:CLA:HHC	1.87	0.57
2:B:359:TYR:CE2	21:B:1225:CLA:HED2	2.40	0.57
5:E:46:ARG:NH2	6:F:476:LYS:HE3	2.20	0.57
16:5:129:MET:HG3	21:5:612:CLA:HMC3	1.86	0.57
18:7:219:ASN:ND2	21:7:603:CLA:OBD	2.36	0.57
19:8:76:ASN:HD22	38:8:604:CHL:HBB2	1.69	0.57
1:A:402:ILE:HG23	23:A:4004:BCR:H343	1.87	0.56
2:B:457:GLU:OE1	2:B:462:GLN:NE2	2.35	0.56
21:B:1232:CLA:HAA2	21:G:1603:CLA:HMA2	1.87	0.56
18:7:101:LEU:O	18:7:105:ILE:HG12	2.05	0.56
23:7:503:BCR:H372	38:7:613: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	21:A:1116:CLA:HBD	2.44	0.56
1:A:679:TRP:CD2	20:A:1011:CL0:H5	2.40	0.56
21:A:1131:CLA:H18	23:L:4001:BCR:H343	1.86	0.56
21:B:1235:CLA:HBC2	30: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
21:F:1301:CLA:C2	31:F:5003:LAP:H21	2.34	0.56
9:K:51:ALA:CB	21:K:1403:CLA:C2C	2.83	0.56
12:L:353:VAL:HA	12:L:376:ASN:CG	2.30	0.56
14:3:436:ASN:O	14:3:440:ASN:ND2	2.31	0.56
24:4:801:LHG:H111	24:4:801: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
21:A:1012:CLA:H172	21: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
21:B:1201:CLA:H203	21:B:1201:CLA:H141	1.87	0.56
9:K:64:THR:CG2	21:K:1403:CLA:CMA	2.83	0.56
21:a:615:CLA:HMA1	48:8:806:P5S:H21	1.86	0.56
14:3:439:ARG:HB3	21:3:607:CLA:HMD1	1.87	0.56
17:6:58:TYR:CD1	21:6:609:CLA:CBC	2.86	0.56
17:6:89:GLY:HA2	37:6:502:LUT:H182	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:6:193:LEU:HD13	21:6:603:CLA:C9	2.36	0.56
38:6:610:CHL:CBB	38:6:613:CHL:HBB2	2.35	0.56
21:B:1201:CLA:HBA2	10:M:30:TYR:CD1	2.41	0.56
9:K:58:PRO:HD2	21:K:1403:CLA:CHB	2.35	0.56
13:1:37:LEU:HD21	38:1:609:CHL:HMA3	1.87	0.56
13:1:60:LEU:HD12	21:1:604:CLA:H2	1.88	0.56
38:4:618:CHL:HBD	38:4:618:CHL:HBA1	1.87	0.56
17:6:128:VAL:HG13	23:6:503:BCR:C14	2.35	0.56
4:D:287:HIS:HB3	4:D:288:PRO:HD3	1.86	0.56
12:L:386:LEU:HD22	23:L:4001:BCR:H17C	1.85	0.56
16:5:52:ARG:HG2	21:5:609:CLA:OBD	2.06	0.56
1:A:390:LEU:HD11	21:A:1127:CLA:HED3	1.86	0.56
13:1:107:VAL:HG12	13:1:108:GLN:HG3	1.87	0.56
21:3:606:CLA:H201	24:5:801:LHG:H372	1.87	0.56
1:A:175:PHE:HE1	30:3:802:PTY:H162	1.71	0.56
12:L:436:SER:HB3	23:L:4003:BCR:H312	1.87	0.56
15:4:57:LEU:HD23	37:4:502:LUT:H222	1.86	0.56
19:8:183:SER:O	19:8:185:GLU:N	2.38	0.56
1:A:178:TRP:HZ2	30:3:802: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	37:1:503:LUT:H373	1.87	0.56
16:5:52:ARG:HB2	21:5:604:CLA:HMD1	1.86	0.56
17:6:135:ARG:NE	21:6:617:CLA:HMC1	2.21	0.56
21:7:605:CLA:HBC2	21:7:605:CLA:HHD	1.87	0.56
19:8:235:PHE:HE1	21:8:608:CLA:O1D	1.88	0.56
37:8:501:LUT:H32	38:8:601:CHL:CBB	2.36	0.56
1:A:389:SER:HB3	21:A:1126:CLA:HMA1	1.86	0.56
2:B:646:VAL:HA	21:B:1206:CLA:HBC1	1.87	0.56
21:B:1228:CLA:CBA	6:F:471:MET:HE2	2.36	0.56
9:K:51:ALA:HB2	21:K:1403:CLA:CBC	2.36	0.56
1:A:359:LEU:HG	21:A:1123:CLA:HHB	1.87	0.56
2:B:608:ASN:O	2:B:612:GLU:HG2	2.06	0.56
21:B:1207:CLA:HBB1	21: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
21:B:1221:CLA:HMA2	21:B:1221:CLA:H2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:1222:CLA:H52	21:B:1231:CLA:HBB2	1.88	0.55
17:6:164:TYR:O	21:6:601:CLA:CED	2.52	0.55
17:6:169:PHE:CD1	38:6:611:CHL:H11	2.28	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
23:5:503:BCR:HC41	24:6:801:LHG:HC81	1.87	0.55
21:5:603:CLA:H2	21:5:608:CLA:HMD2	1.88	0.55
19:8:196:ARG:NH1	24:8:801:LHG:O4	2.38	0.55
21:A:1111:CLA:H201	21:3:605:CLA:H62	1.88	0.55
6:F:445:PRO:HD2	35:J:5001:LPX:O3	2.05	0.55
21:7:609:CLA:HBB2	21:7:604:CLA:HBC2	1.89	0.55
21:A:1119:CLA:H152	23:A:4003:BCR:H21C	1.88	0.55
2:B:10:SER:OG	2:B:13:LEU:HB2	2.06	0.55
2:B:478:LEU:HD13	21:B:1231:CLA:HMD1	1.89	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
21:3:616:CLA:HBC3	16:5:227:TRP:CZ3	2.41	0.55
17:6:124:PHE:CZ	38:6:613: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:1:MET:HE1	11:I:7:PRO:HG3	1.87	0.55
11:I:30:ILE:HD13	23:L:4001:BCR:H333	1.86	0.55
21:a:605:CLA:H51	23:8:503:BCR:C34	2.37	0.55
19:8:139:TRP:HZ3	21:8:618:CLA:HAC2	1.70	0.55
21:A:1131:CLA:HMD3	21:A:1136:CLA:H13	1.88	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	25:B:5003:DGD:HB81	2.41	0.55
17:6:189:ARG:CB	24:6:801:LHG:H241	2.36	0.55
1:A:327:GLU:OE1	1:A:339:LYS:HA	2.07	0.55
21:A:1140:CLA:HHC	21:A:1140:CLA:HBB1	1.89	0.55
13:a:36:TRP:NE1	38:a:609:CHL:C2B	2.69	0.55
21:3:616:CLA:H43	16:5:231:ILE:HG12	1.88	0.55
16:5:81:MET:SD	21:5:601:CLA:HAB	2.47	0.55
21:8:610:CLA:CAD	46:8:808:4RF:H66	2.36	0.55
2:B:416:LYS:HB2	2:B:540:LEU:HD23	1.89	0.55
37:1:501:LUT:H162	21:1:608:CLA:HBC1	1.87	0.55
18:7:211:PRO:HG2	21:7:608:CLA:HMB2	1.89	0.55
21:A:1138:CLA:HED2	2:B:425:TRP:HB2	1.89	0.55
17:6:125:GLU:OE2	38:6:613:CHL:HMB2	2.07	0.55
21:A:1120:CLA:C3D	23:K:4001:BCR:H271	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:1236:CLA:HHD	21:B:1236:CLA:HBC2	1.89	0.54
29:B:5004:PCW:O2P	6:F:471:MET:HE1	2.06	0.54
31:B:5007:LAP:O5	31: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
21:A:1125:CLA:H143	21:A:1133:CLA:H13	1.89	0.54
24:F:5002:LHG:H102	21:8:610:CLA:H93	1.89	0.54
13:a:139:SER:HB2	35:a:804:LPX:H5	1.89	0.54
21:4:615:CLA:HAA2	21:4:615:CLA:H2	1.89	0.54
17:6:139:ASP:CG	38:6:611:CHL:HBC1	2.32	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
21:B:1209:CLA:HAA1	7:G:1278:ARG:HD3	1.89	0.54
3:C:54:CYS:HB3	27:C:3002:SF4:S4	2.47	0.54
33:G:5002:ERG:C3	33:G:5002:ERG:HO1	2.14	0.54
19:8:76:ASN:HD22	38:8:604:CHL:CBB	2.20	0.54
1:A:175:PHE:CE1	30:3:802:PTY:H162	2.43	0.54
1:A:197:MET:HE2	21:A:1111:CLA:HBC2	1.90	0.54
21:B:1234:CLA:HHD	21: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	21:K:1403:CLA:CMA	2.37	0.54
15:4:179:TRP:HB3	21:4:601:CLA:HMA2	1.88	0.54
16:5:164:TYR:HB3	21:5:601:CLA:O1D	2.07	0.54
1:A:656:GLN:HG2	1:A:749:ALA:HB3	1.90	0.54
20:A:1011:CL0:CGD	20:A:1011:CL0:H8	2.38	0.54
2:B:423:LEU:HD13	2:B:533:LEU:HA	1.89	0.54
21:B:1023:CLA:H121	23:I:4001:BCR:H281	1.90	0.54
14:3:311:VAL:O	14:3:315:ARG:HG3	2.08	0.54
21:5:604:CLA:HMB3	21:5:604:CLA:HBB1	1.89	0.54
21:A:1109:CLA:H101	21:A:1101:CLA:HBB2	1.88	0.54
12:L:353:VAL:HA	12:L:376:ASN:OD1	2.08	0.54
21:1:605:CLA:HBC1	21:1:612:CLA:HAC1	1.89	0.54
17:6:170:ALA:HB1	21:6:601:CLA:HBA2	1.90	0.54
17:6:186:LYS:HB3	21:6:607:CLA:HMD1	1.89	0.54
2:B:670:GLY:O	2:B:674:GLU:HG3	2.07	0.54
38:a:609:CHL:O1A	15:4:131:ASN:ND2	2.37	0.54
38:6:613:CHL:HMB3	38:6:613:CHL:HBB1	1.89	0.54
23:A:4001:BCR:H362	23:A:4002:BCR:H21C	1.89	0.54
2:B:727:ILE:O	2:B:731:SER:OG	2.19	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:1231:VAL:O	7:G:1235:VAL:HG12	2.08	0.54
13:a:58:LEU:HD12	37:a:502:LUT:C22	2.34	0.54
21:4:602:CLA:H2	21:4:602:CLA:HMA3	1.90	0.54
2:B:88:ILE:O	2:B:122:TYR:OH	2.24	0.54
14:3:271:GLN:O	14:3:274:SER:OG	2.25	0.54
24:4:801:LHG:HC81	23:6:503:BCR:C3	2.38	0.54
24:6:801:LHG:H372	24:6:801: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
21:B:1209:CLA:HBD	7:G:1278:ARG:HD3	1.90	0.53
23:B:4004:BCR:H313	21:1:605:CLA:HED1	1.89	0.53
21:B:1204:CLA:H61	23:I:4001:BCR:C3	2.26	0.53
13:a:94:LEU:HD22	13:a:96:TYR:CE2	2.43	0.53
14:3:421:LEU:HD22	16:5:35:PHE:CD2	2.44	0.53
17:6:41:PRO:O	21:6:609:CLA:HED1	2.08	0.53
17:6:150:PRO:HD2	21:6:617:CLA:CHC	2.38	0.53
37:7:501:LUT:H361	37:7:501:LUT:H28	1.90	0.53
1:A:714:GLN:HG3	1:A:716:ARG:NH2	2.23	0.53
21:A:1102:CLA:HAB	21:A:1104:CLA:CAD	2.39	0.53
22:A:2001:PQN:H291	24:A:5002:LHG:H141	1.88	0.53
2:B:326:THR:OG1	2:B:404:ASN:OD1	2.25	0.53
21:B:1201:CLA:HBA1	21:B:1201:CLA:CHA	2.37	0.53
9:K:56:LEU:HB3	21:K:1403:CLA:CHD	2.38	0.53
37:1:501:LUT:H30	21:1:601:CLA:H52	1.89	0.53
21:6:601:CLA:H62	21:6:602:CLA:HMA2	1.90	0.53
21:7:610:CLA:HBB1	24:7:803:LHG:H312	1.89	0.53
1:A:452:SER:HB3	1:A:538:ILE:HD13	1.90	0.53
21:A:1130:CLA:C2	21:L:1502:CLA:H72	2.38	0.53
4:D:195:GLN:NE2	4:D:197:ASP:O	2.40	0.53
13:a:67:LEU:O	13:a:71:ARG:HG3	2.07	0.53
13:a:210:MET:HE2	13:a:210:MET:HA	1.90	0.53
21:a:603:CLA:HBC2	21:a:615:CLA:HMD2	1.91	0.53
16:5:188:LYS:NZ	24:5:801:LHG:O5	2.40	0.53
18:7:115:ARG:NH1	21:7:612:CLA:O1D	2.37	0.53
21:8:606:CLA:HMA2	38:8:613:CHL:HBC3	1.89	0.53
21:1:607:CLA:H143	13:a:131:PHE:CE1	2.43	0.53
17:6:41:PRO:HG2	21:6:609:CLA:OBD	2.08	0.53
1:A:296:HIS:HB3	21:A:1116:CLA:HMB2	1.91	0.53
1:A:374:MET:HE1	21:A:1125:CLA:HHC	1.90	0.53
1:A:661:TYR:OH	2:B:442:ASP:OD1	2.19	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1104:CLA:H43	24:A:5002:LHG:H262	1.90	0.53
2:B:176:LEU:HD12	2:B:302:MET:CE	2.39	0.53
21:B:1219:CLA:HBB2	23:B:4004:BCR:H343	1.90	0.53
21:F:1302:CLA:HBC3	21:F:1302:CLA:HHD	1.90	0.53
13:1:71:ARG:HH12	13:1:151:TYR:HE2	1.55	0.53
17:6:82:HIS:HD2	37:6:502:LUT:H15	1.74	0.53
1:A:357:LEU:HD23	21:A:1103:CLA:HED1	1.91	0.53
21:A:1111:CLA:HAA2	21:A:1123:CLA:H52	1.91	0.53
21:B:1232:CLA:HMB3	23:B:4005:BCR:HC32	1.90	0.53
21:B:1239:CLA:H11	22:B:2002:PQN:H302	1.90	0.53
4:D:226:SER:OG	4:D:228:LYS:O	2.27	0.53
18:7:91:ARG:HH22	21:7:606:CLA:HED1	1.74	0.53
1:A:421:ASN:ND2	1:A:421:ASN:O	2.42	0.53
16:5:50:GLY:O	16:5:191:ARG:NH1	2.39	0.53
21:6:612:CLA:HHD	21:6:612:CLA:HBC3	1.89	0.53
30:7:804:PTY:O10	30:7:804:PTY:HC12	2.09	0.53
15:4:193:ALA:O	15:4:197:ILE:HG12	2.08	0.53
17:6:233:PRO:HD2	38:6:619:CHL:O1D	2.07	0.53
21:A:1103:CLA:H141	23:A:4002:BCR:H353	1.90	0.53
21:A:1131:CLA:H143	22:B:2002:PQN:H191	1.91	0.53
21:8:611:CLA:HBB1	21:8:611:CLA:HMB3	1.91	0.53
1:A:454:GLY:C	21:A:1132:CLA:HAB	2.34	0.53
1:A:485:GLN:NE2	1:A:528:LEU:O	2.41	0.53
2:B:493:LEU:HD22	21:B:1213:CLA:HED2	1.91	0.53
21:B:1202:CLA:H11	21:B:1203:CLA:CBB	2.39	0.53
21:B:1204:CLA:H2	23:I:4001:BCR:HC31	1.90	0.53
12:L:390:TYR:O	12:L:394:THR:HG22	2.09	0.53
21:3:606:CLA:HMA3	21:3:613:CLA:C3C	2.39	0.53
16:5:55:ASP:HB2	21:5:604:CLA:HBA2	1.89	0.53
16:5:133:GLU:HG3	21:5:612:CLA:C4B	2.38	0.53
16:5:185:LYS:HG3	21:5:607:CLA:HED2	1.90	0.53
17:6:189:ARG:HB2	24:6:801:LHG:H241	1.90	0.53
18:7:161:CYS:SG	21:7:601:CLA:HAA2	2.48	0.53
37:8:501:LUT:H32	38:8:601:CHL:HBB1	1.90	0.53
2:B:30:HIS:HD2	21:B:1202:CLA:HBB2	1.74	0.52
12:L:313:THR:H	12:L:316:THR:HG1	1.57	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
24:7:803:LHG:P	24:7:803: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	21:B:1212:CLA:HAB	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:659:ALA:CB	21:B:1023:CLA:HBB2	2.40	0.52
21:B:1022:CLA:H151	21:B:1207:CLA:HBC3	1.90	0.52
37:a:502:LUT:H183	38:a:606:CHL:C3B	2.39	0.52
38:5:610:CHL:HBB2	21:5:612:CLA:HBC3	1.91	0.52
21:5:612:CLA:H121	21:5:617:CLA:HAB	1.92	0.52
17:6:85:TRP:CE2	38:6:611:CHL:HED3	2.44	0.52
21:A:1120:CLA:HMD2	23:K:4001:BCR:H23C	1.91	0.52
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
21:4:617:CLA:HHC	21:4:617:CLA:HBB1	1.91	0.52
16:5:35:PHE:HB3	16:5:38:VAL:HB	1.90	0.52
44:6:806:SPH:H161	37:6:502:LUT:H361	1.90	0.52
21:B:1224:CLA:CGA	21:B:1224:CLA:H3A	2.35	0.52
21:B:1230:CLA:HMB2	21:B:1229:CLA:CAB	2.40	0.52
13:a:121:PHE:HB3	13:a:126:LEU:CD2	2.39	0.52
13:a:177:GLY:O	13:a:181:MET:HG3	2.09	0.52
17:6:152:PHE:CE1	21:6:617:CLA:HBA2	2.42	0.52
2:B:438:TYR:CD2	21: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	23:I:4001:BCR:H333	1.92	0.52
13:a:102:ALA:HB3	13:a:103:PRO:HD3	1.92	0.52
14:3:258:ALA:HB2	14:3:265:LYS:HD2	1.90	0.52
14:3:382:ARG:NH2	21:3:612:CLA:O1D	2.41	0.52
24:4:802:LHG:H141	24:4:802:LHG:HC92	1.91	0.52
17:6:133:GLU:OE1	17:6:136:ARG:NH2	2.42	0.52
19:8:138:ARG:NH1	21:8:612:CLA:O1D	2.40	0.52
21:A:1128:CLA:H41	24:A:5002:LHG:H111	1.91	0.52
21:A:1138:CLA:CBB	6:F:422:GLY:HA3	2.37	0.52
21:B:1023:CLA:CGA	21: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	38:6:610:CHL:OBD	2.09	0.52
23:7:503:BCR:C19	38:7:613:CHL:HBA2	2.39	0.52
47:7:504:C7Z:C10	19:8:242:ILE:HD13	2.40	0.52
21:B:1209:CLA:H171	21: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	37:5:501: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
21:6:604:CLA:H3A	21:6:604:CLA:CGA	2.39	0.52
38:6:610:CHL:HBB2	38:6:613:CHL:HBB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:VAL:HG13	1:A:524:MET:HB3	1.91	0.52
21:1:604:CLA:H202	21:8:618:CLA:H91	1.91	0.52
37:6:501:LUT:H161	37:6:501: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	38:8:601:CHL:HBD	1.92	0.52
1:A:329:HIS:HB2	1:A:338:HIS:HD2	1.75	0.52
21:A:1114:CLA:H192	24: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
21:3:612:CLA:HBB1	21:3:612:CLA:HMB3	1.90	0.52
16:5:75:GLN:HE22	38:5:611:CHL:CGD	2.16	0.52
17:6:124:PHE:CE2	38:6:613:CHL:HED3	2.44	0.52
24:6:801:LHG:O9	24:6:801:LHG:H261	2.10	0.52
2:B:16:ASP:HB3	2:B:21:ARG:HB2	1.91	0.52
21:B:1225:CLA:H171	23:B:4002:BCR:H352	1.92	0.52
37:5:505:LUT:H173	21:7:608:CLA:CAB	2.37	0.52
17:6:135:ARG:HD3	38:6:611:CHL:HBB1	1.91	0.52
21:B:1209:CLA:HHC	21:B:1209:CLA:HBB1	1.93	0.51
21:B:1230:CLA:H12	30: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	21:K:1404:CLA:OBD	2.11	0.51
13:a:132:ALA:HB2	35:a:804:LPX:H16	1.91	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	21:K:1403:CLA:C1D	2.40	0.51
13:a:121:PHE:HD1	13:a:125:THR:HG21	1.74	0.51
17:6:40:LEU:CG	21:6:609:CLA:HED2	2.40	0.51
17:6:186:LYS:HD2	24:6:801:LHG:O10	2.11	0.51
19:8:92:GLU:HG2	19:8:220:LEU:HD21	1.92	0.51
1:A:395:MET:HE1	21:A:1124:CLA:HMD1	1.91	0.51
2:B:705:GLN:HG3	25:B:5003:DGD:HA31	1.93	0.51
9:K:51:ALA:HB2	21:K:1403:CLA:C3C	2.40	0.51
13:1:169:LEU:HB3	21:1:601:CLA:CMA	2.38	0.51
13:1:170:LYS:O	13:1:174:ILE:HG12	2.10	0.51
14:3:365:TYR:CE1	21:3:610:CLA:HMA2	2.45	0.51
23:6:503:BCR:H21C	38:6:613:CHL:HBA1	1.92	0.51
21:A:1131:CLA:H18	23:L:4001:BCR:C34	2.41	0.51
9:K:96:LEU:CD2	21:K:1403:CLA:HBB1	2.40	0.51
12:L:297:GLN:O	12:L:297:GLN:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:61:ALA:HB1	13:a:67:LEU:HB2	1.92	0.51
18:7:107:MET:CG	21:8:608:CLA:H12	2.41	0.51
1:A:371:MET:HE1	21:A:1127:CLA:O1D	2.11	0.51
1:A:721:THR:HG22	24:A:5002:LHG:HC62	1.93	0.51
21:A:1012:CLA:C4	2:B:439:VAL:HG22	2.40	0.51
13:1:181:MET:HE3	21:1:604:CLA:HMC2	1.92	0.51
14:3:474:VAL:O	14:3:477:ASN:ND2	2.43	0.51
16:5:144:ASP:HA	16:5:147:ASN:HD21	1.74	0.51
25:8:802:DGD:HAS2	21:8:607:CLA:HBB2	1.92	0.51
1:A:128:ASN:HB3	1:A:136:GLN:HB3	1.93	0.51
1:A:178:TRP:HB2	21:A:1109:CLA:HMC2	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	21:A:1136:CLA:O2D	2.11	0.51
21:A:1012:CLA:HAB	2:B:583:TRP:CH2	2.45	0.51
21:A:1107:CLA:H61	25:A:5005:DGD:HB72	1.93	0.51
2:B:312:PRO:C	2:B:314:GLY:H	2.18	0.51
6:F:346:LEU:O	6:F:348:ASN:N	2.38	0.51
21:1:603:CLA:HBB1	21:1:603:CLA:H111	1.93	0.51
14:3:337:PRO:HG3	21:3:616:CLA:OBD	2.11	0.51
21:B:1206:CLA:HBB1	21:B:1206:CLA:HMB3	1.92	0.51
11:I:30:ILE:CD1	23:L:4001:BCR:H332	2.36	0.51
13:a:106:LEU:HD11	13:a:123:LEU:HA	1.92	0.51
17:6:122:LEU:HD12	38:6:610:CHL:HAC2	1.93	0.51
17:6:184:GLU:HB2	21:6:601:CLA:HMB3	1.90	0.51
21:7:601:CLA:H3A	21:7:601:CLA:CGA	2.41	0.51
1:A:136:GLN:HG3	6:F:355:PRO:HB3	1.92	0.51
24:A:5003:LHG:H162	21:3:610:CLA:HAC2	1.92	0.51
21:B:1225:CLA:H8	23:B:4002:BCR:H21C	1.92	0.51
21:B:1207:CLA:HMC2	23:I:4001:BCR:C19	2.41	0.51
21:3:605:CLA:OBD	21:3:612:CLA:HBA2	2.11	0.51
17:6:75:PHE:CB	21:6:604:CLA:CMA	2.89	0.51
23:7:503:BCR:H391	21:7:606:CLA:H12	1.93	0.51
2:B:279:LEU:HG	21:B:1213:CLA:HAB	1.93	0.51
21:B:1216:CLA:HMB2	21:B:1221:CLA:HED1	1.92	0.51
21:F:1301:CLA:HBD	31:F:5003:LAP:H151	1.91	0.51
13:1:119:VAL:HG21	38:1:613:CHL:HMD1	1.92	0.51
14:3:264:TYR:C	14:3:266:ASN:H	2.18	0.51
38:4:609:CHL:H51	17:6:127:PHE:CD1	2.46	0.51
17:6:121:LEU:HD21	38:6:613:CHL:C2D	2.40	0.51
4:D:298:ASN:HB3	4:D:301:ARG:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:607:CLA:H151	13:a:131:PHE:CZ	2.46	0.51
21:3:601:CLA:C2B	21:3:601: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	21:6:604:CLA:CED	2.41	0.51
17:6:62:PRO:HB2	44:6:806:SPH:H101	1.93	0.51
17:6:99:VAL:HG23	17:6:100:LYS:HG3	1.93	0.51
45:7:502:XAT:H183	21:7:606: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	21:A:1136:CLA:HED1	1.93	0.50
1:A:698:GLU:OE2	5:E:82:TYR:OH	2.29	0.50
2:B:698:PRO:O	3:C:81:TYR:OH	2.24	0.50
21: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
13:a:43:PRO:HG2	13:a:56:ASP:HB3	1.93	0.50
13:a:90:GLY:HA3	38:a:606:CHL:HBC3	1.92	0.50
37:a:501:LUT:H30	21:a:601:CLA:H52	1.93	0.50
35:a:804:LPX:H19A	35:a:804:LPX:H14A	1.93	0.50
16:5:110:ARG:NH2	16:5:116:VAL:HB	2.26	0.50
17:6:62:PRO:HD2	37:6:502:LUT:H23	1.93	0.50
1:A:153:ILE:HG21	1:A:159:LEU:HD12	1.93	0.50
21:B:1237:CLA:H203	21:L:1502:CLA:CAB	2.42	0.50
16:5:45:ASP:OD1	16:5:46:GLY:N	2.43	0.50
23:5:504:BCR:H362	38:5:610:CHL:C1C	2.42	0.50
37:6:502:LUT:H24	21:6:604:CLA:O2A	2.11	0.50
21:7:604:CLA:H191	24:7:802:LHG:H131	1.93	0.50
1:A:208:LEU:HD22	23:A:4001:BCR:H361	1.94	0.50
1:A:366:ILE:HG21	21:A:1117:CLA:H191	1.93	0.50
1:A:376:PRO:HG3	21:A:1117:CLA:HBA1	1.92	0.50
21:A:1118:CLA:H92	24:3:801:LHG:H291	1.93	0.50
2:B:331:LEU:HD21	21:B:1202:CLA:H192	1.92	0.50
2:B:692:VAL:HG11	21:B:1237:CLA:HAB	1.93	0.50
9:K:64:THR:CG2	21:K:1403:CLA:HMA1	2.41	0.50
9:K:64:THR:HG22	21:K:1403:CLA:HMA1	1.92	0.50
12:L:382:LEU:O	12:L:385:THR:HG22	2.11	0.50
21:3:601:CLA:H52	21:3:602:CLA:HMA2	1.92	0.50
15:4:77:GLY:HA3	15:4:187:ALA:HB1	1.92	0.50
15:4:236:ASN:N	24:6:802:LHG:HC2	2.27	0.50
1:A:746:ARG:O	1:A:750:VAL:HG22	2.12	0.50
15:4:158:TYR:OH	15:4:161:LEU:HA	2.12	0.50
1:A:650:LEU:HD21	21:B:1021:CLA:CBB	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:686:THR:HG23	2:B:689:ALA:HB3	1.93	0.50
21:1:607:CLA:H143	13:a:131:PHE:HE1	1.77	0.50
17:6:149:ASP:OD1	17:6:151:ILE:N	2.45	0.50
47:7:504:C7Z:C14	21:8:615: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	21:1:605:CLA:O1A	2.45	0.50
38:1:609:CHL:HMB3	30:8:810:PTY:C37	2.42	0.50
21:4:604:CLA:HED2	21:4:604:CLA:H2A	1.92	0.50
38:4:609:CHL:HAC1	24:4:801:LHG:HC41	1.93	0.50
17:6:105:TRP:O	17:6:108:SER:OG	2.27	0.50
18:7:9:LEU:C	18:7:11:PHE:H	2.19	0.50
18:7:60:THR:HG22	21:7:606:CLA:HAB	1.93	0.50
1:A:351:ALA:HB1	23:A:4003:BCR:H391	1.93	0.50
1:A:392:THR:HG23	1:A:607:ILE:HG21	1.92	0.50
21:A:1110:CLA:H92	14:3:289:LEU:HD11	1.94	0.50
6:F:466:LYS:HB2	43:8:803:DGA:HB32	1.93	0.50
13:1:208:ASN:OD1	13:1:211:ALA:HB3	2.12	0.50
18:7:9:LEU:HD22	18:7:17:VAL:HG21	1.93	0.50
19:8:226:HIS:CG	21:8:603:CLA:HAA2	2.47	0.50
1:A:395:MET:HE1	21:A:1124:CLA:CMD	2.42	0.50
1:A:432:ARG:HG3	4:D:238:GLY:HA3	1.93	0.50
1:A:453:PHE:HD2	21:B:1023:CLA:H41	1.76	0.50
21: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
23:5:503:BCR:H271	21:5:606:CLA:C1B	2.42	0.50
1:A:34:HIS:NE2	21:A:1109:CLA:HBA2	2.26	0.50
21:A:1013:CLA:H3A	21:A:1013:CLA:CGA	2.41	0.50
24:F:5001:LHG:H182	38:8:604:CHL:H102	1.94	0.50
21:1:607:CLA:C4C	24:1:801:LHG:HC62	2.42	0.50
37:a:501:LUT:H383	21:a:611:CLA:H11	1.94	0.50
15:4:224:PHE:CE1	21:4:608:CLA:HED2	2.47	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	21:3:605:CLA:H203	1.94	0.49
1:A:680:ALA:HB3	21:A:1013:CLA:HBB2	1.93	0.49
21:A:1114:CLA:H203	24:A:5003:LHG:H251	1.93	0.49
2:B:520:VAL:HG11	2:B:594:TYR:CG	2.47	0.49
21:B:1205:CLA:O1A	21:B:1224:CLA:HBD	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:1245:LEU:HD11	13:1:135:ALA:HB3	1.94	0.49
13:a:122:ASP:O	13:a:126:LEU:HD23	2.12	0.49
17:6:41:PRO:HD2	21:6:609:CLA:O2D	2.12	0.49
18:7:76:ALA:HB2	32:7:805:SQD:H172	1.93	0.49
19:8:132:ASN:O	19:8:136:ILE:HG12	2.12	0.49
1:A:370:HIS:O	1:A:374:MET:HG2	2.13	0.49
21:A:1138:CLA:HAA2	21:B:1228:CLA:HMB1	1.94	0.49
21:B:1021:CLA:HHC	21:B:1021:CLA:HBB1	1.94	0.49
9:K:98:ALA:O	9:K:102:ILE:HG12	2.13	0.49
13:a:60:LEU:HD22	19:8:157:PHE:CE1	2.48	0.49
21:5:616:CLA:HBB2	38:6:619:CHL:H171	1.94	0.49
17:6:132:VAL:HG12	38:6:611: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	21:8:612:CLA:HAB	2.27	0.49
19:8:176:PRO:HD2	37:8:501:LUT:H23	1.93	0.49
1:A:539:HIS:HB3	21: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
14:3:336:ILE:HG22	21:3:616:CLA:CHD	2.41	0.49
30:8:810:PTY:O4	30:8:810:PTY:H112	2.12	0.49
1:A:105:LEU:HD11	1:A:154:THR:HA	1.93	0.49
21:A:1130:CLA:C10	21:L:1502:CLA:H92	2.37	0.49
21:4:601:CLA:HBB1	21:4:601:CLA:HMB1	1.94	0.49
18:7:204:LEU:O	18:7:208:VAL:HG23	2.12	0.49
25:8:802:DGD:O1A	24:8:801:LHG:O1	2.31	0.49
21:8:609:CLA:H51	24:8:801:LHG:H121	1.93	0.49
2:B:686:THR:HG21	21:B:1237:CLA:HMA3	1.94	0.49
21:B:1240:CLA:HBB2	21:1:604:CLA:H52	1.93	0.49
9:K:58:PRO:HD3	21:K:1403:CLA:HMA2	1.95	0.49
12:L:298:VAL:HB	12:L:314:PRO:HG3	1.94	0.49
17:6:169:PHE:HD1	38:6:611:CHL:C1	2.16	0.49
23:6:504:BCR:H352	24:6:802:LHG:H112	1.95	0.49
1:A:14:LYS:HE2	14:3:295:GLU:OE2	2.13	0.49
23:A:4005:BCR:H24C	21:B:1230:CLA:HMC1	1.93	0.49
2:B:55:LEU:HD21	21: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	33:G:5002:ERG:C18	2.42	0.49
21:4:610:CLA:HBB1	21:8:620:CLA:H18	1.95	0.49
16:5:131:PHE:CB	21:6:609:CLA:H42	2.42	0.49
17:6:89:GLY:HA2	37:6:502:LUT:C18	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:6:258:CYS:SG	17:6:261:HIS:HB2	2.52	0.49
38:6:611:CHL:HBB1	38:6:611:CHL:HHC	1.94	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
21:A:1110:CLA:HED2	21:A:1111:CLA:HAC1	1.93	0.49
21:A:1121:CLA:HED1	9:K:66:GLN:HG2	1.95	0.49
21:B:1216:CLA:HBB1	21:B:1221:CLA:H61	1.93	0.49
13:1:82:MET:HE2	13:1:177:GLY:N	2.28	0.49
13:a:114:TYR:HD1	38:a:606:CHL:HAA1	1.78	0.49
14:3:250:ASP:O	14:3:252:ALA:N	2.43	0.49
1:A:303:VAL:HG21	21:A:1115:CLA:HBB2	1.95	0.49
1:A:423:TYR:CE2	4:D:241:ILE:HD11	2.48	0.49
21:A:1124:CLA:H3A	21:A:1124:CLA:HBA2	1.50	0.49
2:B:130:LEU:HD23	21:B:1211:CLA:HED3	1.95	0.49
6:F:359:LEU:O	6:F:363:ILE:HG13	2.13	0.49
24:F:5001:LHG:HC91	19:8:56:PRO:HG3	1.95	0.49
17:6:125:GLU:OE2	38:6:613:CHL:C2B	2.61	0.49
17:6:183:LYS:NZ	21:6:602:CLA:OBD	2.46	0.49
18:7:174:ASN:O	18:7:178:ASN:ND2	2.34	0.49
1:A:702:TRP:CD1	6:F:477:ILE:HG21	2.48	0.49
2:B:668:TRP:HA	22:B:2002:PQN:H8	1.94	0.49
3:C:14:CYS:O	3:C:15:THR:OG1	2.28	0.49
24:4:802:LHG:H102	21:6:618:CLA:CBA	2.42	0.49
19:8:235:PHE:CE1	21:8:608:CLA:O1D	2.66	0.49
1:A:150:ALA:HB2	1:A:378:PRO:HD2	1.94	0.48
21:A:1106:CLA:H62	23:J:4001:BCR:H343	1.95	0.48
25:A:5005:DGD:HA21	25:A:5005:DGD:HG11	1.70	0.48
24:A:5003:LHG:C10	14:3:456:VAL:HG23	2.42	0.48
21:B:1218:CLA:HBB2	28:B:5006:LMT:H112	1.95	0.48
34:J:4002:RRX:H17	34:J:4002:RRX:C23	2.43	0.48
37:5:505:LUT:H181	38:5:610:CHL:H43	1.95	0.48
1:A:448:LEU:HD11	21:A:1136:CLA:HMB2	1.95	0.48
21: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
21:B:1212:CLA:HED2	21:B:1212:CLA:H2A	1.94	0.48
21:a:601:CLA:HBB1	21:a:601:CLA:HMB3	1.94	0.48
35:a:804:LPX:H9	35:a:804:LPX:H13A	1.95	0.48
15:4:200:GLN:HB3	15:4:211:GLN:OE1	2.13	0.48
18:7:192:GLN:HE22	37:7:501:LUT:H42	1.76	0.48
21:7:604:CLA:H3A	21:7:604:CLA:CGA	2.42	0.48
1:A:43:PRO:HG3	6:F:440:ILE:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1117:CLA:H203	21:A:1125:CLA:HBA2	1.95	0.48
2:B:83:LEU:HD21	2:B:364:GLN:HB3	1.95	0.48
2:B:429:PHE:CD1	21:B:1235:CLA:HAB	2.47	0.48
4:D:261:LEU:HG	4:D:265:ARG:HH12	1.79	0.48
21:G:1603:CLA:HHC	21:G:1603:CLA:HBB1	1.95	0.48
37:1:503:LUT:H173	21:1:606:CLA:H101	1.95	0.48
14:3:328:GLU:CD	14:3:463:PHE:HB3	2.38	0.48
16:5:117:ASN:ND2	17:6:227:SER:HB2	2.23	0.48
38:8:604:CHL:HHC	38:8:604:CHL:HBB1	1.95	0.48
8:J:20:MET:HE3	18:7:37:LEU:O	2.13	0.48
13:a:34:GLY:HA3	13:a:53:TYR:CD2	2.48	0.48
16:5:108:LEU:HD22	16:5:118:MET:HE1	1.94	0.48
17:6:194:ALA:HA	37:6:501:LUT:H181	1.95	0.48
19:8:202:MET:HE3	38:8:604:CHL:OMC	2.14	0.48
21:A:1120:CLA:HMA2	21:A:1121:CLA:HBD	1.95	0.48
2:B:231:TRP:HH2	23:G:4001:BCR:HC32	1.78	0.48
13:1:72:GLU:OE2	13:1:149:ARG:HB3	2.13	0.48
37:3:501:LUT:C30	21:3:601:CLA:H101	2.44	0.48
38:6:610:CHL:HMB1	38:6:610:CHL:HBB1	1.95	0.48
18:7:42:GLU:CG	46:7:807:4RF:H41	2.44	0.48
23:8:503:BCR:H271	21:8:606: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
21:A:1120:CLA:O1A	9:K:58:PRO:HG3	2.14	0.48
23:A:4003:BCR:H351	23:A:4003:BCR:H15C	1.58	0.48
2:B:200:ILE:HB	2:B:201:PRO:HD3	1.96	0.48
2:B:304:GLU:HG3	7:G:1261:ALA:HA	1.93	0.48
21:B:1211:CLA:HMA2	23:B:4003:BCR:H292	1.95	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
13:a:71:ARG:O	13:a:75:VAL:HG23	2.14	0.48
13:a:151:TYR:HB3	21:a:601:CLA:HED3	1.95	0.48
38:6:610:CHL:H91	21:6:615:CLA:H202	1.95	0.48
37:8:502:LUT:H32	38:8:604:CHL:HBB1	1.96	0.48
21:8:618:CLA:HBC2	30:8:810: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	21:B:1203:CLA:H112	1.95	0.48
2:B:677:GLU:HG3	3:C:81:TYR:HD2	1.79	0.48
21:B:1215:CLA:HHC	21:B:1215:CLA:HBB1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:K:5001:LAP:H62	31:K:5001:LAP:H31	1.74	0.48
13:a:126:LEU:HD11	38:a:613:CHL:C2D	2.44	0.48
17:6:61:ASP:OD1	17:6:64:GLY:N	2.45	0.48
21:6:617:CLA:HHC	21:6:617:CLA:HBB1	1.94	0.48
18:7:161:CYS:HB3	18:7:168:THR:HG23	1.95	0.48
1:A:598:TRP:CH2	21:B:1022:CLA:HAB	2.49	0.48
21:A:1103:CLA:HBB1	21:A:1103:CLA:HHC	1.96	0.48
30:B:5005:PTY:H151	6:F:407:PRO:HB3	1.95	0.48
21:F:1301:CLA:HAA1	31:F:5003:LAP:H151	1.96	0.48
12:L:318:SER:HB3	12:L:321:ILE:HD13	1.94	0.48
21:1:607:CLA:CBB	21:a:612:CLA:H11	2.44	0.48
37:a:503:LUT:H41	38:a:606:CHL:H2	1.96	0.48
14:3:337:PRO:HG2	21:3:616:CLA:O1D	2.13	0.48
38:4:618: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
37:5:505:LUT:H362	21:5:617: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
21:A:1105:CLA:HBA1	21:A:1107:CLA:H2	1.95	0.48
21:A:1118:CLA:HBA2	21:A:1118:CLA:H3A	1.37	0.48
2:B:722:TYR:HB2	21:B:1021:CLA:HED3	1.96	0.48
13:a:222:PRO:HG3	21:a:615:CLA:HMB2	1.96	0.48
21:3:616:CLA:H102	21:3:616:CLA:H62	1.53	0.48
24:4:802:LHG:O9	24:4:802:LHG:HC61	2.12	0.48
38:6:610:CHL:CAB	38:6:613:CHL:HBB2	2.43	0.48
38:6:619:CHL:HBB1	38:6:619:CHL:HMB1	1.95	0.48
25:8:802:DGD:HG11	25:8:802:DGD:HA91	1.95	0.48
37:8:502:LUT:H34	38:8:604:CHL:HBB2	1.96	0.48
1:A:153:ILE:HG21	1:A:159:LEU:CD1	2.44	0.48
21:A:1127:CLA:HBB1	21:A:1127:CLA:HHC	1.96	0.48
2:B:431:GLY:HA2	2:B:526:LEU:HD22	1.96	0.48
21:B:1022:CLA:H101	21:B:1023:CLA:H141	1.95	0.48
21:B:1204:CLA:HBB1	21:B:1204:CLA:H111	1.95	0.48
4:D:310:ARG:HB2	4:D:313:GLN:HG3	1.95	0.48
21:F:1302:CLA:H62	46:7:807:4RF:H4	1.95	0.48
21:K:1401:CLA:HBB1	23:K:4002:BCR:C11	2.44	0.48
38:1:609:CHL:HBA2	21:8:618:CLA:O1D	2.14	0.48
15:4:119:LYS:HD2	21:4:610: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
21:A:1109:CLA:C10	21:A:1101:CLA:HBB2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:256:LEU:HD21	21:B:1212:CLA:HBC1	1.95	0.47
2:B:662:PHE:HE1	2:B:714:PHE:CE2	2.32	0.47
21:B:1234:CLA:HBA2	21:B:1235:CLA:CAA	2.41	0.47
21:B:1228:CLA:H111	6:F:462:PHE:HD1	1.79	0.47
8:J:24:THR:HB	35:J:5001:LPX:H4	1.95	0.47
21:a:605:CLA:H41	21:a:605:CLA:H93	1.96	0.47
16:5:197:PHE:CD2	37:5:502:LUT:H12	2.48	0.47
17:6:135:ARG:HE	21:6:617:CLA:HMC1	1.79	0.47
17:6:183:LYS:HA	21:6:607:CLA:OBD	2.13	0.47
19:8:208:PHE:HE1	37:8:501:LUT:H41	1.78	0.47
1:A:334:THR:HG1	24:A:5001:LHG:H02	1.61	0.47
1:A:508:PRO:HG2	1:A:523:MET:HB3	1.96	0.47
1:A:677:PHE:HB2	21:A:1012:CLA:O1A	2.14	0.47
21:A:1126:CLA:H3A	21:A:1126:CLA:HBA2	1.45	0.47
2:B:27:ALA:HA	21: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
17:6:78:SER:OG	21:6:604:CLA:HMB1	2.13	0.47
37:6:501:LUT:H373	38:6:611: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
21:B:1206:CLA:H41	21:B:1206:CLA:H61	1.58	0.47
21:B:1212:CLA:HBA2	21:B:1212:CLA:H3A	1.54	0.47
13:1:90:GLY:HA2	13:1:93:VAL:HG12	1.96	0.47
37:a:501:LUT:H28	21:a:601:CLA:H2	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	24:6:801:LHG:HC62	1.94	0.47
37:6:502:LUT:H193	38:6:610:CHL:CBB	2.44	0.47
18:7:110:PHE:HE2	21:7:611:CLA:CBB	2.27	0.47
1:A:18:ASP:CG	1:A:71:ARG:HH22	2.22	0.47
1:A:197:MET:HB2	21:A:1111:CLA:CBC	2.44	0.47
21:A:1133:CLA:H41	21:A:1133:CLA:H61	1.44	0.47
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
21:B:1209:CLA:H162	21:B:1209:CLA:H141	1.64	0.47
21:B:1223:CLA:H2	23:B:4005:BCR:H14C	1.96	0.47
6:F:448:TRP:HZ3	21:F:1302:CLA:C4A	2.28	0.47
13:1:205:HIS:CG	21:1:603:CLA:HAA2	2.50	0.47
24:1:802:LHG:H121	24:1:802:LHG:HC92	1.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:3:328:GLU:OE2	14:3:464:ALA:N	2.47	0.47
21:4:610:CLA:H111	21:4:610:CLA:H142	1.74	0.47
16:5:188:LYS:NZ	24:5:801:LHG:HC41	2.28	0.47
17:6:104:PHE:HB3	17:6:107:THR:OG1	2.14	0.47
37:6:501:LUT:H30	21:6:601:CLA:H72	1.97	0.47
21:7:603:CLA:H143	21:7:603:CLA:H161	1.74	0.47
21:7:605:CLA:H3A	21:7:605: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	21:B:1023:CLA:C9	2.45	0.47
24:A:5002:LHG:H161	21:A:1101:CLA:HMB2	1.96	0.47
2:B:561:ASP:CG	2:B:565:ARG:HH22	2.21	0.47
21:B:1222:CLA:H41	21:B:1234:CLA:H92	1.96	0.47
29:B:5004:PCW:H322	23: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	33:G:5002:ERG:H181	2.43	0.47
21:4:610:CLA:CBB	21:8:620:CLA:H18	2.44	0.47
17:6:61:ASP:OD2	21:6:604:CLA:HBA2	2.15	0.47
1:A:197:MET:HB2	21:A:1111:CLA:HBC3	1.95	0.47
22:A:2001:PQN:H261	22:A:2001:PQN:H222	1.74	0.47
2:B:530:THR:O	2:B:534:ILE:HG13	2.14	0.47
2:B:676:ILE:HG23	21:B:1238:CLA:CMC	2.44	0.47
21:B:1021:CLA:H8	21:B:1021:CLA:H51	1.60	0.47
23:B:4004:BCR:HC22	21:1:612:CLA:H41	1.95	0.47
8:J:32:VAL:HA	34:J:4002:RRX:H49	1.97	0.47
29:6:803:PCW:H141	29:6:803:PCW:H321	1.95	0.47
18:7:21:TYR:CZ	18:7:39:SER:HA	2.50	0.47
21:A:1132:CLA:HBC3	21:B:1023:CLA:H143	1.96	0.47
2:B:463:TRP:CD2	21:F:1301:CLA:HMA3	2.50	0.47
2:B:662:PHE:HE1	2:B:714:PHE:HE2	1.63	0.47
21:B:1208:CLA:H91	21:B:1208:CLA:H112	1.69	0.47
21:B:1212:CLA:H8	23:B:4001:BCR:H24C	1.97	0.47
4:D:254:LYS:HG2	4:D:258:LEU:HD13	1.95	0.47
21:1:605:CLA:H62	21:1:605:CLA:H41	1.41	0.47
13:a:46:LEU:HD22	21:a:604:CLA:O1D	2.15	0.47
13:a:96:TYR:CZ	13:a:115:PHE:HA	2.49	0.47
37:a:503:LUT:H162	38:a:606:CHL:CHC	2.44	0.47
14:3:282:GLY:HA3	14:3:438:ILE:HD13	1.97	0.47
21:5:604:CLA:H62	21:5:605:CLA:HMA3	1.95	0.47
38:5:613:CHL:HBB1	38:5:613:CHL:HMB1	1.96	0.47
17:6:181:LYS:HG3	21:6:601:CLA:HMA1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:6:501:LUT:H35	37:6:501:LUT:H401	1.75	0.47
21:6:603:CLA:H62	21:6:603:CLA:CHC	2.44	0.47
21:6:609:CLA:H3A	21:6:609:CLA:HBA2	1.46	0.47
21:7:603:CLA:H121	24:7:801:LHG:H341	1.96	0.47
24:7:803:LHG:HC12	24:7:803:LHG:O6	2.14	0.47
21:8:618:CLA:H52	21:8:618:CLA:H11	1.57	0.47
21:8:620:CLA:HBB1	21:8:620:CLA:HMB3	1.97	0.47
24:A:5003:LHG:HO1	24:A:5003:LHG:P	2.38	0.47
21:B:1203:CLA:H43	25:B:5003:DGD:HB51	1.96	0.47
13:a:83:LEU:HB3	38:a:606:CHL:CBB	2.45	0.47
13:a:141:ARG:HA	21:a:611:CLA:C3C	2.45	0.47
35:a:804:LPX:H16	35:a:804:LPX:H19A	1.52	0.47
14:3:421:LEU:HD13	16:5:35:PHE:CZ	2.50	0.47
21:4:608: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	21:7:602: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
21:B:1208:CLA:HBB1	21:B:1208:CLA:HMB1	1.97	0.47
31:B:5007:LAP:H162	31:B:5007:LAP:H193	1.68	0.47
4:D:231:ILE:HG12	4:D:241:ILE:HG12	1.97	0.47
31:F:5003:LAP:H62	31:F:5003:LAP:H31	1.63	0.47
21:1:611:CLA:HBA1	39:1:803:OLA:H162	1.97	0.47
14:3:307:SER:O	14:3:311:VAL:HG23	2.15	0.47
21:7:601:CLA:HMB3	21:7:601:CLA:HBB1	1.96	0.47
1:A:219:HIS:CE1	21: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	23:G:4001:BCR:HC32	2.50	0.47
2:B:536:VAL:HG13	23:B:4004:BCR:H282	1.97	0.47
21:B:1220:CLA:H143	21:B:1220:CLA:H111	1.71	0.47
4:D:309:ARG:HB2	4:D:313:GLN:HB2	1.96	0.47
37:1:503:LUT:H15	37:1:503:LUT:H201	1.77	0.47
13:a:36:TRP:HE1	38:a:609:CHL:C3B	2.27	0.47
21:a:612:CLA:H3A	21:a:612:CLA:HBA2	1.56	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
17:6:261:HIS:O	17:6:262:SER:OG	2.22	0.47
37:8:501:LUT:H24	38:8:601:CHL:HBA1	1.97	0.47
1:A:678:VAL:HG11	1:A:733:LEU:HD23	1.97	0.46
21:A:1105:CLA:H8	25:A:5005:DGD:HB52	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1136:CLA:H41	21:A:1136:CLA:H61	1.54	0.46
2:B:386:GLY:HA3	21:B:1226:CLA:C2C	2.45	0.46
2:B:388:PHE:HZ	21: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	23:L:4002:BCR:HC31	2.44	0.46
23:B:4001:BCR:H321	7:G:1301:ALA:HB1	1.97	0.46
21:F:1302:CLA:C3D	46:7:807:4RF:H35	2.45	0.46
14:3:326:ALA:HB2	23:3:504:BCR:H383	1.96	0.46
16:5:207:THR:C	16:5:235:MET:HG3	2.40	0.46
17:6:106:TYR:CE1	17:6:243:ILE:HD13	2.50	0.46
17:6:150:PRO:HD3	21:6:617:CLA:CMC	2.45	0.46
21:7:611:CLA:H61	21:7:611: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
21:A:1102:CLA:HBA1	21:A:1102:CLA:H3A	1.46	0.46
21:A:1105:CLA:H11	21:A:1105:CLA:H51	1.65	0.46
2:B:298:ILE:CD1	7:G:1297:VAL:HG12	2.42	0.46
2:B:358:PRO:HG3	21:B:1215:CLA:HBA1	1.97	0.46
9:K:56:LEU:O	21:K:1403:CLA:C4D	2.63	0.46
38:a:609:CHL:CGA	38:4:618:CHL:O1D	2.63	0.46
37:5:505:LUT:H381	37:5:505:LUT:H27	1.58	0.46
21:6:604:CLA:H192	21:6:604:CLA:H161	1.74	0.46
21:8:606:CLA:H52	21:8:606:CLA:H11	1.73	0.46
1:A:365:ILE:O	1:A:369:HIS:CD2	2.67	0.46
1:A:389:SER:HB3	21:A:1126:CLA:CMA	2.45	0.46
21:A:1133:CLA:H121	21:A:1133:CLA:H161	1.40	0.46
21:B:1201:CLA:HMA3	10:M:29:LEU:HD22	1.97	0.46
21:B:1226:CLA:H193	21:B:1226:CLA:H161	1.73	0.46
3:C:80:ALA:HB2	4:D:253:ARG:HD3	1.97	0.46
21:1:604:CLA:HBA2	21:1:604:CLA:H3A	1.50	0.46
38:1:613:CHL:HMB3	38:1:613:CHL:HBB1	1.97	0.46
13:a:142:GLY:O	13:a:149:ARG:HD3	2.16	0.46
38:6:619:CHL:H121	38:6:619:CHL:H161	1.72	0.46
18:7:113:PHE:CE1	21:7:612:CLA:CMB	2.99	0.46
21:7:603:CLA:H2	21:7:608:CLA:HMD2	1.96	0.46
1:A:198:LEU:HD12	1:A:322:LEU:HD11	1.96	0.46
1:A:396:TRP:HB3	21:A:1126:CLA:HMC2	1.97	0.46
1:A:740:TRP:CG	23:A:4005:BCR:HC42	2.51	0.46
21:B:1201:CLA:H72	11:I:29:TYR:CZ	2.42	0.46
12:L:330:ALA:HB2	21:L:1502:CLA:HMD3	1.97	0.46
13:1:55:PHE:HB3	21:1:604:CLA:CAD	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:193:ALA:HB2	21:1:615:CLA:HED3	1.98	0.46
13:a:60:LEU:CD2	19:8:157:PHE:HE1	2.29	0.46
14:3:315:ARG:NE	14:3:437:GLU:OE2	2.45	0.46
14:3:362:MET:HE2	14:3:366:SER:HB3	1.97	0.46
21:5:603:CLA:H62	21:5:603:CLA:H41	1.69	0.46
17:6:54:LEU:HD12	21:6:604:CLA:HED2	1.98	0.46
17:6:198:PHE:HE1	37:6:501:LUT:C6	2.29	0.46
25:8:802:DGD:HE1	25:8:802:DGD:HD5	1.52	0.46
25:8:802:DGD:HBH2	25:8:802:DGD:HB92	1.97	0.46
2:B:341:SER:HB3	21:B:1221:CLA:H2	1.98	0.46
2:B:478:LEU:O	2:B:484:SER:OG	2.31	0.46
14:3:275:TYR:CE2	14:3:292:CYS:HB3	2.48	0.46
21:4:601:CLA:O1A	21:4:601:CLA:H3A	2.15	0.46
17:6:138:TYR:HB3	17:6:146:MET:HE3	1.96	0.46
21:6:603:CLA:H72	24:6:801:LHG:H172	1.97	0.46
29:6:803:PCW:H321	29:6:803:PCW:H122	1.97	0.46
45:7:502:XAT:C34	21:7:605:CLA:HAB	2.45	0.46
43:8:803:DGA:HB91	21:8:605:CLA:HED3	1.96	0.46
38:8:604:CHL:H3A	38:8:604: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	21:A:1121:CLA:HED1	2.46	0.46
1:A:695:GLU:OE2	2:B:537:LYS:NZ	2.31	0.46
2:B:60:LEU:HD12	36: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	21:B:1234:CLA:H43	1.98	0.46
21:B:1021:CLA:HBA2	21: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	21:L:1503:CLA:HBC3	1.97	0.46
21:1:607:CLA:H93	35:a:804:LPX:C11	2.45	0.46
15:4:56:PRO:O	21:7:617:CLA:H11	2.16	0.46
16:5:35:PHE:HE1	21:5:609:CLA:CBB	2.29	0.46
18:7:56:ARG:HA	18:7:59:MET:HE3	1.97	0.46
21:A:1103:CLA:H51	21:A:1111:CLA:H12	1.98	0.46
21:A:1135:CLA:H102	21:A:1135:CLA:H62	1.56	0.46
2:B:649:TRP:CE3	23:B:4007:BCR:HC31	2.50	0.46
3:C:15:THR:O	3:C:19:ARG:HG3	2.15	0.46
37:a:501:LUT:H35	37:a:501:LUT:H401	1.79	0.46
21:3:601:CLA:H192	21:3:601:CLA:H162	1.75	0.46
21:3:616:CLA:H2	21:5:616:CLA:O2D	2.16	0.46
37:4:502:LUT:H32	21:4:604:CLA:CAB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:4:607:CLA:H3A	21:4:607:CLA:H43	1.98	0.46
16:5:51:ASP:CG	21:5:604:CLA:HED2	2.41	0.46
21:5:605:CLA:OBD	21:5:612: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	21:8:609:CLA:HAA2	2.32	0.46
1:A:169:MET:HE2	1:A:169:MET:HB2	1.80	0.46
4:D:218:GLU:OE2	4:D:277:VAL:N	2.49	0.46
38:4:609:CHL:HBA2	24:4:801:LHG:H161	1.97	0.46
16:5:188:LYS:HZ1	24:5:801:LHG:HC41	1.80	0.46
19:8:98:VAL:HG12	19:8:99:LEU:HG	1.98	0.46
19:8:137:LYS:HE3	21:8:611:CLA:HMC2	1.98	0.46
1:A:116:GLN:NE2	21:A:1107:CLA:OBD	2.45	0.46
28:A:5008:LMT:H12	18:7:225:PHE:HB3	1.97	0.46
2:B:311:PRO:HB2	24: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
13:a:60:LEU:HD22	19:8:157:PHE:HE1	1.80	0.46
13:a:142:GLY:C	13:a:144:ALA:H	2.23	0.46
14:3:454:GLN:HB3	14:3:465:ASN:HD22	1.81	0.46
21:3:607:CLA:C1B	24:3:801:LHG:HC2	2.46	0.46
15:4:230:SER:HB3	15:4:231:PRO:HD2	1.97	0.46
21:6:604:CLA:H2	21:6:604: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	23:7:503:BCR:H16C	1.98	0.46
21:8:610:CLA:H93	21:8:610:CLA:H61	1.66	0.46
1:A:205:LEU:HD11	21:A:1111:CLA:H42	1.97	0.46
1:A:374:MET:O	1:A:374:MET:HG3	2.16	0.46
21:A:1109:CLA:H61	21:A:1109:CLA:H92	1.75	0.46
21:A:1134:CLA:H62	21:A:1134:CLA:H92	1.71	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
2:B:650:MET:HE1	21:B:1205:CLA:HBC3	1.98	0.46
3:C:17:CYS:HB3	27:C:3003:SF4:S4	2.55	0.46
7:G:1260:LYS:O	7:G:1260:LYS:HD3	2.15	0.46
37:1:502:LUT:H24	21:1:604:CLA:O1A	2.17	0.46
21:1:611:CLA:HBB1	39:1:803:OLA:H111	1.98	0.46
13:a:178:ARG:HA	13:a:181:MET:HE3	1.96	0.46
21:a:608:CLA:H8	21:a:608:CLA:H51	1.74	0.46
14:3:481:ASN:ND2	21:3:603:CLA:HED2	2.28	0.46
14:3:486:LEU:HD23	14:3:486:LEU:HA	1.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:8:802:DGD:HA62	25:8:802:DGD:HA32	1.58	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	21:A:1127:CLA:H193	1.97	0.45
1:A:657:VAL:HG21	1:A:742:PHE:HA	1.97	0.45
21:A:1126:CLA:H102	21:A:1126:CLA:H62	1.31	0.45
2:B:669:ARG:HB2	22:B:2002:PQN:H7	1.97	0.45
21:B:1228:CLA:H141	21:B:1228:CLA:H162	1.78	0.45
3:C:27:GLU:CD	4:D:294:PRO:HA	2.39	0.45
21:K:1402:CLA:H51	21:K:1402:CLA:H11	1.71	0.45
37:3:502:LUT:H161	21:3:613:CLA:HAB	1.99	0.45
15:4:127:PHE:CD1	21:4:610:CLA:HED3	2.51	0.45
30:8:810:PTY:H172	30:8:810:PTY:H142	1.63	0.45
21:A:1103:CLA:H3A	21:A:1103:CLA:HBA1	1.57	0.45
21:A:1125:CLA:H2	21:A:1125:CLA:H61	1.84	0.45
21:A:1101:CLA:HHC	21: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
21:B:1205:CLA:H143	21:B:1205:CLA:H161	1.73	0.45
13:1:161:MET:HG3	13:1:169:LEU:HD11	1.98	0.45
13:a:90:GLY:HA2	13:a:93:VAL:HG12	1.97	0.45
14:3:329:ILE:HD13	23:3:504:BCR:H282	1.98	0.45
16:5:41:PRO:HD2	16:5:44:LEU:HB2	1.97	0.45
21:5:603:CLA:H2	21:5:608:CLA:CMD	2.47	0.45
17:6:193:LEU:CD1	24:6:801:LHG:H302	2.45	0.45
37:6:502:LUT:C35	21:6:605:CLA:HAB	2.45	0.45
21:6:602:CLA:H11	21:6:602:CLA:H51	1.61	0.45
21:6:609:CLA:HMB2	24:6:801:LHG:H321	1.98	0.45
46:8:808:4RF:H46	39:8:809: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	21:A:1140:CLA:C1C	2.46	0.45
21:A:1103:CLA:H121	23:A:4002:BCR:H343	1.97	0.45
2:B:649:TRP:CZ3	23:B:4007:BCR:HC31	2.51	0.45
21:B:1229:CLA:H152	21:B:1229:CLA:H112	1.71	0.45
9:K:55:GLY:O	21:K:1403:CLA:HED2	2.16	0.45
37:1:501:LUT:H15	37:1:501:LUT:H201	1.86	0.45
21:1:601:CLA:H92	21:1:601:CLA:H61	1.78	0.45
21:1:604:CLA:H121	21:1:604:CLA:H162	1.74	0.45
14:3:442:ARG:HA	14:3:445:MET:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:4:801:LHG:C8	23:6:503:BCR:HC22	2.46	0.45
18:7:35:LEU:HD12	45:7:502:XAT:H221	1.98	0.45
18:7:107:MET:HG2	21:8:608: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	37:8:502:LUT:H10	2.52	0.45
1:A:157:LEU:HD11	28:A:5008:LMT:H11	1.97	0.45
1:A:299:LEU:HD22	21:A:1113:CLA:HAC1	1.97	0.45
21:A:1121:CLA:H111	23:K:4001:BCR:H381	1.99	0.45
21:A:1122:CLA:HBB1	21:A:1129:CLA:HBC2	1.98	0.45
2:B:231:TRP:CZ2	7:G:1311:PHE:HD2	2.34	0.45
2:B:308:ALA:HB3	21:B:1219:CLA:O1D	2.16	0.45
21:B:1201:CLA:H203	21:B:1201:CLA:H162	1.67	0.45
21:B:1226:CLA:H41	21:B:1226:CLA:H62	1.50	0.45
3:C:23:THR:HG22	3:C:23:THR:O	2.16	0.45
32:G:5001:SQD:H171	32:G:5001:SQD:H321	1.98	0.45
37:4:501:LUT:H35	37:4:501:LUT:H401	1.83	0.45
17:6:125:GLU:OE1	38:6:613:CHL:C1B	2.64	0.45
21:7:601:CLA:H3A	21:7:601:CLA:O1A	2.17	0.45
19:8:203:VAL:HG21	24:8:801:LHG:H261	1.98	0.45
21:A:1103:CLA:H151	23:A:4001:BCR:H323	1.98	0.45
21:A:1121:CLA:CED	9:K:66:GLN:HG2	2.47	0.45
2:B:175:ARG:HH21	21:B:1221:CLA:HMD2	1.82	0.45
24:B:5001:LHG:H131	24:B:5001:LHG:H161	1.81	0.45
24:5:801:LHG:H311	24:5:801:LHG:H281	1.42	0.45
17:6:265:PRO:HB2	38:6:619:CHL:HAB	1.98	0.45
1:A:120:PRO:HA	1:A:125:GLU:HG3	1.98	0.45
1:A:198:LEU:HG	21:A:1123:CLA:HMD2	1.99	0.45
21:A:1104:CLA:H2	21:A:1104:CLA:HED2	1.99	0.45
21:A:1106:CLA:HBA2	21:A:1106:CLA:H3A	1.35	0.45
2:B:38:MET:HE2	2:B:43:LEU:HA	1.99	0.45
2:B:657:ILE:HG12	21:B:1239:CLA:CMB	2.46	0.45
29:B:5004:PCW:H62	29:B:5004:PCW:H42	1.68	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
21:a:607:CLA:H61	21:a:607:CLA:H41	1.60	0.45
14:3:344:VAL:HG21	14:3:347:ARG:HH21	1.81	0.45
14:3:362:MET:HE2	14:3:366:SER:CB	2.47	0.45
16:5:155:LEU:HD13	21:5:618:CLA:CBD	2.47	0.45
37:6:501:LUT:H362	21:6:601:CLA:H42	1.98	0.45
30:7:804:PTY:H142	30:7:804:PTY:H112	1.64	0.45
21:7:617:CLA:HHC	21:7:617:CLA:CBB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ILE:O	1:A:73:VAL:HG23	2.16	0.45
21:A:1107:CLA:HBB1	21:A:1107:CLA:HMB3	1.99	0.45
2:B:577:PHE:CE2	25:B:5003:DGD:HB81	2.52	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	33:G:5002:ERG:H213	2.46	0.45
12:L:350:TYR:OH	21:L:1503:CLA:OBD	2.34	0.45
23:L:4001:BCR:H281	21:L:1502:CLA:CHD	2.47	0.45
38:a:610:CHL:CBB	38:a:613:CHL:HBB2	2.47	0.45
14:3:308:TYR:O	14:3:312:ILE:HG12	2.17	0.45
21:3:606:CLA:H2	21:3:613:CLA:CAD	2.46	0.45
16:5:131:PHE:HB2	21:6:609:CLA:H11	1.98	0.45
16:5:218:HIS:CG	21:5:603:CLA:HAA2	2.52	0.45
17:6:145:SER:OG	17:6:146:MET:N	2.46	0.45
18:7:50:ALA:CA	21:7:612:CLA:HED2	2.46	0.45
18:7:109:GLY:HA2	21:7:612: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	21:A:1127:CLA:HED2	2.52	0.45
2:B:210:TRP:HA	2:B:213:PHE:CD1	2.52	0.45
21:B:1220:CLA:HMA1	21:B:1240:CLA:CGD	2.47	0.45
21:B:1220:CLA:HMD3	21:B:1221:CLA:HAB	1.98	0.45
32:G:5001:SQD:O49	32:G:5001:SQD:H441	2.11	0.45
9:K:89:ASN:N	9:K:92:ASP:OD2	2.41	0.45
21:3:603:CLA:H41	21:3:603:CLA:H62	1.57	0.45
19:8:144:LYS:O	19:8:147:SER:OG	2.33	0.45
1:A:303:VAL:HG21	21:A:1115:CLA:CBB	2.47	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
23:5:504:BCR:H21C	38:5:610:CHL:CGA	2.47	0.45
21:5:612:CLA:H62	21:5:612: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	23:6:503:BCR:C17	2.39	0.45
21:8:609:CLA:H3A	21:8:609:CLA:HBA1	1.63	0.45
21:8:602:CLA:HHC	21:8:602: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
21:A:1109:CLA:H18	21:A:1109:CLA:H152	1.49	0.45
21:A:1131:CLA:HBB2	12:L:359:LEU:HD13	1.99	0.45
2:B:374:THR:HB	21:B:1224:CLA:HMB1	1.98	0.45
2:B:665:LEU:HD23	2:B:665:LEU:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:F:5002:LHG:H271	24:F:5002:LHG:H242	1.51	0.45
11:I:16:LEU:C	11:I:19:PRO:HD2	2.42	0.45
12:L:356:PHE:HD2	12:L:376:ASN:HD21	1.65	0.45
23:L:4002:BCR:H333	21:L:1502:CLA:NB	2.32	0.45
14:3:306:LEU:HD12	21:3:604:CLA:H12	1.99	0.45
14:3:384:GLN:HG2	18:7:11:PHE:CE2	2.52	0.45
15:4:231:PRO:C	15:4:233:LEU:H	2.24	0.45
21:5:609:CLA:HBD	24:5:801:LHG:HC62	1.98	0.45
21:6:603:CLA:H152	21:6:603: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
1:A:15:ILE:HD13	21: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	31:F:5003:LAP:H182	2.31	0.44
13:a:114:TYR:C	13:a:116:GLY:H	2.25	0.44
15:4:171:PHE:HB2	21:4:601:CLA:CGA	2.47	0.44
16:5:132:VAL:HG11	23:5:503:BCR:H16C	1.98	0.44
17:6:41:PRO:HD3	21:6:609:CLA:C3D	2.47	0.44
17:6:62:PRO:CB	44:6:806:SPH:H101	2.48	0.44
17:6:125:GLU:OE1	38:6:613:CHL:C4A	2.66	0.44
21:6:602:CLA:OBD	21:6:607: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	24:7:801:LHG:O5	2.50	0.44
21:7:601:CLA:H62	21:7:602:CLA:HMA2	1.99	0.44
1:A:25:ASN:O	21:A:1109:CLA:HMB3	2.17	0.44
21:A:1114:CLA:H121	21:A:1114:CLA:CBB	2.47	0.44
21:B:1023:CLA:H41	21: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	23:L:4001:BCR:C33	2.47	0.44
37:a:503:LUT:H35	37:a:503:LUT:H401	1.71	0.44
21:a:605:CLA:CGD	21:a:612:CLA:H2	2.47	0.44
21:3:603:CLA:H112	21:3:603:CLA:H72	1.67	0.44
15:4:200:GLN:NE2	15:4:211:GLN:OE1	2.47	0.44
24:4:801:LHG:H321	24:4:801:LHG:H142	1.99	0.44
16:5:195:VAL:HG21	24:5:801:LHG:H131	1.98	0.44
17:6:125:GLU:OE2	38:6:613:CHL:CMB	2.66	0.44
17:6:207:LYS:HE3	17:6:207:LYS:HB3	1.73	0.44
23:6:504:BCR:H351	23:6:504:BCR:H15C	1.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:PHE:CZ	1:A:732:LEU:HD23	2.53	0.44
1:A:457:ILE:HD12	21:B:1023:CLA:H92	2.00	0.44
21:A:1108:CLA:H13	23:A:4002:BCR:H372	1.99	0.44
21:A:1134:CLA:H111	21:A:1134:CLA:H91	1.65	0.44
21:A:1135:CLA:HBA2	21: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
21:B:1239:CLA:H141	21:B:1239:CLA:H162	1.78	0.44
3:C:27:GLU:OE2	4:D:294:PRO:O	2.35	0.44
4:D:218:GLU:CD	4:D:276:ARG:HG3	2.42	0.44
21:G:1603:CLA:HMC1	21:1:610:CLA:HBA2	2.00	0.44
9:K:96:LEU:HD22	21:K:1403:CLA:HBB1	1.99	0.44
13:1:211:ALA:C	13:1:216:THR:HG21	2.43	0.44
38:1:609:CHL:H92	38:1:609:CHL:H62	1.73	0.44
38:a:609:CHL:HBA1	38:4:618:CHL:O1D	2.18	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
16:5:127:ILE:HG23	16:5:127:ILE:HD12	1.72	0.44
38:6:610:CHL:HAB	38:6:613:CHL:HBB2	1.98	0.44
1:A:552:LYS:NZ	2:B:674:GLU:OE1	2.51	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
4:D:287:HIS:O	4:D:289:LYS:N	2.50	0.44
13:a:53:TYR:OH	13:a:175:LYS:HD3	2.17	0.44
14:3:306:LEU:HB3	21:3:604:CLA:CMA	2.45	0.44
14:3:312:ILE:HG21	14:3:382:ARG:HH12	1.82	0.44
15:4:188:ARG:HA	15:4:191:MET:HE2	1.99	0.44
23:4:503:BCR:H271	21:4:606:CLA:NB	2.33	0.44
23:5:503:BCR:H343	21:5:618:CLA:HAB	1.98	0.44
17:6:247:ILE:HD11	17:6:254:ILE:HB	1.98	0.44
37:6:502:LUT:H35	37:6:502:LUT:H401	1.79	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	21:A:1116:CLA:C1B	2.48	0.44
21:A:1128:CLA:H41	21:A:1128:CLA:H61	1.56	0.44
21:A:1131:CLA:H71	21:B:1238:CLA:H71	1.98	0.44
28:A:5008:LMT:H5'	28:A:5008:LMT:H1B	1.64	0.44
21:B:1223:CLA:HBB1	21:B:1231:CLA:HMA2	2.00	0.44
23:B:4007:BCR:H351	23:B:4007:BCR:H15C	1.76	0.44
5:E:69:ILE:HG22	5:E:71:TYR:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:605:CLA:H51	21:1:605:CLA:H11	1.86	0.44
21:1:605:CLA:H61	21:1:605:CLA:H92	1.79	0.44
21:a:602:CLA:CGD	21:a:602:CLA:HBA2	2.47	0.44
38:4:609:CHL:HHD	38:4:609:CHL:CBC	2.44	0.44
38:5:613:CHL:H62	38:5:613:CHL:H41	1.60	0.44
21:5:617:CLA:HED1	24:6:801:LHG:H321	1.98	0.44
38:6:613:CHL:HBA1	38:6:613:CHL:H3A	1.75	0.44
18:7:21:TYR:CE2	18:7:39:SER:HA	2.53	0.44
19:8:171:GLY:O	19:8:174:PHE:HB2	2.17	0.44
1:A:59:PHE:CD2	21:A:1103:CLA:HMC2	2.52	0.44
1:A:423:TYR:CZ	4:D:241:ILE:HD11	2.52	0.44
2:B:438:TYR:CE2	21:B:1021:CLA:H162	2.53	0.44
2:B:490:GLY:O	2:B:495:LEU:HB2	2.17	0.44
2:B:657:ILE:HG12	21:B:1239:CLA:HMB3	1.98	0.44
21:B:1201:CLA:H101	21:B:1201:CLA:C3	2.47	0.44
21:B:1227:CLA:HMB3	21:B:1227:CLA:HBB1	2.00	0.44
21:B:1228:CLA:H192	21: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
6:F:336:LYS:O	6:F:340:LYS:HE2	2.18	0.44
21:G:1602:CLA:HED2	21:G:1602:CLA:H2A	1.99	0.44
15:4:138:MET:HE2	21:4:612:CLA:HMA2	2.00	0.44
21:4:603:CLA:H61	21:4:603:CLA:H101	1.56	0.44
21:4:610:CLA:H62	21:4:610:CLA:H2	1.71	0.44
1:A:355:ILE:O	1:A:359:LEU:HD23	2.17	0.44
1:A:718:LEU:HD22	1:A:722:GLN:CD	2.43	0.44
21:A:1122:CLA:H91	21:A:1122:CLA:H111	1.67	0.44
21:A:1138:CLA:HBA2	21:A:1138:CLA:H3A	1.56	0.44
6:F:379:LEU:O	6:F:387:HIS:N	2.48	0.44
10:M:30:TYR:OH	11:I:29:TYR:OH	2.34	0.44
21:a:605:CLA:H41	21:a:605:CLA:H61	1.47	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
17:6:125:GLU:CD	38:6:613:CHL:C1B	2.91	0.44
19:8:89:ILE:HB	19:8:90:PRO:HD3	2.00	0.44
21:8:603:CLA:C4A	21:8:603:CLA:HBA2	2.47	0.44
1:A:264:PHE:HZ	23:K:4001:BCR:H343	1.83	0.44
1:A:441:LEU:HD13	21:A:1137:CLA:CAB	2.47	0.44
21:B:1221:CLA:H3A	21:B:1221:CLA:HBA1	1.84	0.44
21:B:1226:CLA:H92	21:B:1226:CLA:H61	1.77	0.44
21:B:1234:CLA:H93	21:B:1235:CLA:O1A	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:1228:CLA:CAA	6:F:471:MET:HE2	2.48	0.44
21:B:1229:CLA:HBB1	21:B:1229:CLA:HHC	1.98	0.44
14:3:318:MET:SD	21:3:601:CLA:HAB	2.58	0.44
15:4:168:PRO:HD2	37:4:501: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	38:5:610:CHL:HBC3	1.99	0.44
17:6:41:PRO:HG3	21:6:609:CLA:CMD	2.47	0.44
30:8:810:PTY:H112	30:8:810:PTY:C1	2.47	0.44
1:A:357:LEU:CD2	21:A:1103:CLA:HED1	2.48	0.44
21:A:1013:CLA:H151	21:A:1013:CLA:H112	1.64	0.44
21:A:1135:CLA:H141	21:A:1135:CLA:H162	1.76	0.44
21:B:1235:CLA:H143	21:B:1235:CLA:H111	1.84	0.44
21:B:1237:CLA:H152	21:B:1237:CLA:H112	1.69	0.44
21:a:604:CLA:HBA2	21:a:604:CLA:H3A	1.74	0.44
14:3:420:MET:HE3	16:5:56:PRO:CG	2.47	0.44
14:3:430:MET:HE1	21:3:601:CLA:HED3	1.99	0.44
21:4:607:CLA:H62	21:4:607:CLA:H41	1.76	0.44
24:4:801:LHG:H342	24:4:801:LHG:H372	1.34	0.44
21:5:604:CLA:H2A	21:5:604:CLA:O2D	2.18	0.44
21:5:604:CLA:H3A	21:5:604:CLA:CGA	2.48	0.44
21:7:609:CLA:H142	21:7:609:CLA:H111	1.78	0.44
46:8:807:4RF:C10	21:8:615:CLA:HBA2	2.47	0.44
21:A:1106:CLA:H193	21:A:1106:CLA:H162	1.81	0.43
21:A:1123:CLA:H193	21:A:1123:CLA:H161	1.75	0.43
2:B:258:PHE:HD1	21:B:1214:CLA:HMB3	1.83	0.43
13:1:37:LEU:O	13:1:38:PRO:C	2.60	0.43
21:1:603:CLA:H62	21:1:603:CLA:H41	1.45	0.43
21:1:610:CLA:CAB	38:1:613:CHL:HBB2	2.48	0.43
38:a:613:CHL:HHC	38:a:613:CHL:CBB	2.46	0.43
14:3:413:PRO:HD2	21:3:601:CLA:OBD	2.18	0.43
15:4:134:GLU:HG3	21:4:612:CLA:NB	2.34	0.43
23:5:504:BCR:H402	38:5:610:CHL:H3A	2.00	0.43
23:7:503:BCR:H313	21:8:609:CLA:C2D	2.48	0.43
1:A:425:ASN:O	1:A:429:ARG:HG2	2.18	0.43
1:A:681:PHE:HZ	21:A:1139:CLA:HBC2	1.83	0.43
1:A:744:LEU:HA	1:A:744:LEU:HD23	1.76	0.43
21:A:1119:CLA:OBD	21:A:1121:CLA:HHD	2.18	0.43
2:B:695:ARG:HG3	12:L:393:VAL:CG1	2.48	0.43
21:B:1203:CLA:H41	25:B:5003:DGD:HB72	2.00	0.43
21:B:1208:CLA:HBD	21:B:1208:CLA:HBA1	2.01	0.43
21:B:1213:CLA:H61	21:B:1213:CLA:H102	1.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:F:5001:LHG:H112	24:F:5001:LHG:H311	1.99	0.43
9:K:69:ILE:HG13	21:K:1403:CLA:O1A	2.17	0.43
13:a:55:PHE:HB3	21:a:604:CLA:CAD	2.49	0.43
13:a:214:PHE:HE1	21:a:608:CLA:HED3	1.84	0.43
21:3:601:CLA:H3A	21:3:601:CLA:HBA2	1.43	0.43
15:4:226:ASN:ND2	23:6:504:BCR:HC21	2.33	0.43
15:4:236:ASN:HB2	24:6:802:LHG:C1	2.48	0.43
24:4:801:LHG:H142	24:4:801:LHG:H301	2.01	0.43
16:5:125:GLU:OE1	38:5:610:CHL:HMC	2.18	0.43
21:5:618:CLA:H3A	21:5:618:CLA:HBA2	1.80	0.43
18:7:11:PHE:HD2	18:7:14:ASN:CB	2.30	0.43
18:7:114:LYS:HB3	21:7:611:CLA:HMC2	1.99	0.43
19:8:35:GLN:HB3	19:8:38:VAL:HB	2.00	0.43
19:8:235:PHE:CD1	21:8:603:CLA:H11	2.54	0.43
1:A:442:ASN:ND2	2:B:675:LEU:CD1	2.70	0.43
1:A:736:ILE:HG21	21:A:1126:CLA:HMC1	2.00	0.43
2:B:51:HIS:HE1	21:B:1202:CLA:H171	1.82	0.43
2:B:51:HIS:ND1	21:B:1210:CLA:OBD	2.49	0.43
2:B:701:LEU:HD22	2:B:705:GLN:NE2	2.33	0.43
21:B:1021:CLA:H142	21:B:1021:CLA:H111	1.67	0.43
21:B:1201:CLA:HBC1	25:B:5003:DGD:HAT1	1.99	0.43
21:B:1212:CLA:NB	23:B:4001:BCR:H271	2.33	0.43
7:G:1253:PHE:CE1	28:1:804: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	37:3:501:LUT:H163	2.01	0.43
38:4:609:CHL:H61	38:4:609:CHL:H41	1.47	0.43
16:5:97:GLN:HE22	16:5:107:ASN:HB3	1.83	0.43
17:6:41:PRO:CG	21:6:609:CLA:HMD1	2.48	0.43
17:6:138:TYR:CB	17:6:146:MET:HE3	2.48	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	21:3:605:CLA:H161	2.53	0.43
23:A:4001:BCR:H282	31:K:5001:LAP:H111	1.99	0.43
21:B:1216:CLA:H111	21:B:1216:CLA:H152	1.30	0.43
25:B:5003:DGD:HA81	25: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	21: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	38:1:613:CHL:CMD	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:3:616:CLA:H61	21:3:616:CLA:H41	1.65	0.43
21:4:606:CLA:HBA2	21:4:616:CLA:HMB2	2.01	0.43
21:5:612:CLA:H112	21:5:612: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	24:6:801:LHG:O5	2.66	0.43
17:6:236:ALA:HB2	42:6:804:PLM:H51	2.01	0.43
19:8:123:LEU:HD21	38:8:613:CHL:CHD	2.48	0.43
21:8:612:CLA:H3A	21:8:612: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	23:B:4004:BCR:H291	2.00	0.43
2:B:701:LEU:HD11	21:B:1239:CLA:HMD3	2.00	0.43
2:B:723:ALA:O	2:B:727:ILE:HG12	2.19	0.43
21:B:1215:CLA:H62	21:B:1215:CLA:H41	1.48	0.43
21:B:1231:CLA:H61	23: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
21:K:1401:CLA:HED2	21:K:1401:CLA:H2A	1.99	0.43
36:M:4001:ECH:H15	36:M:4001:ECH:H35	1.78	0.43
13:a:152:PRO:HD2	21:a:601:CLA:OBD	2.18	0.43
13:a:214:PHE:CZ	21:a:615:CLA:HAC2	2.54	0.43
38:4:609:CHL:HAC1	24:4:801:LHG:C4	2.49	0.43
17:6:150:PRO:HG2	21:6:617:CLA:HBB1	2.01	0.43
44:6:806:SPH:H131	44:6:806:SPH:H162	1.36	0.43
37:6:502:LUT:H15	37:6:502:LUT:H201	1.85	0.43
21:6:601:CLA:H61	21:6:601:CLA:H92	1.68	0.43
1:A:706:LYS:NZ	6:F:471:MET:SD	2.92	0.43
21:A:1115:CLA:H3A	21:A:1115:CLA:HBA2	1.76	0.43
21:A:1135:CLA:HED2	21:A:1135:CLA:H2A	2.00	0.43
2:B:107:ARG:O	2:B:109:GLY:N	2.45	0.43
21:B:1225:CLA:H52	23:B:4002:BCR:H23C	2.00	0.43
21:B:1237:CLA:C20	21: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
21:1:607:CLA:CHD	24:1:801:LHG:HC62	2.49	0.43
13:a:121:PHE:HB3	13:a:126:LEU:HD21	2.00	0.43
13:a:137:ALA:O	13:a:141:ARG:HG2	2.18	0.43
13:a:162:SER:O	13:a:166:SER:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:204:SER:OG	13:a:212:VAL:HG11	2.18	0.43
21:3:602:CLA:H3A	21:3:602:CLA:HBA1	1.81	0.43
21:3:607:CLA:H141	21:3:607:CLA:H161	1.67	0.43
38:4:618:CHL:H62	38:4:618:CHL:H41	1.86	0.43
1:A:410:ALA:HB1	1:A:588:ALA:HB1	1.99	0.43
1:A:596:LEU:HD21	21:A:1128:CLA:HBC1	2.00	0.43
29: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
21:K:1401:CLA:HBA2	21:K:1401:CLA:H3A	1.73	0.43
37:1:503:LUT:H11	37:1:503:LUT:H191	1.83	0.43
13:a:107:VAL:HG12	13:a:108:GLN:H	1.84	0.43
13:a:114:TYR:CE2	38:a:606:CHL:H51	2.54	0.43
21:4:615:CLA:H92	21:4:615:CLA:H62	1.83	0.43
17:6:41:PRO:HG2	21:6:609:CLA:CAD	2.48	0.43
1:A:483:PHE:O	1:A:487:VAL:HG23	2.18	0.43
1:A:715:PRO:HG3	21:A:1140:CLA:HBC2	2.00	0.43
21:A:1115:CLA:H42	21:K:1402:CLA:O1D	2.19	0.43
6:F:466:LYS:CB	43:8:803:DGA:HB32	2.49	0.43
31:F:5003:LAP:H132	21:1:615:CLA:HMA1	2.01	0.43
8:J:20:MET:HB2	8:J:20:MET:HE2	1.88	0.43
34:J:4002:RRX:H51	34:J:4002:RRX:C8	2.48	0.43
13:1:72:GLU:OE2	13:1:149:ARG:HD2	2.18	0.43
21:1:602:CLA:HAC2	21:1:603:CLA:H191	2.01	0.43
15:4:142:ILE:HG13	15:4:143:LYS:N	2.34	0.43
38:4:618:CHL:HBA1	38:4:618:CHL:CHA	2.48	0.43
16:5:97:GLN:HG2	21:5:606: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
17:6:265:PRO:CB	38:6:619:CHL:HAB	2.49	0.43
46:8:807:4RF:H2	21:8:615:CLA:HBA2	2.01	0.43
38:8:601:CHL:C4	21:8:602:CLA:HBA1	2.48	0.43
46:8:808:4RF:H10	46:8:808:4RF: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:679:TRP:CG	20:A:1011:CL0:H5	2.53	0.43
20:A:1011:CL0:H15	20:A:1011:CL0:H11	2.00	0.43
2:B:79:VAL:HG13	2:B:126:TYR:HE1	1.83	0.43
2:B:145:VAL:HG11	24:B:5002:LHG:H192	2.01	0.43
2:B:255:ILE:HG13	2:B:256:LEU:HG	2.01	0.43
9:K:59:THR:HB	9:K:92:ASP:OD1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:71:ARG:O	13:1:75:VAL:HG23	2.19	0.43
13:a:214:PHE:CE1	21:a:608:CLA:HED3	2.54	0.43
38:a:613:CHL:HBD	38:a:613:CHL:HAA2	2.00	0.43
14:3:315:ARG:HD2	38:3:611:CHL:OBD	2.19	0.43
21:3:603:CLA:H112	21:3:603:CLA:H151	1.84	0.43
1:A:395:MET:HE3	1:A:395:MET:HB3	1.82	0.43
1:A:407:ALA:HB2	1:A:592:VAL:HG11	2.00	0.43
2:B:348:LEU:HD23	21:B:1215:CLA:H62	2.01	0.43
2:B:349:VAL:HG21	21:B:1225:CLA:HHD	1.99	0.43
2:B:388:PHE:CZ	21:B:1222:CLA:HAB	2.53	0.43
21:B:1023:CLA:C12	23:I:4001:BCR:H281	2.48	0.43
21:B:1239:CLA:H3A	21:B:1239:CLA:HBA2	1.61	0.43
5:E:45:VAL:O	5:E:58:THR:HA	2.19	0.43
12:L:355:PRO:HA	21:L:1503:CLA:HMB2	1.99	0.43
21:4:604:CLA:H62	21:4:604:CLA:H41	1.79	0.43
16:5:200:PHE:HE1	37:5:501:LUT:H41	1.84	0.43
21:5:612:CLA:H71	38:6:619:CHL:H43	2.00	0.43
24:7:801:LHG:H241	24:7:801:LHG:H271	1.44	0.43
1:A:702:TRP:CD1	6:F:477:ILE:CG2	3.02	0.42
21:A:1106:CLA:CBB	21:A:1126:CLA:H171	2.45	0.42
2:B:353:MET:HE2	2:B:353:MET:HB3	1.83	0.42
2:B:520:VAL:HG11	2:B:594:TYR:HB2	2.01	0.42
21:B:1216:CLA:H41	21:B:1216:CLA:H61	1.64	0.42
9:K:69:ILE:HG13	21:K:1403:CLA:CGA	2.49	0.42
37:1:502:LUT:H15	37:1:502:LUT:H201	1.89	0.42
21:1:607:CLA:H61	21:1:607:CLA:H41	1.89	0.42
21:1:607:CLA:H111	21:1:607:CLA:H72	1.53	0.42
37:a:503:LUT:H3	38:a:606:CHL:CHC	2.49	0.42
37:3:501:LUT:H35	37:3:501:LUT:H401	1.89	0.42
38:4:618:CHL:H8	19:8:177:PHE:CE2	2.54	0.42
45:7:502:XAT:H31	45:7:502:XAT:H391	1.77	0.42
1:A:130:ASP:OD1	1:A:136:GLN:NE2	2.51	0.42
21:A:1131:CLA:H72	21:A:1131:CLA:H111	1.61	0.42
21:A:1140:CLA:H62	21:A:1140:CLA:H41	1.67	0.42
21:B:1218:CLA:H41	21:B:1218:CLA:H62	1.48	0.42
21: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
13:a:138:GLU:HG3	21:a:612:CLA:C4B	2.49	0.42
14:3:397:PHE:HD2	14:3:400:LEU:HB2	1.85	0.42
14:3:462:PRO:O	37:3:501:LUT:O3	2.37	0.42
37:5:502:LUT:H15	37:5:502:LUT:H201	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:6:615:CLA:H161	21:6:615:CLA:H122	1.82	0.42
21:7:612:CLA:HBC2	38:7:613:CHL:H192	2.00	0.42
38:7:613:CHL:H152	38:7:613:CHL:H111	1.71	0.42
21:8:608:CLA:O2D	21:8:608: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
2:B:142:PHE:CE2	21:B:1211:CLA:H52	2.54	0.42
21:B:1234:CLA:H2	21:B:1234:CLA:H62	1.71	0.42
21:B:1236:CLA:HBC3	24:B:5001:LHG:H371	2.01	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
21:1:604:CLA:H203	21:1:604:CLA:H161	1.86	0.42
13:a:60:LEU:CD2	19:8:157:PHE:CE1	3.02	0.42
15:4:129:MET:HE3	38:4:613:CHL:CMA	2.47	0.42
37:5:501:LUT:H11	37:5:501:LUT:H191	1.90	0.42
17:6:75:PHE:HB3	21:6:604:CLA:CMA	2.49	0.42
37:6:501:LUT:H191	37:6:501:LUT:H11	1.79	0.42
19:8:120:PHE:CG	46:8:808:4RF:H9	2.54	0.42
21:A:1108:CLA:HHC	21:A:1108:CLA:CBB	2.50	0.42
21:A:1109:CLA:H161	21:A:1109:CLA:H143	1.69	0.42
21:A:1134:CLA:HBA2	21:A:1134:CLA:H3A	1.65	0.42
2:B:600:LEU:O	2:B:604:GLN:HG3	2.20	0.42
9:K:96:LEU:CD2	21:K:1403:CLA:CBB	2.98	0.42
12:L:324:TYR:HD2	12:L:325:LEU:HD22	1.83	0.42
13:a:211:ALA:C	13:a:216:THR:HG21	2.45	0.42
15:4:135:LEU:HD23	15:4:135:LEU:HA	1.89	0.42
23:4:503:BCR:H271	21:4:606:CLA:C4B	2.48	0.42
21:4:604:CLA:H112	21:4:604:CLA:H91	1.82	0.42
21:4:612:CLA:HMB3	21:4:612:CLA:HBB1	2.01	0.42
17:6:112:VAL:HG23	21:6:606:CLA:HED1	2.00	0.42
21:8:610:CLA:HBA2	46:8:808:4RF:H71	2.00	0.42
38:8:613:CHL:HHC	38:8:613:CHL:HBB1	2.00	0.42
1:A:26:PHE:HE1	26:A:5007:3PH:H251	1.85	0.42
1:A:175:PHE:CE2	21:3:605:CLA:H13	2.54	0.42
1:A:698:GLU:CD	2:B:546:LYS:HB3	2.44	0.42
21:A:1013:CLA:H92	21:A:1013:CLA:H61	1.60	0.42
21:A:1111:CLA:H111	21:A:1111:CLA:H91	1.62	0.42
2:B:556:TYR:CD2	21:B:1226:CLA:HED2	2.54	0.42
21:B:1221:CLA:HBB1	21:B:1221:CLA:HMB3	2.01	0.42
6:F:411:PHE:O	6:F:412:ILE:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:6:194:ALA:CB	37:6:501:LUT:H7	2.44	0.42
37:6:502:LUT:H183	21:6:606:CLA:C3B	2.49	0.42
21:6:618:CLA:HHC	21:6:618:CLA:HBB1	2.02	0.42
18:7:125:GLN:HB3	21:7:611:CLA:HMC3	2.02	0.42
18:7:183:MET:SD	21:7:604:CLA:HAB	2.59	0.42
19:8:85:ALA:HB2	37:8:501:LUT:H401	2.01	0.42
21:A:1119:CLA:H171	23: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
21:B:1023:CLA:HBD	21:B:1023:CLA:HED2	1.83	0.42
21:B:1212:CLA:H192	23:B:4003:BCR:HC41	2.01	0.42
21:B:1223:CLA:H61	21:B:1223:CLA:H102	1.66	0.42
30:B:5005:PTY:H202	30:B:5005:PTY:H171	1.90	0.42
13:1:55:PHE:HB3	21:1:604:CLA:C3D	2.49	0.42
13:a:126:LEU:HA	13:a:126:LEU:HD13	1.86	0.42
23:3:505:BCR:H402	21:3:610:CLA:C2D	2.50	0.42
15:4:32:TRP:HH2	24:4:802:LHG:HC42	1.85	0.42
15:4:185:LYS:HD3	21:4:607: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	21:6:609:CLA:CED	2.86	0.42
17:6:189:ARG:HB3	24:6:801:LHG:H251	2.02	0.42
29:6:803:PCW:H83	29:6:803:PCW:H42	1.87	0.42
19:8:188:ASP:O	19:8:192:TRP:HD1	2.02	0.42
21:8:620:CLA:H61	21:8:620: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
21:A:1012:CLA:H122	21:A:1012:CLA:H8	1.72	0.42
21:A:1106:CLA:HBB1	21:A:1126:CLA:H101	2.00	0.42
21:A:1115:CLA:HED2	21:A:1115:CLA:H2A	2.01	0.42
21:B:1209:CLA:H2	21:B:1209:CLA:H61	1.79	0.42
21:B:1239:CLA:H193	23:L:4001:BCR:C14	2.50	0.42
21:B:1239:CLA:H202	21:B:1239:CLA:H161	1.83	0.42
23:B:4003:BCR:H351	23:B:4003:BCR:H15C	1.89	0.42
4:D:226:SER:HB3	4:D:243:ARG:O	2.20	0.42
9:K:58:PRO:HD3	21:K:1403:CLA:C4A	2.47	0.42
14:3:417:TRP:HE3	16:5:56:PRO:O	2.02	0.42
21:4:605:CLA:HBC1	21:4:612:CLA:HBC1	2.01	0.42
16:5:87:ILE:HD13	37:5:502:LUT:H41	2.01	0.42
16:5:175:SER:C	16:5:177:GLY:H	2.28	0.42
37:5:501:LUT:H15	37:5:501:LUT:H201	1.91	0.42
17:6:75:PHE:CB	21:6:604:CLA:HMA2	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:7:617:CLA:CAA	25:8:802:DGD:HA81	2.47	0.42
1:A:307:ILE:HD13	23:K:4001:BCR:H17C	2.01	0.42
1:A:498:THR:OG1	21:A:1133:CLA:OBD	2.35	0.42
21:A:1108:CLA:H93	21:A:1108:CLA:H111	1.86	0.42
21:A:1138:CLA:H202	21:A:1138:CLA:H162	1.75	0.42
21:B:1220:CLA:H52	23:B:4004:BCR:C14	2.50	0.42
21:B:1224:CLA:H141	21:B:1224:CLA:H161	1.76	0.42
21:F:1302:CLA:H51	21:F:1302:CLA:H8	1.81	0.42
7:G:1312:TYR:OH	33:G:5002:ERG:C27	2.68	0.42
33:G:5002:ERG:H272	33:G:5002:ERG:H23	1.65	0.42
21:L:1501:CLA:H12	21:L:1501:CLA:HBA2	1.75	0.42
37:1:503:LUT:H35	37:1:503:LUT:H401	1.72	0.42
13:a:53:TYR:OH	24:a:801:LHG:O5	2.22	0.42
21:4:601:CLA:H61	21:4:601:CLA:H41	1.70	0.42
23:5:504:BCR:H24C	38:5:610:CHL:HBA2	2.00	0.42
17:6:218:ASP:OD1	17:6:219:ASN:N	2.53	0.42
21:6:603:CLA:H91	21:6:603:CLA:H112	1.79	0.42
38:6:619:CHL:H61	38:6:619:CHL:H41	1.53	0.42
19:8:84:VAL:HG11	37:8:501:LUT:H12	2.01	0.42
19:8:196:ARG:NH2	25:8:802:DGD:O5E	2.52	0.42
21:8:605:CLA:HAC1	21:8:610:CLA:HBB2	2.02	0.42
2:B:57:ILE:HD11	36:M:4001:ECH:C39	2.42	0.42
2:B:305:ILE:HD13	21:B:1219:CLA:HMD1	2.01	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
21:3:612:CLA:H112	21:3:612:CLA:H142	1.79	0.42
24:3:801:LHG:H252	24:3:801:LHG:H282	1.85	0.42
16:5:227:TRP:CD1	16:5:227:TRP:H	2.38	0.42
30:5:802:PTY:H382	21:7:603:CLA:H172	2.02	0.42
17:6:215:GLU:O	17:6:223:THR:HG21	2.20	0.42
18:7:91:ARG:NH2	21:7:606:CLA:HED1	2.34	0.42
19:8:138:ARG:O	19:8:141:ASP:HB3	2.20	0.42
46:8:808:4RF:H39	39:8:809: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
21:A:1120:CLA:C4D	23:K:4001:BCR:H271	2.49	0.42
23:A:4003:BCR:H381	23: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:276:HIS:HB3	21:B:1214:CLA:HMB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:699:VAL:HG12	3:C:79:LEU:HD21	2.02	0.42
21:B:1209:CLA:H72	21:B:1209:CLA:H111	1.48	0.42
4:D:242:MET:HB2	4:D:247:ASN:ND2	2.35	0.42
21:K:1402:CLA:H91	21:K:1402:CLA:H111	1.72	0.42
23:L:4001:BCR:H382	21:L:1502:CLA:HAC2	2.01	0.42
21:1:602:CLA:HHC	21:1:602:CLA:CBB	2.47	0.42
21:1:608:CLA:H142	21:a:612:CLA:H112	2.02	0.42
37:a:502:LUT:H35	37:a:502:LUT:H401	1.78	0.42
16:5:171:PRO:HD2	37:5:501:LUT:H23	2.01	0.42
21:5:602:CLA:H61	21:5:602:CLA:H41	1.74	0.42
19:8:120:PHE:CE1	46:8:808:4RF:H41	2.54	0.42
37:8:501:LUT:H11	37:8:501:LUT:H191	1.96	0.42
1:A:441:LEU:HD13	21:A:1137:CLA:C3B	2.49	0.41
1:A:598:TRP:HH2	21:B:1022:CLA:HAB	1.85	0.41
1:A:715:PRO:HB3	21:A:1140:CLA:C2C	2.49	0.41
2:B:416:LYS:CB	2:B:540:LEU:HD23	2.49	0.41
21:B:1021:CLA:O2D	21:B:1021:CLA:HAA2	2.20	0.41
21:B:1207:CLA:H43	12:L:371:ILE:HG23	2.02	0.41
7:G:1253:PHE:CE2	28:1:804:LMT:H2'	2.52	0.41
11:I:30:ILE:HG21	23:L:4001:BCR:H333	2.02	0.41
21:1:603:CLA:HMA1	21:1:608:CLA:HBC3	2.02	0.41
21:1:606:CLA:HMA2	38:1:613:CHL:C2C	2.50	0.41
13:a:159:MET:HE2	37:a:501:LUT:H222	2.02	0.41
13:a:206:LEU:HD23	13:a:206:LEU:HA	1.92	0.41
14:3:442:ARG:O	14:3:446:ILE:HG13	2.20	0.41
23:3:504:BCR:H351	23:3:504:BCR:H15C	1.74	0.41
21:3:607:CLA:H141	21:3:607: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	38:6:611:CHL:C2B	2.97	0.41
17:6:139:ASP:CB	38:6:611:CHL:HAC2	2.50	0.41
21:7:617:CLA:H62	21:7:617:CLA:H93	1.76	0.41
19:8:215:THR:C	19:8:217:LYS:H	2.28	0.41
21:A:1108:CLA:O2D	21:A:1108:CLA:H2A	2.20	0.41
21:A:1139:CLA:HBA2	21:A:1139:CLA:H3A	1.33	0.41
21:B:1226:CLA:CAD	25:B:5003:DGD:HB32	2.50	0.41
21:B:1237:CLA:H62	21:B:1237:CLA:H41	1.66	0.41
21:B:1207:CLA:HHC	21: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
23:3:503:BCR:H282	21:3:616:CLA:HAB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:3:612:CLA:HBC2	21:3:613:CLA:HMB3	2.01	0.41
37:4:501:LUT:H15	37:4:501:LUT:H201	1.91	0.41
23:4:503:BCR:H19C	38:4:613:CHL:O1A	2.20	0.41
16:5:91:GLU:OE1	16:5:211:PRO:HG2	2.19	0.41
21:7:612:CLA:H93	21:7:612:CLA:H111	1.95	0.41
38:8:601:CHL:H61	38:8:601:CHL:H41	1.62	0.41
1:A:578:PRO:HG2	3:C:69:LEU:HD11	2.02	0.41
21:A:1125:CLA:HHB	21:A:1133:CLA:H43	2.03	0.41
23:A:4001:BCR:H392	23:A:4001:BCR:H23C	2.03	0.41
2:B:92:ILE:HG21	2:B:97:PHE:CE2	2.54	0.41
2:B:280:ALA:HA	21:B:1213:CLA:HMC2	2.02	0.41
2:B:449:THR:OG1	2:B:452:LYS:HE2	2.21	0.41
21:B:1224:CLA:H203	21:B:1224:CLA:H162	1.89	0.41
6:F:409:ILE:HG13	24:F:5002:LHG:C15	2.49	0.41
8:J:31:PRO:O	34:J:4002:RRX:H49	2.20	0.41
13:a:72:GLU:HG2	13:a:150:VAL:HB	2.02	0.41
13:a:105:PRO:HB2	13:a:111:GLN:O	2.20	0.41
21:3:607:CLA:H61	21:3:607:CLA:H102	1.82	0.41
15:4:139:GLN:HA	15:4:142:ILE:HG12	2.02	0.41
16:5:129:MET:HA	16:5:132:VAL:HG22	2.03	0.41
17:6:182:VAL:CG1	21:6:607:CLA:CED	2.96	0.41
17:6:182:VAL:O	17:6:186:LYS:HG2	2.21	0.41
44:6:806:SPH:H151	44:6:806:SPH:H182	1.56	0.41
24:7:801:LHG:H322	24:7:801: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
21:A:1102:CLA:HMC1	24:A:5002:LHG:H171	2.02	0.41
21:A:1138:CLA:HBC1	22: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
2:B:632:LEU:HD21	2:B:651:PHE:CD1	2.56	0.41
21:B:1205:CLA:CGA	21:B:1205:CLA:C1A	2.98	0.41
21:B:1209:CLA:HBD	7:G:1278:ARG:CD	2.51	0.41
21:B:1210:CLA:H93	21:B:1210:CLA:H61	1.76	0.41
21:B:1230:CLA:H91	21:B:1230:CLA:H112	1.84	0.41
21:1:603:CLA:C4A	21:1:603:CLA:HBA2	2.50	0.41
15:4:204:GLN:OE1	21:4:603:CLA:HED3	2.21	0.41
16:5:88:LEU:HD21	16:5:200:PHE:CZ	2.55	0.41
37:5:501:LUT:H35	37:5:501:LUT:H401	1.76	0.41
37:5:505:LUT:H401	37:5:505:LUT:H35	1.75	0.41
37:6:502:LUT:H361	37:6:502:LUT:H28	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:8:80:ALA:CB	19:8:202:MET:HG2	2.50	0.41
25:8:802:DGD:HAN2	25:8:802:DGD:HAW1	1.71	0.41
23:8:503:BCR:H15C	23:8:503:BCR:H351	1.75	0.41
1:A:337:GLY:O	1:A:426:LEU:HG	2.20	0.41
21:A:1117:CLA:HBA2	21:A:1117:CLA:H3A	1.36	0.41
4:D:218:GLU:HG3	4:D:278:PHE:CE1	2.55	0.41
36:M:4001:ECH:H11	36:M:4001:ECH:H34	1.83	0.41
37:1:503:LUT:H31	37:1:503:LUT:H391	1.88	0.41
14:3:315:ARG:HD3	21:3:601:CLA:CHD	2.51	0.41
15:4:167:ASP:HA	37:4:501:LUT:O23	2.19	0.41
15:4:192:LEU:HD23	15:4:192:LEU:HA	1.90	0.41
17:6:150:PRO:HD3	21:6:617:CLA:C2C	2.50	0.41
37:6:501:LUT:H15	37:6:501:LUT:H201	1.93	0.41
18:7:153:ARG:H	18:7:153:ARG:HG2	1.65	0.41
37:8:501:LUT:H34	38:8:601:CHL:CBB	2.50	0.41
37:8:502:LUT:H15	37:8:502:LUT:H201	1.93	0.41
1:A:313:ARG:HH21	1:A:321:SER:HB2	1.85	0.41
21:A:1108:CLA:C4C	21:A:1111:CLA:H203	2.50	0.41
21:A:1114:CLA:CAD	28:A:5008:LMT:H4'	2.50	0.41
21:A:1125:CLA:CAB	21:A:1133:CLA:HMA2	2.50	0.41
21:A:1127:CLA:HMD2	21:A:1127:CLA:H71	2.03	0.41
21:A:1130:CLA:H41	21:A:1130:CLA:H61	1.39	0.41
2:B:523:ALA:HB1	21:B:1021:CLA:H171	2.02	0.41
21:B:1212:CLA:O1A	23:B:4001:BCR:H281	2.21	0.41
21:B:1240:CLA:H142	21:B:1240:CLA:H112	1.88	0.41
21:B:1228:CLA:H42	6:F:465:TYR:CD1	2.55	0.41
13:1:57:PRO:HD2	37:1:502:LUT:H23	2.03	0.41
13:1:159:MET:HG2	37:1:501:LUT:H222	2.02	0.41
13:1:222:PRO:HG3	21:1:615:CLA:C2B	2.50	0.41
28:1:804:LMT:H1'	21:1:612: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
37:3:502:LUT:H35	37:3:502:LUT:H401	1.83	0.41
23:3:504:BCR:C11	38:3:611:CHL:HBA1	2.51	0.41
16:5:245:LEU:HD23	23:5:504: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	21:6:604:CLA:H11	2.03	0.41
17:6:90:VAL:CG1	37:6:501:LUT:H14	2.51	0.41
21:6:604:CLA:CBC	21:6:609:CLA:HBB2	2.47	0.41
18:7:152:GLY:O	18:7:162:ARG:NH2	2.53	0.41
21:7:612:CLA:H2	47:7:504:C7Z:C38	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:MET:SD	21:A:1106:CLA:HAA2	2.60	0.41
1:A:358:ALA:HB1	23:A:4004:BCR:H10C	2.02	0.41
1:A:481:PRO:HG3	1:A:533:PHE:HB2	2.03	0.41
21:A:1134:CLA:H143	21:A:1134:CLA:H112	1.70	0.41
21: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	23:B:4005:BCR:H393	2.03	0.41
21:B:1209:CLA:H143	21:B:1217:CLA:C2	2.50	0.41
29:B:5004:PCW:H331	23:F:4001:BCR:H14C	2.03	0.41
6:F:393:GLY:N	6:F:396:LEU:HD12	2.35	0.41
21:F:1302:CLA:C2D	46:7:807:4RF:H35	2.51	0.41
7:G:1247:ARG:HG2	21:G:1602:CLA:C3B	2.50	0.41
13:1:140:PHE:HB3	21:1:611:CLA:HMC2	2.03	0.41
13:a:107:VAL:HG12	13:a:108:GLN:N	2.36	0.41
37:3:501:LUT:H11	37:3:501:LUT:H191	1.93	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
21:7:603:CLA:H8	21:7:608:CLA:HMD3	2.03	0.41
37:8:501:LUT:H401	37:8:501:LUT:H35	1.89	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
21:A:1107:CLA:H93	34:J:4002:RRX:H38	2.02	0.41
21:A:1112:CLA:H62	21:A:1112:CLA:H2	1.82	0.41
2:B:141:ILE:HD13	2:B:141:ILE:HA	1.91	0.41
2:B:663:MET:O	2:B:667:SER:OG	2.36	0.41
2:B:668:TRP:HA	22:B:2002:PQN:C8	2.50	0.41
21:B:1205:CLA:HAB	21:B:1206:CLA:CBA	2.41	0.41
23:B:4004:BCR:H23C	23:B:4004:BCR:H392	2.02	0.41
3:C:31:TRP:CG	3:C:32:ASP:H	2.38	0.41
12:L:313:THR:C	12:L:315:VAL:H	2.28	0.41
13:a:98:ASN:HB2	13:a:101:ASP:CG	2.46	0.41
13:a:141:ARG:HE	13:a:141:ARG:HB2	1.71	0.41
14:3:314:CYS:N	14:3:445:MET:HE2	2.36	0.41
14:3:447:ALA:HA	21:3:603:CLA:HBB1	2.01	0.41
21:3:605:CLA:H3A	21:3:605:CLA:HBA1	1.78	0.41
17:6:41:PRO:HG2	21:6:609:CLA:HMD1	2.03	0.41
38:6:619:CHL:HMA2	38:6:619:CHL:HAA1	1.88	0.41
21:7:615:CLA:HBA1	21:7:615:CLA:H2	2.03	0.41
21:8:606:CLA:H62	21:8:606:CLA:H41	1.64	0.41
1:A:299:LEU:HD22	21:A:1113:CLA:HMC1	2.02	0.41
21:A:1102:CLA:H61	21:A:1102:CLA:H93	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1106:CLA:H142	21:A:1106:CLA:H112	1.79	0.41
21:A:1109:CLA:HBA1	21:A:1109:CLA:CBD	2.51	0.41
21:A:1125:CLA:CBB	21:A:1133:CLA:HMA2	2.51	0.41
21:A:1131:CLA:H172	21: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:173:GLU:CD	7:G:1264:PRO:HB3	2.46	0.41
2:B:184:PHE:CZ	21:B:1210:CLA:H72	2.56	0.41
2:B:687:PRO:C	2:B:689:ALA:H	2.28	0.41
2:B:716:VAL:HG22	25:B:5003:DGD:HBG2	2.03	0.41
21:B:1204:CLA:H111	21:B:1204:CLA:H142	1.74	0.41
7:G:1248:PHE:CD1	37:1:503:LUT:H221	2.55	0.41
9:K:36:THR:O	9:K:40:ILE:HG22	2.21	0.41
12:L:308:ILE:C	12:L:310:MET:H	2.27	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
23:L:4003:BCR:H351	23:L:4003:BCR:H15C	1.78	0.41
13:a:77:HIS:CE1	21:a:612:CLA:HMD2	2.56	0.41
37:a:502:LUT:H183	38:a:606:CHL:C2B	2.51	0.41
14:3:315:ARG:HD3	21:3:601:CLA:C4C	2.51	0.41
43:5:803:DGA:HB51	43:5:803:DGA:HA32	2.03	0.41
17:6:54:LEU:CD1	21:6:604:CLA:HED1	2.51	0.41
17:6:74:TRP:CZ2	21:6:612:CLA:HED1	2.56	0.41
17:6:81:VAL:HG11	17:6:136:ARG:CZ	2.51	0.41
17:6:186:LYS:HZ3	21:6:607:CLA:CGD	2.21	0.41
17:6:195:PHE:CD2	37:6:502:LUT:H12	2.56	0.41
18:7:15:LYS:C	18:7:17:VAL:H	2.29	0.41
18:7:57:LEU:HD21	21:7:612:CLA:HBC3	2.03	0.41
18:7:192:GLN:NE2	37:7:501:LUT:H42	2.36	0.41
21:7:604:CLA:H71	21:7:605:CLA:HMB1	2.03	0.41
21:8:618:CLA:H3A	21:8:618: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	21:A:1013:CLA:HBB2	2.51	0.41
21: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
2:B:61:TRP:HA	21:B:1204:CLA:HAB	2.03	0.41
21:B:1201:CLA:H71	10:M:30:TYR:CE1	2.56	0.41
21:B:1222:CLA:H51	21:B:1234:CLA:H2	2.02	0.41
21:1:608:CLA:H42	38:1:609:CHL:H93	2.03	0.41
13:a:149:ARG:HH12	41:a:805:GG0:C03	2.34	0.41
13:a:200:GLU:OE1	13:a:200:GLU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:3:316:TRP:CZ2	14:3:375:MET:HE1	2.56	0.41
15:4:37:GLU:OE1	15:4:37:GLU:HA	2.20	0.41
16:5:152:ASN:C	16:5:154:ASN:H	2.29	0.41
21:5:609:CLA:CBD	24:5:801:LHG:HC62	2.50	0.41
18:7:121:ASN:ND2	19:8:37:GLY:O	2.54	0.41
25:8:802:DGD:HA91	25:8:802:DGD:C1G	2.50	0.41
21:8:602:CLA:H41	21:8:602: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
21:A:1131:CLA:H193	21:A:1131:CLA:H162	1.82	0.40
21:A:1136:CLA:H3A	21:A:1136:CLA:HBA2	1.79	0.40
21:A:1140:CLA:H92	6:F:451:LEU:HD22	2.03	0.40
21:B:1209:CLA:HED2	21: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
10:M:14:LEU:HD23	10:M:14:LEU:HA	1.91	0.40
13:1:80:TRP:CE2	21:1:612:CLA:HBC3	2.56	0.40
13:1:122:ASP:O	13:1:126:LEU:HG	2.21	0.40
15:4:215:HIS:CG	21:4:603:CLA:HAA2	2.56	0.40
37:4:502:LUT:H11	37:4:502:LUT:H191	1.97	0.40
21:5:607:CLA:HBC1	24:5:801:LHG:H151	2.03	0.40
38:5:610:CHL:HBB2	21:5:612: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
2:B:83:LEU:HD23	2:B:83:LEU:HA	1.85	0.40
2:B:168:TRP:CZ2	21:B:1208:CLA:HMA1	2.56	0.40
2:B:423:LEU:HG	21:B:1236:CLA:CAB	2.51	0.40
2:B:524:ILE:HG21	21:B:1234:CLA:HAB	2.03	0.40
21:B:1218:CLA:HBA1	21:B:1218:CLA:H12	1.80	0.40
4:D:254:LYS:HE3	4:D:286:LEU:HD13	2.03	0.40
32:G:5001:SQD:H132	32:G:5001:SQD:H272	2.03	0.40
32:G:5001:SQD:H461	32:G:5001:SQD:H82	2.02	0.40
12:L:384:LEU:HD11	12:L:431:ALA:HB2	2.03	0.40
21:1:603:CLA:H91	21:1:603:CLA:H111	1.67	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	30:5:802:PTY:H122	2.04	0.40
21:5:601:CLA:HMB3	21:5:601:CLA:HBB1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:6:184:GLU:HB2	21:6:601:CLA:C1B	2.51	0.40
17:6:255:PRO:HG2	24:6:802:LHG:H322	2.03	0.40
19:8:67:ASN:O	19:8:71:ASN:ND2	2.54	0.40
21:8:605:CLA:HHC	21:8:605:CLA:CBB	2.50	0.40
1:A:345:LEU:HD11	1:A:355:ILE:CD1	2.51	0.40
22:A:2001:PQN:H2M1	22:A:2001:PQN:H111	1.86	0.40
21:L:1503:CLA:HED2	21:L:1503:CLA:H2A	2.03	0.40
21:1:607:CLA:HAB	23:8:503:BCR:C31	2.51	0.40
21:1:612:CLA:H193	21:1:612:CLA:H161	1.66	0.40
16:5:31:ARG:NE	16:5:31:ARG:HA	2.37	0.40
21:A:1119:CLA:H72	23:A:4004:BCR:H14C	2.03	0.40
2:B:66:LEU:HD21	23:B:4003:BCR:H281	2.03	0.40
2:B:372:LEU:HD11	21:B:1225:CLA:HED3	2.03	0.40
21:B:1214:CLA:HBA2	21:B:1214:CLA:H3A	1.78	0.40
21:B:1231:CLA:H142	21:B:1231:CLA:H111	1.87	0.40
35:a:804:LPX:H15	35:a:804:LPX:H12A	1.52	0.40
15:4:183:GLU:HB2	21:4:601:CLA:CHB	2.52	0.40
21:5:618:CLA:HHC	21:5:618:CLA:CBB	2.49	0.40
19:8:120:PHE:CE1	46:8:808:4RF:H43	2.56	0.40
21:8:620:CLA:H12	21:8:620: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	30:3:802:PTY:H121	1.86	0.40
21:A:1121:CLA:H61	21:A:1121:CLA:H41	1.67	0.40
21:A:1131:CLA:H141	21:A:1131:CLA:H161	1.76	0.40
21:A:1133:CLA:C2D	21:A:1134:CLA:HAB	2.52	0.40
21:A:1136:CLA:H51	21:A:1136:CLA:H11	1.79	0.40
24:A:5002:LHG:H151	24:A:5002:LHG:H122	1.75	0.40
2:B:345:ILE:HG23	21: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
13:1:82:MET:HE2	13:1:177:GLY:CA	2.52	0.40
24:1:801:LHG:HC81	24:1:801:LHG:H111	1.79	0.40
13:a:148:LYS:HA	13:a:148:LYS:HD3	1.87	0.40
21:3:610:CLA:H62	21:3:610:CLA:H41	1.36	0.40
15:4:119:LYS:CD	21:4:610:CLA:HBC3	2.51	0.40
21:4:607:CLA:H8	21:4:607:CLA:H51	1.58	0.40
16:5:155:LEU:HD13	21:5:618:CLA:HBD	2.04	0.40
17:6:90:VAL:HG23	17:6:198:PHE:CE2	2.56	0.40
18:7:116:LEU:HD13	21:7:612:CLA:HMA1	2.03	0.40
21:7:610:CLA:H41	21:7:610:CLA:H61	1.79	0.40
19:8:208:PHE:CE1	37:8:501:LUT:H41	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	739/741 (100%)	702 (95%)	36 (5%)	1 (0%)	48	82
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%)	12	47
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%)	24	62
13	a	190/192 (99%)	164 (86%)	25 (13%)	1 (0%)	24	62
14	3	239/241 (99%)	219 (92%)	19 (8%)	1 (0%)	30	66
15	4	205/207 (99%)	188 (92%)	16 (8%)	1 (0%)	24	62
16	5	225/227 (99%)	201 (89%)	23 (10%)	1 (0%)	30	66
17	6	229/231 (99%)	208 (91%)	19 (8%)	2 (1%)	14	49
18	7	219/221 (99%)	198 (90%)	20 (9%)	1 (0%)	24	62
19	8	217/219 (99%)	194 (89%)	21 (10%)	2 (1%)	14	49
All	All	4044/4103 (99%)	3732 (92%)	300 (7%)	12 (0%)	37	71

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%)	600 (100%)	0	100	100
2	B	588/588 (100%)	588 (100%)	0	100	100
3	C	69/69 (100%)	69 (100%)	0	100	100
4	D	121/121 (100%)	121 (100%)	0	100	100
5	E	55/55 (100%)	55 (100%)	0	100	100
6	F	126/126 (100%)	126 (100%)	0	100	100
7	G	71/71 (100%)	70 (99%)	1 (1%)	59	70
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%)	134 (100%)	0	100	100
14	3	186/186 (100%)	186 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	3224 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
7	G	1307	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	80	GLN
1	A	94	HIS
1	A	193	ASN
1	A	217	GLN
1	A	225	ASN
1	A	310	HIS
1	A	442	ASN
1	A	568	ASN
2	B	54	GLN
2	B	134	GLN
2	B	364	GLN
2	B	422	HIS
2	B	507	ASN
2	B	609	GLN
2	B	705	GLN
4	D	247	ASN
4	D	284	GLN
7	G	1266	GLN
7	G	1324	ASN
8	J	49	ASN
12	L	396	GLN
14	3	356	GLN
14	3	481	ASN

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Mol	Chain	Res	Type
15	4	112	ASN
15	4	200	GLN
15	4	218	ASN
16	5	97	GLN
16	5	114	GLN
16	5	117	ASN
16	5	152	ASN
16	5	205	GLN
16	5	225	ASN
17	6	51	ASN
17	6	130	HIS
19	8	197	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
21	CLA	K	1401	-	50,54,73	1.60	7 (14%)	59,90,113	2.00	12 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	CHL	a	610	-	42,56,74	1.53	8 (19%)	36,92,114	2.07	11 (30%)
23	BCR	L	4003	-	41,41,41	1.63	4 (9%)	56,56,56	4.51	14 (25%)
21	CLA	A	1012	-	69,73,73	1.39	6 (8%)	82,113,113	1.84	16 (19%)
21	CLA	5	604	-	69,73,73	1.38	6 (8%)	82,113,113	1.92	19 (23%)
23	BCR	K	4002	-	41,41,41	1.64	5 (12%)	56,56,56	4.29	13 (23%)
37	LUT	4	502	-	42,43,43	2.42	1 (2%)	51,60,60	1.79	12 (23%)
21	CLA	7	602	-	47,52,73	1.65	6 (12%)	55,87,113	2.11	17 (30%)
21	CLA	3	612	-	69,73,73	1.39	6 (8%)	82,113,113	1.83	14 (17%)
21	CLA	3	616	-	60,64,73	1.47	7 (11%)	71,102,113	1.95	19 (26%)
21	CLA	B	1216	-	65,69,73	1.42	6 (9%)	77,108,113	1.86	17 (22%)
21	CLA	F	1302	24	59,63,73	1.49	6 (10%)	70,101,113	2.12	21 (30%)
24	LHG	7	801	21	48,48,48	0.38	0	51,54,54	1.24	5 (9%)
21	CLA	4	607	24	59,63,73	1.47	7 (11%)	70,101,113	2.00	16 (22%)
23	BCR	A	4001	-	41,41,41	1.64	5 (12%)	56,56,56	4.15	17 (30%)
21	CLA	B	1235	2	69,73,73	1.39	7 (10%)	82,113,113	1.94	18 (21%)
28	LMT	1	804	-	36,36,36	1.15	5 (13%)	47,47,47	1.06	1 (2%)
37	LUT	a	501	-	42,43,43	2.45	2 (4%)	51,60,60	2.22	15 (29%)
23	BCR	A	4002	-	41,41,41	1.66	6 (14%)	56,56,56	4.47	16 (28%)
21	CLA	6	612	-	54,58,73	1.54	6 (11%)	64,95,113	2.17	19 (29%)
21	CLA	1	615	13	50,54,73	1.59	7 (14%)	59,90,113	2.04	16 (27%)
21	CLA	B	1234	2	60,64,73	1.49	6 (10%)	71,102,113	2.18	20 (28%)
38	CHL	8	601	19	55,69,74	1.74	9 (16%)	52,108,114	1.91	11 (21%)
21	CLA	7	604	-	69,73,73	1.38	6 (8%)	82,113,113	1.91	22 (26%)
37	LUT	1	501	-	42,43,43	2.49	1 (2%)	51,60,60	1.91	16 (31%)
23	BCR	L	4001	-	41,41,41	1.66	5 (12%)	56,56,56	4.41	17 (30%)
24	LHG	B	5002	-	48,48,48	0.41	0	51,54,54	0.98	3 (5%)
21	CLA	B	1202	2	69,73,73	1.36	6 (8%)	82,113,113	1.92	18 (21%)
24	LHG	3	801	21	48,48,48	0.40	0	51,54,54	1.06	4 (7%)
21	CLA	5	601	16	64,68,73	1.41	6 (9%)	76,107,113	1.98	22 (28%)
23	BCR	L	4002	-	41,41,41	1.62	4 (9%)	56,56,56	4.57	17 (30%)
21	CLA	B	1204	2	69,73,73	1.40	6 (8%)	82,113,113	1.94	20 (24%)
21	CLA	B	1209	2	69,73,73	1.37	7 (10%)	82,113,113	2.01	20 (24%)
22	PQN	B	2002	-	34,34,34	0.44	0	43,45,45	1.28	4 (9%)
21	CLA	6	601	-	64,68,73	1.42	6 (9%)	76,107,113	2.02	19 (25%)
21	CLA	A	1132	-	69,73,73	1.36	7 (10%)	82,113,113	1.97	19 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	BCR	G	4001	-	41,41,41	1.61	4 (9%)	56,56,56	4.45	19 (33%)
21	CLA	a	611	-	54,58,73	1.55	6 (11%)	64,95,113	2.06	18 (28%)
21	CLA	B	1240	24	69,73,73	1.39	6 (8%)	82,113,113	1.92	17 (20%)
24	LHG	F	5002	-	35,35,48	0.46	0	38,41,54	1.24	4 (10%)
21	CLA	4	605	-	50,54,73	1.59	6 (12%)	59,90,113	2.16	20 (33%)
21	CLA	7	617	18	58,62,73	1.50	6 (10%)	69,100,113	2.06	17 (24%)
21	CLA	5	616	-	50,54,73	1.61	7 (14%)	59,90,113	2.04	15 (25%)
21	CLA	B	1227	2	54,58,73	1.56	6 (11%)	64,95,113	2.08	18 (28%)
21	CLA	3	618	-	50,54,73	1.63	7 (14%)	59,90,113	2.04	16 (27%)
21	CLA	B	1230	2	62,66,73	1.44	6 (9%)	73,104,113	2.06	20 (27%)
21	CLA	A	1133	1	69,73,73	1.36	6 (8%)	82,113,113	1.88	17 (20%)
21	CLA	B	1205	-	69,73,73	1.36	6 (8%)	82,113,113	2.01	17 (20%)
21	CLA	1	611	-	59,63,73	1.49	6 (10%)	70,101,113	1.99	19 (27%)
38	CHL	4	613	-	46,60,74	1.49	8 (17%)	40,97,114	1.97	11 (27%)
21	CLA	A	1123	-	69,73,73	1.38	7 (10%)	82,113,113	1.91	18 (21%)
38	CHL	a	606	-	50,64,74	1.44	8 (16%)	46,102,114	1.81	10 (21%)
21	CLA	B	1218	2	59,63,73	1.48	7 (11%)	70,101,113	2.10	21 (30%)
21	CLA	8	607	24	50,54,73	1.60	6 (12%)	59,90,113	2.00	12 (20%)
21	CLA	A	1110	1	64,68,73	1.44	7 (10%)	76,107,113	1.93	18 (23%)
41	GG0	a	805	-	7,8,8	1.32	2 (28%)	6,9,9	0.75	0
46	4RF	8	807	-	41,41,56	1.01	6 (14%)	44,44,59	1.09	3 (6%)
21	CLA	B	1222	-	62,66,73	1.47	6 (9%)	73,104,113	1.98	18 (24%)
21	CLA	B	1212	2	69,73,73	1.39	7 (10%)	82,113,113	1.99	22 (26%)
21	CLA	6	603	-	69,73,73	1.38	7 (10%)	82,113,113	1.99	18 (21%)
21	CLA	G	1601	-	54,58,73	1.55	7 (12%)	64,95,113	2.11	17 (26%)
21	CLA	B	1239	2	69,73,73	1.39	6 (8%)	82,113,113	1.88	19 (23%)
21	CLA	A	1105	-	61,65,73	1.47	6 (9%)	72,103,113	2.03	21 (29%)
21	CLA	3	602	14	50,54,73	1.60	7 (14%)	59,90,113	2.09	16 (27%)
21	CLA	1	612	13	69,73,73	1.36	7 (10%)	82,113,113	1.86	18 (21%)
38	CHL	6	613	-	45,59,74	1.38	8 (17%)	40,96,114	2.01	11 (27%)
21	CLA	A	1106	1	69,73,73	1.35	6 (8%)	82,113,113	1.97	20 (24%)
21	CLA	A	1117	1	69,73,73	1.38	6 (8%)	82,113,113	1.86	15 (18%)
21	CLA	1	608	13	64,68,73	1.43	6 (9%)	76,107,113	1.93	17 (22%)
21	CLA	A	1122	-	69,73,73	1.38	7 (10%)	82,113,113	1.87	16 (19%)
21	CLA	B	1221	-	69,73,73	1.39	7 (10%)	82,113,113	1.95	16 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	3	605	-	69,73,73	1.38	6 (8%)	82,113,113	1.97	20 (24%)
21	CLA	A	1107	1	59,63,73	1.50	7 (11%)	70,101,113	2.04	17 (24%)
21	CLA	L	1503	-	49,53,73	1.65	7 (14%)	58,89,113	2.17	21 (36%)
21	CLA	B	1022	-	69,73,73	1.41	6 (8%)	82,113,113	1.84	18 (21%)
23	BCR	J	4001	-	41,41,41	1.63	5 (12%)	56,56,56	4.54	17 (30%)
48	P5S	8	806	-	35,36,53	1.18	3 (8%)	37,43,60	1.19	3 (8%)
21	CLA	a	612	13	61,65,73	1.48	5 (8%)	72,103,113	1.89	18 (25%)
21	CLA	5	609	16	55,59,73	1.55	7 (12%)	64,96,113	2.12	17 (26%)
24	LHG	5	801	21	48,48,48	0.40	0	51,54,54	1.05	3 (5%)
29	PCW	B	5004	-	29,29,53	1.34	3 (10%)	35,37,61	0.96	1 (2%)
21	CLA	a	608	13	59,63,73	1.47	6 (10%)	70,101,113	1.93	16 (22%)
23	BCR	A	4004	-	41,41,41	1.79	6 (14%)	56,56,56	4.67	15 (26%)
21	CLA	A	1109	1,21	69,73,73	1.34	7 (10%)	82,113,113	2.05	21 (25%)
21	CLA	A	1013	-	69,73,73	1.38	6 (8%)	82,113,113	1.86	19 (23%)
24	LHG	7	803	-	42,42,48	0.39	0	45,48,54	1.08	2 (4%)
21	CLA	A	1128	1	69,73,73	1.40	6 (8%)	82,113,113	1.92	17 (20%)
46	4RF	7	807	-	31,31,56	1.18	6 (19%)	34,34,59	1.19	3 (8%)
37	LUT	8	502	-	42,43,43	2.42	2 (4%)	51,60,60	1.78	12 (23%)
21	CLA	B	1229	-	69,73,73	1.36	6 (8%)	82,113,113	1.92	20 (24%)
21	CLA	3	606	-	69,73,73	1.39	6 (8%)	82,113,113	1.87	16 (19%)
21	CLA	B	1226	2	69,73,73	1.38	6 (8%)	82,113,113	1.84	15 (18%)
21	CLA	B	1224	2	69,73,73	1.38	7 (10%)	82,113,113	1.89	17 (20%)
21	CLA	B	1203	-	69,73,73	1.36	6 (8%)	82,113,113	1.89	16 (19%)
24	LHG	B	5001	21	45,45,48	0.41	0	48,51,54	1.06	3 (6%)
23	BCR	6	504	-	41,41,41	1.69	7 (17%)	56,56,56	4.38	20 (35%)
21	CLA	A	1104	-	69,73,73	1.36	6 (8%)	82,113,113	1.93	21 (25%)
23	BCR	3	505	-	41,41,41	1.62	4 (9%)	56,56,56	4.27	16 (28%)
47	C7Z	7	504	-	43,43,43	5.43	26 (60%)	56,60,60	2.79	23 (41%)
21	CLA	A	1129	-	54,58,73	1.56	6 (11%)	64,95,113	2.14	17 (26%)
21	CLA	A	1140	-	59,63,73	1.48	8 (13%)	70,101,113	1.98	13 (18%)
21	CLA	7	608	18	46,50,73	1.66	6 (13%)	53,85,113	2.19	13 (24%)
21	CLA	1	604	-	69,73,73	1.41	7 (10%)	82,113,113	1.89	20 (24%)
29	PCW	6	803	-	35,35,53	1.30	4 (11%)	41,43,61	1.14	2 (4%)
30	PTY	8	810	-	34,34,49	1.03	4 (11%)	37,39,54	1.34	4 (10%)
38	CHL	3	611	-	49,63,74	1.74	9 (18%)	44,100,114	1.88	12 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	XAT	7	502	-	41,47,47	0.73	1 (2%)	54,74,74	2.00	13 (24%)
40	QTB	a	504	-	19,19,19	2.66	4 (21%)	23,26,26	2.98	12 (52%)
21	CLA	7	612	-	64,68,73	1.50	9 (14%)	76,107,113	1.93	18 (23%)
21	CLA	1	601	13	64,68,73	1.42	6 (9%)	76,107,113	1.90	16 (21%)
21	CLA	A	1121	1	61,65,73	1.49	7 (11%)	72,103,113	2.13	18 (25%)
21	CLA	A	1137	1	64,68,73	1.41	6 (9%)	76,107,113	1.95	22 (28%)
31	LAP	B	5007	-	28,28,28	1.24	3 (10%)	33,35,35	0.99	1 (3%)
21	CLA	a	607	-	62,66,73	1.44	7 (11%)	73,104,113	2.09	18 (24%)
21	CLA	4	602	15	56,60,73	1.50	7 (12%)	65,97,113	2.06	19 (29%)
21	CLA	B	1207	2	64,68,73	1.43	6 (9%)	76,107,113	1.94	20 (26%)
21	CLA	5	602	16	56,60,73	1.52	7 (12%)	65,97,113	2.10	19 (29%)
38	CHL	5	610	-	60,74,74	1.32	8 (13%)	58,114,114	1.69	10 (17%)
21	CLA	7	610	-	59,63,73	1.47	6 (10%)	70,101,113	1.96	20 (28%)
21	CLA	A	1124	-	59,63,73	1.52	6 (10%)	70,101,113	1.97	15 (21%)
28	LMT	B	5006	-	36,36,36	1.15	5 (13%)	47,47,47	1.02	2 (4%)
38	CHL	6	619	17	60,74,74	1.60	8 (13%)	58,114,114	1.63	11 (18%)
21	CLA	a	615	13	50,54,73	1.60	7 (14%)	59,90,113	1.99	16 (27%)
37	LUT	8	501	-	42,43,43	2.46	2 (4%)	51,60,60	1.77	15 (29%)
21	CLA	B	1223	2	69,73,73	1.37	7 (10%)	82,113,113	1.91	19 (23%)
21	CLA	B	1214	2	66,70,73	1.41	6 (9%)	78,109,113	1.88	18 (23%)
21	CLA	6	604	-	69,73,73	1.38	6 (8%)	82,113,113	2.04	23 (28%)
21	CLA	J	1901	8	46,50,73	1.62	6 (13%)	53,85,113	2.15	14 (26%)
21	CLA	5	605	-	50,54,73	1.64	6 (12%)	59,90,113	2.06	15 (25%)
21	CLA	5	606	-	54,58,73	1.54	6 (11%)	64,95,113	2.09	20 (31%)
21	CLA	8	605	-	49,53,73	1.65	6 (12%)	58,89,113	2.01	15 (25%)
21	CLA	A	1103	-	69,73,73	1.35	6 (8%)	82,113,113	1.99	20 (24%)
21	CLA	A	1141	24	49,53,73	1.61	7 (14%)	58,89,113	2.07	14 (24%)
21	CLA	5	618	16	56,60,73	1.52	7 (12%)	65,97,113	2.00	20 (30%)
21	CLA	B	1238	-	69,73,73	1.37	6 (8%)	82,113,113	1.87	16 (19%)
21	CLA	A	1139	1	59,63,73	1.51	7 (11%)	70,101,113	1.99	18 (25%)
23	BCR	K	4001	-	41,41,41	1.66	4 (9%)	56,56,56	4.51	16 (28%)
37	LUT	a	503	-	42,43,43	2.47	1 (2%)	51,60,60	2.06	16 (31%)
23	BCR	3	504	-	41,41,41	1.64	4 (9%)	56,56,56	4.42	15 (26%)
28	LMT	A	5008	-	36,36,36	1.09	5 (13%)	47,47,47	1.05	3 (6%)
21	CLA	A	1112	-	59,63,73	1.50	7 (11%)	70,101,113	2.10	20 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	LUT	6	502	-	42,43,43	2.40	2 (4%)	51,60,60	2.30	13 (25%)
24	LHG	8	801	21	36,36,48	0.46	0	39,42,54	1.23	4 (10%)
37	LUT	5	501	-	42,43,43	2.45	1 (2%)	51,60,60	1.94	14 (27%)
21	CLA	5	603	-	60,64,73	1.47	7 (11%)	71,102,113	2.04	17 (23%)
33	ERG	G	5002	-	32,32,32	8.39	19 (59%)	45,50,50	3.41	20 (44%)
21	CLA	6	617	17	49,53,73	1.58	7 (14%)	58,89,113	2.05	18 (31%)
21	CLA	B	1021	-	69,73,73	1.40	6 (8%)	82,113,113	1.88	18 (21%)
21	CLA	8	611	-	54,58,73	1.53	6 (11%)	64,95,113	2.15	17 (26%)
21	CLA	K	1402	-	64,68,73	1.40	7 (10%)	76,107,113	1.98	20 (26%)
23	BCR	B	4002	-	41,41,41	1.65	4 (9%)	56,56,56	4.52	13 (23%)
21	CLA	3	610	14	64,68,73	1.42	6 (9%)	76,107,113	1.94	17 (22%)
21	CLA	6	608	-	49,53,73	1.61	7 (14%)	58,89,113	2.08	17 (29%)
38	CHL	4	618	15	50,64,74	1.81	8 (16%)	46,102,114	1.84	11 (23%)
37	LUT	3	502	-	42,43,43	2.45	1 (2%)	51,60,60	1.89	11 (21%)
26	3PH	A	5007	-	32,32,47	1.02	4 (12%)	35,37,52	1.23	2 (5%)
21	CLA	7	603	18	69,73,73	1.37	6 (8%)	82,113,113	1.90	16 (19%)
21	CLA	4	617	-	49,53,73	1.60	7 (14%)	58,89,113	2.09	18 (31%)
37	LUT	4	501	-	42,43,43	2.37	1 (2%)	51,60,60	1.90	14 (27%)
38	CHL	3	608	-	37,51,74	1.65	9 (24%)	30,86,114	2.31	10 (33%)
37	LUT	7	501	-	42,43,43	2.47	2 (4%)	51,60,60	1.89	13 (25%)
23	BCR	8	503	-	41,41,41	1.65	4 (9%)	56,56,56	4.41	17 (30%)
21	CLA	4	606	-	54,58,73	1.53	7 (12%)	64,95,113	2.09	17 (26%)
21	CLA	B	1219	-	63,67,73	1.46	6 (9%)	74,105,113	1.95	16 (21%)
21	CLA	B	1206	2	59,63,73	1.52	7 (11%)	70,101,113	2.04	16 (22%)
21	CLA	A	1125	1	69,73,73	1.43	8 (11%)	82,113,113	2.18	21 (25%)
42	PLM	6	804	-	17,17,17	0.57	0	17,17,17	1.11	0
24	LHG	F	5001	21	42,42,48	0.43	0	45,48,54	1.14	3 (6%)
21	CLA	7	605	18	47,52,73	1.69	6 (12%)	55,88,113	2.03	12 (21%)
38	CHL	a	613	-	40,54,74	1.59	9 (22%)	34,90,114	1.99	9 (26%)
21	CLA	8	606	-	61,65,73	1.46	7 (11%)	72,103,113	2.07	19 (26%)
21	CLA	B	1228	2	69,73,73	1.40	9 (13%)	82,113,113	2.78	24 (29%)
21	CLA	B	1232	-	49,53,73	1.63	7 (14%)	58,89,113	2.00	13 (22%)
27	SF4	C	3002	3	0,12,12	-	-	-	-	-
38	CHL	5	611	-	45,59,74	1.79	9 (20%)	40,96,114	1.97	12 (30%)
21	CLA	A	1126	1	69,73,73	1.41	6 (8%)	82,113,113	1.92	18 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	LHG	1	801	-	34,34,48	0.46	0	37,40,54	1.26	4 (10%)
21	CLA	3	603	-	69,73,73	1.37	7 (10%)	82,113,113	1.88	15 (18%)
23	BCR	5	504	-	41,41,41	1.65	6 (14%)	56,56,56	4.32	18 (32%)
25	DGD	B	5003	-	67,67,67	1.30	7 (10%)	81,81,81	1.09	5 (6%)
35	LPX	a	804	-	29,29,29	1.03	2 (6%)	31,33,33	0.93	1 (3%)
21	CLA	7	615	18	59,63,73	1.46	6 (10%)	70,101,113	1.94	18 (25%)
21	CLA	7	601	-	64,68,73	1.45	6 (9%)	76,107,113	1.91	20 (26%)
21	CLA	8	612	19	50,54,73	1.61	6 (12%)	59,90,113	2.01	13 (22%)
21	CLA	B	1201	2	69,73,73	1.37	7 (10%)	82,113,113	1.95	22 (26%)
21	CLA	5	617	-	54,58,73	1.55	6 (11%)	64,95,113	2.21	20 (31%)
34	RRX	J	4002	-	42,42,42	4.99	24 (57%)	56,58,58	2.50	21 (37%)
21	CLA	1	610	-	49,53,73	1.63	6 (12%)	58,89,113	2.03	13 (22%)
24	LHG	a	801	-	34,34,48	0.48	0	37,40,54	1.32	5 (13%)
30	PTY	7	804	-	32,32,49	1.07	4 (12%)	35,37,54	1.21	2 (5%)
30	PTY	3	802	-	37,37,49	1.01	4 (10%)	40,42,54	1.10	2 (5%)
21	CLA	3	607	24	69,73,73	1.36	6 (8%)	82,113,113	1.91	16 (19%)
23	BCR	B	4005	-	41,41,41	1.70	6 (14%)	56,56,56	4.45	18 (32%)
21	CLA	A	1127	1	69,73,73	1.39	6 (8%)	82,113,113	1.82	15 (18%)
40	QTB	3	506	-	19,19,19	2.71	5 (26%)	23,26,26	2.93	10 (43%)
21	CLA	a	604	13	69,73,73	1.36	7 (10%)	82,113,113	1.98	20 (24%)
21	CLA	8	609	19	64,68,73	1.42	6 (9%)	76,107,113	1.99	17 (22%)
38	CHL	1	613	-	42,56,74	1.46	8 (19%)	36,92,114	2.18	11 (30%)
43	DGA	8	803	-	29,29,43	1.27	2 (6%)	31,31,45	1.18	3 (9%)
23	BCR	7	503	-	41,41,41	1.64	6 (14%)	56,56,56	4.48	13 (23%)
21	CLA	5	614	-	50,54,73	1.58	7 (14%)	59,90,113	2.07	13 (22%)
23	BCR	5	503	-	41,41,41	1.65	5 (12%)	56,56,56	4.47	18 (32%)
21	CLA	A	1111	-	69,73,73	1.40	6 (8%)	82,113,113	1.89	21 (25%)
21	CLA	8	615	-	50,54,73	1.61	6 (12%)	59,90,113	2.07	17 (28%)
37	LUT	3	501	-	42,43,43	2.42	1 (2%)	51,60,60	1.97	16 (31%)
21	CLA	B	1217	2	60,64,73	1.45	6 (10%)	71,102,113	2.00	16 (22%)
36	ECH	M	4001	-	42,42,42	1.15	3 (7%)	55,58,58	2.06	16 (29%)
38	CHL	1	609	13	60,74,74	1.49	9 (15%)	58,114,114	1.78	14 (24%)
21	CLA	B	1213	2	64,68,73	1.45	7 (10%)	76,107,113	1.98	20 (26%)
21	CLA	4	608	15	55,59,73	1.53	6 (10%)	64,96,113	2.15	19 (29%)
32	SQD	G	5001	-	44,46,54	0.81	0	54,57,65	0.88	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	A	1136	1	69,73,73	1.37	6 (8%)	82,113,113	1.89	16 (19%)
21	CLA	L	1502	12	64,68,73	1.42	7 (10%)	76,107,113	2.03	19 (25%)
21	CLA	A	1138	1	69,73,73	1.39	7 (10%)	82,113,113	1.99	17 (20%)
21	CLA	L	1501	-	54,58,73	1.53	6 (11%)	64,95,113	2.24	21 (32%)
21	CLA	1	602	-	49,53,73	1.60	6 (12%)	58,89,113	2.04	13 (22%)
21	CLA	8	610	-	59,63,73	1.49	6 (10%)	70,101,113	2.00	18 (25%)
24	LHG	1	802	-	41,41,48	0.42	0	44,47,54	1.08	4 (9%)
21	CLA	6	607	24	59,63,73	1.48	8 (13%)	70,101,113	1.95	17 (24%)
23	BCR	F	4001	-	41,41,41	1.67	5 (12%)	56,56,56	4.14	16 (28%)
37	LUT	5	502	-	42,43,43	2.43	2 (4%)	51,60,60	2.01	13 (25%)
21	CLA	5	612	16	69,73,73	1.37	6 (8%)	82,113,113	1.84	16 (19%)
21	CLA	K	1403	9	50,54,73	1.60	7 (14%)	59,90,113	2.04	12 (20%)
21	CLA	a	601	13	64,68,73	1.42	6 (9%)	76,107,113	1.93	20 (26%)
38	CHL	5	613	-	50,64,74	1.28	8 (16%)	46,102,114	1.97	11 (23%)
21	CLA	A	1101	1	69,73,73	1.38	6 (8%)	82,113,113	2.00	19 (23%)
21	CLA	A	1130	1	60,64,73	1.44	6 (10%)	71,102,113	1.98	19 (26%)
32	SQD	7	805	-	37,39,54	0.89	0	47,50,65	0.94	2 (4%)
21	CLA	7	609	-	64,68,73	1.41	6 (9%)	76,107,113	2.02	19 (25%)
23	BCR	B	4004	-	41,41,41	1.64	5 (12%)	56,56,56	4.53	20 (35%)
21	CLA	A	1102	1,21	69,73,73	1.40	6 (8%)	82,113,113	2.15	19 (23%)
21	CLA	a	603	-	69,73,73	1.38	7 (10%)	82,113,113	1.95	19 (23%)
21	CLA	B	1023	-	69,73,73	1.37	6 (8%)	82,113,113	1.87	17 (20%)
21	CLA	8	602	19	56,60,73	1.54	6 (10%)	65,97,113	2.02	16 (24%)
23	BCR	3	503	-	41,41,41	1.70	6 (14%)	56,56,56	4.22	18 (32%)
24	LHG	7	802	-	35,35,48	0.45	0	38,41,54	1.17	4 (10%)
24	LHG	6	801	21	48,48,48	0.40	0	51,54,54	1.14	3 (5%)
38	CHL	4	609	15	60,74,74	1.30	9 (15%)	58,114,114	1.75	11 (18%)
24	LHG	A	5003	-	41,41,48	0.44	0	44,47,54	1.17	3 (6%)
21	CLA	A	1108	1	69,73,73	1.38	6 (8%)	82,113,113	2.02	16 (19%)
21	CLA	B	1236	2	57,61,73	1.54	7 (12%)	67,98,113	2.23	19 (28%)
21	CLA	7	611	-	64,68,73	1.40	6 (9%)	76,107,113	2.07	23 (30%)
21	CLA	1	603	-	69,73,73	1.33	6 (8%)	82,113,113	1.89	18 (21%)
21	CLA	4	610	-	69,73,73	1.39	7 (10%)	82,113,113	1.93	20 (24%)
42	PLM	4	803	-	15,16,17	0.42	0	14,15,17	0.63	0
21	CLA	7	607	24	63,67,73	1.44	6 (9%)	74,105,113	1.97	15 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
44	SPH	6	806	-	19,20,20	0.63	0	18,21,21	1.14	1 (5%)
21	CLA	8	618	-	64,68,73	1.42	6 (9%)	76,107,113	1.99	18 (23%)
21	CLA	K	1404	9	56,60,73	1.53	8 (14%)	65,97,113	2.09	19 (29%)
21	CLA	5	607	24	59,63,73	1.49	6 (10%)	70,101,113	1.93	16 (22%)
21	CLA	6	602	17	56,60,73	1.50	6 (10%)	65,97,113	2.07	18 (27%)
21	CLA	B	1225	2	69,73,73	1.39	6 (8%)	82,113,113	1.81	16 (19%)
21	CLA	4	603	15	60,64,73	1.44	6 (10%)	71,102,113	2.05	19 (26%)
21	CLA	8	620	19	69,73,73	1.36	7 (10%)	82,113,113	1.87	19 (23%)
21	CLA	A	1113	1	56,60,73	1.52	6 (10%)	65,97,113	2.08	19 (29%)
23	BCR	B	4007	-	41,41,41	1.65	5 (12%)	56,56,56	4.28	16 (28%)
38	CHL	6	610	-	50,64,74	1.58	7 (14%)	46,102,114	1.87	11 (23%)
21	CLA	1	606	-	61,65,73	1.47	6 (9%)	72,103,113	2.02	17 (23%)
27	SF4	C	3003	3	0,12,12	-	-	-	-	-
21	CLA	4	615	15	64,68,73	1.43	6 (9%)	76,107,113	1.95	19 (25%)
25	DGD	8	802	-	67,67,67	1.29	7 (10%)	81,81,81	1.12	5 (6%)
38	CHL	a	609	13	47,61,74	1.81	9 (19%)	41,98,114	1.91	10 (24%)
21	CLA	6	605	-	50,54,73	1.59	6 (12%)	59,90,113	2.10	17 (28%)
21	CLA	A	1135	1	69,73,73	1.36	6 (8%)	82,113,113	1.89	18 (21%)
21	CLA	B	1215	2	64,68,73	1.42	6 (9%)	76,107,113	1.85	19 (25%)
21	CLA	5	608	-	49,53,73	1.62	7 (14%)	58,89,113	2.08	16 (27%)
38	CHL	8	613	-	45,59,74	1.81	9 (20%)	40,96,114	2.13	13 (32%)
21	CLA	B	1210	-	69,73,73	1.40	6 (8%)	82,113,113	2.05	18 (21%)
20	CL0	A	1011	1	58,73,73	3.07	18 (31%)	60,113,113	2.87	19 (31%)
37	LUT	a	502	-	42,43,43	2.45	2 (4%)	51,60,60	1.83	13 (25%)
21	CLA	3	604	-	64,68,73	1.42	6 (9%)	76,107,113	2.01	21 (27%)
25	DGD	A	5005	-	52,52,67	0.97	4 (7%)	66,66,81	1.14	5 (7%)
23	BCR	4	503	-	41,41,41	1.64	5 (12%)	56,56,56	4.55	12 (21%)
21	CLA	A	1114	-	69,73,73	1.39	6 (8%)	82,113,113	1.96	21 (25%)
21	CLA	A	1134	1	64,68,73	1.41	6 (9%)	76,107,113	1.96	19 (25%)
21	CLA	A	1118	1	59,63,73	1.48	6 (10%)	70,101,113	2.07	19 (27%)
21	CLA	7	606	-	59,63,73	1.48	7 (11%)	70,101,113	1.97	20 (28%)
23	BCR	A	4005	-	41,41,41	1.66	6 (14%)	56,56,56	4.42	16 (28%)
21	CLA	6	615	-	69,73,73	1.38	7 (10%)	82,113,113	1.88	19 (23%)
37	LUT	5	505	-	42,43,43	2.50	2 (4%)	51,60,60	2.62	18 (35%)
37	LUT	6	501	-	42,43,43	2.45	1 (2%)	51,60,60	2.13	14 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	BCR	A	4003	-	41,41,41	1.63	5 (12%)	56,56,56	4.47	14 (25%)
21	CLA	B	1237	-	69,73,73	1.38	7 (10%)	82,113,113	1.92	18 (21%)
21	CLA	8	603	19	69,73,73	1.38	7 (10%)	82,113,113	2.02	21 (25%)
21	CLA	B	1231	2	69,73,73	1.37	6 (8%)	82,113,113	1.90	17 (20%)
21	CLA	F	1301	6	54,58,73	1.53	6 (11%)	64,95,113	2.18	19 (29%)
21	CLA	4	601	-	64,68,73	1.43	5 (7%)	76,107,113	1.96	19 (25%)
21	CLA	4	604	15	64,68,73	1.45	6 (9%)	76,107,113	1.91	17 (22%)
21	CLA	4	611	-	60,64,73	1.45	6 (10%)	71,102,113	1.99	19 (26%)
21	CLA	4	616	-	54,58,73	1.54	7 (12%)	64,95,113	2.10	17 (26%)
23	BCR	B	4003	-	41,41,41	1.61	5 (12%)	56,56,56	4.63	17 (30%)
23	BCR	6	503	-	41,41,41	1.65	5 (12%)	56,56,56	4.45	15 (26%)
21	CLA	A	1116	-	64,68,73	1.45	6 (9%)	76,107,113	2.02	19 (25%)
37	LUT	1	502	-	42,43,43	2.35	2 (4%)	51,60,60	1.97	17 (33%)
21	CLA	6	606	-	56,60,73	1.50	7 (12%)	65,97,113	2.03	18 (27%)
21	CLA	A	1120	-	53,57,73	1.54	7 (13%)	61,93,113	2.26	19 (31%)
21	CLA	B	1211	-	59,63,73	1.51	6 (10%)	70,101,113	1.99	17 (24%)
23	BCR	I	4001	-	41,41,41	1.62	4 (9%)	56,56,56	4.37	18 (32%)
24	LHG	A	5001	21	28,28,48	0.52	0	31,34,54	1.36	3 (9%)
38	CHL	7	613	-	60,74,74	1.34	10 (16%)	58,114,114	1.63	10 (17%)
43	DGA	5	803	-	22,22,43	1.45	3 (13%)	24,24,45	1.40	2 (8%)
39	OLA	8	809	-	19,19,19	0.57	0	19,19,19	1.06	0
21	CLA	A	1119	-	69,73,73	1.38	6 (8%)	82,113,113	1.73	18 (21%)
39	OLA	1	803	-	19,19,19	0.57	0	19,19,19	1.05	1 (5%)
37	LUT	1	503	-	42,43,43	2.51	1 (2%)	51,60,60	2.26	12 (23%)
22	PQN	A	2001	-	34,34,34	0.36	0	43,45,45	1.29	5 (11%)
21	CLA	3	601	-	69,73,73	1.38	6 (8%)	82,113,113	1.92	20 (24%)
21	CLA	8	608	19	56,60,73	1.53	6 (10%)	65,97,113	2.26	19 (29%)
21	CLA	a	602	-	54,58,73	1.56	8 (14%)	64,95,113	2.06	18 (28%)
46	4RF	8	808	-	53,53,56	0.91	5 (9%)	56,56,59	1.06	3 (5%)
21	CLA	4	612	15	66,70,73	1.39	7 (10%)	78,109,113	2.02	19 (24%)
24	LHG	4	802	-	31,31,48	0.46	0	34,37,54	1.18	2 (5%)
27	SF4	A	3001	1,2	0,12,12	-	-	-	-	-
21	CLA	A	1115	1	64,68,73	1.43	7 (10%)	76,107,113	1.98	18 (23%)
21	CLA	a	605	-	69,73,73	1.36	6 (8%)	82,113,113	1.90	18 (21%)
21	CLA	3	613	-	65,69,73	1.43	6 (9%)	77,108,113	1.89	15 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	CHL	6	611	-	45,59,74	1.64	9 (20%)	40,96,114	2.10	12 (30%)
24	LHG	A	5002	-	48,48,48	0.40	0	51,54,54	1.05	3 (5%)
24	LHG	4	801	21	48,48,48	0.40	0	51,54,54	1.08	3 (5%)
21	CLA	B	1208	2	64,68,73	1.42	6 (9%)	76,107,113	2.00	20 (26%)
21	CLA	6	618	-	50,54,73	1.58	7 (14%)	59,90,113	2.12	15 (25%)
21	CLA	6	609	17	69,73,73	1.38	6 (8%)	82,113,113	1.89	16 (19%)
23	BCR	B	4006	-	41,41,41	1.62	5 (12%)	56,56,56	4.50	14 (25%)
21	CLA	G	1602	-	50,54,73	1.61	7 (14%)	59,90,113	2.00	17 (28%)
21	CLA	B	1220	-	64,68,73	1.44	6 (9%)	76,107,113	1.98	16 (21%)
30	PTY	B	5005	-	40,40,49	0.96	4 (10%)	43,45,54	1.18	3 (6%)
38	CHL	8	604	19	56,70,74	1.77	9 (16%)	53,109,114	1.73	12 (22%)
23	BCR	B	4001	-	41,41,41	1.65	6 (14%)	56,56,56	4.45	16 (28%)
24	LHG	6	802	-	36,36,48	0.43	0	39,42,54	1.18	4 (10%)
21	CLA	1	607	-	69,73,73	1.37	6 (8%)	82,113,113	1.88	18 (21%)
31	LAP	F	5003	-	28,28,28	1.26	3 (10%)	33,35,35	0.95	1 (3%)
21	CLA	1	605	-	69,73,73	1.36	6 (8%)	82,113,113	1.98	20 (24%)
31	LAP	K	5001	-	28,28,28	1.29	3 (10%)	33,35,35	1.08	2 (6%)
21	CLA	G	1603	-	49,53,73	1.60	6 (12%)	58,89,113	1.99	14 (24%)
21	CLA	A	1131	1	69,73,73	1.40	6 (8%)	82,113,113	1.89	16 (19%)
30	PTY	5	802	-	37,37,49	0.99	4 (10%)	40,42,54	1.19	2 (5%)
35	LPX	J	5001	-	16,16,29	1.35	2 (12%)	18,20,33	1.05	1 (5%)

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
21	CLA	K	1401	-	1/1/11/20	9/17/93/115	-
38	CHL	a	610	-	3/3/16/26	6/18/116/137	-
23	BCR	L	4003	-	-	7/29/63/63	0/2/2/2
21	CLA	A	1012	-	1/1/15/20	15/39/115/115	-
21	CLA	5	604	-	1/1/15/20	10/39/115/115	-
23	BCR	K	4002	-	-	12/29/63/63	0/2/2/2
37	LUT	4	502	-	-	1/29/67/67	0/2/2/2
21	CLA	7	602	-	1/1/10/20	8/14/90/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	3	612	-	1/1/15/20	12/39/115/115	-
21	CLA	3	616	-	1/1/13/20	15/29/105/115	-
21	CLA	B	1216	-	1/1/14/20	18/35/111/115	-
21	CLA	F	1302	24	1/1/13/20	12/27/103/115	-
24	LHG	7	801	21	-	26/53/53/53	-
21	CLA	4	607	24	1/1/13/20	10/27/103/115	-
23	BCR	A	4001	-	-	10/29/63/63	0/2/2/2
21	CLA	B	1235	2	1/1/15/20	19/39/115/115	-
28	LMT	1	804	-	-	10/21/61/61	0/2/2/2
37	LUT	a	501	-	-	7/29/67/67	0/2/2/2
23	BCR	A	4002	-	-	11/29/63/63	0/2/2/2
21	CLA	6	612	-	1/1/12/20	11/21/97/115	-
21	CLA	1	615	13	1/1/11/20	7/17/93/115	-
21	CLA	B	1234	2	1/1/13/20	13/29/105/115	-
38	CHL	8	601	19	4/4/19/26	10/33/131/137	-
21	CLA	7	604	-	1/1/15/20	18/39/115/115	-
37	LUT	1	501	-	-	3/29/67/67	0/2/2/2
23	BCR	L	4001	-	-	13/29/63/63	0/2/2/2
24	LHG	B	5002	-	-	36/53/53/53	-
21	CLA	B	1202	2	1/1/15/20	13/39/115/115	-
24	LHG	3	801	21	-	31/53/53/53	-
21	CLA	5	601	16	1/1/14/20	13/33/109/115	-
23	BCR	L	4002	-	-	8/29/63/63	0/2/2/2
21	CLA	B	1204	2	1/1/15/20	25/39/115/115	-
21	CLA	B	1209	2	1/1/15/20	18/39/115/115	-
22	PQN	B	2002	-	-	5/23/43/43	0/2/2/2
21	CLA	6	601	-	1/1/14/20	15/33/109/115	-
21	CLA	A	1132	-	1/1/15/20	19/39/115/115	-
23	BCR	G	4001	-	-	10/29/63/63	0/2/2/2
21	CLA	a	611	-	1/1/12/20	10/21/97/115	-
21	CLA	B	1240	24	1/1/15/20	10/39/115/115	-
24	LHG	F	5002	-	-	27/40/40/53	-
21	CLA	4	605	-	1/1/11/20	6/17/93/115	-
21	CLA	7	617	18	1/1/13/20	13/25/101/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	5	616	-	1/1/11/20	8/17/93/115	-
21	CLA	B	1227	2	1/1/12/20	6/21/97/115	-
21	CLA	3	618	-	1/1/11/20	5/17/93/115	-
21	CLA	B	1230	2	1/1/13/20	13/31/107/115	-
21	CLA	A	1133	1	1/1/15/20	20/39/115/115	-
21	CLA	B	1205	-	1/1/15/20	16/39/115/115	-
21	CLA	1	611	-	1/1/13/20	13/27/103/115	-
38	CHL	4	613	-	3/3/17/26	9/23/121/137	-
21	CLA	A	1123	-	1/1/15/20	11/39/115/115	-
38	CHL	a	606	-	4/4/18/26	7/27/125/137	-
21	CLA	B	1218	2	1/1/13/20	9/27/103/115	-
21	CLA	8	607	24	1/1/11/20	4/17/93/115	-
21	CLA	A	1110	1	1/1/14/20	16/33/109/115	-
41	GG0	a	805	-	-	2/7/7/7	-
46	4RF	8	807	-	-	23/44/44/59	-
21	CLA	B	1222	-	1/1/13/20	5/31/107/115	-
21	CLA	B	1212	2	1/1/15/20	22/39/115/115	-
21	CLA	6	603	-	1/1/15/20	17/39/115/115	-
21	CLA	G	1601	-	1/1/12/20	12/21/97/115	-
21	CLA	B	1239	2	1/1/15/20	17/39/115/115	-
21	CLA	A	1105	-	1/1/13/20	9/30/106/115	-
21	CLA	3	602	14	1/1/11/20	8/17/93/115	-
21	CLA	1	612	13	1/1/15/20	18/39/115/115	-
38	CHL	6	613	-	3/3/17/26	2/21/119/137	-
21	CLA	A	1106	1	1/1/15/20	19/39/115/115	-
21	CLA	A	1117	1	1/1/15/20	19/39/115/115	-
21	CLA	1	608	13	1/1/14/20	12/33/109/115	-
21	CLA	A	1122	-	1/1/15/20	19/39/115/115	-
21	CLA	B	1221	-	1/1/15/20	12/39/115/115	-
21	CLA	3	605	-	1/1/15/20	16/39/115/115	-
21	CLA	A	1107	1	1/1/13/20	8/27/103/115	-
21	CLA	L	1503	-	1/1/11/20	8/15/91/115	-
21	CLA	B	1022	-	1/1/15/20	13/39/115/115	-
23	BCR	J	4001	-	-	13/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	P5S	8	806	-	-	30/42/42/59	-
21	CLA	a	612	13	1/1/13/20	9/30/106/115	-
21	CLA	5	609	16	1/1/12/20	8/23/99/115	-
24	LHG	5	801	21	-	28/53/53/53	-
29	PCW	B	5004	-	-	14/33/33/57	-
21	CLA	a	608	13	1/1/13/20	11/27/103/115	-
23	BCR	A	4004	-	-	11/29/63/63	0/2/2/2
21	CLA	A	1109	1,21	1/1/15/20	22/39/115/115	-
21	CLA	A	1013	-	1/1/15/20	13/39/115/115	-
24	LHG	7	803	-	-	29/47/47/53	-
21	CLA	A	1128	1	1/1/15/20	15/39/115/115	-
46	4RF	7	807	-	-	19/34/34/59	-
37	LUT	8	502	-	-	1/29/67/67	0/2/2/2
21	CLA	B	1229	-	1/1/15/20	8/39/115/115	-
21	CLA	3	606	-	1/1/15/20	9/39/115/115	-
21	CLA	B	1226	2	1/1/15/20	13/39/115/115	-
21	CLA	B	1224	2	1/1/15/20	23/39/115/115	-
21	CLA	B	1203	-	1/1/15/20	19/39/115/115	-
24	LHG	B	5001	21	-	29/50/50/53	-
23	BCR	6	504	-	-	9/29/63/63	0/2/2/2
21	CLA	A	1104	-	1/1/15/20	20/39/115/115	-
23	BCR	3	505	-	-	13/29/63/63	0/2/2/2
47	C7Z	7	504	-	1/1/12/26	8/29/67/67	0/2/2/2
21	CLA	A	1129	-	1/1/12/20	12/21/97/115	-
21	CLA	A	1140	-	1/1/13/20	14/27/103/115	-
21	CLA	7	608	18	1/1/10/20	6/12/88/115	-
21	CLA	1	604	-	1/1/15/20	21/39/115/115	-
29	PCW	6	803	-	-	19/39/39/57	-
30	PTY	8	810	-	-	19/38/38/53	-
38	CHL	3	611	-	3/3/17/26	6/26/124/137	-
45	XAT	7	502	-	3/3/12/26	1/31/93/93	0/4/4/4
40	QTB	a	504	-	-	6/11/28/28	0/1/1/1
21	CLA	7	612	-	1/1/14/20	19/33/109/115	-
21	CLA	1	601	13	1/1/14/20	7/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	1121	1	1/1/13/20	14/30/106/115	-
21	CLA	A	1137	1	1/1/14/20	11/33/109/115	-
31	LAP	B	5007	-	-	17/30/30/30	-
21	CLA	a	607	-	1/1/13/20	13/31/107/115	-
21	CLA	4	602	15	1/1/12/20	5/24/100/115	-
21	CLA	B	1207	2	1/1/14/20	19/33/109/115	-
21	CLA	5	602	16	1/1/12/20	8/24/100/115	-
38	CHL	5	610	-	4/4/20/26	6/39/137/137	-
21	CLA	7	610	-	1/1/13/20	7/27/103/115	-
21	CLA	A	1124	-	1/1/13/20	9/27/103/115	-
28	LMT	B	5006	-	-	10/21/61/61	1/2/2/2
38	CHL	6	619	17	5/5/20/26	13/39/137/137	-
21	CLA	a	615	13	1/1/11/20	4/17/93/115	-
37	LUT	8	501	-	-	0/29/67/67	0/2/2/2
21	CLA	B	1223	2	1/1/15/20	13/39/115/115	-
21	CLA	B	1214	2	1/1/14/20	21/36/112/115	-
21	CLA	6	604	-	1/1/15/20	20/39/115/115	-
21	CLA	J	1901	8	1/1/10/20	3/12/88/115	-
21	CLA	5	605	-	1/1/11/20	7/17/93/115	-
21	CLA	5	606	-	1/1/12/20	7/21/97/115	-
21	CLA	8	605	-	1/1/11/20	4/15/91/115	-
21	CLA	A	1103	-	1/1/15/20	15/39/115/115	-
21	CLA	A	1141	24	1/1/11/20	10/15/91/115	-
21	CLA	5	618	16	1/1/12/20	4/24/100/115	-
21	CLA	B	1238	-	1/1/15/20	13/39/115/115	-
21	CLA	A	1139	1	1/1/13/20	14/27/103/115	-
23	BCR	K	4001	-	-	10/29/63/63	0/2/2/2
37	LUT	a	503	-	-	4/29/67/67	0/2/2/2
23	BCR	3	504	-	-	11/29/63/63	0/2/2/2
28	LMT	A	5008	-	-	8/21/61/61	0/2/2/2
21	CLA	A	1112	-	1/1/13/20	8/27/103/115	-
37	LUT	6	502	-	1/1/12/27	8/29/67/67	0/2/2/2
24	LHG	8	801	21	-	26/41/41/53	-
37	LUT	5	501	-	-	1/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	5	603	-	1/1/13/20	14/29/105/115	-
33	ERG	G	5002	-	4/4/11/15	10/13/71/71	0/4/4/4
21	CLA	6	617	17	1/1/11/20	4/15/91/115	-
21	CLA	B	1021	-	1/1/15/20	22/39/115/115	-
21	CLA	8	611	-	1/1/12/20	5/21/97/115	-
21	CLA	K	1402	-	1/1/14/20	10/33/109/115	-
23	BCR	B	4002	-	-	13/29/63/63	0/2/2/2
21	CLA	3	610	14	1/1/14/20	15/33/109/115	-
21	CLA	6	608	-	1/1/11/20	6/15/91/115	-
38	CHL	4	618	15	4/4/18/26	7/27/125/137	-
37	LUT	3	502	-	-	3/29/67/67	0/2/2/2
26	3PH	A	5007	-	-	10/34/34/49	-
21	CLA	7	603	18	1/1/15/20	18/39/115/115	-
21	CLA	4	617	-	1/1/11/20	5/15/91/115	-
37	LUT	4	501	-	-	1/29/67/67	0/2/2/2
38	CHL	3	608	-	4/4/15/26	2/12/110/137	-
37	LUT	7	501	-	1/1/12/27	5/29/67/67	0/2/2/2
23	BCR	8	503	-	-	10/29/63/63	0/2/2/2
21	CLA	4	606	-	1/1/12/20	5/21/97/115	-
21	CLA	B	1219	-	1/1/13/20	10/32/108/115	-
21	CLA	B	1206	2	1/1/13/20	12/27/103/115	-
21	CLA	A	1125	1	1/1/15/20	20/39/115/115	-
42	PLM	6	804	-	-	7/15/15/15	-
24	LHG	F	5001	21	-	30/47/47/53	-
21	CLA	7	605	18	1/1/11/20	8/13/89/115	-
38	CHL	a	613	-	3/3/16/26	8/15/113/137	-
21	CLA	8	606	-	1/1/13/20	12/30/106/115	-
21	CLA	B	1228	2	1/1/15/20	18/39/115/115	-
21	CLA	B	1232	-	1/1/11/20	7/15/91/115	-
27	SF4	C	3002	3	-	-	0/6/5/5
38	CHL	5	611	-	3/3/17/26	3/21/119/137	-
21	CLA	A	1126	1	1/1/15/20	21/39/115/115	-
24	LHG	1	801	-	-	25/39/39/53	-
21	CLA	3	603	-	1/1/15/20	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	5	504	-	-	9/29/63/63	0/2/2/2
25	DGD	B	5003	-	-	18/55/95/95	0/2/2/2
35	LPX	a	804	-	-	13/31/31/31	-
21	CLA	7	615	18	1/1/13/20	13/27/103/115	-
21	CLA	7	601	-	1/1/14/20	14/33/109/115	-
21	CLA	8	612	19	1/1/11/20	9/17/93/115	-
21	CLA	B	1201	2	1/1/15/20	17/39/115/115	-
21	CLA	5	617	-	1/1/12/20	13/21/97/115	-
34	RRX	J	4002	-	1/1/11/25	12/29/65/65	0/2/2/2
21	CLA	1	610	-	1/1/11/20	4/15/91/115	-
24	LHG	a	801	-	-	25/39/39/53	-
30	PTY	7	804	-	-	16/36/36/53	-
30	PTY	3	802	-	-	24/41/41/53	-
21	CLA	3	607	24	1/1/15/20	10/39/115/115	-
23	BCR	B	4005	-	-	11/29/63/63	0/2/2/2
21	CLA	A	1127	1	1/1/15/20	11/39/115/115	-
40	QTB	3	506	-	2/2/5/10	3/11/28/28	0/1/1/1
21	CLA	a	604	13	1/1/15/20	19/39/115/115	-
21	CLA	8	609	19	1/1/14/20	21/33/109/115	-
38	CHL	1	613	-	3/3/16/26	0/18/116/137	-
43	DGA	8	803	-	-	11/31/31/45	-
23	BCR	7	503	-	-	16/29/63/63	0/2/2/2
21	CLA	5	614	-	1/1/11/20	5/17/93/115	-
23	BCR	5	503	-	-	16/29/63/63	0/2/2/2
21	CLA	A	1111	-	1/1/15/20	22/39/115/115	-
21	CLA	8	615	-	1/1/11/20	6/17/93/115	-
37	LUT	3	501	-	-	1/29/67/67	0/2/2/2
21	CLA	B	1217	2	1/1/13/20	13/29/105/115	-
36	ECH	M	4001	-	-	9/29/66/66	0/2/2/2
38	CHL	1	609	13	4/4/20/26	10/39/137/137	-
21	CLA	B	1213	2	1/1/14/20	16/33/109/115	-
21	CLA	4	608	15	1/1/12/20	7/23/99/115	-
32	SQD	G	5001	-	-	21/41/61/69	0/1/1/1
21	CLA	A	1136	1	1/1/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	L	1502	12	1/1/14/20	10/33/109/115	-
21	CLA	A	1138	1	1/1/15/20	16/39/115/115	-
21	CLA	L	1501	-	1/1/12/20	8/21/97/115	-
21	CLA	1	602	-	1/1/11/20	7/15/91/115	-
21	CLA	8	610	-	1/1/13/20	13/27/103/115	-
24	LHG	1	802	-	-	28/46/46/53	-
21	CLA	6	607	24	1/1/13/20	7/27/103/115	-
23	BCR	F	4001	-	-	9/29/63/63	0/2/2/2
37	LUT	5	502	-	-	1/29/67/67	0/2/2/2
21	CLA	5	612	16	1/1/15/20	21/39/115/115	-
21	CLA	K	1403	9	1/1/11/20	8/17/93/115	-
21	CLA	a	601	13	1/1/14/20	6/33/109/115	-
38	CHL	5	613	-	4/4/18/26	4/27/125/137	-
21	CLA	A	1101	1	1/1/15/20	22/39/115/115	-
21	CLA	A	1130	1	1/1/13/20	13/29/105/115	-
32	SQD	7	805	-	-	14/34/54/69	0/1/1/1
21	CLA	7	609	-	1/1/14/20	14/33/109/115	-
23	BCR	B	4004	-	-	11/29/63/63	0/2/2/2
21	CLA	A	1102	1,21	1/1/15/20	17/39/115/115	-
21	CLA	a	603	-	1/1/15/20	14/39/115/115	-
21	CLA	B	1023	-	1/1/15/20	17/39/115/115	-
21	CLA	8	602	19	1/1/12/20	8/24/100/115	-
23	BCR	3	503	-	-	9/29/63/63	0/2/2/2
24	LHG	7	802	-	-	21/40/40/53	-
24	LHG	6	801	21	-	28/53/53/53	-
38	CHL	4	609	15	4/4/20/26	18/39/137/137	-
24	LHG	A	5003	-	-	31/46/46/53	-
21	CLA	A	1108	1	1/1/15/20	14/39/115/115	-
21	CLA	B	1236	2	1/1/12/20	14/25/101/115	-
21	CLA	7	611	-	1/1/14/20	10/33/109/115	-
21	CLA	1	603	-	1/1/15/20	21/39/115/115	-
21	CLA	4	610	-	1/1/15/20	21/39/115/115	-
42	PLM	4	803	-	-	9/14/14/15	-
21	CLA	7	607	24	1/1/13/20	11/31/107/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	SPH	6	806	-	-	13/21/21/21	-
21	CLA	8	618	-	1/1/14/20	15/33/109/115	-
21	CLA	K	1404	9	1/1/12/20	11/24/100/115	-
21	CLA	5	607	24	1/1/13/20	10/27/103/115	-
21	CLA	6	602	17	1/1/12/20	6/24/100/115	-
21	CLA	B	1225	2	1/1/15/20	10/39/115/115	-
21	CLA	4	603	15	1/1/13/20	12/29/105/115	-
21	CLA	8	620	19	1/1/15/20	17/39/115/115	-
21	CLA	A	1113	1	1/1/12/20	10/24/100/115	-
23	BCR	B	4007	-	-	9/29/63/63	0/2/2/2
38	CHL	6	610	-	4/4/18/26	4/27/125/137	-
21	CLA	1	606	-	1/1/13/20	11/30/106/115	-
27	SF4	C	3003	3	-	-	0/6/5/5
21	CLA	4	615	15	1/1/14/20	12/33/109/115	-
25	DGD	8	802	-	-	27/55/95/95	0/2/2/2
38	CHL	a	609	13	3/3/17/26	3/24/122/137	-
21	CLA	6	605	-	1/1/11/20	6/17/93/115	-
21	CLA	A	1135	1	1/1/15/20	20/39/115/115	-
21	CLA	B	1215	2	1/1/14/20	17/33/109/115	-
21	CLA	5	608	-	1/1/11/20	6/15/91/115	-
38	CHL	8	613	-	3/3/17/26	1/21/119/137	-
21	CLA	B	1210	-	1/1/15/20	20/39/115/115	-
20	CL0	A	1011	1	3/3/20/25	13/37/135/135	-
37	LUT	a	502	-	1/1/12/27	11/29/67/67	0/2/2/2
21	CLA	3	604	-	1/1/14/20	13/33/109/115	-
25	DGD	A	5005	-	-	20/40/80/95	0/2/2/2
23	BCR	4	503	-	-	15/29/63/63	0/2/2/2
21	CLA	A	1114	-	1/1/15/20	16/39/115/115	-
21	CLA	A	1134	1	1/1/14/20	19/33/109/115	-
21	CLA	A	1118	1	1/1/13/20	14/27/103/115	-
21	CLA	7	606	-	1/1/13/20	9/27/103/115	-
23	BCR	A	4005	-	-	14/29/63/63	0/2/2/2
21	CLA	6	615	-	1/1/15/20	19/39/115/115	-
37	LUT	5	505	-	1/1/12/27	9/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	LUT	6	501	-	1/1/12/27	7/29/67/67	0/2/2/2
23	BCR	A	4003	-	-	11/29/63/63	0/2/2/2
21	CLA	B	1237	-	1/1/15/20	16/39/115/115	-
21	CLA	8	603	19	1/1/15/20	20/39/115/115	-
21	CLA	B	1231	2	1/1/15/20	17/39/115/115	-
21	CLA	F	1301	6	1/1/12/20	4/21/97/115	-
21	CLA	4	601	-	1/1/14/20	8/33/109/115	-
21	CLA	4	604	15	1/1/14/20	15/33/109/115	-
21	CLA	4	611	-	1/1/13/20	9/29/105/115	-
21	CLA	4	616	-	1/1/12/20	8/21/97/115	-
23	BCR	B	4003	-	-	7/29/63/63	0/2/2/2
23	BCR	6	503	-	-	14/29/63/63	0/2/2/2
21	CLA	A	1116	-	1/1/14/20	14/33/109/115	-
37	LUT	1	502	-	-	2/29/67/67	0/2/2/2
21	CLA	6	606	-	1/1/12/20	10/24/100/115	-
21	CLA	A	1120	-	1/1/11/20	11/20/96/115	-
21	CLA	B	1211	-	1/1/13/20	11/27/103/115	-
23	BCR	I	4001	-	-	10/29/63/63	0/2/2/2
38	CHL	7	613	-	4/4/20/26	11/39/137/137	-
24	LHG	A	5001	21	-	19/33/33/53	-
43	DGA	5	803	-	-	13/24/24/45	-
39	OLA	8	809	-	-	8/17/17/17	-
21	CLA	A	1119	-	1/1/15/20	12/39/115/115	-
39	OLA	1	803	-	-	8/17/17/17	-
37	LUT	1	503	-	1/1/12/27	8/29/67/67	0/2/2/2
22	PQN	A	2001	-	-	8/23/43/43	0/2/2/2
21	CLA	3	601	-	1/1/15/20	12/39/115/115	-
21	CLA	8	608	19	1/1/12/20	10/24/100/115	-
21	CLA	a	602	-	1/1/12/20	6/21/97/115	-
46	4RF	8	808	-	-	25/56/56/59	-
21	CLA	4	612	15	1/1/14/20	16/36/112/115	-
24	LHG	4	802	-	-	19/36/36/53	-
27	SF4	A	3001	1,2	-	-	0/6/5/5
21	CLA	A	1115	1	1/1/14/20	9/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	a	605	-	1/1/15/20	12/39/115/115	-
21	CLA	3	613	-	1/1/14/20	12/35/111/115	-
38	CHL	6	611	-	3/3/17/26	5/21/119/137	-
24	LHG	A	5002	-	-	34/53/53/53	-
24	LHG	4	801	21	-	35/53/53/53	-
21	CLA	B	1208	2	1/1/14/20	11/33/109/115	-
21	CLA	6	618	-	1/1/11/20	6/17/93/115	-
21	CLA	6	609	17	1/1/15/20	18/39/115/115	-
23	BCR	B	4006	-	-	13/29/63/63	0/2/2/2
21	CLA	G	1602	-	1/1/11/20	9/17/93/115	-
21	CLA	B	1220	-	1/1/14/20	18/33/109/115	-
30	PTY	B	5005	-	-	22/44/44/53	-
38	CHL	8	604	19	4/4/19/26	11/35/133/137	-
23	BCR	B	4001	-	-	15/29/63/63	0/2/2/2
24	LHG	6	802	-	-	26/41/41/53	-
21	CLA	1	607	-	1/1/15/20	16/39/115/115	-
31	LAP	F	5003	-	-	20/30/30/30	-
21	CLA	1	605	-	1/1/15/20	15/39/115/115	-
31	LAP	K	5001	-	-	18/30/30/30	-
21	CLA	G	1603	-	1/1/11/20	6/15/91/115	-
21	CLA	A	1131	1	1/1/15/20	22/39/115/115	-
30	PTY	5	802	-	-	18/41/41/53	-
35	LPX	J	5001	-	-	11/18/18/31	-

All (1857) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	G	5002	ERG	C1-C10	-25.22	1.08	1.54
33	G	5002	ERG	C10-C9	-23.42	1.26	1.55
47	7	504	C7Z	C25-C26	16.36	1.61	1.34
33	G	5002	ERG	C10-C5	-16.33	1.21	1.52
34	J	4002	RRX	C26-C25	16.13	1.61	1.34
47	7	504	C7Z	C5-C6	16.00	1.61	1.34
37	1	503	LUT	C24-C25	15.45	1.51	1.33
37	5	505	LUT	C24-C25	15.27	1.51	1.33
37	a	503	LUT	C24-C25	15.22	1.51	1.33
37	1	501	LUT	C24-C25	15.19	1.51	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	6	501	LUT	C24-C25	15.11	1.51	1.33
37	7	501	LUT	C24-C25	15.05	1.51	1.33
37	5	501	LUT	C24-C25	15.04	1.51	1.33
37	a	501	LUT	C24-C25	14.99	1.51	1.33
37	3	502	LUT	C24-C25	14.90	1.50	1.33
34	J	4002	RRX	C5-C6	14.85	1.59	1.34
37	8	501	LUT	C24-C25	14.84	1.50	1.33
37	4	502	LUT	C24-C25	14.81	1.50	1.33
37	a	502	LUT	C24-C25	14.80	1.50	1.33
37	3	501	LUT	C24-C25	14.79	1.50	1.33
37	5	502	LUT	C24-C25	14.76	1.50	1.33
37	8	502	LUT	C24-C25	14.70	1.50	1.33
37	6	502	LUT	C24-C25	14.43	1.50	1.33
37	4	501	LUT	C24-C25	14.40	1.50	1.33
37	1	502	LUT	C24-C25	14.30	1.50	1.33
33	G	5002	ERG	C4-C3	-14.00	1.27	1.52
33	G	5002	ERG	C2-C3	-11.85	1.24	1.51
47	7	504	C7Z	C22-C23	-10.76	1.37	1.52
47	7	504	C7Z	C24-C23	10.71	1.71	1.52
34	J	4002	RRX	C29-C28	-10.41	1.37	1.52
47	7	504	C7Z	C2-C3	-9.77	1.38	1.52
33	G	5002	ERG	C12-C13	9.47	1.70	1.54
33	G	5002	ERG	O1-C3	9.42	1.70	1.43
38	4	618	CHL	C3A-C2A	-9.36	1.46	1.54
47	7	504	C7Z	C4-C3	9.08	1.68	1.52
20	A	1011	CL0	C1A-CHA	8.90	1.50	1.40
38	6	619	CHL	C3A-C2A	-8.81	1.47	1.54
33	G	5002	ERG	C6-C5	8.48	1.54	1.34
40	3	506	QTB	C11-C12	-8.40	1.36	1.54
20	A	1011	CL0	C1B-C2B	8.34	1.49	1.39
20	A	1011	CL0	C1D-C2D	8.25	1.48	1.39
40	a	504	QTB	C11-C12	-8.23	1.36	1.54
38	a	609	CHL	C3A-C2A	-8.23	1.47	1.54
38	8	604	CHL	C3A-C2A	-7.91	1.47	1.54
38	6	610	CHL	C3A-C2A	-7.86	1.47	1.54
34	J	4002	RRX	C27-C28	7.74	1.65	1.52
38	8	601	CHL	C3A-C2A	-7.46	1.48	1.54
38	5	611	CHL	C3A-C2A	-7.22	1.48	1.54
34	J	4002	RRX	C2-C3	-7.06	1.35	1.52
38	8	613	CHL	C3A-C2A	-7.06	1.48	1.54
38	1	609	CHL	C3A-C2A	-6.91	1.48	1.54
21	4	615	CLA	MG-NA	6.37	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	618	CLA	MG-NA	6.36	2.21	2.06
21	5	608	CLA	MG-NA	6.34	2.21	2.06
21	B	1240	CLA	MG-NA	6.33	2.21	2.06
21	K	1404	CLA	MG-NA	6.32	2.21	2.06
21	4	617	CLA	MG-NA	6.32	2.21	2.06
21	a	603	CLA	MG-NA	6.32	2.21	2.06
21	a	602	CLA	MG-NA	6.31	2.21	2.06
34	J	4002	RRX	C1-C6	-6.30	1.45	1.53
21	G	1602	CLA	MG-NA	6.30	2.21	2.06
21	4	610	CLA	MG-NA	6.29	2.21	2.06
21	5	602	CLA	MG-NA	6.28	2.21	2.06
21	5	607	CLA	MG-NA	6.28	2.21	2.06
21	A	1114	CLA	MG-NA	6.27	2.21	2.06
21	5	609	CLA	MG-NA	6.27	2.21	2.06
23	A	4004	BCR	C11-C12	-6.26	1.18	1.34
21	3	618	CLA	MG-NA	6.26	2.21	2.06
21	1	608	CLA	MG-NA	6.26	2.21	2.06
21	4	616	CLA	MG-NA	6.26	2.21	2.06
21	K	1402	CLA	MG-NA	6.25	2.21	2.06
21	a	611	CLA	MG-NA	6.24	2.21	2.06
21	8	602	CLA	MG-NA	6.24	2.21	2.06
21	8	605	CLA	MG-NA	6.24	2.21	2.06
21	7	602	CLA	MG-NA	6.24	2.21	2.06
21	3	602	CLA	MG-NA	6.24	2.21	2.06
21	5	614	CLA	MG-NA	6.23	2.21	2.06
21	7	606	CLA	MG-NA	6.23	2.21	2.06
21	A	1139	CLA	MG-NA	6.22	2.21	2.06
21	6	617	CLA	MG-NA	6.22	2.21	2.06
21	A	1101	CLA	MG-NA	6.21	2.21	2.06
21	3	616	CLA	MG-NA	6.21	2.21	2.06
21	6	601	CLA	MG-NA	6.21	2.21	2.06
21	K	1403	CLA	MG-NA	6.20	2.21	2.06
21	a	608	CLA	MG-NA	6.20	2.21	2.06
21	7	605	CLA	MG-NA	6.20	2.21	2.06
21	A	1127	CLA	MG-NA	6.20	2.21	2.06
21	7	603	CLA	MG-NA	6.20	2.21	2.06
21	5	605	CLA	MG-NA	6.19	2.21	2.06
21	a	607	CLA	MG-NA	6.19	2.21	2.06
21	A	1137	CLA	MG-NA	6.19	2.21	2.06
21	A	1141	CLA	MG-NA	6.19	2.21	2.06
21	L	1503	CLA	MG-NA	6.19	2.21	2.06
21	B	1219	CLA	MG-NA	6.19	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	611	CLA	MG-NA	6.19	2.21	2.06
21	B	1213	CLA	MG-NA	6.19	2.21	2.06
34	J	4002	RRX	C30-C25	-6.19	1.45	1.53
21	6	606	CLA	MG-NA	6.18	2.21	2.06
21	A	1115	CLA	MG-NA	6.18	2.21	2.06
21	6	615	CLA	MG-NA	6.18	2.21	2.06
21	4	602	CLA	MG-NA	6.18	2.20	2.06
21	B	1218	CLA	MG-NA	6.18	2.20	2.06
21	A	1123	CLA	MG-NA	6.18	2.20	2.06
21	6	609	CLA	MG-NA	6.18	2.20	2.06
21	L	1501	CLA	MG-NA	6.17	2.20	2.06
21	G	1601	CLA	MG-NA	6.17	2.20	2.06
21	K	1401	CLA	MG-NA	6.17	2.20	2.06
21	4	608	CLA	MG-NA	6.17	2.20	2.06
21	A	1140	CLA	MG-NA	6.16	2.20	2.06
21	B	1206	CLA	MG-NA	6.16	2.20	2.06
21	A	1012	CLA	MG-NA	6.16	2.20	2.06
21	G	1603	CLA	MG-NA	6.15	2.20	2.06
21	3	603	CLA	MG-NA	6.15	2.20	2.06
21	8	620	CLA	MG-NA	6.15	2.20	2.06
21	A	1110	CLA	MG-NA	6.15	2.20	2.06
21	8	610	CLA	MG-NA	6.15	2.20	2.06
21	A	1134	CLA	MG-NA	6.15	2.20	2.06
21	5	616	CLA	MG-NA	6.15	2.20	2.06
21	A	1121	CLA	MG-NA	6.15	2.20	2.06
21	a	605	CLA	MG-NA	6.14	2.20	2.06
21	B	1229	CLA	MG-NA	6.14	2.20	2.06
21	A	1125	CLA	MG-NA	6.14	2.20	2.06
21	B	1237	CLA	MG-NA	6.14	2.20	2.06
21	1	607	CLA	MG-NA	6.14	2.20	2.06
21	B	1022	CLA	MG-NA	6.13	2.20	2.06
21	a	604	CLA	MG-NA	6.13	2.20	2.06
21	4	605	CLA	MG-NA	6.13	2.20	2.06
21	5	606	CLA	MG-NA	6.13	2.20	2.06
21	A	1122	CLA	MG-NA	6.12	2.20	2.06
21	B	1227	CLA	MG-NA	6.12	2.20	2.06
21	F	1302	CLA	MG-NA	6.12	2.20	2.06
21	6	605	CLA	MG-NA	6.12	2.20	2.06
21	8	608	CLA	MG-NA	6.12	2.20	2.06
21	7	615	CLA	MG-NA	6.11	2.20	2.06
21	A	1112	CLA	MG-NA	6.11	2.20	2.06
21	3	607	CLA	MG-NA	6.11	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	603	CLA	MG-NA	6.11	2.20	2.06
21	8	615	CLA	MG-NA	6.11	2.20	2.06
21	6	607	CLA	MG-NA	6.11	2.20	2.06
21	A	1105	CLA	MG-NA	6.10	2.20	2.06
21	B	1220	CLA	MG-NA	6.10	2.20	2.06
21	3	613	CLA	MG-NA	6.10	2.20	2.06
21	A	1107	CLA	MG-NA	6.10	2.20	2.06
21	B	1209	CLA	MG-NA	6.09	2.20	2.06
21	7	617	CLA	MG-NA	6.09	2.20	2.06
33	G	5002	ERG	C16-C17	-6.09	1.42	1.54
21	4	612	CLA	MG-NA	6.09	2.20	2.06
21	J	1901	CLA	MG-NA	6.09	2.20	2.06
21	7	608	CLA	MG-NA	6.09	2.20	2.06
21	A	1129	CLA	MG-NA	6.08	2.20	2.06
21	B	1238	CLA	MG-NA	6.08	2.20	2.06
21	6	604	CLA	MG-NA	6.08	2.20	2.06
21	8	606	CLA	MG-NA	6.08	2.20	2.06
21	1	601	CLA	MG-NA	6.08	2.20	2.06
21	1	602	CLA	MG-NA	6.08	2.20	2.06
21	A	1124	CLA	MG-NA	6.07	2.20	2.06
21	A	1136	CLA	MG-NA	6.07	2.20	2.06
21	A	1126	CLA	MG-NA	6.07	2.20	2.06
21	1	615	CLA	MG-NA	6.07	2.20	2.06
21	A	1135	CLA	MG-NA	6.07	2.20	2.06
21	B	1223	CLA	MG-NA	6.07	2.20	2.06
21	B	1212	CLA	MG-NA	6.07	2.20	2.06
21	B	1232	CLA	MG-NA	6.07	2.20	2.06
21	A	1113	CLA	MG-NA	6.07	2.20	2.06
21	4	607	CLA	MG-NA	6.06	2.20	2.06
21	F	1301	CLA	MG-NA	6.06	2.20	2.06
21	7	604	CLA	MG-NA	6.06	2.20	2.06
21	6	618	CLA	MG-NA	6.06	2.20	2.06
21	7	610	CLA	MG-NA	6.06	2.20	2.06
21	1	612	CLA	MG-NA	6.06	2.20	2.06
21	5	617	CLA	MG-NA	6.06	2.20	2.06
21	8	603	CLA	MG-NA	6.06	2.20	2.06
21	A	1109	CLA	MG-NA	6.06	2.20	2.06
21	3	605	CLA	MG-NA	6.06	2.20	2.06
21	B	1221	CLA	MG-NA	6.05	2.20	2.06
21	1	605	CLA	MG-NA	6.05	2.20	2.06
21	6	602	CLA	MG-NA	6.05	2.20	2.06
21	1	606	CLA	MG-NA	6.05	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	601	CLA	MG-NA	6.05	2.20	2.06
21	1	603	CLA	MG-NA	6.05	2.20	2.06
21	4	611	CLA	MG-NA	6.05	2.20	2.06
21	4	604	CLA	MG-NA	6.05	2.20	2.06
21	B	1208	CLA	MG-NA	6.05	2.20	2.06
21	A	1116	CLA	MG-NA	6.04	2.20	2.06
21	B	1236	CLA	MG-NA	6.04	2.20	2.06
47	7	504	C7Z	C1-C6	-6.04	1.46	1.53
21	B	1225	CLA	MG-NA	6.04	2.20	2.06
21	A	1118	CLA	MG-NA	6.03	2.20	2.06
21	4	603	CLA	MG-NA	6.03	2.20	2.06
21	5	601	CLA	MG-NA	6.03	2.20	2.06
21	4	606	CLA	MG-NA	6.03	2.20	2.06
21	A	1131	CLA	MG-NA	6.03	2.20	2.06
21	B	1234	CLA	MG-NA	6.03	2.20	2.06
21	1	610	CLA	MG-NA	6.03	2.20	2.06
21	7	607	CLA	MG-NA	6.03	2.20	2.06
21	6	608	CLA	MG-NA	6.03	2.20	2.06
21	B	1207	CLA	MG-NA	6.02	2.20	2.06
21	B	1217	CLA	MG-NA	6.02	2.20	2.06
21	B	1239	CLA	MG-NA	6.02	2.20	2.06
21	A	1111	CLA	MG-NA	6.02	2.20	2.06
21	8	611	CLA	MG-NA	6.02	2.20	2.06
38	3	611	CHL	C3A-C2A	-6.01	1.49	1.54
21	3	610	CLA	MG-NA	6.01	2.20	2.06
21	B	1224	CLA	MG-NA	6.01	2.20	2.06
21	8	618	CLA	MG-NA	6.01	2.20	2.06
21	5	612	CLA	MG-NA	6.01	2.20	2.06
21	B	1203	CLA	MG-NA	6.01	2.20	2.06
21	3	601	CLA	MG-NA	6.01	2.20	2.06
21	B	1222	CLA	MG-NA	6.00	2.20	2.06
21	A	1120	CLA	MG-NA	6.00	2.20	2.06
21	A	1104	CLA	MG-NA	6.00	2.20	2.06
21	3	604	CLA	MG-NA	6.00	2.20	2.06
21	A	1119	CLA	MG-NA	6.00	2.20	2.06
21	3	612	CLA	MG-NA	6.00	2.20	2.06
21	B	1204	CLA	MG-NA	5.99	2.20	2.06
21	A	1013	CLA	MG-NA	5.99	2.20	2.06
21	B	1211	CLA	MG-NA	5.99	2.20	2.06
21	A	1130	CLA	MG-NA	5.99	2.20	2.06
21	a	612	CLA	MG-NA	5.99	2.20	2.06
21	8	609	CLA	MG-NA	5.98	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1214	CLA	MG-NA	5.98	2.20	2.06
21	5	604	CLA	MG-NA	5.98	2.20	2.06
21	1	604	CLA	MG-NA	5.98	2.20	2.06
21	a	601	CLA	MG-NA	5.97	2.20	2.06
21	L	1502	CLA	MG-NA	5.97	2.20	2.06
21	a	615	CLA	MG-NA	5.96	2.20	2.06
21	3	606	CLA	MG-NA	5.95	2.20	2.06
21	B	1230	CLA	MG-NA	5.95	2.20	2.06
21	B	1226	CLA	MG-NA	5.94	2.20	2.06
21	A	1133	CLA	MG-NA	5.94	2.20	2.06
21	B	1202	CLA	MG-NA	5.93	2.20	2.06
21	B	1201	CLA	MG-NA	5.93	2.20	2.06
21	A	1128	CLA	MG-NA	5.93	2.20	2.06
21	7	611	CLA	MG-NA	5.93	2.20	2.06
21	A	1138	CLA	MG-NA	5.93	2.20	2.06
21	A	1117	CLA	MG-NA	5.92	2.20	2.06
21	6	612	CLA	MG-NA	5.92	2.20	2.06
23	L	4003	BCR	C24-C23	5.91	1.50	1.33
23	L	4001	BCR	C24-C23	5.91	1.50	1.33
21	8	607	CLA	MG-NA	5.91	2.20	2.06
21	A	1108	CLA	MG-NA	5.90	2.20	2.06
23	G	4001	BCR	C24-C23	5.90	1.50	1.33
21	B	1235	CLA	MG-NA	5.90	2.20	2.06
21	B	1231	CLA	MG-NA	5.90	2.20	2.06
21	B	1216	CLA	MG-NA	5.90	2.20	2.06
21	B	1023	CLA	MG-NA	5.87	2.20	2.06
21	B	1215	CLA	MG-NA	5.87	2.20	2.06
21	7	612	CLA	MG-NA	5.87	2.20	2.06
21	A	1103	CLA	MG-NA	5.86	2.20	2.06
21	B	1021	CLA	MG-NA	5.86	2.20	2.06
21	A	1132	CLA	MG-NA	5.84	2.20	2.06
23	6	503	BCR	C24-C23	5.84	1.50	1.33
21	7	609	CLA	MG-NA	5.83	2.20	2.06
23	3	504	BCR	C24-C23	5.83	1.50	1.33
21	B	1205	CLA	MG-NA	5.81	2.20	2.06
21	7	601	CLA	MG-NA	5.80	2.20	2.06
21	A	1106	CLA	MG-NA	5.79	2.20	2.06
23	K	4002	BCR	C24-C23	5.79	1.50	1.33
23	L	4002	BCR	C24-C23	5.77	1.50	1.33
23	8	503	BCR	C24-C23	5.75	1.50	1.33
21	A	1102	CLA	MG-NA	5.74	2.19	2.06
21	8	612	CLA	MG-NA	5.74	2.19	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	5	503	BCR	C24-C23	5.71	1.50	1.33
23	6	504	BCR	C24-C23	5.70	1.50	1.33
23	3	503	BCR	C24-C23	5.69	1.50	1.33
20	A	1011	CL0	C3B-C4B	5.68	1.46	1.41
40	a	504	QTB	C17-C11	-5.65	1.50	1.55
23	4	503	BCR	C24-C23	5.63	1.49	1.33
23	F	4001	BCR	C24-C23	5.63	1.49	1.33
23	B	4002	BCR	C24-C23	5.62	1.49	1.33
23	B	4006	BCR	C24-C23	5.62	1.49	1.33
23	5	504	BCR	C24-C23	5.61	1.49	1.33
23	B	4001	BCR	C24-C23	5.60	1.49	1.33
23	A	4001	BCR	C24-C23	5.60	1.49	1.33
23	3	505	BCR	C24-C23	5.59	1.49	1.33
23	I	4001	BCR	C24-C23	5.59	1.49	1.33
23	B	4007	BCR	C24-C23	5.58	1.49	1.33
21	B	1210	CLA	MG-NA	5.58	2.19	2.06
23	B	4005	BCR	C11-C12	-5.57	1.20	1.34
21	6	603	CLA	MG-NA	5.57	2.19	2.06
23	J	4001	BCR	C24-C23	5.56	1.49	1.33
23	A	4003	BCR	C24-C23	5.56	1.49	1.33
23	A	4001	BCR	C11-C12	-5.55	1.20	1.34
23	6	504	BCR	C11-C12	-5.54	1.20	1.34
33	G	5002	ERG	C13-C14	-5.54	1.47	1.56
23	K	4001	BCR	C24-C23	5.53	1.49	1.33
23	A	4005	BCR	C24-C23	5.53	1.49	1.33
47	7	504	C7Z	C24-C25	-5.53	1.42	1.51
47	7	504	C7Z	C12-C13	5.50	1.57	1.46
23	3	503	BCR	C11-C12	-5.50	1.20	1.34
23	B	4003	BCR	C24-C23	5.50	1.49	1.33
23	A	4002	BCR	C24-C23	5.50	1.49	1.33
23	A	4004	BCR	C24-C23	5.48	1.49	1.33
23	B	4005	BCR	C24-C23	5.47	1.49	1.33
20	A	1011	CL0	O2A-C1	5.47	1.60	1.46
23	B	4007	BCR	C11-C12	-5.45	1.20	1.34
23	B	4001	BCR	C11-C12	-5.45	1.20	1.34
38	8	604	CHL	C3B-C4B	5.43	1.46	1.41
23	B	4004	BCR	C24-C23	5.42	1.49	1.33
23	7	503	BCR	C24-C23	5.41	1.49	1.33
23	5	503	BCR	C11-C12	-5.41	1.20	1.34
23	A	4002	BCR	C11-C12	-5.40	1.20	1.34
23	8	503	BCR	C11-C12	-5.39	1.20	1.34
23	5	504	BCR	C11-C12	-5.39	1.20	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	4003	BCR	C11-C12	-5.38	1.20	1.34
23	B	4006	BCR	C11-C12	-5.36	1.20	1.34
38	8	601	CHL	C3B-C4B	5.35	1.46	1.41
23	K	4001	BCR	C11-C12	-5.34	1.20	1.34
23	J	4001	BCR	C11-C12	-5.32	1.20	1.34
23	7	503	BCR	C11-C12	-5.32	1.20	1.34
23	A	4005	BCR	C11-C12	-5.28	1.20	1.34
23	4	503	BCR	C11-C12	-5.28	1.20	1.34
33	G	5002	ERG	C7-C6	-5.28	1.27	1.41
23	3	504	BCR	C11-C12	-5.26	1.20	1.34
38	6	611	CHL	C3A-C2A	-5.26	1.50	1.54
23	B	4004	BCR	C11-C12	-5.26	1.20	1.34
23	L	4001	BCR	C11-C12	-5.26	1.21	1.34
23	I	4001	BCR	C11-C12	-5.24	1.21	1.34
23	K	4002	BCR	C11-C12	-5.19	1.21	1.34
33	G	5002	ERG	C12-C11	-5.19	1.43	1.53
20	A	1011	CL0	C3D-C4D	-5.19	1.33	1.41
23	B	4002	BCR	C11-C12	-5.17	1.21	1.34
23	L	4002	BCR	C11-C12	-5.15	1.21	1.34
33	G	5002	ERG	C1-C2	5.14	1.63	1.53
23	6	503	BCR	C11-C12	-5.14	1.21	1.34
20	A	1011	CL0	CHB-C1B	5.14	1.47	1.39
38	3	611	CHL	C3B-C4B	5.13	1.46	1.41
23	F	4001	BCR	C11-C12	-5.12	1.21	1.34
38	5	610	CHL	C3A-C2A	-5.11	1.50	1.54
34	J	4002	RRX	C2-C1	5.07	1.65	1.54
23	L	4003	BCR	C11-C12	-5.06	1.21	1.34
23	B	4003	BCR	C11-C12	-5.05	1.21	1.34
23	G	4001	BCR	C11-C12	-4.98	1.21	1.34
40	3	506	QTB	C17-C11	-4.97	1.50	1.55
34	J	4002	RRX	C19-C18	4.92	1.56	1.46
20	A	1011	CL0	O2D-CGD	4.83	1.45	1.33
21	B	1228	CLA	MG-NA	4.78	2.17	2.06
40	3	506	QTB	C11-C10	-4.78	1.44	1.50
20	A	1011	CL0	C3A-C2A	-4.78	1.50	1.54
23	3	505	BCR	C11-C12	-4.75	1.22	1.34
38	3	608	CHL	C3A-C2A	-4.73	1.50	1.54
20	A	1011	CL0	OBD-CAD	4.71	1.28	1.22
38	4	613	CHL	C3B-C4B	4.71	1.46	1.41
23	B	4005	BCR	C16-C17	-4.67	1.28	1.43
38	8	613	CHL	C3B-C4B	4.62	1.45	1.41
38	a	613	CHL	C3A-C2A	-4.61	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	3	503	BCR	C16-C17	-4.60	1.28	1.43
38	3	611	CHL	C3B-C2B	-4.57	1.34	1.40
40	a	504	QTB	C11-C10	-4.56	1.44	1.50
20	A	1011	CL0	CHC-C4B	4.55	1.47	1.39
23	7	503	BCR	C16-C17	-4.51	1.29	1.43
20	A	1011	CL0	CHD-C1D	4.51	1.46	1.39
21	a	612	CLA	MG-ND	-4.50	1.96	2.05
38	a	606	CHL	C3B-C4B	4.50	1.45	1.41
38	6	613	CHL	C3A-C2A	-4.49	1.50	1.54
23	F	4001	BCR	C16-C17	-4.49	1.29	1.43
33	G	5002	ERG	C13-C17	4.49	1.63	1.55
23	A	4004	BCR	C16-C17	-4.48	1.29	1.43
38	a	606	CHL	C3A-C2A	-4.47	1.50	1.54
38	6	611	CHL	C3B-C4B	4.45	1.45	1.41
21	A	1128	CLA	MG-ND	-4.44	1.97	2.05
23	K	4001	BCR	C16-C17	-4.44	1.29	1.43
23	B	4004	BCR	C16-C17	-4.44	1.29	1.43
23	A	4005	BCR	C16-C17	-4.44	1.29	1.43
20	A	1011	CL0	CHD-C4C	4.43	1.47	1.39
21	L	1501	CLA	CBB-CAB	4.43	1.51	1.30
21	a	602	CLA	CBB-CAB	4.43	1.51	1.30
21	6	618	CLA	CBB-CAB	4.43	1.51	1.30
21	5	608	CLA	CBB-CAB	4.43	1.51	1.30
38	a	610	CHL	C3B-C4B	4.42	1.45	1.41
21	A	1012	CLA	CBB-CAB	4.42	1.51	1.30
47	7	504	C7Z	C31-C30	4.42	1.56	1.43
21	A	1123	CLA	CBB-CAB	4.42	1.51	1.30
21	6	607	CLA	CBB-CAB	4.41	1.51	1.30
21	B	1219	CLA	CBB-CAB	4.41	1.51	1.30
21	a	608	CLA	CBB-CAB	4.41	1.51	1.30
21	1	615	CLA	CBB-CAB	4.41	1.51	1.30
21	8	620	CLA	CBB-CAB	4.41	1.51	1.30
21	4	615	CLA	CBB-CAB	4.40	1.51	1.30
21	6	615	CLA	CBB-CAB	4.40	1.51	1.30
21	5	617	CLA	CBB-CAB	4.40	1.51	1.30
21	6	608	CLA	CBB-CAB	4.40	1.51	1.30
21	4	602	CLA	CBB-CAB	4.40	1.51	1.30
23	5	503	BCR	C16-C17	-4.40	1.29	1.43
21	a	607	CLA	CBB-CAB	4.40	1.51	1.30
21	5	607	CLA	CBB-CAB	4.40	1.51	1.30
47	7	504	C7Z	C28-C29	4.40	1.55	1.46
23	A	4002	BCR	C16-C17	-4.40	1.29	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	602	CLA	CBB-CAB	4.40	1.51	1.30
21	B	1222	CLA	CBB-CAB	4.40	1.51	1.30
21	A	1013	CLA	CBB-CAB	4.39	1.51	1.30
21	A	1139	CLA	MG-ND	-4.39	1.97	2.05
21	B	1221	CLA	CBB-CAB	4.39	1.51	1.30
21	7	617	CLA	CBB-CAB	4.39	1.51	1.30
21	5	616	CLA	CBB-CAB	4.39	1.51	1.30
21	4	617	CLA	CBB-CAB	4.39	1.51	1.30
21	8	618	CLA	CBB-CAB	4.39	1.51	1.30
21	3	602	CLA	CBB-CAB	4.39	1.51	1.30
21	L	1503	CLA	CBB-CAB	4.39	1.51	1.30
21	F	1301	CLA	CBB-CAB	4.39	1.51	1.30
21	8	602	CLA	CBB-CAB	4.39	1.51	1.30
21	8	605	CLA	CBB-CAB	4.39	1.51	1.30
21	6	617	CLA	CBB-CAB	4.38	1.51	1.30
21	3	618	CLA	CBB-CAB	4.38	1.51	1.30
38	4	609	CHL	C3B-C4B	4.38	1.45	1.41
21	B	1231	CLA	CBB-CAB	4.38	1.51	1.30
38	7	613	CHL	C3A-C2A	-4.38	1.50	1.54
21	G	1602	CLA	CBB-CAB	4.38	1.51	1.30
21	6	604	CLA	CBB-CAB	4.38	1.51	1.30
21	5	601	CLA	CBB-CAB	4.38	1.51	1.30
21	8	608	CLA	CBB-CAB	4.38	1.51	1.30
21	5	609	CLA	CBB-CAB	4.38	1.51	1.30
21	L	1502	CLA	CBB-CAB	4.38	1.51	1.30
21	5	618	CLA	CBB-CAB	4.37	1.51	1.30
21	6	601	CLA	CBB-CAB	4.37	1.51	1.30
21	B	1206	CLA	CBB-CAB	4.37	1.51	1.30
21	5	603	CLA	CBB-CAB	4.37	1.51	1.30
21	a	612	CLA	CBB-CAB	4.37	1.51	1.30
21	3	616	CLA	CBB-CAB	4.37	1.51	1.30
21	B	1210	CLA	C1C-NC	-4.37	1.31	1.37
21	5	602	CLA	CBB-CAB	4.37	1.51	1.30
21	1	607	CLA	CBB-CAB	4.37	1.51	1.30
21	1	612	CLA	CBB-CAB	4.37	1.51	1.30
21	A	1117	CLA	CBB-CAB	4.37	1.51	1.30
21	B	1207	CLA	CBB-CAB	4.37	1.51	1.30
21	a	603	CLA	CBB-CAB	4.37	1.51	1.30
21	A	1137	CLA	CBB-CAB	4.37	1.51	1.30
21	4	607	CLA	CBB-CAB	4.37	1.51	1.30
21	3	607	CLA	CBB-CAB	4.37	1.51	1.30
21	5	612	CLA	CBB-CAB	4.37	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	G	1603	CLA	CBB-CAB	4.37	1.51	1.30
23	8	503	BCR	C16-C17	-4.37	1.29	1.43
21	A	1139	CLA	CBB-CAB	4.36	1.51	1.30
21	1	605	CLA	CBB-CAB	4.36	1.51	1.30
21	1	602	CLA	CBB-CAB	4.36	1.51	1.30
21	B	1205	CLA	CBB-CAB	4.36	1.51	1.30
21	B	1236	CLA	CBB-CAB	4.36	1.51	1.30
21	7	615	CLA	CBB-CAB	4.36	1.51	1.30
21	K	1404	CLA	CBB-CAB	4.36	1.51	1.30
21	F	1302	CLA	CBB-CAB	4.36	1.51	1.30
21	B	1227	CLA	CBB-CAB	4.36	1.51	1.30
21	A	1110	CLA	CBB-CAB	4.36	1.51	1.30
21	A	1132	CLA	CBB-CAB	4.36	1.51	1.30
21	5	614	CLA	CBB-CAB	4.36	1.51	1.30
21	8	615	CLA	CBB-CAB	4.36	1.51	1.30
21	7	610	CLA	CBB-CAB	4.36	1.51	1.30
21	7	607	CLA	CBB-CAB	4.36	1.51	1.30
21	6	605	CLA	CBB-CAB	4.36	1.51	1.30
21	J	1901	CLA	CBB-CAB	4.35	1.51	1.30
21	A	1101	CLA	CBB-CAB	4.35	1.51	1.30
21	4	616	CLA	CBB-CAB	4.35	1.51	1.30
21	A	1140	CLA	CBB-CAB	4.35	1.51	1.30
21	1	611	CLA	CBB-CAB	4.35	1.51	1.30
38	a	609	CHL	C3B-C4B	4.35	1.45	1.41
21	B	1210	CLA	CBB-CAB	4.35	1.51	1.30
21	B	1217	CLA	CBB-CAB	4.35	1.51	1.30
21	3	605	CLA	CBB-CAB	4.35	1.51	1.30
21	1	610	CLA	CBB-CAB	4.35	1.51	1.30
23	B	4002	BCR	C16-C17	-4.35	1.29	1.43
21	a	615	CLA	CBB-CAB	4.35	1.51	1.30
21	B	1201	CLA	CBB-CAB	4.35	1.51	1.30
21	B	1215	CLA	CBB-CAB	4.35	1.51	1.30
21	1	601	CLA	CBB-CAB	4.35	1.51	1.30
21	A	1107	CLA	CBB-CAB	4.35	1.51	1.30
21	B	1211	CLA	CBB-CAB	4.35	1.51	1.30
21	A	1126	CLA	CBB-CAB	4.35	1.51	1.30
21	G	1601	CLA	CBB-CAB	4.35	1.51	1.30
21	7	612	CLA	CBB-CAB	4.35	1.51	1.30
21	4	605	CLA	CBB-CAB	4.35	1.51	1.30
34	J	4002	RRX	C8-C9	4.35	1.55	1.46
21	8	611	CLA	CBB-CAB	4.35	1.51	1.30
21	K	1401	CLA	CBB-CAB	4.35	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	606	CLA	CBB-CAB	4.35	1.51	1.30
23	3	505	BCR	C10-C9	4.34	1.45	1.35
23	K	4002	BCR	C16-C17	-4.34	1.29	1.43
21	4	610	CLA	CBB-CAB	4.34	1.51	1.30
21	B	1216	CLA	CBB-CAB	4.34	1.51	1.30
21	7	603	CLA	CBB-CAB	4.34	1.51	1.30
21	A	1111	CLA	CBB-CAB	4.34	1.51	1.30
21	A	1122	CLA	CBB-CAB	4.34	1.51	1.30
21	3	613	CLA	CBB-CAB	4.34	1.51	1.30
21	a	601	CLA	CBB-CAB	4.34	1.51	1.30
21	8	607	CLA	CBB-CAB	4.34	1.51	1.30
21	A	1120	CLA	CBB-CAB	4.34	1.51	1.30
21	3	601	CLA	CBB-CAB	4.34	1.51	1.30
21	4	601	CLA	CBB-CAB	4.34	1.51	1.30
21	A	1121	CLA	CBB-CAB	4.34	1.51	1.30
21	A	1131	CLA	CBB-CAB	4.34	1.51	1.30
21	1	608	CLA	CBB-CAB	4.34	1.51	1.30
21	7	606	CLA	CBB-CAB	4.34	1.51	1.30
21	A	1119	CLA	CBB-CAB	4.34	1.51	1.30
21	4	608	CLA	CBB-CAB	4.34	1.51	1.30
21	4	612	CLA	CBB-CAB	4.33	1.51	1.30
21	B	1223	CLA	CBB-CAB	4.33	1.51	1.30
21	B	1224	CLA	CBB-CAB	4.33	1.51	1.30
21	B	1023	CLA	CBB-CAB	4.33	1.51	1.30
21	B	1228	CLA	CBB-CAB	4.33	1.51	1.30
21	5	605	CLA	CBB-CAB	4.33	1.51	1.30
34	J	4002	RRX	C27-C26	-4.33	1.44	1.51
21	A	1118	CLA	CBB-CAB	4.33	1.51	1.30
21	K	1402	CLA	CBB-CAB	4.33	1.51	1.30
21	3	612	CLA	CBB-CAB	4.33	1.51	1.30
21	4	606	CLA	CBB-CAB	4.33	1.51	1.30
21	B	1229	CLA	CBB-CAB	4.33	1.51	1.30
21	B	1226	CLA	CBB-CAB	4.33	1.51	1.30
21	B	1230	CLA	CBB-CAB	4.32	1.51	1.30
21	A	1108	CLA	CBB-CAB	4.32	1.51	1.30
21	1	606	CLA	CBB-CAB	4.32	1.51	1.30
21	B	1232	CLA	CBB-CAB	4.32	1.51	1.30
21	8	603	CLA	CBB-CAB	4.32	1.51	1.30
21	A	1109	CLA	CBB-CAB	4.32	1.51	1.30
21	7	601	CLA	CBB-CAB	4.32	1.51	1.30
21	A	1141	CLA	CBB-CAB	4.32	1.51	1.30
21	B	1218	CLA	CBB-CAB	4.32	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	611	CLA	CBB-CAB	4.32	1.51	1.30
21	B	1239	CLA	CBB-CAB	4.32	1.51	1.30
21	B	1209	CLA	CBB-CAB	4.32	1.51	1.30
21	7	608	CLA	CBB-CAB	4.32	1.51	1.30
20	A	1011	CL0	C3B-C2B	4.32	1.46	1.40
21	a	605	CLA	CBB-CAB	4.32	1.51	1.30
21	A	1102	CLA	CBB-CAB	4.32	1.51	1.30
21	K	1403	CLA	CBB-CAB	4.31	1.51	1.30
23	A	4003	BCR	C16-C17	-4.31	1.29	1.43
21	B	1238	CLA	CBB-CAB	4.31	1.51	1.30
23	B	4007	BCR	C16-C17	-4.31	1.29	1.43
21	5	604	CLA	CBB-CAB	4.31	1.51	1.30
21	A	1124	CLA	CBB-CAB	4.31	1.51	1.30
21	A	1113	CLA	CBB-CAB	4.31	1.51	1.30
21	A	1135	CLA	CBB-CAB	4.31	1.51	1.30
21	A	1134	CLA	CBB-CAB	4.31	1.51	1.30
21	7	602	CLA	CBB-CAB	4.31	1.51	1.30
21	A	1131	CLA	MG-ND	-4.31	1.97	2.05
21	4	603	CLA	CBB-CAB	4.31	1.51	1.30
21	8	606	CLA	CBB-CAB	4.31	1.51	1.30
21	A	1105	CLA	CBB-CAB	4.31	1.51	1.30
21	B	1214	CLA	CBB-CAB	4.31	1.51	1.30
21	7	611	CLA	CBB-CAB	4.31	1.51	1.30
21	B	1022	CLA	MG-ND	-4.30	1.97	2.05
21	B	1208	CLA	CBB-CAB	4.30	1.51	1.30
21	A	1138	CLA	CBB-CAB	4.30	1.51	1.30
21	A	1136	CLA	CBB-CAB	4.30	1.51	1.30
21	B	1204	CLA	CBB-CAB	4.30	1.51	1.30
21	8	610	CLA	CBB-CAB	4.30	1.51	1.30
21	B	1212	CLA	CBB-CAB	4.30	1.51	1.30
21	4	604	CLA	CBB-CAB	4.30	1.51	1.30
21	7	604	CLA	CBB-CAB	4.30	1.51	1.30
21	3	603	CLA	CBB-CAB	4.30	1.51	1.30
21	A	1127	CLA	CBB-CAB	4.30	1.51	1.30
21	6	606	CLA	CBB-CAB	4.30	1.51	1.30
23	J	4001	BCR	C16-C17	-4.30	1.29	1.43
21	3	610	CLA	CBB-CAB	4.30	1.51	1.30
21	4	611	CLA	CBB-CAB	4.29	1.51	1.30
23	B	4001	BCR	C16-C17	-4.29	1.29	1.43
21	A	1129	CLA	CBB-CAB	4.29	1.51	1.30
23	I	4001	BCR	C16-C17	-4.29	1.29	1.43
21	B	1235	CLA	CBB-CAB	4.29	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	604	CLA	CBB-CAB	4.29	1.51	1.30
21	B	1213	CLA	CBB-CAB	4.29	1.51	1.30
21	A	1103	CLA	CBB-CAB	4.29	1.51	1.30
21	B	1021	CLA	MG-ND	-4.28	1.97	2.05
21	6	612	CLA	CBB-CAB	4.28	1.51	1.30
21	B	1221	CLA	MG-ND	-4.28	1.97	2.05
21	B	1237	CLA	CBB-CAB	4.28	1.50	1.30
23	A	4001	BCR	C16-C17	-4.28	1.29	1.43
21	A	1115	CLA	CBB-CAB	4.27	1.50	1.30
21	A	1112	CLA	CBB-CAB	4.27	1.50	1.30
25	A	5005	DGD	O1G-C1A	4.27	1.45	1.33
21	A	1104	CLA	CBB-CAB	4.27	1.50	1.30
21	A	1106	CLA	CBB-CAB	4.27	1.50	1.30
23	3	505	BCR	C16-C17	-4.27	1.29	1.43
21	A	1128	CLA	CBB-CAB	4.27	1.50	1.30
38	a	613	CHL	C3B-C4B	4.27	1.45	1.41
21	3	606	CLA	CBB-CAB	4.27	1.50	1.30
21	B	1214	CLA	MG-ND	-4.27	1.97	2.05
21	B	1220	CLA	CBB-CAB	4.27	1.50	1.30
23	4	503	BCR	C16-C17	-4.27	1.29	1.43
21	1	603	CLA	CBB-CAB	4.27	1.50	1.30
21	B	1022	CLA	CBB-CAB	4.26	1.50	1.30
21	B	1021	CLA	CBB-CAB	4.26	1.50	1.30
21	A	1130	CLA	CBB-CAB	4.26	1.50	1.30
21	7	612	CLA	MG-ND	-4.26	1.97	2.05
21	5	605	CLA	MG-ND	-4.26	1.97	2.05
21	6	603	CLA	CBB-CAB	4.26	1.50	1.30
21	7	607	CLA	MG-ND	-4.25	1.97	2.05
21	B	1240	CLA	CBB-CAB	4.25	1.50	1.30
21	8	612	CLA	CBB-CAB	4.25	1.50	1.30
21	B	1023	CLA	MG-ND	-4.25	1.97	2.05
23	6	504	BCR	C16-C17	-4.25	1.30	1.43
21	1	604	CLA	CBB-CAB	4.25	1.50	1.30
21	B	1202	CLA	CBB-CAB	4.25	1.50	1.30
21	8	609	CLA	CBB-CAB	4.25	1.50	1.30
21	A	1126	CLA	MG-ND	-4.24	1.97	2.05
23	L	4002	BCR	C16-C17	-4.24	1.30	1.43
21	B	1239	CLA	MG-ND	-4.24	1.97	2.05
23	B	4003	BCR	C16-C17	-4.24	1.30	1.43
23	L	4003	BCR	C16-C17	-4.24	1.30	1.43
21	7	605	CLA	CBB-CAB	4.23	1.50	1.30
21	A	1116	CLA	MG-ND	-4.23	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	7	504	C7Z	C8-C9	4.23	1.55	1.46
21	B	1225	CLA	CBB-CAB	4.23	1.50	1.30
23	3	504	BCR	C16-C17	-4.23	1.30	1.43
21	A	1114	CLA	CBB-CAB	4.22	1.50	1.30
21	6	609	CLA	MG-ND	-4.22	1.97	2.05
21	B	1206	CLA	MG-ND	-4.22	1.97	2.05
21	7	609	CLA	CBB-CAB	4.22	1.50	1.30
21	B	1225	CLA	MG-ND	-4.22	1.97	2.05
23	B	4006	BCR	C16-C17	-4.21	1.30	1.43
21	A	1124	CLA	MG-ND	-4.21	1.97	2.05
47	7	504	C7Z	C32-C33	4.21	1.55	1.46
21	A	1133	CLA	CBB-CAB	4.21	1.50	1.30
21	B	1234	CLA	CBB-CAB	4.21	1.50	1.30
21	A	1125	CLA	CBB-CAB	4.21	1.50	1.30
21	A	1116	CLA	CBB-CAB	4.21	1.50	1.30
21	A	1129	CLA	MG-ND	-4.21	1.97	2.05
20	A	1011	CL0	C3D-C2D	4.20	1.46	1.39
21	8	612	CLA	MG-ND	-4.20	1.97	2.05
21	3	606	CLA	MG-ND	-4.19	1.97	2.05
23	L	4003	BCR	C10-C9	4.19	1.45	1.35
21	4	610	CLA	MG-ND	-4.19	1.97	2.05
21	a	604	CLA	CBB-CAB	4.19	1.50	1.30
38	a	610	CHL	C3A-C2A	-4.19	1.51	1.54
21	8	610	CLA	MG-ND	-4.19	1.97	2.05
21	A	1114	CLA	MG-ND	-4.18	1.97	2.05
21	7	608	CLA	MG-ND	-4.18	1.97	2.05
23	G	4001	BCR	C10-C9	4.18	1.45	1.35
21	5	616	CLA	MG-ND	-4.18	1.97	2.05
21	B	1213	CLA	MG-ND	-4.18	1.97	2.05
21	A	1121	CLA	MG-ND	-4.17	1.97	2.05
21	A	1012	CLA	MG-ND	-4.17	1.97	2.05
21	A	1013	CLA	MG-ND	-4.17	1.97	2.05
38	8	601	CHL	C1A-CHA	-4.16	1.35	1.40
21	6	609	CLA	CBB-CAB	4.16	1.50	1.30
23	5	504	BCR	C16-C17	-4.15	1.30	1.43
21	B	1219	CLA	MG-ND	-4.15	1.97	2.05
21	7	609	CLA	MG-ND	-4.15	1.97	2.05
21	B	1204	CLA	MG-ND	-4.15	1.97	2.05
21	5	609	CLA	MG-ND	-4.15	1.97	2.05
23	G	4001	BCR	C16-C17	-4.14	1.30	1.43
21	B	1203	CLA	CBB-CAB	4.13	1.50	1.30
21	A	1117	CLA	MG-ND	-4.13	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1237	CLA	MG-ND	-4.13	1.97	2.05
21	a	615	CLA	MG-ND	-4.13	1.97	2.05
21	6	607	CLA	MG-ND	-4.13	1.97	2.05
21	B	1212	CLA	MG-ND	-4.13	1.97	2.05
21	4	615	CLA	MG-ND	-4.12	1.97	2.05
21	B	1216	CLA	MG-ND	-4.12	1.97	2.05
25	B	5003	DGD	O1G-C1A	4.12	1.45	1.33
23	6	503	BCR	C10-C9	4.12	1.45	1.35
21	A	1112	CLA	MG-ND	-4.11	1.97	2.05
38	8	601	CHL	C3B-C2B	-4.11	1.34	1.40
21	B	1220	CLA	MG-ND	-4.11	1.97	2.05
21	B	1232	CLA	MG-ND	-4.11	1.97	2.05
21	B	1235	CLA	MG-ND	-4.11	1.97	2.05
21	4	607	CLA	MG-ND	-4.11	1.97	2.05
34	J	4002	RRX	C23-C22	4.11	1.54	1.46
21	K	1404	CLA	MG-ND	-4.11	1.97	2.05
21	A	1111	CLA	MG-ND	-4.11	1.97	2.05
21	B	1207	CLA	MG-ND	-4.11	1.97	2.05
21	B	1202	CLA	MG-ND	-4.10	1.97	2.05
21	B	1223	CLA	MG-ND	-4.10	1.97	2.05
23	6	503	BCR	C16-C17	-4.10	1.30	1.43
21	5	608	CLA	MG-ND	-4.10	1.97	2.05
21	1	608	CLA	MG-ND	-4.10	1.97	2.05
20	A	1011	CL0	CHC-C1C	4.10	1.47	1.39
21	4	608	CLA	MG-ND	-4.10	1.97	2.05
21	K	1401	CLA	MG-ND	-4.10	1.97	2.05
21	A	1133	CLA	MG-ND	-4.09	1.97	2.05
21	6	615	CLA	MG-ND	-4.09	1.97	2.05
21	B	1208	CLA	MG-ND	-4.09	1.97	2.05
21	B	1210	CLA	MG-ND	-4.09	1.97	2.05
34	J	4002	RRX	C3-C4	4.07	1.65	1.52
21	B	1238	CLA	MG-ND	-4.07	1.97	2.05
21	1	615	CLA	MG-ND	-4.07	1.97	2.05
21	3	613	CLA	MG-ND	-4.07	1.97	2.05
21	A	1136	CLA	MG-ND	-4.07	1.97	2.05
21	A	1119	CLA	MG-ND	-4.07	1.97	2.05
21	A	1118	CLA	MG-ND	-4.06	1.97	2.05
21	8	608	CLA	MG-ND	-4.06	1.97	2.05
21	A	1138	CLA	MG-ND	-4.06	1.97	2.05
25	8	802	DGD	O1G-C1A	4.06	1.45	1.33
21	1	610	CLA	MG-ND	-4.06	1.97	2.05
21	B	1211	CLA	MG-ND	-4.06	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1209	CLA	MG-ND	-4.06	1.97	2.05
21	5	618	CLA	MG-ND	-4.06	1.97	2.05
21	a	603	CLA	MG-ND	-4.05	1.97	2.05
21	8	609	CLA	MG-ND	-4.05	1.97	2.05
21	A	1141	CLA	MG-ND	-4.05	1.97	2.05
34	J	4002	RRX	C12-C13	4.05	1.54	1.46
21	B	1222	CLA	MG-ND	-4.05	1.97	2.05
23	F	4001	BCR	C10-C9	4.04	1.45	1.35
21	4	605	CLA	MG-ND	-4.04	1.97	2.05
21	A	1123	CLA	MG-ND	-4.04	1.97	2.05
21	B	1226	CLA	MG-ND	-4.04	1.97	2.05
47	7	504	C7Z	C11-C10	4.04	1.55	1.43
33	G	5002	ERG	C16-C15	4.04	1.65	1.54
21	B	1240	CLA	MG-ND	-4.04	1.97	2.05
21	4	604	CLA	MG-ND	-4.04	1.97	2.05
21	8	607	CLA	MG-ND	-4.04	1.97	2.05
21	A	1110	CLA	MG-ND	-4.04	1.97	2.05
21	6	605	CLA	MG-ND	-4.04	1.97	2.05
21	A	1135	CLA	MG-ND	-4.03	1.97	2.05
23	L	4001	BCR	C16-C17	-4.03	1.30	1.43
21	6	601	CLA	MG-ND	-4.03	1.97	2.05
21	7	601	CLA	MG-ND	-4.03	1.97	2.05
21	5	612	CLA	MG-ND	-4.03	1.97	2.05
21	8	606	CLA	MG-ND	-4.03	1.97	2.05
21	1	612	CLA	MG-ND	-4.03	1.97	2.05
23	B	4003	BCR	C10-C9	4.02	1.45	1.35
21	7	615	CLA	MG-ND	-4.02	1.97	2.05
21	5	607	CLA	MG-ND	-4.02	1.97	2.05
21	3	603	CLA	MG-ND	-4.02	1.97	2.05
21	3	612	CLA	MG-ND	-4.02	1.97	2.05
21	5	602	CLA	MG-ND	-4.02	1.97	2.05
21	6	603	CLA	C1C-NC	-4.02	1.31	1.37
21	8	602	CLA	MG-ND	-4.02	1.97	2.05
38	8	604	CHL	C3B-C2B	-4.02	1.34	1.40
21	7	610	CLA	MG-ND	-4.02	1.97	2.05
21	1	604	CLA	MG-ND	-4.02	1.97	2.05
21	4	606	CLA	MG-ND	-4.02	1.97	2.05
21	a	602	CLA	MG-ND	-4.02	1.97	2.05
21	8	605	CLA	MG-ND	-4.01	1.97	2.05
23	K	4002	BCR	C10-C9	4.01	1.45	1.35
21	1	606	CLA	MG-ND	-4.01	1.97	2.05
38	5	611	CHL	C3B-C4B	4.01	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	L	1503	CLA	MG-ND	-4.01	1.97	2.05
21	B	1215	CLA	MG-ND	-4.00	1.97	2.05
34	J	4002	RRX	C20-C21	4.00	1.55	1.43
21	G	1601	CLA	MG-ND	-4.00	1.97	2.05
21	3	618	CLA	MG-ND	-4.00	1.97	2.05
21	B	1203	CLA	MG-ND	-3.99	1.97	2.05
21	L	1502	CLA	MG-ND	-3.99	1.97	2.05
21	A	1134	CLA	MG-ND	-3.99	1.97	2.05
21	A	1115	CLA	MG-ND	-3.98	1.97	2.05
21	8	618	CLA	MG-ND	-3.98	1.97	2.05
21	A	1113	CLA	MG-ND	-3.98	1.97	2.05
38	5	611	CHL	C3B-C2B	-3.98	1.35	1.40
21	A	1108	CLA	MG-ND	-3.98	1.97	2.05
21	B	1205	CLA	MG-ND	-3.97	1.97	2.05
21	3	602	CLA	MG-ND	-3.97	1.97	2.05
21	4	601	CLA	MG-ND	-3.97	1.97	2.05
21	4	612	CLA	MG-ND	-3.97	1.97	2.05
21	3	610	CLA	MG-ND	-3.97	1.97	2.05
21	3	604	CLA	MG-ND	-3.97	1.97	2.05
21	8	603	CLA	MG-ND	-3.96	1.97	2.05
21	4	611	CLA	MG-ND	-3.96	1.97	2.05
21	B	1224	CLA	MG-ND	-3.96	1.97	2.05
21	3	616	CLA	MG-ND	-3.96	1.97	2.05
21	L	1501	CLA	MG-ND	-3.96	1.97	2.05
21	3	605	CLA	MG-ND	-3.95	1.97	2.05
38	8	604	CHL	C1A-CHA	-3.95	1.35	1.40
21	B	1229	CLA	MG-ND	-3.95	1.98	2.05
21	a	611	CLA	MG-ND	-3.95	1.98	2.05
21	A	1102	CLA	MG-ND	-3.95	1.98	2.05
21	A	1132	CLA	MG-ND	-3.95	1.98	2.05
21	A	1127	CLA	MG-ND	-3.94	1.98	2.05
21	7	603	CLA	MG-ND	-3.94	1.98	2.05
21	A	1130	CLA	MG-ND	-3.94	1.98	2.05
21	G	1602	CLA	MG-ND	-3.94	1.98	2.05
21	a	608	CLA	MG-ND	-3.94	1.98	2.05
21	3	607	CLA	MG-ND	-3.94	1.98	2.05
23	8	503	BCR	C10-C9	3.94	1.44	1.35
21	A	1104	CLA	MG-ND	-3.93	1.98	2.05
21	8	620	CLA	MG-ND	-3.93	1.98	2.05
23	B	4002	BCR	C10-C9	3.93	1.44	1.35
21	7	605	CLA	MG-ND	-3.93	1.98	2.05
21	A	1128	CLA	C1C-NC	-3.93	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1201	CLA	MG-ND	-3.93	1.98	2.05
21	K	1402	CLA	MG-ND	-3.93	1.98	2.05
21	G	1603	CLA	MG-ND	-3.93	1.98	2.05
21	A	1122	CLA	MG-ND	-3.92	1.98	2.05
21	5	604	CLA	MG-ND	-3.92	1.98	2.05
21	a	607	CLA	MG-ND	-3.92	1.98	2.05
21	B	1217	CLA	MG-ND	-3.92	1.98	2.05
21	A	1140	CLA	MG-ND	-3.92	1.98	2.05
21	5	606	CLA	MG-ND	-3.92	1.98	2.05
21	3	601	CLA	MG-ND	-3.92	1.98	2.05
38	1	613	CHL	C3B-C4B	3.92	1.45	1.41
21	8	611	CLA	MG-ND	-3.92	1.98	2.05
23	4	503	BCR	C10-C9	3.91	1.44	1.35
21	7	602	CLA	MG-ND	-3.91	1.98	2.05
21	5	614	CLA	MG-ND	-3.91	1.98	2.05
21	1	611	CLA	MG-ND	-3.91	1.98	2.05
21	4	616	CLA	MG-ND	-3.91	1.98	2.05
21	6	606	CLA	MG-ND	-3.90	1.98	2.05
21	6	608	CLA	MG-ND	-3.90	1.98	2.05
21	B	1231	CLA	MG-ND	-3.90	1.98	2.05
21	A	1108	CLA	C1C-NC	-3.89	1.31	1.37
21	6	602	CLA	MG-ND	-3.89	1.98	2.05
21	5	601	CLA	MG-ND	-3.88	1.98	2.05
23	I	4001	BCR	C10-C9	3.88	1.44	1.35
21	A	1125	CLA	MG-ND	-3.88	1.98	2.05
21	6	612	CLA	MG-ND	-3.88	1.98	2.05
21	B	1218	CLA	MG-ND	-3.87	1.98	2.05
21	B	1230	CLA	MG-ND	-3.87	1.98	2.05
38	5	613	CHL	C3A-C2A	-3.87	1.51	1.54
21	B	1228	CLA	MG-ND	-3.87	1.98	2.05
21	4	617	CLA	MG-ND	-3.86	1.98	2.05
21	A	1137	CLA	MG-ND	-3.86	1.98	2.05
21	4	603	CLA	MG-ND	-3.86	1.98	2.05
23	A	4003	BCR	C10-C9	3.86	1.44	1.35
21	K	1403	CLA	MG-ND	-3.86	1.98	2.05
23	3	504	BCR	C10-C9	3.85	1.44	1.35
21	A	1103	CLA	MG-ND	-3.85	1.98	2.05
21	B	1234	CLA	MG-ND	-3.84	1.98	2.05
21	6	617	CLA	MG-ND	-3.84	1.98	2.05
21	B	1207	CLA	C1C-NC	-3.84	1.31	1.37
21	B	1210	CLA	C4B-NB	-3.83	1.32	1.37
21	A	1120	CLA	MG-ND	-3.82	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	L	4001	BCR	C10-C9	3.82	1.44	1.35
21	1	605	CLA	MG-ND	-3.82	1.98	2.05
21	5	603	CLA	MG-ND	-3.82	1.98	2.05
47	7	504	C7Z	C38-C25	3.82	1.57	1.50
21	B	1212	CLA	C1C-NC	-3.81	1.31	1.37
47	7	504	C7Z	C7-C6	3.81	1.58	1.45
21	8	615	CLA	MG-ND	-3.81	1.98	2.05
38	6	611	CHL	C3B-C2B	-3.81	1.35	1.40
31	F	5003	LAP	P9-O6	3.80	1.74	1.59
21	A	1107	CLA	MG-ND	-3.80	1.98	2.05
21	1	601	CLA	MG-ND	-3.80	1.98	2.05
34	J	4002	RRX	C24-C25	3.80	1.58	1.45
21	B	1021	CLA	C1C-NC	-3.80	1.31	1.37
21	A	1112	CLA	C1C-NC	-3.79	1.31	1.37
23	K	4001	BCR	C10-C9	3.79	1.44	1.35
47	7	504	C7Z	C15-C14	3.79	1.54	1.43
21	a	612	CLA	C1C-NC	-3.79	1.31	1.37
23	J	4001	BCR	C10-C9	3.79	1.44	1.35
21	B	1236	CLA	C1C-NC	-3.79	1.31	1.37
21	4	602	CLA	MG-ND	-3.79	1.98	2.05
21	8	609	CLA	C1C-NC	-3.79	1.31	1.37
47	7	504	C7Z	C22-C21	3.77	1.66	1.54
21	1	607	CLA	MG-ND	-3.77	1.98	2.05
25	B	5003	DGD	CAA-C9A	-3.77	1.33	1.51
21	7	617	CLA	MG-ND	-3.77	1.98	2.05
25	B	5003	DGD	CGB-CFB	-3.76	1.33	1.51
21	a	601	CLA	MG-ND	-3.76	1.98	2.05
25	8	802	DGD	CAA-C9A	-3.76	1.33	1.51
23	B	4001	BCR	C10-C9	3.76	1.44	1.35
21	A	1101	CLA	MG-ND	-3.76	1.98	2.05
23	5	504	BCR	C10-C9	3.76	1.44	1.35
21	7	604	CLA	MG-ND	-3.76	1.98	2.05
21	B	1239	CLA	C1C-NC	-3.75	1.32	1.37
21	L	1503	CLA	C1C-NC	-3.75	1.32	1.37
25	B	5003	DGD	CDB-CCB	-3.75	1.33	1.51
21	7	601	CLA	C1C-NC	-3.74	1.32	1.37
21	6	604	CLA	MG-ND	-3.74	1.98	2.05
38	a	609	CHL	C1A-CHA	-3.73	1.35	1.40
23	B	4004	BCR	C10-C9	3.73	1.44	1.35
21	A	1139	CLA	C1C-NC	-3.73	1.32	1.37
21	A	1105	CLA	MG-ND	-3.73	1.98	2.05
23	5	503	BCR	C10-C9	3.73	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	7	504	C7Z	C2-C1	3.73	1.66	1.54
34	J	4002	RRX	C15-C14	3.73	1.54	1.43
21	B	1209	CLA	C1C-NC	-3.73	1.32	1.37
38	7	613	CHL	C3B-C4B	3.73	1.45	1.41
21	a	605	CLA	MG-ND	-3.73	1.98	2.05
21	F	1302	CLA	MG-ND	-3.72	1.98	2.05
31	K	5001	LAP	P9-O6	3.72	1.74	1.59
21	A	1131	CLA	C1C-NC	-3.72	1.32	1.37
21	B	1227	CLA	MG-ND	-3.72	1.98	2.05
21	A	1106	CLA	C1C-NC	-3.72	1.32	1.37
25	B	5003	DGD	CGA-CFA	-3.71	1.33	1.51
21	8	612	CLA	C1C-NC	-3.71	1.32	1.37
21	A	1138	CLA	C1C-NC	-3.71	1.32	1.37
21	8	605	CLA	C1C-NC	-3.71	1.32	1.37
21	F	1301	CLA	MG-ND	-3.71	1.98	2.05
21	A	1116	CLA	C1C-NC	-3.70	1.32	1.37
21	8	610	CLA	C1C-NC	-3.70	1.32	1.37
25	8	802	DGD	CGA-CFA	-3.70	1.33	1.51
21	5	617	CLA	MG-ND	-3.70	1.98	2.05
25	8	802	DGD	CDA-CCA	-3.70	1.33	1.51
25	8	802	DGD	CGB-CFB	-3.69	1.33	1.51
21	A	1106	CLA	MG-ND	-3.69	1.98	2.05
25	8	802	DGD	CAB-C9B	-3.69	1.33	1.51
21	B	1222	CLA	C1C-NC	-3.69	1.32	1.37
25	B	5003	DGD	CAB-C9B	-3.68	1.33	1.51
38	8	613	CHL	C3B-C2B	-3.68	1.35	1.40
21	A	1117	CLA	C1C-NC	-3.68	1.32	1.37
21	5	617	CLA	C1C-NC	-3.68	1.32	1.37
21	B	1228	CLA	C1C-NC	-3.68	1.32	1.37
23	A	4005	BCR	C10-C9	3.67	1.44	1.35
21	A	1102	CLA	C4B-NB	-3.67	1.33	1.37
21	1	610	CLA	C1C-NC	-3.67	1.32	1.37
21	1	602	CLA	MG-ND	-3.67	1.98	2.05
38	3	608	CHL	C3B-C4B	3.67	1.45	1.41
21	6	618	CLA	MG-ND	-3.67	1.98	2.05
21	B	1204	CLA	C1C-NC	-3.67	1.32	1.37
21	1	603	CLA	MG-ND	-3.66	1.98	2.05
21	7	611	CLA	MG-ND	-3.66	1.98	2.05
25	B	5003	DGD	CDA-CCA	-3.66	1.33	1.51
21	B	1230	CLA	C1C-NC	-3.66	1.32	1.37
21	B	1215	CLA	C1C-NC	-3.65	1.32	1.37
21	B	1236	CLA	MG-ND	-3.65	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	6	619	CHL	C1A-CHA	-3.65	1.35	1.40
21	A	1101	CLA	C1C-NC	-3.64	1.32	1.37
21	7	606	CLA	MG-ND	-3.64	1.98	2.05
21	6	603	CLA	MG-ND	-3.64	1.98	2.05
21	B	1223	CLA	C1C-NC	-3.63	1.32	1.37
21	B	1201	CLA	C1C-NC	-3.63	1.32	1.37
38	4	613	CHL	C3B-C2B	-3.63	1.35	1.40
21	6	603	CLA	C4B-NB	-3.63	1.33	1.37
23	B	4006	BCR	C10-C9	3.63	1.44	1.35
23	L	4002	BCR	C10-C9	3.62	1.44	1.35
21	8	602	CLA	C1C-NC	-3.62	1.32	1.37
23	7	503	BCR	C10-C9	3.62	1.44	1.35
21	3	605	CLA	C1C-NC	-3.62	1.32	1.37
21	a	615	CLA	C1C-NC	-3.61	1.32	1.37
21	3	613	CLA	C1C-NC	-3.61	1.32	1.37
21	4	601	CLA	C1C-NC	-3.61	1.32	1.37
21	B	1225	CLA	C1C-NC	-3.61	1.32	1.37
21	7	610	CLA	C1C-NC	-3.61	1.32	1.37
21	A	1124	CLA	C1C-NC	-3.61	1.32	1.37
21	7	617	CLA	C1C-NC	-3.61	1.32	1.37
21	A	1111	CLA	C1C-NC	-3.61	1.32	1.37
23	A	4002	BCR	C10-C9	3.60	1.44	1.35
21	B	1234	CLA	C1C-NC	-3.60	1.32	1.37
23	B	4005	BCR	C10-C9	3.60	1.44	1.35
21	7	609	CLA	C1C-NC	-3.59	1.32	1.37
25	8	802	DGD	CDB-CCB	-3.59	1.33	1.51
21	4	604	CLA	C1C-NC	-3.59	1.32	1.37
21	1	602	CLA	C1C-NC	-3.59	1.32	1.37
21	A	1133	CLA	C1C-NC	-3.59	1.32	1.37
21	A	1113	CLA	C1C-NC	-3.59	1.32	1.37
21	B	1205	CLA	C1C-NC	-3.59	1.32	1.37
21	J	1901	CLA	MG-ND	-3.59	1.98	2.05
38	4	618	CHL	C3B-C2B	-3.59	1.35	1.40
21	A	1132	CLA	C1C-NC	-3.59	1.32	1.37
21	3	618	CLA	C1C-NC	-3.58	1.32	1.37
21	A	1104	CLA	C1C-NC	-3.58	1.32	1.37
23	B	4007	BCR	C10-C9	3.57	1.44	1.35
21	A	1109	CLA	MG-ND	-3.57	1.98	2.05
21	3	606	CLA	C1C-NC	-3.57	1.32	1.37
21	8	608	CLA	C1C-NC	-3.57	1.32	1.37
21	B	1211	CLA	C1C-NC	-3.57	1.32	1.37
21	L	1501	CLA	C1C-NC	-3.57	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	607	CLA	C1C-NC	-3.56	1.32	1.37
21	B	1206	CLA	C1C-NC	-3.56	1.32	1.37
21	A	1102	CLA	C1C-NC	-3.56	1.32	1.37
21	3	616	CLA	C1C-NC	-3.56	1.32	1.37
23	6	504	BCR	C10-C9	3.55	1.44	1.35
38	1	613	CHL	CBB-CAB	3.55	1.51	1.29
21	B	1240	CLA	C1C-NC	-3.55	1.32	1.37
21	B	1224	CLA	C1C-NC	-3.55	1.32	1.37
21	7	605	CLA	C1C-NC	-3.55	1.32	1.37
43	8	803	DGA	OG2-CB1	3.55	1.44	1.34
38	1	609	CHL	C3B-C4B	3.55	1.44	1.41
21	7	607	CLA	C1C-NC	-3.54	1.32	1.37
21	A	1107	CLA	C1C-NC	-3.54	1.32	1.37
21	A	1121	CLA	C1C-NC	-3.54	1.32	1.37
21	A	1136	CLA	C1C-NC	-3.54	1.32	1.37
21	A	1103	CLA	C1C-NC	-3.54	1.32	1.37
21	B	1202	CLA	C1C-NC	-3.53	1.32	1.37
21	A	1110	CLA	C1C-NC	-3.53	1.32	1.37
21	B	1232	CLA	C1C-NC	-3.53	1.32	1.37
21	7	604	CLA	C4B-NB	-3.53	1.33	1.37
21	7	601	CLA	C4B-NB	-3.53	1.33	1.37
38	a	610	CHL	CBB-CAB	3.52	1.51	1.29
21	A	1126	CLA	C1C-NC	-3.52	1.32	1.37
43	5	803	DGA	OG2-CB1	3.52	1.44	1.34
21	7	605	CLA	C4B-NB	-3.51	1.33	1.37
21	5	603	CLA	C1C-NC	-3.51	1.32	1.37
38	1	613	CHL	C3A-C2A	-3.51	1.51	1.54
38	5	610	CHL	C3B-C4B	3.51	1.44	1.41
23	3	503	BCR	C10-C9	3.51	1.43	1.35
34	J	4002	RRX	C29-C30	3.50	1.65	1.54
21	4	611	CLA	C1C-NC	-3.50	1.32	1.37
21	4	603	CLA	C1C-NC	-3.50	1.32	1.37
21	8	606	CLA	C1C-NC	-3.50	1.32	1.37
21	A	1122	CLA	C1C-NC	-3.50	1.32	1.37
21	5	604	CLA	C1C-NC	-3.50	1.32	1.37
21	8	618	CLA	C1C-NC	-3.49	1.32	1.37
21	A	1013	CLA	C1C-NC	-3.49	1.32	1.37
38	3	608	CHL	CBB-CAB	3.48	1.51	1.29
20	A	1011	CL0	CHB-C4A	-3.48	1.34	1.38
21	A	1137	CLA	C1C-NC	-3.48	1.32	1.37
21	B	1235	CLA	C1C-NC	-3.47	1.32	1.37
21	A	1115	CLA	C1C-NC	-3.47	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	6	619	CHL	CBB-CAB	3.47	1.51	1.29
21	5	601	CLA	C1C-NC	-3.47	1.32	1.37
47	7	504	C7Z	C27-C26	3.47	1.56	1.45
21	1	605	CLA	C1C-NC	-3.47	1.32	1.37
21	B	1219	CLA	C1C-NC	-3.47	1.32	1.37
38	7	613	CHL	C3B-C2B	-3.47	1.35	1.40
21	3	607	CLA	C1C-NC	-3.47	1.32	1.37
21	4	605	CLA	C1C-NC	-3.46	1.32	1.37
38	5	613	CHL	CBB-CAB	3.46	1.51	1.29
21	3	612	CLA	C1C-NC	-3.46	1.32	1.37
21	A	1114	CLA	C1C-NC	-3.46	1.32	1.37
21	a	611	CLA	C1C-NC	-3.46	1.32	1.37
21	8	607	CLA	C1C-NC	-3.46	1.32	1.37
21	A	1135	CLA	C1C-NC	-3.45	1.32	1.37
21	B	1231	CLA	C1C-NC	-3.45	1.32	1.37
47	7	504	C7Z	C35-C34	3.45	1.53	1.43
21	B	1220	CLA	C1C-NC	-3.45	1.32	1.37
38	a	613	CHL	CBB-CAB	3.45	1.50	1.29
21	B	1214	CLA	C1C-NC	-3.45	1.32	1.37
21	3	601	CLA	C1C-NC	-3.45	1.32	1.37
21	3	603	CLA	C1C-NC	-3.44	1.32	1.37
38	4	609	CHL	C3A-C2A	-3.44	1.51	1.54
21	B	1208	CLA	C1C-NC	-3.44	1.32	1.37
21	B	1023	CLA	C1C-NC	-3.44	1.32	1.37
21	K	1403	CLA	C1C-NC	-3.44	1.32	1.37
21	7	611	CLA	C4B-NB	-3.44	1.33	1.37
21	6	607	CLA	C1C-NC	-3.44	1.32	1.37
21	B	1227	CLA	C4B-NB	-3.43	1.33	1.37
21	3	604	CLA	C1C-NC	-3.43	1.32	1.37
21	A	1127	CLA	C1C-NC	-3.43	1.32	1.37
38	6	619	CHL	C3B-C4B	3.43	1.44	1.41
21	A	1140	CLA	C1C-NC	-3.43	1.32	1.37
21	a	604	CLA	MG-ND	-3.43	1.99	2.05
38	4	613	CHL	CBB-CAB	3.43	1.50	1.29
21	5	609	CLA	C1C-NC	-3.43	1.32	1.37
21	8	603	CLA	C1C-NC	-3.43	1.32	1.37
21	1	611	CLA	C1C-NC	-3.42	1.32	1.37
47	7	504	C7Z	C4-C5	-3.42	1.45	1.51
21	A	1105	CLA	C1C-NC	-3.42	1.32	1.37
21	6	601	CLA	C1C-NC	-3.42	1.32	1.37
21	a	601	CLA	C1C-NC	-3.42	1.32	1.37
21	7	604	CLA	C1C-NC	-3.41	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	a	606	CHL	CBB-CAB	3.41	1.50	1.29
21	1	604	CLA	C1C-NC	-3.41	1.32	1.37
21	1	612	CLA	C1C-NC	-3.41	1.32	1.37
21	5	616	CLA	C1C-NC	-3.41	1.32	1.37
21	6	606	CLA	C1C-NC	-3.41	1.32	1.37
38	1	609	CHL	CBB-CAB	3.40	1.50	1.29
21	4	604	CLA	C4B-NB	-3.40	1.33	1.37
21	B	1237	CLA	C1C-NC	-3.40	1.32	1.37
21	7	603	CLA	C1C-NC	-3.40	1.32	1.37
21	A	1109	CLA	C1C-NC	-3.40	1.32	1.37
21	6	609	CLA	C4B-NB	-3.40	1.33	1.37
34	J	4002	RRX	C11-C10	3.40	1.53	1.43
21	4	606	CLA	C1C-NC	-3.39	1.32	1.37
21	B	1218	CLA	C1C-NC	-3.39	1.32	1.37
21	A	1126	CLA	C4B-NB	-3.39	1.33	1.37
21	B	1229	CLA	C1C-NC	-3.39	1.32	1.37
21	A	1112	CLA	C4B-NB	-3.39	1.33	1.37
21	1	615	CLA	C1C-NC	-3.39	1.32	1.37
38	4	609	CHL	CBB-CAB	3.39	1.50	1.29
38	5	610	CHL	CBB-CAB	3.39	1.50	1.29
38	4	618	CHL	CBB-CAB	3.38	1.50	1.29
21	B	1216	CLA	C1C-NC	-3.38	1.32	1.37
21	B	1226	CLA	C1C-NC	-3.38	1.32	1.37
21	6	604	CLA	C4B-NB	-3.38	1.33	1.37
21	A	1134	CLA	C1C-NC	-3.38	1.32	1.37
21	A	1118	CLA	C1C-NC	-3.37	1.32	1.37
21	B	1022	CLA	C1C-NC	-3.37	1.32	1.37
36	M	4001	ECH	C30-C25	-3.37	1.49	1.53
21	B	1221	CLA	C1C-NC	-3.37	1.32	1.37
21	a	602	CLA	C1C-NC	-3.37	1.32	1.37
21	L	1502	CLA	C1C-NC	-3.37	1.32	1.37
21	3	610	CLA	C1C-NC	-3.37	1.32	1.37
21	6	612	CLA	C1C-NC	-3.37	1.32	1.37
21	B	1213	CLA	C1C-NC	-3.37	1.32	1.37
21	K	1401	CLA	C1C-NC	-3.37	1.32	1.37
21	A	1107	CLA	C4B-NB	-3.37	1.33	1.37
21	B	1203	CLA	C1C-NC	-3.37	1.32	1.37
21	A	1138	CLA	C4B-NB	-3.36	1.33	1.37
21	5	605	CLA	C1C-NC	-3.36	1.32	1.37
21	A	1130	CLA	C1C-NC	-3.36	1.32	1.37
21	8	620	CLA	C1C-NC	-3.36	1.32	1.37
43	5	803	DGA	OG1-CA1	3.35	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	1	609	CHL	CHB-C4A	-3.35	1.34	1.38
21	A	1125	CLA	C4B-NB	-3.35	1.33	1.37
21	6	615	CLA	C1C-NC	-3.35	1.32	1.37
38	5	611	CHL	C1A-CHA	-3.35	1.36	1.40
21	5	602	CLA	C1C-NC	-3.35	1.32	1.37
21	B	1217	CLA	C1C-NC	-3.35	1.32	1.37
21	B	1238	CLA	C1C-NC	-3.34	1.32	1.37
21	G	1603	CLA	C1C-NC	-3.34	1.32	1.37
38	6	610	CHL	CBB-CAB	3.34	1.50	1.29
21	A	1111	CLA	C4B-NB	-3.34	1.33	1.37
21	A	1105	CLA	C4B-NB	-3.34	1.33	1.37
21	6	618	CLA	C1C-NC	-3.34	1.32	1.37
21	1	606	CLA	C1C-NC	-3.33	1.32	1.37
21	7	608	CLA	C1C-NC	-3.33	1.32	1.37
21	6	602	CLA	C1C-NC	-3.33	1.32	1.37
21	A	1123	CLA	C1C-NC	-3.33	1.32	1.37
21	7	612	CLA	C1C-NC	-3.33	1.32	1.37
21	B	1234	CLA	C4B-NB	-3.33	1.33	1.37
21	F	1301	CLA	C1C-NC	-3.33	1.32	1.37
21	7	615	CLA	C1C-NC	-3.33	1.32	1.37
21	7	602	CLA	C1C-NC	-3.33	1.32	1.37
21	1	610	CLA	C4B-NB	-3.32	1.33	1.37
21	A	1129	CLA	C1C-NC	-3.32	1.32	1.37
38	a	609	CHL	CBB-CAB	3.32	1.50	1.29
21	4	602	CLA	C1C-NC	-3.32	1.32	1.37
21	B	1211	CLA	C4B-NB	-3.31	1.33	1.37
21	5	612	CLA	C1C-NC	-3.31	1.32	1.37
21	5	617	CLA	C4B-NB	-3.31	1.33	1.37
21	A	1120	CLA	C1C-NC	-3.31	1.32	1.37
38	8	613	CHL	CBB-CAB	3.30	1.50	1.29
21	4	610	CLA	C1C-NC	-3.30	1.32	1.37
34	J	4002	RRX	C16-C17	3.30	1.53	1.43
38	6	613	CHL	CBB-CAB	3.30	1.50	1.29
21	4	617	CLA	C1C-NC	-3.30	1.32	1.37
21	3	606	CLA	C4B-NB	-3.29	1.33	1.37
21	A	1119	CLA	C1C-NC	-3.29	1.32	1.37
38	6	611	CHL	CBB-CAB	3.29	1.50	1.29
21	6	604	CLA	C1C-NC	-3.29	1.32	1.37
21	1	603	CLA	C1C-NC	-3.29	1.32	1.37
21	A	1125	CLA	C1C-C2C	3.29	1.51	1.44
21	B	1204	CLA	C4B-NB	-3.29	1.33	1.37
38	4	618	CHL	C3B-C4B	3.28	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	601	CLA	C4B-NB	-3.28	1.33	1.37
21	6	605	CLA	C1C-NC	-3.28	1.32	1.37
21	8	611	CLA	C1C-NC	-3.28	1.32	1.37
21	a	605	CLA	C1C-NC	-3.28	1.32	1.37
38	4	613	CHL	CHB-C4A	-3.28	1.34	1.38
21	1	601	CLA	C1C-NC	-3.27	1.32	1.37
21	a	603	CLA	C1C-NC	-3.27	1.32	1.37
21	4	615	CLA	C1C-NC	-3.27	1.32	1.37
21	5	618	CLA	C1C-NC	-3.27	1.32	1.37
21	5	606	CLA	C1C-NC	-3.27	1.32	1.37
21	K	1404	CLA	C1C-NC	-3.26	1.32	1.37
38	7	613	CHL	CBB-CAB	3.26	1.49	1.29
38	a	606	CHL	C3B-C2B	-3.26	1.36	1.40
34	J	4002	RRX	C4-C5	-3.26	1.44	1.51
21	3	601	CLA	C4B-NB	-3.26	1.33	1.37
21	8	615	CLA	C4B-NB	-3.25	1.33	1.37
21	3	602	CLA	C1C-NC	-3.25	1.32	1.37
21	G	1601	CLA	C1C-NC	-3.25	1.32	1.37
21	B	1201	CLA	C4B-NB	-3.25	1.33	1.37
21	4	608	CLA	C1C-NC	-3.25	1.32	1.37
38	3	611	CHL	C1A-CHA	-3.25	1.36	1.40
21	J	1901	CLA	C1C-NC	-3.25	1.32	1.37
21	6	612	CLA	C4B-NB	-3.25	1.33	1.37
47	7	504	C7Z	C21-C26	-3.24	1.49	1.53
21	7	611	CLA	C1C-NC	-3.23	1.32	1.37
21	4	612	CLA	C1C-NC	-3.23	1.32	1.37
21	a	608	CLA	C1C-NC	-3.23	1.32	1.37
21	G	1602	CLA	C1C-NC	-3.23	1.32	1.37
21	6	608	CLA	C1C-NC	-3.23	1.32	1.37
21	3	613	CLA	C4B-NB	-3.22	1.33	1.37
21	A	1141	CLA	C1C-NC	-3.22	1.32	1.37
21	B	1240	CLA	C4B-NB	-3.22	1.33	1.37
21	a	605	CLA	C4B-NB	-3.22	1.33	1.37
31	B	5007	LAP	P9-O6	3.22	1.72	1.59
21	a	604	CLA	C1C-NC	-3.21	1.32	1.37
21	B	1212	CLA	C4B-NB	-3.21	1.33	1.37
21	8	615	CLA	C1C-NC	-3.21	1.32	1.37
29	6	803	PCW	O3-C11	3.20	1.42	1.33
21	7	606	CLA	C4B-NB	-3.20	1.33	1.37
21	3	604	CLA	C4B-NB	-3.20	1.33	1.37
21	4	607	CLA	C1C-NC	-3.20	1.32	1.37
21	8	606	CLA	C4B-NB	-3.20	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	604	CLA	C4B-NB	-3.20	1.33	1.37
21	B	1227	CLA	C1C-NC	-3.20	1.32	1.37
38	3	611	CHL	CHB-C4A	-3.19	1.34	1.38
21	A	1132	CLA	C4B-NB	-3.19	1.33	1.37
38	8	601	CHL	CBB-CAB	3.19	1.49	1.29
21	6	617	CLA	C1C-NC	-3.18	1.32	1.37
21	A	1012	CLA	C1C-NC	-3.18	1.32	1.37
21	1	607	CLA	C1C-NC	-3.18	1.32	1.37
38	5	611	CHL	CBB-CAB	3.18	1.49	1.29
21	1	608	CLA	C1C-NC	-3.18	1.32	1.37
23	A	4001	BCR	C10-C9	3.18	1.43	1.35
21	7	606	CLA	C1C-NC	-3.18	1.32	1.37
21	K	1402	CLA	C1C-NC	-3.17	1.32	1.37
38	8	604	CHL	CBB-CAB	3.17	1.49	1.29
31	K	5001	LAP	P9-O4	3.17	1.71	1.59
21	B	1206	CLA	C4B-NB	-3.17	1.33	1.37
21	A	1101	CLA	C4B-NB	-3.17	1.33	1.37
21	A	1124	CLA	C4B-NB	-3.17	1.33	1.37
34	J	4002	RRX	C7-C6	3.17	1.55	1.45
21	a	607	CLA	C1C-NC	-3.16	1.32	1.37
21	A	1110	CLA	C4B-NB	-3.16	1.33	1.37
21	A	1113	CLA	C4B-NB	-3.16	1.33	1.37
21	B	1235	CLA	C4B-NB	-3.16	1.33	1.37
21	8	607	CLA	C4B-NB	-3.16	1.33	1.37
21	B	1230	CLA	C4B-NB	-3.16	1.33	1.37
29	B	5004	PCW	O3-C11	3.15	1.42	1.33
21	B	1214	CLA	C4B-NB	-3.15	1.33	1.37
21	B	1224	CLA	C4B-NB	-3.15	1.33	1.37
21	B	1208	CLA	C4B-NB	-3.15	1.33	1.37
23	A	4004	BCR	C10-C9	3.15	1.43	1.35
21	A	1131	CLA	C4B-NB	-3.15	1.33	1.37
21	5	604	CLA	C4B-NB	-3.15	1.33	1.37
31	B	5007	LAP	P9-O4	3.15	1.71	1.59
21	8	603	CLA	C4B-NB	-3.14	1.33	1.37
21	F	1302	CLA	C4B-NB	-3.14	1.33	1.37
21	5	612	CLA	C4B-NB	-3.14	1.33	1.37
21	8	612	CLA	C4B-NB	-3.14	1.33	1.37
21	1	607	CLA	C4B-NB	-3.13	1.33	1.37
21	5	608	CLA	C1C-NC	-3.13	1.33	1.37
21	3	605	CLA	C4B-NB	-3.13	1.33	1.37
21	8	610	CLA	C4B-NB	-3.13	1.33	1.37
21	5	614	CLA	C1C-NC	-3.12	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	616	CLA	C1C-NC	-3.12	1.33	1.37
38	5	610	CHL	C3B-C2B	-3.12	1.36	1.40
21	5	603	CLA	C4B-NB	-3.11	1.33	1.37
38	8	613	CHL	C1A-CHA	-3.11	1.36	1.40
21	B	1219	CLA	C4B-NB	-3.11	1.33	1.37
21	3	610	CLA	C4B-NB	-3.10	1.33	1.37
21	B	1222	CLA	C4B-NB	-3.10	1.33	1.37
21	a	601	CLA	C4B-NB	-3.10	1.33	1.37
38	5	611	CHL	CHB-C4A	-3.09	1.34	1.38
21	A	1129	CLA	C4B-NB	-3.09	1.33	1.37
21	A	1106	CLA	C4B-NB	-3.09	1.33	1.37
21	A	1013	CLA	C4B-NB	-3.09	1.33	1.37
21	7	609	CLA	C4B-NB	-3.09	1.33	1.37
21	B	1022	CLA	C4B-NB	-3.08	1.33	1.37
21	5	605	CLA	C4B-NB	-3.08	1.33	1.37
38	3	611	CHL	CBB-CAB	3.08	1.48	1.29
21	1	606	CLA	C4B-NB	-3.07	1.33	1.37
21	A	1122	CLA	C4B-NB	-3.07	1.33	1.37
21	3	612	CLA	C4B-NB	-3.07	1.33	1.37
21	5	609	CLA	C4B-NB	-3.07	1.33	1.37
21	B	1216	CLA	C4B-NB	-3.07	1.33	1.37
21	B	1226	CLA	C4B-NB	-3.06	1.33	1.37
38	7	613	CHL	CHB-C4A	-3.06	1.35	1.38
21	A	1117	CLA	C4B-NB	-3.06	1.33	1.37
21	A	1109	CLA	C4B-NB	-3.05	1.33	1.37
21	8	609	CLA	C4B-NB	-3.05	1.33	1.37
21	B	1209	CLA	C4B-NB	-3.05	1.33	1.37
21	B	1221	CLA	C4B-NB	-3.05	1.33	1.37
21	A	1125	CLA	C1C-NC	-3.05	1.33	1.37
21	3	607	CLA	C4B-NB	-3.04	1.33	1.37
21	B	1218	CLA	C4B-NB	-3.04	1.33	1.37
36	M	4001	ECH	C25-C26	-3.03	1.31	1.35
21	B	1220	CLA	C4B-NB	-3.03	1.33	1.37
21	4	612	CLA	C4B-NB	-3.02	1.33	1.37
21	A	1123	CLA	C4B-NB	-3.02	1.33	1.37
21	B	1239	CLA	C4B-NB	-3.02	1.33	1.37
21	1	605	CLA	C4B-NB	-3.02	1.33	1.37
21	B	1232	CLA	C4B-NB	-3.02	1.33	1.37
21	A	1121	CLA	C4B-NB	-3.02	1.33	1.37
48	8	806	P5S	O37-C38	3.01	1.42	1.34
21	8	618	CLA	C4B-NB	-3.01	1.33	1.37
21	A	1135	CLA	C4B-NB	-3.01	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1021	CLA	C4B-NB	-3.01	1.33	1.37
21	G	1601	CLA	C4B-NB	-3.01	1.33	1.37
21	6	608	CLA	C4B-NB	-3.01	1.33	1.37
21	F	1302	CLA	C1C-NC	-3.01	1.33	1.37
21	B	1236	CLA	C4B-NB	-3.01	1.33	1.37
21	5	601	CLA	C4B-NB	-3.00	1.33	1.37
21	B	1207	CLA	C4B-NB	-3.00	1.33	1.37
21	6	607	CLA	C4B-NB	-3.00	1.33	1.37
21	B	1228	CLA	C4B-NB	-3.00	1.33	1.37
21	7	603	CLA	C4B-NB	-3.00	1.33	1.37
21	B	1023	CLA	C4B-NB	-2.99	1.33	1.37
21	A	1116	CLA	C4B-NB	-2.99	1.33	1.37
25	A	5005	DGD	CAB-C9B	-2.99	1.33	1.51
21	8	611	CLA	C4B-NB	-2.99	1.33	1.37
21	1	601	CLA	C4B-NB	-2.99	1.33	1.37
21	A	1115	CLA	C4B-NB	-2.98	1.33	1.37
38	a	606	CHL	CHB-C4A	-2.98	1.35	1.38
21	A	1119	CLA	C4B-NB	-2.98	1.33	1.37
21	6	601	CLA	C4B-NB	-2.98	1.33	1.37
38	6	613	CHL	C1A-CHA	-2.98	1.36	1.40
21	B	1202	CLA	C4B-NB	-2.98	1.34	1.37
21	7	612	CLA	C4B-NB	-2.97	1.34	1.37
21	B	1238	CLA	C4B-NB	-2.96	1.34	1.37
21	4	606	CLA	C4B-NB	-2.96	1.34	1.37
21	8	602	CLA	C4B-NB	-2.96	1.34	1.37
38	5	613	CHL	CHB-C4A	-2.96	1.35	1.38
21	a	615	CLA	C4B-NB	-2.95	1.34	1.37
38	8	604	CHL	CHB-C4A	-2.95	1.35	1.38
21	K	1404	CLA	C4B-NB	-2.94	1.34	1.37
21	3	603	CLA	C4B-NB	-2.94	1.34	1.37
21	A	1012	CLA	C4B-NB	-2.93	1.34	1.37
21	1	602	CLA	C4B-NB	-2.93	1.34	1.37
21	1	611	CLA	C4B-NB	-2.93	1.34	1.37
21	B	1213	CLA	C4B-NB	-2.93	1.34	1.37
21	6	618	CLA	C4B-NB	-2.93	1.34	1.37
21	4	610	CLA	C4B-NB	-2.93	1.34	1.37
21	J	1901	CLA	C4B-NB	-2.93	1.34	1.37
38	8	613	CHL	CHB-C4A	-2.92	1.35	1.38
21	L	1503	CLA	C4B-NB	-2.92	1.34	1.37
21	7	607	CLA	C4B-NB	-2.92	1.34	1.37
21	3	602	CLA	C4B-NB	-2.91	1.34	1.37
43	8	803	DGA	OG1-CA1	2.91	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1104	CLA	C4B-NB	-2.91	1.34	1.37
38	5	613	CHL	C3B-C4B	2.91	1.44	1.41
21	6	615	CLA	C4B-NB	-2.91	1.34	1.37
21	a	611	CLA	C4B-NB	-2.91	1.34	1.37
35	J	5001	LPX	P1-O1	2.90	1.70	1.59
21	7	617	CLA	C4B-NB	-2.90	1.34	1.37
21	A	1118	CLA	C4B-NB	-2.89	1.34	1.37
21	B	1215	CLA	C4B-NB	-2.89	1.34	1.37
38	a	609	CHL	CHB-C4A	-2.89	1.35	1.38
21	6	609	CLA	C1C-NC	-2.89	1.33	1.37
21	7	608	CLA	C4B-NB	-2.89	1.34	1.37
21	B	1225	CLA	C4B-NB	-2.88	1.34	1.37
35	a	804	LPX	P1-O1	2.88	1.70	1.59
21	7	610	CLA	C4B-NB	-2.88	1.34	1.37
38	5	610	CHL	CHB-C4A	-2.88	1.35	1.38
21	a	612	CLA	C4B-NB	-2.88	1.34	1.37
21	K	1401	CLA	C4B-NB	-2.87	1.34	1.37
21	4	608	CLA	C4B-NB	-2.87	1.34	1.37
21	a	603	CLA	C4B-NB	-2.87	1.34	1.37
21	a	604	CLA	C4B-NB	-2.87	1.34	1.37
21	F	1301	CLA	C4B-NB	-2.86	1.34	1.37
21	A	1108	CLA	C4B-NB	-2.86	1.34	1.37
21	7	602	CLA	C4B-NB	-2.86	1.34	1.37
23	A	4004	BCR	C12-C13	-2.85	1.39	1.46
21	L	1502	CLA	C4B-NB	-2.85	1.34	1.37
21	6	605	CLA	C4B-NB	-2.85	1.34	1.37
21	8	620	CLA	C4B-NB	-2.85	1.34	1.37
21	A	1120	CLA	C4B-NB	-2.85	1.34	1.37
21	A	1136	CLA	C4B-NB	-2.85	1.34	1.37
38	6	619	CHL	CHB-C4A	-2.85	1.35	1.38
45	7	502	XAT	O24-C25	-2.84	1.42	1.46
38	6	611	CHL	CHB-C4A	-2.84	1.35	1.38
21	5	616	CLA	C4B-NB	-2.84	1.34	1.37
21	a	607	CLA	C4B-NB	-2.84	1.34	1.37
21	3	616	CLA	C4B-NB	-2.84	1.34	1.37
21	G	1602	CLA	C4B-NB	-2.84	1.34	1.37
21	4	616	CLA	C4B-NB	-2.83	1.34	1.37
38	a	610	CHL	C3B-C2B	-2.83	1.36	1.40
21	5	606	CLA	C4B-NB	-2.83	1.34	1.37
21	A	1141	CLA	C4B-NB	-2.82	1.34	1.37
21	A	1134	CLA	C4B-NB	-2.82	1.34	1.37
21	1	612	CLA	C4B-NB	-2.82	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	4	613	CHL	C1A-CHA	-2.81	1.36	1.40
38	3	608	CHL	C1A-CHA	-2.81	1.36	1.40
21	A	1133	CLA	C4B-NB	-2.81	1.34	1.37
21	B	1203	CLA	C4B-NB	-2.81	1.34	1.37
21	4	603	CLA	C4B-NB	-2.81	1.34	1.37
21	4	607	CLA	C4B-NB	-2.81	1.34	1.37
38	a	613	CHL	CHB-C4A	-2.81	1.35	1.38
21	A	1128	CLA	C4B-NB	-2.80	1.34	1.37
38	6	610	CHL	CHB-C4A	-2.79	1.35	1.38
21	8	605	CLA	C4B-NB	-2.79	1.34	1.37
38	4	609	CHL	CHB-C4A	-2.79	1.35	1.38
21	B	1205	CLA	C4B-NB	-2.79	1.34	1.37
37	5	505	LUT	C1-C6	-2.79	1.50	1.53
21	B	1223	CLA	C4B-NB	-2.79	1.34	1.37
38	8	601	CHL	CHB-C4A	-2.78	1.35	1.38
21	6	602	CLA	C4B-NB	-2.78	1.34	1.37
38	3	608	CHL	C1B-C2B	2.78	1.42	1.39
21	A	1127	CLA	C4B-NB	-2.78	1.34	1.37
38	4	609	CHL	C3B-C2B	-2.78	1.36	1.40
21	3	618	CLA	C4B-NB	-2.77	1.34	1.37
21	1	615	CLA	C4B-NB	-2.77	1.34	1.37
38	a	610	CHL	CHB-C4A	-2.77	1.35	1.38
21	A	1103	CLA	C4B-NB	-2.77	1.34	1.37
38	6	611	CHL	C1A-CHA	-2.77	1.36	1.40
38	4	618	CHL	CHB-C4A	-2.76	1.35	1.38
21	5	602	CLA	C4B-NB	-2.76	1.34	1.37
40	3	506	QTB	C14-C12	-2.76	1.46	1.53
21	L	1501	CLA	C4B-NB	-2.76	1.34	1.37
21	8	608	CLA	C4B-NB	-2.75	1.34	1.37
46	7	807	4RF	O21-C20	-2.75	1.40	1.46
38	6	613	CHL	CHB-C4A	-2.75	1.35	1.38
38	1	609	CHL	C3B-C2B	-2.75	1.36	1.40
21	1	604	CLA	C1C-C2C	2.75	1.50	1.44
21	4	615	CLA	C4B-NB	-2.74	1.34	1.37
21	6	606	CLA	C4B-NB	-2.74	1.34	1.37
21	K	1403	CLA	C4B-NB	-2.74	1.34	1.37
21	4	605	CLA	C4B-NB	-2.74	1.34	1.37
21	B	1231	CLA	C4B-NB	-2.74	1.34	1.37
38	a	610	CHL	C1D-C2D	2.74	1.42	1.39
21	B	1228	CLA	CAA-C2A	-2.73	1.49	1.54
21	a	608	CLA	C4B-NB	-2.73	1.34	1.37
21	6	603	CLA	C3D-C4D	-2.72	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1139	CLA	C4B-NB	-2.71	1.34	1.37
21	A	1130	CLA	C4B-NB	-2.71	1.34	1.37
38	1	613	CHL	C1A-CHA	-2.70	1.36	1.40
21	1	608	CLA	C4B-NB	-2.70	1.34	1.37
48	8	806	P5S	O19-C17	2.69	1.41	1.33
38	6	619	CHL	C1D-C2D	2.69	1.42	1.39
21	B	1228	CLA	C2A-C1A	-2.68	1.46	1.52
38	6	613	CHL	C3B-C4B	2.68	1.44	1.41
38	6	611	CHL	C1D-C2D	2.68	1.42	1.39
38	a	610	CHL	C1B-C2B	2.68	1.42	1.39
29	B	5004	PCW	O2-C2	-2.67	1.40	1.46
21	5	604	CLA	C3D-C4D	-2.66	1.38	1.44
38	4	613	CHL	C1D-C2D	2.66	1.42	1.39
21	A	1137	CLA	C4B-NB	-2.66	1.34	1.37
38	8	604	CHL	C1D-C2D	2.66	1.42	1.39
21	B	1229	CLA	C4B-NB	-2.66	1.34	1.37
38	3	608	CHL	CHB-C4A	-2.65	1.35	1.38
38	6	610	CHL	C1D-C2D	2.64	1.42	1.39
21	B	1237	CLA	C4B-NB	-2.64	1.34	1.37
38	1	609	CHL	C1A-CHA	-2.64	1.37	1.40
38	a	613	CHL	C1D-C2D	2.64	1.42	1.39
21	5	608	CLA	C4B-NB	-2.64	1.34	1.37
21	7	615	CLA	C4B-NB	-2.64	1.34	1.37
38	a	613	CHL	C1B-C2B	2.63	1.42	1.39
21	4	602	CLA	C4B-NB	-2.63	1.34	1.37
30	B	5005	PTY	O7-C6	-2.63	1.40	1.46
29	6	803	PCW	O2-C2	-2.63	1.40	1.46
21	5	614	CLA	C4B-NB	-2.63	1.34	1.37
21	B	1228	CLA	C3D-C4D	-2.63	1.38	1.44
37	a	502	LUT	C22-C21	-2.63	1.51	1.54
38	6	610	CHL	C1B-C2B	2.63	1.42	1.39
21	B	1217	CLA	C4B-NB	-2.62	1.34	1.37
38	4	618	CHL	C1D-C2D	2.62	1.42	1.39
38	a	606	CHL	C1B-C2B	2.62	1.42	1.39
28	B	5006	LMT	O3'-C3'	-2.62	1.36	1.43
26	A	5007	3PH	O21-C2	-2.62	1.40	1.46
33	G	5002	ERG	C7-C8	-2.62	1.28	1.34
38	8	613	CHL	C1D-C2D	2.61	1.42	1.39
38	6	613	CHL	C1D-C2D	2.61	1.42	1.39
38	4	618	CHL	C1B-C2B	2.61	1.42	1.39
38	8	601	CHL	C1D-C2D	2.61	1.42	1.39
34	J	4002	RRX	C32-C1	2.61	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	6	619	CHL	C1B-C2B	2.61	1.42	1.39
38	7	613	CHL	C1D-C2D	2.61	1.42	1.39
21	4	611	CLA	C4B-NB	-2.61	1.34	1.37
38	a	609	CHL	C1D-C2D	2.60	1.42	1.39
38	5	610	CHL	C1B-C2B	2.60	1.42	1.39
46	8	808	4RF	O18-C16	2.60	1.40	1.33
38	6	610	CHL	C3B-C4B	2.60	1.43	1.41
38	a	613	CHL	C3B-C2B	-2.60	1.36	1.40
38	5	610	CHL	C1D-C2D	2.59	1.42	1.39
21	a	602	CLA	C4B-NB	-2.59	1.34	1.37
38	1	613	CHL	CHB-C4A	-2.58	1.35	1.38
38	1	613	CHL	C1B-C2B	2.58	1.42	1.39
21	A	1114	CLA	C4B-NB	-2.57	1.34	1.37
38	a	609	CHL	C1B-C2B	2.57	1.42	1.39
23	A	4005	BCR	C1-C6	-2.56	1.50	1.53
28	1	804	LMT	O2'-C2'	-2.56	1.36	1.43
38	4	609	CHL	C1D-C2D	2.55	1.42	1.39
38	a	606	CHL	C1D-C2D	2.55	1.42	1.39
38	6	613	CHL	C1B-C2B	2.54	1.42	1.39
47	7	504	C7Z	C18-C5	2.53	1.55	1.50
38	1	609	CHL	C1D-C2D	2.52	1.42	1.39
38	4	609	CHL	C1B-C2B	2.52	1.42	1.39
21	A	1131	CLA	C3D-C4D	-2.52	1.38	1.44
38	5	611	CHL	C1D-C2D	2.51	1.42	1.39
21	5	607	CLA	C4B-NB	-2.51	1.34	1.37
38	3	608	CHL	C1D-C2D	2.51	1.42	1.39
21	1	603	CLA	C4B-NB	-2.50	1.34	1.37
23	A	4004	BCR	C35-C13	-2.50	1.45	1.50
38	a	609	CHL	C3B-C2B	-2.50	1.37	1.40
46	8	807	4RF	O18-C16	2.49	1.40	1.33
38	4	613	CHL	CHB-C1B	-2.48	1.35	1.39
21	6	617	CLA	C4B-NB	-2.48	1.34	1.37
23	A	4002	BCR	C1-C6	-2.48	1.50	1.53
38	5	613	CHL	C1B-C2B	2.47	1.42	1.39
38	5	613	CHL	C1D-C2D	2.47	1.42	1.39
21	A	1124	CLA	C3D-C4D	-2.47	1.38	1.44
21	B	1205	CLA	C3D-C4D	-2.47	1.38	1.44
33	G	5002	ERG	C9-C8	2.47	1.57	1.51
21	G	1603	CLA	C4B-NB	-2.47	1.34	1.37
28	1	804	LMT	O3'-C3'	-2.46	1.36	1.43
38	7	613	CHL	C1A-CHA	-2.46	1.37	1.40
21	A	1114	CLA	C3D-C4D	-2.45	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1022	CLA	C3D-C4D	-2.45	1.38	1.44
38	5	611	CHL	C1B-C2B	2.45	1.42	1.39
38	8	613	CHL	C1B-C2B	2.45	1.42	1.39
38	4	609	CHL	C1A-CHA	-2.44	1.37	1.40
30	3	802	PTY	O4-C30	2.44	1.40	1.33
23	6	503	BCR	C1-C6	-2.44	1.50	1.53
38	3	611	CHL	C1D-C2D	2.44	1.42	1.39
30	8	810	PTY	O7-C8	2.44	1.41	1.34
46	7	807	4RF	O18-C19	-2.44	1.39	1.45
38	8	604	CHL	C1B-C2B	2.43	1.42	1.39
21	B	1225	CLA	C3D-C4D	-2.43	1.38	1.44
21	5	605	CLA	C3D-C4D	-2.43	1.38	1.44
21	6	603	CLA	C1D-ND	-2.43	1.34	1.37
23	6	504	BCR	C1-C6	-2.43	1.50	1.53
38	5	613	CHL	C1A-CHA	-2.42	1.37	1.40
29	6	803	PCW	O2-C31	2.42	1.41	1.34
23	F	4001	BCR	C1-C6	-2.42	1.50	1.53
21	3	612	CLA	C3D-C4D	-2.42	1.38	1.44
21	5	618	CLA	C4B-NB	-2.41	1.34	1.37
30	7	804	PTY	O7-C6	-2.41	1.40	1.46
38	1	613	CHL	C1D-C2D	2.41	1.42	1.39
38	6	611	CHL	C1B-C2B	2.41	1.42	1.39
21	4	617	CLA	C4B-NB	-2.41	1.34	1.37
46	7	807	4RF	O40-C39	-2.41	1.39	1.45
30	5	802	PTY	O7-C6	-2.40	1.40	1.46
28	A	5008	LMT	O3'-C3'	-2.40	1.37	1.43
46	8	807	4RF	O21-C20	-2.40	1.41	1.46
21	7	601	CLA	C3D-C4D	-2.40	1.38	1.44
21	A	1111	CLA	C3D-C4D	-2.40	1.38	1.44
34	J	4002	RRX	C35-C13	2.40	1.55	1.50
31	F	5003	LAP	P9-O4	2.40	1.68	1.59
21	8	605	CLA	C3D-C4D	-2.40	1.38	1.44
46	8	808	4RF	O21-C20	-2.40	1.41	1.46
38	4	613	CHL	C1B-C2B	2.39	1.42	1.39
21	8	607	CLA	C3D-C4D	-2.38	1.38	1.44
21	A	1140	CLA	C4B-NB	-2.38	1.34	1.37
21	A	1126	CLA	C3D-C4D	-2.38	1.38	1.44
29	B	5004	PCW	O2-C31	2.38	1.41	1.34
21	7	612	CLA	C3D-C4D	-2.38	1.38	1.44
25	A	5005	DGD	CAA-C9A	-2.37	1.33	1.50
21	B	1213	CLA	C3D-C4D	-2.36	1.38	1.44
30	3	802	PTY	O7-C6	-2.36	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1012	CLA	C3D-C4D	-2.36	1.38	1.44
38	7	613	CHL	C1B-C2B	2.36	1.42	1.39
20	A	1011	CL0	CBD-CGD	-2.35	1.49	1.52
21	B	1231	CLA	C3D-C4D	-2.35	1.38	1.44
21	A	1135	CLA	C3D-C4D	-2.35	1.38	1.44
21	B	1211	CLA	C3D-C4D	-2.34	1.38	1.44
21	A	1127	CLA	C3D-C4D	-2.34	1.38	1.44
46	7	807	4RF	O21-C22	2.34	1.40	1.34
33	G	5002	ERG	C14-C8	2.34	1.57	1.51
23	B	4005	BCR	C12-C13	-2.34	1.40	1.46
37	8	501	LUT	C22-C21	-2.34	1.51	1.54
21	A	1132	CLA	C3D-C4D	-2.34	1.38	1.44
21	A	1118	CLA	C3D-C4D	-2.34	1.38	1.44
21	B	1224	CLA	C3D-C4D	-2.33	1.38	1.44
21	7	609	CLA	C3D-C4D	-2.33	1.38	1.44
21	4	605	CLA	C3D-C4D	-2.33	1.38	1.44
46	8	807	4RF	O40-C41	2.33	1.40	1.33
37	5	502	LUT	C1-C6	-2.33	1.50	1.53
21	B	1237	CLA	C3D-C4D	-2.33	1.39	1.44
21	A	1138	CLA	C3D-C4D	-2.33	1.39	1.44
21	8	611	CLA	C3D-C4D	-2.33	1.39	1.44
21	3	605	CLA	C3D-C4D	-2.32	1.39	1.44
21	B	1236	CLA	C3D-C4D	-2.32	1.39	1.44
21	3	606	CLA	C3D-C4D	-2.32	1.39	1.44
21	B	1229	CLA	C3D-C4D	-2.32	1.39	1.44
21	B	1216	CLA	C3D-C4D	-2.32	1.39	1.44
46	8	808	4RF	O40-C39	-2.32	1.40	1.45
21	1	604	CLA	C3D-C4D	-2.32	1.39	1.44
21	A	1119	CLA	C3D-C4D	-2.31	1.39	1.44
35	a	804	LPX	P1-O2	2.31	1.68	1.59
21	8	602	CLA	C3D-C4D	-2.31	1.39	1.44
30	7	804	PTY	O4-C30	2.31	1.40	1.33
28	B	5006	LMT	O2B-C2B	-2.31	1.37	1.43
21	7	608	CLA	C3D-C4D	-2.31	1.39	1.44
23	A	4001	BCR	C12-C13	-2.30	1.41	1.46
21	a	601	CLA	C3D-C4D	-2.30	1.39	1.44
21	A	1140	CLA	C3D-C4D	-2.30	1.39	1.44
46	7	807	4RF	O18-C16	2.30	1.40	1.33
38	3	608	CHL	C3B-C2B	-2.30	1.37	1.40
21	A	1117	CLA	C3D-C4D	-2.30	1.39	1.44
28	B	5006	LMT	O2'-C2'	-2.30	1.37	1.43
28	A	5008	LMT	O2B-C2B	-2.30	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	608	CLA	C3D-C4D	-2.30	1.39	1.44
38	3	611	CHL	C1B-C2B	2.30	1.42	1.39
21	B	1235	CLA	C3D-C4D	-2.30	1.39	1.44
46	8	808	4RF	O21-C22	2.30	1.40	1.34
21	B	1238	CLA	C3D-C4D	-2.30	1.39	1.44
21	B	1206	CLA	C3D-C4D	-2.30	1.39	1.44
21	6	605	CLA	C3D-C4D	-2.29	1.39	1.44
21	B	1234	CLA	C3D-C4D	-2.29	1.39	1.44
21	B	1202	CLA	C3D-C4D	-2.29	1.39	1.44
21	A	1106	CLA	C3D-C4D	-2.29	1.39	1.44
21	A	1108	CLA	C3D-C4D	-2.29	1.39	1.44
21	B	1227	CLA	C3D-C4D	-2.29	1.39	1.44
21	5	606	CLA	C3D-C4D	-2.29	1.39	1.44
23	B	4007	BCR	C12-C13	-2.29	1.41	1.46
21	B	1222	CLA	C3D-C4D	-2.29	1.39	1.44
21	B	1239	CLA	C3D-C4D	-2.29	1.39	1.44
30	5	802	PTY	O4-C30	2.29	1.40	1.33
21	B	1220	CLA	C3D-C4D	-2.28	1.39	1.44
38	8	601	CHL	C1B-C2B	2.28	1.42	1.39
21	1	607	CLA	C3D-C4D	-2.28	1.39	1.44
35	J	5001	LPX	P1-O2	2.28	1.68	1.59
28	1	804	LMT	O2B-C2B	-2.28	1.37	1.43
21	A	1104	CLA	C3D-C4D	-2.28	1.39	1.44
26	A	5007	3PH	O31-C31	2.28	1.40	1.33
33	G	5002	ERG	C4-C5	2.28	1.56	1.51
30	3	802	PTY	O7-C8	2.28	1.40	1.34
21	A	1139	CLA	C3D-C4D	-2.28	1.39	1.44
30	5	802	PTY	O7-C8	2.28	1.40	1.34
21	B	1214	CLA	C3D-C4D	-2.27	1.39	1.44
21	7	617	CLA	C3D-C4D	-2.27	1.39	1.44
46	8	807	4RF	O21-C22	2.27	1.40	1.34
21	A	1101	CLA	C3D-C4D	-2.27	1.39	1.44
21	K	1403	CLA	C3D-C4D	-2.27	1.39	1.44
21	1	606	CLA	C3D-C4D	-2.27	1.39	1.44
21	5	603	CLA	C3D-C4D	-2.27	1.39	1.44
21	B	1204	CLA	C3D-C4D	-2.26	1.39	1.44
21	A	1116	CLA	C3D-C4D	-2.26	1.39	1.44
30	7	804	PTY	O4-C1	-2.26	1.40	1.45
21	A	1109	CLA	C3D-C4D	-2.26	1.39	1.44
36	M	4001	ECH	C1-C6	-2.26	1.50	1.53
21	A	1133	CLA	C3D-C4D	-2.26	1.39	1.44
21	a	605	CLA	C3D-C4D	-2.26	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	604	CLA	C3D-C4D	-2.26	1.39	1.44
21	4	616	CLA	C3D-C4D	-2.26	1.39	1.44
30	B	5005	PTY	O4-C30	2.26	1.39	1.33
21	B	1023	CLA	C3D-C4D	-2.26	1.39	1.44
28	A	5008	LMT	O2'-C2'	-2.26	1.37	1.43
21	3	613	CLA	C3D-C4D	-2.26	1.39	1.44
46	8	808	4RF	O40-C41	2.26	1.39	1.33
21	A	1128	CLA	C3D-C4D	-2.26	1.39	1.44
21	A	1113	CLA	C3D-C4D	-2.26	1.39	1.44
21	B	1219	CLA	C3D-C4D	-2.26	1.39	1.44
21	4	611	CLA	C3D-C4D	-2.26	1.39	1.44
21	B	1232	CLA	C3D-C4D	-2.26	1.39	1.44
21	7	604	CLA	C3D-C4D	-2.26	1.39	1.44
26	A	5007	3PH	O31-C3	-2.25	1.40	1.45
21	7	612	CLA	C1B-NB	-2.25	1.34	1.37
21	B	1207	CLA	C3D-C4D	-2.25	1.39	1.44
46	8	807	4RF	O18-C19	-2.25	1.40	1.45
38	3	608	CHL	CHA-CBD	2.25	1.54	1.51
21	5	617	CLA	C3D-C4D	-2.25	1.39	1.44
21	A	1107	CLA	C1A-CHA	2.25	1.52	1.43
21	8	618	CLA	C3D-C4D	-2.24	1.39	1.44
48	8	806	P5S	O37-C2	-2.24	1.41	1.46
21	6	604	CLA	C3D-C4D	-2.24	1.39	1.44
21	8	609	CLA	C3D-C4D	-2.24	1.39	1.44
21	B	1203	CLA	C3D-C4D	-2.24	1.39	1.44
21	B	1021	CLA	C3D-C4D	-2.24	1.39	1.44
21	A	1129	CLA	C3D-C4D	-2.24	1.39	1.44
21	B	1210	CLA	C3D-C4D	-2.24	1.39	1.44
21	A	1121	CLA	C3D-C4D	-2.24	1.39	1.44
21	8	612	CLA	C3D-C4D	-2.24	1.39	1.44
21	B	1226	CLA	C3D-C4D	-2.24	1.39	1.44
21	7	615	CLA	C3D-C4D	-2.24	1.39	1.44
43	5	803	DGA	OG2-CG2	-2.23	1.41	1.46
21	B	1217	CLA	C3D-C4D	-2.23	1.39	1.44
23	B	4006	BCR	C12-C13	-2.23	1.41	1.46
21	7	607	CLA	C3D-C4D	-2.23	1.39	1.44
21	A	1109	CLA	C1A-CHA	2.23	1.52	1.43
21	A	1136	CLA	C3D-C4D	-2.22	1.39	1.44
21	3	602	CLA	C3D-C4D	-2.22	1.39	1.44
21	A	1130	CLA	C3D-C4D	-2.22	1.39	1.44
21	4	606	CLA	C3D-C4D	-2.22	1.39	1.44
46	8	807	4RF	O40-C39	-2.22	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	4005	BCR	C1-C6	-2.22	1.50	1.53
21	7	605	CLA	C3D-C4D	-2.22	1.39	1.44
21	B	1230	CLA	C3D-C4D	-2.22	1.39	1.44
31	K	5001	LAP	O1-C13	-2.22	1.40	1.45
23	5	504	BCR	C1-C6	-2.22	1.50	1.53
21	3	610	CLA	C3D-C4D	-2.22	1.39	1.44
21	7	612	CLA	MG-NB	-2.22	2.01	2.05
38	8	601	CHL	CHA-CBD	2.22	1.54	1.51
21	A	1107	CLA	C3D-C4D	-2.22	1.39	1.44
21	F	1301	CLA	C3D-C4D	-2.22	1.39	1.44
21	1	610	CLA	C3D-C4D	-2.22	1.39	1.44
38	7	613	CHL	C3D-C2D	-2.21	1.35	1.39
21	B	1228	CLA	C2-C3	-2.21	1.28	1.33
46	7	807	4RF	O40-C41	2.21	1.39	1.33
21	A	1103	CLA	C3D-C4D	-2.21	1.39	1.44
21	4	615	CLA	C3D-C4D	-2.21	1.39	1.44
38	6	610	CHL	CHA-CBD	2.21	1.54	1.51
21	a	611	CLA	C3D-C4D	-2.21	1.39	1.44
30	5	802	PTY	O4-C1	-2.21	1.40	1.45
30	8	810	PTY	O4-C30	2.21	1.39	1.33
23	B	4003	BCR	C1-C6	-2.20	1.51	1.53
21	6	618	CLA	C3D-C4D	-2.20	1.39	1.44
25	A	5005	DGD	O3G-C1D	2.20	1.43	1.40
21	7	603	CLA	C3D-C4D	-2.20	1.39	1.44
21	B	1215	CLA	C3D-C4D	-2.20	1.39	1.44
21	7	606	CLA	C3D-C4D	-2.20	1.39	1.44
21	4	604	CLA	C3D-C4D	-2.20	1.39	1.44
21	B	1209	CLA	C1A-CHA	2.20	1.52	1.43
21	A	1112	CLA	C3D-C4D	-2.20	1.39	1.44
21	7	602	CLA	C3D-C4D	-2.20	1.39	1.44
21	B	1201	CLA	C3D-C4D	-2.20	1.39	1.44
21	G	1601	CLA	C3D-C4D	-2.20	1.39	1.44
30	3	802	PTY	O4-C1	-2.19	1.40	1.45
21	4	612	CLA	C1A-CHA	2.19	1.52	1.43
31	F	5003	LAP	O4-C15	-2.19	1.36	1.44
21	1	608	CLA	C3D-C4D	-2.19	1.39	1.44
21	B	1221	CLA	C3D-C4D	-2.19	1.39	1.44
21	3	616	CLA	C3D-C4D	-2.19	1.39	1.44
23	3	503	BCR	C1-C6	-2.19	1.51	1.53
21	A	1122	CLA	C3D-C4D	-2.19	1.39	1.44
21	1	601	CLA	C3D-C4D	-2.19	1.39	1.44
30	8	810	PTY	O7-C6	-2.19	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	604	CLA	C3D-C4D	-2.19	1.39	1.44
21	1	602	CLA	C3D-C4D	-2.19	1.39	1.44
21	K	1402	CLA	C4B-NB	-2.18	1.35	1.37
21	B	1223	CLA	C3D-C4D	-2.18	1.39	1.44
21	7	611	CLA	C3D-C4D	-2.18	1.39	1.44
38	8	613	CHL	CHA-CBD	2.18	1.54	1.51
21	L	1501	CLA	C1A-CHA	2.18	1.52	1.43
21	1	615	CLA	C3D-C4D	-2.18	1.39	1.44
28	1	804	LMT	O4'-C4B	-2.18	1.37	1.43
21	A	1013	CLA	C3D-C4D	-2.18	1.39	1.44
21	F	1302	CLA	C3D-C4D	-2.18	1.39	1.44
23	5	504	BCR	C12-C13	-2.18	1.41	1.46
21	8	606	CLA	C3D-C4D	-2.18	1.39	1.44
38	a	610	CHL	CHA-CBD	2.18	1.54	1.51
21	B	1208	CLA	C3D-C4D	-2.18	1.39	1.44
21	1	605	CLA	C3D-C4D	-2.18	1.39	1.44
21	4	602	CLA	C3D-C4D	-2.17	1.39	1.44
21	8	603	CLA	C3D-C4D	-2.17	1.39	1.44
21	1	611	CLA	C3D-C4D	-2.17	1.39	1.44
21	3	601	CLA	C3D-C4D	-2.17	1.39	1.44
47	7	504	C7Z	C40-C33	2.17	1.55	1.50
21	A	1105	CLA	C3D-C4D	-2.17	1.39	1.44
38	7	613	CHL	CHA-CBD	2.16	1.54	1.51
29	6	803	PCW	P-O4P	2.16	1.67	1.59
21	A	1115	CLA	C3D-C4D	-2.16	1.39	1.44
21	8	615	CLA	C3D-C4D	-2.16	1.39	1.44
21	B	1218	CLA	C3D-C4D	-2.16	1.39	1.44
21	A	1102	CLA	C3D-C4D	-2.16	1.39	1.44
21	A	1137	CLA	C3D-C4D	-2.16	1.39	1.44
21	K	1402	CLA	C1C-C2C	2.16	1.48	1.44
21	8	610	CLA	C3D-C4D	-2.16	1.39	1.44
21	4	603	CLA	C3D-C4D	-2.16	1.39	1.44
21	A	1125	CLA	C3D-C4D	-2.15	1.39	1.44
28	1	804	LMT	O1'-C1'	-2.15	1.36	1.40
21	A	1110	CLA	C3D-C4D	-2.15	1.39	1.44
37	6	502	LUT	C22-C21	-2.15	1.52	1.54
21	a	615	CLA	C3D-C4D	-2.15	1.39	1.44
26	A	5007	3PH	O21-C21	2.14	1.40	1.34
37	1	502	LUT	C1-C6	-2.14	1.51	1.53
21	4	610	CLA	C3D-C4D	-2.14	1.39	1.44
21	A	1141	CLA	C3D-C4D	-2.14	1.39	1.44
21	B	1212	CLA	C3D-C4D	-2.14	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	G	1602	CLA	C3D-C4D	-2.14	1.39	1.44
21	8	603	CLA	C1A-CHA	2.14	1.51	1.43
38	a	609	CHL	CHA-CBD	2.13	1.54	1.51
21	L	1502	CLA	C3D-C4D	-2.13	1.39	1.44
21	6	606	CLA	C3D-C4D	-2.13	1.39	1.44
21	7	610	CLA	C3D-C4D	-2.13	1.39	1.44
21	A	1140	CLA	C1C-C2C	2.13	1.48	1.44
21	L	1503	CLA	C3D-C4D	-2.13	1.39	1.44
30	B	5005	PTY	O4-C1	-2.13	1.40	1.45
38	5	611	CHL	CHA-CBD	2.13	1.54	1.51
47	7	504	C7Z	C20-C13	2.13	1.55	1.50
21	6	602	CLA	C3D-C4D	-2.12	1.39	1.44
21	6	615	CLA	C1A-CHA	2.12	1.51	1.43
21	A	1141	CLA	C1A-CHA	2.12	1.51	1.43
21	4	616	CLA	C1A-CHA	2.12	1.51	1.43
23	B	4001	BCR	C12-C13	-2.12	1.41	1.46
21	6	615	CLA	C3D-C4D	-2.12	1.39	1.44
21	6	609	CLA	C3D-C4D	-2.12	1.39	1.44
21	K	1404	CLA	C3D-C4D	-2.12	1.39	1.44
21	6	601	CLA	C3D-C4D	-2.12	1.39	1.44
21	5	618	CLA	C1C-C2C	2.12	1.48	1.44
21	A	1134	CLA	C3D-C4D	-2.11	1.39	1.44
21	4	608	CLA	C3D-C4D	-2.11	1.39	1.44
21	3	618	CLA	C3D-C4D	-2.11	1.39	1.44
38	1	613	CHL	CHA-CBD	2.11	1.54	1.51
21	5	612	CLA	C3D-C4D	-2.11	1.39	1.44
30	B	5005	PTY	O7-C8	2.11	1.40	1.34
30	7	804	PTY	O7-C8	2.11	1.40	1.34
21	a	602	CLA	C3D-C4D	-2.11	1.39	1.44
21	1	603	CLA	C3D-C4D	-2.11	1.39	1.44
23	L	4001	BCR	C1-C6	-2.11	1.51	1.53
21	4	607	CLA	C3D-C4D	-2.11	1.39	1.44
38	8	604	CHL	CHA-CBD	2.11	1.54	1.51
21	3	618	CLA	C1A-CHA	2.11	1.51	1.43
21	5	602	CLA	C3D-C4D	-2.10	1.39	1.44
21	K	1401	CLA	C3D-C4D	-2.10	1.39	1.44
21	A	1123	CLA	C3D-C4D	-2.10	1.39	1.44
38	4	609	CHL	CHA-CBD	2.10	1.54	1.51
21	a	603	CLA	C3D-C4D	-2.10	1.39	1.44
21	5	607	CLA	C3D-C4D	-2.10	1.39	1.44
21	B	1212	CLA	C1A-CHA	2.10	1.51	1.43
23	6	504	BCR	C12-C13	-2.10	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	8	620	CLA	C3D-C4D	-2.10	1.39	1.44
21	B	1232	CLA	C1A-CHA	2.10	1.51	1.43
21	B	1240	CLA	C3D-C4D	-2.10	1.39	1.44
38	a	613	CHL	C1A-CHA	-2.10	1.37	1.40
23	7	503	BCR	C12-C13	-2.09	1.41	1.46
37	7	501	LUT	C22-C21	-2.09	1.52	1.54
28	A	5008	LMT	O3B-C3B	-2.09	1.37	1.43
21	3	607	CLA	C3D-C4D	-2.08	1.39	1.44
38	3	611	CHL	CHA-CBD	2.08	1.54	1.51
21	a	604	CLA	C1C-C2C	2.08	1.48	1.44
21	a	608	CLA	C3D-C4D	-2.08	1.39	1.44
21	K	1402	CLA	C1A-CHA	2.08	1.51	1.43
21	4	610	CLA	C1A-CHA	2.08	1.51	1.43
21	A	1122	CLA	C1A-CHA	2.08	1.51	1.43
21	8	620	CLA	C1A-CHA	2.08	1.51	1.43
21	a	607	CLA	C3D-C4D	-2.08	1.39	1.44
38	6	613	CHL	CHA-CBD	2.08	1.54	1.51
21	5	601	CLA	C3D-C4D	-2.08	1.39	1.44
21	1	612	CLA	C3D-C4D	-2.08	1.39	1.44
38	a	613	CHL	CHA-CBD	2.08	1.54	1.51
21	5	616	CLA	C3D-C4D	-2.08	1.39	1.44
21	B	1213	CLA	C1C-C2C	2.08	1.48	1.44
21	G	1603	CLA	C3D-C4D	-2.08	1.39	1.44
23	3	503	BCR	C12-C13	-2.08	1.41	1.46
21	5	609	CLA	C3D-C4D	-2.07	1.39	1.44
38	4	618	CHL	CHA-CBD	2.07	1.54	1.51
21	8	608	CLA	C3D-C4D	-2.07	1.39	1.44
21	5	614	CLA	C1A-CHA	2.07	1.51	1.43
21	6	607	CLA	C1A-CHA	2.07	1.51	1.43
23	J	4001	BCR	C12-C13	-2.07	1.41	1.46
28	B	5006	LMT	O1'-C1'	-2.06	1.36	1.40
41	a	805	GG0	C03-N05	2.06	1.38	1.33
21	3	603	CLA	C3D-C4D	-2.06	1.39	1.44
21	A	1140	CLA	C1A-CHA	2.06	1.51	1.43
21	A	1115	CLA	C1A-CHA	2.06	1.51	1.43
21	K	1401	CLA	C1A-CHA	2.06	1.51	1.43
38	a	606	CHL	CHA-CBD	2.06	1.54	1.51
21	6	612	CLA	C3D-C4D	-2.06	1.39	1.44
21	A	1120	CLA	C3D-C4D	-2.05	1.39	1.44
21	B	1206	CLA	C1A-CHA	2.05	1.51	1.43
21	4	617	CLA	C3D-C4D	-2.05	1.39	1.44
41	a	805	GG0	C06-C07	2.05	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	1	609	CHL	CHA-CBD	2.05	1.54	1.51
21	A	1120	CLA	C1C-C2C	2.05	1.48	1.44
38	6	611	CHL	CHA-CBD	2.05	1.54	1.51
23	7	503	BCR	C1-C6	-2.05	1.51	1.53
31	B	5007	LAP	O1-C13	-2.05	1.40	1.45
21	6	617	CLA	C3D-C4D	-2.05	1.39	1.44
28	B	5006	LMT	O3B-C3B	-2.05	1.37	1.43
28	A	5008	LMT	O4'-C4B	-2.05	1.37	1.43
21	B	1221	CLA	C1A-CHA	2.05	1.51	1.43
21	A	1138	CLA	C1A-CHA	2.04	1.51	1.43
21	A	1125	CLA	CHC-C1C	2.04	1.42	1.38
37	a	501	LUT	C1-C6	-2.04	1.51	1.53
38	5	610	CHL	CHA-CBD	2.04	1.54	1.51
23	6	504	BCR	C5-C6	-2.04	1.31	1.34
21	B	1201	CLA	C1A-CHA	2.04	1.51	1.43
23	A	4003	BCR	C12-C13	-2.04	1.41	1.46
21	a	602	CLA	C1C-C2C	2.04	1.48	1.44
23	A	4005	BCR	C12-C13	-2.04	1.41	1.46
21	B	1209	CLA	C3D-C4D	-2.04	1.39	1.44
21	A	1112	CLA	C1A-CHA	2.04	1.51	1.43
21	3	603	CLA	C1A-CHA	2.04	1.51	1.43
23	K	4002	BCR	C12-C13	-2.04	1.41	1.46
21	5	614	CLA	C3D-C4D	-2.04	1.39	1.44
21	K	1403	CLA	C1A-CHA	2.04	1.51	1.43
21	B	1224	CLA	C1A-CHA	2.03	1.51	1.43
21	K	1404	CLA	C1A-CHA	2.03	1.51	1.43
21	3	602	CLA	C1A-CHA	2.03	1.51	1.43
30	8	810	PTY	O4-C1	-2.03	1.40	1.45
23	B	4004	BCR	C1-C6	-2.03	1.51	1.53
23	B	4001	BCR	C1-C6	-2.03	1.51	1.53
21	5	608	CLA	C1C-C2C	2.03	1.48	1.44
38	6	619	CHL	CHA-CBD	2.03	1.54	1.51
23	4	503	BCR	C12-C13	-2.03	1.41	1.46
21	B	1235	CLA	C1A-CHA	2.03	1.51	1.43
21	5	603	CLA	C1A-CHA	2.03	1.51	1.43
21	a	607	CLA	C1A-CHA	2.03	1.51	1.43
21	A	1121	CLA	C1A-CHA	2.03	1.51	1.43
21	A	1123	CLA	C1A-CHA	2.03	1.51	1.43
21	5	616	CLA	C1A-CHA	2.02	1.51	1.43
21	L	1503	CLA	C1A-CHA	2.02	1.51	1.43
21	B	1223	CLA	C1A-CHA	2.02	1.51	1.43
21	7	612	CLA	CMB-C2B	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	8	502	LUT	C1-C6	-2.02	1.51	1.53
21	B	1236	CLA	O2D-CED	-2.02	1.40	1.45
21	A	1110	CLA	C1A-CHA	2.02	1.51	1.43
23	A	4002	BCR	C12-C13	-2.02	1.41	1.46
21	5	618	CLA	C3D-C4D	-2.02	1.39	1.44
21	B	1218	CLA	C1A-CHA	2.02	1.51	1.43
21	5	608	CLA	C1A-CHA	2.02	1.51	1.43
23	5	503	BCR	C12-C13	-2.02	1.41	1.46
21	J	1901	CLA	C3D-C4D	-2.02	1.39	1.44
21	4	612	CLA	C3D-C4D	-2.02	1.39	1.44
21	a	603	CLA	C1A-CHA	2.02	1.51	1.43
21	4	617	CLA	C1A-CHA	2.01	1.51	1.43
21	6	606	CLA	C1A-CHA	2.01	1.51	1.43
21	4	607	CLA	C1A-CHA	2.01	1.51	1.43
21	5	602	CLA	C1A-CHA	2.01	1.51	1.43
21	4	606	CLA	C1A-CHA	2.01	1.51	1.43
21	A	1139	CLA	C1A-CHA	2.01	1.51	1.43
21	8	606	CLA	C1A-CHA	2.01	1.51	1.43
21	5	609	CLA	C1C-C2C	2.01	1.48	1.44
38	1	609	CHL	C1B-C2B	2.01	1.41	1.39
21	G	1602	CLA	C1C-C2C	2.01	1.48	1.44
21	B	1237	CLA	C1A-CHA	2.01	1.51	1.43
21	3	616	CLA	C1A-CHA	2.01	1.51	1.43
21	A	1132	CLA	C1A-CHA	2.01	1.51	1.43
21	6	608	CLA	C1A-CHA	2.01	1.51	1.43
21	7	606	CLA	C1A-CHA	2.01	1.51	1.43
21	a	615	CLA	C1A-CHA	2.01	1.51	1.43
21	a	602	CLA	C1A-CHA	2.01	1.51	1.43
21	K	1404	CLA	C1C-C2C	2.01	1.48	1.44
40	3	506	QTB	C13-C12	-2.01	1.47	1.53
21	6	618	CLA	C1A-CHA	2.01	1.51	1.43
21	G	1601	CLA	C1A-CHA	2.01	1.51	1.43
21	1	612	CLA	C1A-CHA	2.01	1.51	1.43
21	6	617	CLA	C1A-CHA	2.01	1.51	1.43
21	4	602	CLA	C1A-CHA	2.01	1.51	1.43
21	6	607	CLA	C1C-C2C	2.00	1.48	1.44
40	a	504	QTB	C14-C12	-2.00	1.48	1.53
21	1	615	CLA	C1A-CHA	2.00	1.51	1.43
21	6	607	CLA	C3D-C4D	-2.00	1.39	1.44
38	5	613	CHL	CHA-CBD	2.00	1.54	1.51
21	L	1502	CLA	C1C-C2C	2.00	1.48	1.44

All (4845) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	J	4001	BCR	C10-C11-C12	19.43	179.50	123.20
23	A	4004	BCR	C10-C11-C12	19.20	178.83	123.20
23	A	4002	BCR	C10-C11-C12	19.09	178.51	123.20
23	4	503	BCR	C10-C11-C12	19.07	178.47	123.20
23	F	4001	BCR	C10-C11-C12	19.04	178.36	123.20
23	K	4001	BCR	C10-C11-C12	18.84	177.79	123.20
23	B	4004	BCR	C10-C11-C12	18.81	177.71	123.20
23	7	503	BCR	C10-C11-C12	18.53	176.90	123.20
23	B	4001	BCR	C10-C11-C12	18.49	176.77	123.20
23	8	503	BCR	C10-C11-C12	18.21	175.97	123.20
23	L	4002	BCR	C10-C11-C12	18.19	175.91	123.20
23	I	4001	BCR	C10-C11-C12	18.14	175.75	123.20
23	5	503	BCR	C10-C11-C12	18.04	175.48	123.20
23	B	4002	BCR	C10-C11-C12	18.03	175.44	123.20
23	3	504	BCR	C10-C11-C12	18.01	175.37	123.20
23	B	4007	BCR	C10-C11-C12	17.89	175.03	123.20
23	K	4002	BCR	C10-C11-C12	17.86	174.96	123.20
23	L	4003	BCR	C10-C11-C12	17.79	174.76	123.20
23	6	503	BCR	C10-C11-C12	17.77	174.69	123.20
23	B	4006	BCR	C10-C11-C12	17.76	174.66	123.20
23	A	4003	BCR	C10-C11-C12	17.66	174.36	123.20
23	B	4003	BCR	C10-C11-C12	17.42	173.69	123.20
23	L	4001	BCR	C10-C11-C12	17.31	173.35	123.20
23	A	4005	BCR	C10-C11-C12	17.22	173.10	123.20
23	5	504	BCR	C10-C11-C12	17.19	173.02	123.20
23	G	4001	BCR	C10-C11-C12	17.09	172.73	123.20
23	3	503	BCR	C10-C11-C12	17.02	172.50	123.20
23	6	503	BCR	C16-C15-C14	17.01	158.32	123.52
23	B	4005	BCR	C10-C11-C12	16.96	172.35	123.20
23	3	505	BCR	C10-C11-C12	16.74	171.72	123.20
23	B	4003	BCR	C11-C10-C9	16.40	150.28	127.28
21	B	1228	CLA	C4A-NA-C1A	15.45	113.73	106.68
23	5	504	BCR	C16-C15-C14	14.92	154.04	123.52
23	3	504	BCR	C21-C20-C19	14.50	165.20	123.20
23	6	504	BCR	C10-C11-C12	14.41	164.96	123.20
23	G	4001	BCR	C21-C20-C19	14.21	164.37	123.20
23	K	4001	BCR	C21-C20-C19	14.19	164.30	123.20
23	K	4002	BCR	C16-C15-C14	14.15	152.47	123.52
23	A	4001	BCR	C10-C11-C12	14.09	164.01	123.20
23	A	4005	BCR	C11-C10-C9	14.00	146.91	127.28
23	B	4001	BCR	C21-C20-C19	13.99	163.75	123.20
23	L	4003	BCR	C11-C10-C9	13.97	146.88	127.28
23	A	4001	BCR	C21-C20-C19	13.94	163.59	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	4003	BCR	C21-C20-C19	13.94	163.58	123.20
23	B	4006	BCR	C11-C10-C9	13.93	146.82	127.28
23	B	4004	BCR	C11-C10-C9	13.88	146.74	127.28
20	A	1011	CL0	C1B-CHB-C4A	13.80	130.20	121.32
23	J	4001	BCR	C16-C15-C14	13.74	151.63	123.52
23	A	4003	BCR	C11-C10-C9	13.72	146.53	127.28
23	L	4001	BCR	C11-C10-C9	13.61	146.36	127.28
23	7	503	BCR	C16-C15-C14	13.57	151.28	123.52
23	B	4002	BCR	C11-C10-C9	13.56	146.30	127.28
23	K	4001	BCR	C11-C10-C9	13.51	146.22	127.28
23	B	4005	BCR	C21-C20-C19	13.48	162.26	123.20
23	5	503	BCR	C16-C15-C14	13.44	151.01	123.52
23	B	4006	BCR	C16-C15-C14	13.35	150.84	123.52
23	6	504	BCR	C16-C15-C14	13.28	150.69	123.52
23	A	4004	BCR	C21-C20-C19	13.23	161.52	123.20
23	G	4001	BCR	C11-C10-C9	13.21	145.81	127.28
23	L	4002	BCR	C11-C12-C13	13.20	162.55	126.36
23	3	504	BCR	C11-C10-C9	13.19	145.77	127.28
23	A	4004	BCR	C11-C10-C9	13.18	145.76	127.28
23	3	505	BCR	C21-C20-C19	13.13	161.25	123.20
23	A	4004	BCR	C11-C12-C13	13.06	162.18	126.36
23	8	503	BCR	C11-C10-C9	13.06	145.59	127.28
23	B	4003	BCR	C11-C12-C13	13.02	162.07	126.36
23	8	503	BCR	C21-C20-C19	13.00	160.88	123.20
23	4	503	BCR	C16-C15-C14	12.99	150.09	123.52
23	L	4002	BCR	C21-C20-C19	12.96	160.76	123.20
23	A	4002	BCR	C11-C10-C9	12.95	145.44	127.28
23	L	4002	BCR	C11-C10-C9	12.92	145.40	127.28
23	A	4003	BCR	C16-C15-C14	12.87	149.85	123.52
23	A	4004	BCR	C16-C15-C14	12.81	149.74	123.52
23	5	504	BCR	C21-C20-C19	12.80	160.30	123.20
23	5	503	BCR	C11-C10-C9	12.80	145.23	127.28
23	7	503	BCR	C11-C10-C9	12.78	145.20	127.28
23	K	4002	BCR	C21-C20-C19	12.64	159.82	123.20
23	B	4004	BCR	C21-C20-C19	12.60	159.72	123.20
23	B	4002	BCR	C16-C15-C14	12.58	149.27	123.52
23	I	4001	BCR	C11-C12-C13	12.58	160.87	126.36
23	4	503	BCR	C11-C12-C13	12.57	160.84	126.36
23	B	4005	BCR	C16-C15-C14	12.53	149.17	123.52
23	6	504	BCR	C21-C20-C19	12.47	159.34	123.20
23	3	505	BCR	C16-C15-C14	12.44	148.97	123.52
23	A	4001	BCR	C11-C10-C9	12.43	144.71	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	L	4003	BCR	C21-C20-C19	12.42	159.18	123.20
23	B	4006	BCR	C21-C20-C19	12.40	159.14	123.20
23	A	4005	BCR	C11-C12-C13	12.40	160.37	126.36
33	G	5002	ERG	C15-C14-C8	-12.39	103.60	120.42
23	L	4003	BCR	C16-C15-C14	12.38	148.86	123.52
23	B	4001	BCR	C11-C10-C9	12.29	144.52	127.28
23	L	4002	BCR	C16-C15-C14	12.22	148.53	123.52
23	J	4001	BCR	C21-C20-C19	12.19	158.52	123.20
23	3	504	BCR	C16-C15-C14	12.18	148.43	123.52
23	B	4005	BCR	C11-C12-C13	12.13	159.63	126.36
23	B	4001	BCR	C11-C12-C13	12.12	159.59	126.36
23	L	4001	BCR	C16-C15-C14	12.09	148.26	123.52
23	B	4004	BCR	C11-C12-C13	12.03	159.36	126.36
23	B	4005	BCR	C11-C10-C9	12.02	144.13	127.28
23	A	4001	BCR	C11-C12-C13	11.95	159.13	126.36
23	L	4003	BCR	C11-C12-C13	11.91	159.01	126.36
23	B	4002	BCR	C11-C12-C13	11.89	158.95	126.36
23	4	503	BCR	C21-C20-C19	11.86	157.56	123.20
23	F	4001	BCR	C21-C20-C19	11.84	157.50	123.20
23	G	4001	BCR	C11-C12-C13	11.84	158.82	126.36
23	3	503	BCR	C21-C20-C19	11.83	157.49	123.20
23	8	503	BCR	C16-C15-C14	11.75	147.55	123.52
23	3	503	BCR	C11-C12-C13	11.74	158.56	126.36
23	B	4002	BCR	C21-C20-C19	11.70	157.09	123.20
23	L	4001	BCR	C21-C20-C19	11.69	157.06	123.20
23	A	4002	BCR	C21-C20-C19	11.67	157.02	123.20
23	A	4002	BCR	C16-C15-C14	11.66	147.37	123.52
23	B	4007	BCR	C21-C20-C19	11.63	156.90	123.20
23	7	503	BCR	C21-C20-C19	11.58	156.76	123.20
23	K	4001	BCR	C16-C15-C14	11.57	147.19	123.52
23	I	4001	BCR	C11-C10-C9	11.55	143.48	127.28
23	B	4007	BCR	C11-C10-C9	11.55	143.47	127.28
23	A	4002	BCR	C11-C12-C13	11.52	157.94	126.36
23	4	503	BCR	C11-C10-C9	11.46	143.35	127.28
23	A	4005	BCR	C21-C20-C19	11.43	156.32	123.20
23	B	4003	BCR	C16-C15-C14	11.35	146.74	123.52
23	B	4007	BCR	C16-C15-C14	11.31	146.66	123.52
23	5	503	BCR	C21-C20-C19	11.30	155.94	123.20
23	3	505	BCR	C11-C10-C9	11.26	143.07	127.28
23	3	503	BCR	C16-C15-C14	11.26	146.55	123.52
23	J	4001	BCR	C11-C10-C9	11.10	142.84	127.28
23	6	503	BCR	C21-C20-C19	11.05	155.20	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	4005	BCR	C16-C15-C14	10.88	145.78	123.52
23	K	4001	BCR	C11-C12-C13	10.86	156.15	126.36
23	I	4001	BCR	C21-C20-C19	10.78	154.45	123.20
23	B	4007	BCR	C11-C12-C13	10.69	155.67	126.36
23	B	4003	BCR	C21-C20-C19	10.67	154.11	123.20
23	K	4002	BCR	C11-C12-C13	10.64	155.53	126.36
23	L	4001	BCR	C11-C12-C13	10.63	155.52	126.36
23	B	4004	BCR	C16-C15-C14	10.58	145.16	123.52
23	B	4006	BCR	C11-C12-C13	10.54	155.26	126.36
23	F	4001	BCR	C16-C15-C14	10.50	145.00	123.52
23	8	503	BCR	C11-C12-C13	10.43	154.97	126.36
23	3	504	BCR	C11-C12-C13	10.43	154.96	126.36
23	5	503	BCR	C11-C12-C13	10.27	154.51	126.36
23	I	4001	BCR	C16-C15-C14	10.25	144.50	123.52
23	3	503	BCR	C11-C10-C9	10.25	141.65	127.28
21	B	1205	CLA	C4A-NA-C1A	10.17	111.32	106.68
21	B	1210	CLA	C4A-NA-C1A	10.15	111.31	106.68
23	6	503	BCR	C11-C10-C9	10.14	141.50	127.28
23	J	4001	BCR	C11-C12-C13	10.14	154.16	126.36
21	A	1106	CLA	C4A-NA-C1A	9.92	111.20	106.68
23	G	4001	BCR	C16-C15-C14	9.90	143.78	123.52
23	A	4001	BCR	C16-C15-C14	9.88	143.73	123.52
21	L	1501	CLA	C4A-NA-C1A	9.87	111.18	106.68
23	6	504	BCR	C11-C12-C13	9.83	153.31	126.36
23	3	505	BCR	C11-C12-C13	9.77	153.16	126.36
21	4	612	CLA	C4A-NA-C1A	9.71	111.11	106.68
21	A	1103	CLA	C4A-NA-C1A	9.69	111.10	106.68
23	6	504	BCR	C33-C5-C6	-9.67	113.94	124.48
23	B	4001	BCR	C16-C15-C14	9.66	143.29	123.52
23	7	503	BCR	C11-C12-C13	9.63	152.78	126.36
21	F	1301	CLA	C4A-NA-C1A	9.62	111.07	106.68
21	A	1109	CLA	C4A-NA-C1A	9.60	111.06	106.68
21	8	611	CLA	C4A-NA-C1A	9.57	111.04	106.68
21	L	1502	CLA	C4A-NA-C1A	9.53	111.03	106.68
21	7	611	CLA	C4A-NA-C1A	9.52	111.02	106.68
21	a	604	CLA	C4A-NA-C1A	9.52	111.02	106.68
23	L	4001	BCR	C20-C19-C18	9.50	152.41	126.36
23	5	503	BCR	C20-C19-C18	9.48	152.36	126.36
23	5	504	BCR	C11-C12-C13	9.44	152.26	126.36
23	6	504	BCR	C11-C10-C9	9.44	140.52	127.28
23	A	4005	BCR	C20-C19-C18	9.43	152.23	126.36
23	B	4003	BCR	C20-C19-C18	9.41	152.16	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	1235	CLA	C4A-NA-C1A	9.40	110.97	106.68
21	A	1141	CLA	C4A-NA-C1A	9.39	110.96	106.68
21	6	618	CLA	C4A-NA-C1A	9.37	110.96	106.68
23	7	503	BCR	C20-C19-C18	9.34	151.98	126.36
23	I	4001	BCR	C20-C19-C18	9.34	151.96	126.36
21	8	606	CLA	C4A-NA-C1A	9.33	110.94	106.68
23	6	503	BCR	C11-C12-C13	9.32	151.92	126.36
21	A	1132	CLA	C4A-NA-C1A	9.31	110.93	106.68
21	A	1101	CLA	C4A-NA-C1A	9.26	110.91	106.68
21	B	1221	CLA	C4A-NA-C1A	9.25	110.90	106.68
21	B	1237	CLA	C4A-NA-C1A	9.25	110.90	106.68
21	1	612	CLA	C4A-NA-C1A	9.22	110.89	106.68
23	4	503	BCR	C20-C19-C18	9.20	151.60	126.36
21	A	1120	CLA	C4A-NA-C1A	9.20	110.88	106.68
21	B	1212	CLA	C4A-NA-C1A	9.19	110.87	106.68
21	a	607	CLA	C4A-NA-C1A	9.17	110.86	106.68
21	1	605	CLA	C4A-NA-C1A	9.16	110.86	106.68
21	6	603	CLA	C4A-NA-C1A	9.14	110.85	106.68
21	A	1102	CLA	C4A-NA-C1A	9.14	110.85	106.68
21	3	612	CLA	C4A-NA-C1A	9.14	110.85	106.68
21	6	601	CLA	C4A-NA-C1A	9.12	110.84	106.68
21	5	617	CLA	C4A-NA-C1A	9.12	110.84	106.68
21	B	1202	CLA	C4A-NA-C1A	9.11	110.83	106.68
21	a	615	CLA	C4A-NA-C1A	9.10	110.83	106.68
21	5	616	CLA	C4A-NA-C1A	9.09	110.83	106.68
21	A	1115	CLA	C4A-NA-C1A	9.09	110.83	106.68
21	3	602	CLA	C4A-NA-C1A	9.09	110.82	106.68
23	B	4002	BCR	C20-C19-C18	9.07	151.24	126.36
21	4	603	CLA	C4A-NA-C1A	9.07	110.82	106.68
21	A	1121	CLA	C4A-NA-C1A	9.07	110.82	106.68
21	7	608	CLA	C4A-NA-C1A	9.07	110.82	106.68
21	3	605	CLA	C4A-NA-C1A	9.06	110.81	106.68
23	A	4003	BCR	C11-C12-C13	9.05	151.18	126.36
21	5	603	CLA	C4A-NA-C1A	9.05	110.81	106.68
21	A	1107	CLA	C4A-NA-C1A	9.04	110.80	106.68
21	8	609	CLA	C4A-NA-C1A	9.03	110.80	106.68
21	4	616	CLA	C4A-NA-C1A	9.02	110.79	106.68
21	A	1113	CLA	C4A-NA-C1A	9.00	110.78	106.68
21	B	1224	CLA	C4A-NA-C1A	8.99	110.78	106.68
21	3	603	CLA	C4A-NA-C1A	8.97	110.77	106.68
21	3	604	CLA	C4A-NA-C1A	8.97	110.77	106.68
21	8	612	CLA	C4A-NA-C1A	8.97	110.77	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	1234	CLA	C4A-NA-C1A	8.97	110.77	106.68
21	B	1206	CLA	C4A-NA-C1A	8.96	110.77	106.68
21	8	620	CLA	C4A-NA-C1A	8.96	110.77	106.68
21	B	1222	CLA	C4A-NA-C1A	8.96	110.77	106.68
21	J	1901	CLA	C4A-NA-C1A	8.96	110.77	106.68
47	7	504	C7Z	C27-C28-C29	-8.96	112.98	126.23
21	8	607	CLA	C4A-NA-C1A	8.96	110.77	106.68
20	A	1011	CL0	O2D-CGD-CBD	8.91	120.74	110.95
21	A	1117	CLA	C4A-NA-C1A	8.91	110.75	106.68
21	B	1230	CLA	C4A-NA-C1A	8.91	110.75	106.68
21	4	602	CLA	C4A-NA-C1A	8.89	110.74	106.68
21	6	612	CLA	C4A-NA-C1A	8.89	110.73	106.68
21	8	610	CLA	C4A-NA-C1A	8.89	110.73	106.68
21	7	610	CLA	C4A-NA-C1A	8.88	110.73	106.68
21	8	603	CLA	C4A-NA-C1A	8.88	110.73	106.68
21	1	615	CLA	C4A-NA-C1A	8.86	110.72	106.68
21	3	601	CLA	C4A-NA-C1A	8.86	110.72	106.68
21	A	1108	CLA	C4A-NA-C1A	8.86	110.72	106.68
21	A	1126	CLA	C4A-NA-C1A	8.85	110.72	106.68
21	A	1013	CLA	C4A-NA-C1A	8.84	110.71	106.68
21	B	1236	CLA	C4A-NA-C1A	8.84	110.71	106.68
21	4	605	CLA	C4A-NA-C1A	8.84	110.71	106.68
21	7	612	CLA	C4A-NA-C1A	8.84	110.71	106.68
21	A	1118	CLA	C4A-NA-C1A	8.83	110.71	106.68
21	A	1112	CLA	C4A-NA-C1A	8.83	110.71	106.68
21	B	1209	CLA	C4A-NA-C1A	8.82	110.70	106.68
21	3	607	CLA	C4A-NA-C1A	8.82	110.70	106.68
21	B	1211	CLA	C4A-NA-C1A	8.82	110.70	106.68
21	B	1021	CLA	C4A-NA-C1A	8.81	110.70	106.68
21	B	1201	CLA	C4A-NA-C1A	8.81	110.70	106.68
21	1	611	CLA	C4A-NA-C1A	8.81	110.70	106.68
21	4	610	CLA	C4A-NA-C1A	8.80	110.69	106.68
21	6	605	CLA	C4A-NA-C1A	8.80	110.69	106.68
21	6	608	CLA	C4A-NA-C1A	8.79	110.69	106.68
21	A	1111	CLA	C4A-NA-C1A	8.78	110.69	106.68
21	7	607	CLA	C4A-NA-C1A	8.78	110.69	106.68
21	a	608	CLA	C4A-NA-C1A	8.77	110.68	106.68
21	A	1110	CLA	C4A-NA-C1A	8.77	110.68	106.68
23	F	4001	BCR	C20-C19-C18	8.77	150.41	126.36
21	6	607	CLA	C4A-NA-C1A	8.76	110.68	106.68
21	6	617	CLA	C4A-NA-C1A	8.76	110.67	106.68
21	3	606	CLA	C4A-NA-C1A	8.75	110.67	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	J	4001	BCR	C20-C19-C18	8.74	150.33	126.36
21	8	605	CLA	C4A-NA-C1A	8.74	110.67	106.68
21	5	614	CLA	C4A-NA-C1A	8.73	110.66	106.68
21	1	602	CLA	C4A-NA-C1A	8.73	110.66	106.68
21	7	609	CLA	C4A-NA-C1A	8.73	110.66	106.68
21	a	602	CLA	C4A-NA-C1A	8.72	110.66	106.68
21	7	617	CLA	C4A-NA-C1A	8.72	110.66	106.68
21	4	606	CLA	C4A-NA-C1A	8.72	110.66	106.68
21	A	1140	CLA	C4A-NA-C1A	8.71	110.66	106.68
21	5	604	CLA	C4A-NA-C1A	8.71	110.66	106.68
21	5	612	CLA	C4A-NA-C1A	8.70	110.65	106.68
21	1	603	CLA	C4A-NA-C1A	8.70	110.65	106.68
21	B	1226	CLA	C4A-NA-C1A	8.69	110.64	106.68
21	K	1404	CLA	C4A-NA-C1A	8.69	110.64	106.68
21	3	613	CLA	C4A-NA-C1A	8.68	110.64	106.68
21	A	1129	CLA	C4A-NA-C1A	8.68	110.64	106.68
21	5	601	CLA	C4A-NA-C1A	8.66	110.63	106.68
21	A	1104	CLA	C4A-NA-C1A	8.65	110.63	106.68
21	A	1138	CLA	C4A-NA-C1A	8.65	110.62	106.68
21	1	608	CLA	C4A-NA-C1A	8.64	110.62	106.68
21	B	1207	CLA	C4A-NA-C1A	8.64	110.62	106.68
21	G	1601	CLA	C4A-NA-C1A	8.64	110.62	106.68
21	A	1133	CLA	C4A-NA-C1A	8.63	110.61	106.68
21	3	616	CLA	C4A-NA-C1A	8.62	110.61	106.68
21	3	618	CLA	C4A-NA-C1A	8.62	110.61	106.68
21	A	1122	CLA	C4A-NA-C1A	8.61	110.61	106.68
21	B	1223	CLA	C4A-NA-C1A	8.61	110.61	106.68
23	A	4002	BCR	C20-C19-C18	8.60	149.94	126.36
21	B	1239	CLA	C4A-NA-C1A	8.59	110.60	106.68
47	7	504	C7Z	C15-C14-C13	-8.59	115.23	127.28
21	4	608	CLA	C4A-NA-C1A	8.59	110.60	106.68
21	A	1134	CLA	C4A-NA-C1A	8.58	110.59	106.68
21	B	1219	CLA	C4A-NA-C1A	8.58	110.59	106.68
21	B	1217	CLA	C4A-NA-C1A	8.58	110.59	106.68
21	7	605	CLA	C4A-NA-C1A	8.57	110.59	106.68
21	A	1123	CLA	C4A-NA-C1A	8.57	110.59	106.68
21	8	618	CLA	C4A-NA-C1A	8.57	110.59	106.68
23	K	4002	BCR	C11-C10-C9	8.57	139.29	127.28
21	1	610	CLA	C4A-NA-C1A	8.56	110.58	106.68
21	6	606	CLA	C4A-NA-C1A	8.56	110.58	106.68
21	B	1218	CLA	C4A-NA-C1A	8.55	110.58	106.68
21	B	1220	CLA	C4A-NA-C1A	8.55	110.58	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	L	1503	CLA	C4A-NA-C1A	8.55	110.58	106.68
21	a	603	CLA	C4A-NA-C1A	8.55	110.58	106.68
21	4	611	CLA	C4A-NA-C1A	8.55	110.58	106.68
21	B	1023	CLA	C4A-NA-C1A	8.54	110.58	106.68
21	4	601	CLA	C4A-NA-C1A	8.54	110.58	106.68
23	L	4003	BCR	C20-C19-C18	8.54	149.77	126.36
21	5	609	CLA	C4A-NA-C1A	8.54	110.57	106.68
21	4	604	CLA	C4A-NA-C1A	8.53	110.57	106.68
21	A	1116	CLA	C4A-NA-C1A	8.53	110.57	106.68
21	6	615	CLA	C4A-NA-C1A	8.52	110.56	106.68
21	7	601	CLA	C4A-NA-C1A	8.52	110.56	106.68
21	A	1136	CLA	C4A-NA-C1A	8.51	110.56	106.68
21	A	1139	CLA	C4A-NA-C1A	8.51	110.56	106.68
21	B	1232	CLA	C4A-NA-C1A	8.49	110.55	106.68
23	5	504	BCR	C11-C10-C9	8.49	139.19	127.28
21	A	1131	CLA	C4A-NA-C1A	8.49	110.55	106.68
21	5	602	CLA	C4A-NA-C1A	8.48	110.55	106.68
21	5	608	CLA	C4A-NA-C1A	8.48	110.55	106.68
21	B	1229	CLA	C4A-NA-C1A	8.47	110.55	106.68
21	4	607	CLA	C4A-NA-C1A	8.47	110.54	106.68
21	4	617	CLA	C4A-NA-C1A	8.46	110.54	106.68
23	F	4001	BCR	C11-C10-C9	8.44	139.11	127.28
21	A	1130	CLA	C4A-NA-C1A	8.44	110.53	106.68
21	B	1208	CLA	C4A-NA-C1A	8.44	110.53	106.68
21	8	615	CLA	C4A-NA-C1A	8.44	110.53	106.68
21	A	1124	CLA	C4A-NA-C1A	8.43	110.53	106.68
21	6	602	CLA	C4A-NA-C1A	8.43	110.53	106.68
21	1	607	CLA	C4A-NA-C1A	8.42	110.52	106.68
21	a	605	CLA	C4A-NA-C1A	8.42	110.52	106.68
21	a	612	CLA	C4A-NA-C1A	8.42	110.52	106.68
21	A	1128	CLA	C4A-NA-C1A	8.40	110.51	106.68
21	K	1402	CLA	C4A-NA-C1A	8.38	110.50	106.68
21	a	611	CLA	C4A-NA-C1A	8.36	110.49	106.68
21	B	1240	CLA	C4A-NA-C1A	8.36	110.49	106.68
21	B	1204	CLA	C4A-NA-C1A	8.36	110.49	106.68
21	1	601	CLA	C4A-NA-C1A	8.35	110.49	106.68
21	A	1105	CLA	C4A-NA-C1A	8.35	110.49	106.68
21	B	1213	CLA	C4A-NA-C1A	8.35	110.49	106.68
37	5	505	LUT	C21-C26-C27	8.34	122.42	112.83
21	5	606	CLA	C4A-NA-C1A	8.34	110.48	106.68
21	K	1401	CLA	C4A-NA-C1A	8.31	110.47	106.68
23	6	504	BCR	C20-C19-C18	8.31	149.14	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1114	CLA	C4A-NA-C1A	8.30	110.47	106.68
21	7	606	CLA	C4A-NA-C1A	8.29	110.46	106.68
21	B	1203	CLA	C4A-NA-C1A	8.29	110.46	106.68
21	B	1231	CLA	C4A-NA-C1A	8.29	110.46	106.68
21	1	606	CLA	C4A-NA-C1A	8.28	110.46	106.68
21	1	604	CLA	C4A-NA-C1A	8.28	110.46	106.68
23	B	4006	BCR	C20-C19-C18	8.27	149.04	126.36
21	B	1215	CLA	C4A-NA-C1A	8.27	110.45	106.68
21	5	605	CLA	C4A-NA-C1A	8.25	110.44	106.68
21	8	602	CLA	C4A-NA-C1A	8.25	110.44	106.68
38	8	601	CHL	C1B-CHB-C4A	8.24	126.62	121.32
21	3	610	CLA	C4A-NA-C1A	8.23	110.43	106.68
21	7	603	CLA	C4A-NA-C1A	8.23	110.43	106.68
21	A	1137	CLA	C4A-NA-C1A	8.22	110.43	106.68
21	A	1012	CLA	C4A-NA-C1A	8.22	110.43	106.68
21	G	1603	CLA	C4A-NA-C1A	8.21	110.42	106.68
21	G	1602	CLA	C4A-NA-C1A	8.20	110.42	106.68
21	7	602	CLA	C4A-NA-C1A	8.19	110.42	106.68
21	B	1216	CLA	C4A-NA-C1A	8.18	110.41	106.68
21	F	1302	CLA	C4A-NA-C1A	8.15	110.40	106.68
21	5	607	CLA	C4A-NA-C1A	8.13	110.39	106.68
21	A	1135	CLA	C4A-NA-C1A	8.12	110.38	106.68
21	4	615	CLA	C4A-NA-C1A	8.11	110.38	106.68
23	B	4007	BCR	C20-C19-C18	8.09	148.54	126.36
21	A	1125	CLA	C4A-NA-C1A	8.09	110.37	106.68
21	a	601	CLA	C4A-NA-C1A	8.09	110.37	106.68
23	3	503	BCR	C20-C19-C18	8.08	148.53	126.36
23	K	4002	BCR	C20-C19-C18	8.04	148.41	126.36
21	B	1238	CLA	C4A-NA-C1A	8.03	110.34	106.68
23	L	4002	BCR	C20-C19-C18	8.03	148.39	126.36
21	B	1214	CLA	C4A-NA-C1A	8.01	110.33	106.68
21	K	1403	CLA	C4A-NA-C1A	8.01	110.33	106.68
37	6	502	LUT	C21-C26-C27	8.00	122.02	112.83
21	6	604	CLA	C4A-NA-C1A	7.99	110.33	106.68
23	3	505	BCR	C20-C19-C18	7.97	148.23	126.36
21	5	618	CLA	C4A-NA-C1A	7.97	110.31	106.68
21	A	1127	CLA	C4A-NA-C1A	7.96	110.31	106.68
21	7	604	CLA	C4A-NA-C1A	7.93	110.30	106.68
38	1	613	CHL	C1B-CHB-C4A	7.93	126.42	121.32
21	B	1225	CLA	C4A-NA-C1A	7.87	110.27	106.68
21	B	1227	CLA	C4A-NA-C1A	7.87	110.27	106.68
33	G	5002	ERG	C19-C10-C9	-7.82	98.00	110.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	609	CLA	C4A-NA-C1A	7.79	110.23	106.68
21	7	615	CLA	C4A-NA-C1A	7.78	110.23	106.68
23	8	503	BCR	C20-C19-C18	7.77	147.66	126.36
21	A	1119	CLA	C4A-NA-C1A	7.71	110.20	106.68
23	B	4004	BCR	C20-C19-C18	7.71	147.51	126.36
21	8	608	CLA	O2D-CGD-CBD	7.64	124.58	111.23
38	8	613	CHL	C1B-CHB-C4A	7.58	126.20	121.32
38	6	611	CHL	C1B-CHB-C4A	7.53	126.17	121.32
21	B	1022	CLA	C4A-NA-C1A	7.51	110.10	106.68
37	5	505	LUT	C15-C14-C13	-7.44	116.85	127.28
38	3	608	CHL	C1B-CHB-C4A	7.39	126.08	121.32
23	B	4005	BCR	C20-C19-C18	7.35	146.51	126.36
23	F	4001	BCR	C11-C12-C13	7.30	146.38	126.36
23	A	4003	BCR	C20-C19-C18	7.21	146.14	126.36
37	1	503	LUT	C21-C26-C27	7.21	121.11	112.83
21	B	1228	CLA	C1-C2-C3	-7.16	114.47	126.20
38	5	613	CHL	C1B-CHB-C4A	7.14	125.92	121.32
34	J	4002	RRX	C38-C26-C25	-7.13	116.71	124.48
21	6	604	CLA	O2D-CGD-CBD	7.06	123.58	111.23
23	G	4001	BCR	C20-C19-C18	7.05	145.70	126.36
33	G	5002	ERG	C14-C13-C17	6.97	107.00	99.72
37	6	501	LUT	C21-C26-C27	6.97	120.83	112.83
23	A	4004	BCR	C20-C19-C18	6.96	145.46	126.36
23	6	503	BCR	C15-C14-C13	-6.85	117.67	127.28
23	K	4001	BCR	C20-C19-C18	6.81	145.03	126.36
21	8	608	CLA	C4A-NA-C1A	6.81	109.78	106.68
38	1	609	CHL	C1B-CHB-C4A	6.74	125.66	121.32
21	4	612	CLA	O2D-CGD-CBD	6.74	123.01	111.23
21	B	1221	CLA	O2D-CGD-CBD	6.68	122.90	111.23
23	A	4001	BCR	C20-C19-C18	6.67	144.65	126.36
21	B	1218	CLA	O2D-CGD-CBD	6.67	122.88	111.23
21	A	1102	CLA	CAC-C3C-C4C	6.66	133.46	124.79
21	B	1205	CLA	O2D-CGD-CBD	6.65	122.86	111.23
23	6	503	BCR	C20-C19-C18	6.65	144.60	126.36
21	A	1125	CLA	CMC-C2C-C1C	6.64	135.41	125.03
21	A	1108	CLA	O2D-CGD-CBD	6.63	122.82	111.23
37	7	501	LUT	C21-C26-C27	6.63	120.45	112.83
23	5	504	BCR	C20-C19-C18	6.57	144.37	126.36
21	A	1138	CLA	O2D-CGD-CBD	6.54	122.66	111.23
33	G	5002	ERG	C12-C13-C14	6.48	116.98	107.19
38	4	609	CHL	C1B-CHB-C4A	6.48	125.49	121.32
21	a	607	CLA	O2D-CGD-CBD	6.46	122.52	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	1228	CLA	C1-O2A-CGA	6.42	132.19	116.65
23	6	504	BCR	C33-C5-C4	6.42	127.28	113.60
21	6	609	CLA	O2D-CGD-CBD	6.40	122.42	111.23
38	5	610	CHL	C1B-CHB-C4A	6.37	125.42	121.32
37	6	502	LUT	C31-C30-C29	-6.36	118.35	127.28
40	3	506	QTB	C04-C03-C02	6.36	136.20	127.28
21	8	608	CLA	O1D-CGD-CBD	-6.35	111.99	124.52
21	B	1210	CLA	O2D-CGD-CBD	6.33	122.30	111.23
21	A	1121	CLA	O2D-CGD-CBD	6.32	122.27	111.23
37	5	505	LUT	C11-C10-C9	-6.28	118.47	127.28
21	A	1112	CLA	O2D-CGD-CBD	6.28	122.21	111.23
21	B	1201	CLA	O2D-CGD-CBD	6.27	122.19	111.23
21	5	608	CLA	O2D-CGD-CBD	6.24	122.14	111.23
21	A	1132	CLA	O2D-CGD-CBD	6.23	122.12	111.23
21	4	607	CLA	O2D-CGD-CBD	6.21	122.09	111.23
21	B	1231	CLA	CMD-C2D-C1D	6.19	135.62	124.73
47	7	504	C7Z	C18-C5-C6	-6.17	117.75	124.48
23	3	504	BCR	C20-C19-C18	6.16	143.25	126.36
21	B	1228	CLA	C3A-C2A-C1A	6.13	110.52	101.34
21	B	1236	CLA	O2D-CGD-CBD	6.12	121.93	111.23
21	A	1121	CLA	CMD-C2D-C1D	6.12	135.50	124.73
21	A	1120	CLA	O2D-CGD-CBD	6.11	121.92	111.23
21	7	604	CLA	O2D-CGD-CBD	6.09	121.88	111.23
21	A	1134	CLA	O2D-CGD-CBD	6.08	121.87	111.23
21	B	1230	CLA	O2D-CGD-CBD	6.06	121.83	111.23
21	A	1137	CLA	O2D-CGD-CBD	6.05	121.81	111.23
38	a	610	CHL	C1B-CHB-C4A	6.05	125.22	121.32
21	A	1118	CLA	O2D-CGD-CBD	6.03	121.78	111.23
21	A	1101	CLA	O2D-CGD-CBD	6.02	121.75	111.23
37	3	501	LUT	C21-C26-C27	6.01	119.73	112.83
21	A	1129	CLA	O2D-CGD-CBD	6.00	121.73	111.23
21	B	1227	CLA	O2D-CGD-CBD	6.00	121.72	111.23
21	1	606	CLA	CMD-C2D-C1D	6.00	135.29	124.73
21	A	1128	CLA	O2D-CGD-CBD	5.99	121.71	111.23
23	B	4001	BCR	C20-C19-C18	5.98	142.75	126.36
21	B	1220	CLA	O2D-CGD-CBD	5.98	121.68	111.23
36	M	4001	ECH	C20-C21-C22	-5.98	118.90	127.28
21	A	1114	CLA	CMD-C2D-C1D	5.97	135.25	124.73
21	7	608	CLA	O2D-CGD-CBD	5.97	121.66	111.23
21	4	605	CLA	O2D-CGD-CBD	5.96	121.66	111.23
21	4	608	CLA	O2D-CGD-CBD	5.95	121.62	111.23
21	7	609	CLA	O2D-CGD-CBD	5.94	121.62	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	8	609	CLA	O2D-CGD-CBD	5.94	121.62	111.23
38	7	613	CHL	C1B-CHB-C4A	5.94	125.14	121.32
21	B	1208	CLA	O2D-CGD-CBD	5.94	121.61	111.23
21	4	611	CLA	CMD-C2D-C1D	5.93	135.16	124.73
21	A	1115	CLA	O2D-CGD-CBD	5.93	121.59	111.23
21	A	1131	CLA	CMD-C2D-C1D	5.92	135.15	124.73
21	A	1116	CLA	O2D-CGD-CBD	5.91	121.56	111.23
37	5	502	LUT	C21-C26-C27	5.90	119.61	112.83
21	4	617	CLA	CMD-C2D-C1D	5.89	135.11	124.73
21	A	1139	CLA	O2D-CGD-CBD	5.89	121.53	111.23
21	K	1403	CLA	CMD-C2D-C1D	5.88	135.08	124.73
21	1	605	CLA	O2D-CGD-CBD	5.86	121.47	111.23
21	8	618	CLA	O2D-CGD-CBD	5.86	121.47	111.23
21	A	1133	CLA	O2D-CGD-CBD	5.85	121.47	111.23
21	1	604	CLA	O2D-CGD-CBD	5.85	121.45	111.23
21	8	611	CLA	CMD-C2D-C1D	5.85	135.03	124.73
21	7	606	CLA	CMD-C2D-C1D	5.85	135.02	124.73
21	L	1502	CLA	O2D-CGD-CBD	5.84	121.45	111.23
21	3	604	CLA	O2D-CGD-CBD	5.84	121.44	111.23
21	B	1223	CLA	O2D-CGD-CBD	5.84	121.43	111.23
21	5	604	CLA	CMD-C2D-C1D	5.82	134.98	124.73
21	A	1101	CLA	CMD-C2D-C1D	5.82	134.98	124.73
21	7	609	CLA	CMD-C2D-C1D	5.81	134.97	124.73
21	a	611	CLA	CMD-C2D-C1D	5.81	134.97	124.73
21	B	1229	CLA	O2D-CGD-CBD	5.81	121.39	111.23
21	F	1302	CLA	O2D-CGD-CBD	5.81	121.39	111.23
21	B	1202	CLA	O2D-CGD-CBD	5.81	121.39	111.23
21	A	1103	CLA	O2D-CGD-CBD	5.81	121.38	111.23
40	a	504	QTB	C09-C02-C03	5.80	128.14	119.01
21	A	1125	CLA	O2D-CGD-CBD	5.80	121.37	111.23
38	3	611	CHL	C1B-CHB-C4A	5.79	125.05	121.32
21	5	603	CLA	CMD-C2D-C1D	5.79	134.92	124.73
21	6	608	CLA	CMD-C2D-C1D	5.78	134.91	124.73
21	B	1219	CLA	O2D-CGD-CBD	5.78	121.34	111.23
34	J	4002	RRX	C11-C10-C9	-5.77	119.18	127.28
21	A	1120	CLA	O2A-C1-C2	5.77	122.73	108.99
21	B	1209	CLA	CMD-C2D-C1D	5.76	134.87	124.73
21	A	1123	CLA	CMD-C2D-C1D	5.76	134.87	124.73
21	3	602	CLA	O2D-CGD-CBD	5.74	121.27	111.23
21	5	617	CLA	CMD-C2D-C1D	5.74	134.84	124.73
21	B	1212	CLA	O2D-CGD-CBD	5.74	121.26	111.23
21	L	1501	CLA	O2D-CGD-CBD	5.73	121.25	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	1228	CLA	C4-C3-C5	5.73	125.17	115.23
21	B	1213	CLA	CMD-C2D-C1D	5.72	134.80	124.73
21	B	1240	CLA	O2D-CGD-CBD	5.71	121.20	111.23
21	7	607	CLA	O2A-C1-C2	5.70	122.56	108.99
40	a	504	QTB	C04-C03-C02	5.70	135.27	127.28
21	5	609	CLA	O2D-CGD-CBD	5.70	121.20	111.23
21	5	601	CLA	CMD-C2D-C1D	5.70	134.76	124.73
23	4	503	BCR	C15-C14-C13	-5.70	119.29	127.28
21	A	1102	CLA	O2D-CGD-CBD	5.70	121.19	111.23
21	B	1208	CLA	CMD-C2D-C1D	5.69	134.76	124.73
21	8	602	CLA	CMD-C2D-C1D	5.69	134.75	124.73
21	A	1104	CLA	CMD-C2D-C1D	5.68	134.73	124.73
21	B	1231	CLA	O2D-CGD-CBD	5.68	121.16	111.23
21	B	1211	CLA	O2D-CGD-CBD	5.68	121.16	111.23
21	4	608	CLA	CMD-C2D-C1D	5.68	134.73	124.73
38	6	613	CHL	C1B-CHB-C4A	5.67	124.97	121.32
21	7	617	CLA	O2D-CGD-CBD	5.67	121.14	111.23
21	3	602	CLA	CMD-C2D-C1D	5.66	134.70	124.73
21	B	1217	CLA	O2D-CGD-CBD	5.66	121.12	111.23
21	B	1227	CLA	CMD-C2D-C1D	5.66	134.69	124.73
21	8	606	CLA	O2D-CGD-CBD	5.65	121.11	111.23
21	5	614	CLA	CMD-C2D-C1D	5.64	134.66	124.73
21	A	1130	CLA	O2D-CGD-CBD	5.64	121.09	111.23
21	4	610	CLA	CMD-C2D-C1D	5.64	134.66	124.73
21	A	1135	CLA	O2D-CGD-CBD	5.63	121.08	111.23
21	B	1213	CLA	O2D-CGD-CBD	5.63	121.07	111.23
38	4	613	CHL	C1B-CHB-C4A	5.62	124.94	121.32
21	3	604	CLA	CMD-C2D-C1D	5.62	134.63	124.73
21	5	617	CLA	O2D-CGD-CBD	5.62	121.06	111.23
21	6	602	CLA	O2D-CGD-CBD	5.62	121.06	111.23
21	3	606	CLA	CMD-C2D-C1D	5.62	134.62	124.73
40	a	504	QTB	C01-C02-C09	-5.62	109.51	118.09
21	B	1203	CLA	CMD-C2D-C1D	5.62	134.62	124.73
21	7	602	CLA	CMD-C2D-C1D	5.62	134.62	124.73
21	B	1216	CLA	O2D-CGD-CBD	5.61	121.04	111.23
21	A	1124	CLA	O2D-CGD-CBD	5.61	121.04	111.23
21	5	606	CLA	O2D-CGD-CBD	5.61	121.04	111.23
21	B	1234	CLA	O2D-CGD-CBD	5.61	121.03	111.23
21	B	1239	CLA	O2D-CGD-CBD	5.60	121.02	111.23
21	7	603	CLA	O2D-CGD-CBD	5.60	121.02	111.23
21	B	1230	CLA	CMD-C2D-C1D	5.60	134.59	124.73
21	4	603	CLA	CMD-C2D-C1D	5.60	134.59	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	608	CLA	O2D-CGD-CBD	5.60	121.02	111.23
21	K	1402	CLA	CMD-C2D-C1D	5.60	134.58	124.73
21	8	615	CLA	CMD-C2D-C1D	5.59	134.57	124.73
21	L	1501	CLA	CMD-C2D-C1D	5.59	134.57	124.73
21	B	1211	CLA	CMD-C2D-C1D	5.59	134.57	124.73
21	a	604	CLA	CMD-C2D-C1D	5.59	134.57	124.73
37	1	503	LUT	C35-C34-C33	-5.59	119.44	127.28
21	a	605	CLA	CMD-C2D-C1D	5.58	134.55	124.73
21	8	605	CLA	CMD-C2D-C1D	5.58	134.55	124.73
21	A	1140	CLA	O2D-CGD-CBD	5.58	120.98	111.23
21	1	610	CLA	O2D-CGD-CBD	5.58	120.98	111.23
21	8	603	CLA	C1-C2-C3	-5.57	117.07	126.20
21	F	1301	CLA	CMD-C2D-C1D	5.57	134.54	124.73
21	A	1106	CLA	O2D-CGD-CBD	5.56	120.95	111.23
21	B	1214	CLA	CMD-C2D-C1D	5.56	134.52	124.73
21	B	1212	CLA	CMD-C2D-C1D	5.55	134.51	124.73
21	A	1126	CLA	CMD-C2D-C1D	5.55	134.51	124.73
21	3	605	CLA	CMD-C2D-C1D	5.55	134.50	124.73
21	a	601	CLA	CMD-C2D-C1D	5.55	134.50	124.73
21	6	605	CLA	CMD-C2D-C1D	5.55	134.50	124.73
21	A	1113	CLA	CMD-C2D-C1D	5.54	134.49	124.73
21	A	1110	CLA	O2D-CGD-CBD	5.54	120.92	111.23
21	4	606	CLA	O2D-CGD-CBD	5.54	120.92	111.23
21	A	1125	CLA	CMD-C2D-C1D	5.54	134.48	124.73
21	A	1108	CLA	CMD-C2D-C1D	5.53	134.47	124.73
21	F	1302	CLA	CMD-C2D-C1D	5.53	134.46	124.73
21	7	603	CLA	CMD-C2D-C1D	5.53	134.46	124.73
34	J	4002	RRX	C33-C5-C6	-5.52	118.46	124.48
21	A	1132	CLA	CMD-C2D-C1D	5.52	134.46	124.73
21	3	610	CLA	O2D-CGD-CBD	5.52	120.89	111.23
21	7	601	CLA	CMD-C2D-C1D	5.52	134.45	124.73
21	L	1503	CLA	CMD-C2D-C1D	5.52	134.45	124.73
21	L	1503	CLA	O2D-CGD-CBD	5.51	120.87	111.23
21	B	1224	CLA	O2D-CGD-CBD	5.51	120.87	111.23
21	A	1111	CLA	CMD-C2D-C1D	5.51	134.43	124.73
21	4	616	CLA	CMD-C2D-C1D	5.51	134.43	124.73
21	7	608	CLA	CMD-C2D-C1D	5.51	134.43	124.73
21	A	1113	CLA	O2D-CGD-CBD	5.51	120.86	111.23
21	7	604	CLA	CMD-C2D-C1D	5.50	134.42	124.73
21	B	1214	CLA	O2D-CGD-CBD	5.50	120.85	111.23
21	4	602	CLA	CMD-C2D-C1D	5.50	134.41	124.73
21	K	1404	CLA	CMD-C2D-C1D	5.49	134.40	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	5	611	CHL	C1B-CHB-C4A	5.49	124.86	121.32
21	A	1116	CLA	CMD-C2D-C1D	5.49	134.40	124.73
21	6	617	CLA	CMD-C2D-C1D	5.49	134.40	124.73
21	6	604	CLA	CMD-C2D-C1D	5.49	134.40	124.73
21	8	608	CLA	CMD-C2D-C1D	5.48	134.39	124.73
21	8	609	CLA	CMD-C2D-C1D	5.48	134.39	124.73
21	4	615	CLA	CMD-C2D-C1D	5.48	134.38	124.73
21	4	606	CLA	CMD-C2D-C1D	5.48	134.38	124.73
21	1	605	CLA	CMD-C2D-C1D	5.48	134.38	124.73
21	8	603	CLA	CMD-C2D-C1D	5.48	134.38	124.73
21	B	1204	CLA	O2D-CGD-CBD	5.48	120.81	111.23
21	6	615	CLA	CMD-C2D-C1D	5.48	134.37	124.73
21	7	617	CLA	CMD-C2D-C1D	5.48	134.37	124.73
21	3	607	CLA	O2D-CGD-CBD	5.47	120.80	111.23
21	A	1129	CLA	CMD-C2D-C1D	5.47	134.35	124.73
21	B	1223	CLA	CMD-C2D-C1D	5.46	134.35	124.73
21	B	1207	CLA	O2D-CGD-CBD	5.46	120.77	111.23
21	A	1137	CLA	CMD-C2D-C1D	5.46	134.34	124.73
21	B	1239	CLA	CMD-C2D-C1D	5.45	134.33	124.73
21	K	1402	CLA	O2D-CGD-CBD	5.45	120.76	111.23
21	4	601	CLA	O2D-CGD-CBD	5.45	120.76	111.23
21	1	602	CLA	CMD-C2D-C1D	5.45	134.32	124.73
21	7	610	CLA	CMD-C2D-C1D	5.45	134.32	124.73
21	A	1135	CLA	CMD-C2D-C1D	5.45	134.32	124.73
21	B	1201	CLA	CMD-C2D-C1D	5.44	134.32	124.73
21	A	1134	CLA	CMD-C2D-C1D	5.44	134.31	124.73
21	1	615	CLA	O2D-CGD-CBD	5.44	120.73	111.23
21	1	601	CLA	CMD-C2D-C1D	5.43	134.29	124.73
21	B	1226	CLA	O2D-CGD-CBD	5.43	120.72	111.23
21	8	607	CLA	O2D-CGD-CBD	5.43	120.72	111.23
21	8	602	CLA	O2D-CGD-CBD	5.43	120.72	111.23
21	1	611	CLA	CMD-C2D-C1D	5.43	134.29	124.73
21	6	608	CLA	O2D-CGD-CBD	5.43	120.72	111.23
21	B	1226	CLA	CMD-C2D-C1D	5.43	134.28	124.73
21	A	1126	CLA	C1-C2-C3	-5.42	117.31	126.20
21	5	606	CLA	CMD-C2D-C1D	5.42	134.27	124.73
21	a	604	CLA	O2D-CGD-CBD	5.42	120.70	111.23
21	5	609	CLA	CMD-C2D-C1D	5.42	134.27	124.73
21	6	601	CLA	C1-C2-C3	-5.42	117.32	126.20
21	5	605	CLA	CMD-C2D-C1D	5.42	134.27	124.73
21	3	603	CLA	O2D-CGD-CBD	5.42	120.70	111.23
21	3	610	CLA	CMD-C2D-C1D	5.41	134.26	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1111	CLA	O2D-CGD-CBD	5.41	120.69	111.23
21	B	1218	CLA	CMD-C2D-C1D	5.41	134.25	124.73
24	7	801	LHG	O7-C7-C8	5.41	123.18	111.48
21	A	1103	CLA	CMD-C2D-C1D	5.40	134.24	124.73
21	K	1404	CLA	O2D-CGD-CBD	5.40	120.67	111.23
21	B	1229	CLA	CMD-C2D-C1D	5.40	134.24	124.73
21	B	1220	CLA	CMD-C2D-C1D	5.40	134.23	124.73
21	B	1021	CLA	O2D-CGD-CBD	5.40	120.66	111.23
36	M	4001	ECH	C15-C14-C13	-5.40	119.71	127.28
21	A	1108	CLA	C1-C2-C3	-5.39	117.36	126.20
21	B	1237	CLA	O2D-CGD-CBD	5.39	120.65	111.23
21	A	1012	CLA	O2D-CGD-CBD	5.39	120.65	111.23
21	a	603	CLA	CMD-C2D-C1D	5.39	134.21	124.73
21	6	606	CLA	CMD-C2D-C1D	5.38	134.21	124.73
21	B	1238	CLA	CMD-C2D-C1D	5.38	134.21	124.73
21	B	1232	CLA	CMD-C2D-C1D	5.38	134.20	124.73
21	J	1901	CLA	CMD-C2D-C1D	5.38	134.20	124.73
21	4	615	CLA	O2D-CGD-CBD	5.38	120.63	111.23
21	5	605	CLA	O2D-CGD-CBD	5.38	120.63	111.23
21	a	605	CLA	O2D-CGD-CBD	5.38	120.63	111.23
21	B	1228	CLA	CMD-C2D-C1D	5.38	134.19	124.73
21	A	1109	CLA	CMD-C2D-C1D	5.38	134.19	124.73
21	6	601	CLA	CMD-C2D-C1D	5.37	134.19	124.73
21	B	1215	CLA	O2D-CGD-CBD	5.37	120.62	111.23
21	6	618	CLA	CMD-C2D-C1D	5.37	134.18	124.73
21	B	1217	CLA	CMD-C2D-C1D	5.36	134.17	124.73
21	7	611	CLA	CMD-C2D-C1D	5.36	134.17	124.73
21	4	605	CLA	CMD-C2D-C1D	5.36	134.16	124.73
21	A	1102	CLA	CMD-C2D-C1D	5.35	134.15	124.73
21	A	1104	CLA	O2D-CGD-CBD	5.35	120.58	111.23
21	A	1139	CLA	CMD-C2D-C1D	5.35	134.15	124.73
21	1	603	CLA	CMD-C2D-C1D	5.35	134.14	124.73
21	5	618	CLA	CMD-C2D-C1D	5.34	134.14	124.73
21	a	601	CLA	O2D-CGD-CBD	5.34	120.57	111.23
21	A	1105	CLA	CMD-C2D-C1D	5.33	134.12	124.73
21	B	1225	CLA	CMD-C2D-C1D	5.33	134.12	124.73
21	K	1403	CLA	O2D-CGD-CBD	5.32	120.54	111.23
21	B	1209	CLA	O2D-CGD-CBD	5.32	120.54	111.23
21	8	610	CLA	CMD-C2D-C1D	5.32	134.09	124.73
21	G	1603	CLA	O2D-CGD-CBD	5.31	120.52	111.23
21	G	1602	CLA	CMD-C2D-C1D	5.31	134.09	124.73
21	4	610	CLA	O2D-CGD-CBD	5.31	120.52	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	5	602	CLA	O2D-CGD-CBD	5.31	120.52	111.23
21	a	602	CLA	CMD-C2D-C1D	5.31	134.08	124.73
21	A	1109	CLA	O2D-CGD-CBD	5.31	120.51	111.23
21	A	1128	CLA	CMD-C2D-C1D	5.31	134.07	124.73
21	6	602	CLA	CMD-C2D-C1D	5.30	134.07	124.73
21	B	1215	CLA	CMD-C2D-C1D	5.30	134.06	124.73
21	5	616	CLA	CMD-C2D-C1D	5.30	134.06	124.73
21	B	1210	CLA	CMD-C2D-C1D	5.30	134.06	124.73
21	A	1114	CLA	O2D-CGD-CBD	5.30	120.49	111.23
21	5	602	CLA	CMD-C2D-C1D	5.30	134.06	124.73
21	A	1136	CLA	CMD-C2D-C1D	5.30	134.06	124.73
21	B	1237	CLA	CMD-C2D-C1D	5.30	134.06	124.73
21	a	603	CLA	O2D-CGD-CBD	5.30	120.49	111.23
37	a	501	LUT	C21-C26-C27	5.29	118.91	112.83
21	B	1222	CLA	CMD-C2D-C1D	5.29	134.05	124.73
21	G	1601	CLA	O2D-CGD-CBD	5.29	120.48	111.23
21	B	1207	CLA	CMD-C2D-C1D	5.29	134.05	124.73
21	B	1206	CLA	O2D-CGD-CBD	5.29	120.48	111.23
21	8	620	CLA	CMD-C2D-C1D	5.29	134.04	124.73
21	7	615	CLA	CMD-C2D-C1D	5.29	134.04	124.73
21	5	614	CLA	O2D-CGD-CBD	5.29	120.48	111.23
21	B	1234	CLA	CMD-C2D-C1D	5.28	134.03	124.73
21	G	1601	CLA	CMD-C2D-C1D	5.28	134.03	124.73
21	3	612	CLA	O2D-CGD-CBD	5.28	120.47	111.23
21	A	1138	CLA	CMD-C2D-C1D	5.27	134.02	124.73
37	3	502	LUT	C21-C26-C27	5.27	118.89	112.83
21	A	1119	CLA	CMD-C2D-C1D	5.27	134.01	124.73
47	7	504	C7Z	C11-C10-C9	-5.27	119.89	127.28
21	6	612	CLA	CMD-C2D-C1D	5.26	134.00	124.73
21	B	1206	CLA	CMD-C2D-C1D	5.26	134.00	124.73
21	A	1127	CLA	O2D-CGD-CBD	5.26	120.43	111.23
21	7	602	CLA	O2D-CGD-CBD	5.26	120.43	111.23
37	6	502	LUT	C35-C34-C33	-5.26	119.90	127.28
37	a	503	LUT	C35-C34-C33	-5.26	119.90	127.28
21	1	607	CLA	CMD-C2D-C1D	5.26	133.99	124.73
21	A	1122	CLA	O2D-CGD-CBD	5.26	120.42	111.23
21	7	607	CLA	O2D-CGD-CBD	5.25	120.41	111.23
23	6	504	BCR	C15-C14-C13	-5.25	119.91	127.28
40	3	506	QTB	C13-C12-C11	5.25	122.50	112.57
21	B	1216	CLA	CMD-C2D-C1D	5.25	133.97	124.73
21	1	612	CLA	CMD-C2D-C1D	5.25	133.97	124.73
21	B	1203	CLA	O2D-CGD-CBD	5.24	120.40	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	7	611	CLA	O2D-CGD-CBD	5.24	120.40	111.23
21	K	1401	CLA	O2D-CGD-CBD	5.23	120.38	111.23
21	A	1120	CLA	CMD-C2D-C1D	5.23	133.94	124.73
21	5	603	CLA	O2D-CGD-CBD	5.22	120.35	111.23
21	3	601	CLA	CMD-C2D-C1D	5.22	133.91	124.73
21	3	607	CLA	CMD-C2D-C1D	5.21	133.91	124.73
21	A	1105	CLA	O2D-CGD-CBD	5.21	120.34	111.23
21	8	615	CLA	O2D-CGD-CBD	5.21	120.33	111.23
21	A	1141	CLA	CMD-C2D-C1D	5.20	133.89	124.73
21	6	615	CLA	O2D-CGD-CBD	5.20	120.32	111.23
38	a	609	CHL	C1B-CHB-C4A	5.20	124.67	121.32
21	3	613	CLA	CMD-C2D-C1D	5.20	133.88	124.73
21	B	1224	CLA	CMD-C2D-C1D	5.19	133.87	124.73
21	4	604	CLA	CMD-C2D-C1D	5.19	133.87	124.73
37	1	502	LUT	C21-C26-C27	5.19	118.80	112.83
21	B	1225	CLA	O2D-CGD-CBD	5.19	120.31	111.23
21	A	1118	CLA	CMD-C2D-C1D	5.19	133.87	124.73
21	B	1235	CLA	CMD-C2D-C1D	5.19	133.87	124.73
21	B	1202	CLA	CMD-C2D-C1D	5.19	133.87	124.73
21	1	608	CLA	CMD-C2D-C1D	5.18	133.86	124.73
21	8	610	CLA	O2D-CGD-CBD	5.18	120.29	111.23
21	A	1138	CLA	C1-C2-C3	-5.18	117.71	126.20
21	7	615	CLA	O2D-CGD-CBD	5.18	120.28	111.23
21	5	608	CLA	CMD-C2D-C1D	5.18	133.84	124.73
21	6	612	CLA	O2D-CGD-CBD	5.17	120.27	111.23
21	A	1122	CLA	CMD-C2D-C1D	5.17	133.83	124.73
21	a	608	CLA	CMD-C2D-C1D	5.17	133.83	124.73
21	a	607	CLA	CMD-C2D-C1D	5.17	133.82	124.73
21	8	603	CLA	O2D-CGD-CBD	5.17	120.26	111.23
21	A	1130	CLA	CMD-C2D-C1D	5.16	133.82	124.73
21	A	1131	CLA	O2D-CGD-CBD	5.16	120.26	111.23
21	8	618	CLA	CMD-C2D-C1D	5.16	133.82	124.73
21	8	611	CLA	O2D-CGD-CBD	5.15	120.24	111.23
21	8	606	CLA	CMD-C2D-C1D	5.15	133.80	124.73
21	6	601	CLA	O2D-CGD-CBD	5.14	120.22	111.23
21	6	607	CLA	O2D-CGD-CBD	5.14	120.22	111.23
21	3	616	CLA	CMD-C2D-C1D	5.14	133.78	124.73
21	6	605	CLA	O2D-CGD-CBD	5.13	120.20	111.23
21	3	618	CLA	CMD-C2D-C1D	5.13	133.76	124.73
21	5	612	CLA	CMD-C2D-C1D	5.12	133.75	124.73
38	8	604	CHL	C1B-CHB-C4A	5.12	124.62	121.32
21	A	1133	CLA	CMD-C2D-C1D	5.12	133.74	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	M	4001	ECH	C11-C10-C9	-5.11	120.11	127.28
21	B	1023	CLA	CMD-C2D-C1D	5.11	133.73	124.73
40	3	506	QTB	C09-C02-C03	5.11	127.05	119.01
21	B	1238	CLA	O2D-CGD-CBD	5.11	120.16	111.23
21	5	607	CLA	CMD-C2D-C1D	5.11	133.72	124.73
21	A	1107	CLA	O2D-CGD-CBD	5.11	120.16	111.23
21	1	610	CLA	CMD-C2D-C1D	5.10	133.72	124.73
21	B	1221	CLA	CMD-C2D-C1D	5.10	133.71	124.73
21	6	617	CLA	O2D-CGD-CBD	5.10	120.14	111.23
21	B	1236	CLA	CMD-C2D-C1D	5.10	133.70	124.73
21	A	1013	CLA	CMD-C2D-C1D	5.09	133.70	124.73
21	B	1205	CLA	CMD-C2D-C1D	5.09	133.70	124.73
21	1	606	CLA	O2D-CGD-CBD	5.09	120.12	111.23
34	J	4002	RRX	C20-C21-C22	-5.08	120.15	127.28
21	3	605	CLA	O2D-CGD-CBD	5.08	120.11	111.23
21	B	1204	CLA	CMD-C2D-C1D	5.08	133.67	124.73
21	A	1112	CLA	CMD-C2D-C1D	5.08	133.67	124.73
37	6	501	LUT	C18-C5-C6	-5.07	118.95	124.48
33	G	5002	ERG	C1-C10-C9	5.06	118.23	108.39
21	B	1023	CLA	O2D-CGD-CBD	5.06	120.08	111.23
21	3	618	CLA	O2D-CGD-CBD	5.06	120.08	111.23
21	3	601	CLA	O2D-CGD-CBD	5.06	120.07	111.23
38	a	613	CHL	C1C-CHC-C4B	5.05	134.15	116.07
21	4	603	CLA	O2D-CGD-CBD	5.04	120.05	111.23
40	3	506	QTB	C01-C02-C09	-5.03	110.40	118.09
21	4	607	CLA	CMD-C2D-C1D	5.03	133.59	124.73
21	5	607	CLA	O2D-CGD-CBD	5.03	120.02	111.23
21	A	1106	CLA	CMD-C2D-C1D	5.03	133.59	124.73
21	A	1136	CLA	O2D-CGD-CBD	5.03	120.02	111.23
21	A	1126	CLA	O2D-CGD-CBD	5.03	120.02	111.23
21	B	1228	CLA	O2D-CGD-CBD	5.02	120.01	111.23
37	8	502	LUT	C21-C26-C27	5.02	118.59	112.83
21	A	1117	CLA	CMD-C2D-C1D	5.02	133.56	124.73
21	1	607	CLA	O2D-CGD-CBD	5.01	120.00	111.23
21	J	1901	CLA	O2D-CGD-CBD	5.01	119.99	111.23
21	4	602	CLA	O2D-CGD-CBD	5.01	119.99	111.23
21	a	615	CLA	CMD-C2D-C1D	5.01	133.55	124.73
21	1	611	CLA	O2D-CGD-CBD	5.00	119.98	111.23
21	A	1013	CLA	O2D-CGD-CBD	5.00	119.97	111.23
21	A	1140	CLA	CMD-C2D-C1D	5.00	133.53	124.73
21	A	1127	CLA	CMD-C2D-C1D	4.99	133.52	124.73
20	A	1011	CL0	O2A-CGA-O1A	-4.99	111.14	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	K	1401	CLA	CMD-C2D-C1D	4.99	133.51	124.73
21	A	1123	CLA	O2D-CGD-CBD	4.98	119.93	111.23
21	a	603	CLA	C1-C2-C3	-4.97	118.05	126.20
21	8	612	CLA	CMD-C2D-C1D	4.97	133.49	124.73
21	5	601	CLA	O2D-CGD-CBD	4.97	119.92	111.23
21	8	607	CLA	CMD-C2D-C1D	4.96	133.47	124.73
37	a	501	LUT	C15-C14-C13	-4.96	120.32	127.28
21	a	612	CLA	CMD-C2D-C1D	4.95	133.45	124.73
21	A	1141	CLA	O2D-CGD-CBD	4.95	119.89	111.23
21	4	601	CLA	CMD-C2D-C1D	4.95	133.44	124.73
21	F	1301	CLA	O2D-CGD-CBD	4.95	119.88	111.23
37	a	501	LUT	C18-C5-C6	-4.94	119.10	124.48
21	A	1119	CLA	O2D-CGD-CBD	4.93	119.85	111.23
21	6	606	CLA	O2D-CGD-CBD	4.93	119.85	111.23
21	B	1022	CLA	CMD-C2D-C1D	4.93	133.40	124.73
21	3	613	CLA	O2D-CGD-CBD	4.92	119.84	111.23
45	7	502	XAT	C38-C25-C24	4.92	119.77	114.24
21	4	612	CLA	CMD-C2D-C1D	4.92	133.40	124.73
21	7	601	CLA	O2D-CGD-CBD	4.92	119.83	111.23
38	a	606	CHL	C1C-CHC-C4B	4.92	133.66	116.07
21	4	604	CLA	O2D-CGD-CBD	4.91	119.82	111.23
21	1	601	CLA	O2D-CGD-CBD	4.91	119.82	111.23
38	4	618	CHL	C1B-CHB-C4A	4.91	124.48	121.32
40	a	504	QTB	C13-C12-C11	4.91	121.86	112.57
21	4	611	CLA	O2D-CGD-CBD	4.91	119.81	111.23
37	a	503	LUT	C21-C26-C27	4.90	118.46	112.83
21	6	618	CLA	O2D-CGD-CBD	4.89	119.79	111.23
33	G	5002	ERG	C19-C10-C1	-4.89	101.98	109.43
21	B	1021	CLA	C1-C2-C3	-4.89	118.18	126.20
37	1	503	LUT	C31-C30-C29	-4.89	120.42	127.28
23	F	4001	BCR	C12-C13-C14	4.89	126.70	119.01
38	6	619	CHL	C1C-CHC-C4B	4.89	133.56	116.07
21	A	1107	CLA	CMD-C2D-C1D	4.89	133.34	124.73
21	B	1219	CLA	CMD-C2D-C1D	4.89	133.33	124.73
21	A	1117	CLA	O2D-CGD-CBD	4.88	119.76	111.23
25	8	802	DGD	O2G-C1B-C2B	4.88	122.03	111.48
38	6	610	CHL	C1C-CHC-C4B	4.88	133.51	116.07
21	B	1240	CLA	CMD-C2D-C1D	4.87	133.31	124.73
21	1	604	CLA	CMD-C2D-C1D	4.87	133.30	124.73
23	5	504	BCR	C15-C14-C13	-4.87	120.45	127.28
21	8	612	CLA	O2D-CGD-CBD	4.87	119.74	111.23
21	a	615	CLA	O2D-CGD-CBD	4.86	119.73	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1115	CLA	CMD-C2D-C1D	4.86	133.29	124.73
38	8	604	CHL	C1C-CHC-C4B	4.86	133.46	116.07
46	8	808	4RF	O21-C22-C24	4.86	121.99	111.48
21	1	615	CLA	CMD-C2D-C1D	4.86	133.28	124.73
23	7	503	BCR	C15-C14-C13	-4.85	120.47	127.28
21	5	612	CLA	O2D-CGD-CBD	4.85	119.71	111.23
21	G	1602	CLA	O2D-CGD-CBD	4.85	119.71	111.23
37	5	505	LUT	C35-C34-C33	-4.85	120.48	127.28
38	4	618	CHL	C1C-CHC-C4B	4.85	133.41	116.07
21	A	1110	CLA	CMD-C2D-C1D	4.84	133.26	124.73
21	1	602	CLA	O2D-CGD-CBD	4.83	119.68	111.23
20	A	1011	CL0	CBC-CAC-C3C	-4.83	105.96	112.87
37	4	501	LUT	C21-C26-C27	4.83	118.37	112.83
21	B	1234	CLA	CAC-C3C-C4C	4.82	131.07	124.79
38	4	609	CHL	C1C-CHC-C4B	4.82	133.33	116.07
21	8	620	CLA	O2D-CGD-CBD	4.82	119.66	111.23
21	B	1022	CLA	O2D-CGD-CBD	4.81	119.64	111.23
21	5	604	CLA	O2D-CGD-CBD	4.80	119.62	111.23
37	6	501	LUT	C35-C34-C33	-4.80	120.55	127.28
38	a	610	CHL	C1C-CHC-C4B	4.79	133.22	116.07
38	a	609	CHL	C1C-CHC-C4B	4.79	133.21	116.07
21	B	1203	CLA	C1-C2-C3	-4.79	118.35	126.20
21	7	606	CLA	O2D-CGD-CBD	4.79	119.60	111.23
21	7	607	CLA	CMD-C2D-C1D	4.78	133.15	124.73
34	J	4002	RRX	C15-C14-C13	-4.78	120.57	127.28
21	B	1235	CLA	O2D-CGD-CBD	4.78	119.58	111.23
21	B	1222	CLA	O2D-CGD-CBD	4.78	119.58	111.23
38	a	606	CHL	C1B-CHB-C4A	4.77	124.39	121.32
21	A	1116	CLA	C1-C2-C3	-4.76	118.39	126.20
21	a	611	CLA	O2D-CGD-CBD	4.76	119.54	111.23
37	5	501	LUT	C35-C34-C33	-4.75	120.61	127.28
21	5	618	CLA	O2D-CGD-CBD	4.75	119.54	111.23
37	5	502	LUT	C7-C8-C9	-4.75	119.21	126.23
38	6	619	CHL	C1B-CHB-C4A	4.75	124.38	121.32
21	B	1204	CLA	C1-C2-C3	-4.75	118.42	126.20
21	A	1128	CLA	C1-C2-C3	-4.74	118.42	126.20
21	3	606	CLA	O2D-CGD-CBD	4.74	119.52	111.23
38	5	610	CHL	C1C-CHC-C4B	4.73	132.99	116.07
21	7	605	CLA	CMD-C2D-C1D	4.72	133.05	124.73
21	4	616	CLA	O2D-CGD-CBD	4.72	119.49	111.23
21	8	603	CLA	O2A-C1-C2	4.72	126.27	108.11
21	G	1603	CLA	CMD-C2D-C1D	4.72	133.03	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	a	502	LUT	C35-C34-C33	-4.71	120.67	127.28
21	4	617	CLA	O2D-CGD-CBD	4.70	119.45	111.23
21	3	605	CLA	C1-C2-C3	-4.70	118.50	126.20
38	7	613	CHL	C1C-CHC-C4B	4.69	132.85	116.07
24	a	801	LHG	O7-C7-C8	4.69	121.62	111.48
21	B	1220	CLA	O2A-C1-C2	4.68	126.10	108.11
21	8	608	CLA	C1-C2-C3	-4.66	118.55	126.20
38	6	613	CHL	C1C-CHC-C4B	4.66	132.75	116.07
21	7	612	CLA	CMD-C2D-C1D	4.65	132.91	124.73
21	1	603	CLA	O2D-CGD-CBD	4.65	119.35	111.23
38	4	613	CHL	C1C-CHC-C4B	4.64	132.66	116.07
21	7	605	CLA	CAC-C3C-C4C	4.63	130.82	124.79
21	a	608	CLA	O2D-CGD-CBD	4.63	119.32	111.23
21	A	1124	CLA	CMD-C2D-C1D	4.62	132.87	124.73
21	6	609	CLA	CMD-C2D-C1D	4.62	132.86	124.73
24	6	801	LHG	O7-C7-C8	4.61	121.46	111.48
37	6	501	LUT	C11-C10-C9	-4.61	120.81	127.28
21	A	1136	CLA	C1-C2-C3	-4.61	118.64	126.20
21	a	602	CLA	O2D-CGD-CBD	4.61	119.29	111.23
21	7	612	CLA	O2D-CGD-CBD	4.61	119.29	111.23
37	4	501	LUT	C26-C27-C28	-4.60	117.41	124.58
37	1	502	LUT	C26-C27-C28	-4.60	117.42	124.58
21	3	612	CLA	CMD-C2D-C1D	4.60	132.82	124.73
38	5	611	CHL	C1C-CHC-C4B	4.60	132.52	116.07
21	L	1502	CLA	CMD-C2D-C1D	4.59	132.82	124.73
21	6	607	CLA	CMD-C2D-C1D	4.59	132.81	124.73
34	J	4002	RRX	C16-C17-C18	-4.59	120.84	127.28
45	7	502	XAT	O4-C5-C18	-4.59	109.92	115.05
38	1	613	CHL	C1C-CHC-C4B	4.58	132.47	116.07
21	a	602	CLA	C1-C2-C3	-4.58	119.36	126.76
38	3	608	CHL	C1C-CHC-C4B	4.58	132.45	116.07
40	a	504	QTB	C17-C11-C10	4.57	120.53	113.07
21	B	1021	CLA	CMD-C2D-C1D	4.56	132.76	124.73
21	A	1118	CLA	C1-C2-C3	-4.56	118.73	126.20
21	B	1232	CLA	O2D-CGD-CBD	4.56	119.20	111.23
21	B	1023	CLA	O2A-C1-C2	4.56	125.64	108.11
24	A	5003	LHG	O7-C7-C8	4.55	121.32	111.48
21	3	601	CLA	C1-C2-C3	-4.54	118.76	126.20
38	8	613	CHL	C1C-CHC-C4B	4.54	132.31	116.07
21	3	616	CLA	O2D-CGD-CBD	4.53	119.15	111.23
38	3	611	CHL	C1C-CHC-C4B	4.53	132.28	116.07
24	4	801	LHG	O7-C7-C8	4.52	121.27	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	7	502	XAT	C31-C30-C29	-4.52	120.94	127.28
37	1	501	LUT	C35-C34-C33	-4.52	120.94	127.28
21	F	1302	CLA	CAC-C3C-C4C	4.51	130.66	124.79
45	7	502	XAT	C7-C8-C9	-4.50	118.54	125.53
37	a	501	LUT	C35-C34-C33	-4.50	120.97	127.28
21	1	612	CLA	O2D-CGD-CBD	4.50	119.09	111.23
23	F	4001	BCR	C33-C5-C6	-4.50	119.58	124.48
21	1	605	CLA	C1-C2-C3	-4.49	118.83	126.20
23	B	4007	BCR	C8-C9-C10	4.49	126.07	119.01
23	I	4001	BCR	C23-C24-C25	-4.49	115.00	127.00
21	6	603	CLA	O2D-CGD-CBD	4.49	119.08	111.23
40	3	506	QTB	C17-C11-C10	4.49	120.40	113.07
47	7	504	C7Z	C31-C30-C29	-4.49	120.98	127.28
37	1	501	LUT	C21-C26-C27	4.48	117.98	112.83
21	8	618	CLA	C1-C2-C3	-4.48	118.86	126.20
23	G	4001	BCR	C33-C5-C6	-4.47	119.60	124.48
37	1	503	LUT	C18-C5-C6	-4.47	119.61	124.48
21	1	606	CLA	C1-C2-C3	-4.47	118.87	126.20
21	3	603	CLA	CMD-C2D-C1D	4.47	132.60	124.73
23	B	4007	BCR	C33-C5-C6	-4.47	119.61	124.48
24	F	5001	LHG	O7-C7-C8	4.46	121.13	111.48
24	1	801	LHG	O7-C7-C8	4.45	121.12	111.48
21	6	602	CLA	C1-C2-C3	-4.44	118.92	126.20
23	J	4001	BCR	C15-C14-C13	-4.44	121.06	127.28
34	J	4002	RRX	C1-C6-C5	-4.43	116.58	122.64
38	1	609	CHL	C1C-CHC-C4B	4.42	131.90	116.07
38	1	609	CHL	C1-C2-C3	-4.42	118.96	126.20
24	7	803	LHG	O7-C7-C8	4.42	121.03	111.48
38	5	613	CHL	C1C-CHC-C4B	4.41	131.86	116.07
21	A	1012	CLA	CMD-C2D-C1D	4.41	132.49	124.73
21	A	1125	CLA	C1-C2-C3	-4.41	118.97	126.20
23	B	4007	BCR	C34-C9-C10	-4.41	115.67	122.82
21	A	1112	CLA	C1-C2-C3	-4.41	118.97	126.20
30	5	802	PTY	O7-C8-C11	4.41	121.01	111.48
21	3	606	CLA	C1-C2-C3	-4.40	118.98	126.20
45	7	502	XAT	C18-C5-C4	4.39	119.17	114.24
37	1	503	LUT	C7-C8-C9	-4.39	119.74	126.23
37	a	503	LUT	C31-C30-C29	-4.38	121.14	127.28
37	7	501	LUT	C7-C8-C9	-4.38	119.76	126.23
21	A	1109	CLA	C1-C2-C3	-4.38	119.03	126.20
37	a	501	LUT	C11-C10-C9	-4.36	121.16	127.28
38	6	611	CHL	C1C-CHC-C4B	4.36	131.66	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	8	810	PTY	O7-C8-C11	4.34	120.87	111.48
37	5	505	LUT	C8-C7-C6	-4.33	115.44	127.00
21	B	1206	CLA	C1-C2-C3	-4.32	119.11	126.20
37	1	503	LUT	C15-C14-C13	-4.32	121.22	127.28
37	a	503	LUT	C15-C14-C13	-4.30	121.25	127.28
38	8	601	CHL	C1C-CHC-C4B	4.30	131.45	116.07
25	B	5003	DGD	O2G-C1B-C2B	4.29	120.77	111.48
21	7	610	CLA	O2D-CGD-CBD	4.29	118.73	111.23
23	A	4004	BCR	C23-C24-C25	-4.29	115.54	127.00
21	A	1129	CLA	C1-C2-C3	-4.29	119.82	126.76
23	G	4001	BCR	C27-C26-C25	-4.29	116.91	122.70
40	a	504	QTB	C10-C09-C02	-4.29	117.11	126.32
37	5	502	LUT	C26-C27-C28	-4.28	117.91	124.58
33	G	5002	ERG	C13-C17-C20	-4.28	114.25	119.38
38	6	610	CHL	C1B-CHB-C4A	4.28	124.08	121.32
29	6	803	PCW	O2-C31-C32	4.28	120.74	111.48
33	G	5002	ERG	C1-C10-C5	4.28	116.12	108.74
38	a	606	CHL	C3D-C4D-CHA	4.27	115.03	108.54
37	a	501	LUT	C7-C8-C9	-4.27	119.92	126.23
21	6	603	CLA	CMA-C3A-C4A	4.26	123.23	111.77
20	A	1011	CL0	CHA-C1A-C2A	-4.26	123.31	133.31
30	B	5005	PTY	O7-C8-C11	4.26	120.69	111.48
23	A	4003	BCR	C15-C14-C13	-4.25	121.31	127.28
21	6	615	CLA	C1-C2-C3	-4.25	119.23	126.20
21	5	601	CLA	C1-C2-C3	-4.24	119.25	126.20
21	6	603	CLA	CMD-C2D-C1D	4.24	132.19	124.73
21	5	616	CLA	O2D-CGD-CBD	4.23	118.63	111.23
21	B	1238	CLA	O2A-C1-C2	4.23	124.38	108.11
21	A	1135	CLA	C1-C2-C3	-4.23	119.27	126.20
21	8	606	CLA	C1-C2-C3	-4.21	119.29	126.20
20	A	1011	CL0	O2A-CGA-CBA	4.21	124.68	111.83
37	4	502	LUT	C21-C26-C27	4.20	117.66	112.83
38	6	610	CHL	C3D-C4D-CHA	4.20	114.93	108.54
38	6	610	CHL	C1-O2A-CGA	4.20	126.82	116.65
21	B	1235	CLA	C1-C2-C3	-4.20	119.32	126.20
23	L	4003	BCR	C33-C5-C6	-4.20	119.91	124.48
46	7	807	4RF	O21-C22-C24	4.19	120.55	111.48
21	B	1209	CLA	C1-C2-C3	-4.19	119.34	126.20
46	8	807	4RF	O21-C22-C24	4.18	120.52	111.48
37	a	502	LUT	C31-C30-C29	-4.18	121.42	127.28
24	A	5001	LHG	O7-C7-C8	4.17	120.51	111.48
21	1	605	CLA	O2A-C1-C2	4.17	124.16	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	618	CHL	C3D-C4D-CHA	4.17	114.87	108.54
21	8	605	CLA	O2D-CGD-CBD	4.16	118.51	111.23
37	a	502	LUT	C11-C10-C9	-4.15	121.45	127.28
37	5	501	LUT	C26-C27-C28	-4.15	118.13	124.58
37	8	501	LUT	C21-C26-C27	4.14	117.58	112.83
31	F	5003	LAP	O7-P9-O5	4.13	131.67	112.44
37	5	501	LUT	C7-C8-C9	-4.12	120.14	126.23
24	8	801	LHG	O7-C7-C8	4.12	120.40	111.48
21	6	604	CLA	CAC-C3C-C4C	4.12	130.15	124.79
23	I	4001	BCR	C34-C9-C10	-4.11	116.15	122.82
38	8	601	CHL	C3D-C4D-CHA	4.11	114.79	108.54
38	5	613	CHL	C3D-C4D-CHA	4.11	114.79	108.54
37	3	502	LUT	C15-C14-C13	-4.11	121.52	127.28
21	A	1114	CLA	C1-C2-C3	-4.11	119.47	126.20
21	A	1123	CLA	C1-C2-C3	-4.11	119.47	126.20
24	4	802	LHG	O7-C7-C8	4.11	120.36	111.48
31	B	5007	LAP	O7-P9-O5	4.10	131.53	112.44
38	5	610	CHL	C3D-C4D-CHA	4.10	114.78	108.54
21	a	612	CLA	O2D-CGD-CBD	4.10	118.40	111.23
24	3	801	LHG	O7-C7-C8	4.10	120.34	111.48
23	B	4002	BCR	C23-C24-C25	-4.08	116.09	127.00
23	B	4001	BCR	C12-C13-C14	-4.08	112.60	119.01
21	B	1222	CLA	C1-C2-C3	-4.07	119.52	126.20
21	1	603	CLA	C1-C2-C3	-4.07	119.52	126.20
21	A	1105	CLA	C1-C2-C3	-4.07	119.53	126.20
24	6	802	LHG	O7-C7-C8	4.07	120.29	111.48
21	5	602	CLA	C1-C2-C3	-4.07	119.53	126.20
21	A	1127	CLA	C1-C2-C3	-4.07	119.53	126.20
21	B	1212	CLA	C1-C2-C3	-4.07	119.53	126.20
21	B	1224	CLA	C1-C2-C3	-4.07	119.53	126.20
21	A	1121	CLA	C1-C2-C3	-4.07	119.53	126.20
30	7	804	PTY	O7-C8-C11	4.07	120.28	111.48
38	a	609	CHL	C3D-C4D-CHA	4.07	114.72	108.54
21	3	605	CLA	O2A-C1-C2	4.06	123.75	108.11
40	3	506	QTB	C19-C17-C11	-4.06	104.86	110.58
38	1	613	CHL	C3D-C4D-CHA	4.06	114.71	108.54
23	3	505	BCR	C35-C13-C12	4.06	124.29	118.09
38	a	610	CHL	C3D-C4D-CHA	4.05	114.70	108.54
23	B	4001	BCR	C33-C5-C6	-4.05	120.06	124.48
21	4	606	CLA	C1-C2-C3	-4.04	120.22	126.76
23	B	4005	BCR	C23-C24-C25	-4.04	116.20	127.00
37	5	502	LUT	C35-C34-C33	-4.04	121.62	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	8	613	CHL	C3D-C4D-CHA	4.03	114.67	108.54
21	B	1210	CLA	C1-C2-C3	-4.03	119.59	126.20
38	6	611	CHL	C3D-C4D-CHA	4.03	114.66	108.54
38	3	608	CHL	C3D-C4D-CHA	4.02	114.66	108.54
21	8	608	CLA	O2A-C1-C2	4.02	123.59	108.11
37	a	501	LUT	C31-C30-C29	-4.02	121.64	127.28
26	A	5007	3PH	O21-C21-C22	4.02	120.18	111.48
21	4	608	CLA	C1-C2-C3	-4.02	119.61	126.20
24	5	801	LHG	O7-C7-C8	4.02	120.17	111.48
21	B	1225	CLA	C1-C2-C3	-4.01	119.62	126.20
21	8	609	CLA	C1-C2-C3	-4.01	119.62	126.20
21	B	1231	CLA	O2A-C1-C2	4.01	123.53	108.11
21	6	612	CLA	C1-C2-C3	-4.01	120.28	126.76
21	A	1103	CLA	C1-C2-C3	-4.01	119.63	126.20
21	7	612	CLA	CAC-C3C-C4C	4.00	130.00	124.79
21	8	606	CLA	O2A-C1-C2	4.00	123.51	108.11
23	3	505	BCR	C12-C13-C14	-4.00	112.72	119.01
38	3	611	CHL	C3D-C4D-CHA	4.00	114.62	108.54
36	M	4001	ECH	C28-C27-C26	-4.00	115.05	118.64
21	a	607	CLA	C1-C2-C3	-4.00	119.65	126.20
38	5	611	CHL	C3D-C4D-CHA	4.00	114.61	108.54
21	4	607	CLA	O2A-C1-C2	4.00	123.48	108.11
21	a	601	CLA	O2A-C1-C2	3.99	123.48	108.11
38	6	613	CHL	C3D-C4D-CHA	3.99	114.61	108.54
24	7	802	LHG	O7-C7-C8	3.99	120.11	111.48
37	5	501	LUT	C18-C5-C6	-3.98	120.14	124.48
37	6	502	LUT	C18-C5-C6	-3.98	120.14	124.48
23	A	4001	BCR	C19-C18-C17	3.98	125.27	119.01
21	4	601	CLA	C1-C2-C3	-3.98	119.67	126.20
24	A	5002	LHG	O7-C7-C8	3.98	120.09	111.48
21	L	1502	CLA	O2A-C1-C2	3.98	123.41	108.11
38	8	604	CHL	CHA-C1A-C2A	-3.98	123.97	133.31
38	1	609	CHL	C3D-C4D-CHA	3.98	114.58	108.54
23	B	4001	BCR	C19-C18-C17	3.97	125.26	119.01
37	8	502	LUT	C35-C34-C33	-3.97	121.71	127.28
37	a	501	LUT	C26-C27-C28	-3.97	118.40	124.58
21	3	606	CLA	O2A-C1-C2	3.96	123.36	108.11
24	1	802	LHG	O7-C7-C8	3.96	120.05	111.48
21	B	1230	CLA	O2A-C1-C2	3.96	123.34	108.11
31	K	5001	LAP	O7-P9-O5	3.96	130.85	112.44
21	A	1109	CLA	O2D-CGD-O1D	-3.96	116.15	123.85
23	B	4004	BCR	C33-C5-C6	-3.95	120.17	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	1240	CLA	C1-C2-C3	-3.95	119.72	126.20
21	A	1102	CLA	CAC-C3C-C2C	-3.95	120.30	127.56
21	B	1238	CLA	C1-C2-C3	-3.95	119.72	126.20
21	A	1115	CLA	O2A-C1-C2	3.95	123.30	108.11
38	4	613	CHL	C3D-C4D-CHA	3.95	114.54	108.54
21	L	1501	CLA	C1-C2-C3	-3.94	120.38	126.76
20	A	1011	CL0	O2A-C1-C2	3.94	123.28	108.11
37	7	501	LUT	C35-C34-C33	-3.94	121.75	127.28
34	J	4002	RRX	C30-C25-C26	-3.94	117.25	122.64
47	7	504	C7Z	C30-C31-C32	-3.94	111.79	123.20
38	5	610	CHL	C1-C2-C3	-3.94	119.75	126.20
21	A	1117	CLA	O2A-C1-C2	3.93	123.25	108.11
21	G	1601	CLA	C1-C2-C3	-3.93	120.40	126.76
21	4	615	CLA	O2A-C1-C2	3.93	123.24	108.11
21	A	1109	CLA	O2A-C1-C2	3.93	123.22	108.11
21	K	1404	CLA	C1-C2-C3	-3.93	119.76	126.20
37	4	501	LUT	C7-C8-C9	-3.93	120.42	126.23
21	1	604	CLA	O2A-C1-C2	3.92	123.21	108.11
38	a	613	CHL	C1A-CHA-C4D	3.92	125.52	118.98
21	A	1117	CLA	C1-C2-C3	-3.92	119.78	126.20
37	a	502	LUT	C38-C25-C24	-3.91	114.10	123.36
21	B	1217	CLA	O2A-C1-C2	3.90	123.13	108.11
23	F	4001	BCR	C35-C13-C14	-3.90	116.49	122.82
38	6	619	CHL	C3D-C4D-CHA	3.90	114.47	108.54
21	a	605	CLA	C1-C2-C3	-3.90	119.81	126.20
21	6	603	CLA	C1-C2-C3	-3.90	119.81	126.20
37	4	502	LUT	C35-C34-C33	-3.90	121.81	127.28
37	4	502	LUT	C18-C5-C6	-3.89	120.23	124.48
38	a	613	CHL	C3D-C4D-CHA	3.89	114.46	108.54
23	3	503	BCR	C33-C5-C6	-3.89	120.23	124.48
21	B	1218	CLA	O2A-C1-C2	3.89	123.08	108.11
21	A	1131	CLA	C1-C2-C3	-3.89	119.82	126.20
47	7	504	C7Z	C1-C6-C5	-3.89	117.33	122.64
21	L	1502	CLA	C1-C2-C3	-3.88	119.83	126.20
21	G	1601	CLA	O2A-C1-C2	3.88	123.03	108.11
21	B	1230	CLA	C1-C2-C3	-3.88	119.84	126.20
24	B	5001	LHG	O7-C7-C8	3.87	119.86	111.48
21	A	1108	CLA	O2A-C1-C2	3.87	123.01	108.11
21	A	1125	CLA	C4B-CHC-C1C	3.87	135.35	126.25
38	4	618	CHL	C1-C2-C3	-3.87	119.85	126.20
21	B	1228	CLA	CMA-C3A-C4A	3.87	122.18	111.77
38	8	604	CHL	C3D-C4D-CHA	3.87	114.42	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	4	502	LUT	C7-C8-C9	-3.87	120.52	126.23
38	6	619	CHL	CHA-C1A-C2A	-3.86	124.23	133.31
37	a	503	LUT	C7-C8-C9	-3.85	120.53	126.23
21	B	1234	CLA	C3B-C4B-NB	-3.85	107.09	110.53
20	A	1011	CL0	C1C-CHC-C4B	3.85	129.86	116.07
21	a	612	CLA	O2A-C1-C2	3.85	122.93	108.11
23	B	4001	BCR	C28-C27-C26	-3.85	107.19	114.06
21	B	1240	CLA	O2A-C1-C2	3.85	122.93	108.11
21	3	613	CLA	C1-C2-C3	-3.85	119.89	126.20
23	3	504	BCR	C33-C5-C6	-3.85	120.29	124.48
21	A	1116	CLA	O2A-C1-C2	3.85	122.91	108.11
21	a	601	CLA	C1-C2-C3	-3.85	119.90	126.20
21	K	1402	CLA	O2A-C1-C2	3.85	122.91	108.11
30	3	802	PTY	O7-C8-C11	3.84	119.79	111.48
24	B	5002	LHG	O7-C7-C8	3.84	119.78	111.48
21	B	1225	CLA	O2A-C1-C2	3.84	122.88	108.11
22	B	2002	PQN	C11-C12-C13	-3.84	120.22	126.83
21	7	603	CLA	C1-C2-C3	-3.83	119.92	126.20
24	F	5002	LHG	O7-C7-C8	3.83	119.77	111.48
21	A	1128	CLA	O2A-C1-C2	3.82	122.83	108.11
23	B	4002	BCR	C33-C5-C6	-3.82	120.31	124.48
37	a	503	LUT	C11-C10-C9	-3.82	121.92	127.28
21	F	1301	CLA	C1-C2-C3	-3.82	120.58	126.76
21	5	602	CLA	O2A-C1-C2	3.82	122.81	108.11
21	3	603	CLA	C1-C2-C3	-3.82	119.94	126.20
21	B	1213	CLA	C1-C2-C3	-3.82	119.94	126.20
21	1	601	CLA	O2A-C1-C2	3.82	122.79	108.11
21	6	601	CLA	O2A-C1-C2	3.81	122.78	108.11
21	K	1402	CLA	C1-C2-C3	-3.81	119.95	126.20
21	B	1203	CLA	O2A-C1-C2	3.81	122.77	108.11
33	G	5002	ERG	C18-C13-C12	-3.81	104.99	110.61
38	8	604	CHL	C1-C2-C3	-3.81	119.96	126.20
37	3	502	LUT	C7-C8-C9	-3.80	120.61	126.23
23	5	504	BCR	C19-C18-C17	3.80	124.99	119.01
21	a	608	CLA	C1-C2-C3	-3.80	119.96	126.20
23	8	503	BCR	C33-C5-C6	-3.80	120.33	124.48
37	a	502	LUT	C15-C14-C13	-3.80	121.95	127.28
38	a	606	CHL	C1A-CHA-C4D	3.80	125.32	118.98
21	3	601	CLA	O2A-C1-C2	3.79	122.71	108.11
21	6	609	CLA	O2D-CGD-O1D	-3.79	116.46	123.85
21	B	1229	CLA	C1-C2-C3	-3.79	119.98	126.20
21	B	1212	CLA	O2A-C1-C2	3.79	122.70	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	3	506	QTB	C10-C09-C02	-3.79	118.17	126.32
21	5	606	CLA	O2A-C1-C2	3.78	122.67	108.11
38	7	613	CHL	C3D-C4D-CHA	3.78	114.29	108.54
38	a	613	CHL	C1B-CHB-C4A	3.78	123.76	121.32
21	A	1137	CLA	O2A-C1-C2	3.78	122.66	108.11
37	5	501	LUT	C21-C26-C27	3.78	117.17	112.83
21	5	612	CLA	C1-C2-C3	-3.78	120.01	126.20
21	8	611	CLA	O2A-C1-C2	3.78	122.64	108.11
21	B	1208	CLA	O2A-C1-C2	3.77	122.63	108.11
43	5	803	DGA	OG2-CB1-CB2	3.77	119.64	111.48
21	B	1205	CLA	C1-C2-C3	-3.77	120.02	126.20
38	4	609	CHL	C3D-C4D-CHA	3.77	114.27	108.54
21	B	1223	CLA	O2A-C1-C2	3.76	122.59	108.11
21	B	1227	CLA	O2A-C1-C2	3.76	122.58	108.11
21	A	1124	CLA	C1-C2-C3	-3.76	120.04	126.20
38	a	613	CHL	CHA-C1A-C2A	-3.76	124.48	133.31
21	A	1130	CLA	O2A-C1-C2	3.76	122.57	108.11
23	5	504	BCR	C33-C5-C6	-3.76	120.39	124.48
23	B	4003	BCR	C33-C5-C6	-3.75	120.39	124.48
25	A	5005	DGD	O2G-C1B-C2B	3.75	119.60	111.48
23	B	4003	BCR	C23-C22-C21	3.75	124.91	119.01
21	B	1226	CLA	O2A-C1-C2	3.75	122.53	108.11
21	7	601	CLA	O2A-C1-C2	3.74	122.52	108.11
21	3	607	CLA	C1-C2-C3	-3.74	120.07	126.20
36	M	4001	ECH	C33-C5-C6	-3.74	120.40	124.48
37	6	501	LUT	C35-C15-C14	-3.73	115.88	123.52
33	G	5002	ERG	C18-C13-C14	-3.73	104.15	110.35
38	6	610	CHL	CHA-C1A-C2A	-3.73	124.55	133.31
21	4	601	CLA	O2A-C1-C2	3.73	122.45	108.11
36	M	4001	ECH	C23-C24-C25	-3.73	117.04	127.00
36	M	4001	ECH	C16-C17-C18	-3.73	122.05	127.28
23	B	4002	BCR	C27-C26-C25	-3.73	117.67	122.70
37	4	501	LUT	C35-C34-C33	-3.72	122.05	127.28
23	5	504	BCR	C28-C27-C26	-3.72	107.42	114.06
45	7	502	XAT	C15-C14-C13	-3.72	122.06	127.28
21	A	1134	CLA	O2A-C1-C2	3.72	122.42	108.11
38	6	613	CHL	CHA-C1A-C2A	-3.72	124.58	133.31
21	5	603	CLA	O2A-C1-C2	3.72	122.41	108.11
47	7	504	C7Z	C11-C12-C13	-3.72	116.18	126.36
37	1	502	LUT	C10-C11-C12	-3.71	112.44	123.20
21	B	1207	CLA	C1-C2-C3	-3.71	120.12	126.20
38	8	613	CHL	C1-C2-C3	-3.71	120.76	126.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	1	501	LUT	C18-C5-C6	-3.71	120.44	124.48
37	3	501	LUT	C7-C8-C9	-3.71	120.75	126.23
21	a	607	CLA	O2A-C1-C2	3.71	122.37	108.11
21	A	1140	CLA	O2A-C1-C2	3.71	122.37	108.11
21	B	1223	CLA	C1-C2-C3	-3.70	120.13	126.20
21	A	1125	CLA	O2A-C1-C2	3.70	122.36	108.11
21	F	1301	CLA	O2A-C1-C2	3.70	122.35	108.11
21	A	1114	CLA	O2A-C1-C2	3.70	122.34	108.11
21	6	603	CLA	O2D-CGD-O1D	-3.70	116.65	123.85
21	1	601	CLA	C1-C2-C3	-3.69	120.15	126.20
21	B	1201	CLA	O2A-C1-C2	3.69	122.31	108.11
21	3	610	CLA	C1-C2-C3	-3.69	120.15	126.20
38	a	609	CHL	CHA-C1A-C2A	-3.69	124.65	133.31
23	A	4002	BCR	C23-C24-C25	-3.69	117.15	127.00
23	3	505	BCR	C33-C5-C6	-3.69	120.46	124.48
21	A	1123	CLA	O2A-C1-C2	3.68	122.28	108.11
21	A	1138	CLA	O2A-C1-C2	3.68	122.27	108.11
23	A	4004	BCR	C33-C5-C6	-3.67	120.47	124.48
21	4	610	CLA	O2A-C1-C2	3.67	122.25	108.11
21	B	1210	CLA	O2A-C1-C2	3.67	122.24	108.11
38	8	601	CHL	C1-C2-C3	-3.67	120.18	126.20
23	5	504	BCR	C36-C18-C17	-3.67	116.87	122.82
21	A	1140	CLA	C1-C2-C3	-3.67	120.19	126.20
21	1	603	CLA	O2A-C1-C2	3.67	122.23	108.11
37	8	502	LUT	C7-C8-C9	-3.67	120.81	126.23
21	8	610	CLA	O2A-C1-C2	3.66	122.20	108.11
23	5	503	BCR	C33-C5-C6	-3.66	120.49	124.48
21	3	607	CLA	O2A-C1-C2	3.66	122.20	108.11
37	4	501	LUT	C18-C5-C6	-3.66	120.49	124.48
21	4	610	CLA	O1D-CGD-CBD	-3.66	117.30	124.52
37	3	502	LUT	C35-C34-C33	-3.66	122.15	127.28
37	1	503	LUT	C11-C10-C9	-3.66	122.15	127.28
21	B	1236	CLA	CED-O2D-CGD	-3.65	107.64	115.92
21	a	603	CLA	O2A-C1-C2	3.64	122.13	108.11
21	5	618	CLA	O2A-C1-C2	3.64	122.12	108.11
37	7	501	LUT	C35-C15-C14	-3.64	116.08	123.52
21	A	1106	CLA	C1-C2-C3	-3.64	120.24	126.20
21	A	1133	CLA	O2A-C1-C2	3.63	122.08	108.11
21	B	1234	CLA	O2A-C1-C2	3.63	122.07	108.11
38	a	610	CHL	CHA-C1A-C2A	-3.63	124.79	133.31
37	3	501	LUT	C35-C34-C33	-3.62	122.20	127.28
38	4	609	CHL	CHA-C1A-C2A	-3.62	124.81	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	8	501	LUT	C7-C8-C9	-3.62	120.89	126.23
21	B	1222	CLA	O2A-C1-C2	3.62	122.02	108.11
21	6	602	CLA	O2A-C1-C2	3.61	122.02	108.11
21	3	603	CLA	O2A-C1-C2	3.61	122.00	108.11
21	6	609	CLA	O2A-C1-C2	3.61	122.00	108.11
21	B	1204	CLA	O2A-C1-C2	3.60	121.98	108.11
21	6	607	CLA	O2A-C1-C2	3.60	121.98	108.11
23	B	4007	BCR	C23-C24-C25	-3.60	117.37	127.00
38	4	609	CHL	C3C-C4C-NC	-3.60	105.85	114.65
37	3	501	LUT	C35-C15-C14	-3.60	116.15	123.52
21	3	610	CLA	O2A-C1-C2	3.60	121.97	108.11
37	6	502	LUT	C11-C10-C9	-3.60	122.23	127.28
21	B	1219	CLA	C1-C2-C3	-3.60	120.30	126.20
21	3	616	CLA	O2A-C1-C2	3.60	121.96	108.11
21	4	606	CLA	O2A-C1-C2	3.60	121.96	108.11
21	B	1022	CLA	C3B-C4B-NB	-3.60	107.32	110.53
21	5	601	CLA	O2A-C1-C2	3.60	121.94	108.11
21	8	618	CLA	O2A-C1-C2	3.60	121.94	108.11
21	K	1404	CLA	O2A-C1-C2	3.59	121.93	108.11
37	8	502	LUT	C26-C27-C28	-3.59	118.99	124.58
37	5	505	LUT	C11-C12-C13	-3.59	116.52	126.36
21	B	1022	CLA	O2A-C1-C2	3.59	121.91	108.11
21	L	1501	CLA	O2A-C1-C2	3.59	121.91	108.11
38	5	611	CHL	CHA-C1A-C2A	-3.58	124.89	133.31
21	A	1112	CLA	O2A-C1-C2	3.58	121.88	108.11
21	A	1105	CLA	O2A-C1-C2	3.58	121.88	108.11
21	5	606	CLA	C1-C2-C3	-3.57	120.98	126.76
21	B	1021	CLA	O2A-C1-C2	3.57	121.85	108.11
37	1	502	LUT	C18-C5-C6	-3.57	120.59	124.48
21	4	602	CLA	O2A-C1-C2	3.57	121.83	108.11
38	a	606	CHL	CHA-C1A-C2A	-3.57	124.94	133.31
37	5	505	LUT	C18-C5-C6	-3.56	120.60	124.48
38	6	610	CHL	C1A-CHA-C4D	3.56	124.92	118.98
37	5	505	LUT	C22-C23-C24	-3.56	105.90	111.18
37	6	502	LUT	C15-C14-C13	-3.56	122.29	127.28
21	B	1236	CLA	CAC-C3C-C4C	3.55	129.41	124.79
21	B	1213	CLA	O2A-C1-C2	3.55	121.78	108.11
45	7	502	XAT	C26-C27-C28	-3.55	118.48	125.99
38	a	610	CHL	C1A-CHA-C4D	3.55	124.91	118.98
37	3	502	LUT	C11-C10-C9	-3.55	122.30	127.28
38	3	611	CHL	CHA-C1A-C2A	-3.55	124.97	133.31
21	A	1104	CLA	O2A-C1-C2	3.55	121.77	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	602	CLA	C1-C2-C3	-3.55	120.39	126.20
23	L	4002	BCR	C33-C5-C6	-3.54	120.62	124.48
21	A	1136	CLA	O2A-C1-C2	3.54	121.75	108.11
21	3	604	CLA	O2A-C1-C2	3.54	121.74	108.11
21	a	611	CLA	C1-C2-C3	-3.54	121.03	126.76
21	4	616	CLA	O2A-C1-C2	3.54	121.73	108.11
37	4	502	LUT	C26-C27-C28	-3.54	119.07	124.58
21	A	1134	CLA	C1-C2-C3	-3.54	120.40	126.20
21	A	1132	CLA	O2A-C1-C2	3.54	121.71	108.11
21	6	603	CLA	O2A-C1-C2	3.53	121.71	108.11
37	8	501	LUT	C18-C5-C6	-3.53	120.63	124.48
21	B	1228	CLA	C5-C3-C2	-3.53	113.24	121.17
21	7	611	CLA	O2A-C1-C2	3.53	121.68	108.11
21	A	1101	CLA	C1-C2-C3	-3.53	120.42	126.20
22	A	2001	PQN	C11-C12-C13	-3.53	120.76	126.83
38	a	609	CHL	C1A-CHA-C4D	3.52	124.86	118.98
21	B	1219	CLA	O2A-C1-C2	3.52	121.66	108.11
21	B	1205	CLA	O2A-C1-C2	3.52	121.65	108.11
21	5	617	CLA	C2C-C1C-NC	3.52	113.68	109.98
21	1	612	CLA	O2A-C1-C2	3.52	121.65	108.11
21	B	1236	CLA	C1-C2-C3	-3.52	120.43	126.20
21	3	613	CLA	O2A-C1-C2	3.51	121.63	108.11
23	A	4005	BCR	C12-C13-C14	-3.51	113.48	119.01
21	B	1209	CLA	C1-O2A-CGA	3.51	125.16	116.65
23	A	4003	BCR	C33-C5-C6	-3.51	120.65	124.48
21	A	1104	CLA	C1-C2-C3	-3.51	120.44	126.20
21	A	1107	CLA	C1-C2-C3	-3.51	120.44	126.20
38	4	613	CHL	C1-C2-C3	-3.51	120.45	126.20
37	8	502	LUT	C18-C5-C6	-3.51	120.66	124.48
21	B	1218	CLA	C1-C2-C3	-3.51	120.45	126.20
21	a	611	CLA	O2A-C1-C2	3.50	121.60	108.11
37	3	501	LUT	C18-C5-C6	-3.50	120.66	124.48
21	B	1221	CLA	O2A-C1-C2	3.50	121.59	108.11
23	G	4001	BCR	C19-C18-C17	3.50	124.51	119.01
23	B	4006	BCR	C28-C27-C26	-3.50	107.82	114.06
37	7	501	LUT	C18-C5-C6	-3.50	120.67	124.48
21	B	1237	CLA	C1-C2-C3	-3.49	120.47	126.20
21	7	615	CLA	C1-C2-C3	-3.49	120.47	126.20
37	5	502	LUT	C11-C10-C9	-3.49	122.38	127.28
21	B	1206	CLA	O2A-C1-C2	3.49	121.54	108.11
47	7	504	C7Z	O3-C3-C2	3.49	116.88	109.75
23	6	504	BCR	C28-C27-C26	-3.49	107.83	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	J	4001	BCR	C33-C5-C6	-3.49	120.68	124.48
38	4	618	CHL	C1A-CHA-C4D	3.49	124.80	118.98
21	6	606	CLA	C1-C2-C3	-3.48	120.49	126.20
21	A	1121	CLA	O2A-C1-C2	3.48	121.51	108.11
21	B	1022	CLA	C1-C2-C3	-3.48	120.49	126.20
21	5	603	CLA	C1-C2-C3	-3.48	120.49	126.20
37	a	503	LUT	C18-C5-C6	-3.48	120.69	124.48
37	5	502	LUT	C18-C5-C6	-3.48	120.69	124.48
21	7	615	CLA	O2A-C1-C2	3.48	121.50	108.11
21	a	602	CLA	O2A-C1-C2	3.47	121.48	108.11
21	B	1236	CLA	O2A-C1-C2	3.47	121.47	108.11
21	F	1302	CLA	C1D-ND-C4D	-3.47	103.88	106.31
38	5	611	CHL	C1-C2-C3	-3.47	121.15	126.76
23	B	4005	BCR	C33-C5-C6	-3.47	120.70	124.48
37	1	501	LUT	C15-C14-C13	-3.46	122.42	127.28
37	1	503	LUT	C27-C28-C29	-3.46	118.88	126.32
21	B	1211	CLA	O2A-C1-C2	3.46	121.42	108.11
21	6	612	CLA	C1D-ND-C4D	-3.46	103.88	106.31
21	4	603	CLA	C1-C2-C3	-3.46	120.53	126.20
21	6	603	CLA	C2C-C1C-NC	3.46	113.61	109.98
21	a	604	CLA	C3B-C4B-NB	-3.46	107.44	110.53
21	5	612	CLA	O2A-C1-C2	3.45	121.40	108.11
21	F	1302	CLA	O2A-C1-C2	3.45	121.39	108.11
23	G	4001	BCR	C28-C27-C26	-3.45	107.90	114.06
38	6	613	CHL	C1A-CHA-C4D	3.45	124.74	118.98
21	6	615	CLA	O2A-C1-C2	3.45	121.38	108.11
21	5	609	CLA	C1-C2-C3	-3.44	120.56	126.20
21	B	1202	CLA	C1-C2-C3	-3.44	120.56	126.20
43	8	803	DGA	OG2-CB1-CB2	3.44	118.92	111.48
21	a	604	CLA	O2A-C1-C2	3.44	121.33	108.11
34	J	4002	RRX	C32-C1-C6	-3.43	104.86	110.24
21	1	608	CLA	C1-C2-C3	-3.43	120.57	126.20
47	7	504	C7Z	O3-C3-C4	3.43	117.44	109.71
38	6	619	CHL	C1A-CHA-C4D	3.43	124.71	118.98
21	B	1229	CLA	C3B-C4B-NB	-3.43	107.47	110.53
21	A	1133	CLA	C1-C2-C3	-3.43	120.57	126.20
21	A	1107	CLA	O2A-C1-C2	3.43	121.31	108.11
23	A	4001	BCR	C36-C18-C17	-3.43	117.26	122.82
21	B	1216	CLA	O2A-C1-C2	3.43	121.30	108.11
38	5	610	CHL	C1A-CHA-C4D	3.43	124.70	118.98
21	6	609	CLA	C3B-C4B-NB	-3.43	107.47	110.53
25	A	5005	DGD	O6D-C5D-C6D	3.43	113.49	106.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	1213	CLA	C3B-C4B-NB	-3.42	107.48	110.53
21	1	604	CLA	CMC-C2C-C1C	3.42	130.38	125.03
22	A	2001	PQN	C14-C13-C15	3.42	121.17	115.23
21	1	607	CLA	O2A-C1-C2	3.42	121.27	108.11
21	A	1130	CLA	C1-C2-C3	-3.42	120.60	126.20
21	A	1124	CLA	O2A-C1-C2	3.42	121.25	108.11
21	A	1139	CLA	O2A-C1-C2	3.41	121.25	108.11
21	7	604	CLA	C1-C2-C3	-3.41	120.61	126.20
38	8	613	CHL	CHA-C1A-C2A	-3.41	125.31	133.31
21	B	1236	CLA	C1D-ND-C4D	-3.41	103.92	106.31
21	a	605	CLA	O2A-C1-C2	3.41	121.22	108.11
23	6	503	BCR	C28-C27-C26	-3.41	107.98	114.06
38	7	613	CHL	CHA-C1A-C2A	-3.40	125.31	133.31
21	7	603	CLA	O2A-C1-C2	3.40	121.21	108.11
21	A	1127	CLA	O2A-C1-C2	3.40	121.20	108.11
23	A	4003	BCR	C34-C9-C10	-3.40	117.31	122.82
21	B	1202	CLA	O2A-C1-C2	3.40	121.18	108.11
21	B	1209	CLA	C3B-C4B-NB	-3.40	107.50	110.53
38	7	613	CHL	C3C-C4C-NC	-3.39	106.36	114.65
21	3	612	CLA	O2A-C1-C2	3.39	121.17	108.11
21	1	608	CLA	O2A-C1-C2	3.39	121.16	108.11
21	A	1131	CLA	O2A-C1-C2	3.39	121.16	108.11
21	1	607	CLA	C3B-C4B-NB	-3.39	107.50	110.53
23	B	4001	BCR	C35-C13-C12	3.39	123.27	118.09
38	a	609	CHL	C3C-C4C-NC	-3.39	106.37	114.65
21	A	1012	CLA	C1-C2-C3	-3.39	120.65	126.20
21	A	1129	CLA	O2A-C1-C2	3.39	121.14	108.11
21	6	606	CLA	O2A-C1-C2	3.39	121.14	108.11
21	A	1135	CLA	O2A-C1-C2	3.39	121.14	108.11
33	G	5002	ERG	C19-C10-C5	-3.39	103.21	108.38
21	a	608	CLA	O2A-C1-C2	3.38	121.13	108.11
23	7	503	BCR	C23-C24-C25	-3.38	117.96	127.00
21	A	1118	CLA	O2A-C1-C2	3.38	121.12	108.11
21	B	1224	CLA	O2A-C1-C2	3.38	121.12	108.11
21	6	612	CLA	O2A-C1-C2	3.38	121.11	108.11
23	B	4006	BCR	C23-C24-C25	-3.38	117.98	127.00
38	3	608	CHL	CHA-C1A-C2A	-3.38	125.38	133.31
38	4	613	CHL	C3C-C4C-NC	-3.38	106.40	114.65
24	A	5001	LHG	C5-O7-C7	-3.37	109.72	117.80
21	7	606	CLA	O2A-C1-C2	3.37	121.09	108.11
21	B	1217	CLA	C1-C2-C3	-3.37	120.67	126.20
21	8	610	CLA	C1-C2-C3	-3.37	120.67	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	611	CLA	O2A-C1-C2	3.37	121.07	108.11
21	4	608	CLA	O2A-C1-C2	3.37	121.06	108.11
24	F	5002	LHG	O8-C23-C24	3.36	122.09	111.83
38	6	611	CHL	CHA-C1A-C2A	-3.36	125.41	133.31
21	7	610	CLA	O2A-C1-C2	3.36	121.04	108.11
21	1	604	CLA	C4B-CHC-C1C	3.36	134.15	126.25
21	A	1013	CLA	O2A-C1-C2	3.36	121.02	108.11
21	a	604	CLA	C1D-ND-C4D	-3.35	103.96	106.31
37	1	502	LUT	C7-C8-C9	-3.35	121.27	126.23
37	5	505	LUT	C18-C5-C4	3.35	120.59	114.42
48	8	806	P5S	O37-C38-C39	3.35	118.73	111.48
45	7	502	XAT	C38-C25-C26	-3.35	116.78	122.30
21	4	604	CLA	O2A-C1-C2	3.35	121.00	108.11
21	L	1503	CLA	C2C-C1C-NC	3.35	113.50	109.98
38	3	611	CHL	C3C-C4C-NC	-3.35	106.47	114.65
21	A	1125	CLA	CHC-C1C-NC	-3.35	119.27	124.31
38	5	613	CHL	C1-O2A-CGA	3.34	124.74	116.65
33	G	5002	ERG	C2-C1-C10	3.34	119.90	112.78
38	3	611	CHL	C1A-CHA-C4D	3.34	124.55	118.98
21	A	1111	CLA	O2A-C1-C2	3.34	120.96	108.11
37	8	502	LUT	C10-C11-C12	-3.34	113.53	123.20
38	5	613	CHL	CHA-C1A-C2A	-3.34	125.47	133.31
21	5	607	CLA	O2A-C1-C2	3.34	120.95	108.11
21	6	604	CLA	O2D-CGD-O1D	-3.34	117.35	123.85
21	A	1127	CLA	C3B-C4B-NB	-3.34	107.55	110.53
24	6	801	LHG	O8-C23-C24	3.34	122.00	111.83
38	1	609	CHL	C3C-C4C-NC	-3.33	106.50	114.65
21	A	1110	CLA	O2A-C1-C2	3.33	120.94	108.11
21	B	1237	CLA	O2A-C1-C2	3.33	120.93	108.11
21	A	1122	CLA	O2A-C1-C2	3.33	120.91	108.11
21	3	616	CLA	C1-C2-C3	-3.32	120.76	126.20
38	6	613	CHL	C1-C2-C3	-3.32	121.39	126.76
37	8	501	LUT	C27-C28-C29	-3.32	119.19	126.32
21	B	1203	CLA	C3B-C4B-NB	-3.32	107.57	110.53
38	8	604	CHL	C3C-C4C-NC	-3.31	106.55	114.65
21	4	604	CLA	C1-C2-C3	-3.31	120.77	126.20
47	7	504	C7Z	C15-C35-C34	-3.31	116.74	123.52
38	5	611	CHL	C3C-C4C-NC	-3.31	106.56	114.65
21	A	1132	CLA	C1-C2-C3	-3.31	120.77	126.20
23	I	4001	BCR	C34-C9-C8	3.31	123.14	118.09
21	B	1236	CLA	O2D-CGD-O1D	-3.31	117.41	123.85
21	6	618	CLA	C1D-ND-C4D	-3.31	103.99	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	1206	CLA	C2C-C1C-NC	3.31	113.46	109.98
21	5	607	CLA	C1-C2-C3	-3.31	120.78	126.20
23	K	4001	BCR	C33-C5-C6	-3.31	120.88	124.48
37	1	501	LUT	C35-C15-C14	-3.31	116.75	123.52
21	B	1239	CLA	C1-C2-C3	-3.31	120.78	126.20
23	K	4002	BCR	C8-C9-C10	3.30	124.21	119.01
21	A	1101	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
21	1	604	CLA	C1-C2-C3	-3.30	120.79	126.20
21	A	1106	CLA	C1D-ND-C4D	-3.30	104.00	106.31
21	A	1114	CLA	C3B-C4B-NB	-3.30	107.58	110.53
23	J	4001	BCR	C28-C27-C26	-3.30	108.17	114.06
23	L	4001	BCR	C27-C26-C25	-3.30	118.25	122.70
21	8	611	CLA	C1-C2-C3	-3.30	121.43	126.76
37	5	501	LUT	C35-C15-C14	-3.30	116.77	123.52
21	7	617	CLA	O2A-C1-C2	3.30	120.79	108.11
21	B	1239	CLA	O2A-C1-C2	3.29	120.78	108.11
21	B	1208	CLA	C1-O2A-CGA	3.29	124.62	116.65
23	7	503	BCR	C33-C5-C6	-3.29	120.89	124.48
21	B	1234	CLA	C1D-ND-C4D	-3.29	104.00	106.31
38	8	613	CHL	C3C-C4C-NC	-3.29	106.61	114.65
21	A	1102	CLA	C1-C2-C3	-3.29	120.81	126.20
21	6	604	CLA	CMA-C3A-C4A	3.29	120.60	111.77
21	1	611	CLA	C1-C2-C3	-3.28	120.82	126.20
21	7	607	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
21	4	603	CLA	O2A-C1-C2	3.28	120.74	108.11
21	B	1237	CLA	C3B-C4B-NB	-3.28	107.60	110.53
23	J	4001	BCR	C29-C30-C25	-3.28	105.67	110.44
21	A	1139	CLA	C1-C2-C3	-3.28	120.82	126.20
21	5	604	CLA	O2A-C1-C2	3.28	120.73	108.11
37	3	502	LUT	C26-C27-C28	-3.28	119.48	124.58
38	5	613	CHL	C1A-CHA-C4D	3.28	124.45	118.98
21	A	1113	CLA	O2A-C1-C2	3.28	120.72	108.11
33	G	5002	ERG	C1-C2-C3	3.28	114.82	110.48
21	A	1012	CLA	OBD-CAD-C3D	-3.28	120.76	128.42
23	7	503	BCR	C29-C30-C25	-3.28	105.68	110.44
33	G	5002	ERG	C9-C10-C5	3.28	114.88	109.66
23	A	4003	BCR	C28-C27-C26	-3.28	108.22	114.06
21	B	1229	CLA	O2A-C1-C2	3.27	120.71	108.11
21	B	1209	CLA	O2A-C1-C2	3.27	120.69	108.11
21	1	606	CLA	O2A-C1-C2	3.27	120.69	108.11
38	5	613	CHL	C3C-C4C-NC	-3.27	106.66	114.65
23	A	4002	BCR	C33-C5-C6	-3.27	120.92	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	7	604	CLA	O2A-C1-C2	3.27	120.68	108.11
38	6	611	CHL	C3C-C4C-NC	-3.26	106.68	114.65
21	8	609	CLA	O2A-C1-C2	3.26	120.64	108.11
23	3	504	BCR	C19-C18-C17	3.26	124.13	119.01
21	B	1206	CLA	C1C-C2C-C3C	-3.26	103.56	106.98
38	6	619	CHL	C3C-C4C-NC	-3.25	106.70	114.65
21	5	617	CLA	O2A-C1-C2	3.25	120.61	108.11
23	L	4001	BCR	C33-C5-C6	-3.25	120.94	124.48
21	4	617	CLA	CMA-C3A-C4A	3.25	120.50	111.77
21	1	607	CLA	C1-C2-C3	-3.24	120.88	126.20
23	B	4001	BCR	C36-C18-C17	-3.24	117.56	122.82
23	A	4003	BCR	C8-C9-C10	3.24	124.10	119.01
21	5	609	CLA	O2A-C1-C2	3.24	120.56	108.11
21	a	612	CLA	C1-C2-C3	-3.23	120.90	126.20
21	B	1238	CLA	C3B-C4B-NB	-3.23	107.64	110.53
21	7	605	CLA	C3B-C4B-NB	-3.23	107.64	110.53
21	8	609	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
23	6	503	BCR	C33-C5-C6	-3.23	120.96	124.48
21	B	1235	CLA	O2A-C1-C2	3.23	120.54	108.11
38	8	604	CHL	C1A-CHA-C4D	3.23	124.37	118.98
37	1	501	LUT	C26-C27-C28	-3.23	119.55	124.58
21	7	609	CLA	O2A-CGA-CBA	3.23	121.69	111.83
37	3	502	LUT	C18-C5-C6	-3.23	120.96	124.48
37	5	502	LUT	C15-C14-C13	-3.23	122.75	127.28
21	7	609	CLA	O2A-C1-C2	3.23	120.53	108.11
23	G	4001	BCR	C30-C25-C26	-3.23	118.23	122.64
37	1	502	LUT	C35-C15-C14	-3.23	116.92	123.52
21	B	1208	CLA	CAA-C2A-C3A	-3.23	104.28	113.00
23	L	4002	BCR	C8-C7-C6	-3.22	118.39	127.00
23	6	504	BCR	C31-C1-C6	-3.22	105.19	110.24
21	1	612	CLA	C1-C2-C3	-3.22	120.92	126.20
38	5	610	CHL	C3C-C4C-NC	-3.22	106.79	114.65
21	B	1215	CLA	O2A-C1-C2	3.22	120.48	108.11
23	A	4001	BCR	C33-C5-C6	-3.21	120.98	124.48
21	B	1022	CLA	OBD-CAD-C3D	-3.21	120.91	128.42
21	A	1115	CLA	C1-C2-C3	-3.21	120.94	126.20
21	8	615	CLA	C1D-ND-C4D	-3.21	104.06	106.31
21	A	1118	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
21	6	612	CLA	CAC-C3C-C4C	3.20	128.96	124.79
37	5	502	LUT	C10-C11-C12	-3.20	113.93	123.20
21	A	1012	CLA	O2A-C1-C2	3.20	120.42	108.11
25	B	5003	DGD	C2G-O2G-C1B	-3.20	110.14	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1103	CLA	O2A-C1-C2	3.19	120.40	108.11
21	A	1106	CLA	C3B-C4B-NB	-3.19	107.68	110.53
21	A	1138	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
23	I	4001	BCR	C27-C26-C25	-3.19	118.39	122.70
38	1	609	CHL	C1A-CHA-C4D	3.19	124.30	118.98
23	A	4004	BCR	C34-C9-C10	-3.19	117.65	122.82
21	7	609	CLA	O2D-CGD-O1D	-3.19	117.65	123.85
21	A	1111	CLA	C1-C2-C3	-3.19	120.98	126.20
21	7	617	CLA	O2D-CGD-O1D	-3.19	117.65	123.85
21	A	1112	CLA	C2C-C1C-NC	3.18	113.33	109.98
21	B	1205	CLA	O2D-CGD-O1D	-3.18	117.65	123.85
21	A	1125	CLA	C3B-C4B-NB	-3.18	107.69	110.53
21	A	1108	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
36	M	4001	ECH	C24-C23-C22	-3.18	121.53	126.23
38	5	611	CHL	C1A-CHA-C4D	3.18	124.28	118.98
21	A	1115	CLA	C3B-C4B-NB	-3.18	107.69	110.53
38	6	610	CHL	C4D-CHA-CBD	-3.17	105.77	108.97
38	8	601	CHL	C3C-C4C-NC	-3.17	106.90	114.65
21	A	1116	CLA	C3B-C4B-NB	-3.17	107.70	110.53
21	A	1130	CLA	C3B-C4B-NB	-3.17	107.70	110.53
23	B	4005	BCR	C35-C13-C12	3.17	122.93	118.09
21	8	602	CLA	O2A-C1-C2	3.17	120.31	108.11
23	B	4005	BCR	C12-C13-C14	-3.17	114.02	119.01
21	4	615	CLA	CMA-C3A-C4A	3.17	120.30	111.77
21	A	1137	CLA	C1-C2-C3	-3.17	121.00	126.20
21	B	1227	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
21	6	604	CLA	O2A-C1-C2	3.17	120.30	108.11
21	8	620	CLA	O2A-C1-C2	3.17	120.30	108.11
21	7	611	CLA	CAC-C3C-C4C	3.17	128.91	124.79
23	B	4006	BCR	C33-C5-C6	-3.16	121.03	124.48
38	4	613	CHL	CMA-C3A-C2A	3.16	126.35	114.13
21	A	1125	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
21	A	1101	CLA	C3B-C4B-NB	-3.16	107.71	110.53
23	K	4002	BCR	C34-C9-C10	-3.16	117.69	122.82
38	a	610	CHL	C3C-C4C-NC	-3.16	106.92	114.65
21	A	1106	CLA	O2A-C1-C2	3.16	120.27	108.11
21	A	1102	CLA	C1D-ND-C4D	-3.16	104.09	106.31
37	1	502	LUT	C35-C34-C33	-3.16	122.85	127.28
21	6	612	CLA	C2D-C1D-ND	3.15	113.25	110.13
38	1	613	CHL	C4D-CHA-CBD	-3.15	105.79	108.97
21	6	612	CLA	O2D-CGD-O1D	-3.15	117.71	123.85
21	A	1013	CLA	C1-C2-C3	-3.15	121.03	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	8	620	CLA	CMA-C3A-C4A	3.15	120.25	111.77
21	B	1201	CLA	C1-C2-C3	-3.15	121.03	126.20
21	7	611	CLA	C1-C2-C3	-3.15	121.03	126.20
40	a	504	QTB	C19-C17-C16	3.15	115.56	109.01
21	7	612	CLA	O2A-C1-C2	3.15	120.23	108.11
21	A	1135	CLA	C3B-C4B-NB	-3.15	107.72	110.53
38	3	608	CHL	C3C-C4C-NC	-3.15	106.95	114.65
21	6	603	CLA	C3B-C4B-NB	-3.15	107.72	110.53
46	8	808	4RF	O18-C16-C15	3.15	121.43	111.83
23	G	4001	BCR	C36-C18-C17	-3.14	117.72	122.82
38	a	613	CHL	C3C-C4C-NC	-3.14	106.96	114.65
21	5	618	CLA	C3B-C4B-NB	-3.14	107.72	110.53
21	L	1501	CLA	CMA-C3A-C4A	3.14	120.22	111.77
38	1	609	CHL	C4D-CHA-CBD	-3.14	105.80	108.97
21	4	603	CLA	CMA-C3A-C4A	3.14	120.22	111.77
21	8	615	CLA	C3B-C4B-NB	-3.14	107.73	110.53
21	A	1112	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
21	7	612	CLA	C2C-C1C-NC	3.14	113.28	109.98
21	A	1105	CLA	C3B-C4B-NB	-3.14	107.73	110.53
21	7	604	CLA	O1D-CGD-CBD	-3.14	118.33	124.52
23	J	4001	BCR	C27-C26-C25	-3.14	118.46	122.70
38	6	619	CHL	C1-O2A-CGA	3.14	124.25	116.65
30	8	810	PTY	C5-C6-C1	-3.14	104.47	111.78
21	B	1222	CLA	CMA-C3A-C4A	3.13	120.19	111.77
38	5	610	CHL	CHA-C1A-C2A	-3.13	125.95	133.31
21	7	617	CLA	C1C-C2C-C3C	-3.13	104.17	107.09
21	F	1302	CLA	C1-C2-C3	-3.13	121.07	126.20
23	5	503	BCR	C36-C18-C17	-3.13	117.75	122.82
38	6	613	CHL	C3C-C4C-NC	-3.12	107.02	114.65
38	3	608	CHL	C1A-CHA-C4D	3.12	124.18	118.98
21	B	1205	CLA	O2A-CGA-CBA	3.12	121.34	111.83
38	1	613	CHL	CHA-C1A-C2A	-3.12	125.99	133.31
21	B	1207	CLA	O2A-C1-C2	3.11	120.09	108.11
38	4	618	CHL	C3C-C4C-NC	-3.11	107.05	114.65
37	5	501	LUT	C11-C10-C9	-3.11	122.92	127.28
38	1	609	CHL	CHA-C1A-C2A	-3.11	126.01	133.31
23	5	504	BCR	C27-C26-C25	-3.11	118.50	122.70
38	8	601	CHL	CHA-C1A-C2A	-3.11	126.01	133.31
21	4	615	CLA	O2A-CGA-CBA	3.11	121.31	111.83
38	7	613	CHL	C4D-CHA-CBD	-3.10	105.84	108.97
23	G	4001	BCR	C12-C13-C14	-3.10	114.13	119.01
47	7	504	C7Z	C20-C13-C14	-3.10	117.79	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	609	CHL	C4D-CHA-CBD	-3.10	105.84	108.97
21	3	618	CLA	C2C-C1C-NC	3.10	113.24	109.98
21	B	1023	CLA	C3B-C4B-NB	-3.10	107.76	110.53
23	8	503	BCR	C33-C5-C4	3.10	120.20	113.60
38	5	610	CHL	C4D-CHA-CBD	-3.10	105.84	108.97
21	J	1901	CLA	C3B-C4B-NB	-3.10	107.77	110.53
23	L	4002	BCR	C12-C13-C14	-3.10	114.14	119.01
21	A	1103	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
21	A	1114	CLA	CMA-C3A-C4A	3.10	120.09	111.77
23	G	4001	BCR	C35-C13-C12	3.09	122.81	118.09
21	B	1209	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
21	B	1227	CLA	C1-C2-C3	-3.09	121.76	126.76
24	7	801	LHG	C6-C5-C4	-3.09	104.58	111.78
21	7	602	CLA	C3B-C4B-NB	-3.09	107.77	110.53
21	4	617	CLA	C2C-C1C-NC	3.09	113.23	109.98
34	J	4002	RRX	C20-C19-C18	-3.09	117.89	126.36
21	5	617	CLA	C1-C2-C3	-3.09	121.76	126.76
21	A	1141	CLA	C2C-C1C-NC	3.09	113.23	109.98
21	B	1202	CLA	C3B-C4B-NB	-3.09	107.77	110.53
21	7	609	CLA	C3B-C4B-NB	-3.09	107.77	110.53
21	6	607	CLA	C1-C2-C3	-3.09	121.14	126.20
21	A	1012	CLA	C3B-C4B-NB	-3.09	107.77	110.53
21	B	1214	CLA	O2A-C1-C2	3.09	119.98	108.11
23	3	503	BCR	C38-C26-C25	-3.08	121.12	124.48
21	5	609	CLA	CMA-C3A-C4A	3.08	120.06	111.77
38	6	610	CHL	C3C-C4C-NC	-3.08	107.11	114.65
21	8	608	CLA	C3B-C4B-NB	-3.08	107.78	110.53
21	3	603	CLA	C3B-C4B-NB	-3.08	107.78	110.53
21	B	1214	CLA	C1-C2-C3	-3.08	121.15	126.20
23	A	4003	BCR	C27-C26-C25	-3.08	118.54	122.70
23	A	4005	BCR	C23-C24-C25	-3.08	118.77	127.00
21	B	1217	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
21	4	612	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
21	A	1120	CLA	C3B-C4B-NB	-3.07	107.79	110.53
38	3	611	CHL	C1-C2-C3	-3.07	121.16	126.20
37	6	502	LUT	C36-C21-C26	3.07	114.20	109.55
21	A	1102	CLA	O2A-CGA-CBA	3.07	121.19	111.83
38	6	611	CHL	C1A-CHA-C4D	3.07	124.10	118.98
21	A	1119	CLA	C3B-C4B-NB	-3.07	107.79	110.53
21	4	608	CLA	O2A-CGA-CBA	3.07	121.18	111.83
23	6	504	BCR	C8-C9-C10	3.06	123.83	119.01
21	7	617	CLA	C2C-C1C-NC	3.06	113.20	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1102	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
21	8	612	CLA	C3B-C4B-NB	-3.06	107.80	110.53
34	J	4002	RRX	C7-C6-C5	-3.06	114.51	121.56
23	K	4002	BCR	C15-C14-C13	-3.06	122.99	127.28
38	7	613	CHL	C1A-CHA-C4D	3.06	124.08	118.98
34	J	4002	RRX	C11-C12-C13	-3.06	117.98	126.36
21	4	615	CLA	C1-O2A-CGA	3.05	124.04	116.65
21	A	1113	CLA	C1-C2-C3	-3.05	121.19	126.20
21	B	1221	CLA	O2D-CGD-O1D	-3.05	117.90	123.85
21	B	1236	CLA	C3B-C4B-NB	-3.05	107.80	110.53
21	K	1402	CLA	C3B-C4B-NB	-3.05	107.81	110.53
21	4	612	CLA	O2A-C1-C2	3.05	119.85	108.11
21	A	1140	CLA	C3B-C4B-NB	-3.05	107.81	110.53
20	A	1011	CL0	CAA-C2A-C3A	-3.05	104.75	113.00
23	A	4002	BCR	C36-C18-C17	-3.05	117.88	122.82
21	B	1225	CLA	C3B-C4B-NB	-3.05	107.81	110.53
21	1	602	CLA	C4B-CHC-C1C	3.05	133.41	126.25
36	M	4001	ECH	C7-C8-C9	-3.05	121.73	126.23
21	A	1123	CLA	CMA-C3A-C4A	3.05	119.96	111.77
24	F	5001	LHG	O8-C23-C24	3.04	121.12	111.83
38	1	613	CHL	C3C-C4C-NC	-3.04	107.21	114.65
21	1	602	CLA	C3B-C4B-NB	-3.04	107.81	110.53
21	1	612	CLA	O2A-CGA-CBA	3.04	121.11	111.83
21	B	1240	CLA	C2C-C1C-NC	3.04	113.17	109.98
38	6	611	CHL	C1-C2-C3	-3.04	121.84	126.76
21	6	602	CLA	C3B-C4B-NB	-3.04	107.82	110.53
37	a	503	LUT	C26-C27-C28	-3.04	119.85	124.58
21	A	1104	CLA	C1C-C2C-C3C	-3.04	103.78	106.98
21	G	1603	CLA	C3B-C4B-NB	-3.04	107.82	110.53
23	B	4003	BCR	C37-C22-C21	-3.04	117.90	122.82
34	J	4002	RRX	C38-C26-C27	-3.04	108.84	114.42
21	a	612	CLA	C2C-C1C-NC	3.04	113.17	109.98
21	A	1101	CLA	O2A-C1-C2	3.03	119.79	108.11
21	A	1122	CLA	C1-C2-C3	-3.03	121.22	126.20
21	8	618	CLA	CAC-C3C-C4C	3.03	128.74	124.79
21	8	609	CLA	C3B-C4B-NB	-3.03	107.82	110.53
21	6	604	CLA	C1-C2-C3	-3.03	121.23	126.20
37	4	502	LUT	C10-C11-C12	-3.03	114.42	123.20
37	8	501	LUT	C26-C27-C28	-3.03	119.87	124.58
21	B	1217	CLA	C3B-C4B-NB	-3.03	107.83	110.53
23	A	4001	BCR	C34-C9-C10	-3.03	117.91	122.82
21	A	1122	CLA	C3B-C4B-NB	-3.03	107.83	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	1	501	LUT	C7-C8-C9	-3.03	121.76	126.23
37	3	502	LUT	C35-C15-C14	-3.02	117.33	123.52
21	B	1023	CLA	C1-C2-C3	-3.02	121.25	126.20
43	8	803	DGA	CDB-CCB-CBB	-3.02	88.75	115.25
21	K	1402	CLA	CMA-C3A-C4A	3.02	119.89	111.77
21	8	618	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
21	6	603	CLA	C1-O2A-CGA	3.02	123.96	116.65
25	B	5003	DGD	O1G-C1A-C2A	3.02	121.04	111.83
21	B	1234	CLA	O2A-CGA-CBA	3.02	121.03	111.83
21	8	605	CLA	C3B-C4B-NB	-3.02	107.84	110.53
23	B	4006	BCR	C12-C13-C14	-3.01	114.27	119.01
21	7	611	CLA	C1D-ND-C4D	-3.01	104.20	106.31
21	A	1102	CLA	O2A-C1-C2	3.01	119.71	108.11
21	A	1135	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
23	B	4004	BCR	C33-C5-C4	3.01	120.02	113.60
21	7	610	CLA	C1-C2-C3	-3.01	121.27	126.20
23	F	4001	BCR	C28-C27-C26	-3.01	108.69	114.06
21	B	1231	CLA	CMD-C2D-C3D	-3.01	120.79	127.69
30	8	810	PTY	O4-C30-C31	3.01	121.00	111.83
38	a	613	CHL	C4D-CHA-CBD	-3.01	105.94	108.97
34	J	4002	RRX	C33-C5-C4	3.01	120.01	113.60
21	B	1236	CLA	C4B-CHC-C1C	3.01	133.32	126.25
21	A	1113	CLA	O2A-CGA-CBA	3.01	121.00	111.83
38	4	609	CHL	C1A-CHA-C4D	3.01	124.00	118.98
21	B	1223	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
38	4	618	CHL	CHA-C1A-C2A	-3.00	126.25	133.31
23	F	4001	BCR	C27-C26-C25	-3.00	118.65	122.70
21	A	1114	CLA	O2A-CGA-CBA	3.00	120.99	111.83
21	B	1235	CLA	O2A-CGA-CBA	3.00	120.98	111.83
21	6	603	CLA	C4D-C3D-CAD	3.00	111.36	108.11
38	4	613	CHL	CHA-C1A-C2A	-3.00	126.27	133.31
21	B	1201	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
21	B	1226	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
38	a	606	CHL	C4D-CHA-CBD	-2.99	105.95	108.97
21	A	1101	CLA	C4B-CHC-C1C	2.99	133.29	126.25
21	L	1503	CLA	CAC-C3C-C2C	2.99	133.06	127.56
21	4	616	CLA	C1-C2-C3	-2.99	121.92	126.76
21	B	1227	CLA	C3B-C4B-NB	-2.99	107.86	110.53
21	4	601	CLA	CAA-C2A-C3A	-2.99	104.91	113.00
21	4	607	CLA	C1-C2-C3	-2.99	121.29	126.20
21	4	602	CLA	C3B-C4B-NB	-2.99	107.86	110.53
21	5	602	CLA	C2C-C1C-NC	2.99	113.12	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	612	CLA	C3B-C4B-NB	-2.99	107.86	110.53
38	5	613	CHL	C4D-CHA-CBD	-2.99	105.95	108.97
21	4	605	CLA	C1C-C2C-C3C	-2.99	103.84	106.98
38	a	609	CHL	C1-O2A-CGA	2.99	123.89	116.65
37	3	501	LUT	C26-C27-C28	-2.99	119.93	124.58
21	7	606	CLA	C1-C2-C3	-2.99	121.30	126.20
21	a	607	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
48	8	806	P5S	O19-C17-C20	2.99	120.94	111.83
37	1	502	LUT	C15-C14-C13	-2.99	123.09	127.28
21	B	1220	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
23	5	504	BCR	C33-C5-C4	2.98	119.96	113.60
21	A	1101	CLA	C1D-ND-C4D	-2.98	104.22	106.31
38	4	609	CHL	C1-C2-C3	-2.98	121.31	126.20
23	L	4002	BCR	C36-C18-C17	-2.98	117.98	122.82
21	4	605	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
38	a	610	CHL	C4D-CHA-CBD	-2.98	105.96	108.97
21	7	604	CLA	C3B-C4B-NB	-2.98	107.87	110.53
38	4	609	CHL	C1-O2A-CGA	2.98	123.87	116.65
21	B	1218	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
21	6	618	CLA	C3B-C4B-NB	-2.98	107.87	110.53
21	A	1139	CLA	C3B-C4B-NB	-2.98	107.87	110.53
21	5	617	CLA	C1C-C2C-C3C	-2.98	103.85	106.98
21	a	602	CLA	CMA-C3A-C4A	2.97	119.77	111.77
21	A	1105	CLA	CAC-C3C-C4C	2.97	128.66	124.79
23	L	4001	BCR	C28-C27-C26	-2.97	108.75	114.06
21	A	1121	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
21	1	611	CLA	O2A-C1-C2	2.97	119.55	108.11
21	F	1302	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
21	B	1212	CLA	C2C-C1C-NC	2.97	113.10	109.98
21	a	602	CLA	C3B-C4B-NB	-2.97	107.88	110.53
21	B	1236	CLA	C2D-C1D-ND	2.97	113.06	110.13
23	B	4003	BCR	C34-C9-C10	-2.96	118.01	122.82
21	A	1129	CLA	C3B-C4B-NB	-2.96	107.88	110.53
23	6	504	BCR	C34-C9-C10	-2.96	118.02	122.82
23	B	4005	BCR	C33-C5-C4	2.96	119.91	113.60
21	6	618	CLA	CMA-C3A-C4A	2.96	119.74	111.77
21	7	604	CLA	O2A-CGA-CBA	2.96	120.87	111.83
21	7	617	CLA	C4B-CHC-C1C	2.96	133.21	126.25
21	5	604	CLA	C1-C2-C3	-2.96	121.34	126.20
21	4	611	CLA	C3B-C4B-NB	-2.96	107.89	110.53
24	8	801	LHG	C5-O7-C7	-2.96	110.72	117.80
24	3	801	LHG	O8-C23-C24	2.96	120.86	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	4002	BCR	C35-C13-C12	2.96	122.61	118.09
21	3	618	CLA	C1C-C2C-C3C	-2.96	103.87	106.98
23	3	503	BCR	C36-C18-C17	-2.95	118.03	122.82
21	7	605	CLA	C1D-ND-C4D	-2.95	104.24	106.31
23	B	4006	BCR	C35-C13-C12	2.95	122.60	118.09
21	4	604	CLA	C4B-CHC-C1C	2.95	133.19	126.25
21	B	1230	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
37	a	503	LUT	C31-C32-C33	-2.95	118.28	126.36
21	B	1239	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
21	6	604	CLA	C1D-ND-C4D	-2.95	104.25	106.31
21	K	1401	CLA	C3B-C4B-NB	-2.95	107.90	110.53
37	6	501	LUT	C15-C14-C13	-2.94	123.15	127.28
21	A	1108	CLA	CMA-C3A-C4A	2.94	119.69	111.77
21	5	602	CLA	C3B-C4B-NB	-2.94	107.90	110.53
21	A	1125	CLA	CAC-C3C-C4C	2.94	128.62	124.79
21	a	603	CLA	CMA-C3A-C4A	2.94	119.68	111.77
23	B	4003	BCR	C8-C9-C10	2.94	123.63	119.01
37	4	501	LUT	C35-C15-C14	-2.94	117.50	123.52
21	A	1110	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
37	4	501	LUT	C15-C14-C13	-2.94	123.16	127.28
38	4	618	CHL	C4D-CHA-CBD	-2.94	106.01	108.97
21	A	1115	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
21	B	1228	CLA	C1D-ND-C4D	-2.94	104.25	106.31
21	5	608	CLA	O1D-CGD-CBD	-2.94	118.73	124.52
21	A	1129	CLA	O2D-CGD-O1D	-2.94	118.14	123.85
21	A	1125	CLA	C1D-ND-C4D	-2.93	104.25	106.31
21	5	617	CLA	C3B-C4B-NB	-2.93	107.91	110.53
21	A	1110	CLA	C1-C2-C3	-2.93	121.39	126.20
21	A	1105	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
23	K	4001	BCR	C15-C14-C13	-2.93	123.17	127.28
21	4	605	CLA	C2C-C1C-NC	2.93	113.06	109.98
38	a	606	CHL	C3C-C4C-NC	-2.93	107.49	114.65
21	B	1202	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
23	B	4003	BCR	C33-C5-C4	2.93	119.84	113.60
21	1	605	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
21	F	1301	CLA	C3B-C4B-NB	-2.93	107.92	110.53
23	6	504	BCR	C27-C26-C25	-2.93	118.75	122.70
23	6	503	BCR	C19-C18-C17	2.93	123.61	119.01
21	B	1231	CLA	C3B-C4B-NB	-2.93	107.92	110.53
21	A	1136	CLA	CMA-C3A-C4A	2.93	119.64	111.77
21	B	1228	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
21	8	606	CLA	C2C-C1C-NC	2.92	113.05	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	5	609	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
21	1	606	CLA	CMD-C2D-C3D	-2.92	120.99	127.69
21	5	603	CLA	C1-O2A-CGA	2.92	123.72	116.65
21	B	1234	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
21	A	1105	CLA	C1D-ND-C4D	-2.92	104.26	106.31
21	B	1222	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
21	7	603	CLA	CMA-C3A-C4A	2.92	119.61	111.77
21	A	1140	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
24	A	5001	LHG	O8-C23-C24	2.92	120.72	111.83
21	8	609	CLA	O2A-CGA-CBA	2.91	120.72	111.83
21	K	1403	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
21	F	1301	CLA	C4B-CHC-C1C	2.91	133.10	126.25
23	3	503	BCR	C35-C13-C12	2.91	122.54	118.09
37	3	502	LUT	C10-C11-C12	-2.91	114.76	123.20
21	B	1229	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
21	B	1202	CLA	O2A-CGA-CBA	2.91	120.71	111.83
24	6	802	LHG	O8-C23-C24	2.91	120.71	111.83
21	A	1109	CLA	C2C-C1C-NC	2.91	113.04	109.98
21	A	1102	CLA	CHD-C4C-C3C	2.91	129.02	124.77
21	4	607	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
21	A	1118	CLA	C3B-C4B-NB	-2.91	107.93	110.53
21	7	617	CLA	C1-C2-C3	-2.91	121.43	126.20
21	A	1105	CLA	C4B-CHC-C1C	2.91	133.09	126.25
23	6	504	BCR	C4-C5-C6	-2.91	118.78	122.70
21	A	1106	CLA	C4B-CHC-C1C	2.91	133.08	126.25
37	a	502	LUT	C22-C23-C24	-2.91	106.87	111.18
21	A	1132	CLA	O2D-CGD-O1D	-2.90	118.19	123.85
21	B	1239	CLA	C3B-C4B-NB	-2.90	107.94	110.53
21	4	617	CLA	C1C-C2C-C3C	-2.90	103.92	106.98
21	A	1102	CLA	C2D-C1D-ND	2.90	113.00	110.13
21	A	1137	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
21	1	604	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
30	B	5005	PTY	O4-C30-C31	2.90	120.68	111.83
28	A	5008	LMT	O1'-C1'-C2'	2.90	112.68	108.27
21	A	1107	CLA	C3B-C4B-NB	-2.90	107.94	110.53
21	a	607	CLA	C3B-C4B-NB	-2.90	107.94	110.53
38	3	608	CHL	C4D-CHA-CBD	-2.90	106.04	108.97
21	8	618	CLA	C2C-C1C-NC	2.90	113.03	109.98
21	4	611	CLA	CMA-C3A-C4A	2.90	119.57	111.77
21	1	603	CLA	C3B-C4B-NB	-2.90	107.94	110.53
21	7	604	CLA	C1D-ND-C4D	-2.90	104.28	106.31
21	a	604	CLA	O2A-CGA-CBA	2.90	120.67	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	618	CLA	C4B-CHC-C1C	2.90	133.06	126.25
21	B	1232	CLA	C2C-C1C-NC	2.90	113.02	109.98
38	6	611	CHL	C4D-CHA-CBD	-2.90	106.05	108.97
21	A	1125	CLA	C2D-C1D-ND	2.89	112.99	110.13
21	A	1121	CLA	CMD-C2D-C3D	-2.89	121.05	127.69
21	6	606	CLA	CMA-C3A-C4A	2.89	119.55	111.77
21	B	1219	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
21	8	602	CLA	C3B-C4B-NB	-2.89	107.95	110.53
21	7	606	CLA	C1D-ND-C4D	-2.89	104.28	106.31
21	B	1209	CLA	C4B-CHC-C1C	2.89	133.04	126.25
21	B	1214	CLA	C1C-C2C-C3C	-2.89	103.94	106.98
38	6	613	CHL	C4D-CHA-CBD	-2.89	106.06	108.97
21	3	616	CLA	C2C-C1C-NC	2.89	113.01	109.98
37	7	501	LUT	C31-C30-C29	-2.89	123.23	127.28
21	3	604	CLA	C1-C2-C3	-2.89	121.47	126.20
21	6	603	CLA	O2A-CGA-CBA	2.88	120.63	111.83
38	3	611	CHL	C4D-CHA-CBD	-2.88	106.06	108.97
37	8	502	LUT	C35-C15-C14	-2.88	117.62	123.52
21	8	606	CLA	C1C-C2C-C3C	-2.88	103.95	106.98
21	A	1122	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
46	8	807	4RF	O18-C16-C15	2.88	120.62	111.83
37	3	501	LUT	C11-C10-C9	-2.88	123.24	127.28
21	5	617	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
47	7	504	C7Z	C7-C8-C9	-2.88	121.97	126.23
21	3	616	CLA	O2A-CGA-CBA	2.88	120.61	111.83
21	6	604	CLA	O1D-CGD-CBD	-2.88	118.84	124.52
21	1	602	CLA	C2C-C1C-NC	2.88	113.00	109.98
21	4	610	CLA	C2C-C1C-NC	2.88	113.00	109.98
21	5	606	CLA	C3B-C4B-NB	-2.88	107.96	110.53
28	1	804	LMT	C1'-O5'-C5'	-2.88	108.10	113.72
21	5	616	CLA	C3B-C4B-NB	-2.88	107.96	110.53
23	5	503	BCR	C33-C5-C4	2.88	119.73	113.60
21	K	1403	CLA	C2C-C1C-NC	2.88	113.00	109.98
21	5	609	CLA	C2C-C1C-NC	2.88	113.00	109.98
21	7	615	CLA	O2A-CGA-CBA	2.88	120.60	111.83
21	A	1134	CLA	C2C-C1C-NC	2.87	113.00	109.98
21	1	607	CLA	C2C-C1C-NC	2.87	113.00	109.98
37	5	501	LUT	C10-C11-C12	-2.87	114.87	123.20
23	3	503	BCR	C37-C22-C23	2.87	122.48	118.09
24	5	801	LHG	O8-C23-C24	2.87	120.59	111.83
21	6	603	CLA	CHA-C4D-ND	2.87	138.47	132.55
21	B	1204	CLA	C2C-C1C-NC	2.87	113.00	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	801	LHG	O8-C23-C24	2.87	120.58	111.83
37	6	502	LUT	C7-C8-C9	-2.87	121.99	126.23
21	1	611	CLA	C1C-C2C-C3C	-2.87	103.97	106.98
38	6	619	CHL	CMA-C3A-C4A	2.87	120.79	114.61
21	7	601	CLA	C1-C2-C3	-2.86	121.50	126.20
21	4	602	CLA	CMA-C3A-C4A	2.86	119.47	111.77
21	A	1133	CLA	C3B-C4B-NB	-2.86	107.97	110.53
21	6	604	CLA	O2A-CGA-CBA	2.86	120.57	111.83
21	3	604	CLA	O2A-CGA-CBA	2.86	120.56	111.83
22	B	2002	PQN	C14-C13-C15	2.86	120.19	115.23
21	B	1210	CLA	O1D-CGD-CBD	-2.86	118.87	124.52
21	F	1301	CLA	C2C-C1C-NC	2.86	112.99	109.98
21	A	1137	CLA	C3B-C4B-NB	-2.86	107.98	110.53
43	5	803	DGA	OG1-CA1-CA2	2.86	120.55	111.83
21	a	611	CLA	CMA-C3A-C4A	2.86	119.45	111.77
21	K	1402	CLA	C1D-ND-C4D	-2.86	104.31	106.31
21	B	1239	CLA	C2C-C1C-NC	2.86	112.98	109.98
21	8	620	CLA	CAA-CBA-CGA	-2.86	105.10	113.21
21	5	607	CLA	C4B-CHC-C1C	2.86	132.96	126.25
21	B	1236	CLA	C2C-C1C-NC	2.86	112.98	109.98
21	G	1601	CLA	C2C-C1C-NC	2.86	112.98	109.98
21	B	1215	CLA	C1-C2-C3	-2.86	121.52	126.20
21	A	1130	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
21	A	1141	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
21	4	603	CLA	C1-O2A-CGA	2.85	123.56	116.65
21	3	602	CLA	C2C-C1C-NC	2.85	112.98	109.98
37	8	501	LUT	C10-C11-C12	-2.85	114.94	123.20
21	7	610	CLA	C2C-C1C-NC	2.85	112.98	109.98
21	A	1101	CLA	C2C-C1C-NC	2.85	112.98	109.98
21	L	1502	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
21	B	1215	CLA	C3B-C4B-NB	-2.85	107.99	110.53
21	A	1121	CLA	C2C-C1C-NC	2.85	112.97	109.98
21	1	602	CLA	C1D-ND-C4D	-2.85	104.31	106.31
24	A	5003	LHG	O8-C23-C24	2.85	120.52	111.83
21	B	1210	CLA	C2C-C1C-NC	2.85	112.97	109.98
21	B	1234	CLA	C4B-CHC-C1C	2.84	132.93	126.25
21	5	604	CLA	O2A-CGA-CBA	2.84	120.50	111.83
24	A	5002	LHG	O8-C23-C24	2.84	120.50	111.83
24	7	802	LHG	O8-C23-C24	2.84	120.50	111.83
21	A	1109	CLA	CMA-C3A-C4A	2.84	119.41	111.77
21	G	1602	CLA	C3B-C4B-NB	-2.84	107.99	110.53
21	3	603	CLA	O2D-CGD-O1D	-2.84	118.32	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	601	CLA	C4B-CHC-C1C	2.84	132.93	126.25
21	K	1404	CLA	C2C-C1C-NC	2.84	112.96	109.98
21	7	608	CLA	C2C-C1C-NC	2.84	112.96	109.98
21	8	610	CLA	C2C-C1C-NC	2.84	112.96	109.98
21	3	607	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
21	6	603	CLA	C4B-CHC-C1C	2.84	132.92	126.25
21	F	1301	CLA	C1D-ND-C4D	-2.84	104.32	106.31
21	F	1301	CLA	O2A-CGA-CBA	2.83	120.48	111.83
21	1	604	CLA	C1C-C2C-C3C	-2.83	104.00	106.98
47	7	504	C7Z	C12-C13-C14	2.83	123.46	119.01
23	B	4003	BCR	C27-C26-C25	-2.83	118.88	122.70
25	A	5005	DGD	C6D-O5D-C1E	-2.83	107.73	113.80
21	B	1234	CLA	C2D-C1D-ND	2.83	112.93	110.13
21	B	1213	CLA	O2A-CGA-CBA	2.83	120.46	111.83
21	L	1503	CLA	CMA-C3A-C4A	2.83	119.38	111.77
21	B	1239	CLA	C1C-C2C-C3C	-2.83	104.00	106.98
37	8	501	LUT	C31-C30-C29	-2.83	123.31	127.28
21	B	1240	CLA	C1C-C2C-C3C	-2.83	104.00	106.98
21	3	616	CLA	CMA-C3A-C4A	2.83	119.37	111.77
21	F	1302	CLA	C3B-C4B-NB	-2.83	108.01	110.53
21	5	612	CLA	C3B-C4B-NB	-2.83	108.01	110.53
21	4	604	CLA	O2A-CGA-CBA	2.83	120.45	111.83
21	A	1122	CLA	O2A-CGA-CBA	2.83	120.45	111.83
21	6	617	CLA	C1C-C2C-C3C	-2.83	104.01	106.98
35	J	5001	LPX	O3-P1-O4	2.83	125.59	112.44
23	I	4001	BCR	C12-C13-C14	-2.83	114.56	119.01
21	A	1012	CLA	O2A-CGA-CBA	2.83	120.45	111.83
37	8	501	LUT	C35-C34-C33	-2.83	123.32	127.28
23	A	4005	BCR	C35-C13-C12	2.82	122.40	118.09
21	B	1223	CLA	C3B-C4B-NB	-2.82	108.01	110.53
21	4	610	CLA	C1C-C2C-C3C	-2.82	104.01	106.98
21	1	605	CLA	C1C-C2C-C3C	-2.82	104.01	106.98
21	5	605	CLA	C3B-C4B-NB	-2.82	108.01	110.53
21	B	1220	CLA	C3B-C4B-NB	-2.82	108.01	110.53
21	A	1012	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
21	1	607	CLA	CMA-C3A-C4A	2.82	119.35	111.77
29	B	5004	PCW	O2-C31-C32	2.82	117.58	111.48
21	3	607	CLA	C1C-C2C-C3C	-2.82	104.02	106.98
21	A	1108	CLA	C4B-CHC-C1C	2.82	132.88	126.25
21	A	1104	CLA	C3B-C4B-NB	-2.82	108.02	110.53
21	5	605	CLA	C1C-C2C-C3C	-2.82	104.02	106.98
21	5	618	CLA	C1C-C2C-C3C	-2.82	104.02	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1141	CLA	CMA-C3A-C4A	2.82	119.34	111.77
21	8	602	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
21	A	1139	CLA	C2C-C1C-NC	2.82	112.94	109.98
21	5	607	CLA	C3B-C4B-NB	-2.82	108.02	110.53
37	5	505	LUT	C31-C30-C29	-2.82	123.33	127.28
21	8	605	CLA	C4B-CHC-C1C	2.82	132.87	126.25
21	4	603	CLA	C2C-C1C-NC	2.81	112.94	109.98
21	4	606	CLA	C2C-C1C-NC	2.81	112.94	109.98
21	4	611	CLA	C1-C2-C3	-2.81	121.59	126.20
21	A	1136	CLA	C3B-C4B-NB	-2.81	108.02	110.53
21	A	1107	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
23	L	4001	BCR	C33-C5-C4	2.81	119.59	113.60
21	B	1021	CLA	C3B-C4B-NB	-2.81	108.02	110.53
21	B	1232	CLA	C3B-C4B-NB	-2.81	108.02	110.53
21	4	604	CLA	C1C-C2C-C3C	-2.81	104.02	106.98
21	3	607	CLA	CMA-C3A-C4A	2.81	119.33	111.77
33	G	5002	ERG	C13-C14-C8	2.81	118.54	113.59
21	A	1134	CLA	C1C-C2C-C3C	-2.81	104.02	106.98
21	A	1133	CLA	C1C-C2C-C3C	-2.81	104.02	106.98
21	7	617	CLA	CMA-C3A-C4A	2.81	119.33	111.77
26	A	5007	3PH	O31-C31-C32	2.81	120.40	111.83
21	1	610	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
21	A	1107	CLA	C1D-ND-C4D	-2.81	104.34	106.31
23	4	503	BCR	C36-C18-C17	-2.81	118.27	122.82
21	A	1133	CLA	C2C-C1C-NC	2.81	112.93	109.98
21	7	615	CLA	C3B-C4B-NB	-2.81	108.03	110.53
21	7	603	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
21	5	608	CLA	C3B-C4B-NB	-2.80	108.03	110.53
23	3	503	BCR	C12-C13-C14	-2.80	114.60	119.01
21	F	1302	CLA	CMA-C3A-C4A	2.80	119.31	111.77
21	7	607	CLA	C2C-C1C-NC	2.80	112.93	109.98
21	3	603	CLA	CMA-C3A-C4A	2.80	119.31	111.77
21	A	1108	CLA	C3B-C4B-NB	-2.80	108.03	110.53
21	F	1302	CLA	C2D-C1D-ND	2.80	112.90	110.13
21	B	1221	CLA	C1-C2-C3	-2.80	121.61	126.20
21	B	1240	CLA	CMA-C3A-C4A	2.80	119.31	111.77
21	K	1403	CLA	CMA-C3A-C4A	2.80	119.31	111.77
21	B	1212	CLA	C1C-C2C-C3C	-2.80	104.03	106.98
21	1	607	CLA	C1D-ND-C4D	-2.80	104.35	106.31
21	A	1114	CLA	OBD-CAD-C3D	-2.80	121.87	128.42
21	B	1226	CLA	C1-C2-C3	-2.80	121.61	126.20
21	B	1211	CLA	C1-C2-C3	-2.80	121.61	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1131	CLA	C3B-C4B-NB	-2.80	108.03	110.53
21	4	611	CLA	C1C-C2C-C3C	-2.80	104.04	106.98
23	L	4002	BCR	C35-C13-C12	2.80	122.36	118.09
46	8	808	4RF	O40-C41-C43	2.80	120.36	111.83
21	5	618	CLA	C1-C2-C3	-2.80	121.61	126.20
21	7	608	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
21	a	607	CLA	C1C-C2C-C3C	-2.80	104.04	106.98
21	B	1207	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
37	6	501	LUT	C1-C6-C7	2.79	123.23	115.65
23	F	4001	BCR	C37-C22-C23	2.79	122.36	118.09
21	5	614	CLA	C2C-C1C-NC	2.79	112.92	109.98
21	3	613	CLA	C1C-C2C-C3C	-2.79	104.04	106.98
23	8	503	BCR	C36-C18-C17	-2.79	118.29	122.82
21	B	1234	CLA	C1-C2-C3	-2.79	121.62	126.20
21	B	1237	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
21	B	1216	CLA	C1-C2-C3	-2.79	121.62	126.20
21	3	618	CLA	C4B-CHC-C1C	2.79	132.81	126.25
24	4	801	LHG	O8-C23-C24	2.79	120.34	111.83
21	A	1109	CLA	C1C-C2C-C3C	-2.79	104.05	106.98
21	1	612	CLA	C1C-C2C-C3C	-2.79	104.05	106.98
23	A	4005	BCR	C4-C5-C6	-2.79	118.93	122.70
24	8	801	LHG	O8-C23-C24	2.79	120.34	111.83
30	5	802	PTY	O4-C30-C31	2.79	120.34	111.83
21	4	615	CLA	C1-C2-C3	-2.79	121.63	126.20
21	5	618	CLA	C4B-CHC-C1C	2.79	132.80	126.25
21	4	605	CLA	OBD-CAD-C3D	-2.79	121.90	128.42
21	B	1210	CLA	O2A-CGA-CBA	2.79	120.33	111.83
21	1	611	CLA	C3B-C4B-NB	-2.79	108.04	110.53
40	3	506	QTB	C03-C04-C05	-2.79	115.13	123.20
35	a	804	LPX	O3-P1-O4	2.79	125.40	112.44
21	8	610	CLA	O2A-CGA-CBA	2.79	120.33	111.83
46	7	807	4RF	O18-C16-C15	2.79	120.33	111.83
21	A	1013	CLA	CHD-C1D-ND	-2.79	120.88	124.80
21	A	1110	CLA	C2C-C1C-NC	2.78	112.91	109.98
21	A	1117	CLA	C2C-C1C-NC	2.78	112.91	109.98
21	8	602	CLA	C2C-C1C-NC	2.78	112.91	109.98
21	B	1231	CLA	C1-C2-C3	-2.78	121.64	126.20
21	A	1113	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
20	A	1011	CL0	C4-C3-C5	2.78	120.06	115.23
21	a	601	CLA	O2A-CGA-CBA	2.78	120.32	111.83
21	A	1120	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
21	L	1503	CLA	CAC-C3C-C4C	-2.78	121.17	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	3	613	CLA	C2C-C1C-NC	2.78	112.90	109.98
21	3	610	CLA	C1C-C2C-C3C	-2.78	104.05	106.98
21	A	1133	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
37	6	501	LUT	C22-C23-C24	-2.78	107.05	111.18
21	a	602	CLA	C4B-CHC-C1C	2.78	132.79	126.25
38	8	604	CHL	C1C-C2C-CMC	2.78	131.81	126.80
21	K	1404	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
21	7	617	CLA	C3B-C4B-NB	-2.78	108.05	110.53
21	1	601	CLA	O2A-CGA-CBA	2.78	120.31	111.83
21	L	1502	CLA	CMA-C3A-C4A	2.78	119.24	111.77
21	3	601	CLA	C1C-C2C-C3C	-2.78	104.06	106.98
37	a	502	LUT	C30-C31-C32	-2.78	115.15	123.20
23	L	4003	BCR	C35-C13-C12	2.78	122.33	118.09
21	B	1232	CLA	CMA-C3A-C4A	2.78	119.24	111.77
21	7	615	CLA	C2C-C1C-NC	2.78	112.90	109.98
21	5	607	CLA	C2C-C1C-NC	2.78	112.90	109.98
21	7	601	CLA	CAA-C2A-C3A	-2.77	105.50	113.00
21	a	603	CLA	C2C-C1C-NC	2.77	112.90	109.98
21	3	602	CLA	C1C-C2C-C3C	-2.77	104.06	106.98
21	5	602	CLA	C1C-C2C-C3C	-2.77	104.06	106.98
23	7	503	BCR	C27-C26-C25	-2.77	118.96	122.70
23	3	504	BCR	C36-C18-C17	-2.77	118.33	122.82
21	4	603	CLA	C3B-C4B-NB	-2.77	108.06	110.53
21	A	1103	CLA	C3B-C4B-NB	-2.77	108.06	110.53
21	A	1134	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
23	3	503	BCR	C19-C18-C17	2.77	123.36	119.01
37	3	501	LUT	C10-C11-C12	-2.77	115.18	123.20
21	G	1601	CLA	C3B-C4B-NB	-2.77	108.06	110.53
30	3	802	PTY	O4-C30-C31	2.77	120.28	111.83
23	3	505	BCR	C19-C18-C17	2.77	123.36	119.01
21	4	606	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
21	G	1603	CLA	CMA-C3A-C4A	2.77	119.21	111.77
23	L	4001	BCR	C29-C30-C25	2.77	114.46	110.44
21	B	1207	CLA	CAA-C2A-C3A	-2.77	105.52	113.00
24	1	802	LHG	O8-C23-C24	2.77	120.27	111.83
21	5	616	CLA	C2C-C1C-NC	2.77	112.89	109.98
37	a	502	LUT	C21-C26-C27	2.77	116.00	112.83
21	8	611	CLA	CMA-C3A-C4A	2.77	119.20	111.77
21	B	1218	CLA	O1D-CGD-CBD	-2.76	119.07	124.52
21	1	608	CLA	C3B-C4B-NB	-2.76	108.06	110.53
21	7	603	CLA	C3B-C4B-NB	-2.76	108.06	110.53
21	3	610	CLA	O2D-CGD-O1D	-2.76	118.47	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	8	603	CLA	C1-O2A-CGA	2.76	123.34	116.65
21	B	1022	CLA	C2C-C1C-NC	2.76	112.88	109.98
21	G	1602	CLA	CMA-C3A-C4A	2.76	119.20	111.77
21	B	1218	CLA	O2A-CGA-CBA	2.76	120.26	111.83
21	A	1131	CLA	CHA-C4D-ND	2.76	138.25	132.55
21	L	1503	CLA	C1C-C2C-C3C	-2.76	104.08	106.98
21	6	605	CLA	C1C-C2C-C3C	-2.76	104.08	106.98
21	3	604	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
21	4	616	CLA	C2C-C1C-NC	2.76	112.88	109.98
38	8	613	CHL	C1A-CHA-C4D	2.76	123.58	118.98
37	6	502	LUT	C27-C28-C29	-2.76	120.39	126.32
21	A	1104	CLA	C2C-C1C-NC	2.76	112.88	109.98
21	A	1109	CLA	C1D-ND-C4D	-2.76	104.38	106.31
37	4	502	LUT	C22-C23-C24	-2.76	107.09	111.18
21	4	603	CLA	C1C-C2C-C3C	-2.76	104.08	106.98
37	6	502	LUT	C26-C27-C28	-2.76	120.29	124.58
23	B	4003	BCR	C35-C13-C12	2.76	122.30	118.09
21	a	611	CLA	C2C-C1C-NC	2.76	112.88	109.98
21	A	1106	CLA	C2D-C1D-ND	2.76	112.85	110.13
37	1	503	LUT	C31-C32-C33	-2.75	118.81	126.36
21	B	1220	CLA	C2C-C1C-NC	2.75	112.88	109.98
36	M	4001	ECH	C8-C7-C6	-2.75	119.64	127.00
23	4	503	BCR	C38-C26-C25	-2.75	121.48	124.48
32	G	5001	SQD	O7-S-C6	-2.75	102.64	106.76
21	a	604	CLA	C4B-CHC-C1C	2.75	132.72	126.25
21	1	607	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
21	8	620	CLA	C1C-C2C-C3C	-2.75	104.09	106.98
21	A	1109	CLA	C3B-C4B-NB	-2.75	108.07	110.53
21	J	1901	CLA	C1D-ND-C4D	-2.75	104.38	106.31
21	B	1230	CLA	O2A-CGA-CBA	2.75	120.22	111.83
21	5	605	CLA	C2C-C1C-NC	2.75	112.87	109.98
37	3	501	LUT	C15-C14-C13	-2.75	123.42	127.28
21	6	602	CLA	C1D-ND-C4D	-2.75	104.38	106.31
21	B	1224	CLA	O2A-CGA-CBA	2.75	120.22	111.83
21	A	1112	CLA	CMA-C3A-C4A	2.75	119.16	111.77
21	6	605	CLA	C3B-C4B-NB	-2.75	108.08	110.53
21	5	617	CLA	CMA-C3A-C4A	2.74	119.15	111.77
21	G	1603	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
21	5	618	CLA	CMA-C3A-C4A	2.74	119.15	111.77
21	a	608	CLA	C1C-C2C-C3C	-2.74	104.09	106.98
23	A	4002	BCR	C19-C18-C17	2.74	123.33	119.01
21	A	1120	CLA	CMA-C3A-C4A	2.74	119.15	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	8	603	CLA	C2C-C1C-NC	2.74	112.86	109.98
21	8	620	CLA	C2C-C1C-NC	2.74	112.86	109.98
20	A	1011	CL0	O1D-CGD-CBD	-2.74	120.56	124.72
21	B	1214	CLA	C2C-C1C-NC	2.74	112.86	109.98
21	B	1224	CLA	C2C-C1C-NC	2.74	112.86	109.98
37	3	501	LUT	C22-C23-C24	-2.74	107.11	111.18
24	B	5001	LHG	O8-C23-C24	2.74	120.18	111.83
21	1	601	CLA	CAA-C2A-C3A	-2.74	105.60	113.00
21	A	1124	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
37	6	501	LUT	C7-C8-C9	-2.74	122.19	126.23
21	4	612	CLA	O1D-CGD-CBD	-2.74	119.12	124.52
21	5	605	CLA	CHA-C4D-ND	2.74	138.19	132.55
23	B	4005	BCR	C8-C7-C6	-2.73	119.69	127.00
21	B	1230	CLA	CAA-CBA-CGA	-2.73	105.44	113.21
21	7	606	CLA	C3B-C4B-NB	-2.73	108.09	110.53
21	B	1219	CLA	C2C-C1C-NC	2.73	112.85	109.98
21	6	609	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
21	4	603	CLA	CHD-C1D-ND	-2.73	120.96	124.80
37	4	502	LUT	C15-C14-C13	-2.73	123.44	127.28
21	B	1231	CLA	C4B-CHC-C1C	2.73	132.67	126.25
21	3	602	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
21	A	1141	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
37	a	502	LUT	C26-C27-C28	-2.73	120.33	124.58
21	A	1104	CLA	O2A-CGA-CBA	2.73	120.17	111.83
37	5	502	LUT	C35-C15-C14	-2.73	117.93	123.52
21	A	1137	CLA	C4B-CHC-C1C	2.73	132.67	126.25
24	4	802	LHG	O8-C23-C24	2.73	120.16	111.83
21	B	1023	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
21	A	1126	CLA	C2C-C1C-NC	2.73	112.85	109.98
21	A	1121	CLA	CHA-C4D-ND	2.73	138.18	132.55
21	B	1240	CLA	C3B-C4B-NB	-2.73	108.09	110.53
40	a	504	QTB	C03-C04-C05	-2.73	115.29	123.20
21	7	610	CLA	O2A-CGA-CBA	2.73	120.16	111.83
21	G	1603	CLA	C4B-CHC-C1C	2.73	132.67	126.25
30	7	804	PTY	O4-C30-C31	2.73	120.16	111.83
21	1	608	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
23	3	503	BCR	C33-C5-C4	2.73	119.41	113.60
21	1	612	CLA	C2C-C1C-NC	2.73	112.85	109.98
21	7	610	CLA	C4B-CHC-C1C	2.73	132.66	126.25
21	A	1117	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
21	F	1301	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
37	5	501	LUT	C15-C14-C13	-2.73	123.46	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	7	617	CLA	C1D-ND-C4D	-2.73	104.40	106.31
21	B	1238	CLA	CMA-C3A-C4A	2.72	119.10	111.77
21	B	1221	CLA	CHA-C4D-ND	2.72	138.17	132.55
21	A	1123	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
21	1	606	CLA	O2A-CGA-CBA	2.72	120.14	111.83
21	7	602	CLA	C2C-C1C-NC	2.72	112.84	109.98
21	A	1132	CLA	C2C-C1C-NC	2.72	112.84	109.98
21	5	609	CLA	C1C-C2C-C3C	-2.72	104.12	106.98
23	A	4005	BCR	C33-C5-C4	2.72	119.39	113.60
38	8	601	CHL	C1-O2A-CGA	2.72	123.23	116.65
21	5	616	CLA	CMA-C3A-C4A	2.72	119.08	111.77
21	B	1223	CLA	OBD-CAD-C3D	-2.72	122.06	128.42
21	A	1128	CLA	CHA-C4D-ND	2.72	138.16	132.55
21	A	1136	CLA	C2C-C1C-NC	2.72	112.84	109.98
21	A	1131	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
21	6	604	CLA	C2C-C1C-NC	2.72	112.83	109.98
23	6	504	BCR	C8-C7-C6	-2.71	119.75	127.00
21	4	601	CLA	C2C-C1C-NC	2.71	112.83	109.98
21	L	1501	CLA	O2A-CGA-CBA	2.71	120.11	111.83
21	8	605	CLA	C1C-C2C-C3C	-2.71	104.13	106.98
23	6	503	BCR	C36-C18-C17	-2.71	118.42	122.82
21	A	1136	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
21	8	603	CLA	CMA-C3A-C4A	2.71	119.06	111.77
21	1	615	CLA	C2C-C1C-NC	2.71	112.83	109.98
21	A	1106	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
23	K	4001	BCR	C36-C18-C17	-2.71	118.42	122.82
21	6	609	CLA	O2A-CGA-CBA	2.71	120.10	111.83
21	6	608	CLA	C1C-C2C-C3C	-2.71	104.13	106.98
21	6	601	CLA	CMA-C3A-C4A	2.71	119.05	111.77
21	3	607	CLA	C2C-C1C-NC	2.71	112.83	109.98
21	7	603	CLA	O2A-CGA-CBA	2.71	120.09	111.83
21	8	603	CLA	C1C-C2C-C3C	-2.71	104.13	106.98
21	1	611	CLA	C2C-C1C-NC	2.71	112.83	109.98
37	8	501	LUT	C15-C14-C13	-2.71	123.48	127.28
21	6	605	CLA	OBD-CAD-C3D	-2.71	122.09	128.42
21	6	603	CLA	CAC-C3C-C4C	2.71	128.31	124.79
23	B	4004	BCR	C38-C26-C25	-2.71	121.53	124.48
21	1	607	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
21	a	601	CLA	CAA-C2A-C3A	-2.70	105.69	113.00
21	B	1022	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
21	B	1217	CLA	C2C-C1C-NC	2.70	112.82	109.98
21	A	1128	CLA	O2D-CGD-O1D	-2.70	118.59	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	601	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
21	A	1139	CLA	CHA-C4D-ND	2.70	138.12	132.55
21	A	1139	CLA	C4B-CHC-C1C	2.70	132.60	126.25
21	1	606	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
21	6	615	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
21	B	1226	CLA	CHD-C1D-ND	-2.70	121.00	124.80
21	B	1215	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
21	4	616	CLA	CMA-C3A-C4A	2.70	119.03	111.77
20	A	1011	CL0	C1-C2-C3	-2.70	121.77	126.20
21	A	1126	CLA	O2A-C1-C2	2.70	118.50	108.11
21	a	602	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
21	J	1901	CLA	C2C-C1C-NC	2.70	112.82	109.98
21	a	602	CLA	C2C-C1C-NC	2.70	112.82	109.98
21	A	1116	CLA	C4B-CHC-C1C	2.70	132.60	126.25
21	4	617	CLA	C3B-C4B-NB	-2.70	108.12	110.53
21	B	1221	CLA	O1D-CGD-CBD	-2.70	119.19	124.52
21	5	616	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
38	1	613	CHL	C1A-CHA-C4D	2.70	123.48	118.98
21	A	1124	CLA	CMA-C3A-C4A	2.70	119.02	111.77
23	B	4004	BCR	C35-C13-C12	2.70	122.21	118.09
21	B	1214	CLA	O2A-CGA-CBA	2.70	120.06	111.83
28	B	5006	LMT	C1'-O5'-C5'	-2.70	108.46	113.72
21	B	1228	CLA	CHD-C1D-ND	-2.69	121.01	124.80
21	B	1240	CLA	C4B-CHC-C1C	2.69	132.58	126.25
21	B	1207	CLA	C4B-CHC-C1C	2.69	132.58	126.25
21	B	1239	CLA	O2A-CGA-CBA	2.69	120.05	111.83
21	4	607	CLA	C3B-C4B-NB	-2.69	108.12	110.53
21	J	1901	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
21	B	1222	CLA	C2C-C1C-NC	2.69	112.81	109.98
21	6	606	CLA	C2C-C1C-NC	2.69	112.81	109.98
21	5	607	CLA	CMA-C3A-C4A	2.69	119.01	111.77
38	a	606	CHL	C1-C2-C3	-2.69	121.78	126.20
21	4	606	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
21	7	609	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
21	L	1501	CLA	C2C-C1C-NC	2.69	112.81	109.98
21	7	608	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
21	G	1603	CLA	C1D-ND-C4D	-2.69	104.42	106.31
21	4	615	CLA	C2C-C1C-NC	2.69	112.81	109.98
21	B	1240	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
21	A	1114	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
21	1	608	CLA	C2C-C1C-NC	2.69	112.81	109.98
21	K	1404	CLA	C3B-C4B-NB	-2.69	108.13	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	8	602	CLA	CMA-C3A-C4A	2.69	118.99	111.77
21	8	620	CLA	O2A-CGA-CBA	2.69	120.03	111.83
21	A	1135	CLA	C1C-C2C-C3C	-2.69	104.16	106.98
23	L	4001	BCR	C40-C30-C25	-2.69	106.03	110.24
21	a	604	CLA	CMA-C3A-C4A	2.69	118.99	111.77
21	8	602	CLA	C4B-CHC-C1C	2.69	132.56	126.25
21	A	1134	CLA	C3B-C4B-NB	-2.69	108.13	110.53
21	7	610	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
21	A	1107	CLA	C2C-C1C-NC	2.68	112.80	109.98
21	B	1228	CLA	C7-C6-C5	-2.68	106.11	113.26
21	B	1216	CLA	C3B-C4B-NB	-2.68	108.13	110.53
21	8	609	CLA	C4B-CHC-C1C	2.68	132.56	126.25
21	B	1218	CLA	CHD-C1D-ND	-2.68	121.03	124.80
37	6	501	LUT	C7-C6-C5	-2.68	115.38	121.56
21	A	1013	CLA	CAA-C2A-C3A	-2.68	105.75	113.00
34	J	4002	RRX	C27-C26-C25	-2.68	115.25	120.76
38	6	613	CHL	C1-O2A-CGA	2.68	123.14	116.65
21	1	602	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
21	3	605	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
21	A	1139	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
21	1	611	CLA	CMA-C3A-C4A	2.68	118.98	111.77
21	5	604	CLA	CED-O2D-CGD	2.68	121.99	115.92
21	a	611	CLA	C3B-C4B-NB	-2.68	108.14	110.53
21	3	616	CLA	C4B-CHC-C1C	2.68	132.55	126.25
21	8	612	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
21	A	1120	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
21	a	607	CLA	C2C-C1C-NC	2.68	112.80	109.98
21	B	1022	CLA	O2A-CGA-CBA	2.68	120.00	111.83
21	1	603	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
21	A	1124	CLA	C3B-C4B-NB	-2.68	108.14	110.53
21	A	1135	CLA	C2C-C1C-NC	2.68	112.79	109.98
21	5	603	CLA	C2C-C1C-NC	2.68	112.79	109.98
38	4	613	CHL	C1A-CHA-C4D	2.68	123.45	118.98
21	A	1110	CLA	C1C-C2C-C3C	-2.68	104.17	106.98
21	6	609	CLA	C2C-C1C-NC	2.68	112.79	109.98
21	a	612	CLA	O2A-CGA-CBA	2.68	120.00	111.83
21	7	608	CLA	C3B-C4B-NB	-2.68	108.14	110.53
46	8	807	4RF	O40-C41-C43	2.67	119.99	111.83
21	7	604	CLA	C4B-CHC-C1C	2.67	132.53	126.25
21	5	617	CLA	CMC-C2C-C3C	2.67	133.38	126.15
21	K	1403	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
21	a	607	CLA	CMA-C3A-C4A	2.67	118.96	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	3	612	CLA	C1-C2-C3	-2.67	121.82	126.20
40	a	504	QTB	C19-C17-C11	-2.67	106.82	110.58
21	6	617	CLA	C2C-C1C-NC	2.67	112.79	109.98
21	7	602	CLA	CMA-C3A-C4A	2.67	118.95	111.77
21	1	615	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
21	1	605	CLA	C2C-C1C-NC	2.67	112.79	109.98
33	G	5002	ERG	C16-C17-C13	2.67	106.98	103.84
21	B	1218	CLA	C3B-C4B-NB	-2.67	108.15	110.53
21	7	606	CLA	C4B-CHC-C1C	2.67	132.52	126.25
47	7	504	C7Z	C1-C6-C7	2.67	122.89	115.65
21	A	1128	CLA	C2C-C1C-NC	2.67	112.78	109.98
21	1	603	CLA	CHD-C1D-ND	-2.67	121.05	124.80
21	A	1112	CLA	O2A-CGA-CBA	2.67	119.97	111.83
21	5	607	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
21	7	611	CLA	C2C-C1C-NC	2.67	112.78	109.98
21	3	603	CLA	O2A-CGA-CBA	2.67	119.97	111.83
21	4	616	CLA	C3B-C4B-NB	-2.67	108.15	110.53
37	6	502	LUT	C31-C32-C33	-2.67	119.05	126.36
21	B	1221	CLA	O2A-CGA-CBA	2.67	119.96	111.83
21	B	1204	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
38	8	601	CHL	C4D-CHA-CBD	-2.67	106.28	108.97
21	6	617	CLA	C3B-C4B-NB	-2.66	108.15	110.53
23	I	4001	BCR	C36-C18-C17	-2.66	118.50	122.82
21	A	1111	CLA	O2A-CGA-CBA	2.66	119.96	111.83
25	8	802	DGD	O1G-C1A-C2A	2.66	119.95	111.83
47	7	504	C7Z	C39-C29-C28	-2.66	114.02	118.09
21	3	605	CLA	CHA-C4D-ND	2.66	138.04	132.55
21	6	604	CLA	CAC-C3C-C2C	-2.66	122.67	127.56
21	B	1235	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
21	B	1204	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
21	A	1140	CLA	C4B-CHC-C1C	2.66	132.51	126.25
23	5	504	BCR	C23-C22-C21	-2.66	114.82	119.01
21	G	1601	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
21	B	1215	CLA	C4B-CHC-C1C	2.66	132.50	126.25
21	B	1231	CLA	CHA-C4D-ND	2.66	138.04	132.55
21	1	603	CLA	O2A-CGA-CBA	2.66	119.95	111.83
21	8	609	CLA	C2C-C1C-NC	2.66	112.78	109.98
37	1	501	LUT	C11-C10-C9	-2.66	123.55	127.28
23	3	505	BCR	C38-C26-C25	-2.66	121.58	124.48
21	8	611	CLA	O2A-CGA-CBA	2.66	119.94	111.83
21	B	1206	CLA	O2A-CGA-CBA	2.66	119.94	111.83
21	G	1601	CLA	O2D-CGD-O1D	-2.66	118.67	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	a	612	CLA	CHA-C4D-ND	2.66	138.03	132.55
21	A	1131	CLA	CMD-C2D-C3D	-2.66	121.60	127.69
21	8	606	CLA	O2A-CGA-CBA	2.66	119.93	111.83
21	8	606	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
37	5	505	LUT	C7-C8-C9	-2.66	122.31	126.23
21	A	1138	CLA	C2C-C1C-NC	2.66	112.77	109.98
21	A	1122	CLA	CMA-C3A-C4A	2.65	118.91	111.77
21	A	1136	CLA	C1C-C2C-C3C	-2.65	104.19	106.98
21	6	607	CLA	C1C-C2C-C3C	-2.65	104.19	106.98
21	6	605	CLA	CMA-C3A-C4A	2.65	118.91	111.77
21	6	608	CLA	C2C-C1C-NC	2.65	112.77	109.98
21	6	607	CLA	C2C-C1C-NC	2.65	112.77	109.98
21	6	601	CLA	C2C-C1C-NC	2.65	112.77	109.98
21	B	1218	CLA	C1C-C2C-C3C	-2.65	104.19	106.98
21	K	1403	CLA	C3B-C4B-NB	-2.65	108.16	110.53
21	3	610	CLA	C3B-C4B-NB	-2.65	108.16	110.53
21	7	607	CLA	C1C-C2C-C3C	-2.65	104.19	106.98
21	a	608	CLA	C2C-C1C-NC	2.65	112.77	109.98
21	4	615	CLA	C1C-C2C-C3C	-2.65	104.19	106.98
21	a	605	CLA	C1D-ND-C4D	-2.65	104.45	106.31
21	6	602	CLA	C1C-C2C-C3C	-2.65	104.19	106.98
21	4	602	CLA	C2C-C1C-NC	2.65	112.76	109.98
21	5	604	CLA	CMA-C3A-C4A	2.65	118.89	111.77
21	A	1114	CLA	CHA-C4D-ND	2.65	138.01	132.55
20	A	1011	CL0	O2D-CGD-O1D	-2.65	118.70	123.85
38	8	604	CHL	C4D-CHA-CBD	-2.65	106.30	108.97
21	6	607	CLA	CMA-C3A-C4A	2.65	118.88	111.77
23	K	4002	BCR	C23-C24-C25	-2.65	119.93	127.00
21	B	1021	CLA	C1C-C2C-C3C	-2.65	104.20	106.98
21	B	1217	CLA	C1C-C2C-C3C	-2.65	104.20	106.98
21	A	1138	CLA	CHA-C4D-ND	2.64	138.00	132.55
21	B	1214	CLA	O2D-CGD-O1D	-2.64	118.70	123.85
21	A	1115	CLA	C4B-CHC-C1C	2.64	132.46	126.25
34	J	4002	RRX	C2-C1-C6	2.64	114.28	110.44
21	B	1223	CLA	CHA-C4D-ND	2.64	138.00	132.55
21	3	604	CLA	CMA-C3A-C4A	2.64	118.87	111.77
21	8	618	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
23	B	4002	BCR	C30-C25-C26	-2.64	119.03	122.64
21	4	608	CLA	CHA-C4D-ND	2.64	138.00	132.55
21	K	1404	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
21	7	612	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
21	B	1225	CLA	O2D-CGD-O1D	-2.64	118.71	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	8	602	CLA	CHA-C4D-ND	2.64	137.99	132.55
21	4	605	CLA	CBC-CAC-C3C	-2.64	105.27	112.42
21	A	1140	CLA	CHA-C4D-ND	2.64	137.99	132.55
21	B	1216	CLA	O2A-CGA-CBA	2.64	119.88	111.83
21	7	609	CLA	CHA-C4D-ND	2.64	137.99	132.55
21	B	1217	CLA	C4B-CHC-C1C	2.64	132.45	126.25
21	B	1208	CLA	O2D-CGD-O1D	-2.64	118.72	123.85
21	1	615	CLA	O2D-CGD-O1D	-2.64	118.72	123.85
21	K	1402	CLA	C4B-CHC-C1C	2.64	132.45	126.25
21	B	1209	CLA	C2D-C1D-ND	2.64	112.73	110.13
24	7	801	LHG	O8-C23-C24	2.64	119.87	111.83
21	B	1222	CLA	C1C-C2C-C3C	-2.64	104.21	106.98
23	A	4004	BCR	C27-C26-C25	-2.64	119.14	122.70
21	4	615	CLA	C3B-C4B-NB	-2.63	108.18	110.53
21	A	1115	CLA	C1C-C2C-C3C	-2.63	104.21	106.98
21	a	612	CLA	C4B-CHC-C1C	2.63	132.44	126.25
21	7	611	CLA	C1-O2A-CGA	2.63	123.03	116.65
37	8	502	LUT	C30-C31-C32	-2.63	115.57	123.20
21	3	607	CLA	O2A-CGA-CBA	2.63	119.86	111.83
21	A	1123	CLA	C2C-C1C-NC	2.63	112.75	109.98
21	B	1224	CLA	C3B-C4B-NB	-2.63	108.18	110.53
21	8	607	CLA	C3B-C4B-NB	-2.63	108.18	110.53
21	A	1013	CLA	C3B-C4B-NB	-2.63	108.18	110.53
21	6	609	CLA	CHA-C4D-ND	2.63	137.98	132.55
38	4	613	CHL	C4D-CHA-CBD	-2.63	106.31	108.97
21	7	609	CLA	C2C-C1C-NC	2.63	112.75	109.98
21	B	1237	CLA	CMA-C3A-C4A	2.63	118.84	111.77
21	1	603	CLA	CMA-C3A-C4A	2.63	118.84	111.77
21	a	604	CLA	C1-C2-C3	-2.63	121.89	126.20
21	4	607	CLA	CHA-C4D-ND	2.63	137.97	132.55
21	5	614	CLA	C1C-C2C-C3C	-2.63	104.21	106.98
21	3	601	CLA	C4B-CHC-C1C	2.63	132.43	126.25
23	B	4006	BCR	C33-C5-C4	2.63	119.20	113.60
21	8	606	CLA	CAA-CBA-CGA	-2.63	105.74	113.21
21	B	1202	CLA	C2C-C1C-NC	2.63	112.74	109.98
21	B	1206	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
21	A	1110	CLA	O2A-CGA-CBA	2.63	119.84	111.83
21	A	1116	CLA	O2D-CGD-O1D	-2.63	118.74	123.85
21	B	1209	CLA	C2C-C1C-NC	2.62	112.74	109.98
21	B	1212	CLA	C3B-C4B-NB	-2.62	108.19	110.53
21	a	605	CLA	CHA-C4D-ND	2.62	137.96	132.55
32	7	805	SQD	O7-S-C6	-2.62	102.84	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	5	608	CLA	C2C-C1C-NC	2.62	112.74	109.98
21	5	603	CLA	CMA-C3A-C4A	2.62	118.82	111.77
21	B	1204	CLA	C3B-C4B-NB	-2.62	108.19	110.53
21	a	605	CLA	C3B-C4B-NB	-2.62	108.19	110.53
21	A	1106	CLA	C2C-C1C-NC	2.62	112.74	109.98
21	4	611	CLA	C2C-C1C-NC	2.62	112.74	109.98
21	A	1105	CLA	C2D-C1D-ND	2.62	112.72	110.13
23	B	4007	BCR	C19-C18-C17	2.62	123.13	119.01
21	G	1602	CLA	C1C-C2C-C3C	-2.62	104.22	106.98
21	1	601	CLA	C3B-C4B-NB	-2.62	108.19	110.53
21	8	608	CLA	C2C-C1C-NC	2.62	112.73	109.98
21	A	1135	CLA	O2A-CGA-CBA	2.62	119.83	111.83
21	B	1240	CLA	O2A-CGA-CBA	2.62	119.83	111.83
21	5	601	CLA	C4B-CHC-C1C	2.62	132.41	126.25
21	4	608	CLA	C3B-C4B-NB	-2.62	108.19	110.53
37	a	501	LUT	C35-C15-C14	-2.62	118.16	123.52
21	6	618	CLA	C2D-C1D-ND	2.62	112.72	110.13
21	A	1114	CLA	CMD-C2D-C3D	-2.62	121.68	127.69
21	A	1104	CLA	CHA-C4D-ND	2.62	137.95	132.55
21	8	618	CLA	CMA-C3A-C4A	2.62	118.81	111.77
21	A	1107	CLA	C2D-C1D-ND	2.62	112.72	110.13
21	J	1901	CLA	C4B-CHC-C1C	2.62	132.40	126.25
21	7	601	CLA	C4B-CHC-C1C	2.62	132.40	126.25
21	J	1901	CLA	CMA-C3A-C4A	2.62	118.81	111.77
21	B	1208	CLA	C1C-C2C-C3C	-2.62	104.23	106.98
21	A	1103	CLA	C4B-CHC-C1C	2.62	132.40	126.25
21	8	611	CLA	CMD-C2D-C3D	-2.62	121.69	127.69
21	B	1220	CLA	CHA-C4D-ND	2.62	137.95	132.55
38	8	601	CHL	C4C-CHD-C1D	2.62	125.43	116.07
21	3	616	CLA	C3B-C4B-NB	-2.62	108.19	110.53
21	5	605	CLA	O2D-CGD-O1D	-2.62	118.76	123.85
21	B	1211	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
21	8	615	CLA	C4B-CHC-C1C	2.61	132.40	126.25
21	7	612	CLA	CAC-C3C-C2C	-2.61	122.75	127.56
21	B	1231	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
21	4	617	CLA	C4B-CHC-C1C	2.61	132.39	126.25
21	A	1129	CLA	C2C-C1C-NC	2.61	112.73	109.98
47	7	504	C7Z	C32-C33-C34	-2.61	114.90	119.01
21	7	601	CLA	O2A-CGA-CBA	2.61	119.80	111.83
37	1	501	LUT	C10-C11-C12	-2.61	115.63	123.20
24	7	803	LHG	O8-C23-C24	2.61	119.80	111.83
47	7	504	C7Z	C38-C25-C24	2.61	119.22	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1107	CLA	CMA-C3A-C4A	2.61	118.79	111.77
21	4	605	CLA	C3B-C4B-NB	-2.61	108.20	110.53
21	7	607	CLA	C3B-C4B-NB	-2.61	108.20	110.53
21	6	605	CLA	CHA-C4D-ND	2.61	137.93	132.55
21	A	1116	CLA	O2A-CGA-CBA	2.61	119.79	111.83
21	5	601	CLA	C1C-C2C-C3C	-2.61	104.24	106.98
21	5	604	CLA	C1C-C2C-C3C	-2.61	104.24	106.98
21	A	1107	CLA	O2A-CGA-CBA	2.61	119.79	111.83
21	8	608	CLA	C4B-CHC-C1C	2.61	132.38	126.25
24	a	801	LHG	C6-C5-C4	-2.61	105.70	111.78
21	5	605	CLA	OBD-CAD-C3D	-2.61	122.32	128.42
21	L	1502	CLA	C1C-C2C-C3C	-2.61	104.24	106.98
21	7	603	CLA	C4B-CHC-C1C	2.61	132.38	126.25
21	7	601	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
21	B	1207	CLA	C3B-C4B-NB	-2.61	108.20	110.53
21	3	604	CLA	C3B-C4B-NB	-2.61	108.20	110.53
21	7	604	CLA	CMA-C3A-C4A	2.61	118.78	111.77
21	B	1216	CLA	O2D-CGD-O1D	-2.61	118.78	123.85
21	B	1202	CLA	C1C-C2C-C3C	-2.61	104.24	106.98
21	8	607	CLA	O2D-CGD-O1D	-2.61	118.78	123.85
21	B	1225	CLA	C1C-C2C-C3C	-2.61	104.24	106.98
23	J	4001	BCR	C33-C5-C4	2.60	119.15	113.60
21	4	611	CLA	CMD-C2D-C3D	-2.60	121.72	127.69
21	8	605	CLA	CHA-C4D-ND	2.60	137.92	132.55
28	B	5006	LMT	C3'-C4'-C5'	-2.60	105.16	110.93
21	A	1127	CLA	O2A-CGA-CBA	2.60	119.77	111.83
21	B	1220	CLA	O2A-CGA-CBA	2.60	119.77	111.83
21	7	611	CLA	O2A-CGA-CBA	2.60	119.77	111.83
21	4	607	CLA	C1C-C2C-C3C	-2.60	104.24	106.98
21	A	1125	CLA	O2A-CGA-CBA	2.60	119.77	111.83
21	7	605	CLA	C2D-C1D-ND	2.60	112.70	110.13
21	a	612	CLA	C3B-C4B-NB	-2.60	108.21	110.53
21	B	1203	CLA	CHA-C4D-ND	2.60	137.91	132.55
21	7	602	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
21	a	603	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
21	A	1114	CLA	C2C-C1C-NC	2.60	112.71	109.98
21	A	1124	CLA	C2C-C1C-NC	2.60	112.71	109.98
21	3	612	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
37	3	501	LUT	C8-C7-C6	-2.60	120.06	127.00
21	3	605	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
24	3	801	LHG	C5-O7-C7	-2.60	111.58	117.80
21	a	601	CLA	C4B-CHC-C1C	2.60	132.35	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	7	502	XAT	C6-C7-C8	-2.60	120.50	125.99
21	B	1221	CLA	C2C-C1C-NC	2.60	112.71	109.98
21	7	610	CLA	C3B-C4B-NB	-2.60	108.21	110.53
21	B	1228	CLA	C2A-C3A-C4A	-2.60	97.68	101.87
25	A	5005	DGD	O1G-C1A-C2A	2.59	119.74	111.83
21	B	1221	CLA	C1C-C2C-C3C	-2.59	104.25	106.98
21	B	1231	CLA	O2A-CGA-CBA	2.59	119.74	111.83
21	A	1127	CLA	C4B-CHC-C1C	2.59	132.34	126.25
21	B	1226	CLA	CMD-C2D-C3D	-2.59	121.74	127.69
21	8	609	CLA	C1C-C2C-C3C	-2.59	104.25	106.98
21	A	1131	CLA	C2C-C1C-NC	2.59	112.70	109.98
21	8	605	CLA	C2C-C1C-NC	2.59	112.70	109.98
29	6	803	PCW	O3-C11-C12	2.59	119.73	111.83
21	1	606	CLA	CHA-C4D-ND	2.59	137.89	132.55
21	A	1116	CLA	C1C-C2C-C3C	-2.59	104.26	106.98
21	3	618	CLA	CMA-C3A-C4A	2.59	118.73	111.77
21	B	1230	CLA	CAA-C2A-C1A	-2.59	103.49	111.97
21	A	1138	CLA	C1C-C2C-C3C	-2.59	104.26	106.98
21	4	615	CLA	CHA-C4D-ND	2.59	137.89	132.55
21	B	1207	CLA	C2C-C1C-NC	2.59	112.70	109.98
21	4	602	CLA	C4B-CHC-C1C	2.59	132.33	126.25
21	B	1223	CLA	CMA-C3A-C4A	2.59	118.73	111.77
21	B	1220	CLA	CMA-C3A-C4A	2.59	118.72	111.77
21	a	605	CLA	C1C-C2C-C3C	-2.59	104.26	106.98
38	8	613	CHL	C4D-CHA-CBD	-2.58	106.36	108.97
23	A	4003	BCR	C39-C30-C25	-2.58	106.19	110.24
21	B	1201	CLA	CAA-C2A-C3A	-2.58	106.02	113.00
21	B	1216	CLA	C1C-C2C-C3C	-2.58	104.26	106.98
21	4	608	CLA	O1D-CGD-CBD	-2.58	119.42	124.52
21	5	617	CLA	C4B-CHC-C1C	2.58	132.32	126.25
21	5	607	CLA	O2A-CGA-CBA	2.58	119.71	111.83
21	5	602	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
21	1	606	CLA	C2C-C1C-NC	2.58	112.69	109.98
21	a	612	CLA	C1C-C2C-C3C	-2.58	104.27	106.98
21	L	1503	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
21	1	608	CLA	CMA-C3A-C4A	2.58	118.71	111.77
21	B	1210	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
21	8	611	CLA	C1C-C2C-C3C	-2.58	104.27	106.98
21	A	1113	CLA	CMA-C3A-C4A	2.58	118.71	111.77
37	8	501	LUT	C30-C31-C32	-2.58	115.72	123.20
21	a	605	CLA	C4B-CHC-C1C	2.58	132.31	126.25
21	A	1101	CLA	CMA-C3A-C4A	2.58	118.70	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	5	611	CHL	C4D-CHA-CBD	-2.58	106.37	108.97
23	A	4005	BCR	C33-C5-C6	-2.58	121.67	124.48
21	A	1106	CLA	C1C-C2C-C3C	-2.58	104.27	106.98
21	6	618	CLA	C1C-C2C-C3C	-2.58	104.27	106.98
21	4	616	CLA	O2A-CGA-CBA	2.58	119.69	111.83
21	A	1118	CLA	C2C-C1C-NC	2.58	112.69	109.98
21	8	602	CLA	C1-O2A-CGA	2.58	122.89	116.65
21	A	1129	CLA	C1C-C2C-C3C	-2.58	104.27	106.98
21	3	610	CLA	CAA-C2A-C3A	-2.58	106.04	113.00
21	K	1403	CLA	CHD-C1D-ND	-2.58	121.18	124.80
23	L	4003	BCR	C8-C7-C6	-2.57	120.12	127.00
21	3	616	CLA	C1C-C2C-C3C	-2.57	104.27	106.98
21	5	604	CLA	CHA-C4D-ND	2.57	137.86	132.55
21	a	607	CLA	O1D-CGD-CBD	-2.57	119.44	124.52
21	7	604	CLA	C6-C5-C3	-2.57	107.20	113.47
21	B	1226	CLA	CHA-C4D-ND	2.57	137.86	132.55
21	K	1404	CLA	CHA-C4D-ND	2.57	137.86	132.55
21	B	1227	CLA	C1D-ND-C4D	-2.57	104.51	106.31
21	A	1123	CLA	C1C-C2C-C3C	-2.57	104.27	106.98
21	5	604	CLA	CHD-C1D-ND	-2.57	121.18	124.80
21	7	611	CLA	CMA-C3A-C4A	2.57	118.69	111.77
23	5	503	BCR	C19-C18-C17	2.57	123.06	119.01
23	3	503	BCR	C34-C9-C10	-2.57	118.65	122.82
21	A	1138	CLA	O2A-CGA-CBA	2.57	119.68	111.83
21	5	618	CLA	C2C-C1C-NC	2.57	112.68	109.98
37	1	502	LUT	C30-C31-C32	-2.57	115.75	123.20
21	B	1229	CLA	CHA-C4D-ND	2.57	137.86	132.55
21	B	1235	CLA	C3B-C4B-NB	-2.57	108.23	110.53
21	K	1403	CLA	CMD-C2D-C3D	-2.57	121.79	127.69
21	G	1602	CLA	C2C-C1C-NC	2.57	112.68	109.98
21	3	604	CLA	C1D-ND-C4D	-2.57	104.51	106.31
21	B	1232	CLA	C1C-C2C-C3C	-2.57	104.28	106.98
21	A	1135	CLA	C4B-CHC-C1C	2.57	132.29	126.25
21	B	1228	CLA	C1C-C2C-C3C	-2.57	104.28	106.98
21	G	1601	CLA	CMA-C3A-C4A	2.57	118.68	111.77
21	6	615	CLA	C2C-C1C-NC	2.57	112.68	109.98
20	A	1011	CL0	C1-O2A-CGA	2.57	122.87	116.65
21	7	606	CLA	CHA-C4D-ND	2.57	137.85	132.55
21	L	1501	CLA	C3B-C4B-NB	-2.57	108.24	110.53
21	6	602	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
23	K	4001	BCR	C2-C1-C6	2.57	114.17	110.44
21	6	617	CLA	C4B-CHC-C1C	2.57	132.28	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	3	618	CLA	C3B-C4B-NB	-2.57	108.24	110.53
21	5	604	CLA	C1D-ND-C4D	-2.57	104.51	106.31
21	4	616	CLA	C1C-C2C-C3C	-2.57	104.28	106.98
21	A	1122	CLA	C2C-C1C-NC	2.56	112.68	109.98
21	A	1126	CLA	C6-C5-C3	-2.56	107.22	113.47
21	B	1225	CLA	CHA-C4D-ND	2.56	137.84	132.55
21	L	1501	CLA	C1C-C2C-C3C	-2.56	104.28	106.98
37	4	501	LUT	C10-C11-C12	-2.56	115.77	123.20
21	7	612	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
38	4	609	CHL	C4C-CHD-C1D	2.56	125.24	116.07
25	8	802	DGD	C1D-O6D-C5D	-2.56	108.72	113.72
21	a	602	CLA	CHA-C4D-ND	2.56	137.83	132.55
21	7	617	CLA	CHA-C4D-ND	2.56	137.83	132.55
21	5	604	CLA	CMD-C2D-C3D	-2.56	121.82	127.69
21	B	1229	CLA	C4B-CHC-C1C	2.56	132.27	126.25
21	A	1113	CLA	C2C-C1C-NC	2.56	112.67	109.98
21	B	1022	CLA	CHA-C4D-ND	2.56	137.83	132.55
21	1	607	CLA	CHA-C4D-ND	2.56	137.83	132.55
21	7	615	CLA	CHA-C4D-ND	2.56	137.82	132.55
25	8	802	DGD	O2G-C1B-O1B	-2.56	117.73	123.70
21	8	611	CLA	CAA-CBA-CGA	-2.56	105.95	113.21
21	B	1213	CLA	CMA-C3A-C4A	2.56	118.64	111.77
21	4	605	CLA	CHA-C4D-ND	2.56	137.82	132.55
21	A	1012	CLA	C1C-C2C-C3C	-2.56	104.29	106.98
21	A	1129	CLA	O2A-CGA-CBA	2.56	119.63	111.83
21	B	1235	CLA	CHD-C1D-ND	-2.56	121.21	124.80
21	K	1402	CLA	C2D-C1D-ND	2.56	112.66	110.13
21	6	615	CLA	C3B-C4B-NB	-2.56	108.25	110.53
21	A	1119	CLA	O2A-C1-C2	2.56	117.94	108.11
21	B	1227	CLA	CHA-C4D-ND	2.55	137.82	132.55
21	5	617	CLA	CHA-C4D-ND	2.55	137.82	132.55
21	5	604	CLA	C2C-C1C-NC	2.55	112.67	109.98
21	6	605	CLA	C2C-C1C-NC	2.55	112.67	109.98
24	1	802	LHG	C5-O7-C7	-2.55	111.68	117.80
21	F	1301	CLA	CHA-C4D-ND	2.55	137.82	132.55
23	8	503	BCR	C19-C18-C17	2.55	123.03	119.01
21	4	610	CLA	CHA-C4D-ND	2.55	137.82	132.55
21	B	1205	CLA	O1D-CGD-CBD	-2.55	119.48	124.52
21	B	1223	CLA	C4B-CHC-C1C	2.55	132.25	126.25
21	7	608	CLA	CHA-C4D-ND	2.55	137.82	132.55
21	A	1108	CLA	CHA-C4D-ND	2.55	137.81	132.55
23	5	503	BCR	C35-C13-C12	2.55	121.99	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	a	603	CLA	CHA-C4D-ND	2.55	137.81	132.55
21	a	611	CLA	C1C-C2C-C3C	-2.55	104.30	106.98
21	A	1012	CLA	CHA-C4D-ND	2.55	137.81	132.55
21	A	1102	CLA	C3B-C4B-NB	-2.55	108.25	110.53
21	A	1101	CLA	CHA-C4D-ND	2.55	137.81	132.55
21	A	1103	CLA	CAA-CBA-CGA	-2.55	105.97	113.21
21	8	608	CLA	C1C-C2C-C3C	-2.55	104.30	106.98
21	B	1235	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
23	K	4001	BCR	C19-C18-C17	2.55	123.02	119.01
21	B	1235	CLA	CMA-C3A-C4A	2.55	118.62	111.77
21	A	1102	CLA	C4B-CHC-C1C	2.55	132.24	126.25
21	B	1211	CLA	O2A-CGA-CBA	2.55	119.60	111.83
21	A	1129	CLA	CHA-C4D-ND	2.55	137.81	132.55
21	5	608	CLA	C1C-C2C-C3C	-2.55	104.30	106.98
21	5	612	CLA	C1C-C2C-C3C	-2.55	104.30	106.98
21	8	607	CLA	C1C-C2C-C3C	-2.55	104.30	106.98
21	3	602	CLA	CHA-C4D-ND	2.55	137.80	132.55
21	4	612	CLA	C1C-C2C-C3C	-2.55	104.30	106.98
21	8	612	CLA	C1C-C2C-C3C	-2.55	104.30	106.98
21	F	1302	CLA	C4B-CHC-C1C	2.55	132.23	126.25
21	5	609	CLA	CHA-C4D-ND	2.55	137.80	132.55
21	B	1225	CLA	C2C-C1C-NC	2.54	112.66	109.98
21	5	614	CLA	O2D-CGD-O1D	-2.54	118.89	123.85
21	B	1211	CLA	CMD-C2D-C3D	-2.54	121.85	127.69
21	6	606	CLA	C1C-C2C-C3C	-2.54	104.30	106.98
21	B	1023	CLA	CHD-C1D-ND	-2.54	121.22	124.80
21	6	615	CLA	CHA-C4D-ND	2.54	137.80	132.55
21	B	1219	CLA	C1C-C2C-C3C	-2.54	104.31	106.98
21	8	602	CLA	C1C-C2C-C3C	-2.54	104.31	106.98
21	A	1133	CLA	C4B-CHC-C1C	2.54	132.23	126.25
21	A	1132	CLA	CAA-C2A-C3A	-2.54	106.13	113.00
21	A	1111	CLA	C4B-CHC-C1C	2.54	132.23	126.25
21	A	1134	CLA	C4B-CHC-C1C	2.54	132.22	126.25
21	5	603	CLA	CMD-C2D-C3D	-2.54	121.86	127.69
21	B	1210	CLA	C4B-CHC-C1C	2.54	132.22	126.25
37	3	501	LUT	C39-C29-C28	2.54	121.97	118.09
21	5	601	CLA	O2A-CGA-CBA	2.54	119.58	111.83
21	A	1111	CLA	C2C-C1C-NC	2.54	112.65	109.98
21	A	1104	CLA	CHD-C1D-ND	-2.54	121.23	124.80
21	B	1231	CLA	CHD-C1D-ND	-2.54	121.23	124.80
21	A	1116	CLA	CHA-C4D-ND	2.54	137.79	132.55
21	A	1132	CLA	C1C-C2C-C3C	-2.54	104.31	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	3	601	CLA	C2C-C1C-NC	2.54	112.65	109.98
21	6	606	CLA	C4B-CHC-C1C	2.54	132.22	126.25
21	4	610	CLA	CHA-C1A-NA	-2.54	120.64	126.39
21	A	1138	CLA	C4B-CHC-C1C	2.54	132.22	126.25
23	L	4001	BCR	C38-C26-C27	2.54	119.01	113.60
21	5	614	CLA	CHA-C4D-ND	2.54	137.78	132.55
21	1	606	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
21	1	610	CLA	CMA-C3A-C4A	2.54	118.59	111.77
21	B	1211	CLA	C1C-C2C-C3C	-2.54	104.31	106.98
21	5	609	CLA	C4B-CHC-C1C	2.54	132.21	126.25
21	A	1108	CLA	O1D-CGD-CBD	-2.54	119.52	124.52
21	5	602	CLA	CHA-C4D-ND	2.54	137.78	132.55
21	4	603	CLA	C4B-CHC-C1C	2.54	132.21	126.25
21	7	609	CLA	C4B-CHC-C1C	2.54	132.21	126.25
21	B	1226	CLA	C1C-C2C-C3C	-2.54	104.31	106.98
21	G	1603	CLA	C2C-C1C-NC	2.53	112.64	109.98
21	B	1021	CLA	CHA-C4D-ND	2.53	137.78	132.55
21	8	610	CLA	CHA-C4D-ND	2.53	137.78	132.55
21	6	606	CLA	C3B-C4B-NB	-2.53	108.27	110.53
21	A	1111	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
21	B	1239	CLA	C4B-CHC-C1C	2.53	132.21	126.25
21	7	612	CLA	CHA-C4D-ND	2.53	137.78	132.55
21	4	603	CLA	C1D-ND-C4D	-2.53	104.53	106.31
21	6	612	CLA	C2C-C1C-NC	2.53	112.64	109.98
23	L	4001	BCR	C37-C22-C21	-2.53	118.71	122.82
21	A	1123	CLA	CHA-C4D-ND	2.53	137.77	132.55
21	4	606	CLA	CHA-C4D-ND	2.53	137.77	132.55
21	8	612	CLA	CHA-C4D-ND	2.53	137.77	132.55
21	7	611	CLA	C1C-C2C-C3C	-2.53	104.32	106.98
21	B	1213	CLA	CHA-C4D-ND	2.53	137.77	132.55
21	7	601	CLA	CHD-C1D-ND	-2.53	121.24	124.80
21	B	1218	CLA	C1D-ND-C4D	-2.53	104.54	106.31
21	B	1209	CLA	CHA-C4D-ND	2.53	137.77	132.55
21	7	609	CLA	C1-C2-C3	-2.53	122.05	126.20
21	B	1021	CLA	C4B-CHC-C1C	2.53	132.20	126.25
21	4	611	CLA	C4B-CHC-C1C	2.53	132.20	126.25
23	G	4001	BCR	C37-C22-C21	-2.53	118.72	122.82
21	A	1132	CLA	C3B-C4B-NB	-2.53	108.27	110.53
21	5	607	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
21	B	1208	CLA	CMD-C2D-C3D	-2.53	121.89	127.69
21	3	605	CLA	C2C-C1C-NC	2.53	112.64	109.98
21	7	615	CLA	CMA-C3A-C4A	2.53	118.57	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	L	1502	CLA	C2C-C1C-NC	2.53	112.64	109.98
21	1	610	CLA	C2C-C1C-NC	2.53	112.64	109.98
21	B	1209	CLA	C3D-C2D-C1D	-2.53	102.38	105.83
21	1	602	CLA	CHA-C4D-ND	2.53	137.76	132.55
21	4	611	CLA	CHA-C4D-ND	2.53	137.76	132.55
21	B	1023	CLA	O2A-CGA-CBA	2.53	119.54	111.83
21	4	617	CLA	CHA-C4D-ND	2.53	137.76	132.55
21	A	1125	CLA	C3D-C2D-C1D	-2.53	102.38	105.83
21	B	1216	CLA	CHA-C4D-ND	2.53	137.76	132.55
23	F	4001	BCR	C38-C26-C27	2.53	118.98	113.60
21	3	601	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
21	B	1224	CLA	C1C-C2C-C3C	-2.53	104.32	106.98
21	B	1238	CLA	C1C-C2C-C3C	-2.53	104.32	106.98
21	4	610	CLA	C3B-C4B-NB	-2.52	108.28	110.53
21	A	1109	CLA	CHA-C4D-ND	2.52	137.76	132.55
21	8	610	CLA	CMA-C3A-C4A	2.52	118.56	111.77
21	5	601	CLA	CHD-C1D-ND	-2.52	121.25	124.80
21	5	612	CLA	CHD-C1D-ND	-2.52	121.25	124.80
21	K	1402	CLA	C1C-C2C-C3C	-2.52	104.33	106.98
21	A	1126	CLA	CHA-C4D-ND	2.52	137.75	132.55
34	J	4002	RRX	C4-C5-C6	-2.52	119.30	122.70
21	8	608	CLA	CHA-C1A-NA	-2.52	120.68	126.39
21	A	1121	CLA	C1C-C2C-C3C	-2.52	104.33	106.98
21	B	1211	CLA	CHA-C4D-ND	2.52	137.75	132.55
21	A	1131	CLA	CMA-C3A-C4A	2.52	118.55	111.77
21	B	1214	CLA	C6-C5-C3	-2.52	107.32	113.47
21	1	611	CLA	CHA-C4D-ND	2.52	137.75	132.55
21	A	1114	CLA	C4B-CHC-C1C	2.52	132.18	126.25
21	5	617	CLA	CMD-C2D-C3D	-2.52	121.91	127.69
21	7	603	CLA	C1C-C2C-C3C	-2.52	104.33	106.98
21	4	604	CLA	C2C-C1C-NC	2.52	112.63	109.98
21	B	1237	CLA	CHA-C4D-ND	2.52	137.75	132.55
21	3	616	CLA	C1-O2A-CGA	2.52	122.75	116.65
21	B	1208	CLA	C3B-C4B-NB	-2.52	108.28	110.53
21	A	1127	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
21	7	603	CLA	CHA-C4D-ND	2.52	137.75	132.55
23	J	4001	BCR	C23-C24-C25	-2.52	120.27	127.00
21	5	607	CLA	CHA-C4D-ND	2.52	137.75	132.55
21	B	1235	CLA	C1D-ND-C4D	-2.52	104.54	106.31
21	L	1502	CLA	C1D-ND-C4D	-2.52	104.54	106.31
21	A	1120	CLA	C4B-CHC-C1C	2.52	132.17	126.25
21	A	1013	CLA	C1C-C2C-C3C	-2.52	104.33	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	a	603	CLA	C3B-C4B-NB	-2.52	108.28	110.53
21	7	603	CLA	C2C-C1C-NC	2.52	112.63	109.98
21	B	1201	CLA	C6-C5-C3	-2.52	107.33	113.47
23	B	4005	BCR	C23-C22-C21	-2.52	115.05	119.01
38	7	613	CHL	C1-O2A-CGA	2.52	122.75	116.65
21	B	1238	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
21	G	1603	CLA	C1C-C2C-C3C	-2.52	104.33	106.98
37	6	501	LUT	C27-C28-C29	-2.52	120.91	126.32
37	5	505	LUT	C1-C6-C5	-2.52	119.20	122.64
21	4	608	CLA	CMA-C3A-C4A	2.52	118.54	111.77
21	7	605	CLA	CHA-C4D-ND	2.52	137.74	132.55
21	1	612	CLA	C3B-C4B-NB	-2.52	108.28	110.53
21	B	1203	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
21	B	1021	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
37	5	501	LUT	C39-C29-C28	2.52	121.93	118.09
21	3	606	CLA	C3B-C4B-NB	-2.51	108.28	110.53
21	4	608	CLA	O2D-CGD-O1D	-2.51	118.95	123.85
21	A	1125	CLA	CHA-C4D-ND	2.51	137.74	132.55
21	B	1208	CLA	C2C-C1C-NC	2.51	112.62	109.98
21	1	603	CLA	C1D-ND-C4D	-2.51	104.55	106.31
21	B	1219	CLA	CHA-C4D-ND	2.51	137.74	132.55
21	B	1213	CLA	O1D-CGD-CBD	-2.51	119.56	124.52
21	B	1227	CLA	C1C-C2C-C3C	-2.51	104.34	106.98
21	7	601	CLA	C3B-C4B-NB	-2.51	108.29	110.53
21	a	611	CLA	O2A-CGA-CBA	2.51	119.50	111.83
21	A	1133	CLA	CHA-C4D-ND	2.51	137.73	132.55
21	3	603	CLA	C4B-CHC-C1C	2.51	132.15	126.25
24	1	801	LHG	O8-C23-C24	2.51	119.49	111.83
21	a	608	CLA	CHA-C4D-ND	2.51	137.73	132.55
21	a	608	CLA	C3B-C4B-NB	-2.51	108.29	110.53
21	4	612	CLA	C3B-C4B-NB	-2.51	108.29	110.53
21	A	1122	CLA	CHA-C4D-ND	2.51	137.73	132.55
21	a	607	CLA	O2A-CGA-CBA	2.51	119.49	111.83
21	7	608	CLA	CMA-C3A-C4A	2.51	118.52	111.77
21	4	601	CLA	O1D-CGD-CBD	-2.51	119.57	124.52
21	B	1022	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
21	B	1238	CLA	O2A-CGA-CBA	2.51	119.48	111.83
21	A	1137	CLA	C1C-C2C-C3C	-2.51	104.34	106.98
21	B	1212	CLA	CMA-C3A-C4A	2.51	118.51	111.77
37	5	505	LUT	C39-C29-C28	2.51	121.92	118.09
21	a	608	CLA	C4B-CHC-C1C	2.51	132.14	126.25
21	B	1201	CLA	C1C-C2C-C3C	-2.51	104.34	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1140	CLA	O2A-CGA-CBA	2.51	119.48	111.83
21	5	606	CLA	O2A-CGA-CBA	2.51	119.48	111.83
21	5	612	CLA	C2C-C1C-NC	2.51	112.61	109.98
21	A	1103	CLA	C2D-C1D-ND	2.51	112.61	110.13
21	B	1219	CLA	CMA-C3A-C4A	2.51	118.51	111.77
21	8	618	CLA	CHA-C4D-ND	2.51	137.72	132.55
21	B	1225	CLA	C4B-CHC-C1C	2.51	132.14	126.25
21	5	606	CLA	O2D-CGD-O1D	-2.50	118.97	123.85
21	L	1501	CLA	O1D-CGD-CBD	-2.50	119.58	124.52
21	A	1122	CLA	C4B-CHC-C1C	2.50	132.13	126.25
21	B	1227	CLA	C4B-CHC-C1C	2.50	132.13	126.25
21	A	1103	CLA	C1D-ND-C4D	-2.50	104.56	106.31
21	7	602	CLA	C1D-ND-C4D	-2.50	104.56	106.31
21	B	1212	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
21	B	1217	CLA	CHA-C4D-ND	2.50	137.71	132.55
23	I	4001	BCR	C19-C18-C17	2.50	122.94	119.01
21	1	604	CLA	C1-O2A-CGA	2.50	122.71	116.65
21	B	1220	CLA	C1C-C2C-C3C	-2.50	104.35	106.98
21	B	1238	CLA	CHA-C4D-ND	2.50	137.71	132.55
21	7	602	CLA	CHA-C4D-ND	2.50	137.71	132.55
21	B	1214	CLA	C3B-C4B-NB	-2.50	108.30	110.53
23	5	503	BCR	C37-C22-C23	2.50	121.91	118.09
21	K	1403	CLA	CHA-C4D-ND	2.50	137.71	132.55
21	5	603	CLA	CHA-C4D-ND	2.50	137.71	132.55
21	B	1220	CLA	C1-O2A-CGA	2.50	122.70	116.65
21	A	1137	CLA	C2C-C1C-NC	2.50	112.61	109.98
21	8	603	CLA	CHA-C4D-ND	2.50	137.71	132.55
21	A	1113	CLA	C1C-C2C-C3C	-2.50	104.35	106.98
21	A	1130	CLA	C1C-C2C-C3C	-2.50	104.35	106.98
21	8	615	CLA	CHA-C4D-ND	2.50	137.70	132.55
21	B	1222	CLA	C4B-CHC-C1C	2.50	132.12	126.25
21	3	613	CLA	CHA-C4D-ND	2.50	137.70	132.55
23	A	4001	BCR	C30-C25-C24	2.50	122.42	115.65
21	B	1204	CLA	CHA-C4D-ND	2.50	137.70	132.55
21	6	608	CLA	CHA-C4D-ND	2.50	137.70	132.55
21	4	612	CLA	CHA-C4D-ND	2.50	137.70	132.55
37	1	502	LUT	C8-C7-C6	-2.50	120.33	127.00
21	7	607	CLA	CAA-C2A-C3A	-2.50	106.25	113.00
21	A	1117	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
21	1	601	CLA	C4B-CHC-C1C	2.50	132.12	126.25
21	B	1022	CLA	CHD-C1D-ND	-2.50	121.29	124.80
21	A	1126	CLA	C1C-C2C-C3C	-2.49	104.36	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	1215	CLA	O2D-CGD-O1D	-2.49	118.99	123.85
38	4	613	CHL	C1-O2A-CGA	2.49	122.69	116.65
21	A	1124	CLA	C4B-CHC-C1C	2.49	132.11	126.25
21	L	1501	CLA	C1-O2A-CGA	2.49	122.69	116.65
21	B	1239	CLA	CHA-C4D-ND	2.49	137.69	132.55
21	A	1111	CLA	CHA-C4D-ND	2.49	137.69	132.55
21	A	1118	CLA	CHA-C4D-ND	2.49	137.69	132.55
37	1	501	LUT	C22-C23-C24	-2.49	107.48	111.18
21	A	1135	CLA	OBD-CAD-C3D	-2.49	122.59	128.42
21	5	609	CLA	CAA-CBA-CGA	-2.49	106.13	113.21
21	3	610	CLA	CHA-C4D-ND	2.49	137.69	132.55
21	B	1205	CLA	C1C-C2C-C3C	-2.49	104.36	106.98
21	B	1234	CLA	CHA-C4D-ND	2.49	137.69	132.55
21	3	616	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
21	1	615	CLA	CMA-C3A-C4A	2.49	118.47	111.77
21	5	605	CLA	C4B-CHC-C1C	2.49	132.10	126.25
21	B	1209	CLA	C1C-C2C-C3C	-2.49	104.36	106.98
21	A	1113	CLA	CHD-C1D-ND	-2.49	121.30	124.80
21	B	1226	CLA	C2C-C1C-NC	2.49	112.60	109.98
21	A	1119	CLA	CHD-C1D-ND	-2.49	121.30	124.80
21	3	610	CLA	CHD-C1D-ND	-2.49	121.30	124.80
21	A	1131	CLA	O2A-CGA-CBA	2.49	119.42	111.83
21	4	608	CLA	CAA-C2A-C3A	-2.49	106.28	113.00
21	B	1229	CLA	CMA-C3A-C4A	2.49	118.46	111.77
21	G	1601	CLA	CHA-C4D-ND	2.49	137.68	132.55
21	6	601	CLA	C1C-C2C-C3C	-2.49	104.37	106.98
21	1	607	CLA	C4B-CHC-C1C	2.48	132.09	126.25
21	a	615	CLA	CHA-C4D-ND	2.48	137.68	132.55
21	a	611	CLA	CMD-C2D-C3D	-2.48	121.99	127.69
21	8	612	CLA	C2C-C1C-NC	2.48	112.59	109.98
21	A	1104	CLA	O2D-CGD-O1D	-2.48	119.01	123.85
21	B	1227	CLA	CMD-C2D-C3D	-2.48	122.00	127.69
21	A	1115	CLA	CMA-C3A-C4A	2.48	118.45	111.77
21	7	612	CLA	C2B-C1B-NB	-2.48	107.75	110.33
21	A	1119	CLA	CHA-C4D-ND	2.48	137.67	132.55
21	A	1107	CLA	C4B-CHC-C1C	2.48	132.08	126.25
23	L	4002	BCR	C19-C18-C17	2.48	122.91	119.01
21	A	1012	CLA	C2C-C1C-NC	2.48	112.59	109.98
21	A	1135	CLA	CHA-C4D-ND	2.48	137.67	132.55
21	6	612	CLA	C4B-CHC-C1C	2.48	132.08	126.25
21	A	1107	CLA	C1C-C2C-C3C	-2.48	104.37	106.98
21	B	1211	CLA	C2C-C1C-NC	2.48	112.59	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1124	CLA	O2A-CGA-CBA	2.48	119.40	111.83
21	B	1224	CLA	O1D-CGD-CBD	-2.48	119.63	124.52
21	6	617	CLA	CHA-C4D-ND	2.48	137.66	132.55
21	8	609	CLA	CHA-C4D-ND	2.48	137.66	132.55
21	4	602	CLA	C1C-C2C-C3C	-2.48	104.37	106.98
37	5	505	LUT	C35-C15-C14	-2.48	118.45	123.52
21	6	618	CLA	C2C-C1C-NC	2.48	112.59	109.98
21	5	608	CLA	CHA-C4D-ND	2.48	137.66	132.55
21	A	1110	CLA	CMA-C3A-C4A	2.48	118.44	111.77
21	4	611	CLA	CHD-C1D-ND	-2.48	121.31	124.80
21	6	604	CLA	CHD-C1D-ND	-2.48	121.31	124.80
21	A	1107	CLA	CHA-C4D-ND	2.48	137.66	132.55
21	6	602	CLA	C2C-C1C-NC	2.48	112.58	109.98
23	A	4002	BCR	C33-C5-C4	2.48	118.88	113.60
21	K	1401	CLA	CHA-C4D-ND	2.48	137.66	132.55
21	7	607	CLA	CMA-C3A-C4A	2.48	118.43	111.77
21	B	1212	CLA	O2A-CGA-CBA	2.48	119.39	111.83
21	5	616	CLA	C4B-CHC-C1C	2.48	132.07	126.25
38	8	613	CHL	C1C-C2C-CMC	2.48	131.26	126.80
21	L	1502	CLA	C3B-C4B-NB	-2.48	108.32	110.53
21	A	1134	CLA	CHA-C4D-ND	2.47	137.66	132.55
38	7	613	CHL	C1-C2-C3	-2.47	122.14	126.20
24	F	5002	LHG	O8-C23-O10	-2.47	117.44	123.63
21	A	1136	CLA	C4B-CHC-C1C	2.47	132.06	126.25
21	5	614	CLA	C4B-CHC-C1C	2.47	132.06	126.25
21	3	606	CLA	CHA-C4D-ND	2.47	137.65	132.55
21	B	1228	CLA	CBA-CAA-C2A	-2.47	106.44	113.79
21	B	1232	CLA	CHA-C4D-ND	2.47	137.65	132.55
37	7	501	LUT	C15-C14-C13	-2.47	123.81	127.28
21	A	1121	CLA	O1D-CGD-CBD	-2.47	119.64	124.52
21	A	1137	CLA	CHA-C4D-ND	2.47	137.65	132.55
21	B	1214	CLA	CHA-C4D-ND	2.47	137.65	132.55
21	B	1217	CLA	O2A-CGA-CBA	2.47	119.37	111.83
46	7	807	4RF	O40-C41-C43	2.47	119.37	111.83
21	a	601	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
21	a	604	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
21	a	601	CLA	CHA-C4D-ND	2.47	137.64	132.55
21	6	609	CLA	CHA-C1A-NA	-2.47	120.80	126.39
21	1	606	CLA	C4B-CHC-C1C	2.47	132.05	126.25
21	3	606	CLA	C4B-CHC-C1C	2.47	132.05	126.25
21	8	615	CLA	CMD-C2D-C3D	-2.47	122.03	127.69
21	B	1209	CLA	CMA-C3A-C4A	2.47	118.41	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1115	CLA	CHA-C4D-ND	2.47	137.64	132.55
21	3	618	CLA	CHA-C4D-ND	2.47	137.64	132.55
21	6	602	CLA	C4B-CHC-C1C	2.47	132.05	126.25
21	7	605	CLA	C4B-CHC-C1C	2.47	132.05	126.25
45	7	502	XAT	O4-C6-C7	-2.47	109.81	116.88
21	L	1503	CLA	C4B-CHC-C1C	2.47	132.05	126.25
21	8	603	CLA	C6-C5-C3	-2.47	107.46	113.47
21	A	1103	CLA	C1-O2A-CGA	2.47	122.62	116.65
21	K	1401	CLA	CMA-C3A-C4A	2.47	118.40	111.77
21	A	1123	CLA	CMD-C2D-C3D	-2.47	122.03	127.69
21	A	1120	CLA	O1D-CGD-CBD	-2.47	119.65	124.52
21	1	606	CLA	C3B-C4B-NB	-2.47	108.33	110.53
21	A	1108	CLA	O2A-CGA-CBA	2.47	119.35	111.83
21	1	605	CLA	CHD-C1D-ND	-2.47	121.33	124.80
21	B	1234	CLA	CAC-C3C-C2C	-2.47	123.03	127.56
21	A	1105	CLA	CHA-C4D-ND	2.47	137.63	132.55
21	A	1141	CLA	CHA-C4D-ND	2.47	137.63	132.55
21	A	1115	CLA	C2C-C1C-NC	2.46	112.57	109.98
21	A	1124	CLA	CHA-C4D-ND	2.46	137.63	132.55
21	8	609	CLA	C1D-ND-C4D	-2.46	104.58	106.31
21	A	1139	CLA	C1-O2A-CGA	2.46	122.61	116.65
21	5	606	CLA	CMA-C3A-C4A	2.46	118.39	111.77
21	7	606	CLA	CMD-C2D-C3D	-2.46	122.04	127.69
21	B	1206	CLA	CHA-C4D-ND	2.46	137.63	132.55
21	4	601	CLA	O2A-CGA-CBA	2.46	119.35	111.83
21	B	1208	CLA	CMA-C3A-C4A	2.46	118.39	111.77
21	7	607	CLA	CHA-C4D-ND	2.46	137.63	132.55
21	4	601	CLA	CMA-C3A-C4A	2.46	118.39	111.77
21	6	608	CLA	CHD-C1D-ND	-2.46	121.34	124.80
21	3	607	CLA	CHA-C4D-ND	2.46	137.63	132.55
23	3	505	BCR	C36-C18-C17	-2.46	118.83	122.82
21	A	1128	CLA	CMA-C3A-C4A	2.46	118.38	111.77
21	B	1208	CLA	O1D-CGD-CBD	-2.46	119.67	124.52
21	5	614	CLA	CMD-C2D-C3D	-2.46	122.05	127.69
21	3	604	CLA	C4B-CHC-C1C	2.46	132.03	126.25
21	6	604	CLA	C4B-CHC-C1C	2.46	132.03	126.25
21	8	611	CLA	C2C-C1C-NC	2.46	112.56	109.98
24	7	802	LHG	C5-O7-C7	-2.46	111.91	117.80
21	6	608	CLA	CMD-C2D-C3D	-2.46	122.05	127.69
21	B	1218	CLA	C4B-CHC-C1C	2.46	132.03	126.25
21	A	1134	CLA	O1D-CGD-CBD	-2.46	119.67	124.52
21	J	1901	CLA	CHA-C4D-ND	2.46	137.62	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	4005	BCR	C4-C5-C6	-2.46	119.38	122.70
21	4	608	CLA	CMD-C2D-C3D	-2.46	122.05	127.69
21	8	615	CLA	C2C-C1C-NC	2.46	112.56	109.98
21	B	1208	CLA	CHD-C1D-ND	-2.46	121.34	124.80
21	A	1128	CLA	C1C-C2C-C3C	-2.46	104.40	106.98
21	B	1231	CLA	C1C-C2C-C3C	-2.46	104.40	106.98
21	1	608	CLA	O2D-CGD-O1D	-2.46	119.07	123.85
21	B	1240	CLA	CHA-C4D-ND	2.46	137.62	132.55
21	3	612	CLA	CHA-C4D-ND	2.46	137.62	132.55
21	B	1202	CLA	C4B-CHC-C1C	2.45	132.02	126.25
21	B	1205	CLA	C2C-C1C-NC	2.45	112.56	109.98
23	B	4004	BCR	C23-C24-C25	-2.45	120.44	127.00
21	7	615	CLA	C1C-C2C-C3C	-2.45	104.40	106.98
21	a	604	CLA	CHA-C4D-ND	2.45	137.61	132.55
21	3	613	CLA	O2D-CGD-O1D	-2.45	119.07	123.85
23	L	4003	BCR	C23-C24-C25	-2.45	120.45	127.00
21	B	1205	CLA	CHA-C4D-ND	2.45	137.61	132.55
21	6	605	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
21	B	1207	CLA	CHA-C4D-ND	2.45	137.61	132.55
21	L	1503	CLA	CHA-C4D-ND	2.45	137.61	132.55
21	3	612	CLA	O2A-CGA-CBA	2.45	119.31	111.83
21	A	1118	CLA	CMA-C3A-C4A	2.45	118.36	111.77
21	A	1124	CLA	C1C-C2C-C3C	-2.45	104.40	106.98
21	5	614	CLA	C3B-C4B-NB	-2.45	108.34	110.53
21	8	606	CLA	CHD-C1D-ND	-2.45	121.36	124.80
47	7	504	C7Z	C24-C25-C26	-2.45	115.72	120.76
21	B	1230	CLA	C1D-ND-C4D	-2.45	104.59	106.31
37	6	502	LUT	C35-C15-C14	-2.45	118.51	123.52
21	F	1302	CLA	CAC-C3C-C2C	-2.45	123.06	127.56
37	1	503	LUT	C35-C15-C14	-2.45	118.51	123.52
21	A	1132	CLA	O1D-CGD-CBD	-2.45	119.69	124.52
21	B	1202	CLA	CHA-C4D-ND	2.45	137.60	132.55
21	A	1126	CLA	C3B-C4B-NB	-2.45	108.34	110.53
21	A	1101	CLA	CMD-C2D-C3D	-2.45	122.08	127.69
21	B	1237	CLA	C4B-CHC-C1C	2.45	132.00	126.25
21	B	1204	CLA	O2A-CGA-CBA	2.45	119.30	111.83
24	6	802	LHG	C5-O7-C7	-2.45	111.94	117.80
21	1	611	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
21	A	1120	CLA	CHD-C1D-ND	-2.45	121.36	124.80
21	8	618	CLA	C4B-CHC-C1C	2.45	132.00	126.25
21	8	618	CLA	C3B-C4B-NB	-2.45	108.35	110.53
21	L	1502	CLA	O2A-CGA-CBA	2.45	119.29	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	601	CLA	CHA-C4D-ND	2.45	137.59	132.55
21	a	611	CLA	CHA-C4D-ND	2.45	137.59	132.55
21	3	601	CLA	CHA-C4D-ND	2.45	137.59	132.55
21	5	618	CLA	CHA-C4D-ND	2.45	137.59	132.55
21	A	1130	CLA	C4B-CHC-C1C	2.45	132.00	126.25
21	6	601	CLA	C4B-CHC-C1C	2.45	132.00	126.25
23	L	4003	BCR	C27-C26-C25	-2.45	119.40	122.70
21	a	612	CLA	CAC-C3C-C4C	2.45	127.97	124.79
23	A	4004	BCR	C34-C9-C8	2.44	121.82	118.09
21	K	1401	CLA	C2C-C1C-NC	2.44	112.55	109.98
21	4	607	CLA	C2C-C1C-NC	2.44	112.55	109.98
21	A	1128	CLA	O1D-CGD-CBD	-2.44	119.70	124.52
21	5	603	CLA	C4B-CHC-C1C	2.44	132.00	126.25
21	1	612	CLA	CHA-C4D-ND	2.44	137.59	132.55
23	F	4001	BCR	C33-C5-C4	2.44	118.80	113.60
21	8	603	CLA	CHD-C1D-ND	-2.44	121.36	124.80
23	L	4003	BCR	C36-C18-C17	-2.44	118.86	122.82
37	6	501	LUT	C31-C32-C33	-2.44	119.67	126.36
23	B	4003	BCR	C12-C13-C14	-2.44	115.17	119.01
21	6	602	CLA	C2D-C1D-ND	2.44	112.54	110.13
21	B	1216	CLA	CAA-C2A-C3A	-2.44	106.40	113.00
24	B	5002	LHG	O8-C23-C24	2.44	119.28	111.83
21	3	604	CLA	CHD-C1D-ND	-2.44	121.37	124.80
21	A	1116	CLA	O1D-CGD-CBD	-2.44	119.71	124.52
21	A	1138	CLA	O1D-CGD-CBD	-2.44	119.71	124.52
21	5	608	CLA	CMA-C3A-C4A	2.44	118.33	111.77
23	I	4001	BCR	C35-C13-C12	2.44	121.81	118.09
23	B	4003	BCR	C29-C28-C27	2.44	116.64	111.28
21	a	603	CLA	C1-O2A-CGA	2.44	122.55	116.65
21	B	1232	CLA	C4B-CHC-C1C	2.44	131.98	126.25
21	A	1116	CLA	C2C-C1C-NC	2.44	112.54	109.98
23	K	4001	BCR	C3-C4-C5	-2.44	109.71	114.06
21	4	610	CLA	CMA-C3A-C4A	2.43	118.32	111.77
21	4	617	CLA	CMD-C2D-C3D	-2.43	122.11	127.69
21	8	602	CLA	CMD-C2D-C3D	-2.43	122.11	127.69
21	7	602	CLA	C2D-C1D-ND	2.43	112.53	110.13
36	M	4001	ECH	C11-C12-C13	-2.43	119.69	126.36
21	A	1109	CLA	CHA-C1A-NA	-2.43	120.88	126.39
21	4	608	CLA	C2C-C1C-NC	2.43	112.54	109.98
38	6	611	CHL	CMA-C3A-C4A	2.43	119.85	114.61
21	4	605	CLA	C4B-CHC-C1C	2.43	131.97	126.25
40	3	506	QTB	C11-C10-C09	2.43	130.45	125.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	615	CLA	CHA-C4D-ND	2.43	137.57	132.55
21	4	607	CLA	O1D-CGD-CBD	-2.43	119.72	124.52
37	1	501	LUT	C8-C7-C6	-2.43	120.50	127.00
21	B	1213	CLA	C4B-CHC-C1C	2.43	131.97	126.25
21	A	1139	CLA	C1C-C2C-C3C	-2.43	104.42	106.98
21	G	1603	CLA	C2D-C1D-ND	2.43	112.53	110.13
21	1	612	CLA	CHD-C1D-ND	-2.43	121.38	124.80
21	4	608	CLA	CHD-C1D-ND	-2.43	121.38	124.80
21	B	1223	CLA	O2A-CGA-CBA	2.43	119.25	111.83
21	B	1201	CLA	C4B-CHC-C1C	2.43	131.96	126.25
21	5	616	CLA	CHA-C4D-ND	2.43	137.56	132.55
21	L	1502	CLA	C2D-C1D-ND	2.43	112.53	110.13
21	A	1138	CLA	CMA-C3A-C4A	2.43	118.30	111.77
21	5	606	CLA	CHA-C4D-ND	2.43	137.56	132.55
21	3	604	CLA	CAA-C2A-C3A	-2.43	106.43	113.00
21	1	605	CLA	CHA-C4D-ND	2.43	137.56	132.55
21	3	606	CLA	CMD-C2D-C3D	-2.43	122.12	127.69
37	a	503	LUT	C22-C23-C24	-2.43	107.58	111.18
21	A	1117	CLA	CMA-C3A-C4A	2.43	118.30	111.77
21	B	1231	CLA	C1-O2A-CGA	2.43	122.53	116.65
21	a	607	CLA	CHA-C4D-ND	2.43	137.56	132.55
21	6	608	CLA	CAA-C2A-C3A	-2.43	106.44	113.00
21	B	1215	CLA	CHD-C1D-ND	-2.43	121.39	124.80
21	A	1127	CLA	C1C-C2C-C3C	-2.43	104.43	106.98
21	5	612	CLA	CHA-C4D-ND	2.43	137.56	132.55
38	a	610	CHL	CMA-C3A-C4A	2.43	119.84	114.61
21	5	608	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
21	4	608	CLA	C1C-C2C-C3C	-2.43	104.43	106.98
21	A	1106	CLA	CHA-C4D-ND	2.43	137.55	132.55
21	6	604	CLA	CHA-C4D-ND	2.43	137.55	132.55
21	B	1210	CLA	CAA-C2A-C1A	-2.43	104.03	111.97
21	7	607	CLA	O2A-CGA-CBA	2.43	119.23	111.83
37	4	501	LUT	C11-C10-C9	-2.43	123.88	127.28
21	B	1225	CLA	CMD-C2D-C3D	-2.42	122.13	127.69
21	8	611	CLA	CHA-C4D-ND	2.42	137.55	132.55
21	a	601	CLA	C1D-ND-C4D	-2.42	104.61	106.31
23	5	504	BCR	C37-C22-C23	2.42	121.79	118.09
23	K	4002	BCR	C33-C5-C6	-2.42	121.84	124.48
21	B	1216	CLA	C2C-C1C-NC	2.42	112.53	109.98
21	B	1228	CLA	CAA-C2A-C1A	-2.42	104.03	111.97
23	B	4004	BCR	C12-C13-C14	-2.42	115.20	119.01
21	8	610	CLA	O2D-CGD-O1D	-2.42	119.13	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	610	CLA	C1-O2A-CGA	2.42	122.52	116.65
21	A	1133	CLA	CAA-C2A-C3A	-2.42	106.45	113.00
21	6	607	CLA	C4B-CHC-C1C	2.42	131.94	126.25
21	B	1230	CLA	C2C-C1C-NC	2.42	112.53	109.98
21	4	615	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
21	6	608	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
23	6	504	BCR	C36-C18-C17	-2.42	118.89	122.82
23	B	4005	BCR	C37-C22-C23	2.42	121.79	118.09
21	B	1226	CLA	O2A-CGA-CBA	2.42	119.22	111.83
21	A	1132	CLA	CHA-C4D-ND	2.42	137.54	132.55
21	7	604	CLA	CHA-C4D-ND	2.42	137.54	132.55
21	A	1111	CLA	C1C-C2C-C3C	-2.42	104.43	106.98
21	7	601	CLA	CHA-C4D-ND	2.42	137.54	132.55
21	B	1211	CLA	C4B-CHC-C1C	2.42	131.94	126.25
37	5	501	LUT	C22-C23-C24	-2.42	107.59	111.18
21	6	607	CLA	C3B-C4B-NB	-2.42	108.37	110.53
21	6	618	CLA	CHA-C4D-ND	2.42	137.54	132.55
21	7	603	CLA	C1-O2A-CGA	2.42	122.51	116.65
21	a	605	CLA	CMD-C2D-C3D	-2.42	122.14	127.69
21	5	601	CLA	CAA-C2A-C3A	-2.42	106.46	113.00
21	B	1204	CLA	C4B-CHC-C1C	2.42	131.93	126.25
21	8	611	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
21	G	1601	CLA	C4B-CHC-C1C	2.42	131.93	126.25
21	7	609	CLA	CMD-C2D-C3D	-2.42	122.14	127.69
21	8	607	CLA	C2C-C1C-NC	2.42	112.52	109.98
21	B	1203	CLA	C1D-ND-C4D	-2.42	104.62	106.31
37	3	502	LUT	C30-C31-C32	-2.42	116.20	123.20
21	K	1401	CLA	C1C-C2C-C3C	-2.42	104.44	106.98
21	a	605	CLA	O2A-CGA-CBA	2.42	119.20	111.83
21	B	1227	CLA	C2C-C1C-NC	2.42	112.52	109.98
21	8	603	CLA	C4B-CHC-C1C	2.42	131.93	126.25
21	a	601	CLA	C3B-C4B-NB	-2.42	108.37	110.53
21	A	1102	CLA	CHA-C4D-ND	2.42	137.53	132.55
21	B	1230	CLA	CHA-C4D-ND	2.42	137.53	132.55
21	B	1218	CLA	CMA-C3A-C4A	2.42	118.27	111.77
21	B	1201	CLA	CHD-C1D-ND	-2.42	121.40	124.80
21	B	1021	CLA	C2C-C1C-NC	2.42	112.52	109.98
21	4	612	CLA	CAA-C2A-C3A	-2.41	106.47	113.00
21	A	1123	CLA	C4B-CHC-C1C	2.41	131.93	126.25
21	3	604	CLA	CHA-C4D-ND	2.41	137.53	132.55
21	L	1501	CLA	C4B-CHC-C1C	2.41	131.92	126.25
21	A	1121	CLA	C3B-C4B-NB	-2.41	108.38	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	5	616	CLA	C2D-C1D-ND	2.41	112.52	110.13
37	8	501	LUT	C35-C15-C14	-2.41	118.58	123.52
21	B	1201	CLA	CHA-C4D-ND	2.41	137.53	132.55
21	B	1201	CLA	C2C-C1C-NC	2.41	112.52	109.98
21	A	1131	CLA	C4B-CHC-C1C	2.41	131.92	126.25
21	6	603	CLA	CMD-C2D-C3D	-2.41	122.16	127.69
21	5	601	CLA	C2C-C1C-NC	2.41	112.52	109.98
21	8	607	CLA	CHA-C4D-ND	2.41	137.52	132.55
21	a	605	CLA	C2C-C1C-NC	2.41	112.51	109.98
21	B	1212	CLA	O1D-CGD-CBD	-2.41	119.76	124.52
21	G	1601	CLA	C1-O2A-CGA	2.41	122.48	116.65
21	A	1126	CLA	CHD-C1D-ND	-2.41	121.41	124.80
21	B	1207	CLA	O2A-CGA-CBA	2.41	119.18	111.83
21	A	1112	CLA	CHA-C4D-ND	2.41	137.52	132.55
21	B	1215	CLA	CHA-C4D-ND	2.41	137.52	132.55
21	A	1132	CLA	CMA-C3A-C4A	2.41	118.25	111.77
21	A	1120	CLA	CHA-C4D-ND	2.41	137.52	132.55
21	G	1602	CLA	CHA-C4D-ND	2.41	137.52	132.55
21	4	601	CLA	CHD-C1D-ND	-2.41	121.41	124.80
21	A	1138	CLA	C3B-C4B-NB	-2.41	108.38	110.53
21	7	610	CLA	CHA-C4D-ND	2.41	137.52	132.55
21	a	604	CLA	CMD-C2D-C3D	-2.41	122.17	127.69
21	B	1224	CLA	CHD-C1D-ND	-2.41	121.41	124.80
21	4	617	CLA	CHD-C1D-ND	-2.41	121.41	124.80
37	4	502	LUT	C35-C15-C14	-2.41	118.59	123.52
21	8	615	CLA	C1C-C2C-C3C	-2.41	104.45	106.98
21	6	617	CLA	CBC-CAC-C3C	-2.41	105.89	112.42
24	A	5002	LHG	C5-O7-C7	-2.41	112.04	117.80
21	1	611	CLA	C4B-CHC-C1C	2.41	131.91	126.25
21	L	1501	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
23	8	503	BCR	C4-C5-C6	-2.41	119.45	122.70
21	7	602	CLA	CAC-C3C-C4C	2.41	127.92	124.79
37	a	503	LUT	C27-C28-C29	-2.41	121.15	126.32
21	A	1136	CLA	CHA-C4D-ND	2.41	137.51	132.55
21	5	601	CLA	CHA-C4D-ND	2.41	137.51	132.55
47	7	504	C7Z	C21-C26-C25	-2.40	119.35	122.64
21	A	1117	CLA	CHD-C1D-ND	-2.40	121.42	124.80
21	B	1201	CLA	O1D-CGD-CBD	-2.40	119.78	124.52
21	3	613	CLA	C4B-CHC-C1C	2.40	131.90	126.25
21	7	611	CLA	CHA-C4D-ND	2.40	137.51	132.55
23	B	4007	BCR	C36-C18-C17	-2.40	118.92	122.82
21	5	601	CLA	C3B-C4B-NB	-2.40	108.39	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	7	603	CLA	CHD-C1D-ND	-2.40	121.42	124.80
21	A	1013	CLA	O2A-CGA-CBA	2.40	119.16	111.83
21	1	604	CLA	CMA-C3A-C4A	2.40	118.23	111.77
21	a	601	CLA	CHD-C1D-ND	-2.40	121.42	124.80
21	B	1212	CLA	CHA-C4D-ND	2.40	137.50	132.55
21	3	605	CLA	C3B-C4B-NB	-2.40	108.39	110.53
23	3	503	BCR	C38-C26-C27	2.40	118.71	113.60
21	B	1201	CLA	O2A-CGA-CBA	2.40	119.15	111.83
37	a	501	LUT	C31-C32-C33	-2.40	119.78	126.36
21	B	1213	CLA	CHD-C1D-ND	-2.40	121.43	124.80
21	4	603	CLA	CHA-C4D-ND	2.40	137.50	132.55
37	3	501	LUT	C30-C31-C32	-2.40	116.25	123.20
21	B	1214	CLA	CMD-C2D-C3D	-2.40	122.19	127.69
21	B	1229	CLA	C1-O2A-CGA	2.40	122.46	116.65
23	L	4001	BCR	C4-C5-C6	-2.40	119.46	122.70
21	5	609	CLA	CHA-C1A-NA	-2.40	120.96	126.39
21	3	610	CLA	C2C-C1C-NC	2.40	112.50	109.98
21	6	604	CLA	C1C-C2C-C3C	-2.40	104.46	106.98
21	A	1013	CLA	C2D-C1D-ND	2.40	112.50	110.13
21	A	1112	CLA	C4B-CHC-C1C	2.40	131.88	126.25
21	F	1301	CLA	CHA-C1A-NA	-2.40	120.96	126.39
37	4	501	LUT	C30-C31-C32	-2.40	116.25	123.20
21	A	1114	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
40	3	506	QTB	C13-C12-C14	2.40	115.53	111.06
21	B	1021	CLA	O2A-CGA-CBA	2.40	119.14	111.83
21	3	613	CLA	C3B-C4B-NB	-2.40	108.39	110.53
21	A	1013	CLA	CHA-C4D-ND	2.40	137.49	132.55
21	B	1235	CLA	C2D-C1D-ND	2.40	112.50	110.13
21	8	618	CLA	O2A-CGA-CBA	2.40	119.14	111.83
21	B	1229	CLA	C2C-C1C-NC	2.40	112.50	109.98
21	K	1404	CLA	O2A-CGA-CBA	2.39	119.14	111.83
21	B	1203	CLA	C4B-CHC-C1C	2.39	131.88	126.25
21	L	1502	CLA	C1-O2A-CGA	2.39	122.45	116.65
21	7	601	CLA	C1-O2A-CGA	2.39	122.45	116.65
37	1	502	LUT	C39-C29-C28	2.39	121.75	118.09
21	4	616	CLA	CHA-C4D-ND	2.39	137.49	132.55
21	B	1208	CLA	CHA-C4D-ND	2.39	137.49	132.55
48	8	806	P5S	OG-CB-CA	2.39	110.14	108.06
23	G	4001	BCR	C15-C14-C13	2.39	130.63	127.28
21	L	1501	CLA	CHA-C4D-ND	2.39	137.49	132.55
21	B	1230	CLA	CHD-C1D-ND	-2.39	121.44	124.80
23	A	4001	BCR	C3-C4-C5	-2.39	109.79	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	603	CLA	C4B-CHC-C1C	2.39	131.87	126.25
21	B	1224	CLA	CHA-C4D-ND	2.39	137.48	132.55
37	a	501	LUT	C36-C21-C26	-2.39	105.92	109.55
21	A	1102	CLA	C2C-C1C-NC	2.39	112.49	109.98
31	K	5001	LAP	O1-C1-O2	-2.39	117.65	123.63
21	A	1118	CLA	C4B-CHC-C1C	2.39	131.86	126.25
21	6	607	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
21	B	1221	CLA	C3B-C4B-NB	-2.39	108.40	110.53
21	4	602	CLA	CHA-C4D-ND	2.39	137.47	132.55
23	B	4001	BCR	C27-C26-C25	-2.39	119.48	122.70
23	G	4001	BCR	C23-C22-C21	2.39	122.76	119.01
21	B	1210	CLA	CAA-C2A-C3A	-2.39	106.55	113.00
21	B	1217	CLA	CMA-C3A-C4A	2.39	118.19	111.77
21	K	1402	CLA	CHA-C4D-ND	2.39	137.47	132.55
21	B	1221	CLA	C4B-CHC-C1C	2.39	131.86	126.25
21	4	604	CLA	CHA-C4D-ND	2.39	137.47	132.55
21	3	606	CLA	C2C-C1C-NC	2.39	112.49	109.98
21	A	1117	CLA	CHA-C4D-ND	2.39	137.47	132.55
21	7	609	CLA	OBD-CAD-C3D	-2.39	122.84	128.42
21	5	603	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
23	8	503	BCR	C15-C14-C13	-2.39	123.93	127.28
21	K	1402	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
21	B	1021	CLA	CAA-C2A-C3A	-2.38	106.56	113.00
21	B	1222	CLA	CHA-C4D-ND	2.38	137.47	132.55
21	1	603	CLA	C2C-C1C-NC	2.38	112.49	109.98
21	A	1119	CLA	C4B-CHC-C1C	2.38	131.85	126.25
21	J	1901	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
23	L	4002	BCR	C34-C9-C10	-2.38	118.95	122.82
21	7	608	CLA	CHD-C1D-ND	-2.38	121.45	124.80
21	1	607	CLA	O2A-CGA-CBA	2.38	119.10	111.83
21	5	603	CLA	C1C-C2C-C3C	-2.38	104.47	106.98
21	1	604	CLA	CHA-C4D-ND	2.38	137.46	132.55
21	1	608	CLA	CHA-C4D-ND	2.38	137.46	132.55
21	7	603	CLA	CMD-C2D-C3D	-2.38	122.23	127.69
21	A	1127	CLA	C2C-C1C-NC	2.38	112.48	109.98
21	A	1108	CLA	CMD-C2D-C3D	-2.38	122.23	127.69
21	8	612	CLA	C4B-CHC-C1C	2.38	131.85	126.25
21	A	1105	CLA	CMA-C3A-C4A	2.38	118.17	111.77
21	7	615	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
21	A	1139	CLA	CMA-C3A-C4A	2.38	118.17	111.77
21	A	1137	CLA	O2A-CGA-CBA	2.38	119.09	111.83
21	F	1302	CLA	CHA-C4D-ND	2.38	137.46	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	1207	CLA	C1C-C2C-C3C	-2.38	104.48	106.98
21	A	1121	CLA	O2A-CGA-CBA	2.38	119.09	111.83
21	6	601	CLA	CHD-C1D-ND	-2.38	121.45	124.80
21	1	615	CLA	C3B-C4B-NB	-2.38	108.41	110.53
21	3	603	CLA	CHA-C4D-ND	2.38	137.46	132.55
37	7	501	LUT	C11-C10-C9	-2.38	123.94	127.28
21	B	1213	CLA	CMD-C2D-C3D	-2.38	122.23	127.69
21	a	602	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
21	A	1101	CLA	C1C-C2C-C3C	-2.38	104.48	106.98
21	8	606	CLA	C4B-CHC-C1C	2.38	131.84	126.25
21	K	1402	CLA	C2C-C1C-NC	2.38	112.48	109.98
23	4	503	BCR	C33-C5-C6	-2.38	121.89	124.48
21	1	606	CLA	CHD-C1D-ND	-2.38	121.46	124.80
21	B	1222	CLA	O2A-CGA-CBA	2.38	119.08	111.83
21	a	603	CLA	C6-C5-C3	-2.38	107.68	113.47
21	B	1208	CLA	C4B-CHC-C1C	2.38	131.84	126.25
21	B	1216	CLA	CHD-C1D-ND	-2.38	121.46	124.80
21	8	603	CLA	CMD-C2D-C3D	-2.38	122.24	127.69
21	3	616	CLA	CHA-C4D-ND	2.38	137.45	132.55
21	F	1302	CLA	O2A-CGA-CBA	2.38	119.08	111.83
37	a	502	LUT	C35-C15-C14	-2.38	118.66	123.52
23	A	4002	BCR	C15-C14-C13	-2.38	123.95	127.28
21	F	1302	CLA	CHD-C1D-ND	-2.38	121.46	124.80
21	B	1236	CLA	C1C-C2C-C3C	-2.38	104.48	106.98
21	B	1212	CLA	C4B-CHC-C1C	2.38	131.83	126.25
21	A	1109	CLA	CAA-C2A-C3A	-2.38	106.58	113.00
21	B	1211	CLA	C3B-C4B-NB	-2.37	108.41	110.53
21	a	603	CLA	CHD-C1D-ND	-2.37	121.46	124.80
21	3	603	CLA	C1C-C2C-C3C	-2.37	104.48	106.98
21	B	1221	CLA	CHA-C1A-NA	-2.37	121.02	126.39
21	a	604	CLA	C2D-C1D-ND	2.37	112.47	110.13
21	A	1125	CLA	CMA-C3A-C4A	2.37	118.15	111.77
21	6	609	CLA	C1-O2A-CGA	2.37	122.39	116.65
21	5	606	CLA	C1D-ND-C4D	-2.37	104.65	106.31
21	A	1117	CLA	C4B-CHC-C1C	2.37	131.83	126.25
21	4	616	CLA	CHD-C1D-ND	-2.37	121.46	124.80
21	A	1128	CLA	O2A-CGA-CBA	2.37	119.07	111.83
21	a	611	CLA	C4B-CHC-C1C	2.37	131.82	126.25
21	4	604	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
40	a	504	QTB	C11-C10-C09	2.37	130.32	125.25
21	7	611	CLA	CAA-CBA-CGA	-2.37	106.47	113.21
38	1	609	CHL	CGD-CBD-CAD	-2.37	103.17	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	5	505	LUT	C1-C6-C7	2.37	122.08	115.65
21	A	1130	CLA	CHD-C1D-ND	-2.37	121.47	124.80
24	B	5002	LHG	C5-O7-C7	-2.37	112.12	117.80
21	A	1103	CLA	CHA-C4D-ND	2.37	137.44	132.55
23	5	503	BCR	C12-C13-C14	-2.37	115.28	119.01
21	8	608	CLA	CAA-C2A-C3A	-2.37	106.59	113.00
21	A	1139	CLA	O1D-CGD-CBD	-2.37	119.84	124.52
21	6	601	CLA	O1D-CGD-CBD	-2.37	119.84	124.52
21	6	601	CLA	CHA-C4D-ND	2.37	137.44	132.55
23	7	503	BCR	C31-C1-C6	-2.37	106.53	110.24
21	8	603	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
21	A	1120	CLA	C1D-ND-C4D	-2.37	104.65	106.31
21	6	612	CLA	CHA-C4D-ND	2.37	137.44	132.55
21	A	1113	CLA	C4B-CHC-C1C	2.37	131.82	126.25
21	A	1106	CLA	CMA-C3A-C4A	2.37	118.14	111.77
21	a	601	CLA	C1C-C2C-C3C	-2.37	104.49	106.98
21	F	1301	CLA	C2D-C1D-ND	2.37	112.47	110.13
33	G	5002	ERG	C20-C22-C23	-2.37	118.65	125.81
21	7	609	CLA	CHD-C1D-ND	-2.37	121.47	124.80
21	A	1101	CLA	CHA-C1A-NA	-2.37	121.03	126.39
21	5	601	CLA	CMD-C2D-C3D	-2.37	122.26	127.69
21	6	606	CLA	CHA-C4D-ND	2.37	137.43	132.55
21	B	1212	CLA	C1-O2A-CGA	2.37	122.38	116.65
23	B	4002	BCR	C38-C26-C27	2.37	118.64	113.60
21	B	1230	CLA	C4B-CHC-C1C	2.37	131.81	126.25
23	5	504	BCR	C38-C26-C27	2.37	118.64	113.60
21	7	602	CLA	CHD-C1D-ND	-2.37	121.47	124.80
21	B	1023	CLA	CHA-C4D-ND	2.37	137.43	132.55
23	B	4005	BCR	C34-C9-C8	2.37	121.70	118.09
21	4	606	CLA	C4B-CHC-C1C	2.37	131.81	126.25
45	7	502	XAT	O4-C5-C4	-2.37	111.27	113.49
21	6	609	CLA	C4B-CHC-C1C	2.37	131.81	126.25
21	a	604	CLA	CMC-C2C-C1C	2.36	128.73	125.03
23	3	505	BCR	C31-C1-C6	-2.36	106.53	110.24
21	K	1402	CLA	CHD-C1D-ND	-2.36	121.47	124.80
21	B	1209	CLA	O2A-CGA-CBA	2.36	119.04	111.83
21	1	608	CLA	O2A-CGA-CBA	2.36	119.04	111.83
21	7	615	CLA	C1-O2A-CGA	2.36	122.37	116.65
22	A	2001	PQN	C11-C3-C2	-2.36	120.84	124.89
23	B	4005	BCR	C29-C28-C27	2.36	116.47	111.28
21	K	1404	CLA	C4B-CHC-C1C	2.36	131.80	126.25
21	4	611	CLA	C1D-ND-C4D	-2.36	104.65	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	601	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
21	1	601	CLA	C1C-C2C-C3C	-2.36	104.50	106.98
21	A	1130	CLA	CHA-C4D-ND	2.36	137.42	132.55
21	B	1229	CLA	C1C-C2C-C3C	-2.36	104.50	106.98
21	4	606	CLA	CMD-C2D-C3D	-2.36	122.27	127.69
23	A	4004	BCR	C33-C5-C4	2.36	118.63	113.60
21	B	1201	CLA	C3B-C4B-NB	-2.36	108.42	110.53
21	B	1222	CLA	C3B-C4B-NB	-2.36	108.42	110.53
21	5	606	CLA	CHD-C1D-ND	-2.36	121.48	124.80
25	B	5003	DGD	O2G-C1B-O1B	-2.36	118.19	123.70
37	6	501	LUT	C38-C25-C24	-2.36	117.78	123.36
22	A	2001	PQN	C2M-C2-C3	-2.36	120.57	124.45
21	B	1236	CLA	CHA-C4D-ND	2.36	137.42	132.55
21	a	603	CLA	C4B-CHC-C1C	2.36	131.79	126.25
21	5	601	CLA	C6-C5-C3	-2.36	107.72	113.47
21	L	1503	CLA	CMC-C2C-C3C	2.36	132.53	126.15
21	3	612	CLA	C2C-C1C-NC	2.36	112.46	109.98
21	5	606	CLA	C2C-C1C-NC	2.36	112.46	109.98
37	a	501	LUT	C8-C7-C6	-2.36	120.70	127.00
21	3	606	CLA	C1C-C2C-C3C	-2.36	104.50	106.98
21	6	608	CLA	C4B-CHC-C1C	2.36	131.79	126.25
21	A	1125	CLA	C1C-C2C-C3C	-2.36	104.50	106.98
23	A	4001	BCR	C38-C26-C25	-2.36	121.91	124.48
21	4	602	CLA	C1D-ND-C4D	-2.36	104.66	106.31
21	A	1126	CLA	CMD-C2D-C3D	-2.35	122.29	127.69
21	B	1203	CLA	CHD-C1D-ND	-2.35	121.49	124.80
21	A	1101	CLA	C2D-C1D-ND	2.35	112.46	110.13
23	B	4001	BCR	C23-C24-C25	-2.35	120.71	127.00
21	5	602	CLA	CMA-C3A-C4A	2.35	118.10	111.77
21	5	606	CLA	C1C-C2C-C3C	-2.35	104.50	106.98
23	L	4001	BCR	C34-C9-C10	-2.35	119.00	122.82
21	A	1110	CLA	C4B-CHC-C1C	2.35	131.78	126.25
21	A	1107	CLA	CHA-C1A-NA	-2.35	121.06	126.39
21	A	1118	CLA	C1C-C2C-C3C	-2.35	104.51	106.98
21	6	615	CLA	C1C-C2C-C3C	-2.35	104.51	106.98
21	6	607	CLA	CHA-C4D-ND	2.35	137.40	132.55
21	B	1228	CLA	C4B-CHC-C1C	2.35	131.78	126.25
21	7	611	CLA	C2D-C1D-ND	2.35	112.45	110.13
21	B	1211	CLA	CHD-C1D-ND	-2.35	121.49	124.80
21	8	611	CLA	CHD-C1D-ND	-2.35	121.49	124.80
21	B	1224	CLA	C4B-CHC-C1C	2.35	131.78	126.25
21	A	1122	CLA	C1C-C2C-C3C	-2.35	104.51	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	a	607	CLA	C2D-C1D-ND	2.35	112.45	110.13
21	B	1228	CLA	C2C-C1C-NC	2.35	112.45	109.98
21	8	608	CLA	C1-O2A-CGA	2.35	122.34	116.65
21	8	610	CLA	CHA-C1A-NA	-2.35	121.07	126.39
21	4	603	CLA	O2A-CGA-CBA	2.35	119.00	111.83
21	B	1225	CLA	O2A-CGA-CBA	2.35	119.00	111.83
21	7	606	CLA	C2C-C1C-NC	2.35	112.45	109.98
21	A	1137	CLA	C2D-C1D-ND	2.35	112.45	110.13
21	B	1222	CLA	C1D-ND-C4D	-2.35	104.67	106.31
21	8	605	CLA	C1D-ND-C4D	-2.35	104.67	106.31
21	4	604	CLA	CMA-C3A-C4A	2.35	118.08	111.77
21	4	607	CLA	CMA-C3A-C4A	2.35	118.08	111.77
21	1	601	CLA	CHD-C1D-ND	-2.35	121.50	124.80
21	A	1120	CLA	C2C-C1C-NC	2.34	112.44	109.98
21	6	602	CLA	CHA-C4D-ND	2.34	137.39	132.55
21	5	604	CLA	C4B-CHC-C1C	2.34	131.76	126.25
21	A	1131	CLA	C1C-C2C-C3C	-2.34	104.51	106.98
21	B	1208	CLA	C1D-ND-C4D	-2.34	104.67	106.31
21	B	1203	CLA	CMD-C2D-C3D	-2.34	122.31	127.69
23	5	504	BCR	C8-C7-C6	-2.34	120.74	127.00
21	a	608	CLA	CMA-C3A-C4A	2.34	118.07	111.77
38	6	611	CHL	C4C-CHD-C1D	2.34	124.45	116.07
21	6	615	CLA	C4B-CHC-C1C	2.34	131.76	126.25
21	B	1218	CLA	CHA-C4D-ND	2.34	137.38	132.55
21	4	611	CLA	CAA-C2A-C3A	-2.34	106.67	113.00
21	a	615	CLA	CAC-C3C-C4C	2.34	127.84	124.79
21	4	615	CLA	CHA-C1A-NA	-2.34	121.09	126.39
21	G	1602	CLA	CHD-C1D-ND	-2.34	121.51	124.80
21	A	1127	CLA	CHA-C4D-ND	2.34	137.38	132.55
21	3	607	CLA	C4B-CHC-C1C	2.34	131.75	126.25
21	B	1214	CLA	CHD-C1D-ND	-2.34	121.51	124.80
21	6	608	CLA	C3B-C4B-NB	-2.34	108.44	110.53
21	6	604	CLA	C2D-C1D-ND	2.34	112.44	110.13
21	3	604	CLA	CMD-C2D-C3D	-2.34	122.32	127.69
21	A	1112	CLA	C1C-C2C-C3C	-2.34	104.52	106.98
36	M	4001	ECH	C37-C22-C23	-2.34	114.52	118.09
21	3	612	CLA	C1C-C2C-C3C	-2.34	104.52	106.98
21	1	608	CLA	O1D-CGD-CBD	-2.34	119.91	124.52
21	G	1603	CLA	CHA-C4D-ND	2.34	137.37	132.55
21	B	1202	CLA	C2D-C1D-ND	2.34	112.44	110.13
21	5	618	CLA	C2D-C1D-ND	2.34	112.44	110.13
21	4	611	CLA	O2D-CGD-O1D	-2.34	119.30	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	8	606	CLA	CHA-C4D-ND	2.34	137.37	132.55
21	7	617	CLA	O2A-CGA-CBA	2.34	118.96	111.83
21	4	603	CLA	C2D-C1D-ND	2.34	112.44	110.13
21	B	1212	CLA	CHD-C1D-ND	-2.34	121.52	124.80
21	5	603	CLA	CHD-C1D-ND	-2.34	121.52	124.80
21	B	1206	CLA	CHD-C1D-ND	-2.34	121.52	124.80
21	4	616	CLA	CMD-C2D-C3D	-2.33	122.33	127.69
21	5	614	CLA	CHD-C1D-ND	-2.33	121.52	124.80
21	5	602	CLA	CHA-C1A-NA	-2.33	121.11	126.39
21	A	1113	CLA	CHA-C4D-ND	2.33	137.37	132.55
21	3	605	CLA	C4B-CHC-C1C	2.33	131.74	126.25
21	1	611	CLA	C6-C5-C3	-2.33	107.78	113.47
21	A	1128	CLA	C4B-CHC-C1C	2.33	131.74	126.25
21	A	1119	CLA	OBD-CAD-C3D	-2.33	122.96	128.42
21	A	1110	CLA	C3B-C4B-NB	-2.33	108.45	110.53
21	L	1503	CLA	CHD-C1D-ND	-2.33	121.52	124.80
21	5	608	CLA	C4B-CHC-C1C	2.33	131.73	126.25
21	A	1109	CLA	O2A-CGA-CBA	2.33	118.95	111.83
21	4	612	CLA	C2C-C1C-NC	2.33	112.43	109.98
21	8	603	CLA	O2A-CGA-CBA	2.33	118.95	111.83
21	A	1126	CLA	C4B-CHC-C1C	2.33	131.73	126.25
23	B	4004	BCR	C8-C7-C6	-2.33	120.77	127.00
21	6	602	CLA	CHD-C1D-ND	-2.33	121.52	124.80
20	A	1011	CL0	CMC-C2C-C1C	2.33	128.93	124.73
21	1	602	CLA	CHA-C1A-NA	-2.33	121.11	126.39
21	8	620	CLA	CHA-C4D-ND	2.33	137.36	132.55
21	6	603	CLA	C1C-C2C-C3C	-2.33	104.53	106.98
21	6	604	CLA	CHA-C1A-NA	-2.33	121.11	126.39
21	B	1218	CLA	C2D-C1D-ND	2.33	112.43	110.13
21	A	1111	CLA	CAA-C2A-C3A	-2.33	106.70	113.00
21	5	612	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
38	a	609	CHL	C4D-CHA-CBD	-2.33	106.62	108.97
21	7	608	CLA	O1D-CGD-CBD	-2.33	119.92	124.52
21	A	1134	CLA	CHD-C1D-ND	-2.33	121.52	124.80
21	6	618	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
21	B	1023	CLA	C2D-C1D-ND	2.33	112.43	110.13
21	8	606	CLA	C3B-C4B-NB	-2.33	108.45	110.53
21	4	605	CLA	C1D-ND-C4D	-2.33	104.68	106.31
21	5	617	CLA	C1D-ND-C4D	-2.33	104.68	106.31
21	B	1210	CLA	CHA-C4D-ND	2.33	137.35	132.55
21	6	612	CLA	C3D-C2D-C1D	-2.33	102.65	105.83
21	B	1240	CLA	CHA-C1A-NA	-2.33	121.12	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	601	CLA	CMD-C2D-C3D	-2.33	122.35	127.69
23	B	4005	BCR	C15-C14-C13	-2.33	124.02	127.28
21	A	1135	CLA	CHD-C1D-ND	-2.33	121.53	124.80
21	6	601	CLA	C1D-ND-C4D	-2.33	104.68	106.31
21	B	1022	CLA	CHA-C1A-NA	-2.33	121.12	126.39
21	L	1502	CLA	C4B-CHC-C1C	2.33	131.72	126.25
33	G	5002	ERG	C16-C15-C14	-2.33	101.46	105.25
38	6	611	CHL	C1-O2A-CGA	2.33	122.28	116.65
21	L	1503	CLA	C3B-C4B-NB	-2.33	108.45	110.53
21	B	1206	CLA	CHA-C1A-NA	-2.33	121.12	126.39
21	A	1110	CLA	CHA-C4D-ND	2.33	137.35	132.55
21	B	1202	CLA	C1D-ND-C4D	-2.32	104.68	106.31
21	A	1104	CLA	CMD-C2D-C3D	-2.32	122.36	127.69
21	L	1502	CLA	CHA-C4D-ND	2.32	137.34	132.55
21	8	620	CLA	C1D-ND-C4D	-2.32	104.68	106.31
21	A	1130	CLA	C2C-C1C-NC	2.32	112.42	109.98
21	B	1238	CLA	C2C-C1C-NC	2.32	112.42	109.98
21	4	610	CLA	CMD-C2D-C3D	-2.32	122.36	127.69
38	a	610	CHL	C1-O2A-CGA	2.32	123.27	116.67
21	B	1236	CLA	C3D-C2D-C1D	-2.32	102.66	105.83
21	B	1223	CLA	CHA-C1A-NA	-2.32	121.13	126.39
21	A	1115	CLA	C2D-C1D-ND	2.32	112.42	110.13
21	B	1220	CLA	C4B-CHC-C1C	2.32	131.71	126.25
21	A	1105	CLA	C2C-C1C-NC	2.32	112.42	109.98
21	A	1123	CLA	CHD-C1D-ND	-2.32	121.54	124.80
21	1	605	CLA	C4B-CHC-C1C	2.32	131.71	126.25
21	A	1125	CLA	C1-O2A-CGA	2.32	122.27	116.65
21	5	602	CLA	C4B-CHC-C1C	2.32	131.70	126.25
21	7	611	CLA	C4B-CHC-C1C	2.32	131.70	126.25
37	a	502	LUT	C7-C8-C9	-2.32	122.80	126.23
37	3	501	LUT	C31-C30-C29	-2.32	124.02	127.28
21	8	620	CLA	C4B-CHC-C1C	2.32	131.70	126.25
38	8	601	CHL	C1A-CHA-C4D	2.32	122.85	118.98
21	A	1102	CLA	CHD-C1D-ND	-2.32	121.54	124.80
21	B	1215	CLA	CMA-C3A-C4A	2.32	118.01	111.77
21	A	1121	CLA	CMA-C3A-C4A	2.32	118.01	111.77
22	B	2002	PQN	C16-C15-C13	-2.32	107.82	113.47
21	7	602	CLA	C4B-CHC-C1C	2.32	131.70	126.25
21	4	606	CLA	C3B-C4B-NB	-2.32	108.46	110.53
23	6	503	BCR	C38-C26-C25	-2.32	121.95	124.48
21	A	1116	CLA	CHD-C1D-ND	-2.32	121.54	124.80
21	3	618	CLA	CHA-C1A-NA	-2.32	121.14	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	1237	CLA	C1D-ND-C4D	-2.32	104.69	106.31
21	A	1120	CLA	C2D-C1D-ND	2.32	112.42	110.13
21	a	605	CLA	O1D-CGD-CBD	-2.32	119.95	124.52
21	A	1129	CLA	C4B-CHC-C1C	2.32	131.69	126.25
21	A	1125	CLA	CHD-C1D-ND	-2.32	121.54	124.80
25	8	802	DGD	O6D-C5D-C6D	2.32	111.29	106.69
21	A	1101	CLA	O2A-CGA-CBA	2.32	118.90	111.83
37	3	502	LUT	C22-C23-C24	-2.32	107.75	111.18
23	6	503	BCR	C33-C5-C4	2.32	118.53	113.60
21	1	605	CLA	CMD-C2D-C3D	-2.32	122.38	127.69
21	5	618	CLA	CMC-C2C-C1C	2.31	128.65	125.03
21	5	618	CLA	C1D-ND-C4D	-2.31	104.69	106.31
21	7	611	CLA	C3B-C4B-NB	-2.31	108.46	110.53
21	B	1215	CLA	C2C-C1C-NC	2.31	112.41	109.98
21	B	1216	CLA	C4B-CHC-C1C	2.31	131.69	126.25
21	3	601	CLA	CHD-C1D-ND	-2.31	121.55	124.80
21	1	610	CLA	C4B-CHC-C1C	2.31	131.69	126.25
21	B	1235	CLA	C4B-CHC-C1C	2.31	131.69	126.25
37	1	501	LUT	C39-C29-C28	2.31	121.62	118.09
21	7	606	CLA	C2D-C1D-ND	2.31	112.41	110.13
21	3	603	CLA	C2C-C1C-NC	2.31	112.41	109.98
21	4	603	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
21	A	1132	CLA	C4B-CHC-C1C	2.31	131.68	126.25
21	K	1402	CLA	O2A-CGA-CBA	2.31	118.88	111.83
21	6	607	CLA	C2D-C1D-ND	2.31	112.41	110.13
24	A	5003	LHG	C5-O7-C7	-2.31	112.27	117.80
21	B	1235	CLA	CHA-C4D-ND	2.31	137.32	132.55
21	A	1132	CLA	CHD-C1D-ND	-2.31	121.55	124.80
21	4	602	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
21	3	602	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
21	1	603	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
21	6	615	CLA	C2D-C1D-ND	2.31	112.41	110.13
21	5	604	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
24	1	801	LHG	C6-C5-C4	-2.31	106.40	111.78
21	G	1602	CLA	C4B-CHC-C1C	2.31	131.68	126.25
21	8	608	CLA	CHD-C1D-ND	-2.31	121.55	124.80
21	B	1235	CLA	C2C-C1C-NC	2.31	112.41	109.98
21	8	615	CLA	O2D-CGD-O1D	-2.31	119.36	123.85
21	3	612	CLA	C3B-C4B-NB	-2.31	108.47	110.53
37	7	501	LUT	C10-C11-C12	-2.31	116.52	123.20
21	6	615	CLA	CHD-C1D-ND	-2.31	121.56	124.80
21	7	610	CLA	CHD-C1D-ND	-2.31	121.56	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	J	4002	RRX	C16-C15-C14	-2.31	118.80	123.52
21	8	620	CLA	CAA-C2A-C1A	-2.31	104.42	111.97
23	K	4002	BCR	C28-C27-C26	-2.31	109.94	114.06
21	A	1115	CLA	O2A-CGA-CBA	2.31	118.86	111.83
21	A	1134	CLA	CMA-C3A-C4A	2.31	117.97	111.77
21	B	1230	CLA	C2D-C1D-ND	2.30	112.41	110.13
21	3	604	CLA	C1C-C2C-C3C	-2.30	104.56	106.98
21	a	608	CLA	O2D-CGD-O1D	-2.30	119.36	123.85
21	B	1223	CLA	C3D-C2D-C1D	-2.30	102.69	105.83
21	4	617	CLA	OBD-CAD-C3D	-2.30	123.03	128.42
21	A	1111	CLA	CHD-C1D-ND	-2.30	121.56	124.80
21	5	606	CLA	C4B-CHC-C1C	2.30	131.66	126.25
21	1	602	CLA	CMD-C2D-C3D	-2.30	122.41	127.69
21	B	1208	CLA	C1-C2-C3	-2.30	122.42	126.20
21	B	1220	CLA	CMD-C2D-C3D	-2.30	122.41	127.69
21	A	1013	CLA	C1D-ND-C4D	-2.30	104.70	106.31
21	A	1137	CLA	C3D-C2D-C1D	-2.30	102.69	105.83
21	6	606	CLA	CHD-C1D-ND	-2.30	121.56	124.80
21	B	1213	CLA	O2D-CGD-O1D	-2.30	119.37	123.85
21	B	1205	CLA	C3B-C4B-NB	-2.30	108.47	110.53
21	4	603	CLA	O2D-CGD-O1D	-2.30	119.37	123.85
21	A	1141	CLA	C4B-CHC-C1C	2.30	131.66	126.25
21	1	608	CLA	C4B-CHC-C1C	2.30	131.66	126.25
37	a	503	LUT	C35-C15-C14	-2.30	118.81	123.52
21	5	601	CLA	CMA-C3A-C4A	2.30	117.95	111.77
21	3	606	CLA	O2D-CGD-O1D	-2.30	119.37	123.85
22	B	2002	PQN	C2M-C2-C3	-2.30	120.67	124.45
21	6	601	CLA	C3B-C4B-NB	-2.30	108.48	110.53
23	A	4004	BCR	C36-C18-C17	-2.30	119.09	122.82
21	7	608	CLA	C4B-CHC-C1C	2.30	131.65	126.25
21	B	1228	CLA	C6-C7-C8	-2.30	108.33	115.97
21	6	615	CLA	O2A-CGA-CBA	2.30	118.84	111.83
21	K	1401	CLA	C4B-CHC-C1C	2.30	131.65	126.25
21	A	1132	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
21	a	615	CLA	C2D-C1D-ND	2.30	112.40	110.13
21	A	1111	CLA	C3B-C4B-NB	-2.30	108.48	110.53
21	7	606	CLA	C1C-C2C-C3C	-2.30	104.56	106.98
21	8	612	CLA	CHD-C1D-ND	-2.30	121.57	124.80
23	3	504	BCR	C8-C9-C10	2.30	122.62	119.01
37	5	505	LUT	C31-C32-C33	-2.30	120.06	126.36
45	7	502	XAT	O24-C26-C27	-2.30	110.30	116.88
21	4	607	CLA	O2A-CGA-CBA	2.30	118.84	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	5	606	CLA	O1D-CGD-CBD	-2.30	119.99	124.52
23	L	4003	BCR	C30-C25-C26	-2.30	119.50	122.64
21	B	1231	CLA	C1D-ND-C4D	-2.30	104.70	106.31
21	A	1137	CLA	O1D-CGD-CBD	-2.30	119.99	124.52
21	B	1228	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
21	K	1404	CLA	C3D-C2D-C1D	-2.30	102.70	105.83
38	3	611	CHL	CMA-C3A-C4A	2.30	119.56	114.61
21	B	1219	CLA	C4B-CHC-C1C	2.29	131.64	126.25
21	B	1227	CLA	C1-O2A-CGA	2.29	122.20	116.65
21	7	608	CLA	CMD-C2D-C3D	-2.29	122.43	127.69
21	6	605	CLA	C4B-CHC-C1C	2.29	131.64	126.25
21	4	601	CLA	CHA-C4D-ND	2.29	137.28	132.55
21	8	607	CLA	C4B-CHC-C1C	2.29	131.64	126.25
21	8	608	CLA	CHA-C4D-ND	2.29	137.28	132.55
21	6	617	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
21	A	1137	CLA	CHD-C1D-ND	-2.29	121.58	124.80
21	B	1230	CLA	CMD-C2D-C3D	-2.29	122.43	127.69
21	A	1103	CLA	CHD-C1D-ND	-2.29	121.58	124.80
21	A	1123	CLA	C1-O2A-CGA	2.29	122.20	116.65
37	5	505	LUT	C38-C25-C24	-2.29	117.94	123.36
21	1	610	CLA	CHA-C4D-ND	2.29	137.27	132.55
37	5	502	LUT	C16-C1-C6	-2.29	106.65	110.24
21	A	1113	CLA	C3B-C4B-NB	-2.29	108.49	110.53
21	8	607	CLA	CHD-C1D-ND	-2.29	121.58	124.80
21	A	1110	CLA	C1-O2A-CGA	2.29	122.19	116.65
37	a	503	LUT	C8-C7-C6	-2.29	120.89	127.00
21	5	603	CLA	O2A-CGA-CBA	2.29	118.81	111.83
21	A	1136	CLA	CHD-C1D-ND	-2.29	121.58	124.80
37	1	502	LUT	C38-C25-C24	-2.29	117.95	123.36
21	6	612	CLA	CHD-C1D-ND	-2.29	121.59	124.80
23	K	4001	BCR	C33-C5-C4	2.29	118.47	113.60
21	3	605	CLA	CMD-C2D-C3D	-2.28	122.45	127.69
21	8	620	CLA	CHD-C1D-ND	-2.28	121.59	124.80
36	M	4001	ECH	C15-C16-C17	-2.28	118.84	123.52
21	5	609	CLA	CMD-C2D-C3D	-2.28	122.45	127.69
21	4	615	CLA	C4B-CHC-C1C	2.28	131.62	126.25
21	L	1502	CLA	CHD-C1D-ND	-2.28	121.59	124.80
21	7	605	CLA	CMA-C3A-C4A	2.28	117.91	111.77
21	A	1123	CLA	O2A-CGA-CBA	2.28	118.80	111.83
21	B	1223	CLA	C2D-C1D-ND	2.28	112.39	110.13
21	K	1402	CLA	O1D-CGD-CBD	-2.28	120.02	124.52
21	B	1229	CLA	CHD-C1D-ND	-2.28	121.59	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	617	CLA	CHD-C1D-ND	-2.28	121.59	124.80
21	a	605	CLA	CMA-C3A-C4A	2.28	117.91	111.77
21	7	606	CLA	CHA-C1A-NA	-2.28	121.22	126.39
21	B	1218	CLA	C2C-C1C-NC	2.28	112.38	109.98
21	a	611	CLA	CHD-C1D-ND	-2.28	121.59	124.80
21	A	1104	CLA	C4B-CHC-C1C	2.28	131.61	126.25
21	4	616	CLA	C4B-CHC-C1C	2.28	131.61	126.25
23	I	4001	BCR	C38-C26-C27	2.28	118.46	113.60
21	A	1103	CLA	C2C-C1C-NC	2.28	112.38	109.98
37	5	501	LUT	C20-C13-C12	2.28	121.57	118.09
21	a	603	CLA	CMD-C2D-C3D	-2.28	122.46	127.69
21	8	608	CLA	C4D-CHA-C1A	2.28	123.96	121.24
21	A	1012	CLA	CHD-C1D-ND	-2.28	121.59	124.80
21	4	602	CLA	C2D-C1D-ND	2.28	112.38	110.13
38	5	611	CHL	CMA-C3A-C4A	2.28	119.52	114.61
21	A	1105	CLA	C1C-C2C-C3C	-2.28	104.58	106.98
21	K	1402	CLA	CHA-C1A-NA	-2.28	121.23	126.39
21	1	608	CLA	CHA-C1A-NA	-2.28	121.23	126.39
21	8	605	CLA	C2D-C1D-ND	2.28	112.38	110.13
21	8	615	CLA	C2D-C1D-ND	2.28	112.38	110.13
23	B	4007	BCR	C33-C5-C4	2.28	118.45	113.60
21	5	605	CLA	CMD-C2D-C3D	-2.28	122.47	127.69
21	7	604	CLA	CHD-C1D-ND	-2.28	121.60	124.80
21	1	615	CLA	C4B-CHC-C1C	2.28	131.60	126.25
21	7	617	CLA	CMD-C2D-C3D	-2.28	122.47	127.69
21	A	1128	CLA	C3B-C4B-NB	-2.28	108.50	110.53
21	B	1239	CLA	CHD-C1D-ND	-2.28	121.60	124.80
23	A	4004	BCR	C38-C26-C27	2.28	118.45	113.60
21	A	1102	CLA	C3D-C2D-C1D	-2.28	102.72	105.83
37	1	501	LUT	C30-C31-C32	-2.28	116.60	123.20
21	4	608	CLA	C4B-CHC-C1C	2.28	131.60	126.25
23	B	4004	BCR	C37-C22-C23	2.28	121.56	118.09
24	5	801	LHG	C5-O7-C7	-2.28	112.35	117.80
24	7	801	LHG	O7-C7-O9	-2.27	118.39	123.70
21	4	610	CLA	CHD-C1D-ND	-2.27	121.60	124.80
21	a	605	CLA	O2D-CGD-O1D	-2.27	119.42	123.85
21	A	1119	CLA	C1C-C2C-C3C	-2.27	104.59	106.98
38	6	619	CHL	C4D-CHA-CBD	-2.27	106.67	108.97
21	5	616	CLA	O2D-CGD-O1D	-2.27	119.42	123.85
21	a	615	CLA	C4B-CHC-C1C	2.27	131.59	126.25
32	7	805	SQD	O3-C3-C2	-2.27	105.02	110.38
21	6	607	CLA	O2A-CGA-CBA	2.27	118.76	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1112	CLA	O1D-CGD-CBD	-2.27	120.04	124.52
21	B	1202	CLA	CHD-C1D-ND	-2.27	121.61	124.80
21	1	603	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
21	5	608	CLA	C2D-C1D-ND	2.27	112.37	110.13
21	3	602	CLA	CHD-C1D-ND	-2.27	121.61	124.80
21	A	1130	CLA	O2A-CGA-CBA	2.27	118.75	111.83
21	K	1404	CLA	C2D-C1D-ND	2.27	112.37	110.13
21	4	604	CLA	CHD-C1D-ND	-2.27	121.61	124.80
21	K	1404	CLA	CHA-C1A-NA	-2.27	121.25	126.39
21	B	1232	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
21	7	611	CLA	O2D-CGD-O1D	-2.27	119.44	123.85
21	a	603	CLA	O1D-CGD-CBD	-2.27	120.05	124.52
21	1	601	CLA	C1D-ND-C4D	-2.27	104.72	106.31
21	F	1302	CLA	C2C-C1C-NC	2.27	112.36	109.98
23	L	4003	BCR	C33-C5-C4	2.27	118.43	113.60
23	6	504	BCR	C37-C22-C23	2.27	121.55	118.09
21	A	1116	CLA	C1D-ND-C4D	-2.26	104.72	106.31
21	a	607	CLA	C1D-ND-C4D	-2.26	104.72	106.31
21	B	1204	CLA	CAA-CBA-CGA	-2.26	106.78	113.21
38	8	613	CHL	C4C-CHD-C1D	2.26	124.17	116.07
21	a	608	CLA	CHD-C1D-ND	-2.26	121.62	124.80
21	7	602	CLA	C1C-C2C-C3C	-2.26	104.60	106.98
21	A	1129	CLA	CMD-C2D-C3D	-2.26	122.50	127.69
21	5	614	CLA	CHA-C1A-NA	-2.26	121.27	126.39
21	B	1228	CLA	C6-C5-C3	-2.26	107.95	113.47
21	B	1204	CLA	CHD-C1D-ND	-2.26	121.62	124.80
23	6	503	BCR	C35-C13-C14	-2.26	119.15	122.82
21	F	1301	CLA	CMD-C2D-C3D	-2.26	122.50	127.69
21	L	1501	CLA	CMD-C2D-C3D	-2.26	122.50	127.69
21	8	608	CLA	CMA-C3A-C4A	2.26	117.85	111.77
21	4	611	CLA	O2A-CGA-CBA	2.26	118.73	111.83
37	5	502	LUT	C40-C33-C32	2.26	121.54	118.09
21	A	1108	CLA	C2C-C1C-NC	2.26	112.36	109.98
37	1	502	LUT	C20-C13-C12	2.26	121.54	118.09
21	B	1204	CLA	CAC-C3C-C4C	2.26	127.73	124.79
21	A	1134	CLA	CMD-C2D-C3D	-2.26	122.50	127.69
21	5	601	CLA	C1D-ND-C4D	-2.26	104.73	106.31
37	5	501	LUT	C30-C31-C32	-2.26	116.65	123.20
38	a	606	CHL	CMD-C2D-C3D	2.26	129.20	124.68
21	5	604	CLA	C1-O2A-CGA	2.26	122.12	116.65
21	B	1230	CLA	O1D-CGD-CBD	-2.26	120.06	124.52
21	B	1215	CLA	O2A-CGA-CBA	2.26	118.72	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	617	CLA	CHA-C1A-NA	-2.26	121.28	126.39
21	A	1127	CLA	CHD-C1D-ND	-2.26	121.63	124.80
23	5	504	BCR	C4-C5-C6	-2.26	119.66	122.70
21	a	612	CLA	C1D-ND-C4D	-2.26	104.73	106.31
21	4	616	CLA	C1D-ND-C4D	-2.26	104.73	106.31
21	a	612	CLA	O2D-CGD-O1D	-2.26	119.46	123.85
21	3	618	CLA	O2D-CGD-O1D	-2.26	119.46	123.85
38	5	613	CHL	C1C-C2C-CMC	2.25	130.87	126.80
21	7	610	CLA	CAA-C2A-C3A	-2.25	106.91	113.00
21	A	1137	CLA	C6-C5-C3	-2.25	107.98	113.47
21	B	1211	CLA	O1D-CGD-CBD	-2.25	120.07	124.52
21	A	1111	CLA	CMD-C2D-C3D	-2.25	122.52	127.69
21	7	605	CLA	CAC-C3C-C2C	-2.25	123.42	127.56
21	A	1126	CLA	O2D-CGD-O1D	-2.25	119.46	123.85
21	K	1401	CLA	O2D-CGD-O1D	-2.25	119.46	123.85
21	a	603	CLA	O2D-CGD-O1D	-2.25	119.46	123.85
21	3	606	CLA	CHD-C1D-ND	-2.25	121.63	124.80
21	B	1205	CLA	CAA-C2A-C3A	-2.25	106.91	113.00
21	B	1223	CLA	C2C-C1C-NC	2.25	112.35	109.98
21	A	1125	CLA	CMC-C2C-C3C	-2.25	120.06	126.15
21	a	605	CLA	CHA-C1A-NA	-2.25	121.29	126.39
21	A	1109	CLA	C2D-C1D-ND	2.25	112.36	110.13
21	1	615	CLA	C2D-C1D-ND	2.25	112.36	110.13
21	6	602	CLA	CMA-C3A-C4A	2.25	117.83	111.77
21	B	1231	CLA	O1D-CGD-CBD	-2.25	120.08	124.52
21	A	1118	CLA	CHD-C1D-ND	-2.25	121.63	124.80
21	B	1205	CLA	CHD-C1D-ND	-2.25	121.63	124.80
23	8	503	BCR	C30-C25-C24	2.25	121.76	115.65
21	B	1214	CLA	C4B-CHC-C1C	2.25	131.54	126.25
21	3	604	CLA	O1D-CGD-CBD	-2.25	120.08	124.52
23	K	4001	BCR	C29-C28-C27	2.25	116.23	111.28
23	K	4002	BCR	C38-C26-C25	-2.25	122.03	124.48
21	a	607	CLA	CHD-C1D-ND	-2.25	121.64	124.80
37	8	502	LUT	C20-C13-C12	2.25	121.53	118.09
21	3	607	CLA	CHD-C1D-ND	-2.25	121.64	124.80
21	B	1212	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
21	5	606	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
21	K	1403	CLA	C4B-CHC-C1C	2.25	131.54	126.25
21	J	1901	CLA	CHA-C1A-NA	-2.25	121.30	126.39
21	B	1228	CLA	CHA-C4D-ND	2.25	137.19	132.55
20	A	1011	CL0	CMB-C2B-C3B	2.25	129.18	124.68
21	1	610	CLA	C3B-C4B-NB	-2.25	108.52	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1129	CLA	CHD-C1D-ND	-2.25	121.64	124.80
21	3	605	CLA	OBD-CAD-C3D	-2.25	123.16	128.42
21	8	615	CLA	CAC-C3C-C4C	2.25	127.72	124.79
21	B	1212	CLA	C1D-ND-C4D	-2.25	104.73	106.31
23	5	503	BCR	C27-C26-C25	-2.25	119.67	122.70
38	a	606	CHL	CMA-C3A-C4A	2.25	119.46	114.61
37	1	502	LUT	C16-C1-C6	-2.25	106.72	110.24
21	3	603	CLA	C2D-C1D-ND	2.25	112.35	110.13
21	A	1114	CLA	CHD-C1D-ND	-2.25	121.64	124.80
21	A	1116	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
21	G	1602	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
21	1	607	CLA	C2D-C1D-ND	2.25	112.35	110.13
21	B	1023	CLA	C1-O2A-CGA	2.25	122.09	116.65
21	a	601	CLA	CMD-C2D-C3D	-2.25	122.54	127.69
21	4	612	CLA	CMC-C2C-C1C	2.25	128.54	125.03
21	8	610	CLA	C1C-C2C-C3C	-2.25	104.62	106.98
21	7	607	CLA	CHD-C1D-ND	-2.25	121.64	124.80
38	1	609	CHL	CMA-C3A-C4A	2.25	119.45	114.61
21	B	1201	CLA	CMA-C3A-C4A	2.25	117.81	111.77
21	6	602	CLA	O1D-CGD-CBD	-2.25	120.09	124.52
23	8	503	BCR	C8-C7-C6	-2.24	121.00	127.00
21	F	1301	CLA	O2D-CGD-O1D	-2.24	119.48	123.85
21	B	1238	CLA	CMD-C2D-C3D	-2.24	122.54	127.69
21	3	610	CLA	CMD-C2D-C3D	-2.24	122.54	127.69
21	A	1118	CLA	C1D-ND-C4D	-2.24	104.74	106.31
21	1	605	CLA	C1D-ND-C4D	-2.24	104.74	106.31
21	7	615	CLA	C4B-CHC-C1C	2.24	131.52	126.25
21	6	604	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
21	A	1113	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
21	4	612	CLA	C4B-CHC-C1C	2.24	131.52	126.25
21	6	617	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
21	4	607	CLA	C4B-CHC-C1C	2.24	131.52	126.25
21	A	1134	CLA	O2A-CGA-CBA	2.24	118.67	111.83
37	4	502	LUT	C11-C10-C9	-2.24	124.14	127.28
21	A	1109	CLA	C4B-CHC-C1C	2.24	131.51	126.25
21	3	601	CLA	O2A-CGA-CBA	2.24	118.67	111.83
21	1	602	CLA	O2D-CGD-O1D	-2.24	119.49	123.85
23	8	503	BCR	C35-C13-C12	2.24	121.51	118.09
21	A	1133	CLA	O1D-CGD-CBD	-2.24	120.10	124.52
21	7	604	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
21	G	1601	CLA	C1D-ND-C4D	-2.24	104.74	106.31
23	G	4001	BCR	C33-C5-C4	2.24	118.37	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1121	CLA	CED-O2D-CGD	-2.24	110.84	115.92
21	6	606	CLA	O2D-CGD-O1D	-2.24	119.49	123.85
24	1	801	LHG	C5-O7-C7	-2.24	112.44	117.80
21	8	609	CLA	CMD-C2D-C3D	-2.24	122.56	127.69
21	4	606	CLA	CAA-C2A-C3A	-2.24	106.95	113.00
21	8	609	CLA	CHD-C1D-ND	-2.24	121.66	124.80
21	1	605	CLA	CMA-C3A-C4A	2.24	117.78	111.77
21	7	615	CLA	CHA-C1A-NA	-2.24	121.33	126.39
21	6	617	CLA	C1D-ND-C4D	-2.24	104.74	106.31
21	B	1209	CLA	CHA-C1A-NA	-2.24	121.33	126.39
21	a	602	CLA	C2D-C1D-ND	2.23	112.34	110.13
37	7	501	LUT	C31-C32-C33	-2.23	120.23	126.36
21	6	604	CLA	C3B-C4B-NB	-2.23	108.53	110.53
21	8	610	CLA	C1-O2A-CGA	2.23	122.06	116.65
21	1	603	CLA	CHA-C4D-ND	2.23	137.16	132.55
21	B	1222	CLA	CHD-C1D-ND	-2.23	121.66	124.80
21	7	605	CLA	C2C-C1C-NC	2.23	112.33	109.98
21	1	604	CLA	CHD-C1D-ND	-2.23	121.66	124.80
21	A	1121	CLA	CHD-C1D-ND	-2.23	121.66	124.80
21	F	1301	CLA	C2A-C1A-CHA	2.23	127.74	123.87
23	3	505	BCR	C23-C24-C25	-2.23	121.03	127.00
21	B	1222	CLA	CMD-C2D-C3D	-2.23	122.57	127.69
21	4	610	CLA	C4B-CHC-C1C	2.23	131.50	126.25
21	4	617	CLA	C3D-C2D-C1D	-2.23	102.79	105.83
21	8	605	CLA	C3D-C2D-C1D	-2.23	102.79	105.83
21	L	1503	CLA	CMD-C2D-C3D	-2.23	122.57	127.69
21	B	1224	CLA	O2D-CGD-O1D	-2.23	119.50	123.85
21	6	617	CLA	CHA-C1A-NA	-2.23	121.34	126.39
21	J	1901	CLA	C2D-C1D-ND	2.23	112.33	110.13
21	A	1112	CLA	CAC-C3C-C4C	2.23	127.69	124.79
21	B	1210	CLA	C3D-C2D-C1D	-2.23	102.79	105.83
21	J	1901	CLA	CMD-C2D-C3D	-2.23	122.57	127.69
21	4	612	CLA	CHD-C1D-ND	-2.23	121.66	124.80
21	5	616	CLA	C3D-C2D-C1D	-2.23	102.79	105.83
21	6	612	CLA	C1C-C2C-C3C	-2.23	104.64	106.98
33	G	5002	ERG	C11-C12-C13	2.23	116.50	112.74
21	7	602	CLA	C3D-C2D-C1D	-2.23	102.79	105.83
21	A	1140	CLA	C1C-C2C-C3C	-2.23	104.64	106.98
21	A	1130	CLA	CMA-C3A-C4A	2.23	117.76	111.77
21	1	610	CLA	C1D-ND-C4D	-2.23	104.75	106.31
21	5	608	CLA	CHA-C1A-NA	-2.23	121.35	126.39
37	a	503	LUT	C10-C11-C12	-2.23	116.75	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	1231	CLA	C2C-C1C-NC	2.23	112.32	109.98
23	F	4001	BCR	C34-C9-C10	-2.23	119.21	122.82
21	A	1112	CLA	CHA-C1A-NA	-2.23	121.35	126.39
21	B	1203	CLA	C1C-C2C-C3C	-2.22	104.64	106.98
21	4	615	CLA	CMD-C2D-C3D	-2.22	122.59	127.69
21	B	1203	CLA	C2D-C1D-ND	2.22	112.33	110.13
21	3	605	CLA	CAA-CBA-CGA	-2.22	106.89	113.21
21	1	604	CLA	C1D-ND-C4D	-2.22	104.75	106.31
21	A	1129	CLA	O1D-CGD-CBD	-2.22	120.13	124.52
21	7	605	CLA	CHA-C1A-NA	-2.22	121.36	126.39
23	B	4007	BCR	C38-C26-C25	-2.22	122.06	124.48
21	7	602	CLA	CMD-C2D-C3D	-2.22	122.59	127.69
21	4	612	CLA	CMA-C3A-C4A	2.22	117.75	111.77
21	A	1110	CLA	CHD-C1D-ND	-2.22	121.68	124.80
21	5	604	CLA	C3B-C4B-NB	-2.22	108.55	110.53
21	B	1207	CLA	CMA-C3A-C4A	2.22	117.74	111.77
21	A	1013	CLA	C1-O2A-CGA	2.22	122.03	116.65
21	B	1219	CLA	C3B-C4B-NB	-2.22	108.55	110.53
21	4	607	CLA	CHD-C1D-ND	-2.22	121.68	124.80
21	A	1103	CLA	CMA-C3A-C4A	2.22	117.74	111.77
21	6	609	CLA	CMA-C3A-C4A	2.22	117.74	111.77
21	7	601	CLA	CMD-C2D-C3D	-2.22	122.60	127.69
23	A	4002	BCR	C38-C26-C25	-2.22	122.06	124.48
21	B	1217	CLA	CHD-C1D-ND	-2.22	121.68	124.80
21	3	602	CLA	C4B-CHC-C1C	2.22	131.47	126.25
21	a	605	CLA	OBD-CAD-C3D	-2.22	123.23	128.42
23	B	4004	BCR	C36-C18-C17	-2.22	119.22	122.82
21	A	1103	CLA	C3D-C2D-C1D	-2.22	102.80	105.83
21	A	1107	CLA	C2A-C1A-CHA	2.22	127.72	123.87
21	B	1212	CLA	C2D-C1D-ND	2.22	112.32	110.13
21	8	607	CLA	CAA-C2A-C3A	-2.22	107.01	113.00
21	6	605	CLA	C3D-C2D-C1D	-2.22	102.81	105.83
21	K	1401	CLA	CHA-C1A-NA	-2.22	121.37	126.39
21	A	1121	CLA	C4B-CHC-C1C	2.22	131.46	126.25
21	7	612	CLA	C3B-C4B-NB	-2.22	108.55	110.53
21	B	1239	CLA	CMA-C3A-C4A	2.22	117.73	111.77
21	7	615	CLA	CHD-C1D-ND	-2.22	121.68	124.80
21	5	601	CLA	O1D-CGD-CBD	-2.22	120.15	124.52
21	A	1114	CLA	CHA-C1A-NA	-2.22	121.37	126.39
21	6	608	CLA	O1D-CGD-CBD	-2.22	120.15	124.52
21	K	1402	CLA	CMD-C2D-C3D	-2.22	122.61	127.69
21	3	602	CLA	C1D-ND-C4D	-2.21	104.76	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	3	612	CLA	CHD-C1D-ND	-2.21	121.69	124.80
21	6	615	CLA	C3D-C2D-C1D	-2.21	102.81	105.83
21	A	1123	CLA	C3B-C4B-NB	-2.21	108.55	110.53
21	5	609	CLA	C3B-C4B-NB	-2.21	108.55	110.53
21	7	606	CLA	CMA-C3A-C4A	2.21	117.72	111.77
21	8	606	CLA	C1D-ND-C4D	-2.21	104.76	106.31
21	B	1219	CLA	CHA-C1A-NA	-2.21	121.38	126.39
21	1	606	CLA	C1-O2A-CGA	2.21	122.01	116.65
21	K	1404	CLA	CHD-C1D-ND	-2.21	121.69	124.80
21	K	1402	CLA	C3D-C2D-C1D	-2.21	102.81	105.83
21	7	606	CLA	O2A-CGA-CBA	2.21	118.58	111.83
23	B	4004	BCR	C31-C1-C6	-2.21	106.77	110.24
47	7	504	C7Z	C40-C33-C32	2.21	121.47	118.09
21	3	610	CLA	C4B-CHC-C1C	2.21	131.45	126.25
37	4	502	LUT	C31-C30-C29	-2.21	124.17	127.28
21	A	1131	CLA	CHA-C1A-NA	-2.21	121.38	126.39
21	a	615	CLA	C1D-ND-C4D	-2.21	104.76	106.31
21	7	601	CLA	C1D-ND-C4D	-2.21	104.76	106.31
21	7	611	CLA	CMD-C2D-C3D	-2.21	122.62	127.69
21	B	1237	CLA	O2A-CGA-CBA	2.21	118.58	111.83
21	K	1401	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
21	4	602	CLA	O2A-CGA-CBA	2.21	118.58	111.83
21	B	1202	CLA	C3D-C2D-C1D	-2.21	102.81	105.83
21	B	1238	CLA	C4B-CHC-C1C	2.21	131.44	126.25
38	1	609	CHL	C3D-C4D-ND	-2.21	109.39	112.94
21	a	607	CLA	C4B-CHC-C1C	2.21	131.44	126.25
21	B	1229	CLA	O2A-CGA-CBA	2.21	118.57	111.83
21	5	605	CLA	CBC-CAC-C3C	-2.21	106.43	112.42
38	1	609	CHL	C4C-CHD-C1D	2.21	123.97	116.07
21	A	1137	CLA	CHA-C1A-NA	-2.21	121.39	126.39
38	1	613	CHL	C4C-CHD-C1D	2.21	123.97	116.07
21	1	603	CLA	C1-O2A-CGA	2.21	122.00	116.65
21	B	1210	CLA	C2D-C1D-ND	2.21	112.31	110.13
21	A	1117	CLA	O2A-CGA-CBA	2.21	118.57	111.83
23	A	4002	BCR	C27-C26-C25	-2.21	119.72	122.70
21	8	618	CLA	CMD-C2D-C3D	-2.21	122.63	127.69
21	7	611	CLA	O1D-CGD-CBD	-2.21	120.17	124.52
21	a	604	CLA	C1C-C2C-C3C	-2.21	104.66	106.98
21	B	1236	CLA	CHA-C1A-NA	-2.21	121.40	126.39
21	B	1220	CLA	CHD-C1D-ND	-2.21	121.70	124.80
21	7	606	CLA	CHD-C1D-ND	-2.21	121.70	124.80
21	B	1234	CLA	C2C-C1C-NC	2.21	112.30	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	3	612	CLA	C4B-CHC-C1C	2.20	131.43	126.25
22	A	2001	PQN	C12-C11-C3	-2.20	106.65	112.08
21	4	612	CLA	C2D-C1D-ND	2.20	112.31	110.13
37	1	503	LUT	C22-C23-C24	-2.20	107.91	111.18
28	A	5008	LMT	O5'-C5'-C6'	2.20	111.90	106.44
21	B	1023	CLA	CHA-C1A-NA	-2.20	121.40	126.39
21	L	1501	CLA	C1D-ND-C4D	-2.20	104.77	106.31
21	1	607	CLA	CHA-C1A-NA	-2.20	121.40	126.39
23	A	4005	BCR	C38-C26-C25	-2.20	122.08	124.48
21	7	612	CLA	CHA-C1A-NA	-2.20	121.40	126.39
20	A	1011	CL0	C4C-CHD-C1D	2.20	123.95	116.07
23	A	4005	BCR	C34-C9-C10	-2.20	119.25	122.82
38	8	613	CHL	C1-O2A-CGA	2.20	121.98	116.65
21	A	1132	CLA	O2A-CGA-CBA	2.20	118.55	111.83
21	7	601	CLA	CMA-C3A-C4A	2.20	117.69	111.77
45	7	502	XAT	C35-C15-C14	-2.20	119.02	123.52
34	J	4002	RRX	C8-C7-C6	-2.20	121.12	127.00
21	A	1121	CLA	CHA-C1A-NA	-2.20	121.41	126.39
21	1	606	CLA	C1D-ND-C4D	-2.20	104.77	106.31
21	A	1109	CLA	CMD-C2D-C3D	-2.20	122.65	127.69
21	A	1136	CLA	CMD-C2D-C3D	-2.20	122.65	127.69
21	a	601	CLA	CMA-C3A-C4A	2.20	117.68	111.77
37	1	502	LUT	C18-C5-C4	2.20	118.46	114.42
21	8	609	CLA	C2D-C1D-ND	2.20	112.30	110.13
21	A	1013	CLA	O1D-CGD-CBD	-2.20	120.18	124.52
21	B	1216	CLA	O1D-CGD-CBD	-2.20	120.18	124.52
21	B	1240	CLA	O1D-CGD-CBD	-2.20	120.18	124.52
21	5	605	CLA	CMA-C3A-C4A	2.20	117.68	111.77
21	7	611	CLA	CHD-C1D-ND	-2.20	121.71	124.80
21	A	1140	CLA	C2C-C1C-NC	2.20	112.29	109.98
21	7	612	CLA	C1-C2-C3	-2.20	122.60	126.20
38	5	611	CHL	C1-O2A-CGA	2.20	121.97	116.65
21	6	618	CLA	CHA-C1A-NA	-2.20	121.42	126.39
21	7	604	CLA	C2D-C1D-ND	2.20	112.30	110.13
38	5	613	CHL	C4C-CHD-C1D	2.20	123.92	116.07
21	F	1302	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
21	4	602	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
24	B	5001	LHG	C5-O7-C7	-2.19	112.54	117.80
38	8	613	CHL	CMA-C3A-C4A	2.19	119.34	114.61
21	5	609	CLA	O2A-CGA-CBA	2.19	118.53	111.83
21	7	604	CLA	CHA-C1A-NA	-2.19	121.42	126.39
21	6	606	CLA	CMD-C2D-C3D	-2.19	122.66	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	605	CLA	CHA-C1A-NA	-2.19	121.42	126.39
23	4	503	BCR	C31-C1-C6	-2.19	106.80	110.24
21	8	605	CLA	CMD-C2D-C3D	-2.19	122.66	127.69
37	5	501	LUT	C8-C7-C6	-2.19	121.14	127.00
38	4	613	CHL	C4C-CHD-C1D	2.19	123.92	116.07
21	7	610	CLA	CMD-C2D-C3D	-2.19	122.66	127.69
21	L	1501	CLA	C2D-C1D-ND	2.19	112.30	110.13
21	A	1012	CLA	CHA-C1A-NA	-2.19	121.43	126.39
23	B	4004	BCR	C19-C18-C17	2.19	122.46	119.01
21	B	1023	CLA	C1D-ND-C4D	-2.19	104.77	106.31
21	4	601	CLA	CHA-C1A-NA	-2.19	121.43	126.39
21	8	603	CLA	CAA-C2A-C3A	-2.19	107.08	113.00
21	3	602	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
21	5	605	CLA	CHA-C1A-NA	-2.19	121.43	126.39
21	3	613	CLA	CHD-C1D-ND	-2.19	121.72	124.80
21	B	1213	CLA	CAA-C2A-C3A	-2.19	107.08	113.00
21	7	615	CLA	CMD-C2D-C3D	-2.19	122.67	127.69
23	A	4001	BCR	C2-C1-C6	2.19	113.62	110.44
21	1	611	CLA	CMD-C2D-C3D	-2.19	122.67	127.69
21	B	1214	CLA	CMA-C3A-C4A	2.19	117.66	111.77
21	5	612	CLA	C4B-CHC-C1C	2.19	131.40	126.25
21	4	617	CLA	C1D-ND-C4D	-2.19	104.78	106.31
21	8	611	CLA	C1D-ND-C4D	-2.19	104.78	106.31
21	4	605	CLA	CHD-C1D-ND	-2.19	121.72	124.80
21	6	604	CLA	CHD-C4C-C3C	2.19	127.97	124.77
21	1	612	CLA	C4B-CHC-C1C	2.19	131.39	126.25
21	B	1234	CLA	C1-O2A-CGA	2.19	121.95	116.65
21	a	601	CLA	C2C-C1C-NC	2.19	112.28	109.98
39	1	803	OLA	C3-C2-C1	-2.19	108.80	114.51
21	8	620	CLA	C2D-C1D-ND	2.19	112.29	110.13
21	6	605	CLA	CHD-C1D-ND	-2.19	121.72	124.80
38	5	611	CHL	C4C-CHD-C1D	2.19	123.89	116.07
21	4	610	CLA	C2A-C1A-CHA	2.19	127.66	123.87
21	1	604	CLA	CHC-C1C-NC	-2.19	121.02	124.31
21	B	1209	CLA	C1D-ND-C4D	-2.19	104.78	106.31
21	3	605	CLA	C1D-ND-C4D	-2.19	104.78	106.31
21	a	611	CLA	O2D-CGD-O1D	-2.19	119.59	123.85
21	6	603	CLA	CAA-C2A-C1A	-2.19	104.81	111.97
21	8	606	CLA	O1D-CGD-CBD	-2.19	120.21	124.52
21	B	1021	CLA	CHA-C1A-NA	-2.18	121.44	126.39
23	8	503	BCR	C38-C26-C25	-2.18	122.10	124.48
23	3	504	BCR	C34-C9-C10	-2.18	119.28	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	1213	CLA	C1D-ND-C4D	-2.18	104.78	106.31
21	1	610	CLA	CHA-C1A-NA	-2.18	121.45	126.39
21	B	1237	CLA	CMD-C2D-C3D	-2.18	122.68	127.69
21	A	1133	CLA	CHD-C1D-ND	-2.18	121.73	124.80
21	A	1116	CLA	C2D-C1D-ND	2.18	112.29	110.13
23	5	503	BCR	C4-C5-C6	-2.18	119.75	122.70
23	3	505	BCR	C38-C26-C27	2.18	118.25	113.60
21	A	1103	CLA	C1C-C2C-C3C	-2.18	104.69	106.98
21	A	1119	CLA	C1-C2-C3	-2.18	122.62	126.20
21	6	601	CLA	CHA-C1A-NA	-2.18	121.45	126.39
21	B	1205	CLA	C4B-CHC-C1C	2.18	131.38	126.25
21	A	1123	CLA	CHA-C1A-NA	-2.18	121.45	126.39
21	3	610	CLA	CHA-C1A-NA	-2.18	121.45	126.39
21	A	1105	CLA	CHD-C1D-ND	-2.18	121.73	124.80
37	a	501	LUT	C18-C5-C4	2.18	118.43	114.42
21	A	1135	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
24	a	801	LHG	C5-O7-C7	-2.18	112.58	117.80
38	1	613	CHL	C1-O2A-CGA	2.18	122.86	116.67
21	5	618	CLA	O2A-CGA-CBA	2.18	118.48	111.83
21	8	615	CLA	CMA-C3A-C4A	2.18	117.63	111.77
21	B	1230	CLA	C3B-C4B-NB	-2.18	108.58	110.53
21	A	1122	CLA	CHD-C1D-ND	-2.18	121.73	124.80
21	5	616	CLA	C1D-ND-C4D	-2.18	104.78	106.31
21	a	612	CLA	CMA-C3A-C4A	2.18	117.63	111.77
21	B	1206	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
21	1	608	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
21	8	608	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
21	A	1141	CLA	C3B-C4B-NB	-2.18	108.58	110.53
21	B	1221	CLA	C3D-C2D-C1D	-2.18	102.86	105.83
21	5	608	CLA	CHD-C1D-ND	-2.18	121.74	124.80
21	6	606	CLA	O2A-CGA-CBA	2.18	118.47	111.83
21	6	615	CLA	CMA-C3A-C4A	2.18	117.63	111.77
37	4	501	LUT	C8-C7-C6	-2.18	121.18	127.00
21	G	1601	CLA	O2A-CGA-CBA	2.18	118.47	111.83
23	3	505	BCR	C33-C5-C4	2.18	118.24	113.60
21	5	607	CLA	CHA-C1A-NA	-2.18	121.46	126.39
21	A	1109	CLA	C2A-C1A-CHA	2.18	127.64	123.87
21	B	1201	CLA	CMD-C2D-C3D	-2.18	122.70	127.69
21	5	601	CLA	CHA-C1A-NA	-2.18	121.46	126.39
21	G	1603	CLA	CHD-C1D-ND	-2.18	121.74	124.80
21	6	605	CLA	CMD-C2D-C3D	-2.18	122.70	127.69
21	6	617	CLA	CMA-C3A-C4A	2.18	117.62	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	5008	LMT	O5'-C5'-C4'	2.18	114.22	109.72
21	B	1207	CLA	CHA-C1A-NA	-2.18	121.47	126.39
21	8	602	CLA	CHA-C1A-NA	-2.18	121.47	126.39
21	F	1302	CLA	CMD-C2D-C3D	-2.18	122.70	127.69
21	4	610	CLA	OBD-CAD-C3D	-2.17	123.33	128.42
21	A	1119	CLA	C2C-C1C-NC	2.17	112.27	109.98
21	B	1021	CLA	C2A-C3A-C4A	2.17	105.38	101.87
21	8	605	CLA	CMA-C3A-C4A	2.17	117.61	111.77
23	B	4006	BCR	C4-C5-C6	-2.17	119.77	122.70
21	B	1217	CLA	CMD-C2D-C3D	-2.17	122.70	127.69
21	B	1229	CLA	CMD-C2D-C3D	-2.17	122.70	127.69
21	6	615	CLA	CHA-C1A-NA	-2.17	121.47	126.39
21	L	1501	CLA	CHD-C1D-ND	-2.17	121.75	124.80
21	4	615	CLA	O1D-CGD-CBD	-2.17	120.23	124.52
21	6	612	CLA	CMA-C3A-C4A	2.17	117.61	111.77
21	A	1132	CLA	C1-O2A-CGA	2.17	121.91	116.65
21	L	1502	CLA	CAA-C2A-C3A	-2.17	107.13	113.00
21	4	617	CLA	O2D-CGD-O1D	-2.17	119.62	123.85
38	8	601	CHL	CMD-C2D-C3D	2.17	129.02	124.68
21	3	610	CLA	O2A-CGA-CBA	2.17	118.46	111.83
21	8	605	CLA	CHA-C1A-NA	-2.17	121.47	126.39
21	A	1133	CLA	O2A-CGA-CBA	2.17	118.46	111.83
21	4	602	CLA	CHD-C1D-ND	-2.17	121.75	124.80
21	B	1239	CLA	CMD-C2D-C3D	-2.17	122.71	127.69
21	5	606	CLA	CAA-C2A-C3A	-2.17	107.13	113.00
21	L	1503	CLA	C1D-ND-C4D	-2.17	104.79	106.31
23	B	4003	BCR	C4-C5-C6	-2.17	119.77	122.70
21	1	608	CLA	CHD-C1D-ND	-2.17	121.75	124.80
21	A	1110	CLA	C2D-C1D-ND	2.17	112.27	110.13
21	3	603	CLA	C1D-ND-C4D	-2.17	104.79	106.31
23	6	504	BCR	C38-C26-C27	2.17	118.22	113.60
21	B	1226	CLA	C3B-C4B-NB	-2.17	108.59	110.53
21	6	618	CLA	CMD-C2D-C3D	-2.17	122.72	127.69
21	5	616	CLA	CHD-C1D-ND	-2.17	121.75	124.80
21	5	603	CLA	C1D-ND-C4D	-2.17	104.79	106.31
21	6	612	CLA	O2A-CGA-CBA	2.17	118.44	111.83
21	A	1119	CLA	O2D-CGD-O1D	-2.17	119.63	123.85
23	J	4001	BCR	C31-C1-C6	-2.17	106.84	110.24
21	F	1302	CLA	CHA-C1A-NA	-2.17	121.48	126.39
21	4	604	CLA	C1D-ND-C4D	-2.17	104.79	106.31
21	1	603	CLA	CAA-C2A-C3A	-2.17	107.15	113.00
21	3	606	CLA	O2A-CGA-CBA	2.17	118.44	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	8	611	CLA	C4B-CHC-C1C	2.17	131.34	126.25
23	A	4002	BCR	C34-C9-C10	-2.17	119.31	122.82
21	3	616	CLA	CHA-C1A-NA	-2.17	121.49	126.39
21	A	1127	CLA	C1D-ND-C4D	-2.16	104.79	106.31
38	3	608	CHL	CMD-C2D-C3D	2.16	129.01	124.68
32	G	5001	SQD	O3-C3-C2	-2.16	105.28	110.38
21	7	617	CLA	CHA-C1A-NA	-2.16	121.49	126.39
23	5	503	BCR	C38-C26-C25	-2.16	122.12	124.48
21	6	601	CLA	CMD-C2D-C3D	-2.16	122.73	127.69
23	A	4002	BCR	C38-C26-C27	2.16	118.21	113.60
23	5	503	BCR	C38-C26-C27	2.16	118.21	113.60
21	G	1601	CLA	CMD-C2D-C3D	-2.16	122.73	127.69
21	a	604	CLA	O1D-CGD-CBD	-2.16	120.25	124.52
21	3	604	CLA	OBD-CAD-C3D	-2.16	123.36	128.42
21	1	602	CLA	C2D-C1D-ND	2.16	112.27	110.13
21	7	607	CLA	C4B-CHC-C1C	2.16	131.33	126.25
21	3	618	CLA	CHD-C1D-ND	-2.16	121.76	124.80
21	L	1502	CLA	O1D-CGD-CBD	-2.16	120.25	124.52
34	J	4002	RRX	C24-C23-C22	-2.16	123.04	126.23
36	M	4001	ECH	C20-C19-C18	-2.16	120.44	126.36
21	1	615	CLA	CHA-C1A-NA	-2.16	121.50	126.39
21	1	604	CLA	C6-C5-C3	-2.16	108.20	113.47
21	1	615	CLA	CHD-C1D-ND	-2.16	121.76	124.80
23	A	4001	BCR	C31-C1-C6	-2.16	106.86	110.24
38	3	608	CHL	CMA-C3A-C4A	2.16	119.27	114.61
21	B	1225	CLA	CHD-C1D-ND	-2.16	121.76	124.80
21	1	605	CLA	C3B-C4B-NB	-2.16	108.60	110.53
38	8	604	CHL	CMD-C2D-C3D	2.16	129.00	124.68
24	1	802	LHG	O7-C7-O9	-2.16	118.66	123.70
21	7	609	CLA	C3D-C2D-C1D	-2.16	102.89	105.83
21	8	618	CLA	CHD-C1D-ND	-2.16	121.77	124.80
24	F	5002	LHG	O8-C6-C5	2.16	114.61	108.40
21	A	1104	CLA	C1D-ND-C4D	-2.16	104.80	106.31
21	7	612	CLA	CHD-C4C-C3C	2.16	127.92	124.77
21	B	1222	CLA	C6-C5-C3	-2.16	108.22	113.47
21	8	610	CLA	C4B-CHC-C1C	2.16	131.32	126.25
23	I	4001	BCR	C33-C5-C6	-2.16	122.13	124.48
21	G	1602	CLA	C2D-C1D-ND	2.16	112.26	110.13
21	a	611	CLA	CHA-C1A-NA	-2.16	121.51	126.39
21	5	616	CLA	CHA-C1A-NA	-2.16	121.51	126.39
21	B	1209	CLA	CMD-C2D-C3D	-2.15	122.75	127.69
37	5	502	LUT	C22-C23-C24	-2.15	107.98	111.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	7	609	CLA	C1-O2A-CGA	2.15	121.86	116.65
21	B	1207	CLA	C1D-ND-C4D	-2.15	104.80	106.31
21	4	601	CLA	O2D-CGD-O1D	-2.15	119.66	123.85
21	1	611	CLA	CHA-C1A-NA	-2.15	121.52	126.39
21	B	1204	CLA	CMA-C3A-C4A	2.15	117.56	111.77
21	4	612	CLA	O2A-CGA-CBA	2.15	118.39	111.83
21	3	607	CLA	CHA-C1A-NA	-2.15	121.52	126.39
21	a	615	CLA	CMA-C3A-C4A	2.15	117.55	111.77
23	5	503	BCR	C3-C4-C5	-2.15	110.22	114.06
21	B	1203	CLA	O2A-CGA-CBA	2.15	118.39	111.83
21	8	603	CLA	C6-C7-C8	-2.15	108.82	115.97
21	A	1115	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
21	4	602	CLA	CMD-C2D-C3D	-2.15	122.76	127.69
21	A	1120	CLA	O2A-CGA-CBA	2.15	118.39	111.83
21	A	1104	CLA	C2D-C1D-ND	2.15	112.25	110.13
21	B	1201	CLA	C2D-C1D-ND	2.15	112.25	110.13
21	a	608	CLA	CMD-C2D-C3D	-2.15	122.76	127.69
21	8	602	CLA	CHD-C1D-ND	-2.15	121.78	124.80
23	B	4004	BCR	C4-C5-C6	-2.15	119.80	122.70
21	4	605	CLA	CHA-C1A-NA	-2.15	121.53	126.39
23	A	4003	BCR	C33-C5-C4	2.15	118.18	113.60
21	B	1227	CLA	CHA-C1A-NA	-2.15	121.53	126.39
21	3	601	CLA	C2D-C1D-ND	2.15	112.25	110.13
21	A	1119	CLA	CMD-C2D-C3D	-2.15	122.76	127.69
21	1	611	CLA	O2A-CGA-CBA	2.15	118.38	111.83
21	A	1137	CLA	C1D-ND-C4D	-2.15	104.81	106.31
21	6	608	CLA	C1D-ND-C4D	-2.15	104.81	106.31
21	B	1220	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
21	7	617	CLA	C2D-C1D-ND	2.15	112.25	110.13
21	B	1236	CLA	CHD-C1D-ND	-2.15	121.78	124.80
21	B	1234	CLA	O1A-CGA-CBA	-2.15	115.39	123.78
21	6	608	CLA	CMA-C3A-C4A	2.15	117.54	111.77
21	1	612	CLA	O2D-CGD-O1D	-2.15	119.67	123.85
21	A	1105	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
21	4	604	CLA	C3B-C4B-NB	-2.15	108.61	110.53
38	8	604	CHL	CMA-C3A-C4A	2.15	119.23	114.61
21	A	1116	CLA	CHA-C1A-NA	-2.14	121.53	126.39
21	B	1216	CLA	CMD-C2D-C3D	-2.14	122.77	127.69
21	B	1207	CLA	C2D-C1D-ND	2.14	112.25	110.13
21	B	1239	CLA	C1D-ND-C4D	-2.14	104.81	106.31
21	A	1104	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
21	3	604	CLA	C2D-C1D-ND	2.14	112.25	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	5005	DGD	C3G-C2G-C1G	-2.14	106.79	111.78
37	8	502	LUT	C15-C14-C13	-2.14	124.28	127.28
23	3	503	BCR	C29-C28-C27	2.14	115.98	111.28
21	6	606	CLA	CHA-C1A-NA	-2.14	121.54	126.39
21	3	604	CLA	C2C-C1C-NC	2.14	112.23	109.98
24	4	801	LHG	C5-O7-C7	-2.14	112.67	117.80
23	3	504	BCR	C15-C14-C13	-2.14	124.28	127.28
21	7	606	CLA	O2D-CGD-O1D	-2.14	119.68	123.85
21	a	607	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
21	3	602	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
21	B	1224	CLA	CAA-C2A-C3A	-2.14	107.22	113.00
38	a	610	CHL	C4C-CHD-C1D	2.14	123.72	116.07
21	B	1210	CLA	CHD-C1D-ND	-2.14	121.79	124.80
23	B	4001	BCR	C33-C5-C4	2.14	118.16	113.60
37	6	502	LUT	C10-C11-C12	-2.14	117.00	123.20
21	4	605	CLA	O1D-CGD-CBD	-2.14	120.30	124.52
24	6	801	LHG	C5-O7-C7	-2.14	112.68	117.80
21	L	1503	CLA	CBC-CAC-C3C	2.14	118.22	112.42
21	B	1227	CLA	CMA-C3A-C4A	2.14	117.52	111.77
21	4	605	CLA	CMA-C3A-C4A	2.14	117.52	111.77
21	B	1202	CLA	C11-C12-C13	-2.14	108.86	115.97
21	B	1022	CLA	C4B-CHC-C1C	2.14	131.27	126.25
21	5	618	CLA	O2D-CGD-O1D	-2.14	119.69	123.85
21	B	1234	CLA	C3D-C2D-C1D	-2.14	102.92	105.83
37	8	501	LUT	C15-C35-C34	-2.14	119.15	123.52
21	L	1503	CLA	O1D-CGD-CBD	-2.14	120.31	124.52
21	a	608	CLA	O2A-CGA-CBA	2.14	118.34	111.83
21	6	617	CLA	C2D-C1D-ND	2.13	112.24	110.13
21	B	1206	CLA	C4B-CHC-C1C	2.13	131.27	126.25
21	5	608	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
23	L	4002	BCR	C37-C22-C23	2.13	121.35	118.09
21	A	1137	CLA	CAA-CBA-CGA	-2.13	107.15	113.21
21	8	615	CLA	O1D-CGD-CBD	-2.13	120.31	124.52
21	1	611	CLA	CHD-C1D-ND	-2.13	121.80	124.80
21	8	620	CLA	O2D-CGD-O1D	-2.13	119.70	123.85
21	8	608	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
38	6	613	CHL	C4C-CHD-C1D	2.13	123.70	116.07
21	B	1219	CLA	CHD-C1D-ND	-2.13	121.80	124.80
21	B	1237	CLA	C2D-C1D-ND	2.13	112.24	110.13
21	8	603	CLA	C3B-C4B-NB	-2.13	108.63	110.53
21	B	1238	CLA	CHD-C1D-ND	-2.13	121.80	124.80
21	B	1212	CLA	CHA-C1A-NA	-2.13	121.56	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	1238	CLA	CHA-C1A-NA	-2.13	121.56	126.39
21	B	1206	CLA	CAA-C2A-C3A	-2.13	107.24	113.00
21	A	1132	CLA	C1D-ND-C4D	-2.13	104.82	106.31
21	3	618	CLA	C1D-ND-C4D	-2.13	104.82	106.31
21	A	1112	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
21	B	1218	CLA	CMD-C2D-C3D	-2.13	122.81	127.69
21	A	1112	CLA	CHD-C1D-ND	-2.13	121.81	124.80
37	8	502	LUT	C22-C23-C24	-2.13	108.02	111.18
21	B	1232	CLA	O2D-CGD-O1D	-2.13	119.70	123.85
21	3	602	CLA	C2D-C1D-ND	2.13	112.23	110.13
21	B	1215	CLA	CMD-C2D-C3D	-2.13	122.81	127.69
21	B	1230	CLA	C1C-C2C-C3C	-2.13	104.74	106.98
23	F	4001	BCR	C8-C9-C10	2.13	122.36	119.01
21	7	604	CLA	O2D-CGD-O1D	-2.13	119.70	123.85
21	G	1602	CLA	CHA-C1A-NA	-2.13	121.57	126.39
37	a	502	LUT	C11-C12-C13	-2.13	120.53	126.36
21	B	1205	CLA	CMD-C2D-C3D	-2.13	122.81	127.69
21	B	1205	CLA	CMA-C3A-C4A	2.13	117.49	111.77
21	L	1501	CLA	C3D-C2D-C1D	-2.13	102.93	105.83
21	5	617	CLA	CAC-C3C-C2C	2.13	131.47	127.56
21	4	606	CLA	CHD-C1D-ND	-2.13	121.81	124.80
21	3	612	CLA	CHA-C1A-NA	-2.13	121.58	126.39
21	B	1207	CLA	C3D-C2D-C1D	-2.13	102.93	105.83
21	3	607	CLA	C3D-C2D-C1D	-2.13	102.93	105.83
37	a	501	LUT	C15-C35-C34	-2.13	119.17	123.52
21	8	605	CLA	CHD-C1D-ND	-2.13	121.81	124.80
21	7	612	CLA	O2A-CGA-CBA	2.13	118.32	111.83
21	A	1140	CLA	CHA-C1A-NA	-2.13	121.58	126.39
21	5	617	CLA	CHA-C1A-NA	-2.13	121.58	126.39
21	A	1114	CLA	O1D-CGD-CBD	-2.13	120.33	124.52
21	6	615	CLA	CMD-C2D-C3D	-2.13	122.81	127.69
21	A	1133	CLA	C1-O2A-CGA	2.13	121.80	116.65
21	3	613	CLA	O2A-CGA-CBA	2.12	118.31	111.83
23	B	4007	BCR	C37-C22-C23	2.12	121.33	118.09
37	4	501	LUT	C39-C29-C28	2.12	121.33	118.09
21	B	1218	CLA	CHA-C1A-NA	-2.12	121.58	126.39
21	B	1221	CLA	C2D-C1D-ND	2.12	112.23	110.13
21	7	609	CLA	CAA-CBA-CGA	-2.12	107.18	113.21
21	3	606	CLA	C1D-ND-C4D	-2.12	104.82	106.31
21	6	606	CLA	C1D-ND-C4D	-2.12	104.82	106.31
21	B	1023	CLA	CAA-C2A-C3A	-2.12	107.26	113.00
21	4	616	CLA	O2D-CGD-O1D	-2.12	119.72	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	1219	CLA	O2A-CGA-CBA	2.12	118.31	111.83
21	5	602	CLA	C1-O2A-CGA	2.12	121.79	116.65
21	B	1209	CLA	CHD-C1D-ND	-2.12	121.82	124.80
21	3	605	CLA	CHD-C1D-ND	-2.12	121.82	124.80
21	A	1012	CLA	C4B-CHC-C1C	2.12	131.24	126.25
21	B	1208	CLA	O2A-CGA-CBA	2.12	118.30	111.83
21	B	1022	CLA	CMA-C3A-C4A	2.12	117.47	111.77
21	A	1129	CLA	CHA-C1A-NA	-2.12	121.59	126.39
21	6	601	CLA	C2D-C1D-ND	2.12	112.22	110.13
21	A	1119	CLA	C1D-ND-C4D	-2.12	104.82	106.31
21	a	611	CLA	C1D-ND-C4D	-2.12	104.82	106.31
21	6	615	CLA	C1D-ND-C4D	-2.12	104.82	106.31
21	7	606	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
21	3	605	CLA	CAA-C2A-C1A	-2.12	105.03	111.97
21	A	1139	CLA	CMD-C2D-C3D	-2.12	122.83	127.69
21	a	604	CLA	CHD-C1D-ND	-2.12	121.82	124.80
21	7	604	CLA	C1C-C2C-C3C	-2.12	104.75	106.98
21	K	1404	CLA	OBD-CAD-C3D	-2.12	123.46	128.42
21	A	1124	CLA	O1D-CGD-CBD	-2.12	120.34	124.52
21	A	1114	CLA	C1-O2A-CGA	2.12	121.78	116.65
21	a	615	CLA	C2C-C1C-NC	2.12	112.21	109.98
21	7	602	CLA	CHA-C1A-NA	-2.12	121.59	126.39
23	K	4001	BCR	C34-C9-C10	-2.12	119.38	122.82
33	G	5002	ERG	C18-C13-C17	-2.12	107.83	111.68
21	1	607	CLA	CMD-C2D-C3D	-2.12	122.83	127.69
21	G	1602	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
21	B	1215	CLA	C2D-C1D-ND	2.12	112.22	110.13
21	1	601	CLA	C6-C5-C3	-2.12	108.31	113.47
21	6	605	CLA	C2D-C1D-ND	2.12	112.22	110.13
21	4	616	CLA	CHA-C1A-NA	-2.12	121.60	126.39
21	8	606	CLA	C1-O2A-CGA	2.12	121.77	116.65
38	a	613	CHL	CMA-C3A-C4A	2.12	119.17	114.61
21	A	1136	CLA	C1-O2A-CGA	2.11	121.77	116.65
38	1	609	CHL	C4D-ND-C1D	2.11	106.82	105.22
21	A	1101	CLA	C3D-C2D-C1D	-2.11	102.94	105.83
21	B	1218	CLA	C3D-C2D-C1D	-2.11	102.94	105.83
21	1	604	CLA	O1D-CGD-CBD	-2.11	120.35	124.52
21	6	607	CLA	CHA-C1A-NA	-2.11	121.60	126.39
21	B	1204	CLA	C2D-C1D-ND	2.11	112.22	110.13
21	1	612	CLA	C2D-C1D-ND	2.11	112.22	110.13
21	3	601	CLA	CMC-C2C-C1C	2.11	128.34	125.03
21	A	1115	CLA	C1D-ND-C4D	-2.11	104.83	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1135	CLA	CMA-C3A-C4A	2.11	117.45	111.77
21	4	607	CLA	CAA-C2A-C3A	-2.11	107.29	113.00
21	G	1601	CLA	CHA-C1A-NA	-2.11	121.61	126.39
21	7	601	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
23	I	4001	BCR	C30-C25-C26	-2.11	119.75	122.64
21	A	1126	CLA	CHA-C1A-NA	-2.11	121.61	126.39
21	5	602	CLA	CHD-C1D-ND	-2.11	121.83	124.80
21	B	1204	CLA	CAA-C2A-C3A	-2.11	107.30	113.00
21	A	1115	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
21	B	1240	CLA	C2D-C1D-ND	2.11	112.21	110.13
21	3	613	CLA	CHA-C1A-NA	-2.11	121.61	126.39
21	5	618	CLA	CHA-C1A-NA	-2.11	121.61	126.39
21	6	609	CLA	C1-C2-C3	-2.11	122.74	126.20
21	A	1113	CLA	C1D-ND-C4D	-2.11	104.83	106.31
44	6	806	SPH	C3-C4-C5	-2.11	120.32	124.69
21	7	601	CLA	C1C-C2C-C3C	-2.11	104.76	106.98
21	B	1235	CLA	CAA-C2A-C3A	-2.11	107.30	113.00
21	A	1106	CLA	CAC-C3C-C4C	2.11	127.53	124.79
21	7	604	CLA	CAC-C3C-C4C	2.11	127.53	124.79
21	A	1113	CLA	C2D-C1D-ND	2.11	112.21	110.13
21	A	1124	CLA	CAA-C2A-C1A	-2.11	105.07	111.97
21	4	615	CLA	CHD-C1D-ND	-2.11	121.84	124.80
38	1	613	CHL	C1C-C2C-CMC	2.11	130.60	126.80
21	a	603	CLA	CAC-C3C-C4C	2.11	127.53	124.79
21	A	1135	CLA	CHA-C1A-NA	-2.11	121.62	126.39
21	4	605	CLA	C3D-C2D-C1D	-2.11	102.96	105.83
21	4	617	CLA	C2D-C1D-ND	2.11	112.21	110.13
21	7	610	CLA	CHA-C1A-NA	-2.11	121.62	126.39
38	4	609	CHL	CMD-C2D-C3D	2.11	128.89	124.68
37	6	501	LUT	C11-C12-C13	-2.11	120.59	126.36
21	3	616	CLA	C2D-C1D-ND	2.11	112.21	110.13
21	A	1110	CLA	C1D-ND-C4D	-2.11	104.83	106.31
38	7	613	CHL	C4C-CHD-C1D	2.10	123.60	116.07
21	A	1113	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
38	5	610	CHL	CMD-C2D-C3D	2.10	128.89	124.68
20	A	1011	CL0	C2C-C1C-NC	2.10	116.41	110.46
21	B	1239	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
21	F	1301	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
23	3	504	BCR	C37-C22-C21	-2.10	119.41	122.82
21	B	1239	CLA	C2D-C1D-ND	2.10	112.21	110.13
23	J	4001	BCR	C38-C26-C27	2.10	118.08	113.60
21	A	1129	CLA	CMA-C3A-C4A	2.10	117.42	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	1229	CLA	CHA-C1A-NA	-2.10	121.63	126.39
21	B	1235	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
21	B	1227	CLA	CHD-C1D-ND	-2.10	121.84	124.80
21	8	606	CLA	C2D-C1D-ND	2.10	112.21	110.13
38	3	608	CHL	C4C-CHD-C1D	2.10	123.59	116.07
21	B	1212	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
21	8	618	CLA	CHA-C1A-NA	-2.10	121.63	126.39
21	6	602	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
21	B	1215	CLA	C1D-ND-C4D	-2.10	104.84	106.31
21	A	1137	CLA	CMA-C3A-C4A	2.10	117.42	111.77
21	a	601	CLA	C2D-C1D-ND	2.10	112.20	110.13
21	a	612	CLA	C2D-C1D-ND	2.10	112.20	110.13
21	5	618	CLA	CHD-C1D-ND	-2.10	121.85	124.80
21	8	610	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
21	7	610	CLA	C1D-ND-C4D	-2.10	104.84	106.31
47	7	504	C7Z	C1-C2-C3	2.10	118.20	113.59
21	B	1226	CLA	C4B-CHC-C1C	2.10	131.18	126.25
21	a	601	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
23	6	504	BCR	C23-C24-C25	-2.10	121.39	127.00
21	1	605	CLA	O1D-CGD-CBD	-2.10	120.38	124.52
21	3	616	CLA	C1D-ND-C4D	-2.10	104.84	106.31
21	8	620	CLA	CMD-C2D-C3D	-2.10	122.88	127.69
21	A	1105	CLA	O2A-CGA-CBA	2.10	118.23	111.83
21	A	1013	CLA	C4B-CHC-C1C	2.10	131.18	126.25
21	B	1213	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
38	3	611	CHL	C1-O2A-CGA	2.10	121.73	116.65
21	B	1227	CLA	O2A-CGA-CBA	2.10	118.23	111.83
21	5	618	CLA	CMD-C2D-C3D	-2.10	122.88	127.69
21	4	605	CLA	CMD-C2D-C3D	-2.10	122.88	127.69
21	B	1201	CLA	C1D-ND-C4D	-2.10	104.84	106.31
38	a	610	CHL	CMD-C2D-C3D	2.10	128.87	124.68
21	B	1021	CLA	O1D-CGD-CBD	-2.10	120.38	124.52
21	a	615	CLA	O1D-CGD-CBD	-2.10	120.38	124.52
38	6	610	CHL	C3D-C4D-ND	-2.10	109.58	112.94
34	J	4002	RRX	C31-C1-C6	2.09	113.53	110.24
38	6	610	CHL	CMD-C2D-C3D	2.09	128.87	124.68
37	4	501	LUT	C20-C13-C12	2.09	121.29	118.09
21	4	608	CLA	C1D-ND-C4D	-2.09	104.84	106.31
37	1	502	LUT	C22-C23-C24	-2.09	108.08	111.18
21	A	1104	CLA	C1-O2A-CGA	2.09	121.72	116.65
21	A	1134	CLA	CHA-C1A-NA	-2.09	121.65	126.39
21	B	1236	CLA	OBD-CAD-C3D	-2.09	123.52	128.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	F	5001	LHG	O7-C7-O9	-2.09	118.81	123.70
21	A	1013	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
21	B	1215	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
21	A	1104	CLA	CBC-CAC-C3C	-2.09	106.75	112.42
21	a	601	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
21	4	608	CLA	CHA-C1A-NA	-2.09	121.65	126.39
21	B	1230	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
21	a	602	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
21	5	601	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
21	A	1104	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
21	A	1111	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
23	L	4002	BCR	C34-C9-C8	2.09	121.28	118.09
21	B	1217	CLA	CHA-C1A-NA	-2.09	121.66	126.39
21	8	615	CLA	CHA-C1A-NA	-2.09	121.66	126.39
37	1	501	LUT	C31-C30-C29	-2.09	124.35	127.28
21	L	1503	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
21	7	610	CLA	C2D-C1D-ND	2.09	112.19	110.13
21	3	601	CLA	C1D-ND-C4D	-2.09	104.85	106.31
21	3	606	CLA	C1-O2A-CGA	2.09	121.71	116.65
21	4	612	CLA	CHA-C1A-NA	-2.09	121.66	126.39
21	4	606	CLA	O2A-CGA-CBA	2.09	118.20	111.83
38	6	610	CHL	CMA-C3A-C4A	2.09	119.11	114.61
21	K	1404	CLA	CMD-C2D-C3D	-2.09	122.90	127.69
21	5	618	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
23	B	4004	BCR	C39-C30-C25	-2.09	106.97	110.24
23	4	503	BCR	C38-C26-C27	2.09	118.05	113.60
21	A	1104	CLA	CHA-C1A-NA	-2.09	121.66	126.39
21	B	1225	CLA	CHA-C1A-NA	-2.09	121.66	126.39
21	1	606	CLA	CAA-CBA-CGA	-2.09	107.28	113.21
21	4	610	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
21	B	1224	CLA	CHA-C1A-NA	-2.09	121.67	126.39
21	B	1213	CLA	C2D-C1D-ND	2.09	112.19	110.13
21	4	610	CLA	CAA-C2A-C3A	-2.09	107.36	113.00
37	8	501	LUT	C22-C23-C24	-2.09	108.09	111.18
21	A	1131	CLA	CHD-C1D-ND	-2.09	121.87	124.80
21	8	602	CLA	OBD-CAD-C3D	-2.09	123.54	128.42
21	A	1138	CLA	CHD-C1D-ND	-2.09	121.87	124.80
21	5	609	CLA	CHD-C1D-ND	-2.09	121.87	124.80
21	A	1138	CLA	CMD-C2D-C3D	-2.09	122.91	127.69
21	B	1201	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
21	A	1106	CLA	CHD-C1D-ND	-2.08	121.87	124.80
21	B	1021	CLA	CHD-C1D-ND	-2.08	121.87	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1117	CLA	CMD-C2D-C3D	-2.08	122.91	127.69
21	4	611	CLA	CHA-C1A-NA	-2.08	121.67	126.39
37	8	501	LUT	C11-C10-C9	-2.08	124.36	127.28
21	3	613	CLA	CMD-C2D-C3D	-2.08	122.91	127.69
21	5	604	CLA	OBD-CAD-C3D	-2.08	123.55	128.42
24	a	801	LHG	O7-C7-O9	-2.08	118.84	123.70
21	7	607	CLA	CHA-C1A-NA	-2.08	121.68	126.39
23	3	503	BCR	C23-C22-C21	-2.08	115.73	119.01
21	A	1128	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
21	4	604	CLA	CMC-C2C-C1C	2.08	128.29	125.03
21	A	1118	CLA	C2D-C1D-ND	2.08	112.19	110.13
21	A	1106	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
21	A	1135	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
21	6	607	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
21	A	1134	CLA	C1D-ND-C4D	-2.08	104.85	106.31
21	a	615	CLA	CHA-C1A-NA	-2.08	121.68	126.39
36	M	4001	ECH	C7-C6-C5	-2.08	116.77	121.56
21	1	615	CLA	C1D-ND-C4D	-2.08	104.85	106.31
21	A	1128	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
21	5	602	CLA	CMD-C2D-C3D	-2.08	122.92	127.69
21	B	1229	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
21	5	612	CLA	CAA-C2A-C3A	-2.08	107.39	113.00
21	8	610	CLA	CHD-C1D-ND	-2.08	121.88	124.80
37	a	503	LUT	C18-C5-C4	2.08	118.24	114.42
21	A	1108	CLA	CHD-C1D-ND	-2.08	121.88	124.80
21	6	607	CLA	CHD-C1D-ND	-2.08	121.88	124.80
38	a	609	CHL	CMA-C3A-C4A	2.08	119.08	114.61
21	3	601	CLA	C3D-C2D-C1D	-2.08	103.00	105.83
21	B	1211	CLA	CMA-C3A-C4A	2.08	117.35	111.77
21	8	610	CLA	C3B-C4B-NB	-2.08	108.68	110.53
21	A	1139	CLA	O2A-CGA-CBA	2.08	118.16	111.83
21	A	1141	CLA	CHD-C1D-ND	-2.08	121.88	124.80
21	A	1130	CLA	C1D-ND-C4D	-2.08	104.86	106.31
21	a	615	CLA	C3B-C4B-NB	-2.07	108.68	110.53
38	4	618	CHL	C3D-C4D-ND	-2.07	109.61	112.94
21	A	1118	CLA	O2A-CGA-CBA	2.07	118.16	111.83
21	A	1119	CLA	O2A-CGA-CBA	2.07	118.16	111.83
21	B	1218	CLA	C1-O2A-CGA	2.07	121.67	116.65
21	4	610	CLA	O2A-CGA-CBA	2.07	118.16	111.83
21	A	1112	CLA	CAA-C2A-C3A	-2.07	107.40	113.00
21	1	605	CLA	CBC-CAC-C3C	-2.07	106.80	112.42
21	a	602	CLA	CHD-C1D-ND	-2.07	121.89	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1106	CLA	O2A-CGA-CBA	2.07	118.15	111.83
21	3	605	CLA	C2D-C1D-ND	2.07	112.18	110.13
38	5	613	CHL	CMD-C2D-C3D	2.07	128.82	124.68
21	3	616	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
21	A	1128	CLA	CMD-C2D-C3D	-2.07	122.94	127.69
21	4	601	CLA	C3B-C4B-NB	-2.07	108.68	110.53
37	8	502	LUT	C19-C9-C8	2.07	121.25	118.09
38	8	604	CHL	C4C-CHD-C1D	2.07	123.48	116.07
21	B	1021	CLA	C1-O2A-CGA	2.07	121.66	116.65
21	5	612	CLA	O2A-CGA-CBA	2.07	118.15	111.83
21	8	610	CLA	CMD-C2D-C3D	-2.07	122.94	127.69
21	A	1127	CLA	CHA-C1A-NA	-2.07	121.70	126.39
21	5	606	CLA	C2D-C1D-ND	2.07	112.17	110.13
38	6	611	CHL	CMD-C2D-C3D	2.07	128.82	124.68
21	a	602	CLA	CMD-C2D-C3D	-2.07	122.94	127.69
21	B	1219	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
21	B	1237	CLA	CAC-C3C-C4C	2.07	127.48	124.79
37	5	505	LUT	C20-C13-C14	-2.07	119.47	122.82
21	3	602	CLA	CMA-C3A-C4A	2.07	117.33	111.77
23	L	4002	BCR	C33-C5-C4	2.07	118.00	113.60
21	A	1109	CLA	C6-C7-C8	-2.07	109.09	115.97
21	1	610	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
21	a	602	CLA	C1D-ND-C4D	-2.07	104.86	106.31
21	B	1214	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
21	L	1503	CLA	C2D-C1D-ND	2.07	112.17	110.13
21	5	603	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
21	A	1111	CLA	CHA-C1A-NA	-2.07	121.71	126.39
21	B	1240	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
38	3	611	CHL	CMD-C2D-C3D	2.07	128.81	124.68
21	A	1139	CLA	CHA-C1A-NA	-2.06	121.72	126.39
38	a	609	CHL	CMD-C2D-C3D	2.06	128.81	124.68
21	A	1012	CLA	C2D-C1D-ND	2.06	112.17	110.13
21	A	1103	CLA	CMD-C2D-C3D	-2.06	122.96	127.69
21	1	612	CLA	CMD-C2D-C3D	-2.06	122.96	127.69
21	a	604	CLA	C3A-C2A-C1A	2.06	104.43	101.34
23	B	4006	BCR	C36-C18-C17	-2.06	119.47	122.82
21	3	601	CLA	C3B-C4B-NB	-2.06	108.69	110.53
21	5	601	CLA	C2D-C1D-ND	2.06	112.17	110.13
21	5	607	CLA	CMD-C2D-C3D	-2.06	122.96	127.69
21	4	604	CLA	CMD-C2D-C3D	-2.06	122.96	127.69
21	3	605	CLA	C1-O2A-CGA	2.06	121.64	116.65
21	B	1211	CLA	C1D-ND-C4D	-2.06	104.87	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	5	602	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
21	A	1110	CLA	CHA-C1A-NA	-2.06	121.72	126.39
21	B	1237	CLA	C1C-C2C-C3C	-2.06	104.81	106.98
21	7	610	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
38	6	613	CHL	CMD-C2D-C3D	2.06	128.80	124.68
21	G	1603	CLA	CHA-C1A-NA	-2.06	121.73	126.39
23	A	4001	BCR	C37-C22-C21	-2.06	119.48	122.82
21	A	1120	CLA	CMD-C2D-C3D	-2.06	122.97	127.69
38	5	610	CHL	C4C-CHD-C1D	2.06	123.44	116.07
21	4	603	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
21	A	1118	CLA	CHA-C1A-NA	-2.06	121.73	126.39
21	5	606	CLA	CHA-C1A-NA	-2.06	121.73	126.39
21	B	1223	CLA	CMD-C2D-C3D	-2.06	122.97	127.69
21	3	607	CLA	C2D-C1D-ND	2.06	112.16	110.13
21	6	602	CLA	CMD-C2D-C3D	-2.06	122.97	127.69
21	A	1013	CLA	O2D-CGD-O1D	-2.06	119.84	123.85
21	B	1207	CLA	CHD-C1D-ND	-2.06	121.91	124.80
21	G	1602	CLA	CMD-C2D-C3D	-2.06	122.97	127.69
21	3	618	CLA	O1D-CGD-CBD	-2.06	120.46	124.52
21	7	604	CLA	C3D-C2D-C1D	-2.06	103.03	105.83
21	5	607	CLA	CHD-C1D-ND	-2.06	121.91	124.80
21	a	608	CLA	CHA-C1A-NA	-2.06	121.74	126.39
21	A	1105	CLA	CMD-C2D-C3D	-2.06	122.98	127.69
21	B	1202	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
21	5	602	CLA	O2A-CGA-CBA	2.05	118.10	111.83
21	A	1139	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
21	1	607	CLA	CHD-C1D-ND	-2.05	121.91	124.80
21	A	1137	CLA	CMD-C2D-C3D	-2.05	122.98	127.69
21	8	603	CLA	C1D-ND-C4D	-2.05	104.87	106.31
21	A	1133	CLA	CMD-C2D-C3D	-2.05	122.98	127.69
21	4	615	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
23	7	503	BCR	C37-C22-C23	2.05	121.22	118.09
21	7	611	CLA	CAC-C3C-C2C	-2.05	123.79	127.56
23	B	4007	BCR	C15-C14-C13	-2.05	124.40	127.28
23	K	4001	BCR	C38-C26-C25	-2.05	122.25	124.48
21	A	1106	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
21	F	1302	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
38	4	618	CHL	C4C-CHD-C1D	2.05	123.41	116.07
20	A	1011	CL0	C4C-C3C-C2C	-2.05	105.27	113.37
21	4	605	CLA	C2D-C1D-ND	2.05	112.16	110.13
21	K	1404	CLA	C1D-ND-C4D	-2.05	104.87	106.31
21	6	617	CLA	O1D-CGD-CBD	-2.05	120.47	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	1224	CLA	CMD-C2D-C3D	-2.05	122.99	127.69
21	6	608	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
37	1	501	LUT	C18-C5-C4	2.05	118.19	114.42
37	7	501	LUT	C18-C5-C4	2.05	118.19	114.42
21	A	1122	CLA	CMD-C2D-C3D	-2.05	122.99	127.69
21	A	1130	CLA	C2D-C1D-ND	2.05	112.15	110.13
21	A	1120	CLA	CMC-C2C-C1C	2.05	128.24	125.03
21	G	1602	CLA	CAA-C2A-C3A	-2.05	107.46	113.00
23	J	4001	BCR	C39-C30-C29	2.05	116.81	108.95
21	4	606	CLA	CHA-C1A-NA	-2.05	121.75	126.39
21	1	612	CLA	C6-C5-C3	-2.05	108.48	113.47
21	A	1105	CLA	CHA-C1A-NA	-2.05	121.76	126.39
21	A	1136	CLA	C1D-ND-C4D	-2.05	104.88	106.31
21	B	1210	CLA	CAA-CBA-CGA	-2.05	107.40	113.21
21	8	612	CLA	CMD-C2D-C3D	-2.05	123.00	127.69
21	7	601	CLA	C2C-C1C-NC	2.05	112.13	109.98
24	7	802	LHG	O7-C7-O9	-2.05	118.92	123.70
21	A	1114	CLA	C1D-ND-C4D	-2.05	104.88	106.31
21	4	601	CLA	C1D-ND-C4D	-2.05	104.88	106.31
21	B	1022	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
23	A	4004	BCR	C8-C7-C6	-2.05	121.53	127.00
21	a	612	CLA	CMD-C2D-C3D	-2.04	123.00	127.69
40	a	504	QTB	C16-C15-C14	2.04	114.64	111.33
21	4	602	CLA	CHA-C1A-NA	-2.04	121.76	126.39
21	B	1232	CLA	CHD-C1D-ND	-2.04	121.93	124.80
21	6	606	CLA	C2D-C1D-ND	2.04	112.15	110.13
21	B	1229	CLA	C1D-ND-C4D	-2.04	104.88	106.31
21	6	618	CLA	CHD-C1D-ND	-2.04	121.93	124.80
38	6	619	CHL	CMD-C2D-C3D	2.04	128.77	124.68
37	5	502	LUT	C30-C31-C32	-2.04	117.28	123.20
21	a	611	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
24	3	801	LHG	O7-C7-O9	-2.04	118.93	123.70
40	a	504	QTB	C13-C12-C14	2.04	114.87	111.06
21	A	1141	CLA	CHA-C1A-NA	-2.04	121.77	126.39
21	8	612	CLA	OBD-CAD-C3D	-2.04	123.64	128.42
21	B	1212	CLA	CAA-CBA-CGA	-2.04	107.41	113.21
21	5	612	CLA	CHA-C1A-NA	-2.04	121.77	126.39
21	A	1111	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
37	a	501	LUT	C11-C12-C13	-2.04	120.77	126.36
21	a	604	CLA	CAC-C3C-C4C	2.04	127.44	124.79
21	1	611	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
30	B	5005	PTY	C6-O7-C8	-2.04	112.91	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	611	CLA	C2D-C1D-ND	2.04	112.14	110.13
37	a	503	LUT	C38-C25-C24	-2.04	118.53	123.36
21	6	612	CLA	CHA-C1A-NA	-2.04	121.77	126.39
21	A	1118	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
21	3	604	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
21	a	615	CLA	O2D-CGD-O1D	-2.04	119.88	123.85
23	I	4001	BCR	C37-C22-C23	2.04	121.20	118.09
21	B	1223	CLA	C1D-ND-C4D	-2.04	104.88	106.31
21	a	602	CLA	CHA-C1A-NA	-2.04	121.78	126.39
21	3	605	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
21	8	607	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
21	B	1216	CLA	CHA-C1A-NA	-2.04	121.78	126.39
21	B	1023	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
21	8	606	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
21	A	1115	CLA	CHA-C1A-NA	-2.04	121.78	126.39
21	3	602	CLA	CHA-C1A-NA	-2.04	121.78	126.39
21	A	1141	CLA	CMD-C2D-C3D	-2.04	123.02	127.69
21	5	612	CLA	CMD-C2D-C3D	-2.04	123.02	127.69
21	5	602	CLA	C2D-C1D-ND	2.04	112.14	110.13
21	A	1013	CLA	CHA-C1A-NA	-2.04	121.78	126.39
21	6	617	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
21	8	603	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
21	A	1130	CLA	CHA-C1A-NA	-2.04	121.78	126.39
38	4	618	CHL	CMD-C2D-C3D	2.04	128.75	124.68
23	B	4004	BCR	C34-C9-C8	2.04	121.20	118.09
21	B	1206	CLA	CBC-CAC-C3C	-2.04	106.90	112.42
21	7	615	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
21	A	1112	CLA	C2D-C1D-ND	2.03	112.14	110.13
21	L	1501	CLA	CAA-C2A-C3A	-2.03	107.50	113.00
21	B	1237	CLA	C2C-C1C-NC	2.03	112.12	109.98
24	8	801	LHG	O8-C23-O10	-2.03	118.54	123.63
21	B	1207	CLA	CMD-C2D-C3D	-2.03	123.03	127.69
21	A	1112	CLA	C3B-C4B-NB	-2.03	108.72	110.53
21	A	1134	CLA	C2D-C1D-ND	2.03	112.14	110.13
21	7	609	CLA	C2D-C1D-ND	2.03	112.14	110.13
21	5	617	CLA	O2A-CGA-CBA	2.03	118.03	111.83
21	6	604	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
21	8	609	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
21	B	1234	CLA	CHD-C1D-ND	-2.03	121.94	124.80
37	a	502	LUT	C15-C35-C34	-2.03	119.36	123.52
37	7	501	LUT	C8-C7-C6	-2.03	121.57	127.00
21	B	1201	CLA	CHA-C1A-NA	-2.03	121.79	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	1237	CLA	CHD-C1D-ND	-2.03	121.94	124.80
21	B	1229	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
21	1	612	CLA	C1D-ND-C4D	-2.03	104.89	106.31
21	6	609	CLA	C2D-C1D-ND	2.03	112.14	110.13
30	8	810	PTY	O4-C30-O30	-2.03	118.55	123.63
21	8	612	CLA	CHA-C1A-NA	-2.03	121.79	126.39
21	A	1111	CLA	C2D-C1D-ND	2.03	112.14	110.13
21	7	604	CLA	C2C-C1C-NC	2.03	112.11	109.98
21	A	1111	CLA	CMA-C3A-C4A	2.03	117.23	111.77
21	a	612	CLA	CHA-C1A-NA	-2.03	121.80	126.39
21	A	1109	CLA	CHD-C1D-ND	-2.03	121.95	124.80
21	A	1126	CLA	O1D-CGD-CBD	-2.03	120.52	124.52
24	7	801	LHG	O4-P-O5	2.03	121.88	112.44
21	B	1208	CLA	CHA-C1A-NA	-2.03	121.80	126.39
38	8	613	CHL	CMD-C2D-C3D	2.03	128.74	124.68
21	B	1203	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
23	3	504	BCR	C23-C24-C25	-2.03	121.58	127.00
21	F	1301	CLA	CHD-C1D-ND	-2.03	121.95	124.80
21	A	1116	CLA	C3D-C2D-C1D	-2.03	103.07	105.83
21	A	1119	CLA	O1D-CGD-CBD	-2.03	120.52	124.52
38	5	611	CHL	CMD-C2D-C3D	2.03	128.73	124.68
21	B	1214	CLA	CHA-C1A-NA	-2.03	121.80	126.39
21	A	1122	CLA	CAA-C2A-C3A	-2.03	107.53	113.00
38	1	613	CHL	CMD-C2D-C3D	2.03	128.73	124.68
21	1	605	CLA	C1-O2A-CGA	2.02	121.55	116.65
37	1	501	LUT	C20-C13-C12	2.02	121.18	118.09
21	A	1114	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
47	7	504	C7Z	C35-C34-C33	-2.02	124.44	127.28
21	1	604	CLA	O2A-CGA-CBA	2.02	118.01	111.83
21	B	1226	CLA	CAA-C2A-C3A	-2.02	107.53	113.00
23	B	4002	BCR	C8-C7-C6	-2.02	121.59	127.00
21	A	1119	CLA	CHA-C1A-NA	-2.02	121.81	126.39
21	A	1117	CLA	CAA-C2A-C3A	-2.02	107.53	113.00
21	B	1204	CLA	C1D-ND-C4D	-2.02	104.89	106.31
21	7	611	CLA	CHD-C4C-C3C	2.02	127.72	124.77
38	a	613	CHL	CMD-C2D-C3D	2.02	128.72	124.68
21	a	615	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
21	B	1234	CLA	CMD-C2D-C3D	-2.02	123.05	127.69
21	3	618	CLA	CMD-C2D-C3D	-2.02	123.05	127.69
21	A	1113	CLA	CAA-CBA-CGA	-2.02	107.47	113.21
21	B	1022	CLA	C2D-C1D-ND	2.02	112.13	110.13
21	3	618	CLA	C2D-C1D-ND	2.02	112.13	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	605	CLA	OBD-CAD-C3D	-2.02	123.69	128.42
21	A	1105	CLA	CMC-C2C-C1C	2.02	128.19	125.03
23	G	4001	BCR	C38-C26-C27	2.02	117.91	113.60
21	B	1204	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
37	4	502	LUT	C38-C25-C24	-2.02	118.58	123.36
21	8	611	CLA	C3B-C4B-NB	-2.02	108.73	110.53
21	4	617	CLA	CMA-C3A-C2A	2.02	121.80	113.98
21	5	614	CLA	CMA-C3A-C4A	2.02	117.20	111.77
21	A	1102	CLA	CHD-C4C-NC	-2.02	121.10	124.23
21	B	1213	CLA	CHA-C1A-NA	-2.02	121.82	126.39
24	6	802	LHG	O8-C23-O10	-2.02	118.58	123.63
21	3	610	CLA	CMA-C3A-C4A	2.02	117.20	111.77
21	A	1103	CLA	CAA-C2A-C1A	-2.02	105.36	111.97
21	A	1126	CLA	CAA-CBA-CGA	-2.02	107.47	113.21
37	7	501	LUT	C26-C27-C28	-2.02	121.44	124.58
23	3	504	BCR	C33-C5-C4	2.02	117.90	113.60
21	B	1215	CLA	CHA-C1A-NA	-2.02	121.82	126.39
21	B	1210	CLA	C6-C5-C3	-2.02	108.55	113.47
21	1	612	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
21	7	610	CLA	O2D-CGD-O1D	-2.02	119.92	123.85
21	A	1108	CLA	CAC-C3C-C4C	2.02	127.42	124.79
21	A	1130	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
21	A	1138	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
21	5	601	CLA	O2D-CGD-O1D	-2.02	119.92	123.85
21	6	601	CLA	O2D-CGD-O1D	-2.02	119.92	123.85
21	8	620	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
21	B	1213	CLA	C1C-C2C-C3C	-2.02	104.86	106.98
21	A	1106	CLA	C6-C5-C3	-2.02	108.56	113.47
21	5	617	CLA	CHD-C1D-ND	-2.02	121.97	124.80
21	B	1228	CLA	C3B-C4B-NB	-2.02	108.73	110.53
23	L	4002	BCR	C27-C26-C25	-2.02	119.98	122.70
21	7	612	CLA	CHD-C1D-ND	-2.01	121.97	124.80
21	8	620	CLA	C1-C2-C3	-2.01	122.90	126.20
21	7	612	CLA	CMA-C3A-C4A	2.01	117.19	111.77
23	A	4005	BCR	C29-C28-C27	2.01	115.70	111.28
21	8	615	CLA	CHD-C1D-ND	-2.01	121.97	124.80
25	B	5003	DGD	O6D-C5D-C6D	2.01	110.69	106.69
21	7	610	CLA	CMA-C3A-C4A	2.01	117.18	111.77
21	B	1232	CLA	CHA-C1A-NA	-2.01	121.83	126.39
21	L	1503	CLA	CHA-C1A-NA	-2.01	121.83	126.39
21	1	615	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
21	B	1222	CLA	C2D-C1D-ND	2.01	112.12	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	8	803	DGA	OG1-CA1-OA1	-2.01	118.59	123.63
37	3	501	LUT	C20-C13-C12	2.01	121.16	118.09
23	L	4001	BCR	C23-C22-C21	2.01	122.17	119.01
21	4	606	CLA	CMA-C3A-C4A	2.01	117.18	111.77
23	B	4001	BCR	C34-C9-C10	-2.01	119.56	122.82
37	3	501	LUT	C38-C25-C24	-2.01	118.60	123.36
21	3	601	CLA	CMA-C3A-C4A	2.01	117.18	111.77
37	1	502	LUT	C19-C9-C8	2.01	121.16	118.09
21	A	1141	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
21	4	612	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
21	6	601	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
21	7	601	CLA	C2D-C1D-ND	2.01	112.12	110.13
21	a	615	CLA	CAA-C2A-C3A	-2.01	107.57	113.00
21	B	1023	CLA	C4B-CHC-C1C	2.01	130.97	126.25
38	3	611	CHL	C4C-CHD-C1D	2.01	123.26	116.07
21	6	608	CLA	C2D-C1D-ND	2.01	112.11	110.13
21	5	605	CLA	C1D-ND-C4D	-2.01	104.90	106.31
23	J	4001	BCR	C1-C6-C7	2.01	121.10	115.65
21	A	1120	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
21	8	618	CLA	O1D-CGD-CBD	-2.01	120.56	124.52
37	4	501	LUT	C18-C5-C4	2.01	118.11	114.42
21	A	1118	CLA	CMD-C2D-C3D	-2.01	123.08	127.69
37	8	501	LUT	C36-C21-C26	-2.01	106.50	109.55
23	8	503	BCR	C3-C4-C5	-2.01	110.47	114.06
21	B	1225	CLA	CMA-C3A-C4A	2.01	117.17	111.77
38	1	609	CHL	CMD-C2D-C3D	2.01	128.70	124.68
38	6	619	CHL	C1-C2-C3	-2.01	122.91	126.20
23	6	503	BCR	C8-C7-C6	-2.01	121.63	127.00
21	1	610	CLA	C2D-C1D-ND	2.01	112.11	110.13
21	4	605	CLA	O2A-CGA-CBA	2.01	119.72	112.14
21	B	1239	CLA	CHA-C1A-NA	-2.01	121.85	126.39
21	1	604	CLA	C2C-C1C-NC	2.01	112.09	109.98
21	3	601	CLA	CMD-C2D-C3D	-2.01	123.09	127.69
37	1	503	LUT	C18-C5-C4	2.01	118.11	114.42
21	7	606	CLA	CAC-C3C-C4C	2.00	127.40	124.79
21	B	1223	CLA	O1D-CGD-CBD	-2.00	120.56	124.52
21	G	1602	CLA	C1D-ND-C4D	-2.00	104.91	106.31
21	1	605	CLA	CAA-C2A-C1A	-2.00	105.41	111.97
21	3	616	CLA	CHD-C1D-ND	-2.00	121.98	124.80
23	A	4005	BCR	C38-C26-C27	2.00	117.87	113.60
21	5	617	CLA	O1D-CGD-CBD	-2.00	120.57	124.52
21	4	601	CLA	C2D-C1D-ND	2.00	112.11	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1111	CLA	C1D-ND-C4D	-2.00	104.91	106.31
21	1	611	CLA	C1D-ND-C4D	-2.00	104.91	106.31
21	5	608	CLA	C1D-ND-C4D	-2.00	104.91	106.31
21	A	1101	CLA	C2A-C1A-CHA	2.00	127.34	123.87
23	A	4001	BCR	C38-C26-C27	2.00	117.86	113.60
21	A	1123	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
21	1	615	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
21	1	604	CLA	C3B-C4B-NB	-2.00	108.74	110.53
36	M	4001	ECH	O27-C27-C26	2.00	122.78	120.98
21	6	605	CLA	CBC-CAC-C3C	-2.00	107.00	112.42
21	A	1130	CLA	CMD-C2D-C3D	-2.00	123.10	127.69
21	a	603	CLA	CHA-C1A-NA	-2.00	121.86	126.39
21	3	601	CLA	CHA-C1A-NA	-2.00	121.86	126.39
21	A	1126	CLA	C1-O2A-CGA	2.00	121.49	116.65

All (299) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	A	1011	CL0	NC
20	A	1011	CL0	ND
20	A	1011	CL0	NA
21	A	1012	CLA	ND
21	A	1013	CLA	ND
21	A	1102	CLA	ND
21	A	1103	CLA	ND
21	A	1104	CLA	ND
21	A	1105	CLA	ND
21	A	1106	CLA	ND
21	A	1107	CLA	ND
21	A	1108	CLA	ND
21	A	1109	CLA	ND
21	A	1110	CLA	ND
21	A	1111	CLA	ND
21	A	1112	CLA	ND
21	A	1113	CLA	ND
21	A	1114	CLA	ND
21	A	1115	CLA	ND
21	A	1116	CLA	ND
21	A	1117	CLA	ND
21	A	1118	CLA	ND
21	A	1119	CLA	ND
21	A	1120	CLA	ND

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Mol	Chain	Res	Type	Atom
21	A	1121	CLA	ND
21	A	1122	CLA	ND
21	A	1123	CLA	ND
21	A	1124	CLA	ND
21	A	1125	CLA	ND
21	A	1126	CLA	ND
21	A	1127	CLA	ND
21	A	1128	CLA	ND
21	A	1129	CLA	ND
21	A	1130	CLA	ND
21	A	1131	CLA	ND
21	A	1132	CLA	ND
21	A	1133	CLA	ND
21	A	1134	CLA	ND
21	A	1135	CLA	ND
21	A	1136	CLA	ND
21	A	1137	CLA	ND
21	A	1138	CLA	ND
21	A	1139	CLA	ND
21	A	1141	CLA	ND
21	A	1140	CLA	ND
21	A	1101	CLA	ND
21	B	1022	CLA	ND
21	B	1021	CLA	ND
21	B	1023	CLA	ND
21	B	1201	CLA	ND
21	B	1202	CLA	ND
21	B	1203	CLA	ND
21	B	1205	CLA	ND
21	B	1206	CLA	ND
21	B	1208	CLA	ND
21	B	1209	CLA	ND
21	B	1210	CLA	ND
21	B	1211	CLA	ND
21	B	1212	CLA	ND
21	B	1213	CLA	ND
21	B	1214	CLA	ND
21	B	1215	CLA	ND
21	B	1216	CLA	ND
21	B	1217	CLA	ND
21	B	1218	CLA	ND
21	B	1219	CLA	ND

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Mol	Chain	Res	Type	Atom
21	B	1220	CLA	ND
21	B	1221	CLA	ND
21	B	1222	CLA	ND
21	B	1223	CLA	ND
21	B	1224	CLA	ND
21	B	1225	CLA	ND
21	B	1226	CLA	ND
21	B	1227	CLA	ND
21	B	1230	CLA	ND
21	B	1231	CLA	ND
21	B	1232	CLA	ND
21	B	1234	CLA	ND
21	B	1235	CLA	ND
21	B	1236	CLA	ND
21	B	1237	CLA	ND
21	B	1238	CLA	ND
21	B	1239	CLA	ND
21	B	1240	CLA	ND
21	B	1228	CLA	ND
21	B	1229	CLA	ND
21	B	1204	CLA	ND
21	B	1207	CLA	ND
21	F	1301	CLA	ND
21	F	1302	CLA	ND
21	G	1601	CLA	ND
21	G	1602	CLA	ND
21	G	1603	CLA	ND
21	J	1901	CLA	ND
21	K	1401	CLA	ND
21	K	1402	CLA	ND
21	K	1403	CLA	ND
21	K	1404	CLA	ND
21	L	1501	CLA	ND
21	L	1502	CLA	ND
21	L	1503	CLA	ND
21	1	601	CLA	ND
21	1	602	CLA	ND
21	1	603	CLA	ND
21	1	604	CLA	ND
21	1	605	CLA	ND
21	1	606	CLA	ND
21	1	607	CLA	ND

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Mol	Chain	Res	Type	Atom
21	1	608	CLA	ND
21	1	610	CLA	ND
21	1	611	CLA	ND
21	1	612	CLA	ND
21	1	615	CLA	ND
21	a	601	CLA	ND
21	a	602	CLA	ND
21	a	603	CLA	ND
21	a	604	CLA	ND
21	a	605	CLA	ND
21	a	607	CLA	ND
21	a	608	CLA	ND
21	a	611	CLA	ND
21	a	612	CLA	ND
21	a	615	CLA	ND
21	3	601	CLA	ND
21	3	602	CLA	ND
21	3	603	CLA	ND
21	3	604	CLA	ND
21	3	605	CLA	ND
21	3	606	CLA	ND
21	3	607	CLA	ND
21	3	610	CLA	ND
21	3	612	CLA	ND
21	3	613	CLA	ND
21	3	616	CLA	ND
21	3	618	CLA	ND
21	4	601	CLA	ND
21	4	602	CLA	ND
21	4	603	CLA	ND
21	4	604	CLA	ND
21	4	605	CLA	ND
21	4	606	CLA	ND
21	4	607	CLA	ND
21	4	610	CLA	ND
21	4	611	CLA	ND
21	4	612	CLA	ND
21	4	615	CLA	ND
21	4	616	CLA	ND
21	4	617	CLA	ND
21	4	608	CLA	ND
21	5	601	CLA	ND

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Mol	Chain	Res	Type	Atom
21	5	602	CLA	ND
21	5	603	CLA	ND
21	5	604	CLA	ND
21	5	605	CLA	ND
21	5	606	CLA	ND
21	5	607	CLA	ND
21	5	608	CLA	ND
21	5	609	CLA	ND
21	5	612	CLA	ND
21	5	614	CLA	ND
21	5	616	CLA	ND
21	5	617	CLA	ND
21	5	618	CLA	ND
21	6	608	CLA	ND
21	6	601	CLA	ND
21	6	602	CLA	ND
21	6	603	CLA	ND
21	6	604	CLA	ND
21	6	605	CLA	ND
21	6	606	CLA	ND
21	6	607	CLA	ND
21	6	609	CLA	ND
21	6	612	CLA	ND
21	6	615	CLA	ND
21	6	617	CLA	ND
21	6	618	CLA	ND
21	7	609	CLA	ND
21	7	601	CLA	ND
21	7	602	CLA	ND
21	7	603	CLA	ND
21	7	604	CLA	ND
21	7	605	CLA	ND
21	7	606	CLA	ND
21	7	607	CLA	ND
21	7	608	CLA	ND
21	7	610	CLA	ND
21	7	611	CLA	ND
21	7	612	CLA	ND
21	7	615	CLA	ND
21	7	617	CLA	ND
21	8	609	CLA	ND
21	8	602	CLA	ND

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Mol	Chain	Res	Type	Atom
21	8	603	CLA	ND
21	8	605	CLA	ND
21	8	606	CLA	ND
21	8	607	CLA	ND
21	8	608	CLA	ND
21	8	610	CLA	ND
21	8	611	CLA	ND
21	8	612	CLA	ND
21	8	615	CLA	ND
21	8	618	CLA	ND
21	8	620	CLA	ND
33	G	5002	ERG	C20
33	G	5002	ERG	C9
33	G	5002	ERG	C24
33	G	5002	ERG	C14
34	J	4002	RRX	C28
37	1	503	LUT	C26
37	a	502	LUT	C26
37	5	505	LUT	C26
37	6	501	LUT	C26
37	6	502	LUT	C26
37	7	501	LUT	C26
38	1	613	CHL	NC
38	1	613	CHL	ND
38	1	613	CHL	NA
38	1	609	CHL	NC
38	1	609	CHL	C8
38	1	609	CHL	ND
38	1	609	CHL	NA
38	a	606	CHL	NC
38	a	606	CHL	C8
38	a	606	CHL	ND
38	a	606	CHL	NA
38	a	609	CHL	NC
38	a	609	CHL	ND
38	a	609	CHL	NA
38	a	610	CHL	NC
38	a	610	CHL	ND
38	a	610	CHL	NA
38	a	613	CHL	NC
38	a	613	CHL	ND
38	a	613	CHL	NA

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Mol	Chain	Res	Type	Atom
38	3	608	CHL	C3A
38	3	608	CHL	ND
38	3	608	CHL	NC
38	3	608	CHL	NA
38	3	611	CHL	NC
38	3	611	CHL	ND
38	3	611	CHL	NA
38	4	609	CHL	NC
38	4	609	CHL	C8
38	4	609	CHL	ND
38	4	609	CHL	NA
38	4	613	CHL	NC
38	4	613	CHL	ND
38	4	613	CHL	NA
38	4	618	CHL	NC
38	4	618	CHL	C8
38	4	618	CHL	ND
38	4	618	CHL	NA
38	5	610	CHL	NC
38	5	610	CHL	C8
38	5	610	CHL	ND
38	5	610	CHL	NA
38	5	611	CHL	NC
38	5	611	CHL	ND
38	5	611	CHL	NA
38	5	613	CHL	NC
38	5	613	CHL	C8
38	5	613	CHL	ND
38	5	613	CHL	NA
38	6	610	CHL	NC
38	6	610	CHL	C8
38	6	610	CHL	ND
38	6	610	CHL	NA
38	6	611	CHL	NC
38	6	611	CHL	ND
38	6	611	CHL	NA
38	6	613	CHL	NC
38	6	613	CHL	ND
38	6	613	CHL	NA
38	6	619	CHL	ND
38	6	619	CHL	C3A
38	6	619	CHL	NC

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Mol	Chain	Res	Type	Atom
38	6	619	CHL	C8
38	6	619	CHL	NA
38	7	613	CHL	NC
38	7	613	CHL	C8
38	7	613	CHL	ND
38	7	613	CHL	NA
38	8	601	CHL	NC
38	8	601	CHL	C8
38	8	601	CHL	ND
38	8	601	CHL	NA
38	8	604	CHL	NC
38	8	604	CHL	C8
38	8	604	CHL	ND
38	8	604	CHL	NA
38	8	613	CHL	NC
38	8	613	CHL	ND
38	8	613	CHL	NA
40	3	506	QTB	C11
40	3	506	QTB	C12
45	7	502	XAT	C6
45	7	502	XAT	C5
45	7	502	XAT	C26
47	7	504	C7Z	C3

All (4229) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	1011	CL0	C2-C1-O2A-CGA
21	A	1013	CLA	CBD-CGD-O2D-CED
21	A	1102	CLA	C1A-C2A-CAA-CBA
21	A	1102	CLA	C3A-C2A-CAA-CBA
21	A	1102	CLA	C2C-C3C-CAC-CBC
21	A	1102	CLA	C4C-C3C-CAC-CBC
21	A	1103	CLA	C1A-C2A-CAA-CBA
21	A	1103	CLA	C3A-C2A-CAA-CBA
21	A	1104	CLA	C2B-C3B-CAB-CBB
21	A	1104	CLA	C4B-C3B-CAB-CBB
21	A	1106	CLA	C3A-C2A-CAA-CBA
21	A	1106	CLA	CHA-CBD-CGD-O1D
21	A	1106	CLA	CHA-CBD-CGD-O2D
21	A	1107	CLA	C1A-C2A-CAA-CBA
21	A	1107	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	A	1108	CLA	C1A-C2A-CAA-CBA
21	A	1108	CLA	C3A-C2A-CAA-CBA
21	A	1109	CLA	C1A-C2A-CAA-CBA
21	A	1109	CLA	C3A-C2A-CAA-CBA
21	A	1109	CLA	C2-C1-O2A-CGA
21	A	1109	CLA	CBD-CGD-O2D-CED
21	A	1110	CLA	CBA-CGA-O2A-C1
21	A	1110	CLA	O1A-CGA-O2A-C1
21	A	1111	CLA	C1A-C2A-CAA-CBA
21	A	1111	CLA	C3A-C2A-CAA-CBA
21	A	1111	CLA	CBD-CGD-O2D-CED
21	A	1112	CLA	CBD-CGD-O2D-CED
21	A	1114	CLA	CBA-CGA-O2A-C1
21	A	1114	CLA	O1A-CGA-O2A-C1
21	A	1114	CLA	CBD-CGD-O2D-CED
21	A	1116	CLA	C3A-C2A-CAA-CBA
21	A	1116	CLA	CBD-CGD-O2D-CED
21	A	1117	CLA	C1A-C2A-CAA-CBA
21	A	1117	CLA	C3A-C2A-CAA-CBA
21	A	1118	CLA	C1A-C2A-CAA-CBA
21	A	1118	CLA	C3A-C2A-CAA-CBA
21	A	1119	CLA	CBD-CGD-O2D-CED
21	A	1120	CLA	CHA-CBD-CGD-O1D
21	A	1120	CLA	CHA-CBD-CGD-O2D
21	A	1121	CLA	CHA-CBD-CGD-O1D
21	A	1121	CLA	CHA-CBD-CGD-O2D
21	A	1121	CLA	CBD-CGD-O2D-CED
21	A	1122	CLA	C6-C7-C8-C9
21	A	1123	CLA	CAD-CBD-CGD-O1D
21	A	1123	CLA	CAD-CBD-CGD-O2D
21	A	1124	CLA	C1A-C2A-CAA-CBA
21	A	1124	CLA	C3A-C2A-CAA-CBA
21	A	1125	CLA	CAD-CBD-CGD-O1D
21	A	1125	CLA	CAD-CBD-CGD-O2D
21	A	1126	CLA	C1A-C2A-CAA-CBA
21	A	1126	CLA	C3A-C2A-CAA-CBA
21	A	1126	CLA	C2-C1-O2A-CGA
21	A	1128	CLA	CHA-CBD-CGD-O1D
21	A	1128	CLA	CHA-CBD-CGD-O2D
21	A	1129	CLA	CAD-CBD-CGD-O1D
21	A	1129	CLA	CAD-CBD-CGD-O2D
21	A	1130	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	A	1130	CLA	C3A-C2A-CAA-CBA
21	A	1132	CLA	CHA-CBD-CGD-O1D
21	A	1132	CLA	CHA-CBD-CGD-O2D
21	A	1133	CLA	C12-C13-C15-C16
21	A	1134	CLA	C1A-C2A-CAA-CBA
21	A	1134	CLA	C3A-C2A-CAA-CBA
21	A	1134	CLA	CHA-CBD-CGD-O1D
21	A	1134	CLA	CHA-CBD-CGD-O2D
21	A	1135	CLA	C6-C7-C8-C10
21	A	1136	CLA	CAD-CBD-CGD-O1D
21	A	1136	CLA	CAD-CBD-CGD-O2D
21	A	1137	CLA	CHA-CBD-CGD-O1D
21	A	1137	CLA	CHA-CBD-CGD-O2D
21	A	1138	CLA	C1A-C2A-CAA-CBA
21	A	1138	CLA	C3A-C2A-CAA-CBA
21	A	1139	CLA	C3A-C2A-CAA-CBA
21	A	1141	CLA	CAD-CBD-CGD-O1D
21	A	1141	CLA	CAD-CBD-CGD-O2D
21	A	1140	CLA	CBD-CGD-O2D-CED
21	A	1101	CLA	C1A-C2A-CAA-CBA
21	A	1101	CLA	CHA-CBD-CGD-O1D
21	A	1101	CLA	CHA-CBD-CGD-O2D
21	B	1022	CLA	CBD-CGD-O2D-CED
21	B	1023	CLA	C2-C1-O2A-CGA
21	B	1023	CLA	CBD-CGD-O2D-CED
21	B	1201	CLA	C1A-C2A-CAA-CBA
21	B	1201	CLA	CHA-CBD-CGD-O1D
21	B	1201	CLA	CHA-CBD-CGD-O2D
21	B	1202	CLA	C1A-C2A-CAA-CBA
21	B	1202	CLA	C3A-C2A-CAA-CBA
21	B	1205	CLA	CHA-CBD-CGD-O1D
21	B	1205	CLA	CHA-CBD-CGD-O2D
21	B	1206	CLA	CBD-CGD-O2D-CED
21	B	1208	CLA	C1A-C2A-CAA-CBA
21	B	1210	CLA	C1A-C2A-CAA-CBA
21	B	1210	CLA	C3A-C2A-CAA-CBA
21	B	1212	CLA	C1A-C2A-CAA-CBA
21	B	1212	CLA	C3A-C2A-CAA-CBA
21	B	1214	CLA	C1A-C2A-CAA-CBA
21	B	1214	CLA	C3A-C2A-CAA-CBA
21	B	1215	CLA	C3A-C2A-CAA-CBA
21	B	1217	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
21	B	1217	CLA	CAD-CBD-CGD-O2D
21	B	1217	CLA	C4-C3-C5-C6
21	B	1218	CLA	CBA-CGA-O2A-C1
21	B	1218	CLA	O1A-CGA-O2A-C1
21	B	1220	CLA	CBD-CGD-O2D-CED
21	B	1221	CLA	CHA-CBD-CGD-O1D
21	B	1221	CLA	CHA-CBD-CGD-O2D
21	B	1223	CLA	C1A-C2A-CAA-CBA
21	B	1223	CLA	C3A-C2A-CAA-CBA
21	B	1224	CLA	C1A-C2A-CAA-CBA
21	B	1224	CLA	CBD-CGD-O2D-CED
21	B	1224	CLA	C11-C10-C8-C9
21	B	1225	CLA	C1A-C2A-CAA-CBA
21	B	1225	CLA	C3A-C2A-CAA-CBA
21	B	1226	CLA	C6-C7-C8-C9
21	B	1227	CLA	C2-C1-O2A-CGA
21	B	1227	CLA	CAD-CBD-CGD-O1D
21	B	1227	CLA	CAD-CBD-CGD-O2D
21	B	1230	CLA	CHA-CBD-CGD-O1D
21	B	1230	CLA	CHA-CBD-CGD-O2D
21	B	1231	CLA	C2-C1-O2A-CGA
21	B	1232	CLA	C3A-C2A-CAA-CBA
21	B	1236	CLA	C1A-C2A-CAA-CBA
21	B	1236	CLA	C3A-C2A-CAA-CBA
21	B	1236	CLA	CHA-CBD-CGD-O2D
21	B	1237	CLA	C2-C1-O2A-CGA
21	B	1238	CLA	C2B-C3B-CAB-CBB
21	B	1238	CLA	C4B-C3B-CAB-CBB
21	B	1228	CLA	C1A-C2A-CAA-CBA
21	B	1229	CLA	CBD-CGD-O2D-CED
21	B	1204	CLA	C2B-C3B-CAB-CBB
21	B	1204	CLA	C4B-C3B-CAB-CBB
21	B	1207	CLA	C2-C1-O2A-CGA
21	B	1207	CLA	CAD-CBD-CGD-O1D
21	B	1207	CLA	CAD-CBD-CGD-O2D
21	B	1207	CLA	CBD-CGD-O2D-CED
21	F	1302	CLA	CBD-CGD-O2D-CED
21	G	1601	CLA	C1A-C2A-CAA-CBA
21	G	1601	CLA	CBD-CGD-O2D-CED
21	G	1602	CLA	CHA-CBD-CGD-O1D
21	G	1602	CLA	CHA-CBD-CGD-O2D
21	G	1603	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	J	1901	CLA	C1A-C2A-CAA-CBA
21	J	1901	CLA	CBD-CGD-O2D-CED
21	K	1401	CLA	CBA-CGA-O2A-C1
21	K	1401	CLA	CHA-CBD-CGD-O1D
21	K	1401	CLA	CHA-CBD-CGD-O2D
21	K	1402	CLA	CBD-CGD-O2D-CED
21	K	1403	CLA	CBA-CGA-O2A-C1
21	K	1403	CLA	C2B-C3B-CAB-CBB
21	K	1403	CLA	C4B-C3B-CAB-CBB
21	K	1403	CLA	CAD-CBD-CGD-O1D
21	K	1403	CLA	CAD-CBD-CGD-O2D
21	K	1404	CLA	CHA-CBD-CGD-O1D
21	K	1404	CLA	CHA-CBD-CGD-O2D
21	L	1501	CLA	CBA-CGA-O2A-C1
21	L	1501	CLA	O1A-CGA-O2A-C1
21	1	602	CLA	C1A-C2A-CAA-CBA
21	1	603	CLA	CBD-CGD-O2D-CED
21	1	604	CLA	C3A-C2A-CAA-CBA
21	1	608	CLA	C2B-C3B-CAB-CBB
21	1	608	CLA	C4B-C3B-CAB-CBB
21	1	611	CLA	CBD-CGD-O2D-CED
21	1	612	CLA	C3A-C2A-CAA-CBA
21	1	615	CLA	CBA-CGA-O2A-C1
21	1	615	CLA	CBD-CGD-O2D-CED
21	a	602	CLA	C1A-C2A-CAA-CBA
21	a	603	CLA	CBD-CGD-O2D-CED
21	a	604	CLA	C1A-C2A-CAA-CBA
21	a	604	CLA	C3A-C2A-CAA-CBA
21	a	607	CLA	C2B-C3B-CAB-CBB
21	a	607	CLA	C4B-C3B-CAB-CBB
21	a	608	CLA	C1A-C2A-CAA-CBA
21	a	608	CLA	C3A-C2A-CAA-CBA
21	a	611	CLA	C1A-C2A-CAA-CBA
21	a	611	CLA	C3A-C2A-CAA-CBA
21	a	611	CLA	C2-C1-O2A-CGA
21	a	611	CLA	CBD-CGD-O2D-CED
21	a	612	CLA	C1A-C2A-CAA-CBA
21	a	612	CLA	C3A-C2A-CAA-CBA
21	a	612	CLA	CBD-CGD-O2D-CED
21	a	615	CLA	CBD-CGD-O2D-CED
21	3	601	CLA	C3A-C2A-CAA-CBA
21	3	602	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
21	3	602	CLA	CHA-CBD-CGD-O2D
21	3	603	CLA	C4-C3-C5-C6
21	3	604	CLA	CHA-CBD-CGD-O1D
21	3	604	CLA	CHA-CBD-CGD-O2D
21	3	605	CLA	CBD-CGD-O2D-CED
21	3	606	CLA	C1A-C2A-CAA-CBA
21	3	606	CLA	C3A-C2A-CAA-CBA
21	3	610	CLA	C1A-C2A-CAA-CBA
21	3	618	CLA	CBA-CGA-O2A-C1
21	3	618	CLA	CBD-CGD-O2D-CED
21	4	602	CLA	CBD-CGD-O2D-CED
21	4	607	CLA	C2B-C3B-CAB-CBB
21	4	607	CLA	C4B-C3B-CAB-CBB
21	4	607	CLA	CBD-CGD-O2D-CED
21	4	610	CLA	CBD-CGD-O2D-CED
21	4	611	CLA	CBD-CGD-O2D-CED
21	4	612	CLA	CHA-CBD-CGD-O1D
21	4	612	CLA	CHA-CBD-CGD-O2D
21	4	615	CLA	CBA-CGA-O2A-C1
21	4	615	CLA	O1A-CGA-O2A-C1
21	4	615	CLA	CBD-CGD-O2D-CED
21	4	616	CLA	C2-C1-O2A-CGA
21	4	608	CLA	C2-C3-C5-C6
21	5	602	CLA	CBD-CGD-O2D-CED
21	5	603	CLA	CBD-CGD-O2D-CED
21	5	605	CLA	CHA-CBD-CGD-O1D
21	5	605	CLA	CHA-CBD-CGD-O2D
21	5	608	CLA	C1A-C2A-CAA-CBA
21	5	608	CLA	C3A-C2A-CAA-CBA
21	5	608	CLA	CHA-CBD-CGD-O1D
21	5	608	CLA	CHA-CBD-CGD-O2D
21	5	609	CLA	C2-C3-C5-C6
21	5	609	CLA	C4-C3-C5-C6
21	5	612	CLA	C2-C1-O2A-CGA
21	5	612	CLA	C11-C10-C8-C7
21	5	614	CLA	CBD-CGD-O2D-CED
21	5	616	CLA	C1A-C2A-CAA-CBA
21	5	616	CLA	C3A-C2A-CAA-CBA
21	5	616	CLA	CBD-CGD-O2D-CED
21	5	617	CLA	C3A-C2A-CAA-CBA
21	5	617	CLA	C2-C1-O2A-CGA
21	5	617	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	5	618	CLA	C3-C5-C6-C7
21	6	608	CLA	CBD-CGD-O2D-CED
21	6	604	CLA	CHA-CBD-CGD-O1D
21	6	604	CLA	CHA-CBD-CGD-O2D
21	6	605	CLA	CBA-CGA-O2A-C1
21	6	606	CLA	CBD-CGD-O2D-CED
21	6	606	CLA	C3-C5-C6-C7
21	6	609	CLA	C1A-C2A-CAA-CBA
21	6	609	CLA	C3A-C2A-CAA-CBA
21	6	609	CLA	C2-C1-O2A-CGA
21	6	609	CLA	CAD-CBD-CGD-O1D
21	6	609	CLA	CAD-CBD-CGD-O2D
21	6	612	CLA	C1A-C2A-CAA-CBA
21	6	612	CLA	C3A-C2A-CAA-CBA
21	6	615	CLA	CAD-CBD-CGD-O1D
21	6	615	CLA	CAD-CBD-CGD-O2D
21	6	617	CLA	C3A-C2A-CAA-CBA
21	6	618	CLA	C1A-C2A-CAA-CBA
21	6	618	CLA	CBA-CGA-O2A-C1
21	6	618	CLA	CBD-CGD-O2D-CED
21	7	609	CLA	CAD-CBD-CGD-O1D
21	7	609	CLA	CAD-CBD-CGD-O2D
21	7	603	CLA	CBD-CGD-O2D-CED
21	7	604	CLA	CHA-CBD-CGD-O1D
21	7	604	CLA	CHA-CBD-CGD-O2D
21	7	605	CLA	C2B-C3B-CAB-CBB
21	7	605	CLA	C4B-C3B-CAB-CBB
21	7	606	CLA	CBD-CGD-O2D-CED
21	7	608	CLA	C1A-C2A-CAA-CBA
21	7	608	CLA	C3A-C2A-CAA-CBA
21	7	610	CLA	CBD-CGD-O2D-CED
21	7	611	CLA	C2-C1-O2A-CGA
21	7	612	CLA	C11-C10-C8-C9
21	7	617	CLA	CAD-CBD-CGD-O2D
21	8	609	CLA	C1A-C2A-CAA-CBA
21	8	603	CLA	CBD-CGD-O2D-CED
21	8	606	CLA	CBD-CGD-O2D-CED
21	8	608	CLA	C2-C1-O2A-CGA
21	8	610	CLA	C1A-C2A-CAA-CBA
21	8	610	CLA	C3A-C2A-CAA-CBA
21	8	611	CLA	C2-C1-O2A-CGA
21	8	611	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	8	612	CLA	C3A-C2A-CAA-CBA
21	8	612	CLA	C2B-C3B-CAB-CBB
21	8	612	CLA	C4B-C3B-CAB-CBB
21	8	620	CLA	C2-C1-O2A-CGA
23	A	4001	BCR	C23-C24-C25-C26
23	A	4001	BCR	C23-C24-C25-C30
23	A	4002	BCR	C7-C8-C9-C10
23	A	4002	BCR	C7-C8-C9-C34
23	A	4002	BCR	C11-C10-C9-C8
23	A	4002	BCR	C11-C10-C9-C34
23	A	4003	BCR	C11-C10-C9-C8
23	A	4003	BCR	C11-C10-C9-C34
23	A	4003	BCR	C10-C11-C12-C13
23	A	4003	BCR	C11-C12-C13-C14
23	A	4003	BCR	C17-C18-C19-C20
23	A	4004	BCR	C11-C10-C9-C8
23	A	4004	BCR	C11-C10-C9-C34
23	A	4004	BCR	C17-C18-C19-C20
23	A	4004	BCR	C36-C18-C19-C20
23	A	4005	BCR	C7-C8-C9-C10
23	A	4005	BCR	C17-C18-C19-C20
23	A	4005	BCR	C36-C18-C19-C20
23	A	4005	BCR	C21-C22-C23-C24
23	A	4005	BCR	C37-C22-C23-C24
23	B	4002	BCR	C7-C8-C9-C10
23	B	4002	BCR	C7-C8-C9-C34
23	B	4002	BCR	C17-C18-C19-C20
23	B	4002	BCR	C36-C18-C19-C20
23	B	4002	BCR	C21-C22-C23-C24
23	B	4003	BCR	C21-C22-C23-C24
23	B	4003	BCR	C37-C22-C23-C24
23	B	4004	BCR	C11-C10-C9-C8
23	B	4004	BCR	C11-C10-C9-C34
23	B	4004	BCR	C10-C11-C12-C13
23	B	4004	BCR	C23-C24-C25-C26
23	B	4004	BCR	C23-C24-C25-C30
23	B	4005	BCR	C7-C8-C9-C10
23	B	4005	BCR	C19-C20-C21-C22
23	B	4007	BCR	C11-C10-C9-C8
23	B	4007	BCR	C11-C10-C9-C34
23	B	4007	BCR	C10-C11-C12-C13
23	B	4006	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
23	B	4006	BCR	C11-C10-C9-C34
23	B	4006	BCR	C10-C11-C12-C13
23	B	4006	BCR	C17-C18-C19-C20
23	B	4006	BCR	C36-C18-C19-C20
23	B	4006	BCR	C21-C22-C23-C24
23	B	4006	BCR	C37-C22-C23-C24
23	B	4001	BCR	C7-C8-C9-C10
23	B	4001	BCR	C11-C10-C9-C8
23	B	4001	BCR	C11-C10-C9-C34
23	B	4001	BCR	C11-C12-C13-C14
23	F	4001	BCR	C23-C24-C25-C26
23	G	4001	BCR	C11-C10-C9-C8
23	G	4001	BCR	C11-C10-C9-C34
23	G	4001	BCR	C17-C18-C19-C20
23	J	4001	BCR	C11-C10-C9-C8
23	J	4001	BCR	C11-C10-C9-C34
23	J	4001	BCR	C10-C11-C12-C13
23	J	4001	BCR	C17-C18-C19-C20
23	J	4001	BCR	C36-C18-C19-C20
23	K	4001	BCR	C7-C8-C9-C10
23	K	4001	BCR	C7-C8-C9-C34
23	K	4001	BCR	C11-C10-C9-C8
23	K	4001	BCR	C11-C10-C9-C34
23	K	4001	BCR	C11-C12-C13-C14
23	K	4001	BCR	C21-C22-C23-C24
23	K	4001	BCR	C37-C22-C23-C24
23	K	4002	BCR	C10-C11-C12-C13
23	K	4002	BCR	C11-C12-C13-C14
23	K	4002	BCR	C11-C12-C13-C35
23	K	4002	BCR	C17-C18-C19-C20
23	K	4002	BCR	C36-C18-C19-C20
23	I	4001	BCR	C7-C8-C9-C10
23	I	4001	BCR	C7-C8-C9-C34
23	I	4001	BCR	C11-C10-C9-C8
23	I	4001	BCR	C11-C10-C9-C34
23	I	4001	BCR	C10-C11-C12-C13
23	L	4002	BCR	C11-C10-C9-C8
23	L	4002	BCR	C11-C10-C9-C34
23	L	4002	BCR	C13-C14-C15-C16
23	L	4002	BCR	C21-C22-C23-C24
23	L	4002	BCR	C37-C22-C23-C24
23	L	4001	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
23	L	4001	BCR	C11-C10-C9-C34
23	L	4001	BCR	C10-C11-C12-C13
23	L	4001	BCR	C13-C14-C15-C16
23	L	4001	BCR	C21-C22-C23-C24
23	L	4001	BCR	C37-C22-C23-C24
23	L	4001	BCR	C23-C24-C25-C26
23	L	4001	BCR	C23-C24-C25-C30
23	3	503	BCR	C23-C24-C25-C26
23	3	503	BCR	C23-C24-C25-C30
23	3	504	BCR	C7-C8-C9-C10
23	3	504	BCR	C7-C8-C9-C34
23	3	504	BCR	C11-C10-C9-C8
23	3	504	BCR	C11-C10-C9-C34
23	3	504	BCR	C9-C10-C11-C12
23	3	504	BCR	C10-C11-C12-C13
23	3	504	BCR	C21-C22-C23-C24
23	3	504	BCR	C37-C22-C23-C24
23	3	505	BCR	C11-C10-C9-C8
23	3	505	BCR	C11-C10-C9-C34
23	3	505	BCR	C17-C18-C19-C20
23	3	505	BCR	C36-C18-C19-C20
23	3	505	BCR	C21-C22-C23-C24
23	3	505	BCR	C37-C22-C23-C24
23	3	505	BCR	C23-C24-C25-C26
23	3	505	BCR	C23-C24-C25-C30
23	4	503	BCR	C7-C8-C9-C10
23	4	503	BCR	C7-C8-C9-C34
23	4	503	BCR	C11-C10-C9-C8
23	4	503	BCR	C11-C10-C9-C34
23	4	503	BCR	C9-C10-C11-C12
23	4	503	BCR	C11-C12-C13-C14
23	4	503	BCR	C11-C12-C13-C35
23	4	503	BCR	C19-C20-C21-C22
23	4	503	BCR	C21-C22-C23-C24
23	4	503	BCR	C37-C22-C23-C24
23	4	503	BCR	C23-C24-C25-C26
23	4	503	BCR	C23-C24-C25-C30
23	5	503	BCR	C11-C10-C9-C8
23	5	503	BCR	C11-C10-C9-C34
23	5	503	BCR	C10-C11-C12-C13
23	5	503	BCR	C11-C12-C13-C14
23	5	503	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
23	5	504	BCR	C10-C11-C12-C13
23	5	504	BCR	C13-C14-C15-C16
23	6	504	BCR	C17-C18-C19-C20
23	6	503	BCR	C17-C18-C19-C20
23	6	503	BCR	C36-C18-C19-C20
23	7	503	BCR	C7-C8-C9-C10
23	7	503	BCR	C7-C8-C9-C34
23	7	503	BCR	C11-C10-C9-C8
23	7	503	BCR	C11-C10-C9-C34
23	7	503	BCR	C21-C22-C23-C24
23	7	503	BCR	C37-C22-C23-C24
23	8	503	BCR	C7-C8-C9-C10
23	8	503	BCR	C11-C10-C9-C8
23	8	503	BCR	C11-C10-C9-C34
23	8	503	BCR	C10-C11-C12-C13
23	8	503	BCR	C21-C22-C23-C24
23	8	503	BCR	C37-C22-C23-C24
23	8	503	BCR	C23-C24-C25-C26
23	8	503	BCR	C23-C24-C25-C30
24	A	5001	LHG	O1-C1-C2-C3
24	A	5001	LHG	C3-O3-P-O6
24	A	5001	LHG	C4-O6-P-O3
24	A	5001	LHG	C4-O6-P-O4
24	A	5001	LHG	C4-O6-P-O5
24	A	5001	LHG	O6-C4-C5-O7
24	A	5002	LHG	O1-C1-C2-O2
24	A	5002	LHG	O1-C1-C2-C3
24	A	5002	LHG	C3-O3-P-O4
24	A	5002	LHG	C3-O3-P-O6
24	A	5002	LHG	C4-O6-P-O3
24	A	5002	LHG	C4-O6-P-O4
24	A	5002	LHG	C4-O6-P-O5
24	A	5003	LHG	O1-C1-C2-C3
24	A	5003	LHG	C3-O3-P-O4
24	A	5003	LHG	C3-O3-P-O6
24	A	5003	LHG	C4-O6-P-O3
24	A	5003	LHG	C4-O6-P-O4
24	A	5003	LHG	C4-O6-P-O5
24	A	5003	LHG	C8-C7-O7-C5
24	B	5002	LHG	O1-C1-C2-C3
24	B	5002	LHG	C3-O3-P-O6
24	B	5002	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
24	B	5002	LHG	C4-O6-P-O4
24	B	5001	LHG	C3-O3-P-O4
24	B	5001	LHG	C3-O3-P-O5
24	B	5001	LHG	C3-O3-P-O6
24	B	5001	LHG	C4-O6-P-O3
24	B	5001	LHG	C4-O6-P-O5
24	F	5002	LHG	O2-C2-C3-O3
24	F	5002	LHG	C3-O3-P-O5
24	F	5002	LHG	C4-O6-P-O3
24	F	5002	LHG	C4-O6-P-O4
24	F	5002	LHG	C4-O6-P-O5
24	F	5002	LHG	C8-C7-O7-C5
24	F	5001	LHG	O1-C1-C2-O2
24	F	5001	LHG	O1-C1-C2-C3
24	F	5001	LHG	C4-O6-P-O3
24	F	5001	LHG	C4-O6-P-O4
24	F	5001	LHG	C8-C7-O7-C5
24	1	801	LHG	C1-C2-C3-O3
24	1	801	LHG	C3-O3-P-O5
24	1	801	LHG	C4-O6-P-O3
24	1	801	LHG	C4-O6-P-O5
24	1	802	LHG	O1-C1-C2-C3
24	1	802	LHG	C4-O6-P-O3
24	1	802	LHG	O7-C5-C6-O8
24	1	802	LHG	C8-C7-O7-C5
24	a	801	LHG	C3-O3-P-O4
24	a	801	LHG	C3-O3-P-O5
24	a	801	LHG	C3-O3-P-O6
24	a	801	LHG	C4-O6-P-O3
24	a	801	LHG	C4-O6-P-O5
24	a	801	LHG	C8-C7-O7-C5
24	3	801	LHG	O1-C1-C2-C3
24	3	801	LHG	C1-C2-C3-O3
24	3	801	LHG	C3-O3-P-O4
24	3	801	LHG	C3-O3-P-O5
24	3	801	LHG	C3-O3-P-O6
24	3	801	LHG	O9-C7-O7-C5
24	4	802	LHG	C3-O3-P-O4
24	4	802	LHG	C3-O3-P-O5
24	4	802	LHG	C3-O3-P-O6
24	4	802	LHG	C4-O6-P-O5
24	4	802	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
24	5	801	LHG	C3-O3-P-O5
24	5	801	LHG	C4-O6-P-O3
24	5	801	LHG	C4-O6-P-O4
24	6	802	LHG	O1-C1-C2-C3
24	6	802	LHG	C1-C2-C3-O3
24	6	802	LHG	C4-O6-P-O3
24	6	801	LHG	C3-O3-P-O4
24	6	801	LHG	C3-O3-P-O5
24	6	801	LHG	C3-O3-P-O6
24	6	801	LHG	C4-O6-P-O5
24	7	801	LHG	O1-C1-C2-C3
24	7	801	LHG	C3-O3-P-O4
24	7	801	LHG	C3-O3-P-O5
24	7	801	LHG	C3-O3-P-O6
24	7	801	LHG	C4-O6-P-O3
24	7	801	LHG	C4-O6-P-O4
24	7	801	LHG	C4-O6-P-O5
24	7	801	LHG	O9-C7-O7-C5
24	7	801	LHG	C8-C7-O7-C5
24	7	802	LHG	O2-C2-C3-O3
24	7	802	LHG	C2-C3-O3-P
24	7	803	LHG	O1-C1-C2-C3
24	7	803	LHG	C3-O3-P-O4
24	7	803	LHG	C3-O3-P-O6
24	7	803	LHG	C4-O6-P-O3
24	7	803	LHG	C4-O6-P-O5
24	8	801	LHG	C4-O6-P-O3
24	8	801	LHG	C4-O6-P-O4
24	8	801	LHG	C4-O6-P-O5
25	A	5005	DGD	C2A-C1A-O1G-C1G
25	A	5005	DGD	O1A-C1A-O1G-C1G
25	A	5005	DGD	O6D-C1D-O3G-C3G
25	8	802	DGD	C2B-C1B-O2G-C2G
26	A	5007	3PH	C22-C21-O21-C2
28	B	5006	LMT	O5'-C1'-O1'-C1
28	1	804	LMT	C2-C1-O1'-C1'
29	B	5004	PCW	C2-C1-O3P-P
29	6	803	PCW	O4P-C4-C5-N
29	6	803	PCW	C1-O3P-P-O2P
29	6	803	PCW	C4-O4P-P-O1P
29	6	803	PCW	C4-O4P-P-O2P
29	6	803	PCW	C4-O4P-P-O3P

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

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Mol	Chain	Res	Type	Atoms
35	J	5001	LPX	C3-O1-P1-O3
35	J	5001	LPX	C3-O1-P1-O2
35	J	5001	LPX	O2-C1-C2-N1
35	a	804	LPX	O2-C1-C2-N1
36	M	4001	ECH	C11-C12-C13-C14
37	1	503	LUT	C21-C26-C27-C28
37	1	503	LUT	C27-C28-C29-C30
37	1	503	LUT	C27-C28-C29-C39
37	1	503	LUT	C31-C32-C33-C34
37	1	503	LUT	C31-C32-C33-C40
37	a	501	LUT	C5-C6-C7-C8
37	a	501	LUT	C31-C32-C33-C34
37	a	502	LUT	C7-C8-C9-C10
37	a	502	LUT	C7-C8-C9-C19
37	a	502	LUT	C21-C26-C27-C28
37	a	502	LUT	C25-C26-C27-C28
37	a	503	LUT	C21-C26-C27-C28
37	a	503	LUT	C31-C32-C33-C34
37	a	503	LUT	C31-C32-C33-C40
37	5	505	LUT	C21-C26-C27-C28
37	5	505	LUT	C25-C26-C27-C28
37	6	501	LUT	C7-C8-C9-C10
37	6	501	LUT	C7-C8-C9-C19
37	6	501	LUT	C21-C26-C27-C28
37	6	501	LUT	C25-C26-C27-C28
37	6	502	LUT	C21-C26-C27-C28
37	7	501	LUT	C21-C26-C27-C28
38	1	609	CHL	C3A-C2A-CAA-CBA
38	a	606	CHL	C3A-C2A-CAA-CBA
38	3	608	CHL	C1A-C2A-CAA-CBA
38	4	609	CHL	C1A-C2A-CAA-CBA
38	4	609	CHL	C3A-C2A-CAA-CBA
38	4	609	CHL	C4C-C3C-CAC-CBC
38	4	613	CHL	C1A-C2A-CAA-CBA
38	4	613	CHL	C2-C3-C5-C6
38	4	613	CHL	C4-C3-C5-C6
38	4	618	CHL	C1A-C2A-CAA-CBA
38	4	618	CHL	C4C-C3C-CAC-CBC
38	6	619	CHL	C1A-C2A-CAA-CBA
38	6	619	CHL	C2-C3-C5-C6
38	6	619	CHL	C4-C3-C5-C6
38	8	601	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
38	8	601	CHL	C4C-C3C-CAC-CBC
38	8	604	CHL	C1A-C2A-CAA-CBA
38	8	604	CHL	C3A-C2A-CAA-CBA
40	a	504	QTB	C01-C02-C09-C10
40	a	504	QTB	C03-C02-C09-C10
40	a	504	QTB	C09-C10-C11-C12
40	3	506	QTB	C04-C05-C06-O07
41	a	805	GG0	N05-C06-C07-O08
41	a	805	GG0	N05-C06-C07-O09
42	4	803	PLM	O2-C1-C2-C3
42	4	803	PLM	C1-C2-C3-C4
43	5	803	DGA	CB2-CB1-OG2-CG2
43	8	803	DGA	CB2-CB1-OG2-CG2
44	6	806	SPH	C2-C3-C4-C5
44	6	806	SPH	O3-C3-C4-C5
46	8	808	4RF	O42-C41-O40-C39
46	8	808	4RF	C43-C41-O40-C39
47	7	504	C7Z	C9-C10-C11-C12
47	7	504	C7Z	C29-C30-C31-C32
48	8	806	P5S	C-CA-CB-OG
48	8	806	P5S	N-CA-CB-OG
48	8	806	P5S	CA-CB-OG-P12
48	8	806	P5S	CB-OG-P12-O15
48	8	806	P5S	C3-O16-P12-OG
48	8	806	P5S	C3-O16-P12-O13
38	4	609	CHL	C2C-C3C-CAC-CBC
21	7	605	CLA	C2C-C3C-CAC-CBC
21	A	1138	CLA	O1D-CGD-O2D-CED
21	B	1021	CLA	O1D-CGD-O2D-CED
21	B	1232	CLA	O1D-CGD-O2D-CED
21	L	1501	CLA	O1D-CGD-O2D-CED
21	a	602	CLA	O1D-CGD-O2D-CED
21	a	608	CLA	O1D-CGD-O2D-CED
21	a	615	CLA	O1D-CGD-O2D-CED
21	4	603	CLA	O1D-CGD-O2D-CED
21	4	610	CLA	O1D-CGD-O2D-CED
21	5	618	CLA	O1D-CGD-O2D-CED
21	6	606	CLA	O1D-CGD-O2D-CED
21	6	617	CLA	O1D-CGD-O2D-CED
21	8	605	CLA	O1D-CGD-O2D-CED
21	5	617	CLA	C4C-C3C-CAC-CBC
21	A	1108	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	A	1109	CLA	O1D-CGD-O2D-CED
21	B	1023	CLA	O1D-CGD-O2D-CED
21	F	1302	CLA	O1D-CGD-O2D-CED
21	a	612	CLA	O1D-CGD-O2D-CED
21	3	606	CLA	O1D-CGD-O2D-CED
21	5	616	CLA	O1D-CGD-O2D-CED
21	7	606	CLA	O1D-CGD-O2D-CED
21	7	615	CLA	O1D-CGD-O2D-CED
20	A	1011	CL0	CBD-CGD-O2D-CED
21	A	1012	CLA	CBD-CGD-O2D-CED
21	A	1108	CLA	CBD-CGD-O2D-CED
21	A	1115	CLA	CBD-CGD-O2D-CED
21	A	1122	CLA	CBD-CGD-O2D-CED
21	A	1123	CLA	CBD-CGD-O2D-CED
21	A	1125	CLA	CBD-CGD-O2D-CED
21	A	1126	CLA	CBD-CGD-O2D-CED
21	A	1127	CLA	CBD-CGD-O2D-CED
21	A	1131	CLA	CBD-CGD-O2D-CED
21	A	1132	CLA	CBD-CGD-O2D-CED
21	A	1134	CLA	CBD-CGD-O2D-CED
21	A	1135	CLA	CBD-CGD-O2D-CED
21	A	1138	CLA	CBD-CGD-O2D-CED
21	A	1139	CLA	CBD-CGD-O2D-CED
21	B	1021	CLA	CBD-CGD-O2D-CED
21	B	1203	CLA	CBD-CGD-O2D-CED
21	B	1210	CLA	CBD-CGD-O2D-CED
21	B	1211	CLA	CBD-CGD-O2D-CED
21	B	1212	CLA	CBD-CGD-O2D-CED
21	B	1213	CLA	CBD-CGD-O2D-CED
21	B	1215	CLA	CBD-CGD-O2D-CED
21	B	1216	CLA	CBD-CGD-O2D-CED
21	B	1219	CLA	CBD-CGD-O2D-CED
21	B	1222	CLA	CBD-CGD-O2D-CED
21	B	1226	CLA	CBD-CGD-O2D-CED
21	B	1227	CLA	CBD-CGD-O2D-CED
21	B	1232	CLA	CBD-CGD-O2D-CED
21	B	1239	CLA	CBD-CGD-O2D-CED
21	G	1602	CLA	CBD-CGD-O2D-CED
21	K	1404	CLA	CBD-CGD-O2D-CED
21	L	1501	CLA	CBD-CGD-O2D-CED
21	1	602	CLA	CBD-CGD-O2D-CED
21	1	605	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	1	612	CLA	CBD-CGD-O2D-CED
21	a	602	CLA	CBD-CGD-O2D-CED
21	a	605	CLA	CBD-CGD-O2D-CED
21	a	607	CLA	CBD-CGD-O2D-CED
21	a	608	CLA	CBD-CGD-O2D-CED
21	3	602	CLA	CBD-CGD-O2D-CED
21	3	606	CLA	CBD-CGD-O2D-CED
21	3	612	CLA	CBD-CGD-O2D-CED
21	3	613	CLA	CBD-CGD-O2D-CED
21	3	616	CLA	CBD-CGD-O2D-CED
21	4	603	CLA	CBD-CGD-O2D-CED
21	4	604	CLA	CBD-CGD-O2D-CED
21	4	606	CLA	CBD-CGD-O2D-CED
21	4	616	CLA	CBD-CGD-O2D-CED
21	4	617	CLA	CBD-CGD-O2D-CED
21	5	601	CLA	CBD-CGD-O2D-CED
21	5	606	CLA	CBD-CGD-O2D-CED
21	5	607	CLA	CBD-CGD-O2D-CED
21	5	608	CLA	CBD-CGD-O2D-CED
21	5	609	CLA	CBD-CGD-O2D-CED
21	5	618	CLA	CBD-CGD-O2D-CED
21	6	602	CLA	CBD-CGD-O2D-CED
21	6	603	CLA	CBD-CGD-O2D-CED
21	6	605	CLA	CBD-CGD-O2D-CED
21	6	617	CLA	CBD-CGD-O2D-CED
21	7	601	CLA	CBD-CGD-O2D-CED
21	7	602	CLA	CBD-CGD-O2D-CED
21	7	608	CLA	CBD-CGD-O2D-CED
21	7	612	CLA	CBD-CGD-O2D-CED
21	7	615	CLA	CBD-CGD-O2D-CED
21	8	605	CLA	CBD-CGD-O2D-CED
21	8	608	CLA	CBD-CGD-O2D-CED
21	8	610	CLA	CBD-CGD-O2D-CED
21	8	615	CLA	CBD-CGD-O2D-CED
21	8	620	CLA	CBD-CGD-O2D-CED
38	4	609	CHL	CBD-CGD-O2D-CED
21	A	1118	CLA	O1A-CGA-O2A-C1
21	F	1301	CLA	O1A-CGA-O2A-C1
21	K	1404	CLA	O1A-CGA-O2A-C1
21	4	607	CLA	O1A-CGA-O2A-C1
21	8	606	CLA	O1A-CGA-O2A-C1
29	6	803	PCW	O11-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
30	B	5005	PTY	O30-C30-O4-C1
31	F	5003	LAP	O2-C1-O1-C13
46	7	807	4RF	O42-C41-O40-C39
46	8	807	4RF	O17-C16-O18-C19
48	8	806	P5S	O18-C17-O19-C1
21	K	1401	CLA	O1A-CGA-O2A-C1
21	1	615	CLA	O1A-CGA-O2A-C1
21	3	618	CLA	O1A-CGA-O2A-C1
21	6	618	CLA	O1A-CGA-O2A-C1
21	B	1234	CLA	C2C-C3C-CAC-CBC
21	F	1302	CLA	C2C-C3C-CAC-CBC
21	5	617	CLA	C2C-C3C-CAC-CBC
21	5	612	CLA	C13-C15-C16-C17
24	F	5002	LHG	C5-C6-O8-C23
25	B	5003	DGD	C2G-C1G-O1G-C1A
31	F	5003	LAP	C14-C13-O1-C1
21	7	605	CLA	C4C-C3C-CAC-CBC
21	A	1126	CLA	O1D-CGD-O2D-CED
21	A	1131	CLA	O1D-CGD-O2D-CED
21	1	602	CLA	O1D-CGD-O2D-CED
21	1	612	CLA	O1D-CGD-O2D-CED
21	4	616	CLA	O1D-CGD-O2D-CED
21	4	617	CLA	O1D-CGD-O2D-CED
21	5	617	CLA	O1D-CGD-O2D-CED
21	8	610	CLA	O1D-CGD-O2D-CED
21	8	615	CLA	O1D-CGD-O2D-CED
21	A	1118	CLA	CBA-CGA-O2A-C1
21	F	1301	CLA	CBA-CGA-O2A-C1
21	K	1404	CLA	CBA-CGA-O2A-C1
21	4	607	CLA	CBA-CGA-O2A-C1
21	7	615	CLA	CBA-CGA-O2A-C1
21	8	606	CLA	CBA-CGA-O2A-C1
30	B	5005	PTY	C31-C30-O4-C1
46	7	807	4RF	C43-C41-O40-C39
46	8	807	4RF	C15-C16-O18-C19
48	8	806	P5S	C20-C17-O19-C1
21	B	1231	CLA	CBD-CGD-O2D-CED
21	B	1237	CLA	CBD-CGD-O2D-CED
21	1	606	CLA	CBD-CGD-O2D-CED
21	5	612	CLA	CBD-CGD-O2D-CED
21	A	1122	CLA	O1A-CGA-O2A-C1
21	A	1101	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	B	1201	CLA	O1A-CGA-O2A-C1
21	B	1206	CLA	O1A-CGA-O2A-C1
21	B	1219	CLA	O1A-CGA-O2A-C1
21	1	607	CLA	O1A-CGA-O2A-C1
21	3	603	CLA	O1A-CGA-O2A-C1
21	3	610	CLA	O1A-CGA-O2A-C1
21	3	612	CLA	O1A-CGA-O2A-C1
21	6	607	CLA	O1A-CGA-O2A-C1
21	6	615	CLA	O1A-CGA-O2A-C1
21	7	610	CLA	O1A-CGA-O2A-C1
21	7	615	CLA	O1A-CGA-O2A-C1
21	8	609	CLA	O1A-CGA-O2A-C1
29	B	5004	PCW	O11-C11-O3-C3
32	G	5001	SQD	O10-C23-O48-C46
32	7	805	SQD	O10-C23-O48-C46
43	5	803	DGA	OA1-CA1-OG1-CG1
46	8	807	4RF	O42-C41-O40-C39
21	A	1109	CLA	C15-C16-C17-C18
21	K	1403	CLA	O1A-CGA-O2A-C1
21	6	605	CLA	O1A-CGA-O2A-C1
21	B	1234	CLA	C4C-C3C-CAC-CBC
21	A	1114	CLA	O1D-CGD-O2D-CED
21	A	1140	CLA	O1D-CGD-O2D-CED
21	B	1206	CLA	O1D-CGD-O2D-CED
21	B	1224	CLA	O1D-CGD-O2D-CED
21	B	1207	CLA	O1D-CGD-O2D-CED
21	G	1603	CLA	O1D-CGD-O2D-CED
21	J	1901	CLA	O1D-CGD-O2D-CED
21	K	1402	CLA	O1D-CGD-O2D-CED
21	1	603	CLA	O1D-CGD-O2D-CED
21	a	611	CLA	O1D-CGD-O2D-CED
21	3	605	CLA	O1D-CGD-O2D-CED
21	4	607	CLA	O1D-CGD-O2D-CED
21	6	603	CLA	O1D-CGD-O2D-CED
21	7	612	CLA	O1D-CGD-O2D-CED
21	8	611	CLA	O1D-CGD-O2D-CED
21	8	620	CLA	O1D-CGD-O2D-CED
21	A	1013	CLA	O1D-CGD-O2D-CED
21	A	1107	CLA	O1D-CGD-O2D-CED
21	A	1111	CLA	O1D-CGD-O2D-CED
21	A	1116	CLA	O1D-CGD-O2D-CED
21	A	1119	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	B	1022	CLA	O1D-CGD-O2D-CED
21	1	611	CLA	O1D-CGD-O2D-CED
21	1	615	CLA	O1D-CGD-O2D-CED
21	a	603	CLA	O1D-CGD-O2D-CED
21	4	602	CLA	O1D-CGD-O2D-CED
21	4	615	CLA	O1D-CGD-O2D-CED
21	5	603	CLA	O1D-CGD-O2D-CED
21	6	608	CLA	O1D-CGD-O2D-CED
21	7	610	CLA	O1D-CGD-O2D-CED
21	A	1135	CLA	C8-C10-C11-C12
21	B	1021	CLA	C5-C6-C7-C8
21	F	1302	CLA	C5-C6-C7-C8
21	B	1217	CLA	CBD-CGD-O2D-CED
21	K	1401	CLA	CBD-CGD-O2D-CED
21	L	1503	CLA	CBD-CGD-O2D-CED
21	1	601	CLA	CBD-CGD-O2D-CED
21	4	612	CLA	CBD-CGD-O2D-CED
24	F	5002	LHG	O10-C23-O8-C6
46	8	808	4RF	O17-C16-O18-C19
21	L	1503	CLA	C4C-C3C-CAC-CBC
24	A	5003	LHG	O9-C7-O7-C5
24	F	5002	LHG	O9-C7-O7-C5
24	F	5001	LHG	O9-C7-O7-C5
24	1	802	LHG	O9-C7-O7-C5
24	a	801	LHG	O9-C7-O7-C5
24	4	802	LHG	O9-C7-O7-C5
25	8	802	DGD	O1B-C1B-O2G-C2G
26	A	5007	3PH	O22-C21-O21-C2
30	5	802	PTY	O10-C8-O7-C6
30	7	804	PTY	O10-C8-O7-C6
43	8	803	DGA	OB1-CB1-OG2-CG2
46	8	807	4RF	O23-C22-O21-C20
46	8	808	4RF	O23-C22-O21-C20
21	5	602	CLA	O1D-CGD-O2D-CED
21	8	603	CLA	O1D-CGD-O2D-CED
21	A	1013	CLA	C3-C5-C6-C7
21	A	1109	CLA	C3-C5-C6-C7
21	A	1110	CLA	C3-C5-C6-C7
21	A	1114	CLA	C3-C5-C6-C7
21	A	1131	CLA	C3-C5-C6-C7
21	A	1133	CLA	C3-C5-C6-C7
21	A	1135	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
21	B	1203	CLA	C3-C5-C6-C7
21	B	1205	CLA	C3-C5-C6-C7
21	B	1206	CLA	C3-C5-C6-C7
21	B	1211	CLA	C3-C5-C6-C7
21	B	1218	CLA	C3-C5-C6-C7
21	B	1234	CLA	C3-C5-C6-C7
21	B	1204	CLA	C3-C5-C6-C7
21	1	604	CLA	C3-C5-C6-C7
21	1	612	CLA	C3-C5-C6-C7
21	a	603	CLA	C3-C5-C6-C7
21	3	603	CLA	C3-C5-C6-C7
21	3	605	CLA	C3-C5-C6-C7
21	3	613	CLA	C3-C5-C6-C7
21	3	616	CLA	C3-C5-C6-C7
21	4	612	CLA	C3-C5-C6-C7
21	6	601	CLA	C3-C5-C6-C7
21	7	609	CLA	C3-C5-C6-C7
21	8	618	CLA	C3-C5-C6-C7
38	4	609	CHL	C3-C5-C6-C7
21	F	1302	CLA	C4C-C3C-CAC-CBC
21	L	1503	CLA	C2C-C3C-CAC-CBC
21	4	611	CLA	O1D-CGD-O2D-CED
21	7	603	CLA	O1D-CGD-O2D-CED
21	A	1122	CLA	CBA-CGA-O2A-C1
21	A	1126	CLA	CBA-CGA-O2A-C1
21	B	1023	CLA	CBA-CGA-O2A-C1
21	B	1201	CLA	CBA-CGA-O2A-C1
21	B	1230	CLA	CBA-CGA-O2A-C1
21	B	1237	CLA	CBA-CGA-O2A-C1
21	B	1228	CLA	CBA-CGA-O2A-C1
21	1	603	CLA	CBA-CGA-O2A-C1
21	3	603	CLA	CBA-CGA-O2A-C1
21	3	610	CLA	CBA-CGA-O2A-C1
21	4	606	CLA	CBA-CGA-O2A-C1
21	6	607	CLA	CBA-CGA-O2A-C1
21	6	615	CLA	CBA-CGA-O2A-C1
21	7	610	CLA	CBA-CGA-O2A-C1
29	B	5004	PCW	C12-C11-O3-C3
29	6	803	PCW	C12-C11-O3-C3
31	F	5003	LAP	C2-C1-O1-C13
32	G	5001	SQD	C24-C23-O48-C46
32	7	805	SQD	C24-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
43	5	803	DGA	CA2-CA1-OG1-CG1
21	A	1103	CLA	CBD-CGD-O2D-CED
21	A	1104	CLA	CBD-CGD-O2D-CED
21	A	1106	CLA	CBD-CGD-O2D-CED
21	A	1110	CLA	CBD-CGD-O2D-CED
21	A	1113	CLA	CBD-CGD-O2D-CED
21	A	1118	CLA	CBD-CGD-O2D-CED
21	A	1128	CLA	CBD-CGD-O2D-CED
21	A	1129	CLA	CBD-CGD-O2D-CED
21	B	1201	CLA	CBD-CGD-O2D-CED
21	B	1205	CLA	CBD-CGD-O2D-CED
21	B	1209	CLA	CBD-CGD-O2D-CED
21	B	1225	CLA	CBD-CGD-O2D-CED
21	B	1230	CLA	CBD-CGD-O2D-CED
21	B	1234	CLA	CBD-CGD-O2D-CED
21	B	1238	CLA	CBD-CGD-O2D-CED
21	B	1228	CLA	CBD-CGD-O2D-CED
21	K	1403	CLA	CBD-CGD-O2D-CED
21	L	1502	CLA	CBD-CGD-O2D-CED
21	1	604	CLA	CBD-CGD-O2D-CED
21	1	608	CLA	CBD-CGD-O2D-CED
21	1	610	CLA	CBD-CGD-O2D-CED
21	a	601	CLA	CBD-CGD-O2D-CED
21	3	604	CLA	CBD-CGD-O2D-CED
21	3	610	CLA	CBD-CGD-O2D-CED
21	6	601	CLA	CBD-CGD-O2D-CED
21	6	615	CLA	CBD-CGD-O2D-CED
21	7	609	CLA	CBD-CGD-O2D-CED
21	8	609	CLA	CBD-CGD-O2D-CED
21	8	602	CLA	CBD-CGD-O2D-CED
21	8	618	CLA	CBD-CGD-O2D-CED
38	a	610	CHL	CBD-CGD-O2D-CED
24	3	801	LHG	C8-C7-O7-C5
30	8	810	PTY	C11-C8-O7-C6
46	8	807	4RF	C24-C22-O21-C20
46	8	808	4RF	C24-C22-O21-C20
21	6	612	CLA	C2C-C3C-CAC-CBC
21	A	1112	CLA	O1D-CGD-O2D-CED
21	A	1121	CLA	O1D-CGD-O2D-CED
21	B	1220	CLA	O1D-CGD-O2D-CED
21	B	1226	CLA	O1D-CGD-O2D-CED
21	B	1229	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	G	1601	CLA	O1D-CGD-O2D-CED
21	a	607	CLA	O1D-CGD-O2D-CED
21	3	618	CLA	O1D-CGD-O2D-CED
21	5	614	CLA	O1D-CGD-O2D-CED
21	6	618	CLA	O1D-CGD-O2D-CED
21	7	601	CLA	O1D-CGD-O2D-CED
21	8	606	CLA	O1D-CGD-O2D-CED
21	5	607	CLA	O1A-CGA-O2A-C1
21	5	609	CLA	O1A-CGA-O2A-C1
28	B	5006	LMT	O5'-C5'-C6'-O6'
21	B	1236	CLA	C2C-C3C-CAC-CBC
21	6	605	CLA	O1D-CGD-O2D-CED
21	A	1115	CLA	C4-C3-C5-C6
21	A	1128	CLA	C4-C3-C5-C6
21	A	1130	CLA	C4-C3-C5-C6
21	A	1133	CLA	C4-C3-C5-C6
21	A	1135	CLA	C4-C3-C5-C6
21	A	1136	CLA	C4-C3-C5-C6
21	B	1206	CLA	C4-C3-C5-C6
21	B	1215	CLA	C4-C3-C5-C6
21	B	1218	CLA	C4-C3-C5-C6
21	B	1226	CLA	C4-C3-C5-C6
21	B	1236	CLA	C4-C3-C5-C6
21	1	603	CLA	C4-C3-C5-C6
21	1	605	CLA	C4-C3-C5-C6
21	a	605	CLA	C4-C3-C5-C6
21	3	616	CLA	C4-C3-C5-C6
21	5	602	CLA	C4-C3-C5-C6
21	5	603	CLA	C4-C3-C5-C6
21	6	615	CLA	C4-C3-C5-C6
21	7	611	CLA	C4-C3-C5-C6
21	8	602	CLA	C4-C3-C5-C6
21	8	606	CLA	C4-C3-C5-C6
38	4	609	CHL	C4-C3-C5-C6
38	4	618	CHL	C4-C3-C5-C6
38	5	610	CHL	C4-C3-C5-C6
38	5	613	CHL	C4-C3-C5-C6
21	A	1115	CLA	C2-C3-C5-C6
21	A	1133	CLA	C2-C3-C5-C6
21	A	1135	CLA	C2-C3-C5-C6
21	A	1136	CLA	C2-C3-C5-C6
21	B	1206	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	B	1215	CLA	C2-C3-C5-C6
21	B	1217	CLA	C2-C3-C5-C6
21	B	1226	CLA	C2-C3-C5-C6
21	1	603	CLA	C2-C3-C5-C6
21	1	605	CLA	C2-C3-C5-C6
21	a	605	CLA	C2-C3-C5-C6
21	3	603	CLA	C2-C3-C5-C6
21	3	616	CLA	C2-C3-C5-C6
21	5	602	CLA	C2-C3-C5-C6
21	6	615	CLA	C2-C3-C5-C6
21	8	602	CLA	C2-C3-C5-C6
21	8	606	CLA	C2-C3-C5-C6
38	4	618	CHL	C2-C3-C5-C6
38	5	610	CHL	C2-C3-C5-C6
38	5	613	CHL	C2-C3-C5-C6
21	a	615	CLA	CBA-CGA-O2A-C1
21	5	616	CLA	CBA-CGA-O2A-C1
21	A	1130	CLA	CBD-CGD-O2D-CED
21	B	1211	CLA	O1D-CGD-O2D-CED
21	B	1239	CLA	O1D-CGD-O2D-CED
21	4	606	CLA	O1D-CGD-O2D-CED
21	5	609	CLA	O1D-CGD-O2D-CED
21	7	608	CLA	O1D-CGD-O2D-CED
21	B	1234	CLA	C2A-CAA-CBA-CGA
21	B	1228	CLA	C2A-CAA-CBA-CGA
21	K	1404	CLA	C3-C5-C6-C7
21	4	602	CLA	C3-C5-C6-C7
21	8	602	CLA	C3-C5-C6-C7
21	B	1212	CLA	O1A-CGA-O2A-C1
21	B	1207	CLA	O1A-CGA-O2A-C1
21	a	611	CLA	O1A-CGA-O2A-C1
21	A	1111	CLA	C3-C5-C6-C7
21	A	1130	CLA	C3-C5-C6-C7
21	A	1134	CLA	C3-C5-C6-C7
21	B	1214	CLA	C3-C5-C6-C7
21	B	1220	CLA	C3-C5-C6-C7
21	a	605	CLA	C3-C5-C6-C7
21	3	610	CLA	C3-C5-C6-C7
21	7	601	CLA	C3-C5-C6-C7
21	7	615	CLA	C3-C5-C6-C7
21	8	606	CLA	C3-C5-C6-C7
21	4	604	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	A	1117	CLA	CBA-CGA-O2A-C1
21	A	1119	CLA	CBA-CGA-O2A-C1
21	A	1125	CLA	CBA-CGA-O2A-C1
21	A	1101	CLA	CBA-CGA-O2A-C1
21	B	1206	CLA	CBA-CGA-O2A-C1
21	B	1219	CLA	CBA-CGA-O2A-C1
21	1	607	CLA	CBA-CGA-O2A-C1
21	1	611	CLA	CBA-CGA-O2A-C1
21	3	604	CLA	CBA-CGA-O2A-C1
21	3	607	CLA	CBA-CGA-O2A-C1
21	3	612	CLA	CBA-CGA-O2A-C1
21	4	604	CLA	CBA-CGA-O2A-C1
21	4	611	CLA	CBA-CGA-O2A-C1
21	8	609	CLA	CBA-CGA-O2A-C1
21	8	603	CLA	CBA-CGA-O2A-C1
24	F	5002	LHG	C24-C23-O8-C6
35	a	804	LPX	C7-C6-O6-C5
46	8	807	4RF	C43-C41-O40-C39
46	8	808	4RF	C15-C16-O18-C19
21	5	616	CLA	O1A-CGA-O2A-C1
25	B	5003	DGD	CBA-CCA-CDA-CEA
23	B	4006	BCR	C9-C10-C11-C12
23	7	503	BCR	C13-C14-C15-C16
23	7	503	BCR	C19-C20-C21-C22
37	5	505	LUT	C29-C30-C31-C32
21	A	1104	CLA	O1A-CGA-O2A-C1
21	A	1119	CLA	O1A-CGA-O2A-C1
21	B	1237	CLA	O1A-CGA-O2A-C1
21	B	1228	CLA	O1A-CGA-O2A-C1
21	1	603	CLA	O1A-CGA-O2A-C1
21	1	606	CLA	O1A-CGA-O2A-C1
21	1	611	CLA	O1A-CGA-O2A-C1
21	4	606	CLA	O1A-CGA-O2A-C1
21	4	611	CLA	O1A-CGA-O2A-C1
21	7	603	CLA	O1A-CGA-O2A-C1
21	8	620	CLA	O1A-CGA-O2A-C1
30	5	802	PTY	O30-C30-O4-C1
32	G	5001	SQD	O49-C7-O47-C45
43	5	803	DGA	OB1-CB1-OG2-CG2
21	a	605	CLA	O1D-CGD-O2D-CED
21	1	603	CLA	C5-C6-C7-C8
25	B	5003	DGD	C8A-C9A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	8	802	DGD	CEA-CFA-CGA-CHA
25	8	802	DGD	CEB-CFB-CGB-CHB
21	B	1219	CLA	O1D-CGD-O2D-CED
21	K	1404	CLA	O1D-CGD-O2D-CED
21	3	613	CLA	O1D-CGD-O2D-CED
21	3	616	CLA	O1D-CGD-O2D-CED
21	B	1208	CLA	C3-C5-C6-C7
21	B	1212	CLA	C3-C5-C6-C7
21	B	1207	CLA	C3-C5-C6-C7
21	K	1402	CLA	C3-C5-C6-C7
21	L	1502	CLA	C3-C5-C6-C7
21	1	603	CLA	C3-C5-C6-C7
21	3	601	CLA	C3-C5-C6-C7
21	4	601	CLA	C3-C5-C6-C7
21	4	615	CLA	C3-C5-C6-C7
21	8	603	CLA	C3-C5-C6-C7
21	8	610	CLA	C3-C5-C6-C7
21	A	1102	CLA	CBD-CGD-O2D-CED
21	B	1214	CLA	CBD-CGD-O2D-CED
21	B	1240	CLA	CBD-CGD-O2D-CED
21	3	601	CLA	CBD-CGD-O2D-CED
21	5	605	CLA	CBD-CGD-O2D-CED
21	6	612	CLA	CBD-CGD-O2D-CED
21	7	617	CLA	CBD-CGD-O2D-CED
31	F	5003	LAP	C5-C6-C7-C8
24	A	5001	LHG	O2-C2-C3-O3
24	A	5003	LHG	O2-C2-C3-O3
24	1	801	LHG	O2-C2-C3-O3
24	a	801	LHG	O2-C2-C3-O3
24	3	801	LHG	O2-C2-C3-O3
24	4	801	LHG	O2-C2-C3-O3
24	5	801	LHG	O2-C2-C3-O3
24	6	801	LHG	O2-C2-C3-O3
24	8	801	LHG	O2-C2-C3-O3
31	F	5003	LAP	O3-C14-C15-O4
31	K	5001	LAP	O3-C14-C15-O4
35	J	5001	LPX	O1-C3-C4-O5
21	A	1122	CLA	O1D-CGD-O2D-CED
21	B	1210	CLA	O1D-CGD-O2D-CED
21	B	1212	CLA	O1D-CGD-O2D-CED
21	B	1215	CLA	O1D-CGD-O2D-CED
21	G	1602	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	1	605	CLA	O1D-CGD-O2D-CED
21	5	601	CLA	O1D-CGD-O2D-CED
21	5	606	CLA	O1D-CGD-O2D-CED
21	5	607	CLA	O1D-CGD-O2D-CED
21	5	608	CLA	O1D-CGD-O2D-CED
21	7	602	CLA	O1D-CGD-O2D-CED
21	A	1104	CLA	CBA-CGA-O2A-C1
21	B	1217	CLA	CBA-CGA-O2A-C1
21	B	1204	CLA	CBA-CGA-O2A-C1
21	1	606	CLA	CBA-CGA-O2A-C1
21	a	604	CLA	CBA-CGA-O2A-C1
21	a	607	CLA	CBA-CGA-O2A-C1
21	a	611	CLA	CBA-CGA-O2A-C1
21	4	616	CLA	CBA-CGA-O2A-C1
21	5	604	CLA	CBA-CGA-O2A-C1
21	5	607	CLA	CBA-CGA-O2A-C1
21	5	609	CLA	CBA-CGA-O2A-C1
21	5	612	CLA	CBA-CGA-O2A-C1
21	7	609	CLA	CBA-CGA-O2A-C1
21	7	607	CLA	CBA-CGA-O2A-C1
21	8	620	CLA	CBA-CGA-O2A-C1
30	5	802	PTY	C31-C30-O4-C1
21	A	1125	CLA	O1A-CGA-O2A-C1
21	A	1126	CLA	O1A-CGA-O2A-C1
21	B	1023	CLA	O1A-CGA-O2A-C1
21	B	1230	CLA	O1A-CGA-O2A-C1
21	5	604	CLA	O1A-CGA-O2A-C1
21	8	603	CLA	O1A-CGA-O2A-C1
31	B	5007	LAP	O1-C13-C14-O3
21	A	1135	CLA	O1D-CGD-O2D-CED
21	B	1216	CLA	O1D-CGD-O2D-CED
21	6	602	CLA	O1D-CGD-O2D-CED
28	A	5008	LMT	C5'-C4'-O1B-C1B
21	B	1202	CLA	CBD-CGD-O2D-CED
21	6	609	CLA	CBD-CGD-O2D-CED
38	a	613	CHL	CBD-CGD-O2D-CED
24	A	5002	LHG	C8-C7-O7-C5
48	8	806	P5S	C39-C38-O37-C2
21	3	612	CLA	O1D-CGD-O2D-CED
21	A	1117	CLA	O1A-CGA-O2A-C1
21	3	607	CLA	O1A-CGA-O2A-C1
21	4	616	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	5	612	CLA	O1A-CGA-O2A-C1
35	a	804	LPX	O7-C6-O6-C5
20	A	1011	CL0	O1D-CGD-O2D-CED
21	A	1123	CLA	O1D-CGD-O2D-CED
21	A	1127	CLA	O1D-CGD-O2D-CED
21	A	1132	CLA	O1D-CGD-O2D-CED
21	B	1203	CLA	O1D-CGD-O2D-CED
21	B	1213	CLA	O1D-CGD-O2D-CED
21	3	602	CLA	O1D-CGD-O2D-CED
21	A	1103	CLA	C3-C5-C6-C7
21	7	617	CLA	C3-C5-C6-C7
21	A	1137	CLA	CBD-CGD-O2D-CED
21	B	1223	CLA	CBD-CGD-O2D-CED
21	3	603	CLA	CBD-CGD-O2D-CED
21	4	601	CLA	CBD-CGD-O2D-CED
28	B	5006	LMT	C4'-C5'-C6'-O6'
21	A	1012	CLA	O1D-CGD-O2D-CED
21	A	1115	CLA	O1D-CGD-O2D-CED
21	A	1139	CLA	O1D-CGD-O2D-CED
21	B	1222	CLA	O1D-CGD-O2D-CED
21	B	1227	CLA	O1D-CGD-O2D-CED
38	4	609	CHL	O1D-CGD-O2D-CED
21	A	1106	CLA	CBA-CGA-O2A-C1
21	B	1212	CLA	CBA-CGA-O2A-C1
21	B	1207	CLA	CBA-CGA-O2A-C1
21	4	612	CLA	CBA-CGA-O2A-C1
21	7	603	CLA	CBA-CGA-O2A-C1
21	A	1110	CLA	C4-C3-C5-C6
21	A	1132	CLA	C4-C3-C5-C6
21	B	1228	CLA	C4-C3-C5-C6
21	a	607	CLA	C4-C3-C5-C6
21	4	612	CLA	C4-C3-C5-C6
21	6	601	CLA	C4-C3-C5-C6
21	A	1128	CLA	C2-C3-C5-C6
21	A	1130	CLA	C2-C3-C5-C6
21	B	1218	CLA	C2-C3-C5-C6
21	B	1228	CLA	C2-C3-C5-C6
21	3	610	CLA	C2-C3-C5-C6
21	4	612	CLA	C2-C3-C5-C6
21	7	611	CLA	C2-C3-C5-C6
38	4	609	CHL	C2-C3-C5-C6
21	B	1217	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	3	604	CLA	O1A-CGA-O2A-C1
21	4	604	CLA	O1A-CGA-O2A-C1
21	7	609	CLA	O1A-CGA-O2A-C1
21	7	607	CLA	O1A-CGA-O2A-C1
48	8	806	P5S	O47-C38-O37-C2
21	A	1105	CLA	CBD-CGD-O2D-CED
21	A	1117	CLA	CBD-CGD-O2D-CED
24	6	801	LHG	C2-C3-O3-P
48	8	806	P5S	C2-C3-O16-P12
28	A	5008	LMT	O5'-C5'-C6'-O6'
21	3	612	CLA	C2A-CAA-CBA-CGA
21	5	616	CLA	C2A-CAA-CBA-CGA
38	4	613	CHL	C2A-CAA-CBA-CGA
24	5	801	LHG	C28-C29-C30-C31
21	A	1125	CLA	O1D-CGD-O2D-CED
21	A	1134	CLA	O1D-CGD-O2D-CED
21	1	601	CLA	O1D-CGD-O2D-CED
21	1	606	CLA	O1D-CGD-O2D-CED
21	5	612	CLA	O1D-CGD-O2D-CED
21	B	1204	CLA	O1A-CGA-O2A-C1
21	a	607	CLA	O1A-CGA-O2A-C1
25	8	802	DGD	O6E-C1E-O5D-C6D
28	A	5008	LMT	O5'-C1'-O1'-C1
32	7	805	SQD	O5-C1-O6-C44
24	F	5002	LHG	C11-C12-C13-C14
21	B	1231	CLA	O1D-CGD-O2D-CED
21	A	1120	CLA	CBA-CGA-O2A-C1
21	4	603	CLA	CBA-CGA-O2A-C1
21	7	601	CLA	CBA-CGA-O2A-C1
21	8	618	CLA	CBA-CGA-O2A-C1
24	6	802	LHG	C24-C23-O8-C6
31	K	5001	LAP	C2-C1-O1-C13
21	A	1120	CLA	CBD-CGD-O2D-CED
21	A	1133	CLA	CBD-CGD-O2D-CED
21	A	1101	CLA	CBD-CGD-O2D-CED
21	3	607	CLA	CBD-CGD-O2D-CED
21	4	605	CLA	CBD-CGD-O2D-CED
21	5	604	CLA	CBD-CGD-O2D-CED
21	7	611	CLA	CBD-CGD-O2D-CED
21	a	615	CLA	O1A-CGA-O2A-C1
21	K	1401	CLA	O1D-CGD-O2D-CED
21	a	604	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	4	612	CLA	O1A-CGA-O2A-C1
21	A	1104	CLA	O1D-CGD-O2D-CED
21	B	1237	CLA	O1D-CGD-O2D-CED
21	B	1236	CLA	CBD-CGD-O2D-CED
24	7	803	LHG	C8-C7-O7-C5
23	A	4002	BCR	C13-C14-C15-C16
23	J	4001	BCR	C9-C10-C11-C12
23	7	503	BCR	C9-C10-C11-C12
34	J	4002	RRX	C9-C10-C11-C12
21	A	1106	CLA	O1A-CGA-O2A-C1
21	A	1120	CLA	O1A-CGA-O2A-C1
31	K	5001	LAP	O2-C1-O1-C13
24	7	803	LHG	O9-C7-O7-C5
24	A	5003	LHG	C1-C2-C3-O3
24	4	801	LHG	C1-C2-C3-O3
24	5	801	LHG	C1-C2-C3-O3
31	F	5003	LAP	C13-C14-C15-O4
21	L	1503	CLA	O1D-CGD-O2D-CED
21	A	1102	CLA	CBA-CGA-O2A-C1
21	A	1113	CLA	CBA-CGA-O2A-C1
21	A	1121	CLA	CBA-CGA-O2A-C1
21	A	1124	CLA	CBA-CGA-O2A-C1
21	A	1136	CLA	CBA-CGA-O2A-C1
21	A	1139	CLA	CBA-CGA-O2A-C1
21	A	1140	CLA	CBA-CGA-O2A-C1
21	B	1213	CLA	CBA-CGA-O2A-C1
21	B	1215	CLA	CBA-CGA-O2A-C1
21	B	1231	CLA	CBA-CGA-O2A-C1
21	F	1302	CLA	CBA-CGA-O2A-C1
21	3	616	CLA	CBA-CGA-O2A-C1
21	4	608	CLA	CBA-CGA-O2A-C1
21	6	603	CLA	CBA-CGA-O2A-C1
21	7	606	CLA	CBA-CGA-O2A-C1
21	8	602	CLA	CBA-CGA-O2A-C1
21	8	610	CLA	CBA-CGA-O2A-C1
21	8	611	CLA	CBA-CGA-O2A-C1
24	7	803	LHG	C24-C23-O8-C6
25	B	5003	DGD	C2A-C1A-O1G-C1G
26	A	5007	3PH	C32-C31-O31-C3
24	7	801	LHG	C24-C25-C26-C27
21	7	604	CLA	CBD-CGD-O2D-CED
24	7	801	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
31	F	5003	LAP	C7-C8-C9-C10
21	B	1217	CLA	O1D-CGD-O2D-CED
21	1	604	CLA	O1D-CGD-O2D-CED
21	1	610	CLA	O1D-CGD-O2D-CED
21	4	612	CLA	O1D-CGD-O2D-CED
21	A	1123	CLA	C8-C10-C11-C12
21	7	606	CLA	O1A-CGA-O2A-C1
24	4	801	LHG	C34-C35-C36-C37
43	8	803	DGA	CB9-CAB-CBB-CCB
21	3	610	CLA	C4-C3-C5-C6
21	A	1110	CLA	C2-C3-C5-C6
21	A	1132	CLA	C2-C3-C5-C6
21	B	1236	CLA	C2-C3-C5-C6
21	a	607	CLA	C2-C3-C5-C6
21	5	603	CLA	C2-C3-C5-C6
21	6	601	CLA	C2-C3-C5-C6
21	A	1013	CLA	C6-C7-C8-C9
21	A	1106	CLA	C6-C7-C8-C9
21	A	1111	CLA	C11-C10-C8-C9
21	A	1121	CLA	C6-C7-C8-C9
21	A	1122	CLA	C11-C10-C8-C9
21	A	1125	CLA	C14-C13-C15-C16
21	A	1126	CLA	C14-C13-C15-C16
21	A	1131	CLA	C11-C12-C13-C14
21	A	1133	CLA	C6-C7-C8-C9
21	B	1021	CLA	C11-C12-C13-C14
21	B	1023	CLA	C6-C7-C8-C9
21	B	1201	CLA	C11-C10-C8-C9
21	B	1202	CLA	C6-C7-C8-C9
21	B	1205	CLA	C14-C13-C15-C16
21	B	1210	CLA	C11-C12-C13-C14
21	B	1234	CLA	C6-C7-C8-C9
21	B	1238	CLA	C11-C10-C8-C9
21	B	1239	CLA	C14-C13-C15-C16
21	B	1204	CLA	C11-C10-C8-C9
21	L	1502	CLA	C11-C10-C8-C9
21	1	603	CLA	C11-C10-C8-C9
21	3	601	CLA	C11-C12-C13-C14
21	4	610	CLA	C11-C12-C13-C14
21	6	601	CLA	C6-C7-C8-C9
21	6	604	CLA	C14-C13-C15-C16
21	6	609	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
21	7	601	CLA	C11-C10-C8-C9
21	7	603	CLA	C14-C13-C15-C16
21	8	603	CLA	C11-C10-C8-C9
38	1	609	CHL	C6-C7-C8-C9
38	8	604	CHL	C11-C12-C13-C14
35	a	804	LPX	C12-C13-C14-C15
21	A	1118	CLA	O1D-CGD-O2D-CED
21	1	608	CLA	O1D-CGD-O2D-CED
21	a	601	CLA	O1D-CGD-O2D-CED
21	8	602	CLA	O1D-CGD-O2D-CED
25	8	802	DGD	C2E-C1E-O5D-C6D
28	A	5008	LMT	C2'-C1'-O1'-C1
32	7	805	SQD	C2-C1-O6-C44
24	6	801	LHG	C23-C24-C25-C26
21	5	614	CLA	CBA-CGA-O2A-C1
21	B	1205	CLA	O1D-CGD-O2D-CED
21	B	1225	CLA	O1D-CGD-O2D-CED
21	3	604	CLA	O1D-CGD-O2D-CED
28	1	804	LMT	O5B-C5B-C6B-O6B
21	A	1113	CLA	O1A-CGA-O2A-C1
21	A	1124	CLA	O1A-CGA-O2A-C1
21	B	1215	CLA	O1A-CGA-O2A-C1
21	B	1231	CLA	O1A-CGA-O2A-C1
21	A	1106	CLA	O1D-CGD-O2D-CED
21	A	1129	CLA	O1D-CGD-O2D-CED
21	B	1230	CLA	O1D-CGD-O2D-CED
21	B	1228	CLA	O1D-CGD-O2D-CED
21	L	1502	CLA	O1D-CGD-O2D-CED
23	A	4003	BCR	C11-C12-C13-C35
23	A	4003	BCR	C36-C18-C19-C20
23	A	4004	BCR	C7-C8-C9-C34
23	A	4004	BCR	C11-C12-C13-C35
23	A	4005	BCR	C7-C8-C9-C34
23	B	4002	BCR	C37-C22-C23-C24
23	B	4004	BCR	C37-C22-C23-C24
23	B	4005	BCR	C7-C8-C9-C34
23	B	4005	BCR	C36-C18-C19-C20
23	B	4007	BCR	C11-C12-C13-C35
23	B	4007	BCR	C36-C18-C19-C20
23	B	4006	BCR	C11-C12-C13-C35
23	B	4001	BCR	C7-C8-C9-C34
23	B	4001	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
23	F	4001	BCR	C37-C22-C23-C24
23	G	4001	BCR	C36-C18-C19-C20
23	J	4001	BCR	C7-C8-C9-C34
23	K	4001	BCR	C11-C12-C13-C35
23	I	4001	BCR	C11-C12-C13-C35
23	3	504	BCR	C36-C18-C19-C20
23	5	503	BCR	C11-C12-C13-C35
23	5	503	BCR	C36-C18-C19-C20
23	5	503	BCR	C37-C22-C23-C24
23	6	504	BCR	C36-C18-C19-C20
23	7	503	BCR	C11-C12-C13-C35
23	7	503	BCR	C36-C18-C19-C20
23	8	503	BCR	C7-C8-C9-C34
34	J	4002	RRX	C37-C22-C23-C24
34	J	4002	RRX	C11-C12-C13-C35
36	M	4001	ECH	C11-C12-C13-C35
37	a	501	LUT	C31-C32-C33-C40
37	a	502	LUT	C11-C12-C13-C20
37	5	505	LUT	C7-C8-C9-C19
23	A	4004	BCR	C7-C8-C9-C10
23	B	4004	BCR	C21-C22-C23-C24
23	B	4005	BCR	C17-C18-C19-C20
23	B	4007	BCR	C11-C12-C13-C14
23	B	4006	BCR	C11-C12-C13-C14
23	F	4001	BCR	C21-C22-C23-C24
23	J	4001	BCR	C7-C8-C9-C10
23	5	503	BCR	C21-C22-C23-C24
23	6	504	BCR	C21-C22-C23-C24
23	7	503	BCR	C17-C18-C19-C20
34	J	4002	RRX	C11-C12-C13-C14
37	a	502	LUT	C11-C12-C13-C14
37	5	505	LUT	C7-C8-C9-C10
30	8	810	PTY	C14-C15-C16-C17
21	A	1113	CLA	C3-C5-C6-C7
21	A	1127	CLA	C2A-CAA-CBA-CGA
21	A	1134	CLA	C2A-CAA-CBA-CGA
21	B	1227	CLA	C2A-CAA-CBA-CGA
21	3	610	CLA	C2A-CAA-CBA-CGA
21	7	615	CLA	C2A-CAA-CBA-CGA
21	6	612	CLA	C4C-C3C-CAC-CBC
29	B	5004	PCW	C31-C32-C33-C34
30	7	804	PTY	C8-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
21	A	1102	CLA	O1A-CGA-O2A-C1
21	A	1121	CLA	O1A-CGA-O2A-C1
21	A	1139	CLA	O1A-CGA-O2A-C1
21	3	616	CLA	O1A-CGA-O2A-C1
21	6	603	CLA	O1A-CGA-O2A-C1
21	8	602	CLA	O1A-CGA-O2A-C1
21	8	610	CLA	O1A-CGA-O2A-C1
21	7	610	CLA	C3-C5-C6-C7
24	A	5002	LHG	O9-C7-O7-C5
21	3	602	CLA	CBA-CGA-O2A-C1
21	B	1212	CLA	C2C-C3C-CAC-CBC
24	A	5002	LHG	O7-C5-C6-O8
24	1	801	LHG	O7-C5-C6-O8
21	B	1201	CLA	O1D-CGD-O2D-CED
21	A	1112	CLA	CBA-CGA-O2A-C1
21	A	1135	CLA	CBA-CGA-O2A-C1
21	4	610	CLA	CBA-CGA-O2A-C1
21	5	606	CLA	CBA-CGA-O2A-C1
21	7	604	CLA	CBA-CGA-O2A-C1
21	A	1102	CLA	C10-C11-C12-C13
21	B	1214	CLA	C8-C10-C11-C12
24	5	801	LHG	C7-C8-C9-C10
21	A	1111	CLA	C2-C1-O2A-CGA
21	A	1120	CLA	C2-C1-O2A-CGA
21	A	1133	CLA	C2-C1-O2A-CGA
21	B	1022	CLA	C2-C1-O2A-CGA
21	B	1220	CLA	C2-C1-O2A-CGA
21	B	1236	CLA	C2-C1-O2A-CGA
21	B	1238	CLA	C2-C1-O2A-CGA
21	B	1228	CLA	C2-C1-O2A-CGA
21	B	1229	CLA	C2-C1-O2A-CGA
21	1	608	CLA	C2-C1-O2A-CGA
21	1	611	CLA	C2-C1-O2A-CGA
21	4	610	CLA	C2-C1-O2A-CGA
21	4	611	CLA	C2-C1-O2A-CGA
21	4	612	CLA	C2-C1-O2A-CGA
21	6	606	CLA	C2-C1-O2A-CGA
21	6	607	CLA	C2-C1-O2A-CGA
21	7	612	CLA	C2-C1-O2A-CGA
21	A	1103	CLA	O1D-CGD-O2D-CED
21	K	1403	CLA	O1D-CGD-O2D-CED
21	1	607	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	A	1013	CLA	C8-C10-C11-C12
21	B	1224	CLA	C8-C10-C11-C12
21	B	1231	CLA	C10-C11-C12-C13
21	3	616	CLA	C5-C6-C7-C8
21	5	607	CLA	C5-C6-C7-C8
21	6	615	CLA	O1D-CGD-O2D-CED
21	8	609	CLA	O1D-CGD-O2D-CED
24	A	5003	LHG	O1-C1-C2-O2
24	a	801	LHG	O1-C1-C2-O2
24	7	802	LHG	O1-C1-C2-O2
21	B	1021	CLA	C3-C5-C6-C7
21	B	1213	CLA	O1A-CGA-O2A-C1
21	F	1302	CLA	O1A-CGA-O2A-C1
21	B	1201	CLA	C15-C16-C17-C18
21	B	1221	CLA	C15-C16-C17-C18
21	A	1141	CLA	CBD-CGD-O2D-CED
21	a	604	CLA	CBD-CGD-O2D-CED
21	7	607	CLA	CBD-CGD-O2D-CED
21	8	612	CLA	CBD-CGD-O2D-CED
21	A	1012	CLA	C6-C7-C8-C10
21	A	1104	CLA	C6-C7-C8-C10
21	A	1126	CLA	C6-C7-C8-C10
21	B	1021	CLA	C12-C13-C15-C16
21	B	1203	CLA	C11-C10-C8-C7
21	B	1213	CLA	C6-C7-C8-C10
21	B	1214	CLA	C6-C7-C8-C10
21	B	1216	CLA	C11-C12-C13-C15
21	B	1220	CLA	C6-C7-C8-C10
21	3	613	CLA	C6-C7-C8-C10
21	3	616	CLA	C6-C7-C8-C10
21	7	604	CLA	C11-C12-C13-C15
38	6	619	CHL	C12-C13-C15-C16
38	7	613	CHL	C11-C10-C8-C7
38	7	613	CHL	C11-C12-C13-C15
21	B	1210	CLA	CBA-CGA-O2A-C1
21	a	602	CLA	CBA-CGA-O2A-C1
25	8	802	DGD	C2A-C1A-O1G-C1G
24	1	802	LHG	C9-C10-C11-C12
38	8	601	CHL	C4-C3-C5-C6
25	8	802	DGD	O6E-C5E-C6E-O5E
24	5	801	LHG	C31-C32-C33-C34
48	8	806	P5S	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
21	A	1105	CLA	C5-C6-C7-C8
21	B	1208	CLA	C10-C11-C12-C13
21	B	1228	CLA	C15-C16-C17-C18
21	7	612	CLA	C10-C11-C12-C13
21	A	1113	CLA	O1D-CGD-O2D-CED
21	6	601	CLA	O1D-CGD-O2D-CED
24	F	5001	LHG	C23-C24-C25-C26
24	7	801	LHG	C23-C24-C25-C26
30	8	810	PTY	C30-C31-C32-C33
23	B	4007	BCR	C9-C10-C11-C12
23	K	4002	BCR	C9-C10-C11-C12
23	K	4002	BCR	C13-C14-C15-C16
23	3	505	BCR	C13-C14-C15-C16
23	5	503	BCR	C13-C14-C15-C16
23	5	504	BCR	C9-C10-C11-C12
23	5	504	BCR	C15-C16-C17-C18
21	A	1110	CLA	O1D-CGD-O2D-CED
21	3	610	CLA	O1D-CGD-O2D-CED
21	5	604	CLA	O1D-CGD-O2D-CED
21	7	609	CLA	O1D-CGD-O2D-CED
21	B	1201	CLA	C3-C5-C6-C7
21	1	606	CLA	C3-C5-C6-C7
21	A	1112	CLA	C5-C6-C7-C8
21	B	1022	CLA	C13-C15-C16-C17
21	B	1205	CLA	C15-C16-C17-C18
21	B	1216	CLA	C5-C6-C7-C8
21	B	1231	CLA	C15-C16-C17-C18
21	3	604	CLA	C10-C11-C12-C13
21	5	612	CLA	C5-C6-C7-C8
21	7	604	CLA	C10-C11-C12-C13
21	B	1234	CLA	O1D-CGD-O2D-CED
21	8	608	CLA	O1D-CGD-O2D-CED
28	1	804	LMT	O5'-C5'-C6'-O6'
24	6	802	LHG	C7-C8-C9-C10
29	B	5004	PCW	C11-C12-C13-C14
43	8	803	DGA	CB1-CB2-CB3-CB4
46	8	808	4RF	C13-C14-C15-C16
21	4	608	CLA	O1A-CGA-O2A-C1
26	A	5007	3PH	O32-C31-O31-C3
21	B	1236	CLA	CBA-CGA-O2A-C1
21	A	1013	CLA	C5-C6-C7-C8
21	A	1133	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
21	A	1134	CLA	C8-C10-C11-C12
21	B	1021	CLA	C10-C11-C12-C13
21	B	1023	CLA	C8-C10-C11-C12
21	B	1203	CLA	C8-C10-C11-C12
21	B	1210	CLA	C8-C10-C11-C12
21	B	1210	CLA	C15-C16-C17-C18
21	B	1215	CLA	C5-C6-C7-C8
21	B	1226	CLA	C10-C11-C12-C13
21	B	1226	CLA	C15-C16-C17-C18
21	B	1235	CLA	C5-C6-C7-C8
21	3	605	CLA	C13-C15-C16-C17
21	3	606	CLA	C5-C6-C7-C8
21	3	607	CLA	C13-C15-C16-C17
21	4	610	CLA	C8-C10-C11-C12
21	6	604	CLA	C5-C6-C7-C8
21	7	603	CLA	C5-C6-C7-C8
38	7	613	CHL	C10-C11-C12-C13
21	A	1110	CLA	C2A-CAA-CBA-CGA
21	A	1114	CLA	C2A-CAA-CBA-CGA
21	A	1125	CLA	C2A-CAA-CBA-CGA
21	A	1129	CLA	C2A-CAA-CBA-CGA
21	A	1130	CLA	C2A-CAA-CBA-CGA
21	A	1140	CLA	C2A-CAA-CBA-CGA
21	B	1225	CLA	C2A-CAA-CBA-CGA
21	B	1232	CLA	C2A-CAA-CBA-CGA
21	B	1237	CLA	C2A-CAA-CBA-CGA
21	B	1204	CLA	C2A-CAA-CBA-CGA
21	F	1302	CLA	C2A-CAA-CBA-CGA
21	1	610	CLA	C2A-CAA-CBA-CGA
21	1	612	CLA	C2A-CAA-CBA-CGA
21	a	611	CLA	C2A-CAA-CBA-CGA
21	3	603	CLA	C2A-CAA-CBA-CGA
21	5	609	CLA	C2A-CAA-CBA-CGA
21	6	606	CLA	C2A-CAA-CBA-CGA
21	7	612	CLA	C2A-CAA-CBA-CGA
21	8	612	CLA	C2A-CAA-CBA-CGA
21	8	618	CLA	C2A-CAA-CBA-CGA
38	1	609	CHL	C2A-CAA-CBA-CGA
38	a	613	CHL	C2A-CAA-CBA-CGA
33	G	5002	ERG	C28-C24-C25-C26
21	B	1238	CLA	O1D-CGD-O2D-CED
23	G	4001	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	4	503	BCR	C10-C11-C12-C13
21	A	1104	CLA	C8-C10-C11-C12
21	A	1106	CLA	C15-C16-C17-C18
21	A	1126	CLA	C10-C11-C12-C13
21	A	1127	CLA	C8-C10-C11-C12
21	A	1101	CLA	C15-C16-C17-C18
21	B	1021	CLA	C8-C10-C11-C12
21	B	1201	CLA	C5-C6-C7-C8
21	B	1210	CLA	C13-C15-C16-C17
21	B	1212	CLA	C5-C6-C7-C8
21	B	1212	CLA	C10-C11-C12-C13
21	B	1239	CLA	C5-C6-C7-C8
21	B	1228	CLA	C13-C15-C16-C17
21	1	605	CLA	C15-C16-C17-C18
21	a	601	CLA	C5-C6-C7-C8
21	3	601	CLA	C15-C16-C17-C18
21	3	605	CLA	C5-C6-C7-C8
21	3	610	CLA	C5-C6-C7-C8
21	8	620	CLA	C10-C11-C12-C13
21	8	620	CLA	C15-C16-C17-C18
24	A	5002	LHG	C23-C24-C25-C26
24	5	801	LHG	C23-C24-C25-C26
24	7	803	LHG	C23-C24-C25-C26
24	8	801	LHG	C23-C24-C25-C26
30	B	5005	PTY	C8-C11-C12-C13
30	8	810	PTY	C8-C11-C12-C13
46	7	807	4RF	C41-C43-C44-C45
21	A	1130	CLA	O1D-CGD-O2D-CED
21	8	618	CLA	O1D-CGD-O2D-CED
21	A	1136	CLA	O1A-CGA-O2A-C1
21	4	603	CLA	O1A-CGA-O2A-C1
21	7	601	CLA	O1A-CGA-O2A-C1
21	8	611	CLA	O1A-CGA-O2A-C1
24	6	802	LHG	O10-C23-O8-C6
24	7	803	LHG	O10-C23-O8-C6
25	B	5003	DGD	O1A-C1A-O1G-C1G
21	A	1122	CLA	C3-C5-C6-C7
21	A	1125	CLA	C3-C5-C6-C7
21	8	609	CLA	C3-C5-C6-C7
21	A	1136	CLA	CBD-CGD-O2D-CED
24	F	5002	LHG	C24-C25-C26-C27
24	3	801	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
21	A	1128	CLA	O1D-CGD-O2D-CED
21	5	605	CLA	O1D-CGD-O2D-CED
38	a	610	CHL	O1D-CGD-O2D-CED
21	A	1106	CLA	C10-C11-C12-C13
21	A	1109	CLA	C13-C15-C16-C17
21	A	1110	CLA	C5-C6-C7-C8
21	A	1114	CLA	C10-C11-C12-C13
21	A	1130	CLA	C5-C6-C7-C8
21	A	1131	CLA	C5-C6-C7-C8
21	A	1135	CLA	C13-C15-C16-C17
21	B	1021	CLA	C13-C15-C16-C17
21	B	1206	CLA	C5-C6-C7-C8
21	B	1209	CLA	C5-C6-C7-C8
21	B	1213	CLA	C5-C6-C7-C8
21	B	1214	CLA	C5-C6-C7-C8
21	B	1216	CLA	C10-C11-C12-C13
21	B	1223	CLA	C8-C10-C11-C12
21	B	1231	CLA	C13-C15-C16-C17
21	B	1229	CLA	C13-C15-C16-C17
21	B	1204	CLA	C10-C11-C12-C13
21	1	606	CLA	C5-C6-C7-C8
21	1	608	CLA	C5-C6-C7-C8
21	1	612	CLA	C15-C16-C17-C18
21	3	601	CLA	C10-C11-C12-C13
21	3	605	CLA	C15-C16-C17-C18
21	4	610	CLA	C15-C16-C17-C18
21	7	601	CLA	C10-C11-C12-C13
21	7	603	CLA	C8-C10-C11-C12
21	7	603	CLA	C13-C15-C16-C17
21	8	603	CLA	C5-C6-C7-C8
35	a	804	LPX	C16-C17-C18-C19
24	B	5002	LHG	O2-C2-C3-O3
24	6	802	LHG	O2-C2-C3-O3
31	B	5007	LAP	O3-C14-C15-O4
21	B	1214	CLA	O1D-CGD-O2D-CED
21	B	1211	CLA	CBA-CGA-O2A-C1
25	A	5005	DGD	C8B-C9B-CAB-CBB
21	4	608	CLA	CBD-CGD-O2D-CED
21	A	1140	CLA	O1A-CGA-O2A-C1
21	8	618	CLA	O1A-CGA-O2A-C1
25	A	5005	DGD	C1A-C2A-C3A-C4A
46	7	807	4RF	C22-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
21	A	1122	CLA	C8-C10-C11-C12
21	A	1136	CLA	C5-C6-C7-C8
21	4	604	CLA	C8-C10-C11-C12
21	7	617	CLA	O1D-CGD-O2D-CED
44	6	806	SPH	C13-C14-C15-C16
21	3	601	CLA	O1D-CGD-O2D-CED
21	3	603	CLA	C5-C6-C7-C8
21	3	612	CLA	C10-C11-C12-C13
38	4	609	CHL	C5-C6-C7-C8
21	A	1135	CLA	O1A-CGA-O2A-C1
21	B	1210	CLA	O1A-CGA-O2A-C1
24	A	5001	LHG	C23-C24-C25-C26
24	B	5001	LHG	C23-C24-C25-C26
21	B	1202	CLA	O1D-CGD-O2D-CED
21	A	1108	CLA	C10-C11-C12-C13
21	A	1111	CLA	C8-C10-C11-C12
21	A	1122	CLA	C15-C16-C17-C18
21	B	1212	CLA	C15-C16-C17-C18
21	B	1226	CLA	C13-C15-C16-C17
21	B	1231	CLA	C5-C6-C7-C8
21	1	601	CLA	C5-C6-C7-C8
21	a	604	CLA	C15-C16-C17-C18
21	3	607	CLA	C15-C16-C17-C18
21	A	1131	CLA	CBA-CGA-O2A-C1
21	5	603	CLA	CBA-CGA-O2A-C1
30	8	810	PTY	C31-C30-O4-C1
24	1	801	LHG	C8-C7-O7-C5
21	5	606	CLA	O1A-CGA-O2A-C1
21	4	601	CLA	O1D-CGD-O2D-CED
21	B	1236	CLA	C4C-C3C-CAC-CBC
21	B	1202	CLA	C8-C10-C11-C12
21	A	1012	CLA	C3-C5-C6-C7
21	5	612	CLA	C3-C5-C6-C7
21	7	603	CLA	C3-C5-C6-C7
38	8	601	CHL	C3-C5-C6-C7
23	A	4003	BCR	C9-C10-C11-C12
23	L	4001	BCR	C19-C20-C21-C22
23	5	503	BCR	C15-C16-C17-C18
37	a	502	LUT	C9-C10-C11-C12
21	A	1012	CLA	C13-C15-C16-C17
24	4	802	LHG	C11-C12-C13-C14
24	7	801	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
24	B	5002	LHG	C7-C8-C9-C10
24	1	801	LHG	O9-C7-O7-C5
24	A	5001	LHG	C1-C2-C3-O3
24	B	5002	LHG	C1-C2-C3-O3
24	F	5002	LHG	C1-C2-C3-O3
24	a	801	LHG	C1-C2-C3-O3
24	7	802	LHG	C1-C2-C3-O3
31	B	5007	LAP	C13-C14-C15-O4
21	A	1139	CLA	C2A-CAA-CBA-CGA
21	G	1602	CLA	C2A-CAA-CBA-CGA
21	K	1404	CLA	C2A-CAA-CBA-CGA
21	1	611	CLA	C2A-CAA-CBA-CGA
38	5	613	CHL	C2A-CAA-CBA-CGA
21	A	1115	CLA	CBA-CGA-O2A-C1
21	B	1221	CLA	CBA-CGA-O2A-C1
21	A	1102	CLA	C15-C16-C17-C18
21	A	1134	CLA	C10-C11-C12-C13
21	B	1023	CLA	C10-C11-C12-C13
21	B	1023	CLA	C13-C15-C16-C17
21	B	1220	CLA	C8-C10-C11-C12
21	B	1238	CLA	C15-C16-C17-C18
21	1	603	CLA	C13-C15-C16-C17
21	4	603	CLA	C5-C6-C7-C8
21	7	603	CLA	C10-C11-C12-C13
21	B	1219	CLA	C3-C5-C6-C7
21	1	605	CLA	C3-C5-C6-C7
46	8	808	4RF	C02-C03-C04-C05
31	F	5003	LAP	C16-C17-N8-C18
31	F	5003	LAP	C16-C17-N8-C19
31	F	5003	LAP	C16-C17-N8-C20
21	B	1209	CLA	O1D-CGD-O2D-CED
21	B	1240	CLA	O1D-CGD-O2D-CED
38	a	613	CHL	O1D-CGD-O2D-CED
21	A	1128	CLA	C15-C16-C17-C18
21	A	1136	CLA	C15-C16-C17-C18
21	B	1215	CLA	C10-C11-C12-C13
21	B	1239	CLA	C13-C15-C16-C17
21	B	1204	CLA	C15-C16-C17-C18
21	3	603	CLA	C10-C11-C12-C13
21	3	606	CLA	C13-C15-C16-C17
21	4	604	CLA	C5-C6-C7-C8
21	5	604	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
21	6	601	CLA	C8-C10-C11-C12
21	6	603	CLA	C15-C16-C17-C18
21	8	618	CLA	C5-C6-C7-C8
38	8	601	CHL	C5-C6-C7-C8
21	A	1102	CLA	O1D-CGD-O2D-CED
21	A	1111	CLA	C10-C11-C12-C13
21	A	1133	CLA	C13-C15-C16-C17
21	A	1138	CLA	C8-C10-C11-C12
21	B	1240	CLA	C5-C6-C7-C8
21	B	1228	CLA	C5-C6-C7-C8
21	B	1207	CLA	C8-C10-C11-C12
21	K	1402	CLA	C8-C10-C11-C12
21	4	612	CLA	C10-C11-C12-C13
21	7	609	CLA	C10-C11-C12-C13
21	8	609	CLA	C5-C6-C7-C8
21	8	603	CLA	C10-C11-C12-C13
38	6	619	CHL	C10-C11-C12-C13
38	7	613	CHL	C5-C6-C7-C8
21	B	1223	CLA	O1D-CGD-O2D-CED
21	A	1133	CLA	CBA-CGA-O2A-C1
21	B	1220	CLA	CBA-CGA-O2A-C1
20	A	1011	CL0	C4-C3-C5-C6
38	8	601	CHL	C2-C3-C5-C6
21	3	603	CLA	O1D-CGD-O2D-CED
21	A	1136	CLA	C13-C15-C16-C17
21	B	1210	CLA	C10-C11-C12-C13
33	G	5002	ERG	C13-C17-C20-C22
24	B	5001	LHG	C8-C7-O7-C5
29	6	803	PCW	C32-C31-O2-C2
21	3	607	CLA	C14-C13-C15-C16
21	6	612	CLA	O1D-CGD-O2D-CED
21	A	1112	CLA	O1A-CGA-O2A-C1
21	a	602	CLA	O1A-CGA-O2A-C1
21	1	607	CLA	C2C-C3C-CAC-CBC
24	4	801	LHG	O9-C7-O7-C5
29	6	803	PCW	O31-C31-O2-C2
28	B	5006	LMT	C2'-C1'-O1'-C1
21	1	604	CLA	C5-C6-C7-C8
21	6	615	CLA	C10-C11-C12-C13
30	5	802	PTY	C30-C31-C32-C33
21	6	609	CLA	O1D-CGD-O2D-CED
21	7	612	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	B	1224	CLA	C13-C15-C16-C17
21	4	601	CLA	C5-C6-C7-C8
25	8	802	DGD	O1A-C1A-O1G-C1G
23	A	4001	BCR	C11-C10-C9-C34
23	A	4005	BCR	C11-C10-C9-C34
23	K	4002	BCR	C11-C10-C9-C34
23	3	503	BCR	C11-C10-C9-C34
23	6	504	BCR	C11-C10-C9-C34
38	5	613	CHL	C3-C5-C6-C7
46	8	808	4RF	C41-C43-C44-C45
21	8	609	CLA	C8-C10-C11-C12
23	A	4002	BCR	C36-C18-C19-C20
23	G	4001	BCR	C37-C22-C23-C24
23	5	504	BCR	C37-C22-C23-C24
23	6	503	BCR	C37-C22-C23-C24
35	a	804	LPX	C4-C3-O1-P1
37	5	505	LUT	C31-C32-C33-C40
37	6	502	LUT	C27-C28-C29-C39
47	7	504	C7Z	C27-C28-C29-C39
24	7	801	LHG	C32-C33-C34-C35
21	4	612	CLA	C13-C15-C16-C17
23	A	4004	BCR	C11-C12-C13-C14
23	B	4007	BCR	C17-C18-C19-C20
23	G	4001	BCR	C21-C22-C23-C24
23	3	504	BCR	C17-C18-C19-C20
23	5	504	BCR	C21-C22-C23-C24
23	6	503	BCR	C21-C22-C23-C24
23	7	503	BCR	C11-C12-C13-C14
34	J	4002	RRX	C21-C22-C23-C24
37	6	502	LUT	C27-C28-C29-C30
37	7	501	LUT	C27-C28-C29-C30
47	7	504	C7Z	C27-C28-C29-C30
21	B	1236	CLA	O1A-CGA-O2A-C1
24	7	803	LHG	C18-C19-C20-C21
21	A	1118	CLA	C2A-CAA-CBA-CGA
21	A	1141	CLA	C2A-CAA-CBA-CGA
21	B	1212	CLA	C2A-CAA-CBA-CGA
21	B	1214	CLA	C2A-CAA-CBA-CGA
21	B	1239	CLA	C2A-CAA-CBA-CGA
21	1	602	CLA	C2A-CAA-CBA-CGA
21	1	603	CLA	C2A-CAA-CBA-CGA
21	3	604	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
21	4	604	CLA	C2A-CAA-CBA-CGA
21	7	603	CLA	C2A-CAA-CBA-CGA
21	8	603	CLA	C2A-CAA-CBA-CGA
38	3	611	CHL	C2A-CAA-CBA-CGA
38	6	611	CHL	C2A-CAA-CBA-CGA
38	8	613	CHL	C2A-CAA-CBA-CGA
21	A	1108	CLA	C8-C10-C11-C12
21	A	1125	CLA	C13-C15-C16-C17
21	A	1132	CLA	C13-C15-C16-C17
24	F	5002	LHG	O1-C1-C2-C3
24	1	801	LHG	O1-C1-C2-C3
24	a	801	LHG	O1-C1-C2-C3
24	7	802	LHG	O1-C1-C2-C3
24	8	801	LHG	O1-C1-C2-C3
39	8	809	OLA	C1-C2-C3-C4
32	G	5001	SQD	C44-C45-O47-C7
43	8	803	DGA	CG1-CG2-OG2-CB1
37	3	502	LUT	C29-C30-C31-C32
21	A	1117	CLA	C16-C17-C18-C20
21	B	1224	CLA	C16-C17-C18-C19
21	B	1231	CLA	C16-C17-C18-C19
21	B	1235	CLA	C16-C17-C18-C19
21	B	1239	CLA	C16-C17-C18-C19
21	a	604	CLA	C16-C17-C18-C20
21	3	603	CLA	C16-C17-C18-C19
21	4	607	CLA	C6-C7-C8-C10
21	6	615	CLA	C16-C17-C18-C19
21	8	609	CLA	C11-C12-C13-C14
21	8	620	CLA	C16-C17-C18-C19
21	A	1137	CLA	O1D-CGD-O2D-CED
21	B	1211	CLA	O1A-CGA-O2A-C1
21	B	1221	CLA	O1A-CGA-O2A-C1
21	4	610	CLA	O1A-CGA-O2A-C1
21	B	1221	CLA	C3-C5-C6-C7
21	B	1208	CLA	C5-C6-C7-C8
23	A	4001	BCR	C11-C10-C9-C8
23	A	4005	BCR	C11-C10-C9-C8
23	K	4002	BCR	C11-C10-C9-C8
23	3	503	BCR	C11-C10-C9-C8
23	6	504	BCR	C11-C10-C9-C8
23	6	503	BCR	C11-C10-C9-C8
28	1	804	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
24	B	5002	LHG	C8-C7-O7-C5
24	A	5003	LHG	C23-C24-C25-C26
21	A	1102	CLA	C5-C6-C7-C8
21	A	1117	CLA	C13-C15-C16-C17
21	8	607	CLA	CBA-CGA-O2A-C1
21	A	1117	CLA	O1D-CGD-O2D-CED
40	a	504	QTB	C04-C05-C06-O07
40	3	506	QTB	C04-C05-C06-C08
21	7	604	CLA	O1D-CGD-O2D-CED
21	6	606	CLA	CBA-CGA-O2A-C1
21	A	1101	CLA	C8-C10-C11-C12
21	B	1213	CLA	C10-C11-C12-C13
21	B	1235	CLA	C8-C10-C11-C12
21	1	605	CLA	C13-C15-C16-C17
21	4	607	CLA	C5-C6-C7-C8
24	F	5002	LHG	C7-C8-C9-C10
21	B	1216	CLA	C3-C5-C6-C7
21	A	1012	CLA	C2-C1-O2A-CGA
21	A	1121	CLA	C2-C1-O2A-CGA
21	A	1123	CLA	C2-C1-O2A-CGA
21	A	1124	CLA	C2-C1-O2A-CGA
21	A	1137	CLA	C2-C1-O2A-CGA
21	A	1140	CLA	C2-C1-O2A-CGA
21	B	1208	CLA	C2-C1-O2A-CGA
21	B	1214	CLA	C2-C1-O2A-CGA
21	B	1216	CLA	C2-C1-O2A-CGA
21	G	1601	CLA	C2-C1-O2A-CGA
21	1	605	CLA	C2-C1-O2A-CGA
21	a	608	CLA	C2-C1-O2A-CGA
21	4	615	CLA	C2-C1-O2A-CGA
21	5	607	CLA	C2-C1-O2A-CGA
21	5	618	CLA	C2-C1-O2A-CGA
21	8	609	CLA	C2-C1-O2A-CGA
21	8	606	CLA	C2-C1-O2A-CGA
21	8	610	CLA	C2-C1-O2A-CGA
20	A	1011	CL0	C16-C17-C18-C20
21	A	1109	CLA	C16-C17-C18-C19
21	A	1118	CLA	C6-C7-C8-C10
21	A	1132	CLA	C16-C17-C18-C19
21	A	1139	CLA	C6-C7-C8-C10
21	B	1022	CLA	C16-C17-C18-C19
21	B	1021	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
21	B	1218	CLA	C6-C7-C8-C9
21	B	1238	CLA	C16-C17-C18-C19
21	1	605	CLA	C16-C17-C18-C19
21	6	603	CLA	C16-C17-C18-C19
21	6	615	CLA	C16-C17-C18-C20
21	7	612	CLA	C11-C12-C13-C14
21	8	609	CLA	C11-C12-C13-C15
21	8	603	CLA	C16-C17-C18-C20
21	8	620	CLA	C16-C17-C18-C20
38	4	609	CHL	C16-C17-C18-C20
38	7	613	CHL	C16-C17-C18-C20
21	5	603	CLA	O1A-CGA-O2A-C1
30	8	810	PTY	O30-C30-O4-C1
21	a	605	CLA	C15-C16-C17-C18
21	6	601	CLA	C5-C6-C7-C8
24	6	802	LHG	C29-C30-C31-C32
29	B	5004	PCW	C13-C14-C15-C16
21	4	605	CLA	CBA-CGA-O2A-C1
24	B	5002	LHG	C34-C35-C36-C37
24	B	5001	LHG	C29-C30-C31-C32
24	4	801	LHG	C28-C29-C30-C31
24	5	801	LHG	C12-C13-C14-C15
24	7	801	LHG	C30-C31-C32-C33
30	5	802	PTY	C11-C12-C13-C14
21	A	1133	CLA	O1D-CGD-O2D-CED
21	A	1101	CLA	O1D-CGD-O2D-CED
21	3	607	CLA	O1D-CGD-O2D-CED
31	F	5003	LAP	C1-C2-C3-C4
21	A	1125	CLA	C8-C10-C11-C12
21	B	1203	CLA	C10-C11-C12-C13
29	6	803	PCW	C12-C13-C14-C15
48	8	806	P5S	C39-C40-C41-C42
21	7	604	CLA	O1A-CGA-O2A-C1
21	B	1236	CLA	O1D-CGD-O2D-CED
21	B	1202	CLA	CBA-CGA-O2A-C1
21	1	604	CLA	CBA-CGA-O2A-C1
21	B	1212	CLA	C4C-C3C-CAC-CBC
24	4	801	LHG	C29-C30-C31-C32
24	5	801	LHG	C16-C17-C18-C19
24	6	801	LHG	C11-C12-C13-C14
24	7	802	LHG	C27-C28-C29-C30
28	1	804	LMT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
43	5	803	DGA	CB2-CB3-CB4-CB5
24	B	5001	LHG	O9-C7-O7-C5
24	B	5002	LHG	O1-C1-C2-O2
24	1	802	LHG	O1-C1-C2-O2
24	6	802	LHG	O1-C1-C2-O2
24	7	803	LHG	O1-C1-C2-O2
24	8	801	LHG	O1-C1-C2-O2
24	4	801	LHG	C27-C28-C29-C30
25	B	5003	DGD	C3A-C4A-C5A-C6A
30	8	810	PTY	C17-C18-C19-C20
44	6	806	SPH	C14-C15-C16-C17
21	A	1105	CLA	O1D-CGD-O2D-CED
21	A	1109	CLA	C4B-C3B-CAB-CBB
21	B	1022	CLA	C4B-C3B-CAB-CBB
21	B	1212	CLA	C4B-C3B-CAB-CBB
21	B	1214	CLA	C4B-C3B-CAB-CBB
21	B	1220	CLA	C4B-C3B-CAB-CBB
21	B	1240	CLA	C4B-C3B-CAB-CBB
21	G	1601	CLA	C4B-C3B-CAB-CBB
21	K	1404	CLA	C4B-C3B-CAB-CBB
21	L	1501	CLA	C4B-C3B-CAB-CBB
21	1	615	CLA	C4B-C3B-CAB-CBB
21	a	603	CLA	C4B-C3B-CAB-CBB
21	a	611	CLA	C4B-C3B-CAB-CBB
21	4	616	CLA	C4B-C3B-CAB-CBB
21	5	602	CLA	C4B-C3B-CAB-CBB
21	5	617	CLA	C4B-C3B-CAB-CBB
21	7	615	CLA	C4B-C3B-CAB-CBB
24	1	801	LHG	C23-C24-C25-C26
24	4	801	LHG	C23-C24-C25-C26
35	a	804	LPX	C6-C7-C8-C9
24	B	5002	LHG	C13-C14-C15-C16
24	6	802	LHG	C11-C12-C13-C14
24	7	801	LHG	C25-C26-C27-C28
20	A	1011	CL0	C16-C17-C18-C19
21	A	1117	CLA	C16-C17-C18-C19
21	A	1136	CLA	C16-C17-C18-C19
21	B	1211	CLA	C6-C7-C8-C9
21	B	1218	CLA	C6-C7-C8-C10
21	B	1231	CLA	C16-C17-C18-C20
21	B	1238	CLA	C16-C17-C18-C20
21	F	1302	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
21	F	1302	CLA	C6-C7-C8-C10
21	1	605	CLA	C16-C17-C18-C20
21	a	604	CLA	C16-C17-C18-C19
21	3	601	CLA	C16-C17-C18-C20
21	6	603	CLA	C16-C17-C18-C20
21	6	607	CLA	C6-C7-C8-C9
21	6	607	CLA	C6-C7-C8-C10
21	7	604	CLA	C16-C17-C18-C20
21	7	615	CLA	C6-C7-C8-C9
21	7	615	CLA	C6-C7-C8-C10
21	8	603	CLA	C16-C17-C18-C19
21	A	1131	CLA	O1A-CGA-O2A-C1
21	B	1220	CLA	O1A-CGA-O2A-C1
21	A	1113	CLA	C2A-CAA-CBA-CGA
21	a	608	CLA	C2A-CAA-CBA-CGA
21	5	607	CLA	C2A-CAA-CBA-CGA
24	A	5003	LHG	C16-C17-C18-C19
21	A	1105	CLA	C8-C10-C11-C12
21	A	1108	CLA	C13-C15-C16-C17
21	B	1201	CLA	C13-C15-C16-C17
21	8	610	CLA	C5-C6-C7-C8
38	6	619	CHL	C13-C15-C16-C17
24	4	801	LHG	C8-C7-O7-C5
24	6	801	LHG	C8-C7-O7-C5
24	7	802	LHG	C8-C7-O7-C5
24	8	801	LHG	C8-C7-O7-C5
26	A	5007	3PH	C22-C23-C24-C25
21	A	1105	CLA	C6-C7-C8-C10
21	1	607	CLA	C11-C12-C13-C15
21	1	608	CLA	C11-C10-C8-C7
22	B	2002	PQN	C21-C22-C23-C25
38	5	610	CHL	C12-C13-C15-C16
24	7	803	LHG	C9-C10-C11-C12
25	8	802	DGD	C3A-C4A-C5A-C6A
24	4	802	LHG	O2-C2-C3-O3
24	3	801	LHG	C7-C8-C9-C10
48	8	806	P5S	OXT-C-CA-N
21	B	1224	CLA	C10-C11-C12-C13
21	B	1237	CLA	C10-C11-C12-C13
21	6	603	CLA	C10-C11-C12-C13
24	A	5002	LHG	C34-C35-C36-C37
24	A	5003	LHG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
42	4	803	PLM	C9-CA-CB-CC
21	A	1115	CLA	O1A-CGA-O2A-C1
21	4	610	CLA	C3-C5-C6-C7
21	5	607	CLA	C3-C5-C6-C7
28	A	5008	LMT	C3'-C4'-O1B-C1B
21	A	1104	CLA	C3A-C2A-CAA-CBA
21	A	1107	CLA	C3A-C2A-CAA-CBA
21	A	1131	CLA	C3A-C2A-CAA-CBA
21	B	1201	CLA	C3A-C2A-CAA-CBA
21	B	1206	CLA	C3A-C2A-CAA-CBA
21	B	1208	CLA	C3A-C2A-CAA-CBA
21	B	1224	CLA	C3A-C2A-CAA-CBA
21	B	1228	CLA	C3A-C2A-CAA-CBA
21	B	1207	CLA	C3A-C2A-CAA-CBA
21	1	602	CLA	C3A-C2A-CAA-CBA
21	a	602	CLA	C3A-C2A-CAA-CBA
21	4	610	CLA	C3A-C2A-CAA-CBA
21	7	602	CLA	C3A-C2A-CAA-CBA
38	4	613	CHL	C3A-C2A-CAA-CBA
38	4	618	CHL	C3A-C2A-CAA-CBA
38	6	611	CHL	C3A-C2A-CAA-CBA
38	6	619	CHL	C3A-C2A-CAA-CBA
21	4	605	CLA	O1D-CGD-O2D-CED
24	5	801	LHG	C9-C10-C11-C12
43	5	803	DGA	CA4-CA5-CA6-CA7
21	A	1134	CLA	C5-C6-C7-C8
21	7	611	CLA	O1D-CGD-O2D-CED
23	5	503	BCR	C9-C10-C11-C12
23	8	503	BCR	C9-C10-C11-C12
37	a	503	LUT	C29-C30-C31-C32
37	3	501	LUT	C29-C30-C31-C32
21	A	1109	CLA	C16-C17-C18-C20
21	A	1136	CLA	C16-C17-C18-C20
21	B	1206	CLA	C6-C7-C8-C10
21	B	1211	CLA	C6-C7-C8-C10
21	B	1215	CLA	C11-C12-C13-C14
21	1	607	CLA	C16-C17-C18-C19
21	1	607	CLA	C16-C17-C18-C20
21	4	607	CLA	C6-C7-C8-C9
21	7	601	CLA	C11-C12-C13-C14
21	7	601	CLA	C11-C12-C13-C15
21	A	1133	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	3	801	LHG	C26-C27-C28-C29
31	K	5001	LAP	C3-C4-C5-C6
24	A	5003	LHG	C12-C13-C14-C15
24	6	801	LHG	C13-C14-C15-C16
24	8	801	LHG	C26-C27-C28-C29
32	G	5001	SQD	C13-C14-C15-C16
21	A	1120	CLA	O1D-CGD-O2D-CED
21	B	1209	CLA	CBA-CGA-O2A-C1
21	B	1226	CLA	CBA-CGA-O2A-C1
21	6	612	CLA	CBA-CGA-O2A-C1
24	A	5002	LHG	C24-C23-O8-C6
24	5	801	LHG	C4-C5-C6-O8
21	B	1219	CLA	C10-C11-C12-C13
24	F	5001	LHG	C16-C17-C18-C19
24	3	801	LHG	C31-C32-C33-C34
24	7	801	LHG	C33-C34-C35-C36
28	B	5006	LMT	C5-C6-C7-C8
30	5	802	PTY	C32-C33-C34-C35
32	G	5001	SQD	C11-C10-C9-C8
42	4	803	PLM	C5-C6-C7-C8
46	7	807	4RF	C08-C09-C10-C11
46	7	807	4RF	C12-C13-C14-C15
21	B	1215	CLA	C3-C5-C6-C7
24	6	802	LHG	C23-C24-C25-C26
31	B	5007	LAP	C1-C2-C3-C4
24	A	5002	LHG	C27-C28-C29-C30
24	A	5003	LHG	C13-C14-C15-C16
24	B	5002	LHG	C33-C34-C35-C36
24	F	5002	LHG	C25-C26-C27-C28
24	a	801	LHG	C30-C31-C32-C33
24	3	801	LHG	C27-C28-C29-C30
24	4	801	LHG	C13-C14-C15-C16
24	4	801	LHG	C26-C27-C28-C29
24	6	802	LHG	C28-C29-C30-C31
29	6	803	PCW	C14-C15-C16-C17
30	B	5005	PTY	C15-C16-C17-C18
21	7	602	CLA	C2C-C3C-CAC-CBC
24	8	801	LHG	C29-C30-C31-C32
30	3	802	PTY	C16-C17-C18-C19
35	a	804	LPX	C7-C8-C9-C10
44	6	806	SPH	C12-C13-C14-C15
21	6	604	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	B	5002	LHG	C31-C32-C33-C34
24	7	803	LHG	C17-C18-C19-C20
25	A	5005	DGD	C2A-C3A-C4A-C5A
31	F	5003	LAP	C3-C4-C5-C6
21	6	604	CLA	C8-C10-C11-C12
24	6	801	LHG	C27-C28-C29-C30
21	A	1118	CLA	C6-C7-C8-C9
21	B	1235	CLA	C16-C17-C18-C20
24	a	801	LHG	C23-C24-C25-C26
24	7	803	LHG	C7-C8-C9-C10
43	5	803	DGA	CB1-CB2-CB3-CB4
21	B	1213	CLA	C2B-C3B-CAB-CBB
21	B	1240	CLA	C2B-C3B-CAB-CBB
21	5	602	CLA	C2B-C3B-CAB-CBB
21	5	617	CLA	C2B-C3B-CAB-CBB
23	F	4001	BCR	C23-C24-C25-C30
23	J	4001	BCR	C1-C6-C7-C8
23	J	4001	BCR	C5-C6-C7-C8
23	K	4002	BCR	C23-C24-C25-C26
23	K	4002	BCR	C23-C24-C25-C30
23	L	4002	BCR	C1-C6-C7-C8
23	L	4002	BCR	C5-C6-C7-C8
23	L	4003	BCR	C23-C24-C25-C26
23	L	4003	BCR	C23-C24-C25-C30
23	5	503	BCR	C1-C6-C7-C8
23	5	503	BCR	C5-C6-C7-C8
23	6	504	BCR	C23-C24-C25-C26
23	6	504	BCR	C23-C24-C25-C30
23	6	503	BCR	C1-C6-C7-C8
23	6	503	BCR	C5-C6-C7-C8
34	J	4002	RRX	C23-C24-C25-C26
36	M	4001	ECH	C23-C24-C25-C26
37	a	501	LUT	C1-C6-C7-C8
47	7	504	C7Z	C1-C6-C7-C8
47	7	504	C7Z	C5-C6-C7-C8
24	A	5003	LHG	C11-C12-C13-C14
24	7	802	LHG	C11-C12-C13-C14
25	B	5003	DGD	C6A-C7A-C8A-C9A
38	a	606	CHL	CBA-CGA-O2A-C1
21	A	1124	CLA	C5-C6-C7-C8
21	1	604	CLA	C15-C16-C17-C18
28	B	5006	LMT	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
24	7	801	LHG	C11-C10-C9-C8
32	G	5001	SQD	C25-C26-C27-C28
44	6	806	SPH	C7-C8-C9-C10
21	A	1138	CLA	C2A-CAA-CBA-CGA
21	B	1023	CLA	C2A-CAA-CBA-CGA
21	5	603	CLA	C2A-CAA-CBA-CGA
21	5	604	CLA	C2A-CAA-CBA-CGA
21	6	603	CLA	C2A-CAA-CBA-CGA
38	8	604	CHL	C2A-CAA-CBA-CGA
38	1	609	CHL	C5-C6-C7-C8
43	8	803	DGA	CA5-CA6-CA7-CA8
24	5	801	LHG	C13-C14-C15-C16
31	K	5001	LAP	C2-C3-C4-C5
35	a	804	LPX	C15-C16-C17-C18
44	6	806	SPH	C10-C11-C12-C13
21	B	1202	CLA	O1A-CGA-O2A-C1
21	B	1209	CLA	O1A-CGA-O2A-C1
21	1	604	CLA	O1A-CGA-O2A-C1
21	6	606	CLA	O1A-CGA-O2A-C1
21	7	612	CLA	O1A-CGA-O2A-C1
21	5	614	CLA	O1A-CGA-O2A-C1
24	F	5001	LHG	C13-C14-C15-C16
30	8	810	PTY	C32-C33-C34-C35
46	8	807	4RF	C27-C28-C29-C30
24	B	5002	LHG	O9-C7-O7-C5
24	7	802	LHG	O9-C7-O7-C5
21	5	603	CLA	C11-C10-C8-C7
24	a	801	LHG	C28-C29-C30-C31
23	A	4001	BCR	C10-C11-C12-C13
23	A	4002	BCR	C10-C11-C12-C13
23	3	505	BCR	C10-C11-C12-C13
21	1	605	CLA	C5-C6-C7-C8
21	A	1012	CLA	C2-C3-C5-C6
21	A	1139	CLA	C6-C7-C8-C9
21	A	1140	CLA	C6-C7-C8-C9
24	B	5001	LHG	C28-C29-C30-C31
35	a	804	LPX	C14-C15-C16-C17
42	4	803	PLM	CA-CB-CC-CD
44	6	806	SPH	C11-C12-C13-C14
24	A	5003	LHG	C7-C8-C9-C10
24	a	801	LHG	C7-C8-C9-C10
20	A	1011	CL0	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	B	1224	CLA	C3-C5-C6-C7
21	B	1225	CLA	C14-C13-C15-C16
21	1	603	CLA	C11-C12-C13-C14
24	A	5002	LHG	C30-C31-C32-C33
24	1	802	LHG	C14-C15-C16-C17
24	6	801	LHG	C31-C32-C33-C34
24	8	801	LHG	C11-C12-C13-C14
30	8	810	PTY	C13-C14-C15-C16
21	7	604	CLA	C15-C16-C17-C18
21	1	607	CLA	O1D-CGD-O2D-CED
24	B	5001	LHG	C9-C10-C11-C12
24	4	801	LHG	C11-C12-C13-C14
25	A	5005	DGD	O6E-C1E-O5D-C6D
24	F	5001	LHG	C11-C12-C13-C14
24	1	802	LHG	C11-C12-C13-C14
24	7	801	LHG	C28-C29-C30-C31
25	B	5003	DGD	C9A-CAA-CBA-CCA
28	1	804	LMT	C3-C4-C5-C6
46	8	808	4RF	C45-C46-C47-C48
25	A	5005	DGD	C2E-C1E-O5D-C6D
28	1	804	LMT	C2'-C1'-O1'-C1
21	B	1022	CLA	C8-C10-C11-C12
21	1	604	CLA	C8-C10-C11-C12
21	6	615	CLA	C8-C10-C11-C12
24	7	802	LHG	C28-C29-C30-C31
24	7	803	LHG	C10-C11-C12-C13
28	B	5006	LMT	C4-C5-C6-C7
30	B	5005	PTY	C24-C25-C26-C27
24	1	801	LHG	C28-C29-C30-C31
24	4	801	LHG	C15-C16-C17-C18
24	4	801	LHG	C31-C32-C33-C34
31	B	5007	LAP	C3-C4-C5-C6
31	B	5007	LAP	C5-C6-C7-C8
21	A	1116	CLA	C10-C11-C12-C13
21	L	1502	CLA	C8-C10-C11-C12
21	4	610	CLA	C5-C6-C7-C8
21	a	612	CLA	C3-C5-C6-C7
21	3	604	CLA	C3-C5-C6-C7
21	B	1239	CLA	C16-C17-C18-C20
21	5	601	CLA	C11-C12-C13-C14
24	5	801	LHG	C34-C35-C36-C37
21	a	612	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	F	5002	LHG	C23-C24-C25-C26
24	F	5001	LHG	C7-C8-C9-C10
44	6	806	SPH	C15-C16-C17-C18
21	B	1205	CLA	C13-C15-C16-C17
21	7	603	CLA	C15-C16-C17-C18
24	8	801	LHG	O9-C7-O7-C5
21	3	602	CLA	O1A-CGA-O2A-C1
24	A	5003	LHG	C14-C15-C16-C17
24	B	5002	LHG	C26-C27-C28-C29
24	6	802	LHG	C26-C27-C28-C29
46	8	807	4RF	C32-C33-C34-C35
21	B	1239	CLA	C2C-C3C-CAC-CBC
23	A	4001	BCR	C37-C22-C23-C24
23	F	4001	BCR	C36-C18-C19-C20
23	6	504	BCR	C37-C22-C23-C24
36	M	4001	ECH	C36-C18-C19-C20
37	a	501	LUT	C7-C8-C9-C19
37	7	501	LUT	C27-C28-C29-C39
24	B	5002	LHG	C11-C10-C9-C8
30	8	810	PTY	C12-C13-C14-C15
30	3	802	PTY	C8-C11-C12-C13
24	5	801	LHG	C15-C16-C17-C18
21	6	603	CLA	C3-C5-C6-C7
23	A	4001	BCR	C21-C22-C23-C24
37	a	501	LUT	C7-C8-C9-C10
47	7	504	C7Z	C7-C8-C9-C10
21	A	1106	CLA	C2A-CAA-CBA-CGA
21	A	1101	CLA	C2A-CAA-CBA-CGA
21	4	612	CLA	C2A-CAA-CBA-CGA
21	A	1116	CLA	C11-C12-C13-C14
21	B	1209	CLA	C16-C17-C18-C19
21	B	1209	CLA	C16-C17-C18-C20
21	5	601	CLA	C11-C12-C13-C15
24	3	801	LHG	C13-C14-C15-C16
24	8	801	LHG	C25-C26-C27-C28
21	A	1012	CLA	C4-C3-C5-C6
21	A	1125	CLA	C4-C3-C5-C6
21	B	1239	CLA	C4-C3-C5-C6
38	6	610	CHL	C4-C3-C5-C6
24	1	802	LHG	C10-C11-C12-C13
24	3	801	LHG	C16-C17-C18-C19
30	5	802	PTY	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
21	A	1103	CLA	C8-C10-C11-C12
21	A	1140	CLA	C5-C6-C7-C8
24	6	801	LHG	C12-C13-C14-C15
21	B	1226	CLA	O1A-CGA-O2A-C1
21	B	1220	CLA	C10-C11-C12-C13
21	1	608	CLA	C8-C10-C11-C12
24	F	5001	LHG	C28-C29-C30-C31
24	5	801	LHG	C24-C25-C26-C27
29	B	5004	PCW	C12-C13-C14-C15
43	8	803	DGA	CB7-CB8-CB9-CAB
24	4	802	LHG	C7-C8-C9-C10
24	4	801	LHG	C18-C19-C20-C21
25	A	5005	DGD	C4B-C5B-C6B-C7B
24	6	801	LHG	O9-C7-O7-C5
48	8	806	P5S	O37-C2-C3-O16
21	A	1105	CLA	C2C-C3C-CAC-CBC
24	B	5001	LHG	C11-C12-C13-C14
21	1	603	CLA	C8-C10-C11-C12
21	3	603	CLA	C8-C10-C11-C12
21	A	1116	CLA	C11-C12-C13-C15
24	A	5002	LHG	C13-C14-C15-C16
24	A	5003	LHG	C26-C27-C28-C29
24	4	802	LHG	C9-C10-C11-C12
21	6	612	CLA	O1A-CGA-O2A-C1
25	B	5003	DGD	C3B-C4B-C5B-C6B
21	A	1106	CLA	C13-C15-C16-C17
21	A	1125	CLA	C15-C16-C17-C18
21	1	605	CLA	C8-C10-C11-C12
22	B	2002	PQN	C23-C25-C26-C27
38	6	619	CHL	C3-C5-C6-C7
24	5	801	LHG	O7-C5-C6-O8
24	7	803	LHG	C16-C17-C18-C19
46	7	807	4RF	C10-C11-C12-C13
46	7	807	4RF	C24-C25-C26-C27
21	A	1108	CLA	C5-C6-C7-C8
21	a	603	CLA	C10-C11-C12-C13
21	a	603	CLA	C15-C16-C17-C18
21	8	612	CLA	CBA-CGA-O2A-C1
24	B	5001	LHG	C33-C34-C35-C36
21	A	1139	CLA	C2-C1-O2A-CGA
21	B	1203	CLA	C2-C1-O2A-CGA
38	3	608	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	B	1206	CLA	C6-C7-C8-C9
21	3	603	CLA	C16-C17-C18-C20
38	4	609	CHL	C16-C17-C18-C19
21	A	1103	CLA	C4-C3-C5-C6
21	1	607	CLA	C10-C11-C12-C13
24	A	5002	LHG	C9-C10-C11-C12
28	A	5008	LMT	C5-C6-C7-C8
46	8	808	4RF	C08-C09-C10-C11
21	A	1012	CLA	C2A-CAA-CBA-CGA
21	A	1109	CLA	C2A-CAA-CBA-CGA
21	A	1116	CLA	C2A-CAA-CBA-CGA
21	B	1213	CLA	C2A-CAA-CBA-CGA
21	B	1217	CLA	C2A-CAA-CBA-CGA
21	7	605	CLA	C2A-CAA-CBA-CGA
38	4	618	CHL	C2A-CAA-CBA-CGA
30	7	804	PTY	C14-C15-C16-C17
43	8	803	DGA	CAB-CBB-CCB-CDB
24	B	5001	LHG	C31-C32-C33-C34
21	B	1223	CLA	C10-C11-C12-C13
24	F	5002	LHG	C28-C29-C30-C31
25	B	5003	DGD	CCA-CDA-CEA-CFA
24	A	5002	LHG	C11-C12-C13-C14
21	B	1224	CLA	C16-C17-C18-C20
21	A	1141	CLA	O1D-CGD-O2D-CED
24	3	801	LHG	O1-C1-C2-O2
24	7	801	LHG	O1-C1-C2-O2
38	a	606	CHL	O1A-CGA-O2A-C1
21	A	1112	CLA	C3-C5-C6-C7
21	A	1104	CLA	C1A-C2A-CAA-CBA
21	A	1106	CLA	C1A-C2A-CAA-CBA
21	A	1116	CLA	C1A-C2A-CAA-CBA
21	A	1131	CLA	C1A-C2A-CAA-CBA
21	A	1132	CLA	C1A-C2A-CAA-CBA
21	A	1139	CLA	C1A-C2A-CAA-CBA
21	B	1021	CLA	C1A-C2A-CAA-CBA
21	B	1206	CLA	C1A-C2A-CAA-CBA
21	B	1211	CLA	C1A-C2A-CAA-CBA
21	B	1215	CLA	C1A-C2A-CAA-CBA
21	B	1216	CLA	C1A-C2A-CAA-CBA
21	B	1217	CLA	C1A-C2A-CAA-CBA
21	B	1218	CLA	C1A-C2A-CAA-CBA
21	B	1219	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	B	1220	CLA	C1A-C2A-CAA-CBA
21	B	1232	CLA	C1A-C2A-CAA-CBA
21	B	1234	CLA	C1A-C2A-CAA-CBA
21	B	1207	CLA	C1A-C2A-CAA-CBA
21	F	1301	CLA	C1A-C2A-CAA-CBA
21	K	1402	CLA	C1A-C2A-CAA-CBA
21	1	601	CLA	C1A-C2A-CAA-CBA
21	1	604	CLA	C1A-C2A-CAA-CBA
21	1	608	CLA	C1A-C2A-CAA-CBA
21	1	612	CLA	C1A-C2A-CAA-CBA
21	a	601	CLA	C1A-C2A-CAA-CBA
21	a	607	CLA	C1A-C2A-CAA-CBA
21	3	601	CLA	C1A-C2A-CAA-CBA
21	3	607	CLA	C1A-C2A-CAA-CBA
21	3	618	CLA	C1A-C2A-CAA-CBA
21	4	601	CLA	C1A-C2A-CAA-CBA
21	4	610	CLA	C1A-C2A-CAA-CBA
21	4	611	CLA	C1A-C2A-CAA-CBA
21	4	612	CLA	C1A-C2A-CAA-CBA
21	4	616	CLA	C1A-C2A-CAA-CBA
21	4	617	CLA	C1A-C2A-CAA-CBA
21	4	608	CLA	C1A-C2A-CAA-CBA
21	5	601	CLA	C1A-C2A-CAA-CBA
21	5	606	CLA	C1A-C2A-CAA-CBA
21	5	617	CLA	C1A-C2A-CAA-CBA
21	6	601	CLA	C1A-C2A-CAA-CBA
21	6	606	CLA	C1A-C2A-CAA-CBA
21	6	617	CLA	C1A-C2A-CAA-CBA
21	7	602	CLA	C1A-C2A-CAA-CBA
21	7	605	CLA	C1A-C2A-CAA-CBA
21	7	606	CLA	C1A-C2A-CAA-CBA
21	7	607	CLA	C1A-C2A-CAA-CBA
21	7	610	CLA	C1A-C2A-CAA-CBA
21	7	612	CLA	C1A-C2A-CAA-CBA
21	8	608	CLA	C1A-C2A-CAA-CBA
21	8	612	CLA	C1A-C2A-CAA-CBA
21	A	1135	CLA	C10-C11-C12-C13
21	B	1202	CLA	C15-C16-C17-C18
24	F	5001	LHG	C9-C10-C11-C12
39	1	803	OLA	C12-C13-C14-C15
24	A	5002	LHG	O10-C23-O8-C6
25	B	5003	DGD	C2B-C3B-C4B-C5B

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Mol	Chain	Res	Type	Atoms
21	3	605	CLA	C8-C10-C11-C12
24	7	802	LHG	O6-C4-C5-C6
31	K	5001	LAP	O1-C13-C14-O3
24	6	802	LHG	C11-C10-C9-C8
21	A	1109	CLA	C11-C12-C13-C15
21	A	1117	CLA	C6-C7-C8-C10
21	A	1123	CLA	C11-C10-C8-C7
21	A	1126	CLA	C11-C10-C8-C7
21	A	1135	CLA	C11-C10-C8-C7
21	B	1023	CLA	C12-C13-C15-C16
21	B	1209	CLA	C6-C7-C8-C10
21	B	1209	CLA	C11-C10-C8-C7
21	B	1210	CLA	C11-C12-C13-C15
21	B	1214	CLA	C12-C13-C15-C16
21	B	1215	CLA	C11-C10-C8-C7
21	B	1223	CLA	C11-C10-C8-C7
21	B	1224	CLA	C11-C10-C8-C7
21	B	1231	CLA	C11-C10-C8-C7
21	1	606	CLA	C11-C10-C8-C7
21	1	607	CLA	C11-C10-C8-C7
21	a	604	CLA	C12-C13-C15-C16
21	3	603	CLA	C11-C10-C8-C7
21	3	612	CLA	C11-C10-C8-C7
21	4	610	CLA	C6-C7-C8-C10
21	6	604	CLA	C12-C13-C15-C16
21	6	615	CLA	C11-C10-C8-C7
21	8	620	CLA	C11-C12-C13-C15
38	4	609	CHL	C12-C13-C15-C16
38	8	604	CHL	C11-C10-C8-C7
24	B	5002	LHG	C16-C17-C18-C19
21	B	1207	CLA	C11-C12-C13-C15
21	3	604	CLA	C11-C12-C13-C15
21	7	617	CLA	C6-C7-C8-C10
21	A	1110	CLA	C10-C11-C12-C13
20	A	1011	CL0	O1A-CGA-O2A-C1
21	G	1602	CLA	CBA-CGA-O2A-C1
21	A	1108	CLA	C15-C16-C17-C18
21	A	1114	CLA	C13-C15-C16-C17
21	1	612	CLA	C8-C10-C11-C12
21	3	610	CLA	C10-C11-C12-C13
21	7	601	CLA	C8-C10-C11-C12
21	A	1109	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	B	1205	CLA	C4-C3-C5-C6
21	A	1103	CLA	C2-C3-C5-C6
21	A	1125	CLA	C2-C3-C5-C6
21	B	1205	CLA	C2-C3-C5-C6
21	B	1209	CLA	C2-C3-C5-C6
21	B	1231	CLA	C2-C3-C5-C6
21	8	620	CLA	C8-C10-C11-C12
24	4	802	LHG	C23-C24-C25-C26
21	A	1104	CLA	C2A-CAA-CBA-CGA
21	A	1135	CLA	C2A-CAA-CBA-CGA
21	B	1224	CLA	C2A-CAA-CBA-CGA
21	6	602	CLA	C3-C5-C6-C7
21	6	615	CLA	C2A-CAA-CBA-CGA
38	a	610	CHL	C2A-CAA-CBA-CGA
21	A	1012	CLA	C6-C7-C8-C9
21	A	1105	CLA	C6-C7-C8-C9
21	A	1109	CLA	C11-C12-C13-C14
21	A	1114	CLA	C11-C10-C8-C9
21	A	1116	CLA	C6-C7-C8-C9
21	A	1117	CLA	C6-C7-C8-C9
21	A	1122	CLA	C14-C13-C15-C16
21	A	1126	CLA	C11-C10-C8-C9
21	B	1202	CLA	C11-C10-C8-C9
21	B	1214	CLA	C14-C13-C15-C16
21	B	1215	CLA	C11-C10-C8-C9
21	B	1221	CLA	C14-C13-C15-C16
21	B	1223	CLA	C11-C10-C8-C9
21	B	1230	CLA	C6-C7-C8-C9
21	B	1237	CLA	C14-C13-C15-C16
21	B	1228	CLA	C6-C7-C8-C9
21	B	1204	CLA	C6-C7-C8-C9
21	B	1207	CLA	C6-C7-C8-C9
21	1	604	CLA	C6-C7-C8-C9
21	a	604	CLA	C14-C13-C15-C16
21	3	612	CLA	C6-C7-C8-C9
21	4	604	CLA	C6-C7-C8-C9
21	5	601	CLA	C11-C10-C8-C9
21	6	609	CLA	C11-C10-C8-C9
21	6	615	CLA	C11-C10-C8-C9
21	7	603	CLA	C11-C12-C13-C14
21	7	611	CLA	C11-C10-C8-C9
21	8	609	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
21	8	620	CLA	C11-C12-C13-C14
31	B	5007	LAP	O1-C13-C14-C15
38	1	609	CHL	C14-C13-C15-C16
42	6	804	PLM	C1-C2-C3-C4
37	5	505	LUT	C13-C14-C15-C35
32	7	805	SQD	C10-C11-C12-C13
21	1	608	CLA	CBA-CGA-O2A-C1
21	6	604	CLA	CBD-CGD-O2D-CED
25	A	5005	DGD	C2D-C1D-O3G-C3G
24	6	801	LHG	C10-C11-C12-C13
26	A	5007	3PH	C33-C34-C35-C36
30	7	804	PTY	C13-C14-C15-C16
46	8	807	4RF	C09-C10-C11-C12
24	7	802	LHG	C23-C24-C25-C26
24	A	5001	LHG	C4-C5-C6-O8
24	1	801	LHG	C4-C5-C6-O8
24	a	801	LHG	C4-C5-C6-O8
30	5	802	PTY	O4-C1-C6-C5
30	7	804	PTY	O4-C1-C6-C5
30	8	810	PTY	O4-C1-C6-C5
43	5	803	DGA	OG1-CG1-CG2-CG3
39	1	803	OLA	C10-C11-C12-C13
21	5	617	CLA	CBA-CGA-O2A-C1
24	3	801	LHG	C24-C23-O8-C6
24	3	801	LHG	C23-C24-C25-C26
21	6	604	CLA	C16-C17-C18-C20
24	F	5001	LHG	C26-C27-C28-C29
24	3	801	LHG	C11-C12-C13-C14
21	1	604	CLA	C2C-C3C-CAC-CBC
21	7	607	CLA	O1D-CGD-O2D-CED
24	F	5001	LHG	C10-C11-C12-C13
21	8	612	CLA	O1D-CGD-O2D-CED
23	B	4003	BCR	C11-C10-C9-C34
23	L	4003	BCR	C11-C10-C9-C34
23	6	503	BCR	C11-C10-C9-C34
21	a	601	CLA	C10-C11-C12-C13
24	8	801	LHG	C28-C29-C30-C31
21	B	1231	CLA	C4-C3-C5-C6
20	A	1011	CL0	C2-C3-C5-C6
21	A	1109	CLA	C2-C3-C5-C6
21	A	1126	CLA	C15-C16-C17-C18
21	6	604	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
23	B	4001	BCR	C37-C22-C23-C24
23	J	4001	BCR	C11-C12-C13-C35
23	3	503	BCR	C37-C22-C23-C24
37	a	502	LUT	C27-C28-C29-C39
47	7	504	C7Z	C7-C8-C9-C19
21	B	1204	CLA	C16-C17-C18-C20
23	B	4001	BCR	C21-C22-C23-C24
23	J	4001	BCR	C11-C12-C13-C14
23	I	4001	BCR	C11-C12-C13-C14
23	3	503	BCR	C21-C22-C23-C24
36	M	4001	ECH	C21-C22-C23-C24
37	5	505	LUT	C31-C32-C33-C34
21	A	1132	CLA	C5-C6-C7-C8
24	A	5002	LHG	C12-C13-C14-C15
24	A	5002	LHG	C31-C32-C33-C34
21	B	1235	CLA	C2A-CAA-CBA-CGA
21	7	609	CLA	C2A-CAA-CBA-CGA
21	8	609	CLA	C2A-CAA-CBA-CGA
21	7	611	CLA	C3-C5-C6-C7
24	1	802	LHG	C27-C28-C29-C30
21	B	1215	CLA	C8-C10-C11-C12
21	B	1226	CLA	C5-C6-C7-C8
24	6	802	LHG	C25-C26-C27-C28
46	8	808	4RF	C22-C24-C25-C26
25	B	5003	DGD	C4B-C5B-C6B-C7B
30	3	802	PTY	C15-C16-C17-C18
21	a	604	CLA	O1D-CGD-O2D-CED
21	4	608	CLA	O1D-CGD-O2D-CED
21	A	1013	CLA	CBA-CGA-O2A-C1
24	a	801	LHG	C24-C23-O8-C6
25	8	802	DGD	C3G-C2G-O2G-C1B
30	3	802	PTY	C5-C6-O7-C8
30	7	804	PTY	C1-C6-O7-C8
46	8	807	4RF	C39-C20-O21-C22
46	8	808	4RF	C39-C20-O21-C22
24	A	5003	LHG	C10-C11-C12-C13
24	B	5002	LHG	C11-C12-C13-C14
35	a	804	LPX	C17-C18-C19-C20
24	F	5001	LHG	C14-C15-C16-C17
24	1	802	LHG	C13-C14-C15-C16
24	6	801	LHG	C30-C31-C32-C33
23	B	4005	BCR	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
23	B	4006	BCR	C13-C14-C15-C16
23	I	4001	BCR	C9-C10-C11-C12
23	L	4003	BCR	C19-C20-C21-C22
34	J	4002	RRX	C19-C20-C21-C22
37	a	501	LUT	C29-C30-C31-C32
21	A	1132	CLA	C16-C17-C18-C20
21	B	1207	CLA	C11-C12-C13-C14
21	3	604	CLA	C11-C12-C13-C14
21	5	607	CLA	C6-C7-C8-C9
24	6	801	LHG	C16-C17-C18-C19
21	B	1231	CLA	C3-C5-C6-C7
21	A	1128	CLA	C10-C11-C12-C13
21	4	611	CLA	C5-C6-C7-C8
21	A	1116	CLA	CBA-CGA-O2A-C1
21	G	1601	CLA	CBA-CGA-O2A-C1
21	4	602	CLA	CBA-CGA-O2A-C1
46	7	807	4RF	C15-C16-O18-C19
24	A	5002	LHG	C28-C29-C30-C31
21	A	1124	CLA	O1D-CGD-O2D-CED
21	A	1136	CLA	O1D-CGD-O2D-CED
21	B	1209	CLA	C4-C3-C5-C6
21	B	1216	CLA	C4-C3-C5-C6
21	B	1230	CLA	C4-C3-C5-C6
21	A	1119	CLA	C2-C3-C5-C6
32	7	805	SQD	C15-C16-C17-C18
24	B	5001	LHG	C27-C28-C29-C30
21	B	1220	CLA	C11-C12-C13-C15
24	A	5002	LHG	C16-C17-C18-C19
24	1	801	LHG	C30-C31-C32-C33
24	A	5003	LHG	C11-C10-C9-C8
24	4	801	LHG	C12-C13-C14-C15
30	8	810	PTY	C33-C34-C35-C36
24	8	801	LHG	O7-C5-C6-O8
46	8	808	4RF	O18-C19-C20-O21
28	1	804	LMT	C4B-C5B-C6B-O6B
40	a	504	QTB	C04-C05-C06-C08
24	B	5002	LHG	C9-C10-C11-C12
24	B	5002	LHG	C27-C28-C29-C30
24	5	801	LHG	C19-C20-C21-C22
31	F	5003	LAP	C9-C10-C11-C12
31	K	5001	LAP	C6-C7-C8-C9
46	8	808	4RF	C46-C47-C48-C49

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Mol	Chain	Res	Type	Atoms
21	B	1238	CLA	C2A-CAA-CBA-CGA
21	6	609	CLA	C2A-CAA-CBA-CGA
21	B	1228	CLA	C3-C5-C6-C7
21	6	609	CLA	C3-C5-C6-C7
24	1	801	LHG	C9-C10-C11-C12
24	6	802	LHG	C30-C31-C32-C33
21	A	1114	CLA	C5-C6-C7-C8
21	B	1204	CLA	C13-C15-C16-C17
21	A	1107	CLA	C2-C1-O2A-CGA
24	F	5001	LHG	C25-C26-C27-C28
24	4	801	LHG	C16-C17-C18-C19
24	8	801	LHG	C24-C25-C26-C27
21	A	1127	CLA	CBA-CGA-O2A-C1
21	A	1129	CLA	CBA-CGA-O2A-C1
21	7	617	CLA	CBA-CGA-O2A-C1
31	B	5007	LAP	C2-C1-O1-C13
46	7	807	4RF	C25-C26-C27-C28
24	B	5001	LHG	C25-C26-C27-C28
42	4	803	PLM	C7-C8-C9-CA
46	7	807	4RF	C24-C22-O21-C20
24	1	802	LHG	C19-C20-C21-C22
21	B	1239	CLA	C4C-C3C-CAC-CBC
24	4	801	LHG	C19-C20-C21-C22
24	1	802	LHG	C23-C24-C25-C26
46	8	808	4RF	C31-C32-C33-C34
20	A	1011	CL0	C13-C15-C16-C17
21	B	1223	CLA	C5-C6-C7-C8
21	7	611	CLA	C8-C10-C11-C12
37	1	502	LUT	C29-C30-C31-C32
21	B	1216	CLA	C14-C13-C15-C16
21	A	1113	CLA	C4-C3-C5-C6
21	A	1118	CLA	C4-C3-C5-C6
21	A	1119	CLA	C4-C3-C5-C6
21	A	1139	CLA	C4-C3-C5-C6
21	B	1203	CLA	C4-C3-C5-C6
21	B	1225	CLA	C4-C3-C5-C6
21	8	603	CLA	C4-C3-C5-C6
21	8	610	CLA	C4-C3-C5-C6
21	B	1204	CLA	C2-C3-C5-C6
21	B	1216	CLA	CBA-CGA-O2A-C1
21	B	1235	CLA	CBA-CGA-O2A-C1
21	L	1502	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
35	J	5001	LPX	C7-C6-O6-C5
21	A	1126	CLA	C5-C6-C7-C8
21	1	611	CLA	C5-C6-C7-C8
21	a	603	CLA	C13-C15-C16-C17
21	5	601	CLA	C8-C10-C11-C12
21	7	612	CLA	C8-C10-C11-C12
24	5	801	LHG	C29-C30-C31-C32
24	7	803	LHG	C25-C26-C27-C28
24	A	5001	LHG	O1-C1-C2-O2
21	A	1109	CLA	C11-C10-C8-C9
21	A	1123	CLA	C11-C10-C8-C9
21	A	1133	CLA	C11-C12-C13-C14
21	A	1134	CLA	C11-C10-C8-C9
21	A	1135	CLA	C11-C10-C8-C9
21	A	1138	CLA	C14-C13-C15-C16
21	B	1022	CLA	C6-C7-C8-C9
21	B	1023	CLA	C14-C13-C15-C16
21	B	1203	CLA	C11-C10-C8-C9
21	B	1209	CLA	C6-C7-C8-C9
21	B	1213	CLA	C11-C10-C8-C9
21	B	1214	CLA	C6-C7-C8-C9
21	B	1217	CLA	C6-C7-C8-C9
21	B	1231	CLA	C11-C10-C8-C9
21	K	1402	CLA	C6-C7-C8-C9
21	1	606	CLA	C11-C10-C8-C9
21	3	612	CLA	C11-C10-C8-C9
21	4	610	CLA	C6-C7-C8-C9
21	4	610	CLA	C14-C13-C15-C16
21	5	603	CLA	C6-C7-C8-C9
21	6	603	CLA	C6-C7-C8-C9
21	7	609	CLA	C11-C10-C8-C9
21	7	603	CLA	C11-C10-C8-C9
21	8	609	CLA	C6-C7-C8-C9
21	8	606	CLA	C11-C10-C8-C9
31	K	5001	LAP	O1-C13-C14-C15
38	1	609	CHL	C11-C12-C13-C14
38	6	619	CHL	C11-C10-C8-C9
38	7	613	CHL	C11-C12-C13-C14
38	8	604	CHL	C11-C10-C8-C9
28	A	5008	LMT	C2-C3-C4-C5
30	7	804	PTY	C11-C12-C13-C14
21	a	604	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
21	8	603	CLA	C15-C16-C17-C18
21	A	1105	CLA	C4B-C3B-CAB-CBB
21	A	1131	CLA	C4B-C3B-CAB-CBB
21	A	1132	CLA	C4B-C3B-CAB-CBB
21	B	1213	CLA	C4B-C3B-CAB-CBB
21	B	1224	CLA	C4B-C3B-CAB-CBB
21	K	1401	CLA	C4B-C3B-CAB-CBB
21	1	612	CLA	C4B-C3B-CAB-CBB
21	3	605	CLA	C4B-C3B-CAB-CBB
21	5	606	CLA	C4B-C3B-CAB-CBB
21	7	607	CLA	C4B-C3B-CAB-CBB
21	8	615	CLA	C4B-C3B-CAB-CBB
48	8	806	P5S	O37-C38-C39-C40
21	B	1219	CLA	C5-C6-C7-C8
24	1	802	LHG	C28-C29-C30-C31
24	4	801	LHG	C35-C36-C37-C38
46	8	807	4RF	C25-C26-C27-C28
21	A	1127	CLA	C15-C16-C17-C18
24	6	801	LHG	C26-C27-C28-C29
30	B	5005	PTY	C11-C12-C13-C14
42	6	804	PLM	CA-CB-CC-CD
43	5	803	DGA	CA6-CA7-CA8-CA9
24	4	801	LHG	O6-C4-C5-C6
24	6	802	LHG	O6-C4-C5-C6
30	B	5005	PTY	O14-C5-C6-C1
30	3	802	PTY	O14-C5-C6-C1
30	7	804	PTY	O14-C5-C6-C1
48	8	806	P5S	C1-C2-C3-O16
31	F	5003	LAP	C2-C3-C4-C5
21	A	1102	CLA	C11-C12-C13-C15
21	A	1106	CLA	C12-C13-C15-C16
21	A	1110	CLA	C11-C10-C8-C7
21	A	1111	CLA	C12-C13-C15-C16
21	A	1114	CLA	C11-C10-C8-C7
21	A	1117	CLA	C11-C12-C13-C15
21	A	1119	CLA	C6-C7-C8-C10
21	A	1122	CLA	C12-C13-C15-C16
21	A	1138	CLA	C12-C13-C15-C16
21	B	1201	CLA	C11-C10-C8-C7
21	B	1202	CLA	C11-C10-C8-C7
21	B	1213	CLA	C11-C10-C8-C7
21	B	1217	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
21	B	1230	CLA	C6-C7-C8-C10
21	B	1234	CLA	C6-C7-C8-C10
21	B	1237	CLA	C12-C13-C15-C16
21	B	1228	CLA	C6-C7-C8-C10
21	B	1204	CLA	C6-C7-C8-C10
21	B	1207	CLA	C6-C7-C8-C10
21	K	1402	CLA	C6-C7-C8-C10
21	1	604	CLA	C6-C7-C8-C10
21	a	604	CLA	C11-C12-C13-C15
21	3	610	CLA	C6-C7-C8-C10
21	4	604	CLA	C6-C7-C8-C10
21	4	610	CLA	C12-C13-C15-C16
21	4	611	CLA	C6-C7-C8-C10
21	5	601	CLA	C11-C10-C8-C7
21	5	603	CLA	C6-C7-C8-C10
21	6	603	CLA	C6-C7-C8-C10
21	6	603	CLA	C12-C13-C15-C16
21	6	609	CLA	C11-C10-C8-C7
21	7	609	CLA	C11-C10-C8-C7
21	7	603	CLA	C11-C10-C8-C7
21	7	603	CLA	C11-C12-C13-C15
21	7	611	CLA	C11-C10-C8-C7
21	7	612	CLA	C11-C10-C8-C7
21	8	609	CLA	C11-C10-C8-C7
21	8	606	CLA	C11-C10-C8-C7
21	8	618	CLA	C11-C10-C8-C7
22	A	2001	PQN	C21-C22-C23-C25
38	1	609	CHL	C12-C13-C15-C16
21	A	1013	CLA	C15-C16-C17-C18
21	A	1131	CLA	C10-C11-C12-C13
21	A	1101	CLA	C5-C6-C7-C8
22	A	2001	PQN	C25-C26-C27-C28
24	1	801	LHG	C31-C32-C33-C34
21	A	1102	CLA	C13-C15-C16-C17
21	3	605	CLA	C10-C11-C12-C13
21	B	1201	CLA	C16-C17-C18-C19
21	8	618	CLA	C11-C12-C13-C14
24	3	801	LHG	C9-C10-C11-C12
21	8	607	CLA	O1A-CGA-O2A-C1
21	1	608	CLA	O1A-CGA-O2A-C1
31	B	5007	LAP	C9-C10-C11-C12
21	A	1127	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	A	1101	CLA	C3A-C2A-CAA-CBA
21	B	1021	CLA	C3A-C2A-CAA-CBA
21	B	1234	CLA	C3A-C2A-CAA-CBA
21	B	1239	CLA	C3A-C2A-CAA-CBA
21	F	1301	CLA	C3A-C2A-CAA-CBA
21	G	1601	CLA	C3A-C2A-CAA-CBA
21	L	1501	CLA	C3A-C2A-CAA-CBA
21	7	605	CLA	C3A-C2A-CAA-CBA
21	8	609	CLA	C3A-C2A-CAA-CBA
21	K	1402	CLA	C5-C6-C7-C8
21	7	617	CLA	C5-C6-C7-C8
22	A	2001	PQN	C15-C16-C17-C18
21	G	1601	CLA	CAA-CBA-CGA-O2A
30	5	802	PTY	C38-C39-C40-C41
21	A	1117	CLA	C10-C11-C12-C13
21	A	1135	CLA	C15-C16-C17-C18
21	8	603	CLA	C13-C15-C16-C17
24	B	5001	LHG	C35-C36-C37-C38
21	7	611	CLA	C2C-C3C-CAC-CBC
24	B	5001	LHG	C16-C17-C18-C19
23	A	4004	BCR	C13-C14-C15-C16
23	A	4005	BCR	C19-C20-C21-C22
23	B	4002	BCR	C15-C16-C17-C18
23	B	4003	BCR	C19-C20-C21-C22
23	K	4001	BCR	C13-C14-C15-C16
23	K	4002	BCR	C19-C20-C21-C22
23	I	4001	BCR	C19-C20-C21-C22
23	3	503	BCR	C13-C14-C15-C16
23	6	503	BCR	C19-C20-C21-C22
23	7	503	BCR	C15-C16-C17-C18
37	a	502	LUT	C29-C30-C31-C32
37	6	501	LUT	C29-C30-C31-C32
37	6	502	LUT	C29-C30-C31-C32
37	7	501	LUT	C29-C30-C31-C32
37	8	502	LUT	C29-C30-C31-C32
21	A	1110	CLA	C11-C12-C13-C14
21	4	608	CLA	C4-C3-C5-C6
40	3	506	QTB	C09-C10-C11-C17
21	A	1013	CLA	O1A-CGA-O2A-C1
21	4	602	CLA	O1A-CGA-O2A-C1
24	7	803	LHG	C27-C28-C29-C30
30	5	802	PTY	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
25	8	802	DGD	C4E-C5E-C6E-O5E
46	8	808	4RF	C50-C51-C52-C53
24	6	801	LHG	C1-C2-C3-O3
21	A	1119	CLA	C2A-CAA-CBA-CGA
24	7	803	LHG	C13-C14-C15-C16
24	A	5002	LHG	C4-C5-C6-O8
24	A	5003	LHG	C4-C5-C6-O8
24	B	5001	LHG	C4-C5-C6-O8
24	F	5001	LHG	C4-C5-C6-O8
24	1	802	LHG	C4-C5-C6-O8
24	4	802	LHG	C4-C5-C6-O8
24	6	802	LHG	C4-C5-C6-O8
24	8	801	LHG	C4-C5-C6-O8
25	B	5003	DGD	O1G-C1G-C2G-C3G
32	7	805	SQD	C44-C45-C46-O48
21	A	1124	CLA	C3-C5-C6-C7
21	A	1132	CLA	C3-C5-C6-C7
21	7	606	CLA	C3-C5-C6-C7
24	B	5001	LHG	C30-C31-C32-C33
21	8	618	CLA	C11-C12-C13-C15
21	A	1104	CLA	C10-C11-C12-C13
21	A	1137	CLA	C10-C11-C12-C13
21	1	612	CLA	C10-C11-C12-C13
21	a	605	CLA	C5-C6-C7-C8
24	F	5002	LHG	C9-C10-C11-C12
24	7	803	LHG	C24-C25-C26-C27
30	3	802	PTY	C12-C13-C14-C15
39	1	803	OLA	C3-C4-C5-C6
46	8	808	4RF	C44-C45-C46-C47
48	8	806	P5S	O-C-CA-N
25	8	802	DGD	O6D-C5D-C6D-O5D
21	A	1121	CLA	C4-C3-C5-C6
21	A	1134	CLA	C4-C3-C5-C6
21	A	1101	CLA	C4-C3-C5-C6
21	B	1234	CLA	C4-C3-C5-C6
21	B	1229	CLA	C4-C3-C5-C6
21	B	1204	CLA	C4-C3-C5-C6
21	1	607	CLA	C4-C3-C5-C6
32	G	5001	SQD	C23-C24-C25-C26
21	a	608	CLA	CBA-CGA-O2A-C1
21	A	1113	CLA	C2-C3-C5-C6
21	A	1118	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	B	1225	CLA	C2-C3-C5-C6
24	3	801	LHG	O10-C23-O8-C6
21	A	1140	CLA	C3-C5-C6-C7
24	6	801	LHG	C35-C36-C37-C38
21	7	604	CLA	C16-C17-C18-C19
24	A	5002	LHG	C7-C8-C9-C10
24	A	5002	LHG	O6-C4-C5-O7
24	6	802	LHG	O6-C4-C5-O7
21	8	615	CLA	C2B-C3B-CAB-CBB
23	A	4001	BCR	C1-C6-C7-C8
23	A	4003	BCR	C1-C6-C7-C8
23	A	4004	BCR	C1-C6-C7-C8
23	A	4005	BCR	C1-C6-C7-C8
23	B	4001	BCR	C23-C24-C25-C30
23	G	4001	BCR	C1-C6-C7-C8
23	L	4001	BCR	C1-C6-C7-C8
23	5	504	BCR	C23-C24-C25-C30
23	6	503	BCR	C23-C24-C25-C30
23	7	503	BCR	C1-C6-C7-C8
37	1	501	LUT	C1-C6-C7-C8
37	1	503	LUT	C1-C6-C7-C8
37	6	502	LUT	C1-C6-C7-C8
30	B	5005	PTY	C13-C14-C15-C16
39	8	809	OLA	C6-C7-C8-C9
39	1	803	OLA	C13-C14-C15-C16
24	A	5003	LHG	C2-C3-O3-P
24	3	801	LHG	C2-C3-O3-P
21	5	603	CLA	C11-C10-C8-C9
24	A	5003	LHG	C15-C16-C17-C18
24	F	5001	LHG	C11-C10-C9-C8
44	6	806	SPH	O1-C1-C2-N2
46	7	807	4RF	O17-C16-O18-C19
24	5	801	LHG	C10-C11-C12-C13
21	1	604	CLA	C10-C11-C12-C13
21	a	612	CLA	C5-C6-C7-C8
30	5	802	PTY	C15-C16-C17-C18
46	8	807	4RF	C11-C12-C13-C14
21	4	605	CLA	O1A-CGA-O2A-C1
38	7	613	CHL	C16-C17-C18-C19
38	8	601	CHL	C11-C12-C13-C14
38	6	610	CHL	CAA-CBA-CGA-O2A
21	3	616	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
21	A	1127	CLA	C5-C6-C7-C8
21	A	1138	CLA	C5-C6-C7-C8
24	A	5003	LHG	O7-C5-C6-O8
24	B	5002	LHG	O7-C5-C6-O8
24	6	802	LHG	O7-C5-C6-O8
24	6	801	LHG	O7-C5-C6-O8
29	B	5004	PCW	O2-C2-C3-O3
32	G	5001	SQD	O6-C44-C45-O47
46	8	807	4RF	O18-C19-C20-O21
46	8	808	4RF	O21-C20-C39-O40
38	8	601	CHL	C2C-C3C-CAC-CBC
28	B	5006	LMT	C5'-C4'-O1B-C1B
33	G	5002	ERG	C28-C24-C25-C27
21	4	603	CLA	C4-C3-C5-C6
23	3	503	BCR	C10-C11-C12-C13
21	A	1109	CLA	C5-C6-C7-C8
21	A	1139	CLA	C2-C3-C5-C6
21	A	1101	CLA	C2-C3-C5-C6
21	B	1234	CLA	C2-C3-C5-C6
21	4	603	CLA	C2-C3-C5-C6
39	8	809	OLA	C15-C16-C17-C18
21	B	1215	CLA	C11-C12-C13-C15
21	B	1204	CLA	C16-C17-C18-C19
21	7	612	CLA	C11-C12-C13-C15
32	G	5001	SQD	C7-C8-C9-C10
21	A	1116	CLA	O1A-CGA-O2A-C1
21	A	1117	CLA	C11-C12-C13-C14
21	A	1119	CLA	C6-C7-C8-C9
21	A	1133	CLA	C14-C13-C15-C16
21	B	1224	CLA	C14-C13-C15-C16
21	3	606	CLA	C14-C13-C15-C16
21	5	612	CLA	C11-C10-C8-C9
22	A	2001	PQN	C21-C22-C23-C24
21	A	1111	CLA	C15-C16-C17-C18
26	A	5007	3PH	O21-C21-C22-C23
35	a	804	LPX	C13-C14-C15-C16
21	B	1021	CLA	C16-C17-C18-C20
21	3	601	CLA	C16-C17-C18-C19
21	4	607	CLA	C2A-CAA-CBA-CGA
29	6	803	PCW	C34-C35-C36-C37
32	G	5001	SQD	C16-C17-C18-C19
21	A	1127	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	G	1601	CLA	O1A-CGA-O2A-C1
21	5	617	CLA	O1A-CGA-O2A-C1
21	B	1224	CLA	C15-C16-C17-C18
21	B	1228	CLA	C8-C10-C11-C12
21	5	604	CLA	C10-C11-C12-C13
21	B	1021	CLA	CBA-CGA-O2A-C1
21	B	1203	CLA	CBA-CGA-O2A-C1
30	3	802	PTY	C31-C30-O4-C1
30	7	804	PTY	C31-C30-O4-C1
38	7	613	CHL	CBA-CGA-O2A-C1
21	7	612	CLA	C4-C3-C5-C6
23	B	4006	BCR	C15-C16-C17-C18
23	L	4001	BCR	C9-C10-C11-C12
37	1	503	LUT	C29-C30-C31-C32
37	5	502	LUT	C29-C30-C31-C32
24	8	801	LHG	C30-C31-C32-C33
21	B	1203	CLA	C2-C3-C5-C6
21	B	1229	CLA	C2-C3-C5-C6
21	8	603	CLA	C2-C3-C5-C6
21	8	610	CLA	C2-C3-C5-C6
21	a	603	CLA	C16-C17-C18-C20
24	A	5001	LHG	C8-C7-O7-C5
21	7	604	CLA	C8-C10-C11-C12
31	B	5007	LAP	C11-C10-C9-C8
21	4	610	CLA	C10-C11-C12-C13
25	A	5005	DGD	O6E-C5E-C6E-O5E
24	F	5001	LHG	C1-C2-C3-O3
24	8	801	LHG	C1-C2-C3-O3
24	B	5001	LHG	C26-C27-C28-C29
24	7	803	LHG	C11-C12-C13-C14
23	B	4005	BCR	C11-C10-C9-C34
24	a	801	LHG	O10-C23-O8-C6
21	B	1223	CLA	C3-C5-C6-C7
21	A	1111	CLA	CBA-CGA-O2A-C1
21	B	1222	CLA	CBA-CGA-O2A-C1
21	B	1225	CLA	CBA-CGA-O2A-C1
21	6	607	CLA	C5-C6-C7-C8
21	8	620	CLA	C13-C15-C16-C17
24	A	5002	LHG	C18-C19-C20-C21
24	A	5001	LHG	O6-C4-C5-C6
24	B	5002	LHG	O6-C4-C5-C6
24	F	5002	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
29	6	803	PCW	O3P-C1-C2-C3
21	A	1140	CLA	C6-C7-C8-C10
21	B	1022	CLA	C16-C17-C18-C20
21	5	607	CLA	C6-C7-C8-C10
21	6	604	CLA	C16-C17-C18-C19
21	7	617	CLA	C6-C7-C8-C9
30	3	802	PTY	O30-C30-O4-C1
21	A	1128	CLA	C8-C10-C11-C12
23	B	4004	BCR	C7-C8-C9-C34
36	M	4001	ECH	C37-C22-C23-C24
21	A	1104	CLA	C11-C10-C8-C7
21	A	1106	CLA	C11-C10-C8-C7
21	A	1125	CLA	C12-C13-C15-C16
21	A	1126	CLA	C12-C13-C15-C16
21	A	1131	CLA	C6-C7-C8-C10
21	A	1132	CLA	C6-C7-C8-C10
21	A	1136	CLA	C12-C13-C15-C16
21	A	1137	CLA	C6-C7-C8-C10
21	B	1219	CLA	C6-C7-C8-C10
21	B	1221	CLA	C12-C13-C15-C16
21	B	1239	CLA	C12-C13-C15-C16
21	a	604	CLA	C11-C10-C8-C7
21	8	620	CLA	C11-C10-C8-C7
38	6	619	CHL	C11-C10-C8-C7
38	8	604	CHL	C11-C12-C13-C15
24	B	5002	LHG	C25-C26-C27-C28
24	A	5002	LHG	C11-C10-C9-C8
24	4	801	LHG	C25-C26-C27-C28
46	8	807	4RF	C10-C11-C12-C13
21	4	604	CLA	C10-C11-C12-C13
21	8	606	CLA	C5-C6-C7-C8
43	5	803	DGA	CB3-CB4-CB5-CB6
23	B	4004	BCR	C7-C8-C9-C10
23	F	4001	BCR	C17-C18-C19-C20
36	M	4001	ECH	C17-C18-C19-C20
21	B	1224	CLA	CBA-CGA-O2A-C1
24	7	802	LHG	C10-C11-C12-C13
21	A	1129	CLA	O1A-CGA-O2A-C1
21	a	608	CLA	O1A-CGA-O2A-C1
21	1	607	CLA	C4C-C3C-CAC-CBC
21	A	1111	CLA	C2A-CAA-CBA-CGA
21	B	1201	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
21	G	1603	CLA	C2A-CAA-CBA-CGA
21	1	615	CLA	C2A-CAA-CBA-CGA
21	5	602	CLA	C2A-CAA-CBA-CGA
38	5	611	CHL	C2A-CAA-CBA-CGA
21	3	616	CLA	C11-C10-C8-C9
21	1	612	CLA	C16-C17-C18-C19
21	B	1207	CLA	C4-C3-C5-C6
21	6	609	CLA	C4-C3-C5-C6
21	a	608	CLA	CAA-CBA-CGA-O2A
21	3	602	CLA	CAA-CBA-CGA-O2A
21	B	1021	CLA	O1A-CGA-O2A-C1
21	L	1502	CLA	O1A-CGA-O2A-C1
21	7	617	CLA	O1A-CGA-O2A-C1
30	7	804	PTY	O30-C30-O4-C1
35	J	5001	LPX	O7-C6-O6-C5
21	A	1131	CLA	C15-C16-C17-C18
24	4	801	LHG	C4-C5-O7-C7
30	5	802	PTY	C1-C6-O7-C8
48	8	806	P5S	C1-C2-O37-C38
31	B	5007	LAP	O2-C1-O1-C13
39	1	803	OLA	C4-C5-C6-C7
21	A	1101	CLA	C13-C15-C16-C17
37	1	501	LUT	C29-C30-C31-C32
37	a	502	LUT	C13-C14-C15-C35
37	6	502	LUT	C9-C10-C11-C12
21	A	1128	CLA	C16-C17-C18-C19
21	B	1201	CLA	C16-C17-C18-C20
21	B	1220	CLA	C11-C12-C13-C14
21	1	611	CLA	C6-C7-C8-C9
21	B	1203	CLA	O1A-CGA-O2A-C1
21	B	1216	CLA	O1A-CGA-O2A-C1
21	B	1235	CLA	O1A-CGA-O2A-C1
21	1	604	CLA	C4C-C3C-CAC-CBC
23	L	4003	BCR	C11-C10-C9-C8
25	A	5005	DGD	C7B-C8B-C9B-CAB
39	1	803	OLA	C2-C3-C4-C5
21	5	612	CLA	C10-C11-C12-C13
46	7	807	4RF	O23-C22-O21-C20
24	1	802	LHG	O8-C23-C24-C25
24	F	5002	LHG	O6-C4-C5-O7
24	4	801	LHG	O6-C4-C5-O7
24	7	802	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
30	B	5005	PTY	O14-C5-C6-O7
24	7	803	LHG	C15-C16-C17-C18
25	8	802	DGD	C5A-C6A-C7A-C8A
25	8	802	DGD	C2B-C3B-C4B-C5B
21	B	1204	CLA	C2C-C3C-CAC-CBC
24	6	801	LHG	C4-C5-C6-O8
32	G	5001	SQD	O6-C44-C45-C46
46	7	807	4RF	C19-C20-C39-O40
46	8	808	4RF	C19-C20-C39-O40
48	8	806	P5S	O19-C1-C2-C3
42	4	803	PLM	CD-CE-CF-CG
21	B	1235	CLA	C15-C16-C17-C18
21	A	1110	CLA	C11-C12-C13-C15
21	A	1114	CLA	C16-C17-C18-C19
21	A	1117	CLA	C4-C3-C5-C6
21	1	611	CLA	C4-C3-C5-C6
21	3	606	CLA	C2A-CAA-CBA-CGA
38	a	609	CHL	C3-C5-C6-C7
31	F	5003	LAP	C17-C16-O6-P9
31	K	5001	LAP	C17-C16-O6-P9
21	A	1110	CLA	C8-C10-C11-C12
21	A	1139	CLA	C3-C5-C6-C7
21	a	601	CLA	C3-C5-C6-C7
21	7	612	CLA	C3-C5-C6-C7
24	A	5001	LHG	O7-C5-C6-O8
24	a	801	LHG	O7-C5-C6-O8
24	4	802	LHG	O7-C5-C6-O8
30	5	802	PTY	O4-C1-C6-O7
30	7	804	PTY	O4-C1-C6-O7
43	5	803	DGA	OG1-CG1-CG2-OG2
46	7	807	4RF	O21-C20-C39-O40
46	8	807	4RF	O21-C20-C39-O40
21	A	1104	CLA	C11-C10-C8-C9
21	A	1135	CLA	C6-C7-C8-C9
21	A	1137	CLA	C6-C7-C8-C9
21	a	604	CLA	C11-C12-C13-C14
21	3	613	CLA	C6-C7-C8-C9
21	6	603	CLA	C14-C13-C15-C16
21	6	609	CLA	C14-C13-C15-C16
21	7	604	CLA	C6-C7-C8-C9
21	8	620	CLA	C11-C10-C8-C9
38	8	604	CHL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
21	A	1134	CLA	C11-C12-C13-C15
21	B	1213	CLA	C11-C12-C13-C14
48	8	806	P5S	C45-C46-C48-C49
24	B	5002	LHG	C28-C29-C30-C31
24	6	802	LHG	C10-C11-C12-C13
24	6	801	LHG	C18-C19-C20-C21
24	8	801	LHG	C27-C28-C29-C30
30	3	802	PTY	C36-C37-C38-C39
24	F	5001	LHG	C24-C25-C26-C27
29	6	803	PCW	C13-C14-C15-C16
21	3	612	CLA	C15-C16-C17-C18
21	A	1111	CLA	O1A-CGA-O2A-C1
46	8	808	4RF	C10-C11-C12-C13
21	B	1211	CLA	C2-C1-O2A-CGA
21	B	1235	CLA	C2-C1-O2A-CGA
21	B	1239	CLA	C2-C1-O2A-CGA
21	3	612	CLA	C2-C1-O2A-CGA
21	3	613	CLA	C2-C1-O2A-CGA
21	7	607	CLA	C2-C1-O2A-CGA
23	A	4003	BCR	C19-C20-C21-C22
21	6	604	CLA	CBA-CGA-O2A-C1
21	A	1134	CLA	C11-C12-C13-C14
21	A	1109	CLA	C10-C11-C12-C13
30	B	5005	PTY	C30-C31-C32-C33
24	1	801	LHG	C25-C26-C27-C28
24	F	5001	LHG	C29-C30-C31-C32
31	F	5003	LAP	O6-C16-C17-N8
31	K	5001	LAP	O6-C16-C17-N8
25	8	802	DGD	C2G-C1G-O1G-C1A
21	B	1023	CLA	C4-C3-C5-C6
21	4	601	CLA	C4-C3-C5-C6
21	6	604	CLA	C2C-C3C-CAC-CBC
21	A	1128	CLA	C3-C5-C6-C7
21	1	611	CLA	C2-C3-C5-C6
21	A	1102	CLA	C8-C10-C11-C12
21	B	1209	CLA	C8-C10-C11-C12
21	4	615	CLA	C5-C6-C7-C8
24	7	801	LHG	O2-C2-C3-O3
21	B	1209	CLA	C2A-CAA-CBA-CGA
21	1	604	CLA	C2A-CAA-CBA-CGA
24	6	801	LHG	C25-C26-C27-C28
21	B	1225	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
38	7	613	CHL	O1A-CGA-O2A-C1
24	7	801	LHG	C31-C32-C33-C34
21	A	1124	CLA	CBD-CGD-O2D-CED
38	a	613	CHL	C2C-C3C-CAC-CBC
21	5	601	CLA	C3-C5-C6-C7
38	3	611	CHL	C3-C5-C6-C7
21	7	612	CLA	C2C-C3C-CAC-CBC
38	a	606	CHL	C4C-C3C-CAC-CBC
21	B	1222	CLA	C10-C11-C12-C13
24	3	801	LHG	C11-C10-C9-C8
35	a	804	LPX	C9-C10-C11-C12
23	B	4001	BCR	C36-C18-C19-C20
24	5	801	LHG	C27-C28-C29-C30
21	A	1118	CLA	C4B-C3B-CAB-CBB
21	A	1120	CLA	C4B-C3B-CAB-CBB
21	A	1121	CLA	C1A-C2A-CAA-CBA
21	A	1122	CLA	C4B-C3B-CAB-CBB
21	A	1130	CLA	C4B-C3B-CAB-CBB
21	B	1203	CLA	C4B-C3B-CAB-CBB
21	B	1205	CLA	C4B-C3B-CAB-CBB
21	B	1232	CLA	C4B-C3B-CAB-CBB
21	B	1239	CLA	C1A-C2A-CAA-CBA
21	1	606	CLA	C1A-C2A-CAA-CBA
21	1	607	CLA	C4B-C3B-CAB-CBB
21	1	610	CLA	C1A-C2A-CAA-CBA
21	1	611	CLA	C4B-C3B-CAB-CBB
21	3	603	CLA	C4B-C3B-CAB-CBB
21	5	605	CLA	C4B-C3B-CAB-CBB
21	7	602	CLA	C4B-C3B-CAB-CBB
21	7	608	CLA	C4B-C3B-CAB-CBB
21	8	618	CLA	C4B-C3B-CAB-CBB
21	A	1140	CLA	C4-C3-C5-C6
48	8	806	P5S	C43-C44-C45-C46
21	B	1239	CLA	C2-C3-C5-C6
38	6	610	CHL	C2-C3-C5-C6
23	A	4002	BCR	C17-C18-C19-C20
46	7	807	4RF	C45-C46-C47-C48
21	B	1224	CLA	O1A-CGA-O2A-C1
21	A	1123	CLA	C2A-CAA-CBA-CGA
24	5	801	LHG	C33-C34-C35-C36
31	K	5001	LAP	C11-C10-C9-C8
24	6	801	LHG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
24	A	5002	LHG	O6-C4-C5-C6
24	A	5003	LHG	O6-C4-C5-C6
24	1	801	LHG	O6-C4-C5-C6
24	8	801	LHG	O6-C4-C5-C6
24	B	5002	LHG	O8-C23-C24-C25
24	7	803	LHG	C28-C29-C30-C31
46	8	808	4RF	C28-C29-C30-C31
24	A	5001	LHG	O9-C7-O7-C5
24	3	801	LHG	C34-C35-C36-C37
21	A	1104	CLA	C11-C12-C13-C15
21	A	1122	CLA	C11-C10-C8-C7
21	A	1101	CLA	C6-C7-C8-C10
21	B	1021	CLA	C6-C7-C8-C10
21	B	1021	CLA	C11-C12-C13-C15
21	B	1202	CLA	C6-C7-C8-C10
21	B	1208	CLA	C6-C7-C8-C10
21	B	1210	CLA	C12-C13-C15-C16
21	B	1235	CLA	C11-C10-C8-C7
21	B	1235	CLA	C12-C13-C15-C16
21	L	1502	CLA	C11-C10-C8-C7
21	1	603	CLA	C6-C7-C8-C10
21	3	605	CLA	C11-C10-C8-C7
21	4	610	CLA	C11-C12-C13-C15
21	5	604	CLA	C12-C13-C15-C16
21	7	601	CLA	C11-C10-C8-C7
38	4	609	CHL	C11-C10-C8-C7
24	3	801	LHG	C30-C31-C32-C33
44	6	806	SPH	C9-C10-C11-C12
21	8	612	CLA	O1A-CGA-O2A-C1
21	A	1128	CLA	CBA-CGA-O2A-C1
21	7	607	CLA	C2C-C3C-CAC-CBC
21	B	1222	CLA	O1A-CGA-O2A-C1
21	6	601	CLA	C10-C11-C12-C13
48	8	806	P5S	C17-C20-C21-C22
24	A	5003	LHG	C5-C4-O6-P
24	a	801	LHG	C2-C3-O3-P
24	7	803	LHG	C2-C3-O3-P
29	6	803	PCW	C2-C1-O3P-P
21	A	1120	CLA	C3A-C2A-CAA-CBA
21	B	1235	CLA	C3A-C2A-CAA-CBA
21	5	612	CLA	C4-C3-C5-C6
21	6	604	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	6	609	CLA	C2-C3-C5-C6
24	7	801	LHG	C18-C19-C20-C21
24	A	5003	LHG	O6-C4-C5-O7
24	F	5001	LHG	O6-C4-C5-O7
24	1	801	LHG	O6-C4-C5-O7
24	8	801	LHG	O6-C4-C5-O7
30	3	802	PTY	O14-C5-C6-O7
30	5	802	PTY	O14-C5-C6-O7
30	7	804	PTY	O14-C5-C6-O7
21	A	1108	CLA	C2A-CAA-CBA-CGA
21	A	1104	CLA	C6-C7-C8-C9
21	A	1131	CLA	C6-C7-C8-C9
21	A	1132	CLA	C6-C7-C8-C9
21	A	1136	CLA	C14-C13-C15-C16
21	B	1219	CLA	C6-C7-C8-C9
21	3	605	CLA	C11-C10-C8-C9
21	3	610	CLA	C6-C7-C8-C9
21	4	611	CLA	C6-C7-C8-C9
21	7	604	CLA	C11-C12-C13-C14
21	A	1132	CLA	O1A-CGA-O2A-C1
39	8	809	OLA	C4-C5-C6-C7
42	6	804	PLM	C6-C7-C8-C9
23	3	505	BCR	C15-C16-C17-C18
37	4	501	LUT	C29-C30-C31-C32
37	4	502	LUT	C29-C30-C31-C32
37	5	505	LUT	C9-C10-C11-C12
25	B	5003	DGD	C4A-C5A-C6A-C7A
21	A	1120	CLA	C1-C2-C3-C4
24	4	801	LHG	C9-C10-C11-C12
46	7	807	4RF	C43-C44-C45-C46
24	B	5001	LHG	O7-C5-C6-O8
24	F	5001	LHG	O7-C5-C6-O8
25	B	5003	DGD	O1G-C1G-C2G-O2G
25	8	802	DGD	O1G-C1G-C2G-O2G
30	B	5005	PTY	O4-C1-C6-O7
30	8	810	PTY	O4-C1-C6-O7
32	7	805	SQD	O47-C45-C46-O48
48	8	806	P5S	O19-C1-C2-O37
21	8	615	CLA	CBA-CGA-O2A-C1
21	6	609	CLA	C15-C16-C17-C18
21	A	1128	CLA	C16-C17-C18-C20
21	B	1213	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
29	B	5004	PCW	C1-C2-C3-O3
30	B	5005	PTY	O4-C1-C6-C5
32	7	805	SQD	O6-C44-C45-C46
46	8	807	4RF	O18-C19-C20-C39
46	8	808	4RF	O18-C19-C20-C39
21	B	1236	CLA	C5-C6-C7-C8
26	A	5007	3PH	C31-C32-C33-C34
46	8	807	4RF	C34-C35-C36-C37
21	A	1102	CLA	CAD-CBD-CGD-O2D
21	A	1111	CLA	CAD-CBD-CGD-O2D
21	A	1113	CLA	CAD-CBD-CGD-O2D
21	B	1210	CLA	CAD-CBD-CGD-O2D
21	B	1235	CLA	CAD-CBD-CGD-O2D
21	8	609	CLA	CAD-CBD-CGD-O2D
38	a	609	CHL	CAD-CBD-CGD-O2D
30	B	5005	PTY	C25-C26-C27-C28
46	8	807	4RF	C24-C25-C26-C27
24	A	5001	LHG	C7-C8-C9-C10
21	B	1237	CLA	C3-C5-C6-C7
21	A	1103	CLA	C2A-CAA-CBA-CGA
24	B	5002	LHG	C15-C16-C17-C18
25	8	802	DGD	CAB-CBB-CCB-CDB
25	B	5003	DGD	C7A-C8A-C9A-CAA
21	A	1102	CLA	CAD-CBD-CGD-O1D
21	A	1111	CLA	CAD-CBD-CGD-O1D
21	A	1113	CLA	CAD-CBD-CGD-O1D
21	A	1133	CLA	CHA-CBD-CGD-O1D
21	A	1133	CLA	CHA-CBD-CGD-O2D
21	A	1135	CLA	CHA-CBD-CGD-O1D
21	A	1135	CLA	CHA-CBD-CGD-O2D
21	A	1138	CLA	CAD-CBD-CGD-O1D
21	B	1210	CLA	CAD-CBD-CGD-O1D
21	B	1235	CLA	CAD-CBD-CGD-O1D
21	B	1236	CLA	CHA-CBD-CGD-O1D
21	L	1503	CLA	CHA-CBD-CGD-O1D
21	L	1503	CLA	CHA-CBD-CGD-O2D
21	a	604	CLA	CHA-CBD-CGD-O1D
21	a	604	CLA	CHA-CBD-CGD-O2D
21	a	605	CLA	CHA-CBD-CGD-O1D
21	a	605	CLA	CHA-CBD-CGD-O2D
21	a	607	CLA	CHA-CBD-CGD-O1D
21	a	607	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	4	604	CLA	CHA-CBD-CGD-O1D
21	4	604	CLA	CHA-CBD-CGD-O2D
21	4	605	CLA	CHA-CBD-CGD-O1D
21	4	605	CLA	CHA-CBD-CGD-O2D
21	7	617	CLA	CAD-CBD-CGD-O1D
21	8	609	CLA	CAD-CBD-CGD-O1D
23	B	4004	BCR	C19-C20-C21-C22
23	F	4001	BCR	C19-C20-C21-C22
23	I	4001	BCR	C13-C14-C15-C16
23	L	4002	BCR	C15-C16-C17-C18
23	4	503	BCR	C13-C14-C15-C16
24	A	5001	LHG	C3-O3-P-O5
24	B	5002	LHG	C3-O3-P-O5
24	B	5001	LHG	C4-O6-P-O4
24	F	5001	LHG	C3-O3-P-O5
24	1	801	LHG	C4-O6-P-O4
24	1	802	LHG	C3-O3-P-O5
24	1	802	LHG	C4-O6-P-O5
24	3	801	LHG	C4-O6-P-O5
24	4	802	LHG	C4-O6-P-O3
24	4	802	LHG	C4-O6-P-O4
24	6	802	LHG	C4-O6-P-O5
24	7	803	LHG	C3-O3-P-O5
24	8	801	LHG	C3-O3-P-O5
29	B	5004	PCW	C1-O3P-P-O2P
29	6	803	PCW	C1-O3P-P-O4P
30	3	802	PTY	C3-O11-P1-O13
30	3	802	PTY	C5-O14-P1-O13
30	7	804	PTY	C5-O14-P1-O12
31	B	5007	LAP	C16-O6-P9-O5
31	F	5003	LAP	C15-O4-P9-O5
31	F	5003	LAP	C16-O6-P9-O4
31	K	5001	LAP	C16-O6-P9-O5
35	J	5001	LPX	C3-O1-P1-O4
35	J	5001	LPX	C1-O2-P1-O1
35	J	5001	LPX	C1-O2-P1-O3
35	J	5001	LPX	C1-O2-P1-O4
37	1	502	LUT	C33-C34-C35-C15
37	5	501	LUT	C29-C30-C31-C32
38	a	609	CHL	CAD-CBD-CGD-O1D
38	6	611	CHL	CHA-CBD-CGD-O1D
38	6	611	CHL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
38	6	613	CHL	CHA-CBD-CGD-O2D
38	8	604	CHL	CHA-CBD-CGD-O1D
38	8	604	CHL	CHA-CBD-CGD-O2D
48	8	806	P5S	CB-OG-P12-O13
48	8	806	P5S	CB-OG-P12-O16
21	B	1221	CLA	C16-C17-C18-C19
24	F	5002	LHG	C26-C27-C28-C29
21	B	1237	CLA	C4-C3-C5-C6
21	7	601	CLA	C4-C3-C5-C6
21	A	1109	CLA	C2B-C3B-CAB-CBB
21	A	1118	CLA	C2B-C3B-CAB-CBB
21	B	1022	CLA	C2B-C3B-CAB-CBB
21	B	1203	CLA	C2B-C3B-CAB-CBB
21	B	1212	CLA	C2B-C3B-CAB-CBB
21	B	1214	CLA	C2B-C3B-CAB-CBB
21	B	1220	CLA	C2B-C3B-CAB-CBB
21	G	1601	CLA	C2B-C3B-CAB-CBB
21	K	1401	CLA	C2B-C3B-CAB-CBB
21	K	1404	CLA	C2B-C3B-CAB-CBB
21	L	1501	CLA	C2B-C3B-CAB-CBB
21	1	607	CLA	C2B-C3B-CAB-CBB
21	1	611	CLA	C2B-C3B-CAB-CBB
21	1	615	CLA	C2B-C3B-CAB-CBB
21	a	603	CLA	C2B-C3B-CAB-CBB
21	a	611	CLA	C2B-C3B-CAB-CBB
21	3	603	CLA	C2B-C3B-CAB-CBB
21	4	616	CLA	C2B-C3B-CAB-CBB
21	7	615	CLA	C2B-C3B-CAB-CBB
23	B	4002	BCR	C1-C6-C7-C8
21	A	1103	CLA	CAA-CBA-CGA-O2A
21	A	1117	CLA	C2-C3-C5-C6
21	B	1216	CLA	C2-C3-C5-C6
21	B	1207	CLA	C2-C3-C5-C6
24	F	5002	LHG	C2-C3-O3-P
24	1	802	LHG	C2-C3-O3-P
24	1	802	LHG	C5-C4-O6-P
38	1	609	CHL	C3-C5-C6-C7
24	5	801	LHG	C26-C27-C28-C29
24	A	5002	LHG	C32-C33-C34-C35
24	6	801	LHG	C9-C10-C11-C12
30	8	810	PTY	C16-C17-C18-C19
25	B	5003	DGD	C5A-C6A-C7A-C8A

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Mol	Chain	Res	Type	Atoms
30	8	810	PTY	C11-C12-C13-C14
24	F	5002	LHG	O1-C1-C2-O2
24	1	801	LHG	O1-C1-C2-O2
21	A	1128	CLA	O1A-CGA-O2A-C1
25	A	5005	DGD	O6D-C5D-C6D-O5D
24	1	801	LHG	C11-C10-C9-C8
21	G	1602	CLA	O1A-CGA-O2A-C1
30	5	802	PTY	C8-C11-C12-C13
21	3	616	CLA	C11-C10-C8-C7
24	B	5001	LHG	C12-C13-C14-C15
24	4	802	LHG	C6-C5-O7-C7
24	1	802	LHG	C26-C27-C28-C29
23	6	503	BCR	C18-C19-C20-C21
21	B	1230	CLA	C2-C3-C5-C6
21	5	612	CLA	C2-C3-C5-C6
24	1	802	LHG	C24-C25-C26-C27
24	5	801	LHG	C11-C10-C9-C8
23	3	505	BCR	C19-C20-C21-C22
23	6	503	BCR	C9-C10-C11-C12
21	1	611	CLA	C6-C7-C8-C10
21	1	612	CLA	C16-C17-C18-C20
21	a	603	CLA	C16-C17-C18-C19
21	A	1132	CLA	C15-C16-C17-C18
25	A	5005	DGD	C3B-C4B-C5B-C6B
21	A	1104	CLA	C3-C5-C6-C7
24	4	802	LHG	C10-C11-C12-C13
21	A	1106	CLA	C11-C10-C8-C9
21	A	1106	CLA	C14-C13-C15-C16
21	A	1110	CLA	C11-C10-C8-C9
21	A	1111	CLA	C14-C13-C15-C16
21	A	1131	CLA	C14-C13-C15-C16
21	B	1210	CLA	C6-C7-C8-C9
21	B	1220	CLA	C6-C7-C8-C9
21	a	604	CLA	C11-C10-C8-C9
21	3	616	CLA	C6-C7-C8-C9
21	8	618	CLA	C11-C10-C8-C9
21	A	1111	CLA	C11-C12-C13-C15
21	B	1023	CLA	C6-C7-C8-C10
21	a	607	CLA	C6-C7-C8-C10
23	B	4003	BCR	C11-C10-C9-C8
24	B	5002	LHG	O6-C4-C5-O7
29	6	803	PCW	O3P-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
20	A	1011	CL0	C5-C6-C7-C8
24	4	801	LHG	C33-C34-C35-C36
21	A	1132	CLA	CBA-CGA-O2A-C1
24	4	802	LHG	C14-C15-C16-C17
21	A	1131	CLA	C4-C3-C5-C6
21	B	1023	CLA	C2-C3-C5-C6
21	1	607	CLA	C2-C3-C5-C6
24	5	801	LHG	C35-C36-C37-C38
30	7	804	PTY	C12-C13-C14-C15
46	8	807	4RF	C41-C43-C44-C45
23	5	504	BCR	C19-C20-C21-C22
21	B	1203	CLA	C16-C17-C18-C19
25	8	802	DGD	C4D-C5D-C6D-O5D
21	G	1601	CLA	C2A-CAA-CBA-CGA
21	A	1133	CLA	C10-C11-C12-C13
21	B	1213	CLA	C3-C5-C6-C7
42	6	804	PLM	C9-CA-CB-CC
21	7	607	CLA	C4C-C3C-CAC-CBC
21	B	1230	CLA	C2-C1-O2A-CGA
21	6	602	CLA	C2-C1-O2A-CGA
21	B	1021	CLA	CAA-CBA-CGA-O2A
46	8	807	4RF	C28-C29-C30-C31
38	a	606	CHL	C3-C5-C6-C7
21	A	1127	CLA	CAA-CBA-CGA-O2A
21	B	1224	CLA	CAA-CBA-CGA-O2A
21	3	613	CLA	CAA-CBA-CGA-O2A
21	B	1226	CLA	C16-C17-C18-C19
24	F	5002	LHG	C29-C30-C31-C32
46	8	807	4RF	C12-C13-C14-C15
21	A	1126	CLA	CAA-CBA-CGA-O2A
25	8	802	DGD	C5D-C6D-O5D-C1E
21	A	1131	CLA	C13-C15-C16-C17
21	B	1203	CLA	C5-C6-C7-C8
24	6	801	LHG	C15-C16-C17-C18
21	7	617	CLA	C2A-CAA-CBA-CGA
23	A	4005	BCR	C13-C14-C15-C16
23	B	4002	BCR	C13-C14-C15-C16
23	B	4001	BCR	C13-C14-C15-C16
23	G	4001	BCR	C13-C14-C15-C16
23	J	4001	BCR	C13-C14-C15-C16
23	L	4001	BCR	C15-C16-C17-C18
37	7	501	LUT	C33-C34-C35-C15

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Mol	Chain	Res	Type	Atoms
24	7	801	LHG	C15-C16-C17-C18
24	A	5003	LHG	C27-C28-C29-C30
46	7	807	4RF	C44-C45-C46-C47
46	8	808	4RF	C12-C13-C14-C15
21	A	1111	CLA	CAA-CBA-CGA-O2A
21	7	612	CLA	C2-C3-C5-C6
21	B	1238	CLA	CBA-CGA-O2A-C1
21	A	1115	CLA	C6-C7-C8-C9
21	B	1021	CLA	C6-C7-C8-C9
21	1	612	CLA	C11-C12-C13-C14
21	5	604	CLA	C14-C13-C15-C16
21	5	612	CLA	C14-C13-C15-C16
38	4	609	CHL	C11-C10-C8-C9
38	5	610	CHL	C14-C13-C15-C16
24	4	801	LHG	C24-C23-O8-C6
21	B	1204	CLA	O1D-CGD-O2D-CED
21	A	1012	CLA	C4B-C3B-CAB-CBB
21	A	1135	CLA	C4B-C3B-CAB-CBB
21	A	1141	CLA	C4B-C3B-CAB-CBB
21	1	604	CLA	C4B-C3B-CAB-CBB
21	4	610	CLA	C4B-C3B-CAB-CBB
21	6	602	CLA	C4B-C3B-CAB-CBB
21	6	612	CLA	C4B-C3B-CAB-CBB
21	7	609	CLA	C4B-C3B-CAB-CBB
21	A	1114	CLA	C8-C10-C11-C12
25	A	5005	DGD	C4D-C5D-C6D-O5D
38	4	609	CHL	CBA-CGA-O2A-C1
21	A	1119	CLA	C13-C15-C16-C17
21	B	1235	CLA	O1D-CGD-O2D-CED
21	B	1218	CLA	C2A-CAA-CBA-CGA
21	A	1126	CLA	C4-C3-C5-C6
21	B	1022	CLA	C4-C3-C5-C6
21	3	607	CLA	C4-C3-C5-C6
32	7	805	SQD	C14-C15-C16-C17
24	B	5001	LHG	O6-C4-C5-O7
24	4	801	LHG	O10-C23-O8-C6
23	A	4001	BCR	C19-C20-C21-C22
24	6	802	LHG	C9-C10-C11-C12
21	A	1121	CLA	C6-C7-C8-C10
21	A	1125	CLA	C6-C7-C8-C10
21	B	1240	CLA	C12-C13-C15-C16
21	B	1204	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
21	a	603	CLA	C6-C7-C8-C10
21	a	605	CLA	C6-C7-C8-C10
21	4	603	CLA	C6-C7-C8-C10
21	6	604	CLA	C11-C10-C8-C7
21	8	606	CLA	C6-C7-C8-C10
21	8	618	CLA	C10-C11-C12-C13
21	A	1116	CLA	C3-C5-C6-C7
21	A	1117	CLA	C3-C5-C6-C7
24	F	5001	LHG	O2-C2-C3-O3
29	6	803	PCW	C33-C34-C35-C36
24	A	5002	LHG	C10-C11-C12-C13
21	B	1214	CLA	C4-C3-C5-C6
21	B	1221	CLA	C4-C3-C5-C6
21	5	609	CLA	C3A-C2A-CAA-CBA
38	5	610	CHL	C3A-C2A-CAA-CBA
38	5	611	CHL	C3A-C2A-CAA-CBA
23	A	4005	BCR	C16-C17-C18-C36
23	B	4003	BCR	C20-C21-C22-C37
23	F	4001	BCR	C35-C13-C14-C15
21	8	605	CLA	CAA-CBA-CGA-O1A
21	8	605	CLA	CAA-CBA-CGA-O2A
21	6	615	CLA	C15-C16-C17-C18
21	1	601	CLA	C2-C1-O2A-CGA
23	A	4002	BCR	C15-C16-C17-C18
23	B	4007	BCR	C19-C20-C21-C22
21	B	1239	CLA	C15-C16-C17-C18
23	B	4002	BCR	C11-C12-C13-C35
31	B	5007	LAP	C6-C7-C8-C9
46	7	807	4RF	C11-C12-C13-C14
21	3	603	CLA	C15-C16-C17-C18
21	B	1212	CLA	C4-C3-C5-C6
21	B	1224	CLA	C4-C3-C5-C6
21	L	1502	CLA	C4-C3-C5-C6
21	4	615	CLA	C4-C3-C5-C6
38	a	606	CHL	C4-C3-C5-C6
21	A	1013	CLA	C16-C17-C18-C19
21	A	1125	CLA	C16-C17-C18-C20
21	A	1115	CLA	C8-C10-C11-C12
21	A	1101	CLA	C10-C11-C12-C13
21	K	1402	CLA	C10-C11-C12-C13
21	4	610	CLA	C13-C15-C16-C17
46	8	807	4RF	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
21	B	1204	CLA	CBD-CGD-O2D-CED
25	8	802	DGD	CAA-CBA-CCA-CDA
43	5	803	DGA	CA5-CA6-CA7-CA8
43	8	803	DGA	CA4-CA5-CA6-CA7
24	B	5002	LHG	C4-C5-C6-O8
32	G	5001	SQD	C44-C45-C46-O48
32	7	805	SQD	C9-C10-C11-C12
21	A	1126	CLA	C3-C5-C6-C7
39	8	809	OLA	O1-C1-C2-C3
21	A	1102	CLA	C11-C12-C13-C14
21	A	1108	CLA	C14-C13-C15-C16
21	A	1109	CLA	C14-C13-C15-C16
21	A	1119	CLA	C11-C10-C8-C9
21	A	1138	CLA	C6-C7-C8-C9
21	A	1138	CLA	C11-C12-C13-C14
21	B	1203	CLA	C6-C7-C8-C9
21	B	1205	CLA	C11-C10-C8-C9
21	B	1216	CLA	C11-C12-C13-C14
21	B	1240	CLA	C14-C13-C15-C16
21	1	601	CLA	C6-C7-C8-C9
21	a	605	CLA	C11-C12-C13-C14
21	a	612	CLA	C6-C7-C8-C9
21	6	604	CLA	C11-C10-C8-C9
38	6	619	CHL	C6-C7-C8-C9
38	6	619	CHL	C14-C13-C15-C16
24	B	5002	LHG	C12-C13-C14-C15
24	A	5001	LHG	C9-C10-C11-C12
30	B	5005	PTY	C12-C13-C14-C15
42	4	803	PLM	C4-C5-C6-C7
38	4	609	CHL	O1A-CGA-O2A-C1
30	3	802	PTY	C13-C14-C15-C16
29	B	5004	PCW	C3-C2-O2-C31
21	A	1107	CLA	C3-C5-C6-C7
38	6	611	CHL	C1A-C2A-CAA-CBA
21	3	613	CLA	C4-C3-C5-C6
32	7	805	SQD	C11-C12-C13-C14
30	3	802	PTY	C12-C11-C8-O7
21	A	1121	CLA	C2-C3-C5-C6
21	B	1217	CLA	C5-C6-C7-C8
21	B	1235	CLA	CBD-CGD-O2D-CED
21	B	1022	CLA	C2A-CAA-CBA-CGA
21	7	601	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
26	A	5007	3PH	C29-C2A-C2B-C2C
21	A	1127	CLA	C1A-C2A-CAA-CBA
21	A	1129	CLA	C1A-C2A-CAA-CBA
21	A	1140	CLA	C1A-C2A-CAA-CBA
21	B	1230	CLA	C1A-C2A-CAA-CBA
21	B	1240	CLA	C1A-C2A-CAA-CBA
21	3	613	CLA	C1A-C2A-CAA-CBA
21	4	606	CLA	C1A-C2A-CAA-CBA
23	A	4005	BCR	C16-C17-C18-C19
23	B	4003	BCR	C20-C21-C22-C23
23	F	4001	BCR	C12-C13-C14-C15
21	8	608	CLA	CBA-CGA-O2A-C1
24	A	5002	LHG	C25-C26-C27-C28
21	B	1221	CLA	C16-C17-C18-C20
21	8	610	CLA	C6-C7-C8-C9
39	1	803	OLA	O1-C1-C2-C3
21	A	1120	CLA	C2B-C3B-CAB-CBB
21	A	1122	CLA	C2B-C3B-CAB-CBB
21	A	1130	CLA	C2B-C3B-CAB-CBB
21	A	1131	CLA	C2B-C3B-CAB-CBB
21	A	1135	CLA	C2B-C3B-CAB-CBB
21	A	1141	CLA	C2B-C3B-CAB-CBB
21	B	1205	CLA	C2B-C3B-CAB-CBB
21	B	1224	CLA	C2B-C3B-CAB-CBB
21	B	1232	CLA	C2B-C3B-CAB-CBB
21	G	1602	CLA	C2B-C3B-CAB-CBB
21	1	604	CLA	C2B-C3B-CAB-CBB
21	4	610	CLA	C2B-C3B-CAB-CBB
21	5	605	CLA	C2B-C3B-CAB-CBB
21	6	602	CLA	C2B-C3B-CAB-CBB
21	7	609	CLA	C2B-C3B-CAB-CBB
21	7	607	CLA	C2B-C3B-CAB-CBB
21	7	608	CLA	C2B-C3B-CAB-CBB
21	8	618	CLA	C2B-C3B-CAB-CBB
23	A	4001	BCR	C5-C6-C7-C8
23	A	4003	BCR	C5-C6-C7-C8
23	A	4004	BCR	C5-C6-C7-C8
23	A	4005	BCR	C5-C6-C7-C8
23	B	4002	BCR	C5-C6-C7-C8
23	B	4005	BCR	C23-C24-C25-C30
23	B	4001	BCR	C1-C6-C7-C8
23	B	4001	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
23	G	4001	BCR	C5-C6-C7-C8
23	L	4001	BCR	C5-C6-C7-C8
23	3	504	BCR	C23-C24-C25-C30
23	5	504	BCR	C23-C24-C25-C26
23	6	503	BCR	C23-C24-C25-C26
23	7	503	BCR	C5-C6-C7-C8
36	M	4001	ECH	C5-C6-C7-C8
36	M	4001	ECH	C23-C24-C25-C30
37	1	501	LUT	C5-C6-C7-C8
37	1	503	LUT	C5-C6-C7-C8
37	6	502	LUT	C5-C6-C7-C8
21	7	604	CLA	C13-C15-C16-C17
24	F	5001	LHG	C27-C28-C29-C30
30	3	802	PTY	C32-C33-C34-C35
21	A	1103	CLA	O1A-CGA-O2A-C1
24	4	801	LHG	C2-C3-O3-P
24	5	801	LHG	C2-C3-O3-P
21	6	604	CLA	C3-C5-C6-C7
24	7	801	LHG	C16-C17-C18-C19
21	A	1122	CLA	C4-C3-C5-C6
21	A	1134	CLA	C2-C3-C5-C6
21	B	1221	CLA	C2-C3-C5-C6
21	4	615	CLA	C2-C3-C5-C6
38	a	606	CHL	C2-C3-C5-C6
24	a	801	LHG	C27-C28-C29-C30
24	6	802	LHG	C24-C25-C26-C27
21	A	1103	CLA	CBA-CGA-O2A-C1
21	A	1108	CLA	C11-C12-C13-C15
21	A	1108	CLA	C12-C13-C15-C16
21	A	1111	CLA	C11-C10-C8-C7
21	A	1114	CLA	C6-C7-C8-C10
21	A	1115	CLA	C6-C7-C8-C10
21	A	1133	CLA	C6-C7-C8-C10
21	A	1101	CLA	C12-C13-C15-C16
21	B	1203	CLA	C11-C12-C13-C15
21	B	1205	CLA	C11-C10-C8-C7
21	B	1223	CLA	C11-C12-C13-C15
21	B	1237	CLA	C6-C7-C8-C10
21	B	1240	CLA	C6-C7-C8-C10
21	B	1204	CLA	C11-C10-C8-C7
21	1	612	CLA	C11-C12-C13-C15
21	3	604	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
21	3	605	CLA	C12-C13-C15-C16
21	5	612	CLA	C12-C13-C15-C16
22	A	2001	PQN	C22-C23-C25-C26
22	B	2002	PQN	C16-C17-C18-C20
38	1	609	CHL	C11-C12-C13-C15
46	8	807	4RF	C33-C34-C35-C36
21	3	601	CLA	C2A-CAA-CBA-CGA
21	4	603	CLA	C2A-CAA-CBA-CGA
21	B	1207	CLA	C5-C6-C7-C8
21	6	604	CLA	C10-C11-C12-C13
24	4	801	LHG	O7-C5-C6-O8
24	7	802	LHG	O7-C5-C6-O8
30	3	802	PTY	O4-C1-C6-O7
32	7	805	SQD	O6-C44-C45-O47
39	8	809	OLA	O2-C1-C2-C3
31	K	5001	LAP	C5-C6-C7-C8
28	1	804	LMT	C5'-C4'-O1B-C1B
21	B	1216	CLA	C12-C13-C15-C16
23	B	4005	BCR	C11-C12-C13-C35
23	L	4003	BCR	C36-C18-C19-C20
21	F	1302	CLA	C4-C3-C5-C6
21	1	612	CLA	C4-C3-C5-C6
21	5	604	CLA	C4-C3-C5-C6
38	6	619	CHL	C8-C10-C11-C12
21	A	1122	CLA	C2-C3-C5-C6
21	A	1126	CLA	C2-C3-C5-C6
21	B	1022	CLA	C2-C3-C5-C6
21	B	1214	CLA	C2-C3-C5-C6
21	L	1502	CLA	C2-C3-C5-C6
21	1	612	CLA	C2-C3-C5-C6
21	3	607	CLA	C2-C3-C5-C6
24	A	5003	LHG	C9-C10-C11-C12
21	B	1238	CLA	O1A-CGA-O2A-C1
21	L	1503	CLA	CAA-CBA-CGA-O2A
22	A	2001	PQN	C26-C27-C28-C29
24	7	801	LHG	C10-C11-C12-C13
30	5	802	PTY	C12-C13-C14-C15
43	8	803	DGA	CBB-CAB-CB9-CB8
24	B	5001	LHG	O2-C2-C3-O3
24	4	801	LHG	C17-C18-C19-C20
38	a	610	CHL	C2-C1-O2A-CGA
21	A	1103	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
21	A	1126	CLA	C6-C7-C8-C9
21	B	1021	CLA	C11-C10-C8-C9
21	B	1204	CLA	C14-C13-C15-C16
24	4	801	LHG	C30-C31-C32-C33
32	G	5001	SQD	C26-C27-C28-C29
48	8	806	P5S	O47-C38-C39-C40
23	A	4002	BCR	C19-C20-C21-C22
24	a	801	LHG	C11-C10-C9-C8
21	B	1212	CLA	C8-C10-C11-C12
21	1	604	CLA	C13-C15-C16-C17
24	a	801	LHG	C9-C10-C11-C12
30	3	802	PTY	C33-C34-C35-C36
39	1	803	OLA	O2-C1-C2-C3
28	B	5006	LMT	C3'-C4'-O1B-C1B
21	a	607	CLA	C8-C10-C11-C12
21	3	612	CLA	C8-C10-C11-C12
21	4	612	CLA	C5-C6-C7-C8
21	4	612	CLA	C8-C10-C11-C12
21	A	1104	CLA	C4-C3-C5-C6
21	B	1220	CLA	C4-C3-C5-C6
21	7	606	CLA	C4-C3-C5-C6
21	A	1140	CLA	C2-C3-C5-C6
21	B	1212	CLA	C2-C3-C5-C6
21	B	1224	CLA	C2-C3-C5-C6
21	4	601	CLA	C2-C3-C5-C6
21	7	601	CLA	C2-C3-C5-C6
21	8	608	CLA	O1A-CGA-O2A-C1
21	A	1133	CLA	C5-C6-C7-C8
21	B	1023	CLA	C5-C6-C7-C8
21	4	615	CLA	C8-C10-C11-C12
21	8	609	CLA	C10-C11-C12-C13
24	7	802	LHG	C29-C30-C31-C32
24	B	5002	LHG	C24-C23-O8-C6
24	7	803	LHG	C19-C20-C21-C22
43	5	803	DGA	CA1-CA2-CA3-CA4
24	3	801	LHG	C4-C5-C6-O8
21	1	602	CLA	CAA-CBA-CGA-O2A
21	8	607	CLA	CBD-CGD-O2D-CED
21	A	1131	CLA	C2A-CAA-CBA-CGA
21	3	613	CLA	C8-C10-C11-C12
21	1	606	CLA	C8-C10-C11-C12
30	3	802	PTY	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
21	A	1116	CLA	CAA-CBA-CGA-O2A
24	a	801	LHG	C29-C30-C31-C32
25	A	5005	DGD	O1B-C1B-O2G-C2G
29	B	5004	PCW	O31-C31-O2-C2
21	A	1122	CLA	C10-C11-C12-C13
24	7	803	LHG	O6-C4-C5-O7
21	B	1021	CLA	C4-C3-C5-C6
21	B	1235	CLA	C4-C3-C5-C6
21	7	610	CLA	C4-C3-C5-C6
21	A	1129	CLA	C4B-C3B-CAB-CBB
21	G	1602	CLA	C4B-C3B-CAB-CBB
21	5	612	CLA	C4B-C3B-CAB-CBB
21	5	614	CLA	C4B-C3B-CAB-CBB
21	6	608	CLA	C4B-C3B-CAB-CBB
21	6	605	CLA	C4B-C3B-CAB-CBB
21	6	608	CLA	CAA-CBA-CGA-O2A
21	1	612	CLA	CAA-CBA-CGA-O2A
21	A	1111	CLA	C13-C15-C16-C17
38	8	601	CHL	C11-C12-C13-C15
38	a	613	CHL	CHA-CBD-CGD-O1D
38	a	613	CHL	CHA-CBD-CGD-O2D
38	3	611	CHL	CHA-CBD-CGD-O1D
38	3	611	CHL	CHA-CBD-CGD-O2D
38	4	613	CHL	CHA-CBD-CGD-O1D
38	4	613	CHL	CHA-CBD-CGD-O2D
38	7	613	CHL	CHA-CBD-CGD-O2D
21	L	1503	CLA	CAA-CBA-CGA-O1A
24	F	5001	LHG	O6-C4-C5-C6
30	5	802	PTY	O14-C5-C6-C1
21	3	610	CLA	C11-C12-C13-C14
21	5	612	CLA	C16-C17-C18-C20
21	6	601	CLA	C11-C12-C13-C14
21	4	617	CLA	CAA-CBA-CGA-O2A
21	G	1601	CLA	CAA-CBA-CGA-O1A
21	A	1104	CLA	C2-C3-C5-C6
48	8	806	P5S	C42-C43-C44-C45
21	B	1229	CLA	C8-C10-C11-C12
24	B	5002	LHG	C2-C3-O3-P
21	A	1103	CLA	C6-C7-C8-C10
21	1	603	CLA	C11-C10-C8-C7
21	B	1211	CLA	C5-C6-C7-C8
23	B	4004	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
37	3	502	LUT	C13-C14-C15-C35
40	a	504	QTB	C02-C03-C04-C05
25	8	802	DGD	CCA-CDA-CEA-CFA
38	6	610	CHL	CAA-CBA-CGA-O1A
21	A	1138	CLA	C11-C10-C8-C9
21	A	1101	CLA	C6-C7-C8-C9
21	B	1212	CLA	C11-C12-C13-C14
21	B	1235	CLA	C14-C13-C15-C16
21	1	604	CLA	C11-C10-C8-C9
38	4	609	CHL	C11-C12-C13-C14
38	7	613	CHL	C11-C10-C8-C9
25	8	802	DGD	C2G-C3G-O3G-C1D
25	8	802	DGD	CDA-CEA-CFA-CGA
21	A	1013	CLA	C2A-CAA-CBA-CGA
21	B	1212	CLA	C2-C1-O2A-CGA
21	4	604	CLA	C2-C1-O2A-CGA
21	7	609	CLA	C2-C1-O2A-CGA
21	7	604	CLA	C2-C1-O2A-CGA
21	B	1208	CLA	C8-C10-C11-C12
21	A	1141	CLA	C3A-C2A-CAA-CBA
21	A	1140	CLA	C3A-C2A-CAA-CBA
21	B	1230	CLA	C3A-C2A-CAA-CBA
21	3	613	CLA	C3A-C2A-CAA-CBA
21	8	618	CLA	C3A-C2A-CAA-CBA
38	6	613	CHL	C3A-C2A-CAA-CBA
38	8	601	CHL	C3A-C2A-CAA-CBA
21	B	1237	CLA	C2-C3-C5-C6
21	7	606	CLA	C2-C3-C5-C6
21	7	615	CLA	C2C-C3C-CAC-CBC
21	G	1603	CLA	CAA-CBA-CGA-O2A
24	B	5002	LHG	C35-C36-C37-C38
28	1	804	LMT	C6-C7-C8-C9
21	A	1134	CLA	CBA-CGA-O2A-C1
21	7	607	CLA	C2-C3-C5-C6
23	B	4002	BCR	C10-C11-C12-C13
23	6	504	BCR	C10-C11-C12-C13
45	7	502	XAT	C10-C11-C12-C13
38	a	610	CHL	CAA-CBA-CGA-O2A
21	B	1231	CLA	C8-C10-C11-C12
24	1	802	LHG	C17-C18-C19-C20
33	G	5002	ERG	C22-C23-C24-C28
30	7	804	PTY	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
21	6	608	CLA	CAA-CBA-CGA-O1A
24	B	5001	LHG	C32-C33-C34-C35
28	B	5006	LMT	C1-C2-C3-C4
39	8	809	OLA	C7-C8-C9-C10
21	G	1603	CLA	CAA-CBA-CGA-O1A
24	a	801	LHG	O6-C4-C5-O7
21	B	1023	CLA	C2C-C3C-CAC-CBC
38	a	613	CHL	CAA-CBA-CGA-O2A
21	A	1134	CLA	O1A-CGA-O2A-C1
21	6	604	CLA	O1A-CGA-O2A-C1
21	A	1103	CLA	C10-C11-C12-C13
21	7	615	CLA	C5-C6-C7-C8
21	6	607	CLA	C3-C5-C6-C7
42	6	804	PLM	C7-C8-C9-CA
21	7	606	CLA	C2A-CAA-CBA-CGA
21	7	612	CLA	CAA-CBA-CGA-O2A
24	B	5002	LHG	O7-C7-C8-C9
24	7	802	LHG	O8-C23-C24-C25
21	3	613	CLA	C2-C3-C5-C6
23	A	4002	BCR	C9-C10-C11-C12
37	6	502	LUT	C33-C34-C35-C15
26	A	5007	3PH	O22-C21-C22-C23
42	6	804	PLM	CC-CD-CE-CF
21	1	602	CLA	CAA-CBA-CGA-O1A
24	F	5002	LHG	O8-C23-C24-C25
24	6	802	LHG	O8-C23-C24-C25
30	B	5005	PTY	C12-C11-C8-O7
21	A	1122	CLA	C13-C15-C16-C17
24	3	801	LHG	O7-C5-C6-O8
21	A	1104	CLA	C11-C12-C13-C14
21	A	1111	CLA	C11-C12-C13-C14
21	B	1203	CLA	C11-C12-C13-C14
21	B	1208	CLA	C6-C7-C8-C9
21	B	1235	CLA	C11-C10-C8-C9
21	B	1237	CLA	C11-C10-C8-C9
21	1	603	CLA	C6-C7-C8-C9
21	1	607	CLA	C11-C12-C13-C14
21	7	604	CLA	C11-C10-C8-C9
22	B	2002	PQN	C16-C17-C18-C19
38	5	610	CHL	C6-C7-C8-C9
21	3	616	CLA	CAA-CBA-CGA-O2A
21	8	620	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
21	5	601	CLA	O1A-CGA-O2A-C1
24	1	802	LHG	O6-C4-C5-C6
24	3	801	LHG	O6-C4-C5-C6
21	4	617	CLA	CAA-CBA-CGA-O1A
23	B	4001	BCR	C17-C18-C19-C20
23	L	4003	BCR	C17-C18-C19-C20
24	1	802	LHG	C25-C26-C27-C28
21	8	608	CLA	C4-C3-C5-C6
21	B	1214	CLA	O1A-CGA-O2A-C1
21	A	1109	CLA	CAA-CBA-CGA-O2A
21	A	1013	CLA	C11-C10-C8-C7
21	A	1106	CLA	C6-C7-C8-C10
21	A	1122	CLA	C6-C7-C8-C10
21	A	1137	CLA	C11-C10-C8-C7
21	A	1138	CLA	C11-C10-C8-C7
21	A	1101	CLA	C11-C10-C8-C7
21	B	1021	CLA	C11-C10-C8-C7
21	B	1205	CLA	C12-C13-C15-C16
21	B	1216	CLA	C6-C7-C8-C10
21	B	1223	CLA	C6-C7-C8-C10
21	B	1226	CLA	C6-C7-C8-C10
21	B	1237	CLA	C11-C12-C13-C15
21	1	604	CLA	C11-C10-C8-C7
21	1	606	CLA	C6-C7-C8-C10
21	6	609	CLA	C6-C7-C8-C10
21	6	615	CLA	C11-C12-C13-C15
21	7	603	CLA	C12-C13-C15-C16
21	8	603	CLA	C11-C12-C13-C15
22	B	2002	PQN	C17-C18-C20-C21
38	1	609	CHL	C6-C7-C8-C10
46	8	808	4RF	C32-C33-C34-C35
21	A	1012	CLA	C2B-C3B-CAB-CBB
21	A	1105	CLA	C2B-C3B-CAB-CBB
21	A	1129	CLA	C2B-C3B-CAB-CBB
21	A	1132	CLA	C2B-C3B-CAB-CBB
21	1	612	CLA	C2B-C3B-CAB-CBB
21	3	605	CLA	C2B-C3B-CAB-CBB
21	5	606	CLA	C2B-C3B-CAB-CBB
21	5	612	CLA	C2B-C3B-CAB-CBB
21	6	608	CLA	C2B-C3B-CAB-CBB
21	6	605	CLA	C2B-C3B-CAB-CBB
21	6	612	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
21	7	602	CLA	C2B-C3B-CAB-CBB
23	B	4005	BCR	C23-C24-C25-C26
23	B	4001	BCR	C5-C6-C7-C8
23	5	503	BCR	C23-C24-C25-C26
23	5	503	BCR	C23-C24-C25-C30
37	6	501	LUT	C1-C6-C7-C8
37	6	501	LUT	C5-C6-C7-C8
21	B	1204	CLA	CAA-CBA-CGA-O2A
21	8	607	CLA	O1D-CGD-O2D-CED
24	4	802	LHG	C13-C14-C15-C16
42	4	803	PLM	C3-C4-C5-C6
21	B	1202	CLA	C2-C1-O2A-CGA
21	1	603	CLA	C2-C1-O2A-CGA
21	8	602	CLA	C2-C1-O2A-CGA
38	3	611	CHL	C2-C1-O2A-CGA
21	8	615	CLA	O1A-CGA-O2A-C1
21	7	602	CLA	C4C-C3C-CAC-CBC
24	4	801	LHG	O7-C7-C8-C9
24	7	802	LHG	O7-C7-C8-C9
24	3	801	LHG	C28-C29-C30-C31
21	A	1125	CLA	C16-C17-C18-C19
21	8	610	CLA	C6-C7-C8-C10
21	A	1131	CLA	C2-C3-C5-C6
21	6	604	CLA	C2-C3-C5-C6
21	8	608	CLA	C2-C3-C5-C6
21	7	615	CLA	C4C-C3C-CAC-CBC
25	B	5003	DGD	O1B-C1B-O2G-C2G
44	6	806	SPH	C4-C5-C6-C7
21	L	1501	CLA	C2A-CAA-CBA-CGA
21	5	601	CLA	C2A-CAA-CBA-CGA
24	B	5002	LHG	O10-C23-O8-C6
21	B	1209	CLA	CAA-CBA-CGA-O2A
21	3	610	CLA	C11-C12-C13-C15
22	A	2001	PQN	C26-C27-C28-C30
29	6	803	PCW	C32-C33-C34-C35
21	3	605	CLA	CAA-CBA-CGA-O2A
21	5	612	CLA	CAA-CBA-CGA-O2A
21	8	609	CLA	CAA-CBA-CGA-O2A
21	8	608	CLA	CAA-CBA-CGA-O2A
23	K	4001	BCR	C10-C11-C12-C13
21	A	1129	CLA	CAA-CBA-CGA-O2A
21	5	617	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	8	801	LHG	O8-C23-C24-C25
44	6	806	SPH	C6-C7-C8-C9
29	B	5004	PCW	C32-C31-O2-C2
21	A	1117	CLA	C2A-CAA-CBA-CGA
21	5	612	CLA	C2A-CAA-CBA-CGA
21	B	1214	CLA	CAA-CBA-CGA-O2A
21	5	603	CLA	CAA-CBA-CGA-O2A
21	B	1237	CLA	C6-C7-C8-C9
21	B	1240	CLA	C6-C7-C8-C9
21	B	1207	CLA	C11-C10-C8-C9
21	8	603	CLA	C11-C12-C13-C14
21	A	1112	CLA	CAA-CBA-CGA-O2A
21	A	1121	CLA	CAA-CBA-CGA-O2A
21	A	1125	CLA	CAA-CBA-CGA-O2A
38	3	611	CHL	CAA-CBA-CGA-O2A
21	A	1012	CLA	C1A-C2A-CAA-CBA
21	A	1110	CLA	C4B-C3B-CAB-CBB
21	A	1134	CLA	C4B-C3B-CAB-CBB
21	B	1234	CLA	C4B-C3B-CAB-CBB
21	G	1603	CLA	C1A-C2A-CAA-CBA
21	K	1401	CLA	C1A-C2A-CAA-CBA
21	1	603	CLA	C4B-C3B-CAB-CBB
21	a	604	CLA	C4B-C3B-CAB-CBB
21	4	603	CLA	C4B-C3B-CAB-CBB
21	5	616	CLA	C4B-C3B-CAB-CBB
21	7	617	CLA	C1A-C2A-CAA-CBA
21	A	1107	CLA	CAA-CBA-CGA-O2A
21	A	1131	CLA	CAA-CBA-CGA-O2A
21	B	1208	CLA	CAA-CBA-CGA-O2A
21	1	603	CLA	CAA-CBA-CGA-O2A
21	1	605	CLA	CAA-CBA-CGA-O2A
21	4	603	CLA	CAA-CBA-CGA-O2A
21	6	603	CLA	CAA-CBA-CGA-O2A
38	4	613	CHL	CAA-CBA-CGA-O2A
21	B	1220	CLA	C2-C3-C5-C6
30	B	5005	PTY	C16-C17-C18-C19
23	B	4002	BCR	C11-C12-C13-C14
23	B	4005	BCR	C11-C12-C13-C14
37	a	502	LUT	C27-C28-C29-C30
23	B	4006	BCR	C19-C20-C21-C22
23	3	503	BCR	C19-C20-C21-C22
23	3	505	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
23	6	503	BCR	C13-C14-C15-C16
21	A	1138	CLA	C16-C17-C18-C20
38	a	613	CHL	CAA-CBA-CGA-O1A
20	A	1011	CL0	CAA-CBA-CGA-O2A
21	B	1210	CLA	CAA-CBA-CGA-O2A
21	a	603	CLA	CAA-CBA-CGA-O2A
21	7	603	CLA	CAA-CBA-CGA-O2A
24	B	5001	LHG	C14-C15-C16-C17
24	1	802	LHG	C12-C13-C14-C15
21	B	1216	CLA	C2A-CAA-CBA-CGA
21	a	603	CLA	C2A-CAA-CBA-CGA
32	G	5001	SQD	C14-C15-C16-C17
21	A	1141	CLA	CAA-CBA-CGA-O2A
21	1	601	CLA	C11-C12-C13-C14
24	B	5001	LHG	O6-C4-C5-C6
21	4	615	CLA	CAA-CBA-CGA-O2A
21	8	603	CLA	CAA-CBA-CGA-O2A
24	1	801	LHG	O7-C7-C8-C9
24	1	801	LHG	O8-C23-C24-C25
21	5	603	CLA	C5-C6-C7-C8
21	A	1137	CLA	C4-C3-C5-C6
21	4	604	CLA	C4-C3-C5-C6
21	a	608	CLA	CAA-CBA-CGA-O1A
21	B	1209	CLA	C2-C1-O2A-CGA
21	B	1210	CLA	C2-C1-O2A-CGA
21	B	1224	CLA	C2-C1-O2A-CGA
21	B	1204	CLA	C2-C1-O2A-CGA
21	3	604	CLA	C2-C1-O2A-CGA
21	4	603	CLA	C2-C1-O2A-CGA
21	5	601	CLA	C2-C1-O2A-CGA
38	4	618	CHL	C2-C1-O2A-CGA
21	A	1130	CLA	CAA-CBA-CGA-O2A
21	6	606	CLA	CAA-CBA-CGA-O2A
32	G	5001	SQD	C12-C13-C14-C15
21	A	1117	CLA	C11-C10-C8-C7
21	B	1212	CLA	C11-C12-C13-C15
21	1	603	CLA	C12-C13-C15-C16
21	6	601	CLA	C6-C7-C8-C10
21	6	601	CLA	C11-C10-C8-C7
21	7	604	CLA	C11-C10-C8-C7
21	8	603	CLA	C11-C10-C8-C7
21	3	606	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
21	A	1119	CLA	C16-C17-C18-C20
21	6	609	CLA	C16-C17-C18-C19
29	B	5004	PCW	C1-C2-O2-C31
21	B	1228	CLA	C10-C11-C12-C13
24	A	5002	LHG	O7-C7-C8-C9
25	A	5005	DGD	O1G-C1A-C2A-C3A
21	1	608	CLA	C10-C11-C12-C13
21	3	602	CLA	CAA-CBA-CGA-O1A
21	B	1215	CLA	C2A-CAA-CBA-CGA
21	a	612	CLA	C2A-CAA-CBA-CGA
21	1	605	CLA	C10-C11-C12-C13
21	A	1114	CLA	C16-C17-C18-C20
21	B	1229	CLA	C10-C11-C12-C13
21	A	1012	CLA	C3A-C2A-CAA-CBA
24	1	802	LHG	O10-C23-C24-C25
21	A	1123	CLA	O1A-CGA-O2A-C1
21	A	1137	CLA	C11-C12-C13-C14
21	a	608	CLA	C6-C7-C8-C10
24	A	5001	LHG	C10-C11-C12-C13
24	8	801	LHG	O7-C7-C8-C9
48	8	806	P5S	C40-C41-C42-C43
21	B	1208	CLA	CAA-CBA-CGA-O1A
43	8	803	DGA	CB2-CB3-CB4-CB5
21	B	1214	CLA	CBA-CGA-O2A-C1
21	A	1106	CLA	C8-C10-C11-C12
21	3	603	CLA	CAA-CBA-CGA-O2A
21	5	612	CLA	CAA-CBA-CGA-O1A
21	5	617	CLA	CAA-CBA-CGA-O1A
21	8	609	CLA	CAA-CBA-CGA-O1A
24	1	801	LHG	O9-C7-C8-C9
24	6	802	LHG	O10-C23-C24-C25
24	7	802	LHG	O9-C7-C8-C9
21	5	601	CLA	CBA-CGA-O2A-C1
21	A	1013	CLA	C11-C10-C8-C9
21	A	1108	CLA	C11-C12-C13-C14
21	A	1114	CLA	C6-C7-C8-C9
21	A	1101	CLA	C11-C12-C13-C14
21	A	1101	CLA	C14-C13-C15-C16
21	B	1210	CLA	C14-C13-C15-C16
21	B	1216	CLA	C6-C7-C8-C9
21	B	1223	CLA	C11-C12-C13-C14
21	3	605	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
21	6	601	CLA	C11-C10-C8-C9
21	5	605	CLA	CAA-CBA-CGA-O2A
21	3	616	CLA	CAA-CBA-CGA-O1A
21	8	620	CLA	CAA-CBA-CGA-O1A
38	4	613	CHL	CAA-CBA-CGA-O1A
24	7	802	LHG	C25-C26-C27-C28
32	G	5001	SQD	C28-C29-C30-C31
21	1	603	CLA	CAA-CBA-CGA-O1A
21	7	612	CLA	CAA-CBA-CGA-O1A
21	8	608	CLA	CAA-CBA-CGA-O1A
24	4	801	LHG	O9-C7-C8-C9
37	3	502	LUT	C21-C26-C27-C28
38	a	610	CHL	C2C-C3C-CAC-CBC
21	A	1112	CLA	CAA-CBA-CGA-O1A
21	B	1210	CLA	CAA-CBA-CGA-O1A
21	3	605	CLA	CAA-CBA-CGA-O1A
21	A	1133	CLA	C15-C16-C17-C18
48	8	806	P5S	C20-C21-C22-C23
21	F	1302	CLA	CAA-CBA-CGA-O2A
21	5	602	CLA	CAA-CBA-CGA-O2A
21	A	1126	CLA	C8-C10-C11-C12
23	4	503	BCR	C17-C18-C19-C20
21	A	1118	CLA	C2C-C3C-CAC-CBC
21	A	1107	CLA	CAA-CBA-CGA-O1A
21	A	1130	CLA	CAA-CBA-CGA-O1A
21	6	603	CLA	CAA-CBA-CGA-O1A
24	F	5002	LHG	O10-C23-C24-C25
24	7	802	LHG	O10-C23-C24-C25
21	B	1205	CLA	C8-C10-C11-C12
25	A	5005	DGD	C2G-C3G-O3G-C1D
24	B	5002	LHG	O9-C7-C8-C9
30	B	5005	PTY	C12-C11-C8-O10
21	K	1402	CLA	CAA-CBA-CGA-O2A
21	3	601	CLA	CAA-CBA-CGA-O2A
25	A	5005	DGD	O2G-C1B-C2B-C3B
25	8	802	DGD	C4A-C5A-C6A-C7A
24	3	801	LHG	C35-C36-C37-C38
25	8	802	DGD	O1G-C1G-C2G-C3G
30	3	802	PTY	O4-C1-C6-C5
21	A	1121	CLA	CAA-CBA-CGA-O1A
21	5	603	CLA	CAA-CBA-CGA-O1A
21	8	603	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
24	A	5002	LHG	O9-C7-C8-C9
21	7	617	CLA	C4-C3-C5-C6
28	A	5008	LMT	C4'-C5'-C6'-O6'
21	B	1209	CLA	C13-C15-C16-C17
21	B	1220	CLA	C5-C6-C7-C8
24	4	801	LHG	C5-C4-O6-P
21	K	1404	CLA	CAA-CBA-CGA-O2A
25	8	802	DGD	O1G-C1A-C2A-C3A
21	A	1141	CLA	CAA-CBA-CGA-O1A
21	7	605	CLA	CAA-CBA-CGA-O2A
21	A	1129	CLA	CAA-CBA-CGA-O1A
21	B	1209	CLA	CAA-CBA-CGA-O1A
21	B	1204	CLA	CAA-CBA-CGA-O1A
24	1	801	LHG	O10-C23-C24-C25
21	A	1138	CLA	CAD-CBD-CGD-O2D
21	a	605	CLA	CAD-CBD-CGD-O2D
21	4	604	CLA	CAD-CBD-CGD-O2D
21	A	1123	CLA	C3-C5-C6-C7
21	4	615	CLA	CAA-CBA-CGA-O1A
21	6	606	CLA	CAA-CBA-CGA-O1A
21	A	1116	CLA	C8-C10-C11-C12
21	A	1012	CLA	C8-C10-C11-C12
21	4	601	CLA	C2-C1-O2A-CGA
24	6	801	LHG	C29-C30-C31-C32
21	A	1125	CLA	CAA-CBA-CGA-O1A
21	A	1131	CLA	CAA-CBA-CGA-O1A
21	B	1214	CLA	CAA-CBA-CGA-O1A
24	8	801	LHG	O10-C23-C24-C25
21	B	1211	CLA	CAA-CBA-CGA-O2A
21	6	615	CLA	CAA-CBA-CGA-O2A
38	5	611	CHL	CAA-CBA-CGA-O2A
21	6	601	CLA	C11-C12-C13-C15
21	A	1128	CLA	C5-C6-C7-C8
42	6	804	PLM	CB-CC-CD-CE
25	A	5005	DGD	O1A-C1A-C2A-C3A
21	6	615	CLA	C5-C6-C7-C8
22	A	2001	PQN	C20-C21-C22-C23
21	6	603	CLA	C11-C12-C13-C15
21	B	1213	CLA	CAA-CBA-CGA-O2A
21	B	1238	CLA	CAA-CBA-CGA-O2A
21	6	618	CLA	CAA-CBA-CGA-O2A
24	4	801	LHG	O8-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
30	8	810	PTY	O4-C30-C31-C32
38	8	604	CHL	CAA-CBA-CGA-O2A
20	A	1011	CL0	CAA-CBA-CGA-O1A
21	1	605	CLA	CAA-CBA-CGA-O1A
21	a	603	CLA	CAA-CBA-CGA-O1A
24	F	5001	LHG	O10-C23-C24-C25
39	8	809	OLA	C9-C10-C11-C12
21	A	1139	CLA	CAA-CBA-CGA-O2A
21	B	1212	CLA	CAA-CBA-CGA-O2A
21	6	612	CLA	CAA-CBA-CGA-O2A
24	F	5001	LHG	O8-C23-C24-C25
24	5	801	LHG	O8-C23-C24-C25
31	B	5007	LAP	O1-C1-C2-C3
24	7	803	LHG	C11-C10-C9-C8

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	B	5006	LMT	C1'-C2'-C3'-C4'-C5'-O5'

328 monomers are involved in 1533 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	K	1401	CLA	3	0
38	a	610	CHL	2	0
23	L	4003	BCR	2	0
21	A	1012	CLA	11	0
21	5	604	CLA	10	0
23	K	4002	BCR	1	0
37	4	502	LUT	4	0
21	7	602	CLA	2	0
21	3	612	CLA	5	0
21	3	616	CLA	10	0
21	B	1216	CLA	5	0
21	F	1302	CLA	7	0
24	7	801	LHG	6	0
21	4	607	CLA	5	0
23	A	4001	BCR	5	0
21	B	1235	CLA	8	0
28	1	804	LMT	9	0
37	a	501	LUT	5	0
23	A	4002	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	6	612	CLA	2	0
21	1	615	CLA	4	0
21	B	1234	CLA	10	0
38	8	601	CHL	8	0
21	7	604	CLA	7	0
37	1	501	LUT	5	0
23	L	4001	BCR	17	0
24	B	5002	LHG	2	0
21	B	1202	CLA	6	0
24	3	801	LHG	5	0
21	5	601	CLA	5	0
23	L	4002	BCR	5	0
21	B	1204	CLA	10	0
21	B	1209	CLA	11	0
22	B	2002	PQN	5	0
21	6	601	CLA	24	0
21	A	1132	CLA	3	0
23	G	4001	BCR	3	0
21	a	611	CLA	2	0
21	B	1240	CLA	5	0
24	F	5002	LHG	3	0
21	4	605	CLA	1	0
21	7	617	CLA	6	0
21	5	616	CLA	2	0
21	B	1227	CLA	3	0
21	3	618	CLA	1	0
21	B	1230	CLA	4	0
21	A	1133	CLA	9	0
21	B	1205	CLA	7	0
21	1	611	CLA	4	0
38	4	613	CHL	4	0
21	A	1123	CLA	4	0
38	a	606	CHL	13	0
21	B	1218	CLA	7	0
21	8	607	CLA	2	0
21	A	1110	CLA	2	0
41	a	805	GG0	1	0
46	8	807	4RF	2	0
21	B	1222	CLA	5	0
21	B	1212	CLA	10	0
21	6	603	CLA	6	0
21	B	1239	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	1105	CLA	3	0
21	3	602	CLA	2	0
21	1	612	CLA	9	0
38	6	613	CHL	19	0
21	A	1106	CLA	9	0
21	A	1117	CLA	5	0
21	1	608	CLA	5	0
21	A	1122	CLA	3	0
21	B	1221	CLA	8	0
21	3	605	CLA	6	0
21	A	1107	CLA	8	0
21	L	1503	CLA	4	0
21	B	1022	CLA	4	0
23	J	4001	BCR	3	0
48	8	806	P5S	1	0
21	a	612	CLA	6	0
21	5	609	CLA	9	0
24	5	801	LHG	10	0
29	B	5004	PCW	6	0
21	a	608	CLA	3	0
23	A	4004	BCR	6	0
21	A	1109	CLA	13	0
21	A	1013	CLA	8	0
24	7	803	LHG	5	0
21	A	1128	CLA	3	0
46	7	807	4RF	6	0
37	8	502	LUT	5	0
21	B	1229	CLA	4	0
21	3	606	CLA	3	0
21	B	1226	CLA	7	0
21	B	1224	CLA	6	0
21	B	1203	CLA	6	0
24	B	5001	LHG	7	0
23	6	504	BCR	5	0
21	A	1104	CLA	6	0
23	3	505	BCR	1	0
47	7	504	C7Z	3	0
21	A	1129	CLA	2	0
21	A	1140	CLA	7	0
21	7	608	CLA	6	0
21	1	604	CLA	12	0
29	6	803	PCW	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	8	810	PTY	6	0
38	3	611	CHL	7	0
45	7	502	XAT	5	0
40	a	504	QTB	1	0
21	7	612	CLA	9	0
21	1	601	CLA	5	0
21	A	1121	CLA	7	0
21	A	1137	CLA	4	0
31	B	5007	LAP	3	0
21	a	607	CLA	1	0
21	4	602	CLA	1	0
21	B	1207	CLA	9	0
21	5	602	CLA	1	0
38	5	610	CHL	10	0
21	7	610	CLA	4	0
21	A	1124	CLA	5	0
28	B	5006	LMT	2	0
38	6	619	CHL	9	0
21	a	615	CLA	4	0
37	8	501	LUT	12	0
21	B	1223	CLA	3	0
21	B	1214	CLA	4	0
21	6	604	CLA	18	0
21	5	605	CLA	2	0
21	5	606	CLA	2	0
21	8	605	CLA	4	0
21	A	1103	CLA	11	0
21	5	618	CLA	7	0
21	B	1238	CLA	5	0
21	A	1139	CLA	2	0
23	K	4001	BCR	6	0
37	a	503	LUT	4	0
23	3	504	BCR	9	0
28	A	5008	LMT	4	0
21	A	1112	CLA	1	0
37	6	502	LUT	13	0
24	8	801	LHG	5	0
37	5	501	LUT	8	0
21	5	603	CLA	4	0
33	G	5002	ERG	16	0
21	6	617	CLA	12	0
21	B	1021	CLA	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	8	611	CLA	3	0
21	K	1402	CLA	6	0
23	B	4002	BCR	4	0
21	3	610	CLA	5	0
38	4	618	CHL	8	0
37	3	502	LUT	3	0
26	A	5007	3PH	1	0
21	7	603	CLA	6	0
21	4	617	CLA	1	0
37	4	501	LUT	5	0
38	3	608	CHL	1	0
37	7	501	LUT	4	0
23	8	503	BCR	5	0
21	4	606	CLA	3	0
21	B	1219	CLA	4	0
21	B	1206	CLA	6	0
21	A	1125	CLA	8	0
42	6	804	PLM	1	0
24	F	5001	LHG	4	0
21	7	605	CLA	5	0
38	a	613	CHL	7	0
21	8	606	CLA	4	0
21	B	1228	CLA	9	0
21	B	1232	CLA	3	0
27	C	3002	SF4	1	0
38	5	611	CHL	4	0
21	A	1126	CLA	11	0
24	1	801	LHG	3	0
21	3	603	CLA	8	0
23	5	504	BCR	5	0
25	B	5003	DGD	10	0
35	a	804	LPX	12	0
21	7	615	CLA	1	0
21	7	601	CLA	6	0
21	8	612	CLA	4	0
21	B	1201	CLA	16	0
21	5	617	CLA	5	0
34	J	4002	RRX	10	0
21	1	610	CLA	2	0
24	a	801	LHG	2	0
30	7	804	PTY	3	0
30	3	802	PTY	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	3	607	CLA	7	0
23	B	4005	BCR	4	0
21	A	1127	CLA	7	0
21	a	604	CLA	4	0
21	8	609	CLA	6	0
38	1	613	CHL	5	0
43	8	803	DGA	5	0
23	7	503	BCR	9	0
23	5	503	BCR	4	0
21	A	1111	CLA	10	0
21	8	615	CLA	3	0
37	3	501	LUT	6	0
21	B	1217	CLA	5	0
36	M	4001	ECH	6	0
38	1	609	CHL	8	0
21	B	1213	CLA	5	0
21	4	608	CLA	3	0
32	G	5001	SQD	4	0
21	A	1136	CLA	10	0
21	L	1502	CLA	15	0
21	A	1138	CLA	8	0
21	L	1501	CLA	3	0
21	1	602	CLA	4	0
21	8	610	CLA	6	0
24	1	802	LHG	2	0
21	6	607	CLA	12	0
23	F	4001	BCR	5	0
37	5	502	LUT	5	0
21	5	612	CLA	9	0
21	K	1403	CLA	28	0
21	a	601	CLA	5	0
38	5	613	CHL	2	0
21	A	1101	CLA	7	0
21	A	1130	CLA	8	0
32	7	805	SQD	1	0
21	7	609	CLA	4	0
23	B	4004	BCR	9	0
21	A	1102	CLA	6	0
21	a	603	CLA	2	0
21	B	1023	CLA	15	0
21	8	602	CLA	3	0
23	3	503	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	7	802	LHG	1	0
24	6	801	LHG	16	0
38	4	609	CHL	9	0
24	A	5003	LHG	7	0
21	A	1108	CLA	10	0
21	B	1236	CLA	5	0
21	7	611	CLA	5	0
21	1	603	CLA	8	0
21	4	610	CLA	8	0
42	4	803	PLM	1	0
44	6	806	SPH	7	0
21	8	618	CLA	7	0
21	K	1404	CLA	2	0
21	5	607	CLA	3	0
21	6	602	CLA	5	0
21	B	1225	CLA	6	0
21	4	603	CLA	3	0
21	8	620	CLA	5	0
21	A	1113	CLA	4	0
23	B	4007	BCR	3	0
38	6	610	CHL	9	0
21	1	606	CLA	2	0
27	C	3003	SF4	1	0
21	4	615	CLA	2	0
25	8	802	DGD	13	0
38	a	609	CHL	7	0
21	6	605	CLA	1	0
21	A	1135	CLA	5	0
21	B	1215	CLA	5	0
21	5	608	CLA	3	0
38	8	613	CHL	3	0
21	B	1210	CLA	7	0
20	A	1011	CL0	4	0
37	a	502	LUT	5	0
21	3	604	CLA	3	0
25	A	5005	DGD	3	0
23	4	503	BCR	3	0
21	A	1114	CLA	6	0
21	A	1134	CLA	6	0
21	A	1118	CLA	5	0
21	7	606	CLA	5	0
23	A	4005	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	6	615	CLA	3	0
37	5	505	LUT	7	0
37	6	501	LUT	16	0
23	A	4003	BCR	5	0
21	B	1237	CLA	8	0
21	8	603	CLA	4	0
21	B	1231	CLA	7	0
21	F	1301	CLA	5	0
21	4	601	CLA	8	0
21	4	604	CLA	5	0
21	4	616	CLA	2	0
23	B	4003	BCR	6	0
23	6	503	BCR	11	0
21	A	1116	CLA	6	0
37	1	502	LUT	3	0
21	6	606	CLA	2	0
21	A	1120	CLA	5	0
21	B	1211	CLA	4	0
23	I	4001	BCR	8	0
24	A	5001	LHG	1	0
38	7	613	CHL	5	0
43	5	803	DGA	3	0
39	8	809	OLA	4	0
21	A	1119	CLA	4	0
39	1	803	OLA	2	0
37	1	503	LUT	8	0
22	A	2001	PQN	6	0
21	3	601	CLA	12	0
21	8	608	CLA	5	0
21	a	602	CLA	2	0
46	8	808	4RF	13	0
21	4	612	CLA	5	0
24	4	802	LHG	5	0
21	A	1115	CLA	5	0
21	a	605	CLA	6	0
21	3	613	CLA	4	0
38	6	611	CHL	19	0
24	A	5002	LHG	8	0
24	4	801	LHG	15	0
21	B	1208	CLA	5	0
21	6	618	CLA	4	0
21	6	609	CLA	23	0

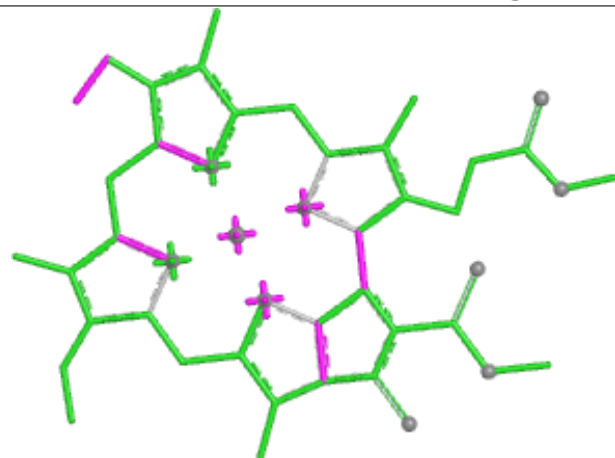
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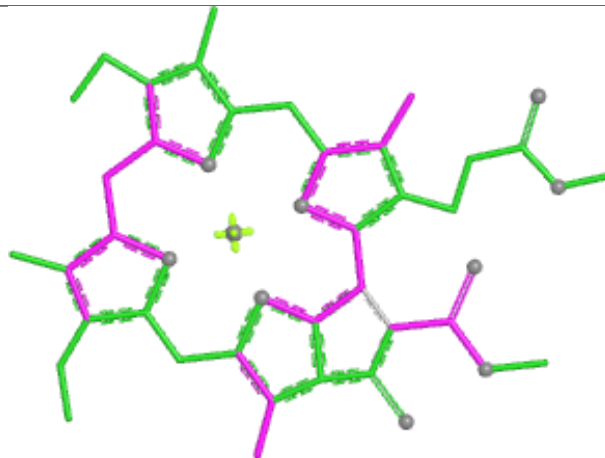
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	4006	BCR	1	0
21	G	1602	CLA	2	0
21	B	1220	CLA	6	0
30	B	5005	PTY	4	0
38	8	604	CHL	9	0
23	B	4001	BCR	5	0
24	6	802	LHG	4	0
21	1	607	CLA	14	0
31	F	5003	LAP	6	0
21	1	605	CLA	8	0
31	K	5001	LAP	3	0
21	G	1603	CLA	5	0
21	A	1131	CLA	11	0
30	5	802	PTY	2	0
35	J	5001	LPX	3	0

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

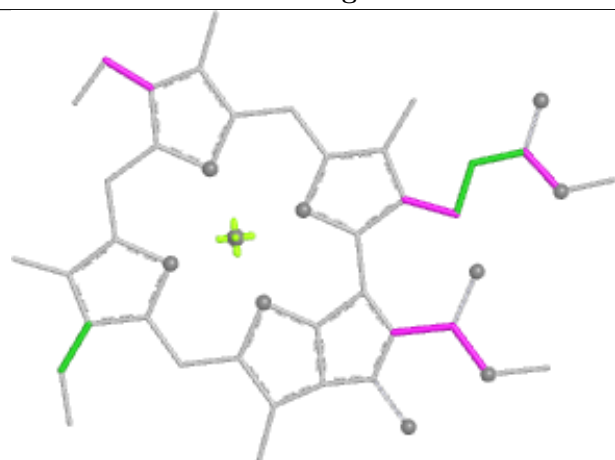
Ligand CLA K 1401



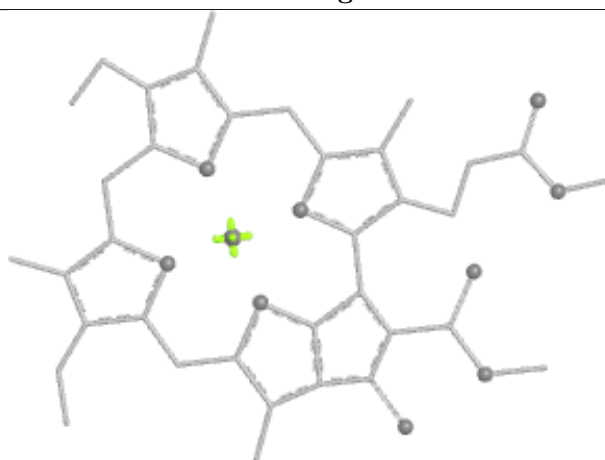
Bond lengths



Bond angles

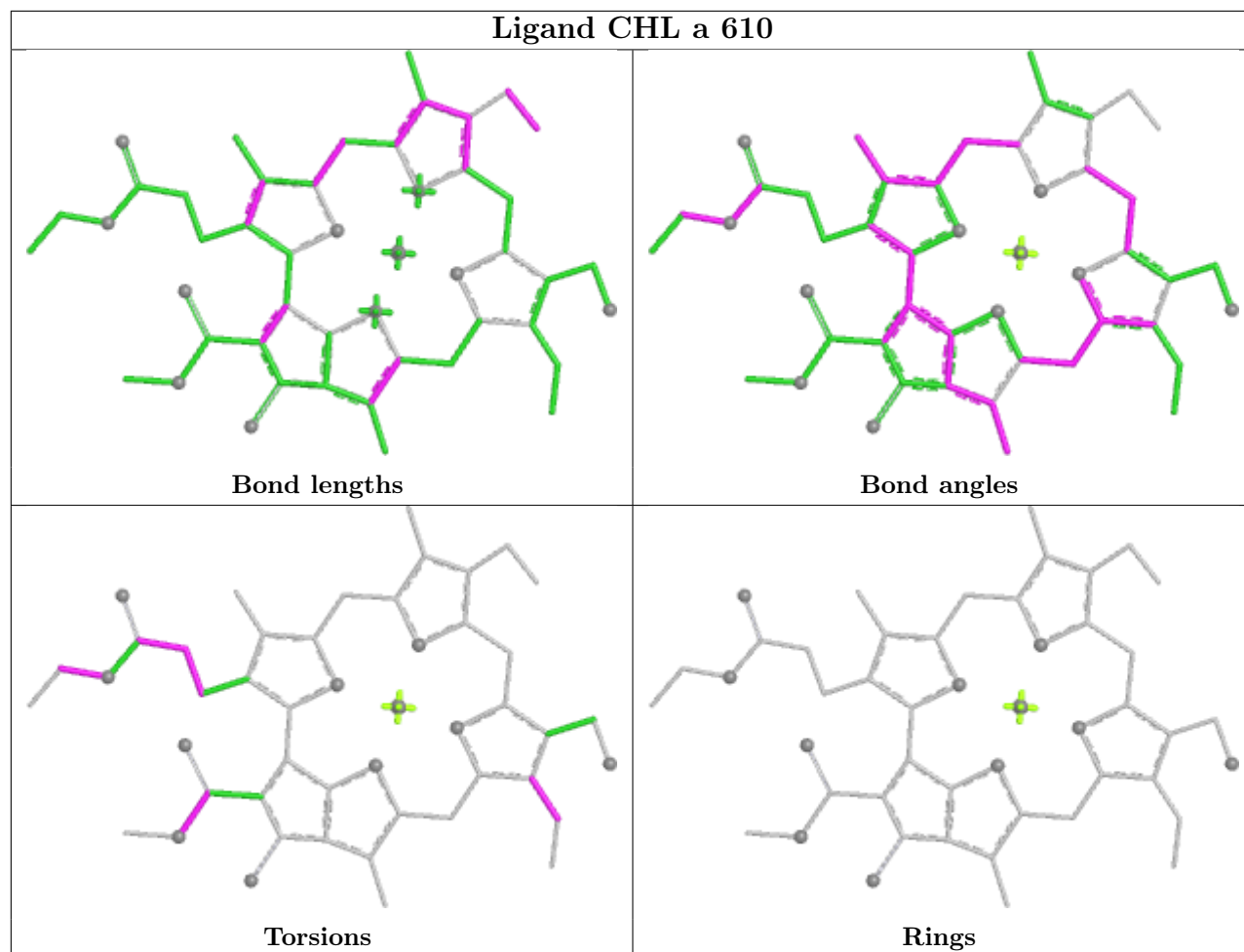


Torsions

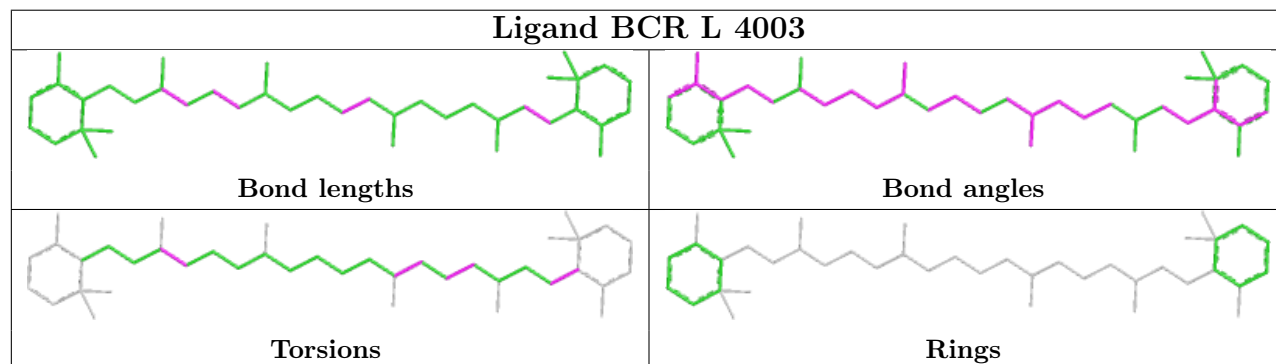


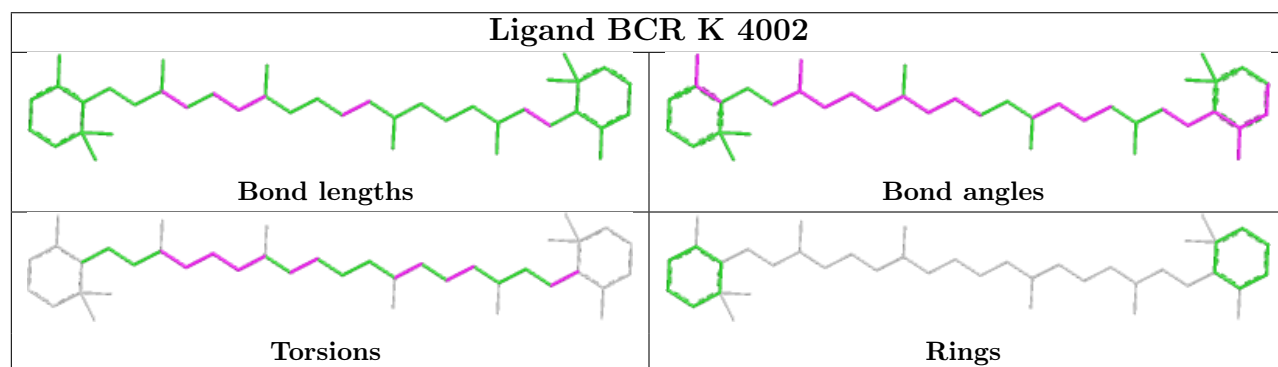
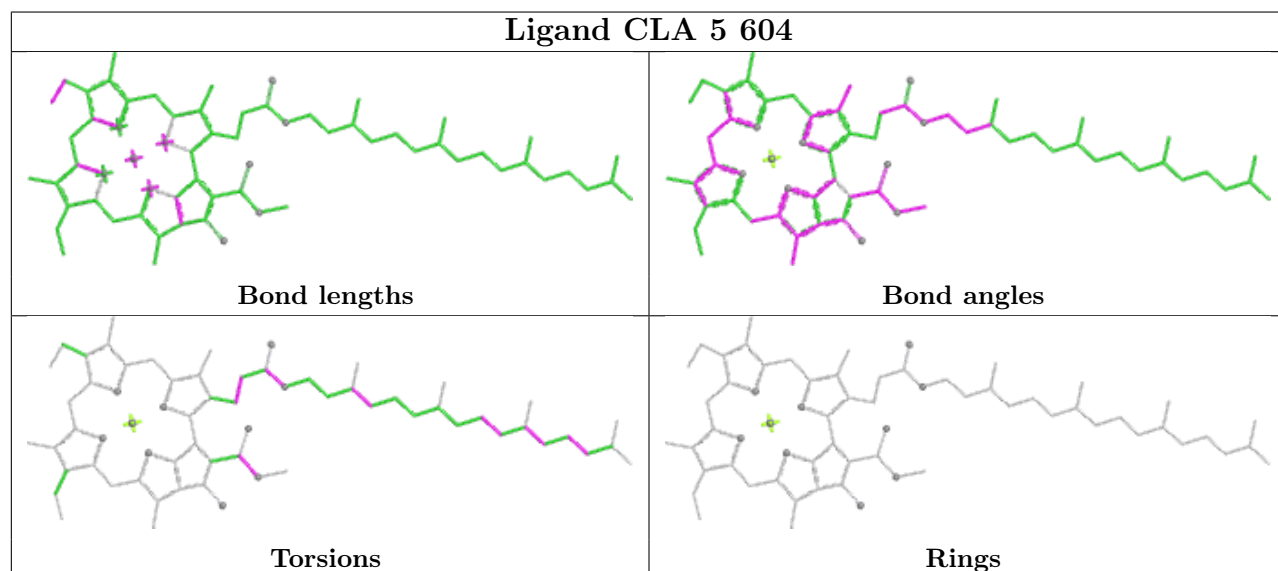
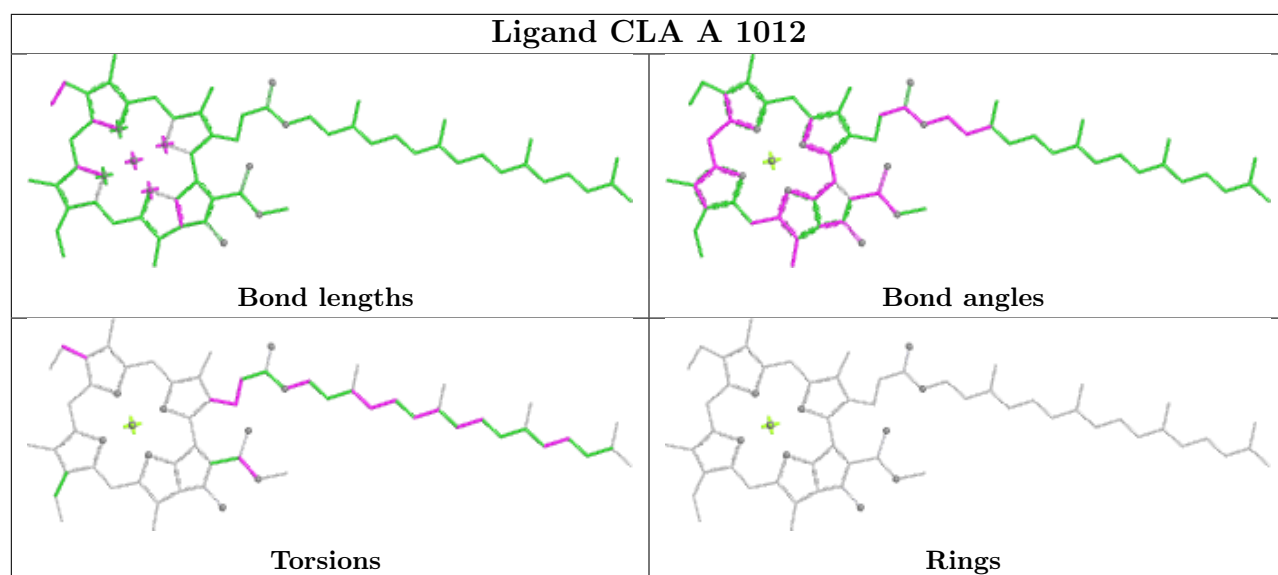
Rings

Ligand CHL a 610

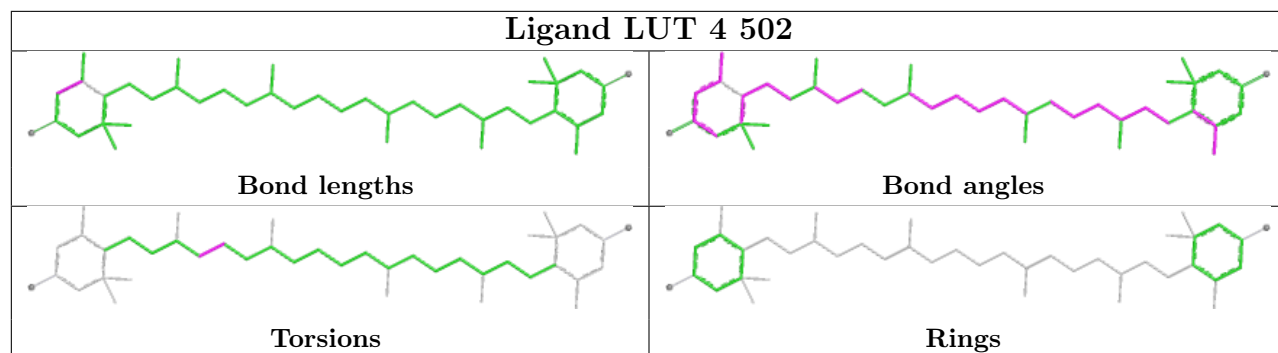


Ligand BCR L 4003

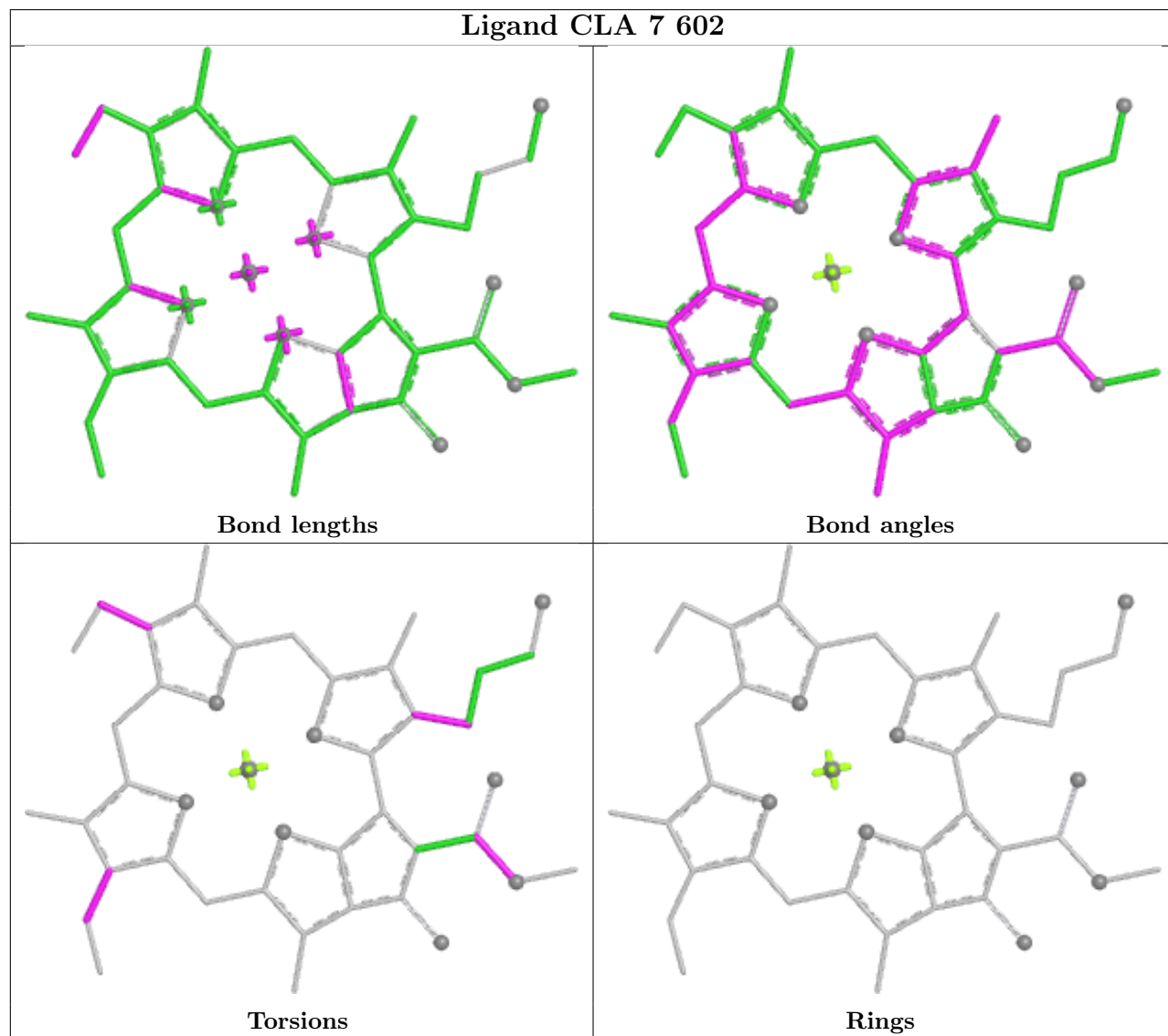


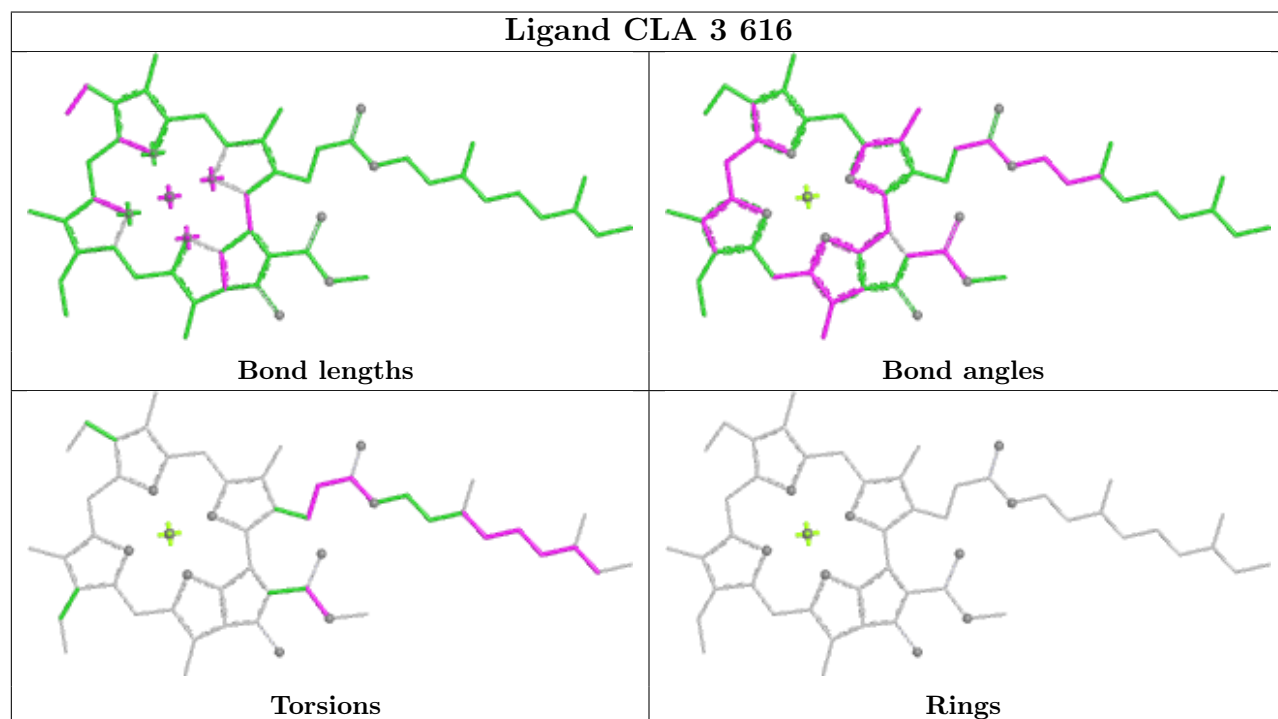
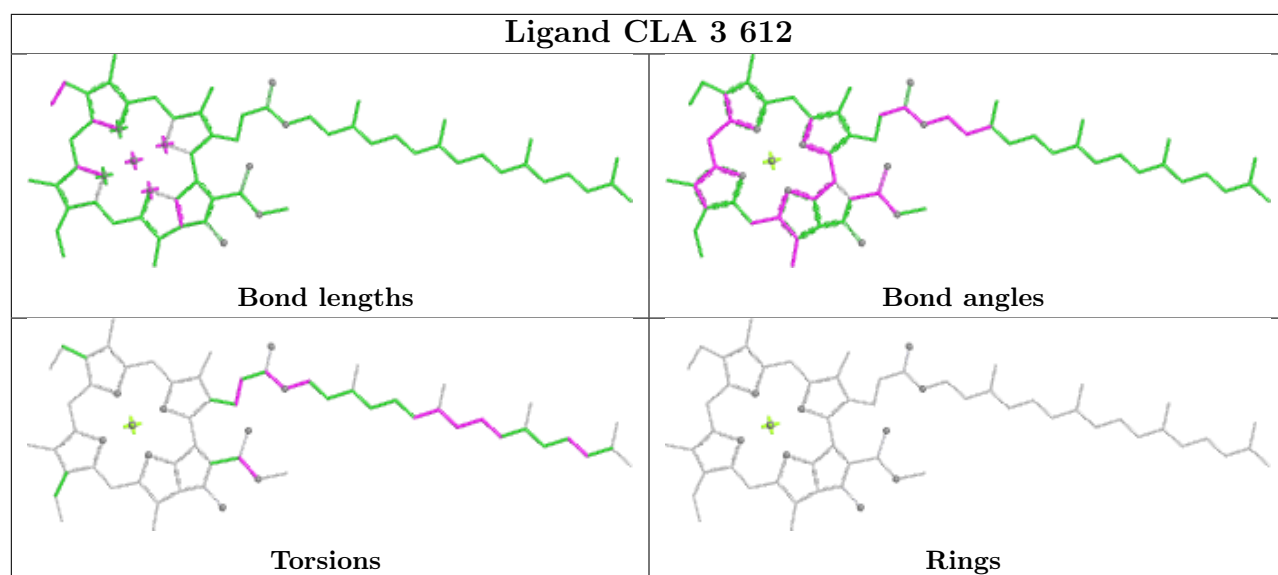


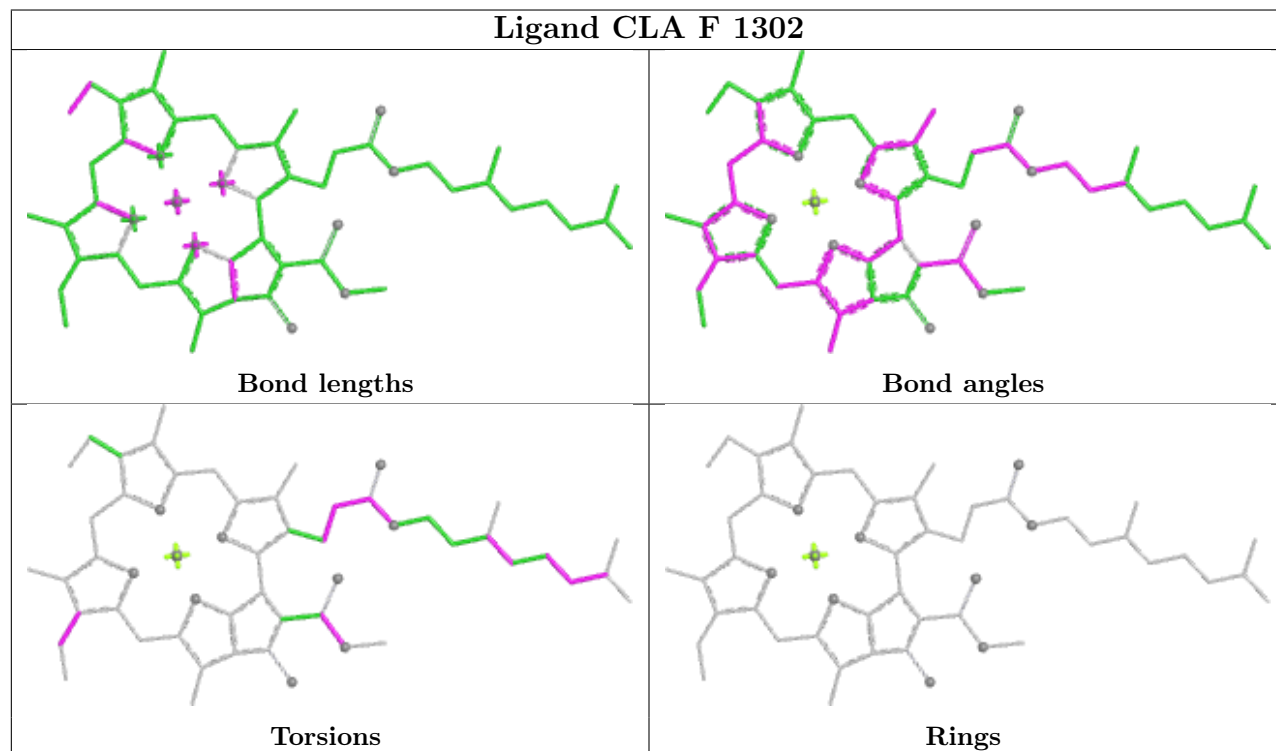
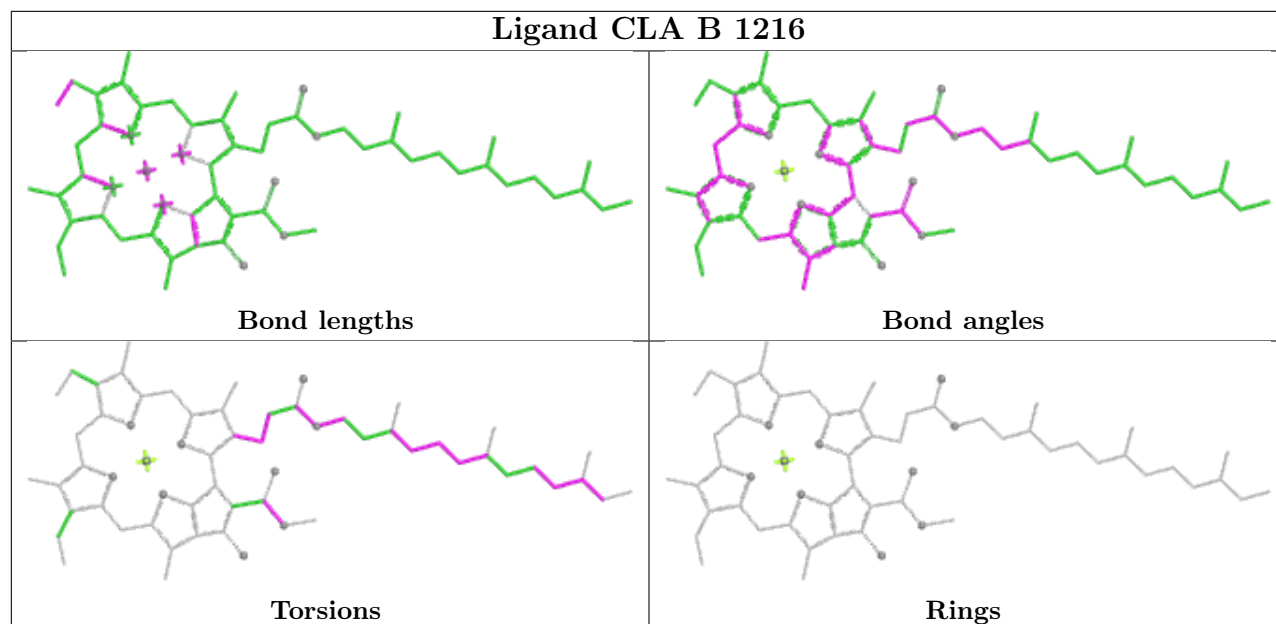
Ligand LUT 4 502

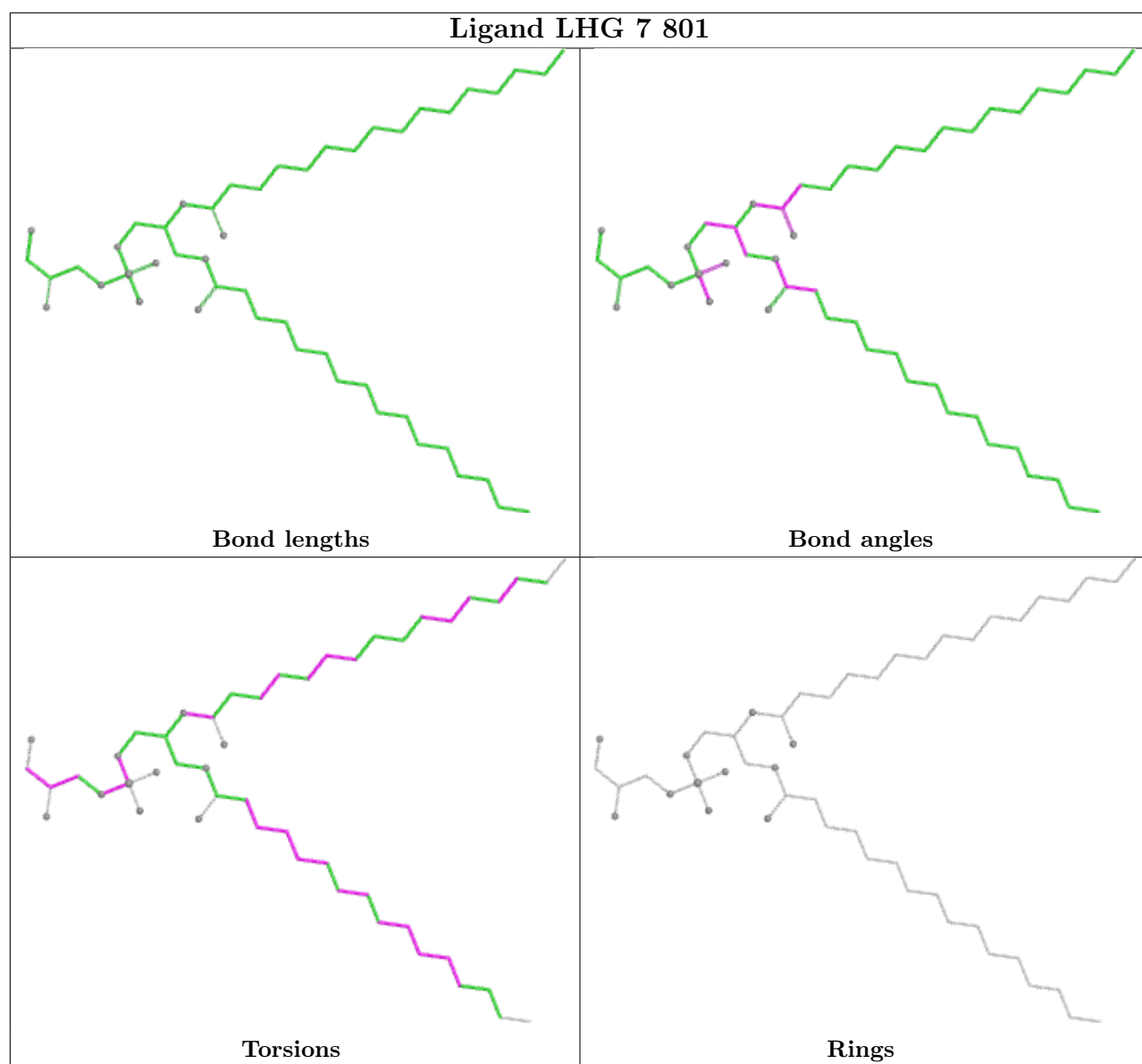


Ligand CLA 7 602

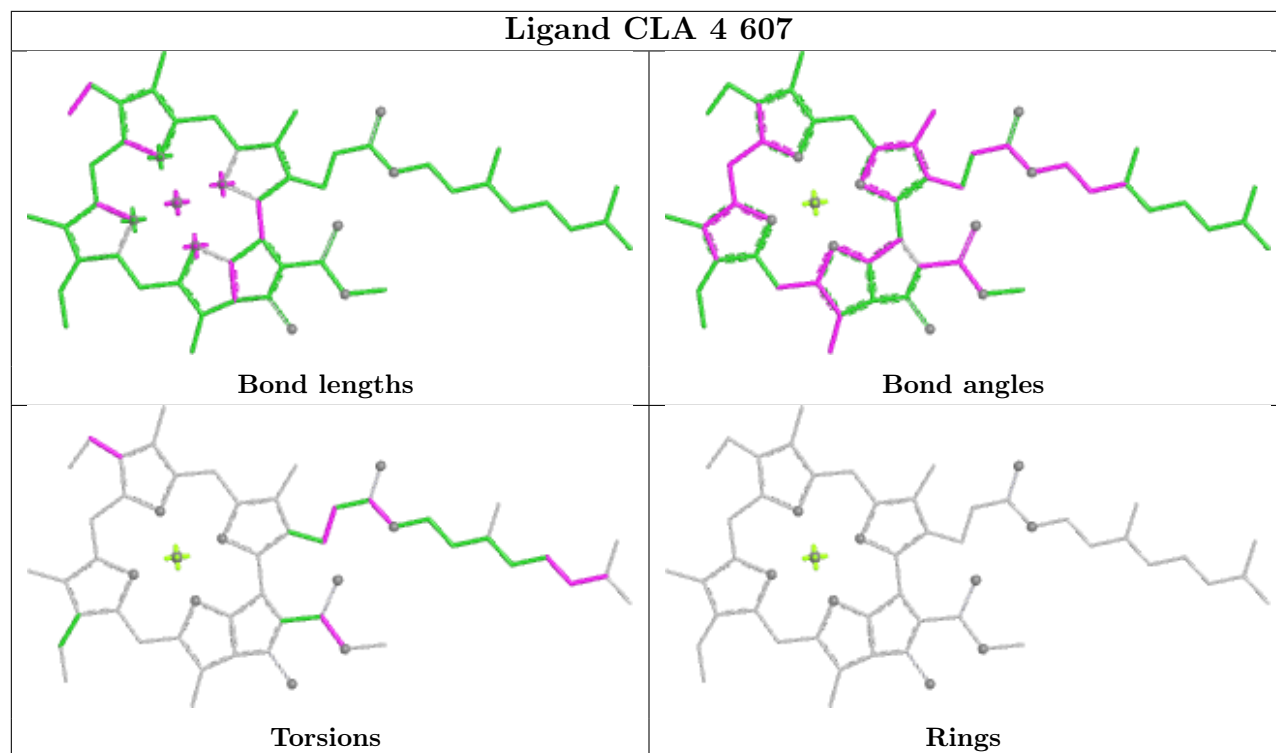




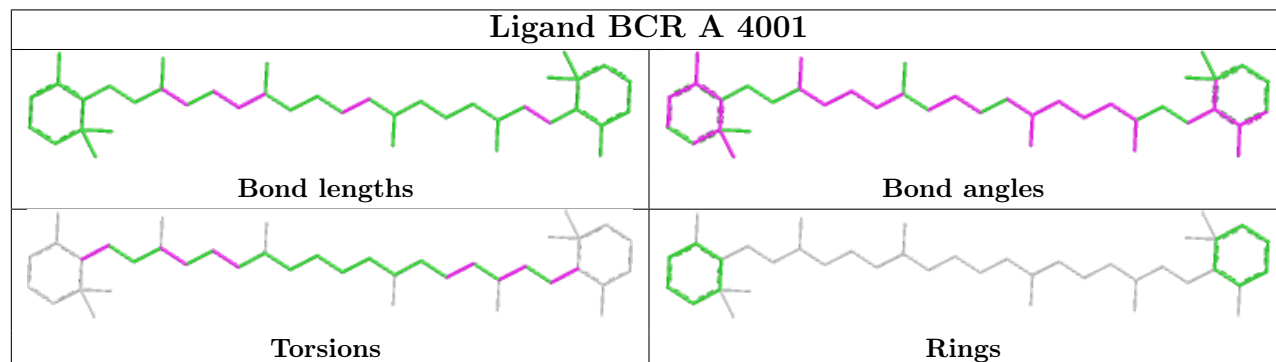




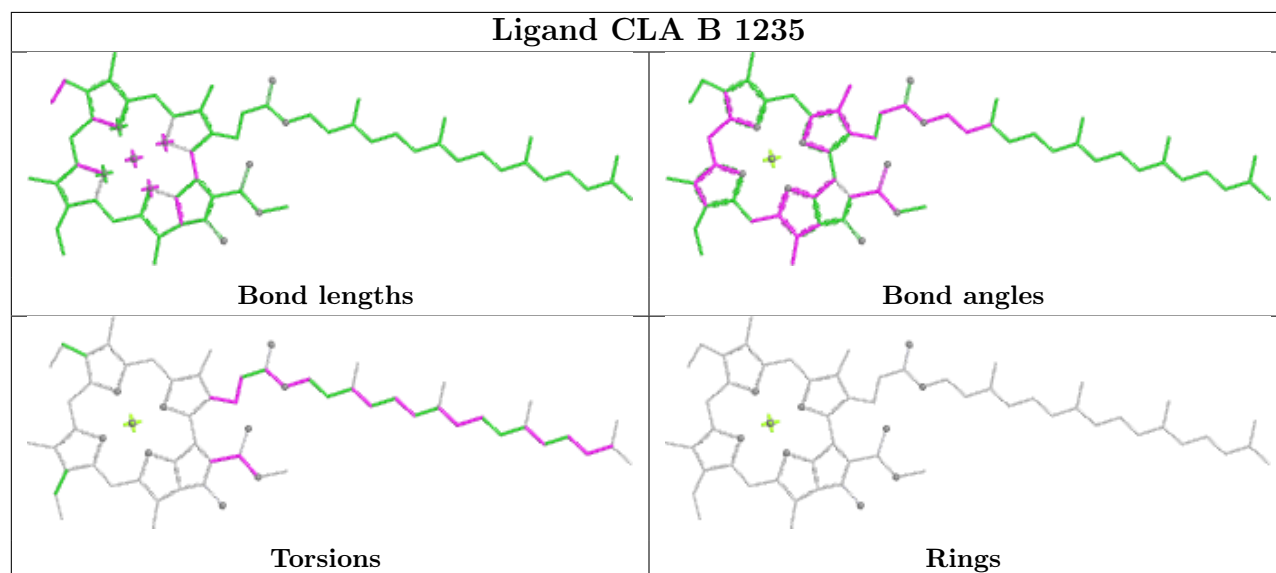
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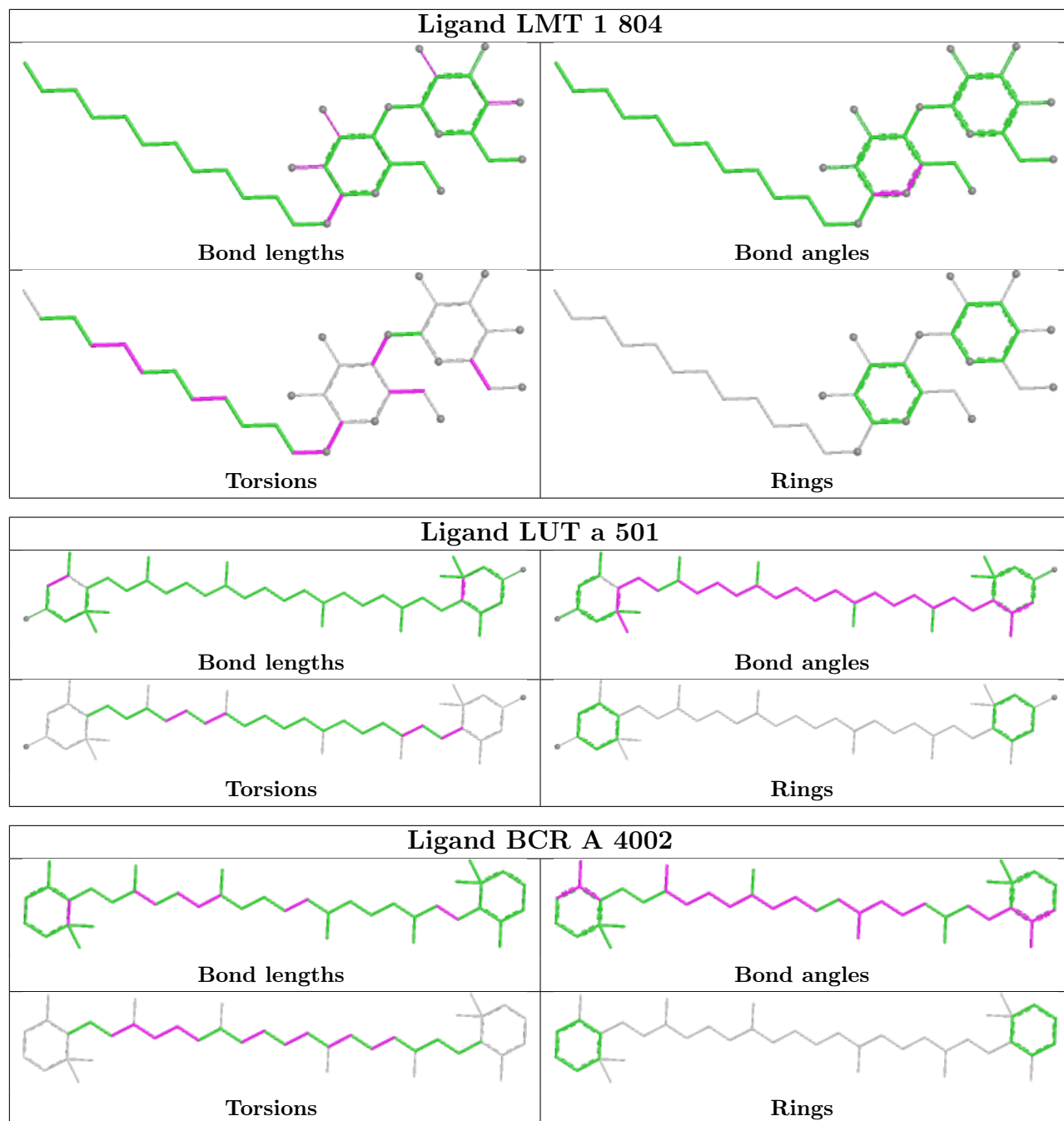


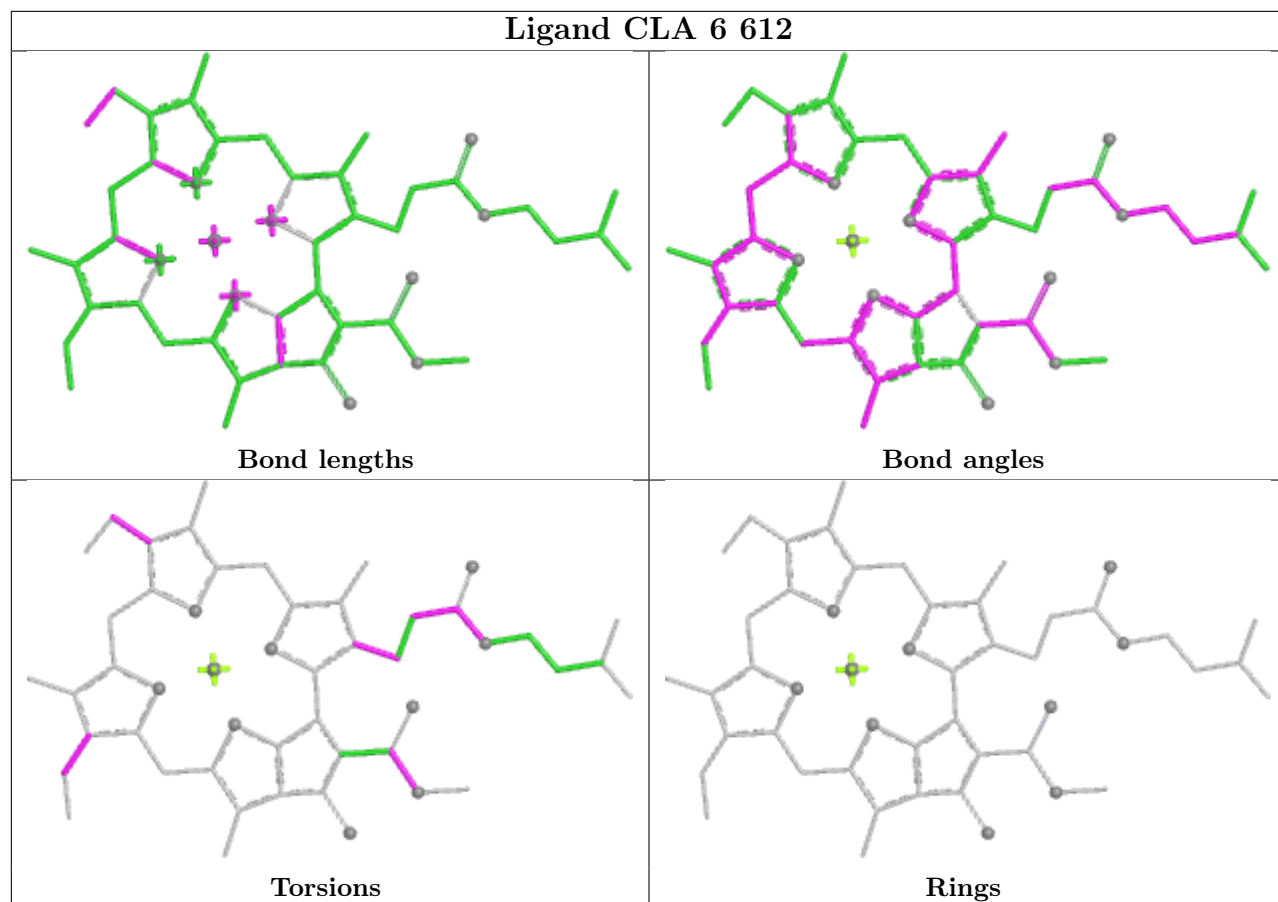
Ligand BCR A 4001



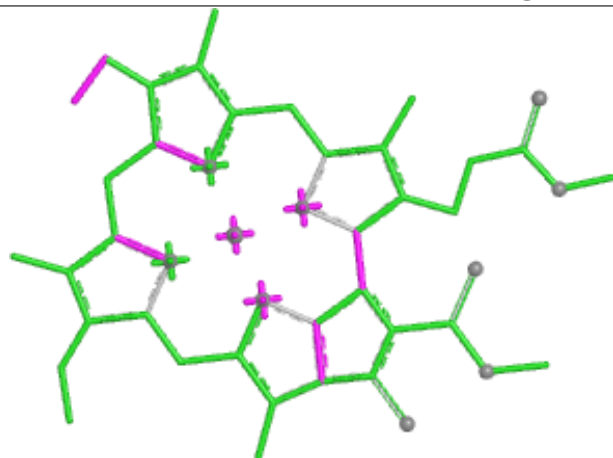
Ligand CLA B 1235



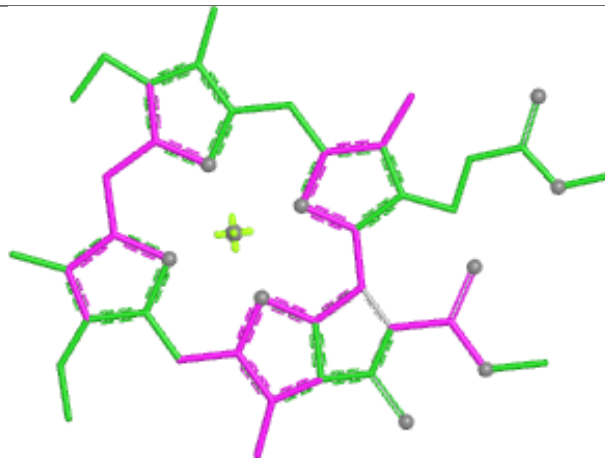




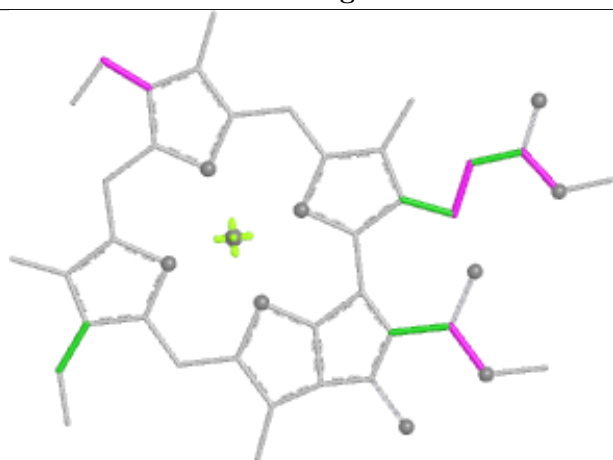
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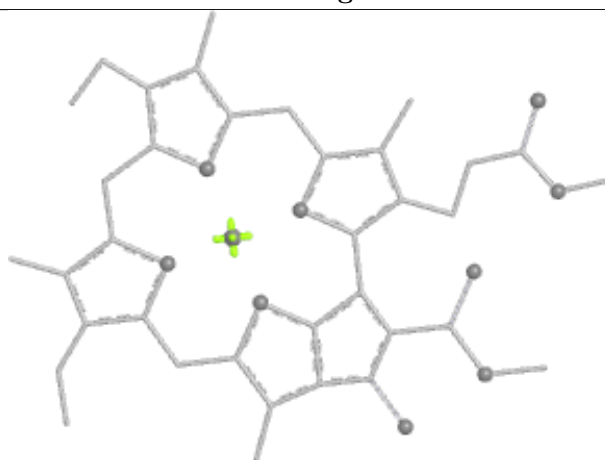
Bond lengths



Bond angles

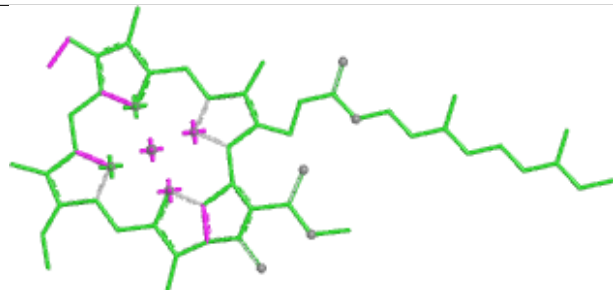


Torsions

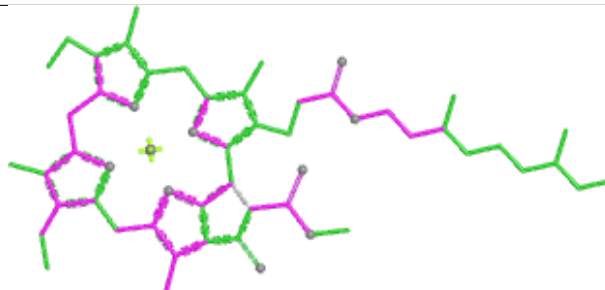


Rings

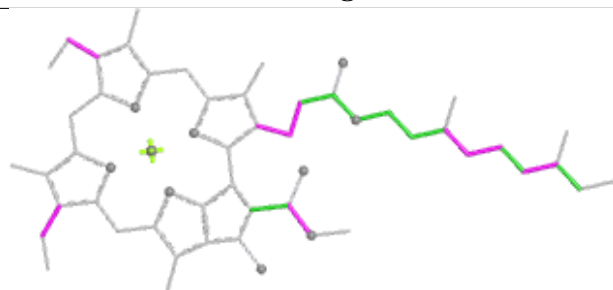
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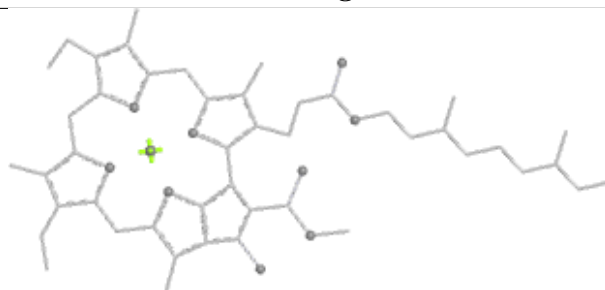
Bond lengths



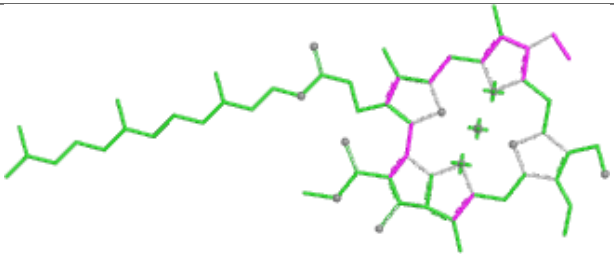
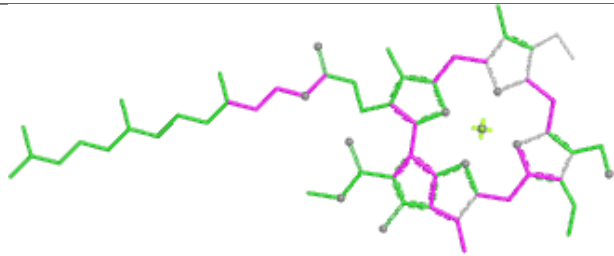
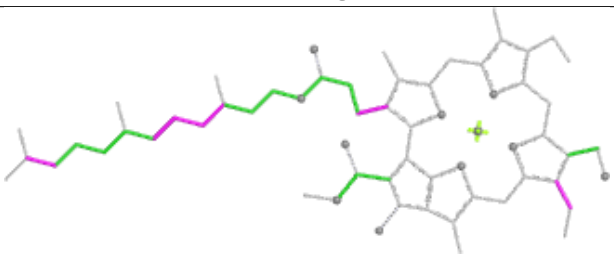
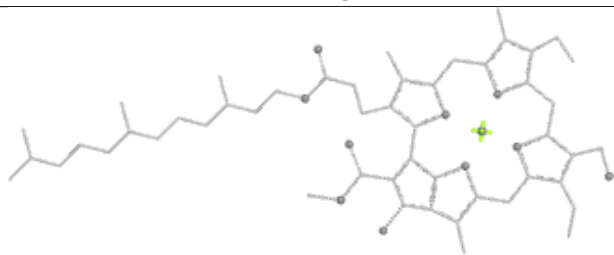
Bond angles

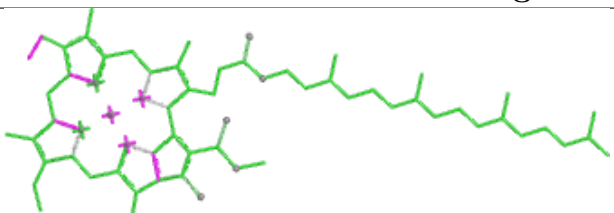
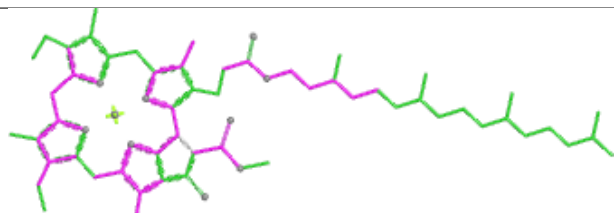
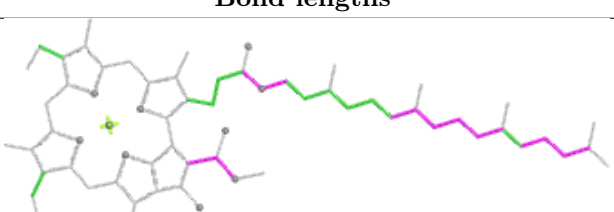
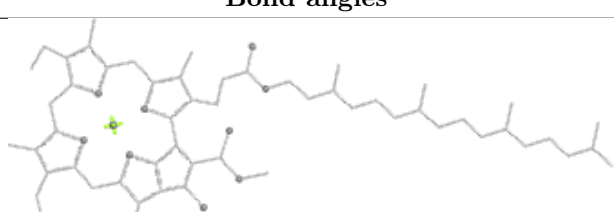


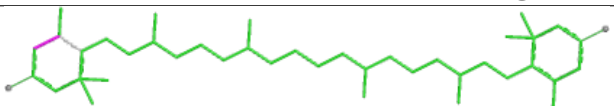
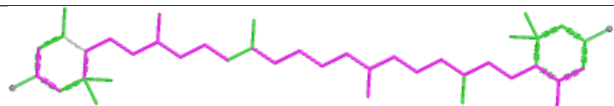
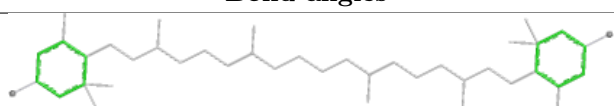
Torsions

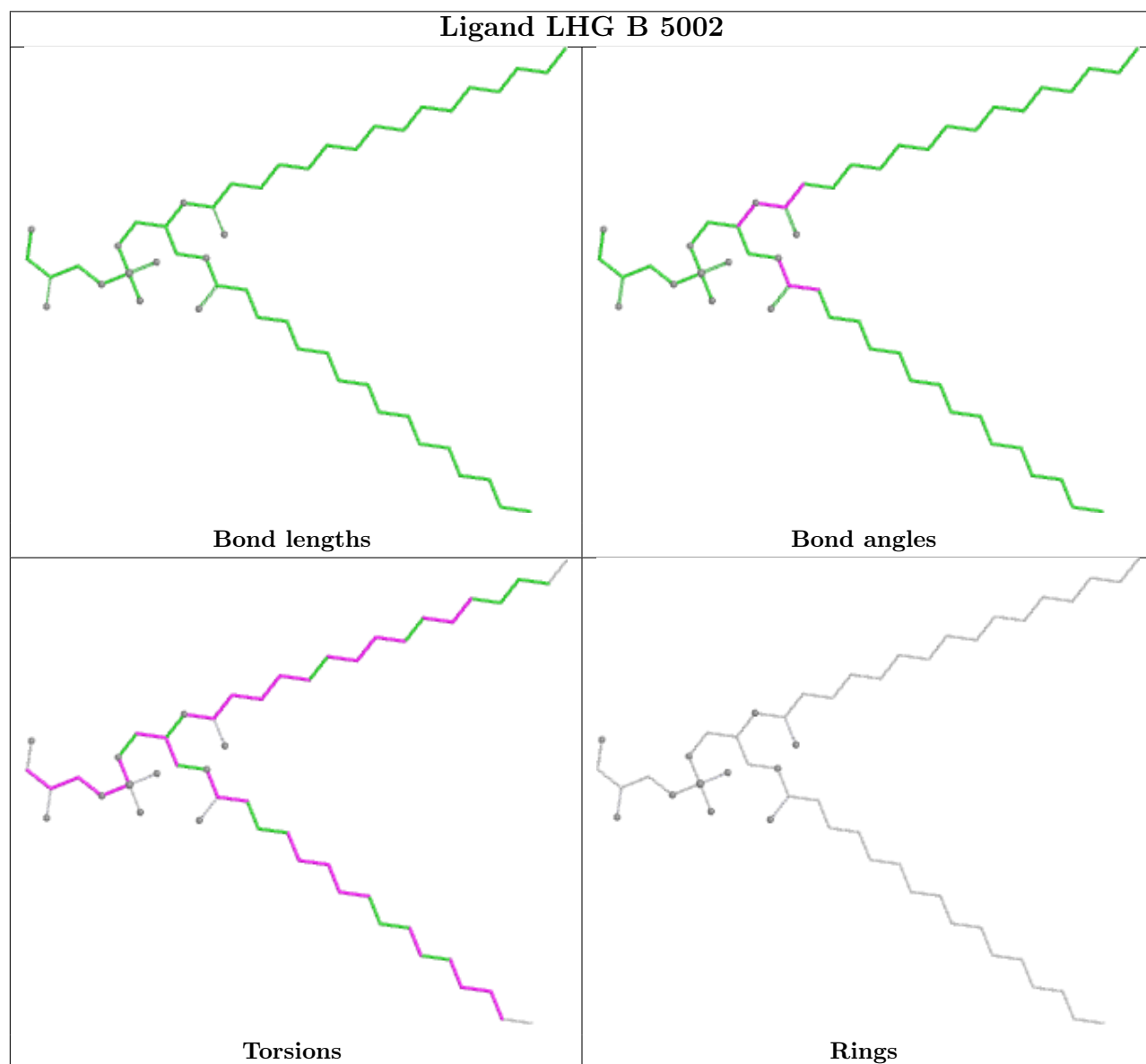
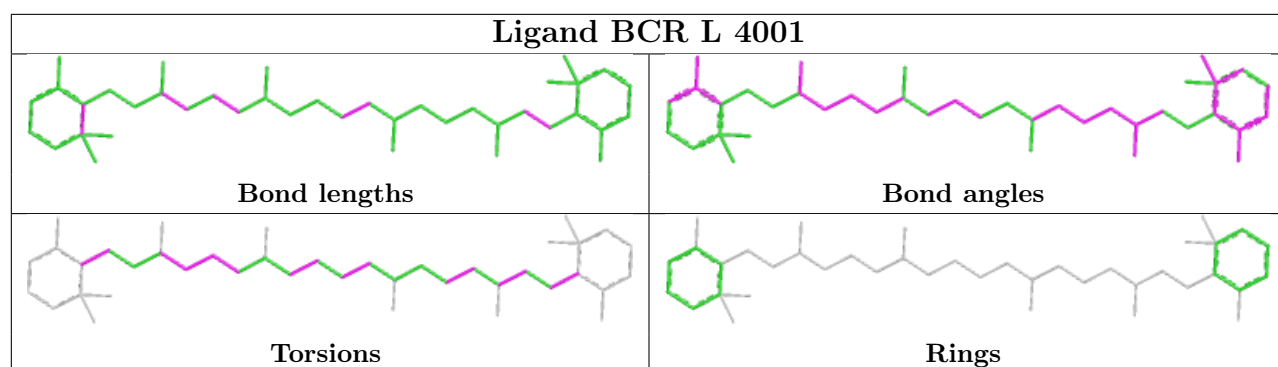


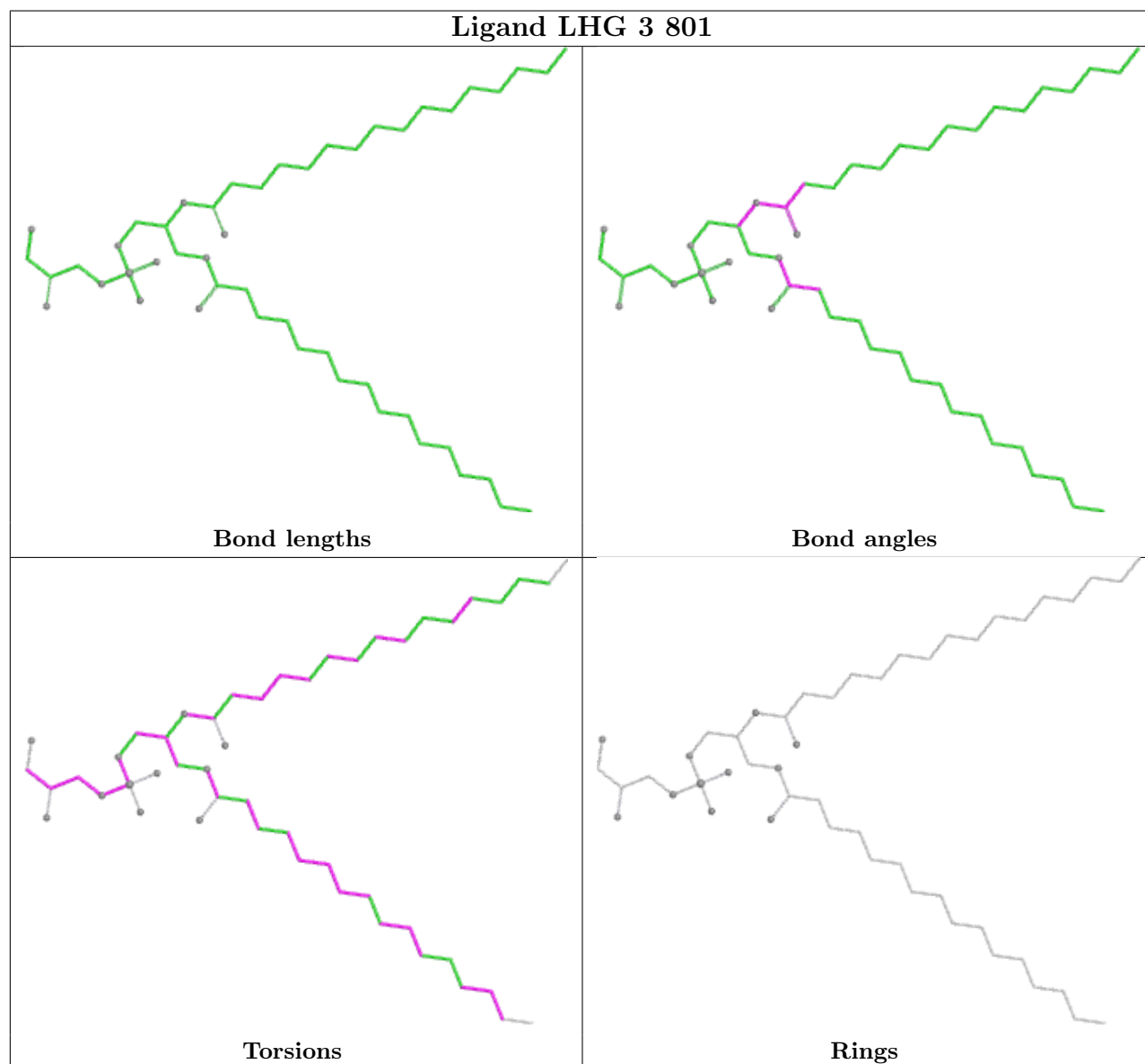
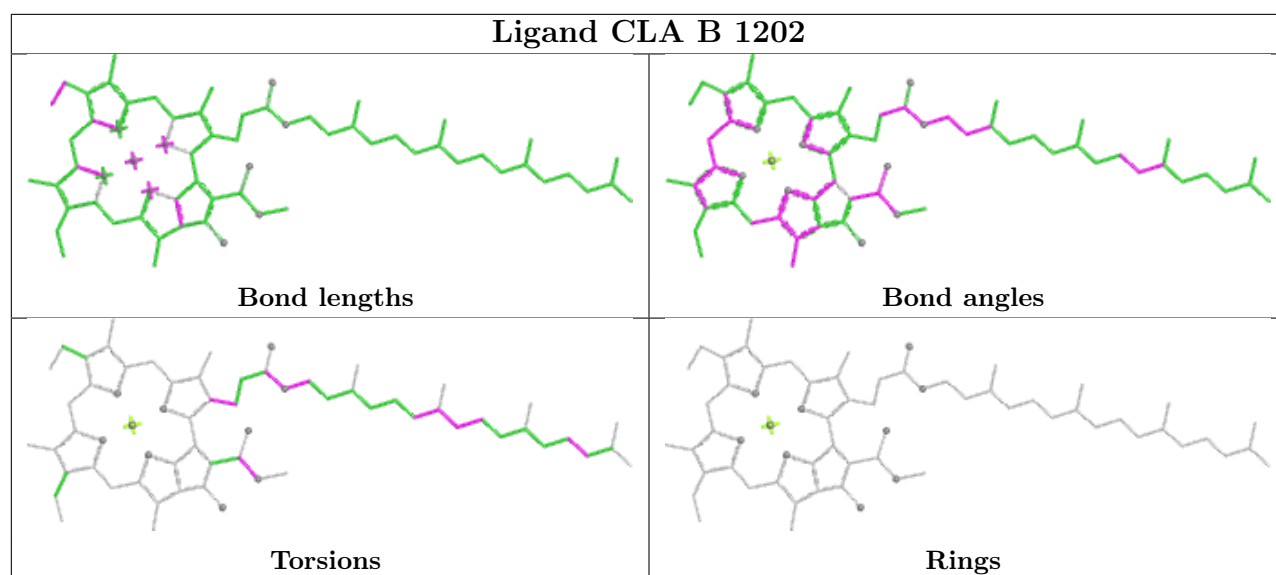
Rings

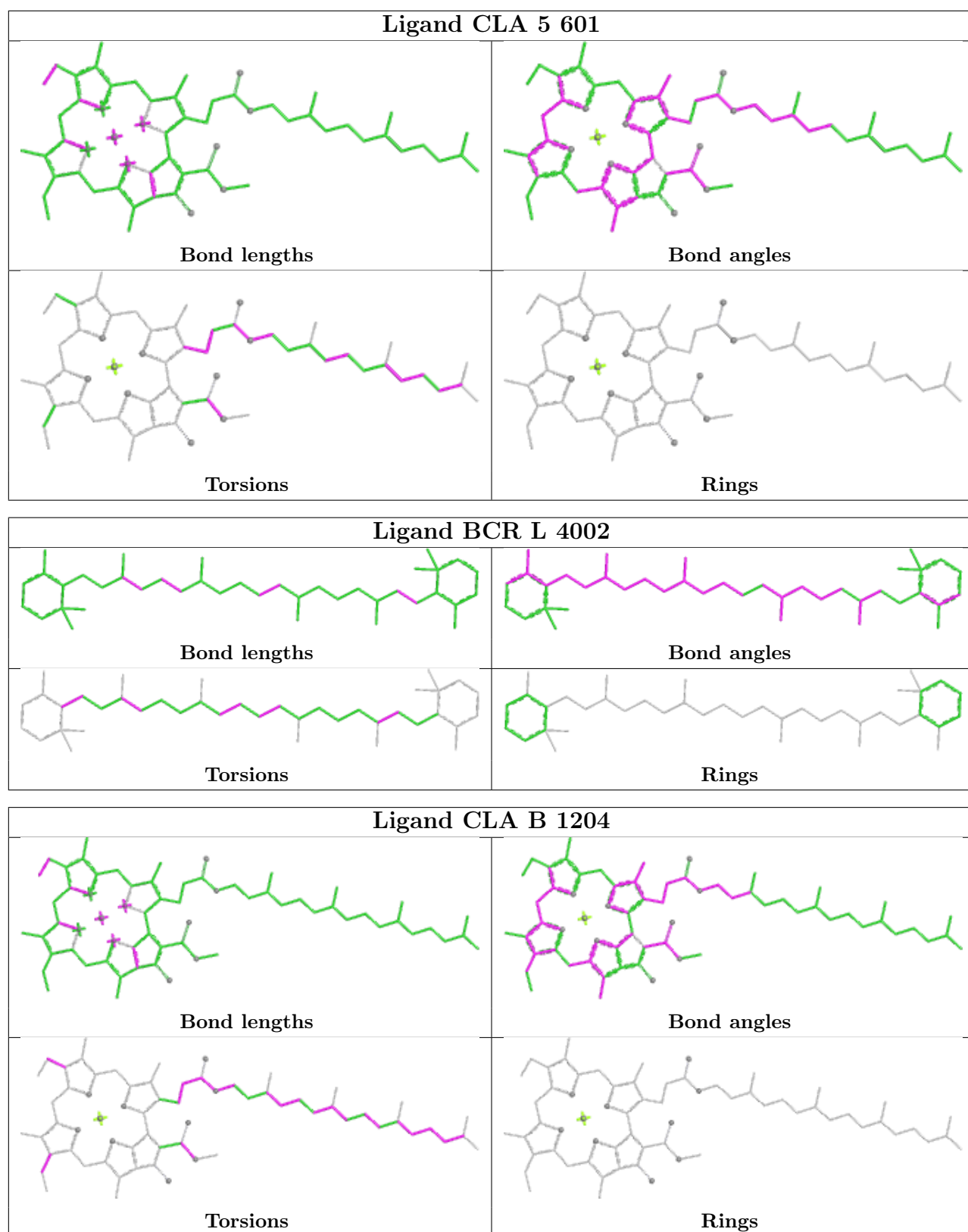
Ligand CHL 8 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

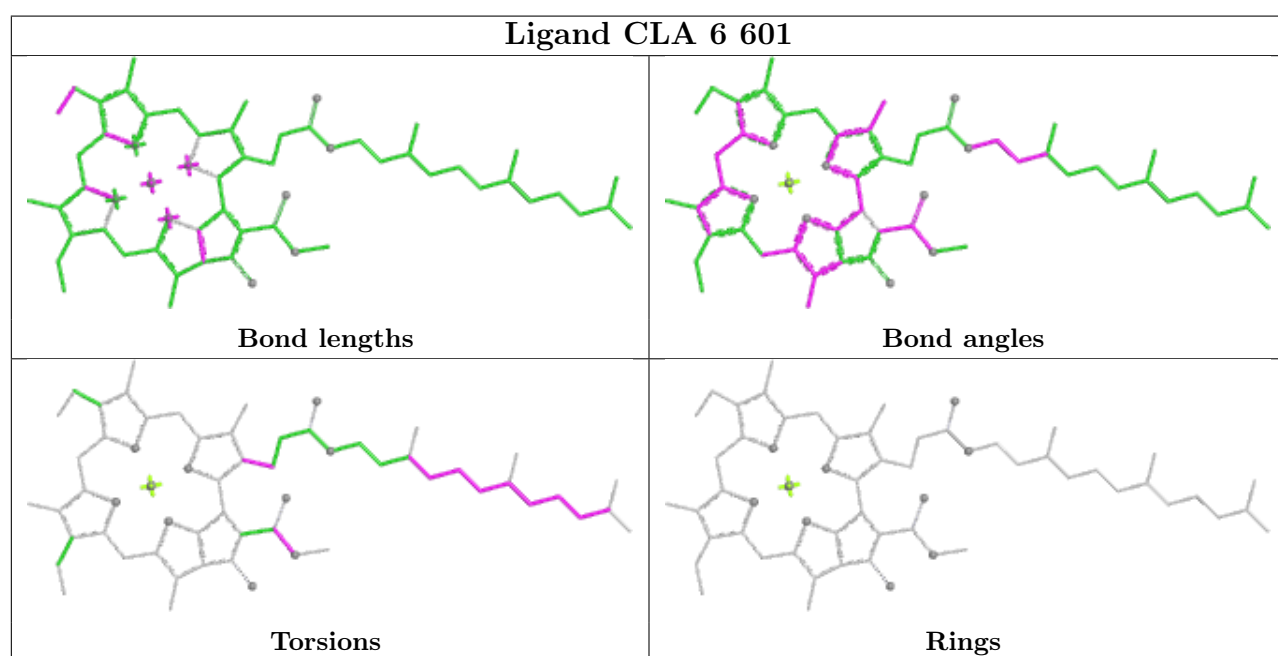
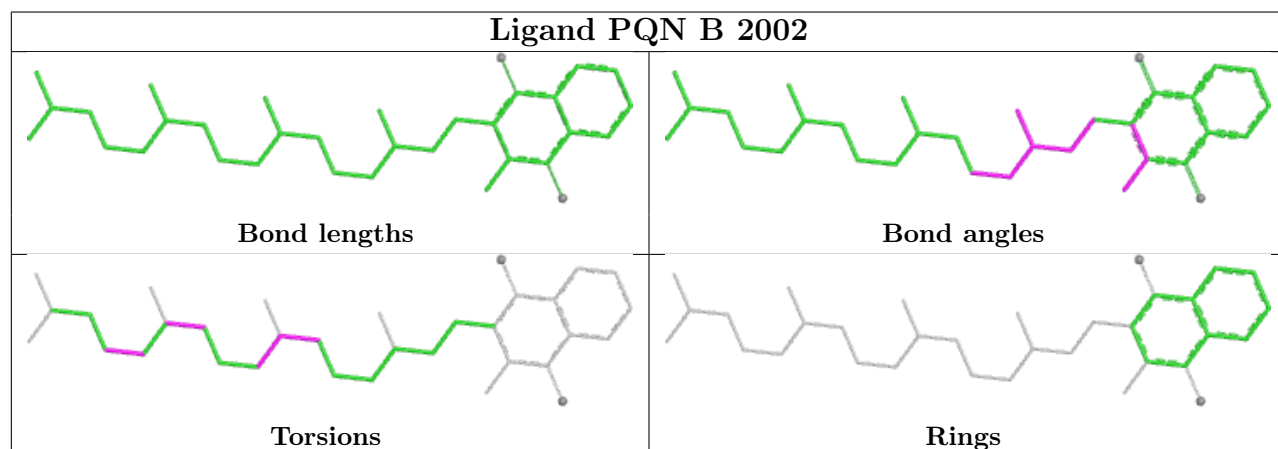
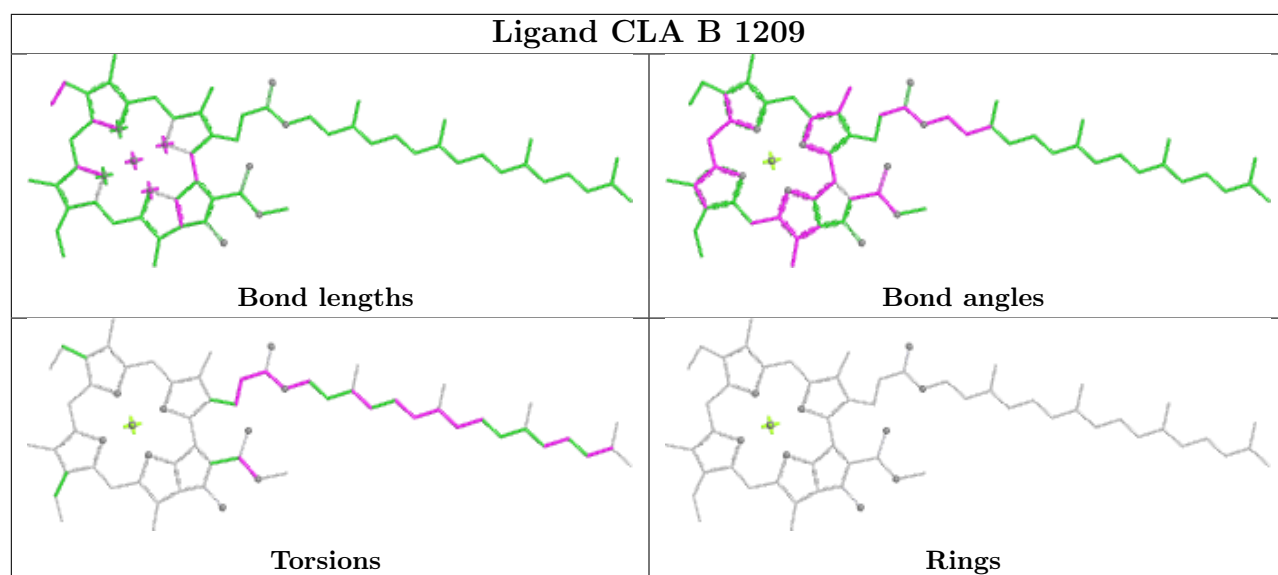
Ligand CLA 7 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

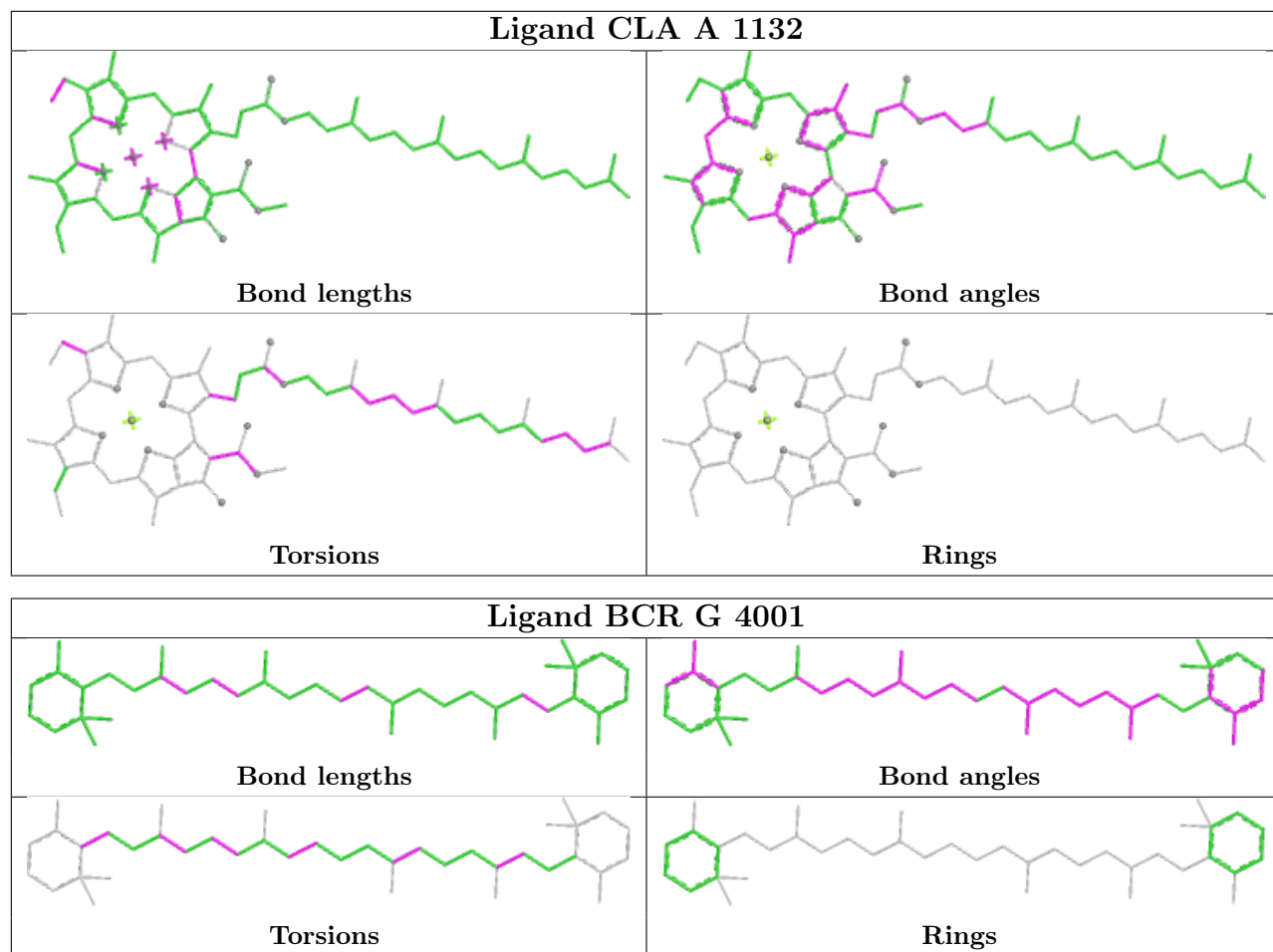
Ligand LUT 1 501	
	
Bond lengths	Bond angles
	
Torsions	Rings



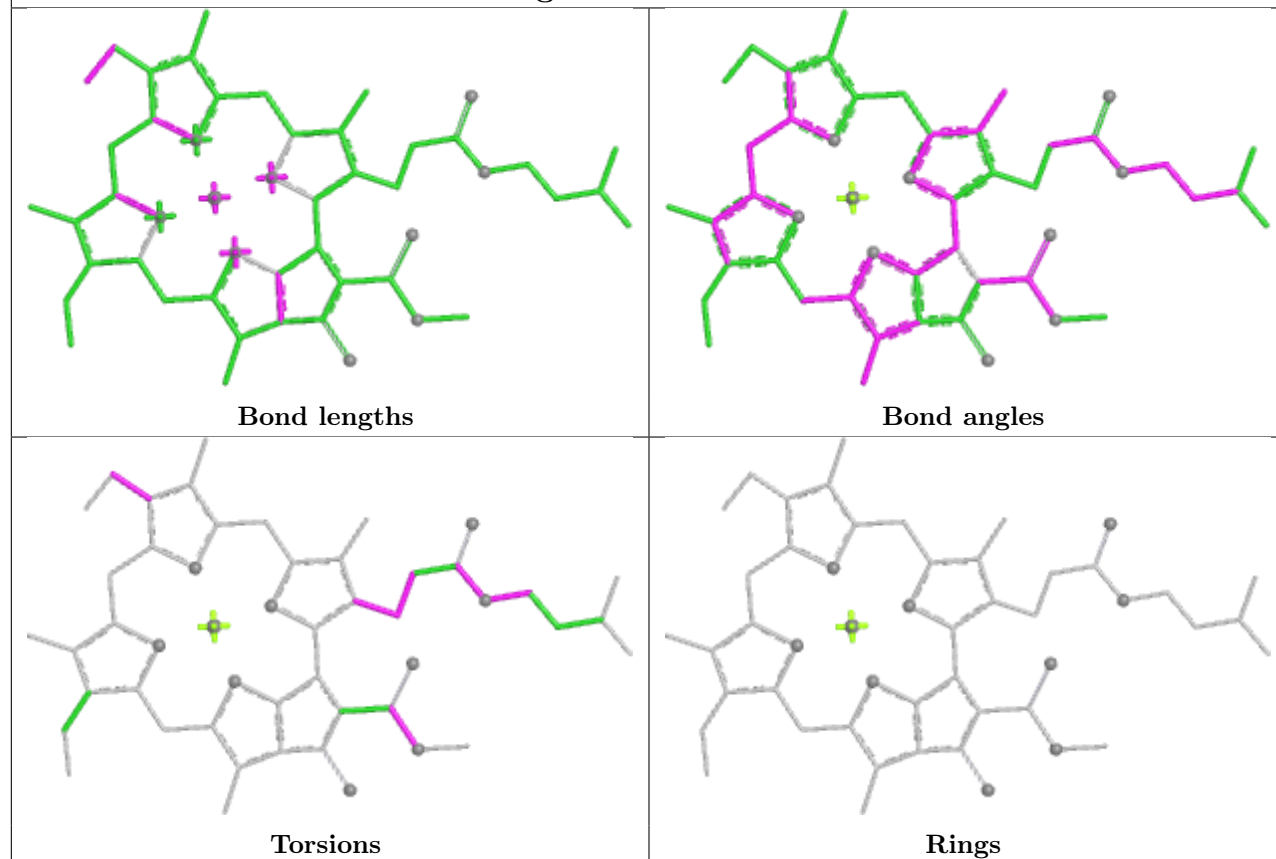




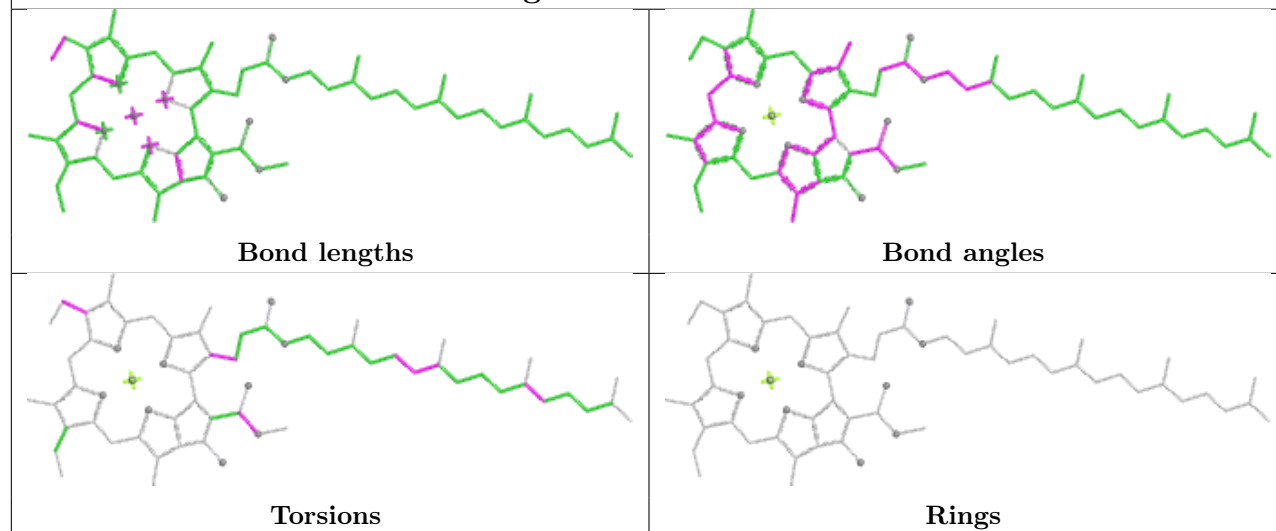


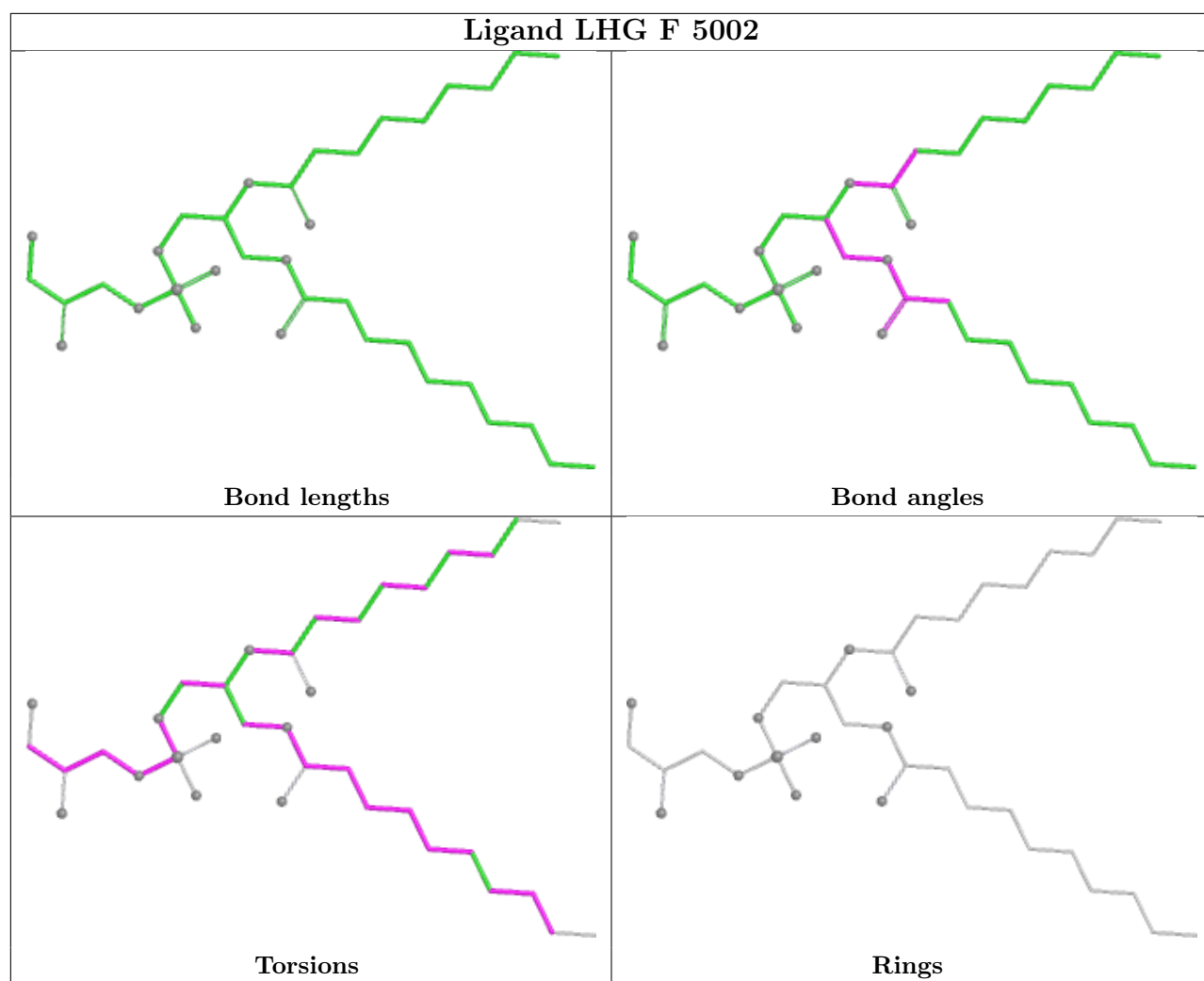


Ligand CLA a 611

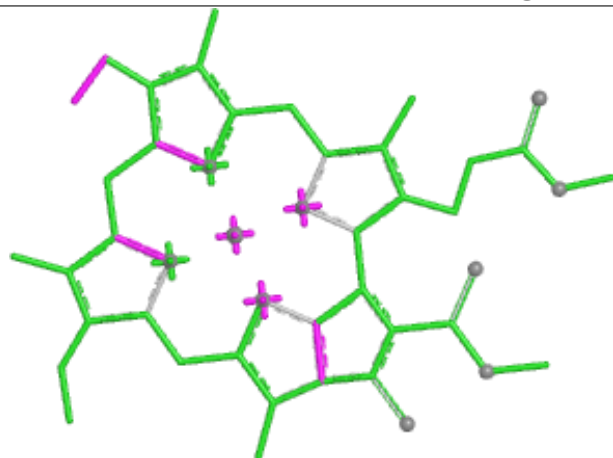


Ligand CLA B 1240

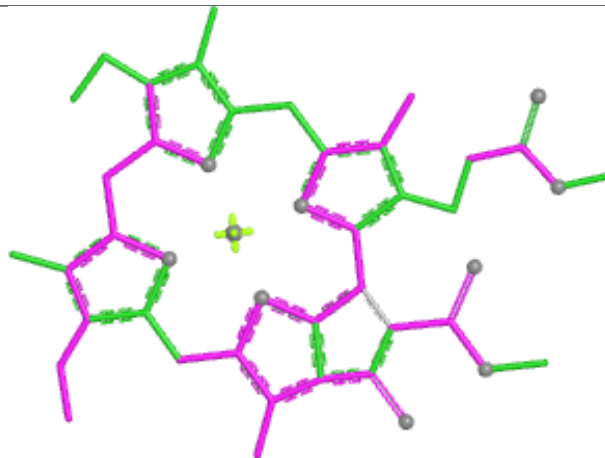




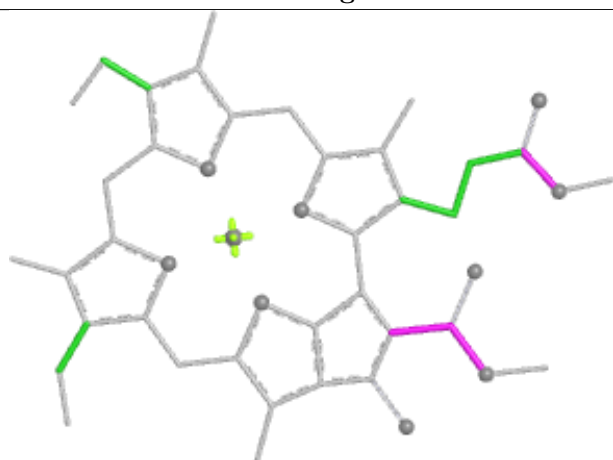
Ligand CLA 4 605



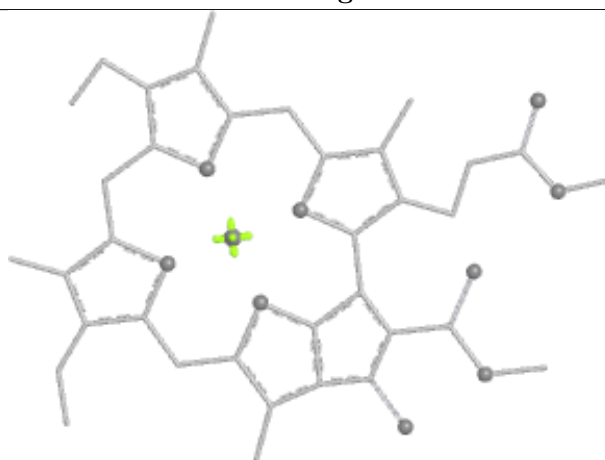
Bond lengths



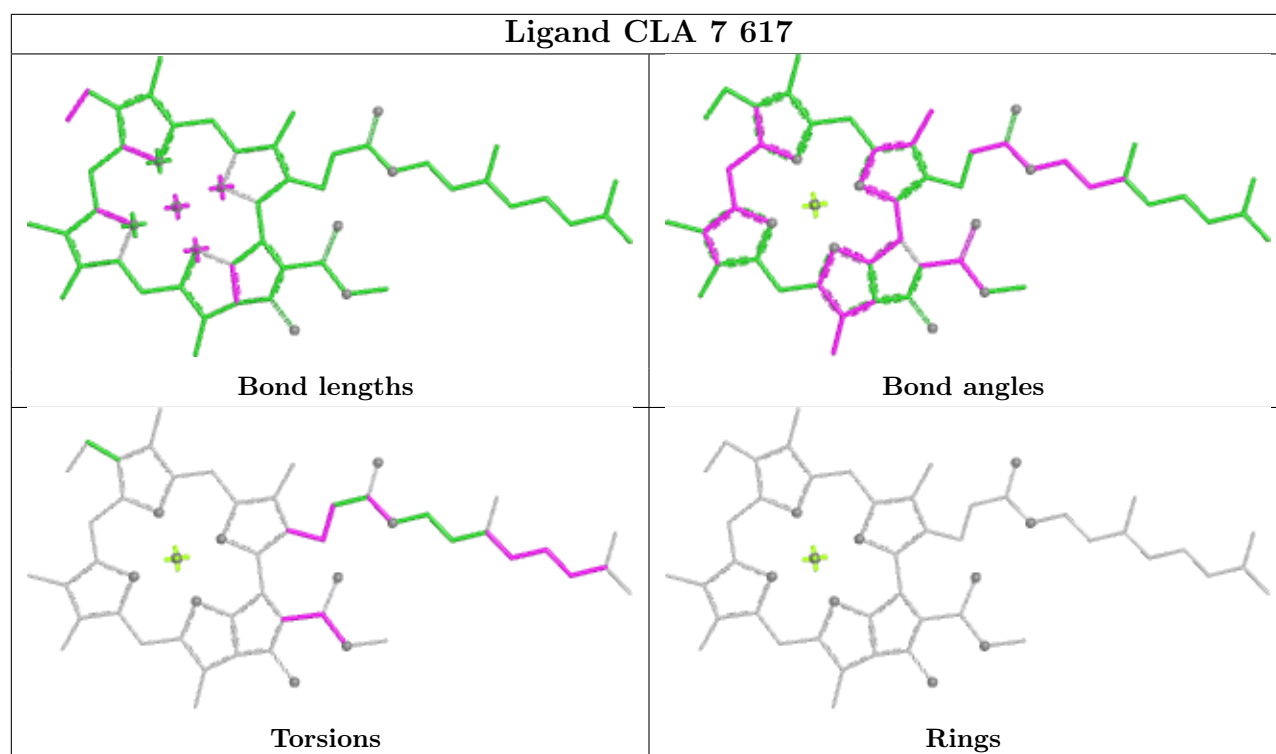
Bond angles



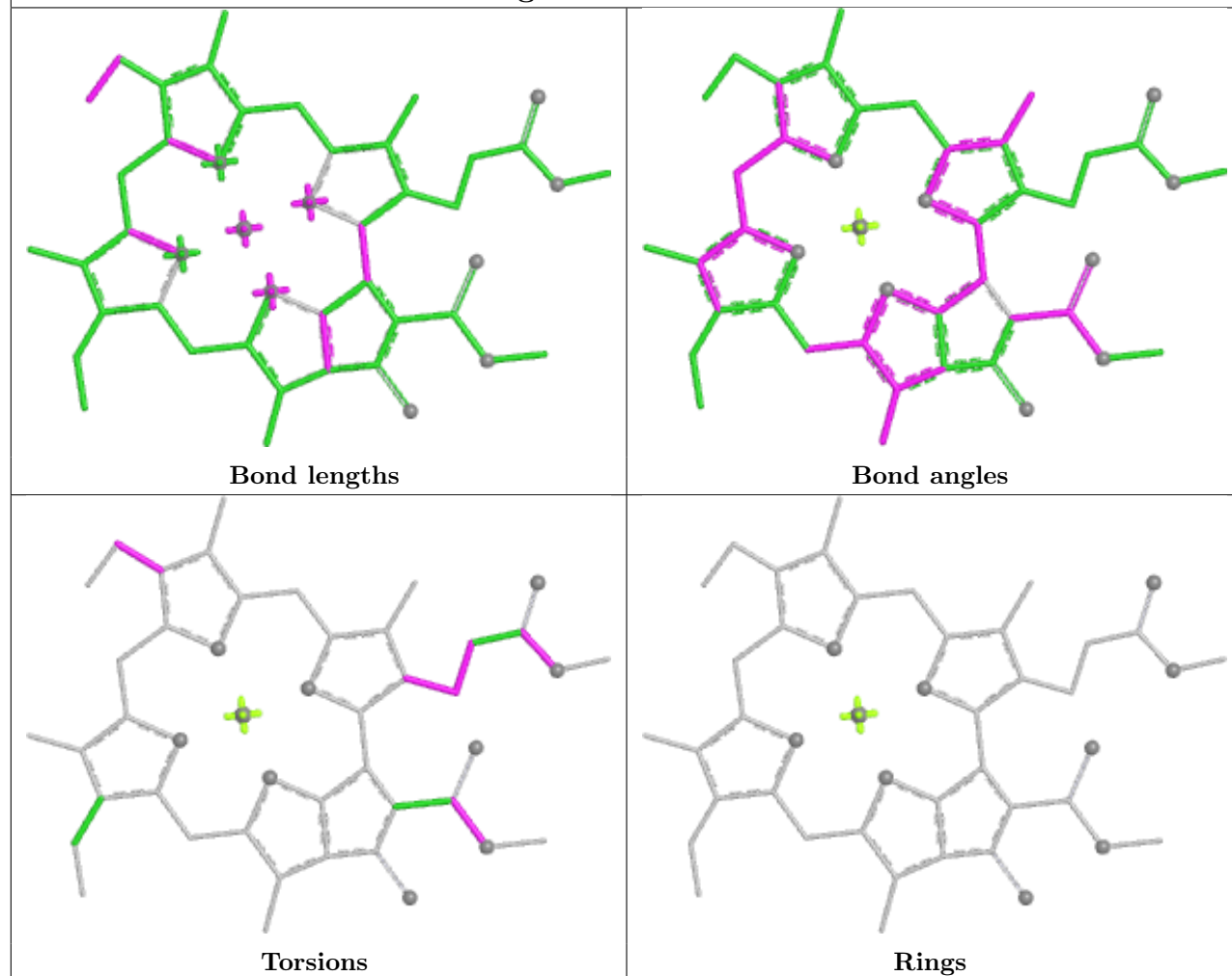
Torsions

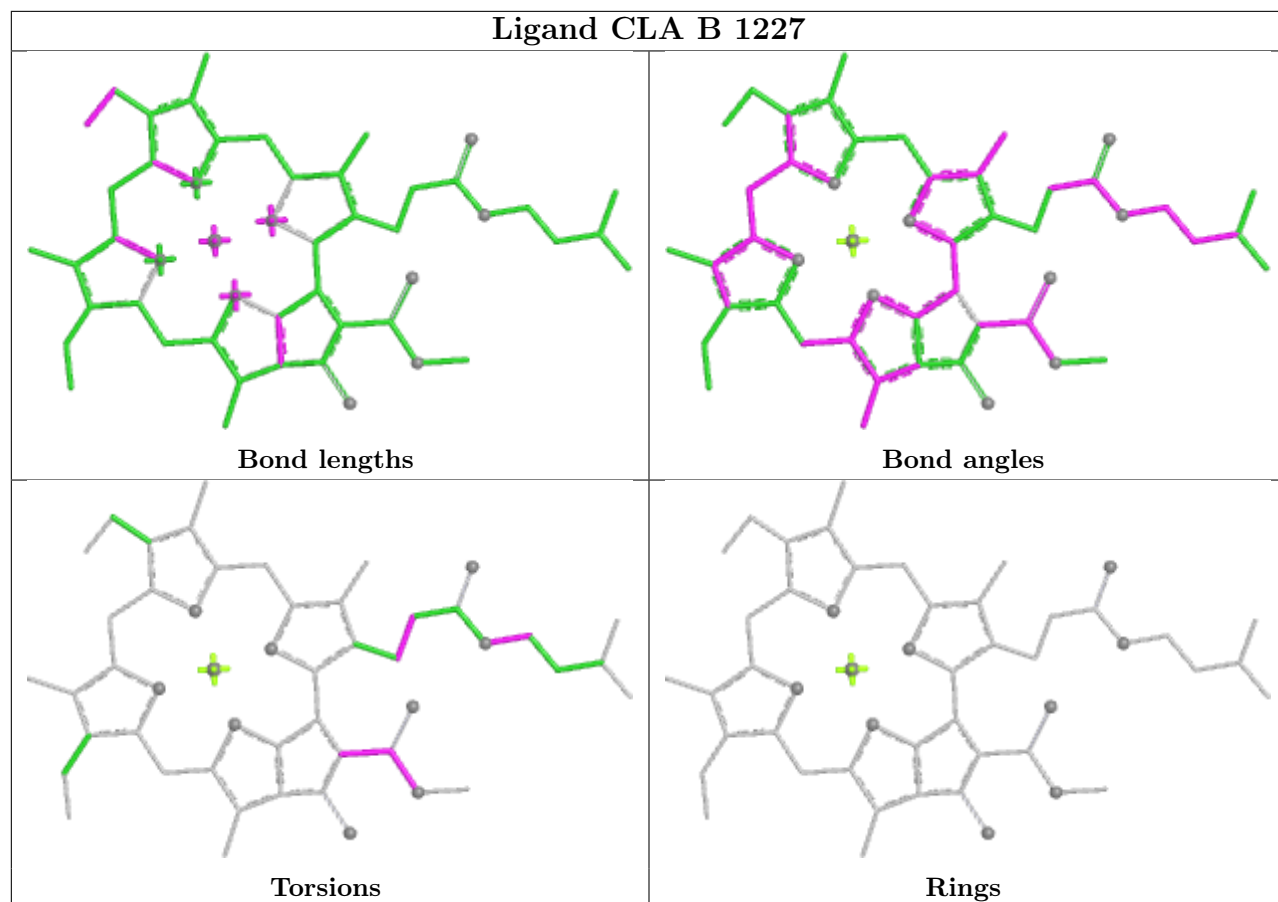


Rings

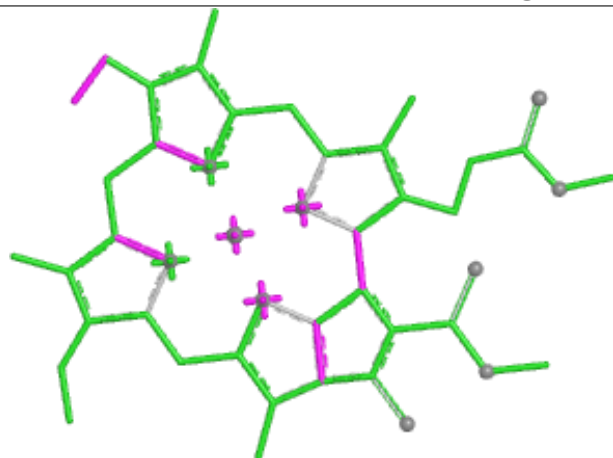


Ligand CLA 5 616

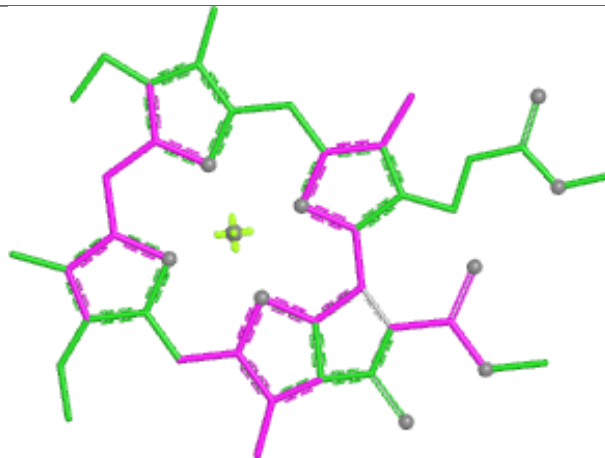




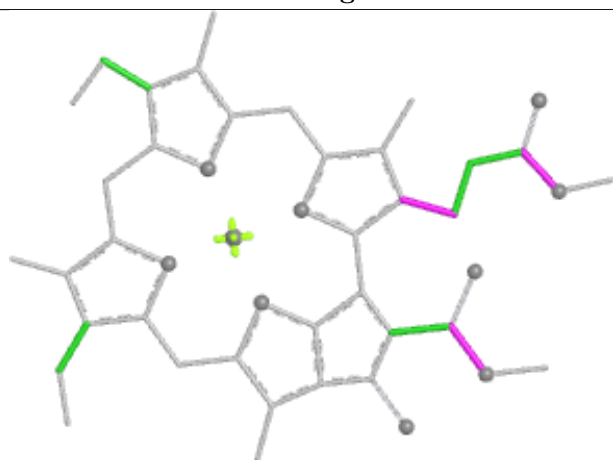
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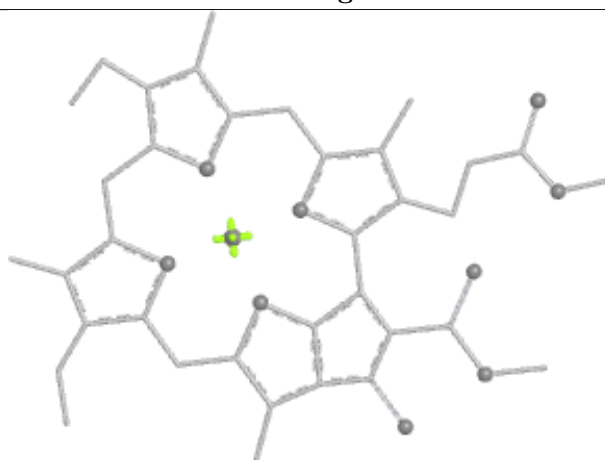
Bond lengths



Bond angles

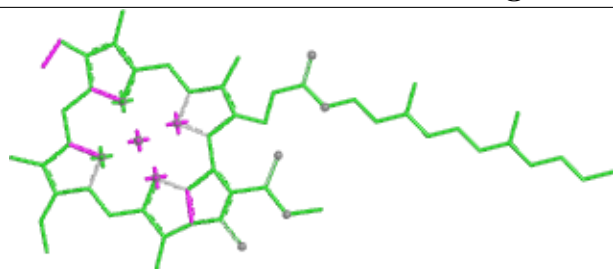


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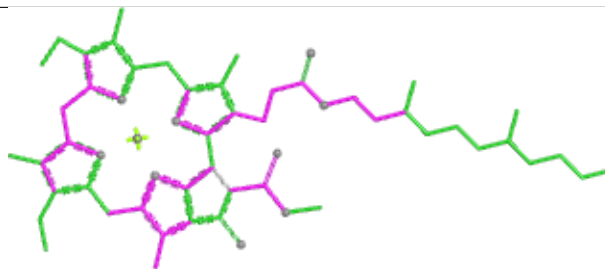


Rings

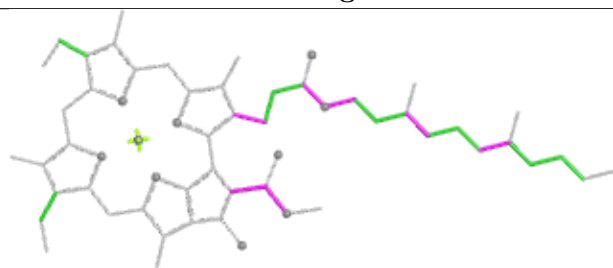
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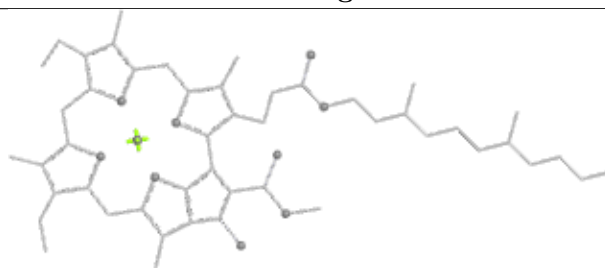
Bond lengths



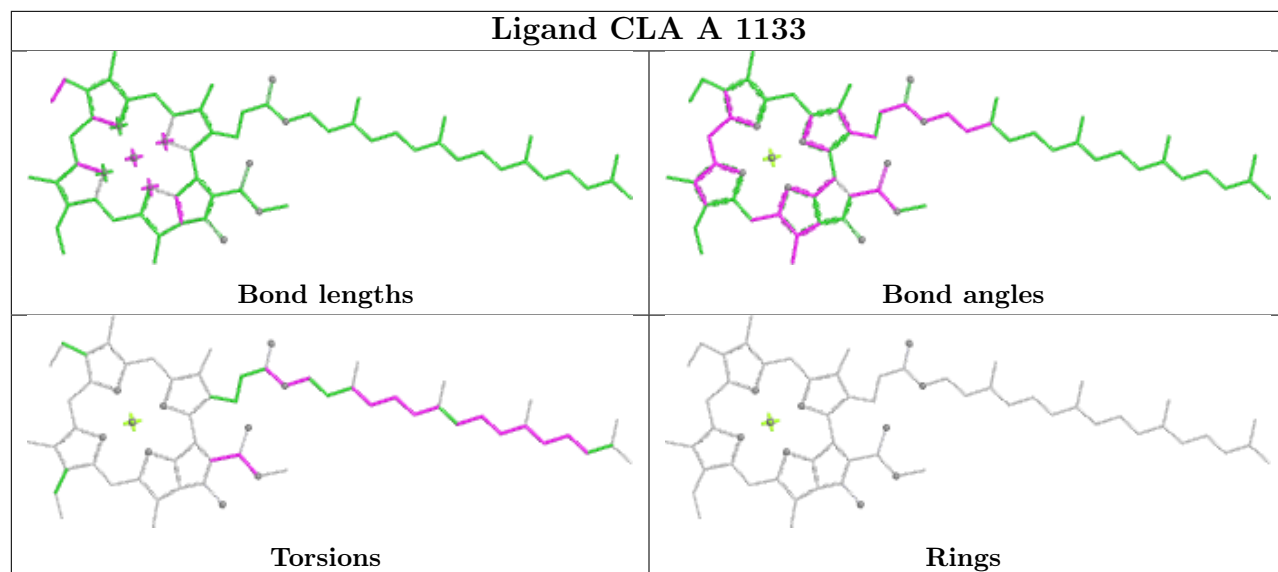
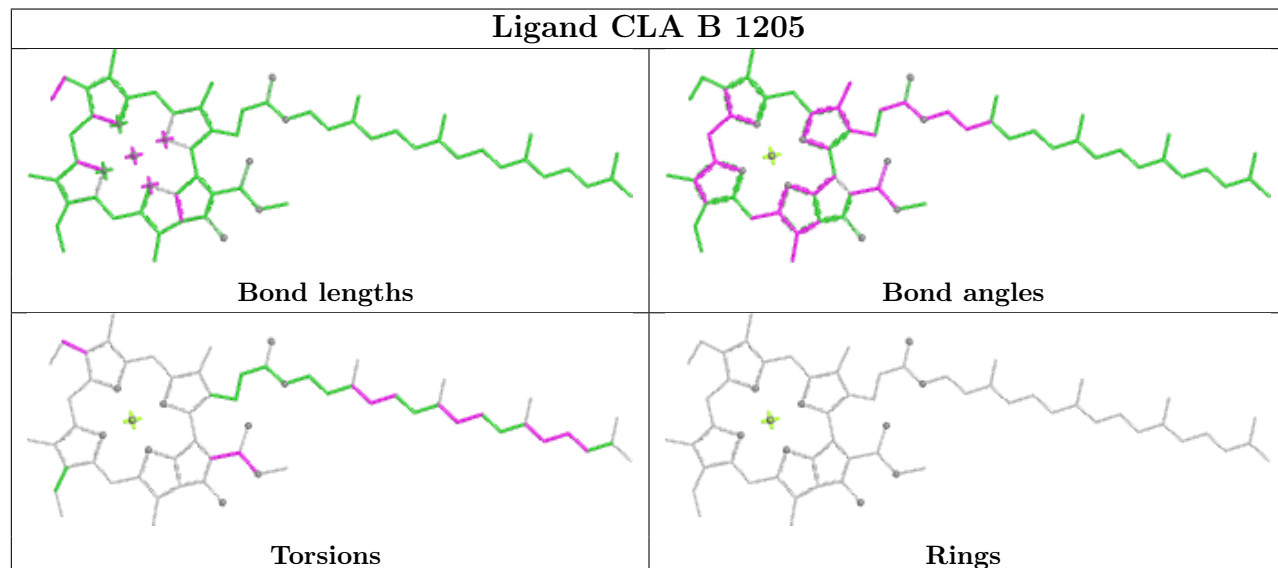
Bond angles



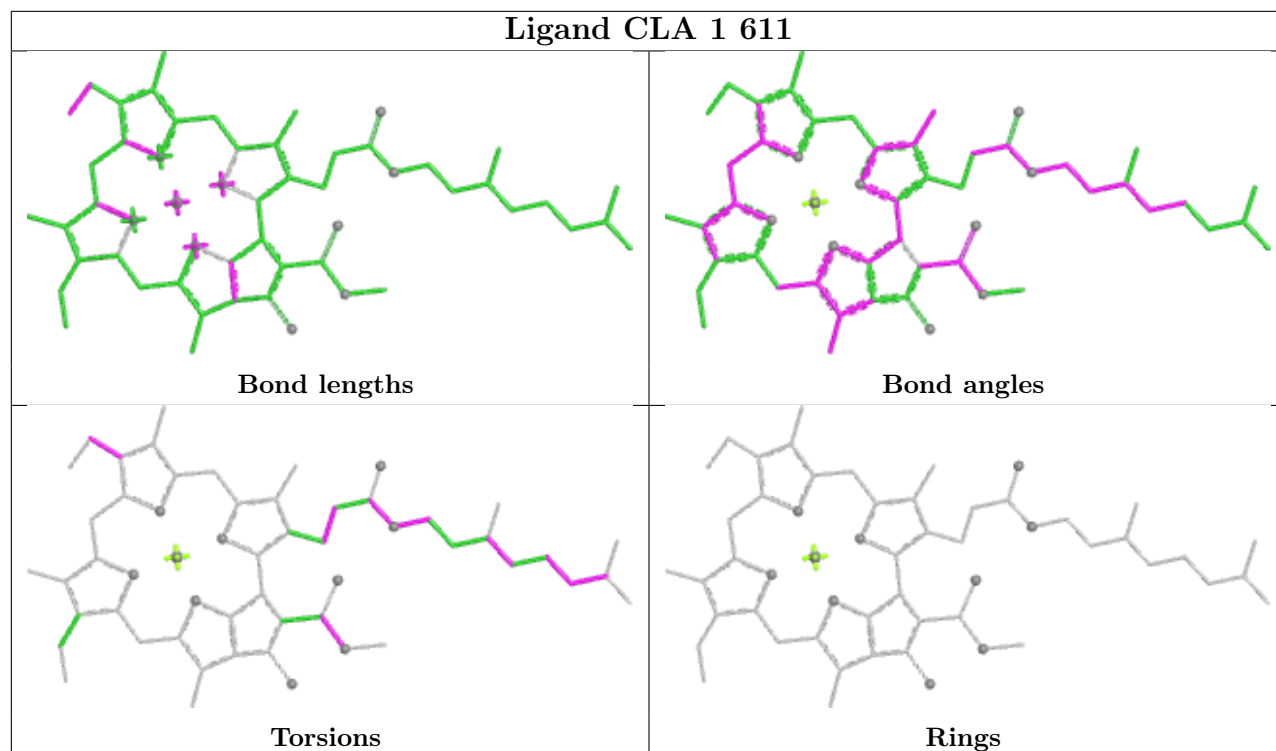
Torsions



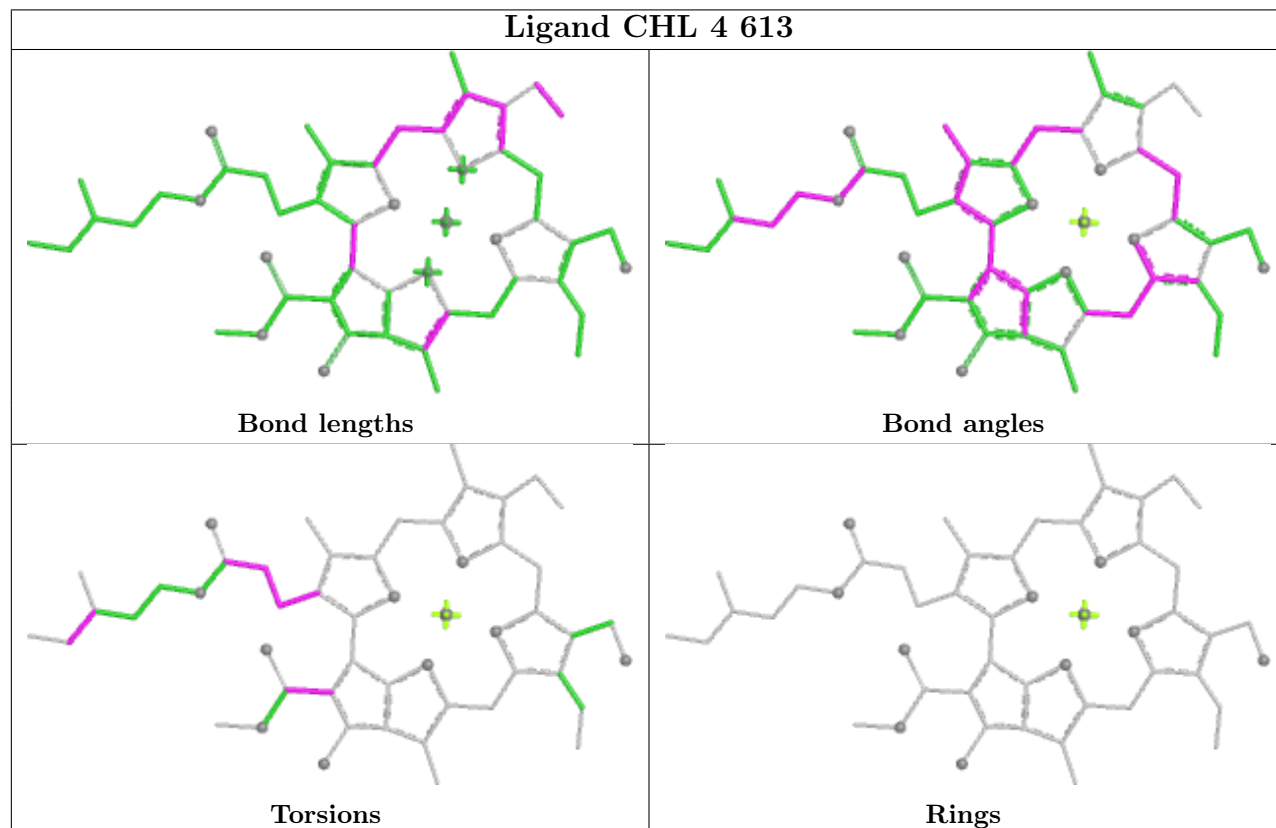
Rings

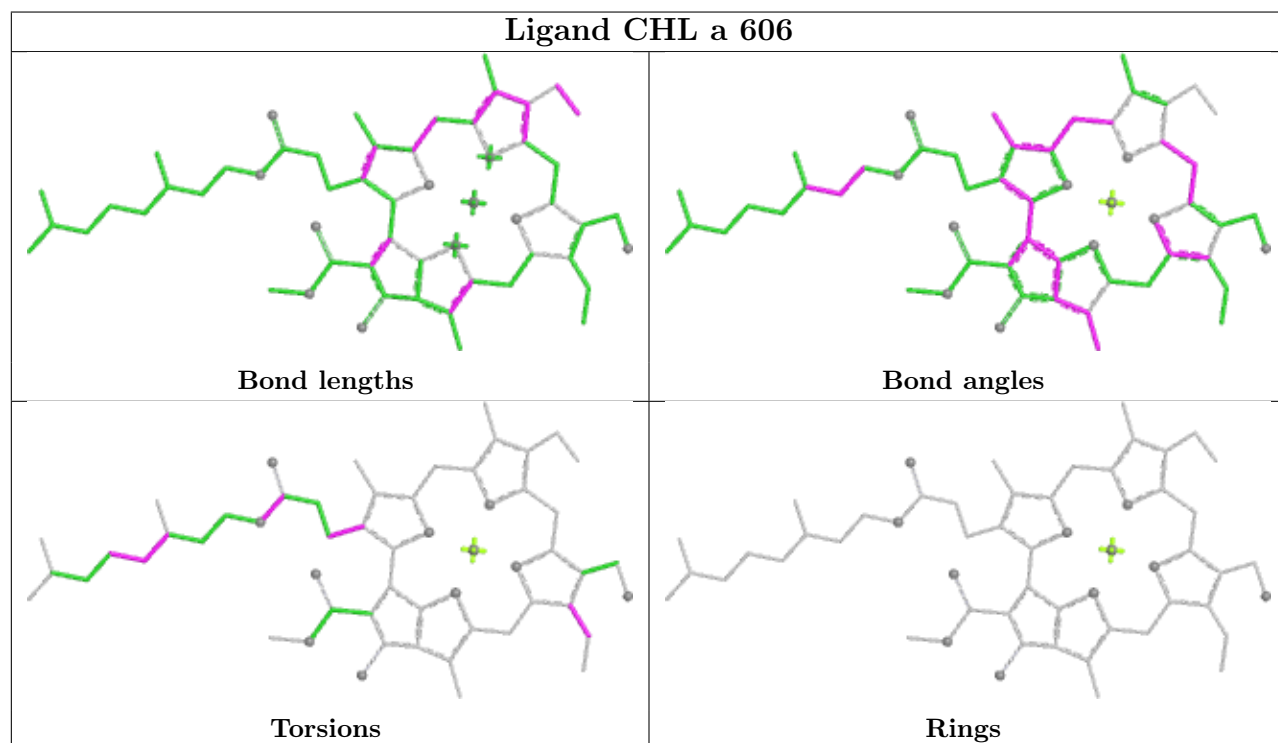
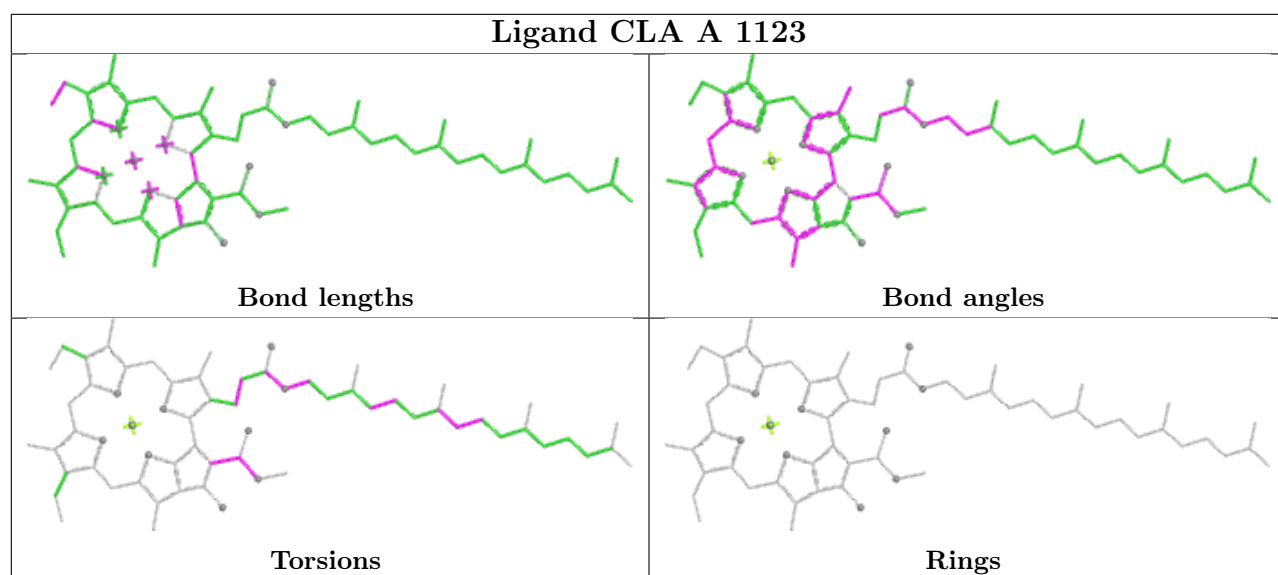
Ligand CLA A 1133**Ligand CLA B 1205**

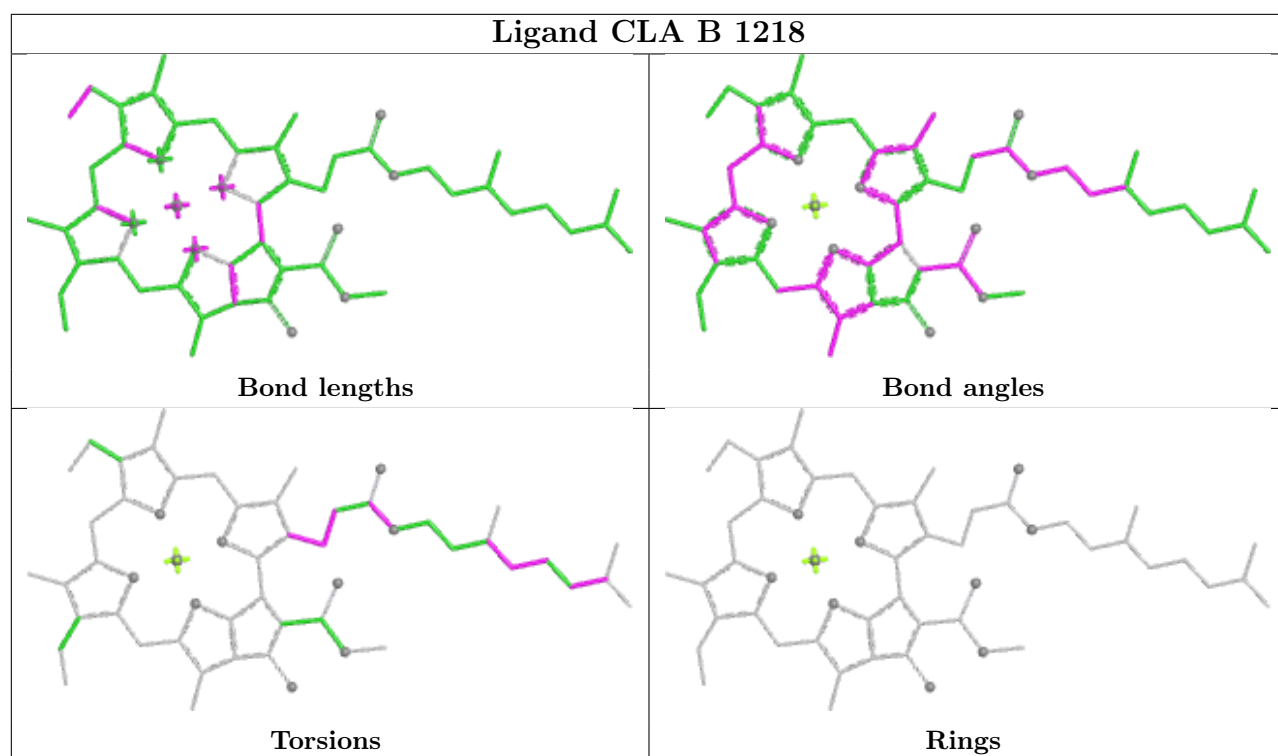
Ligand CLA 1 611



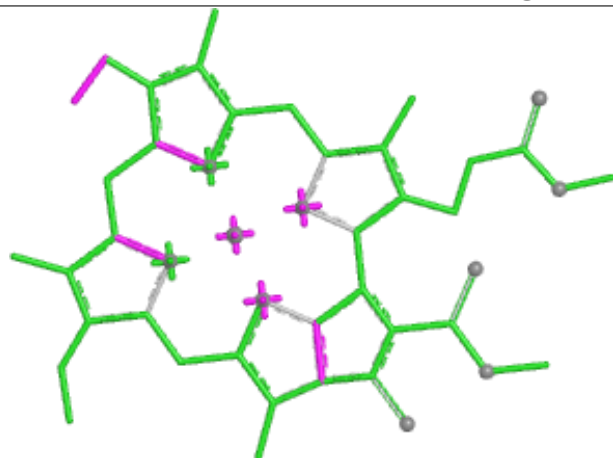
Ligand CHL 4 613



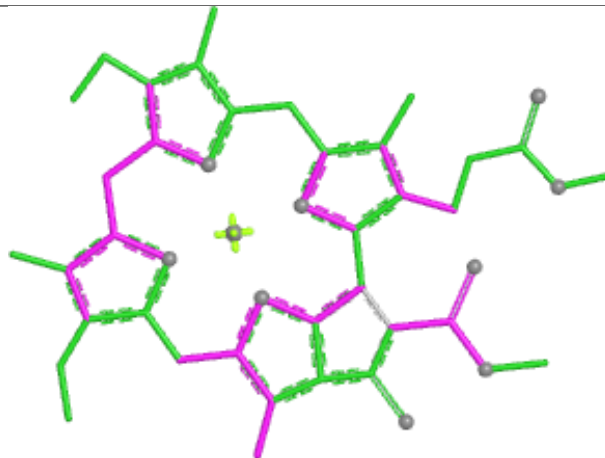




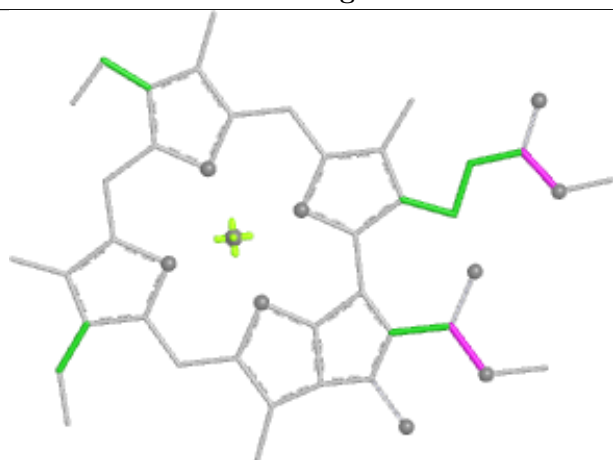
Ligand CLA 8 607



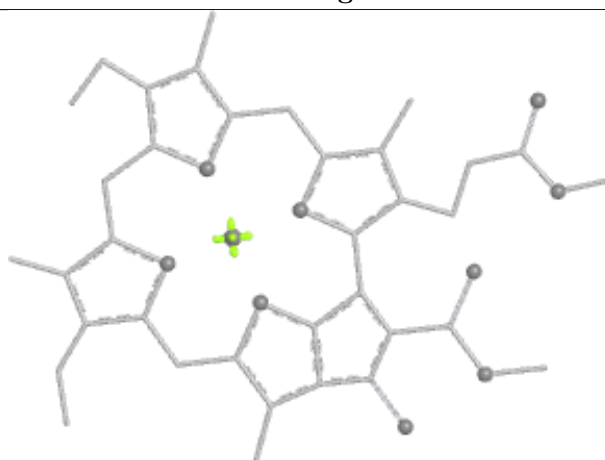
Bond lengths



Bond angles

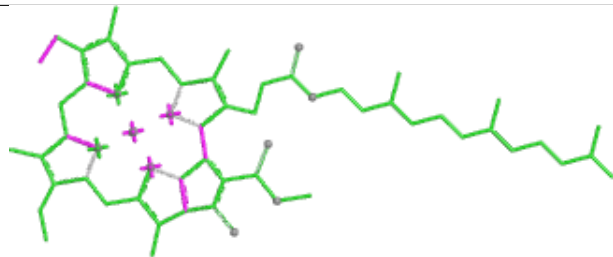


Torsions

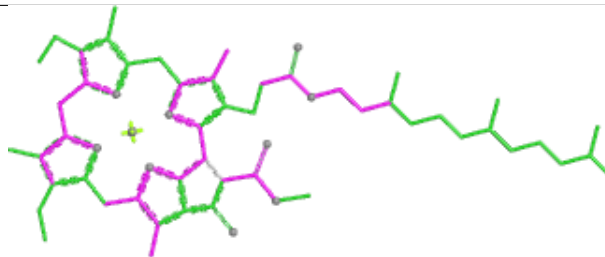


Rings

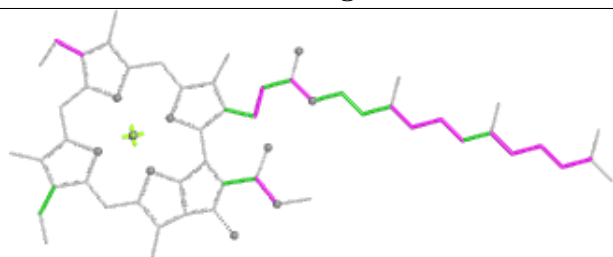
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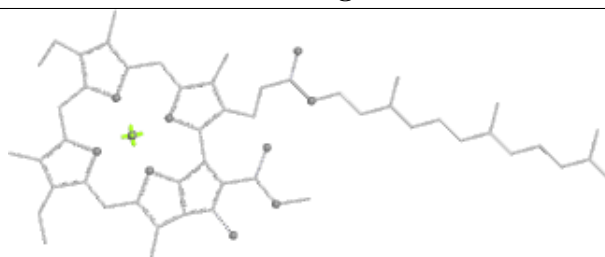
Bond lengths



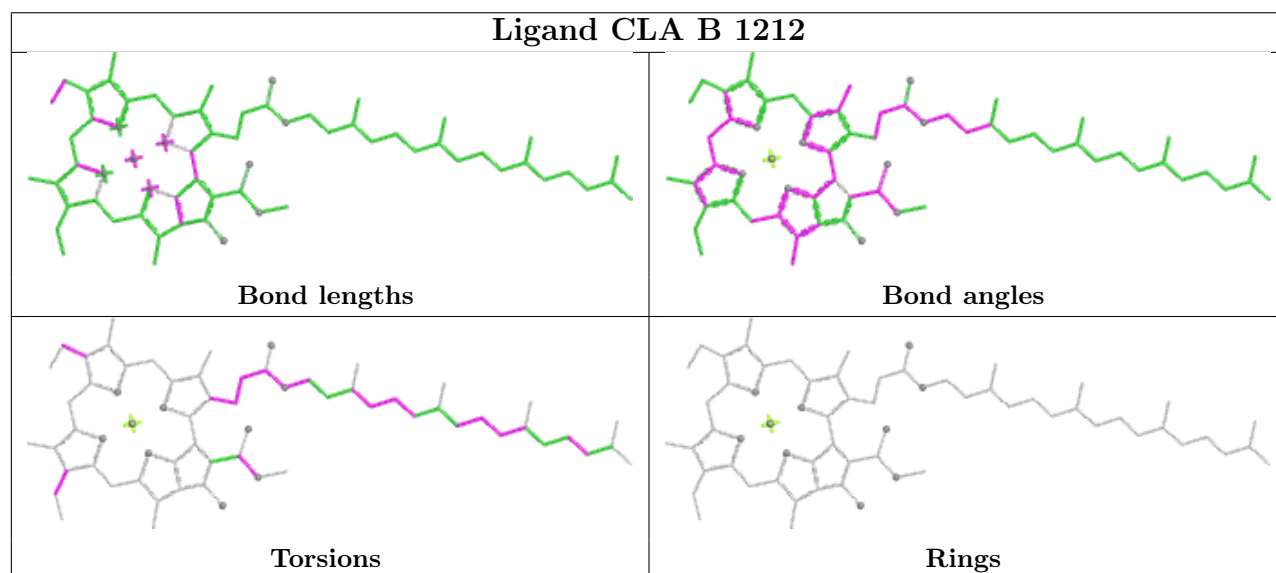
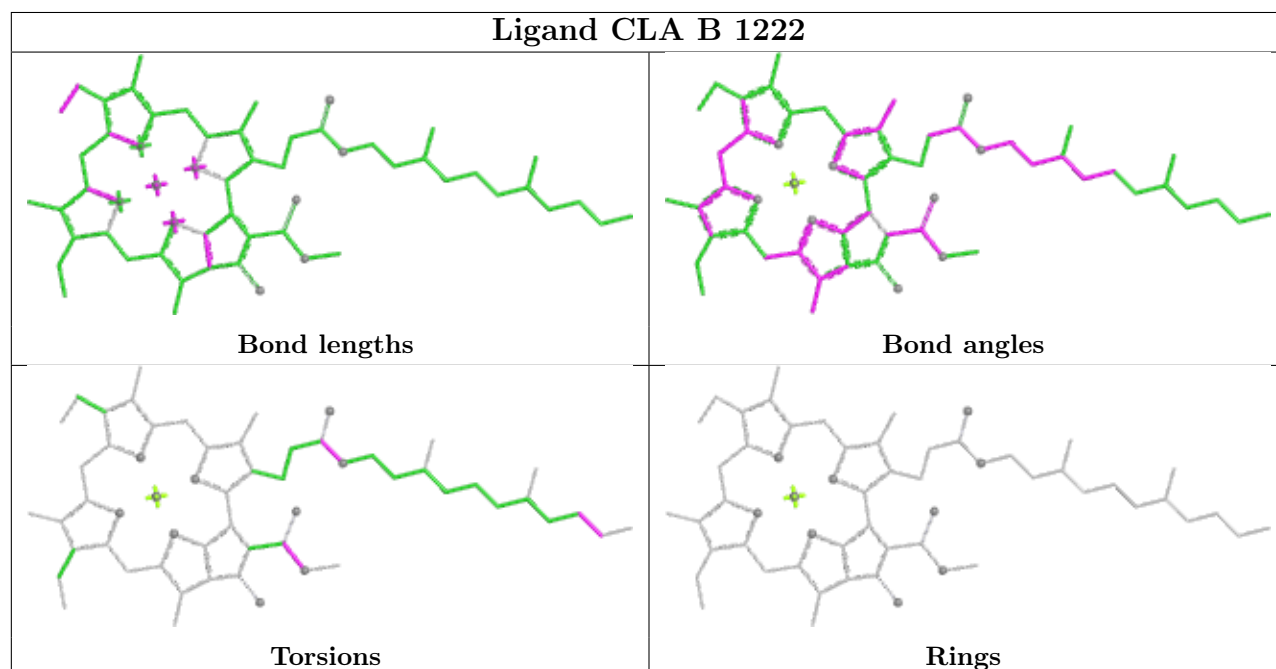
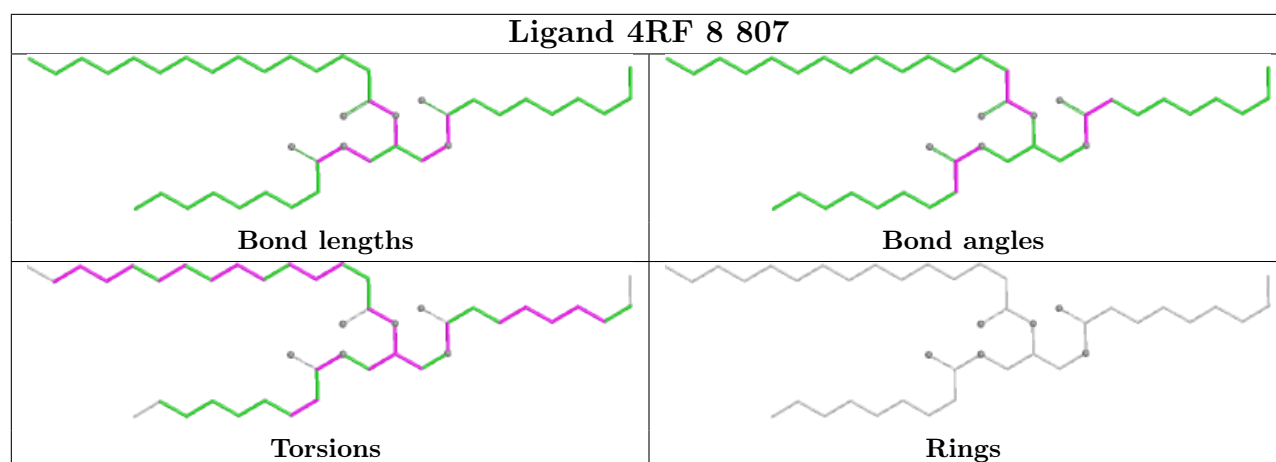
Bond angles



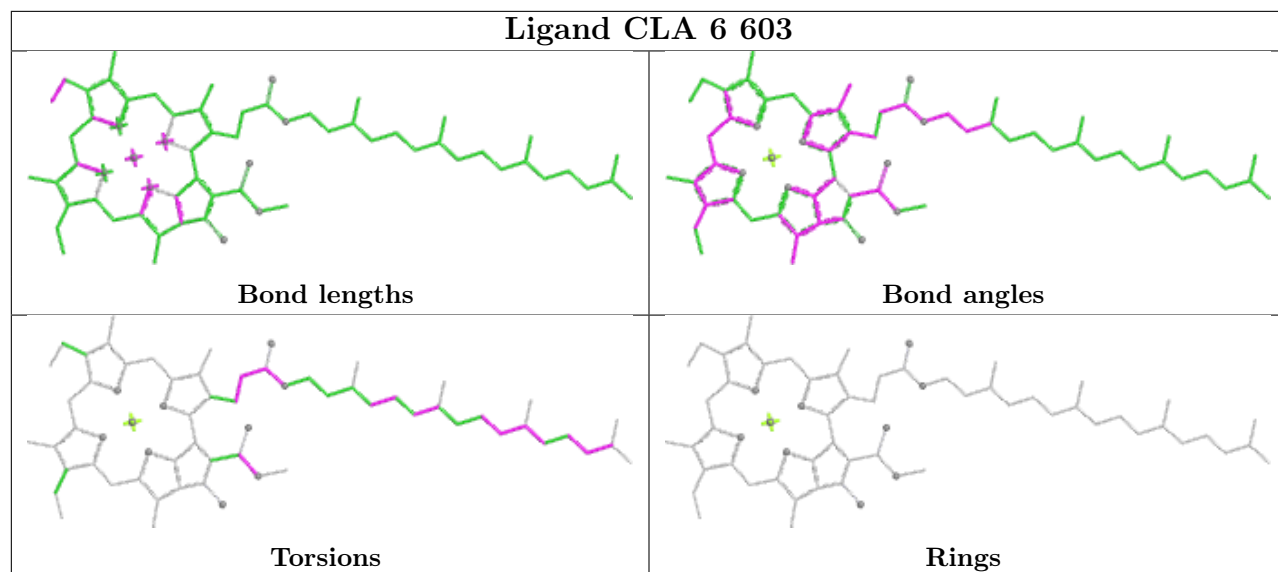
Torsions



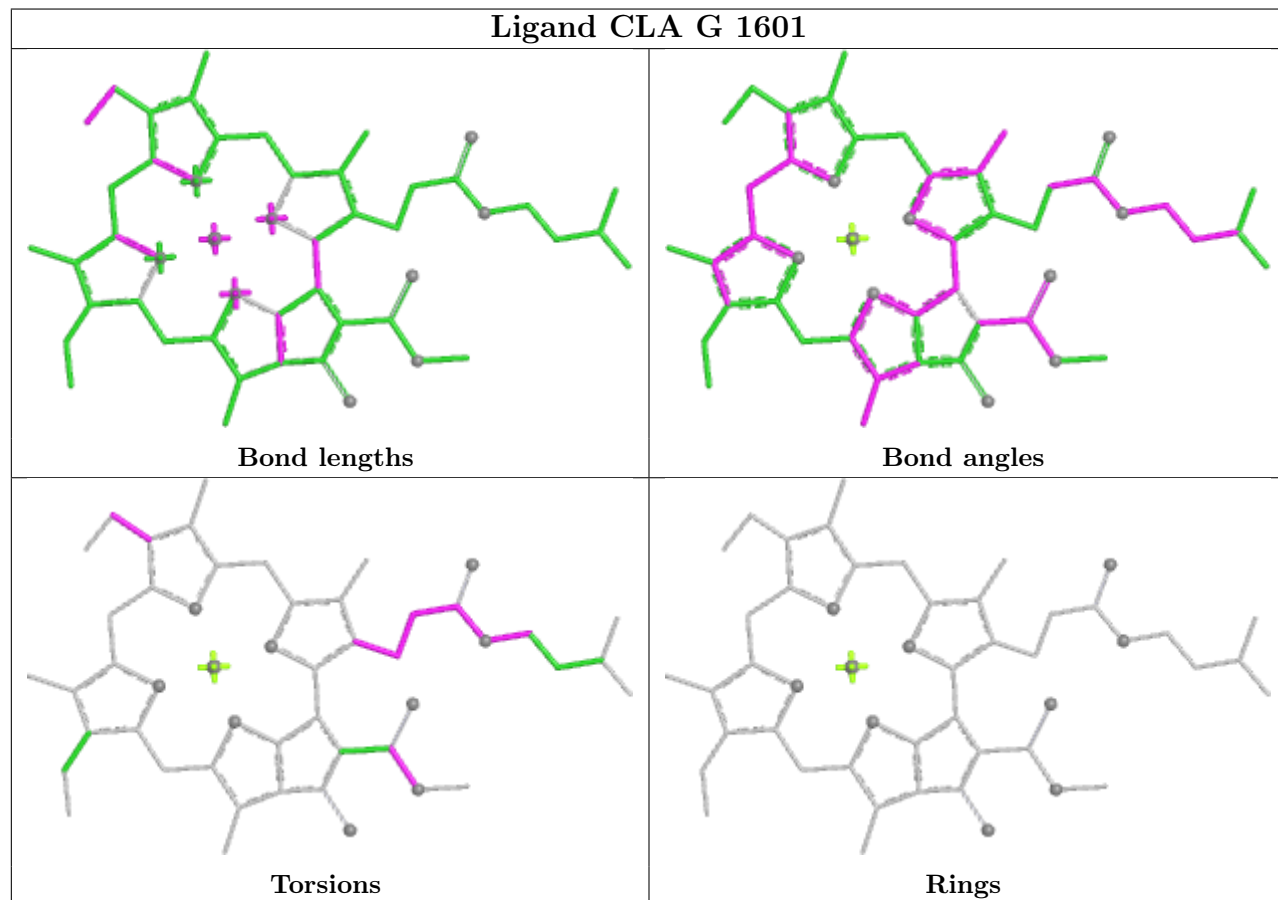
Rings

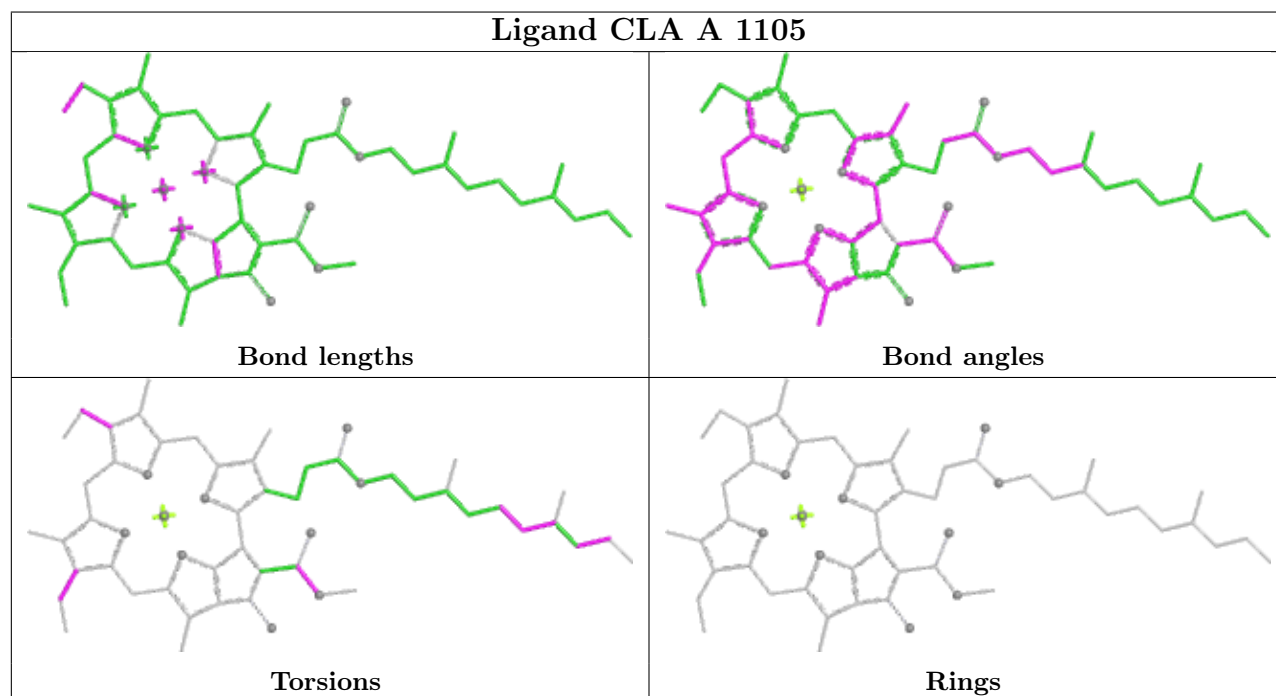
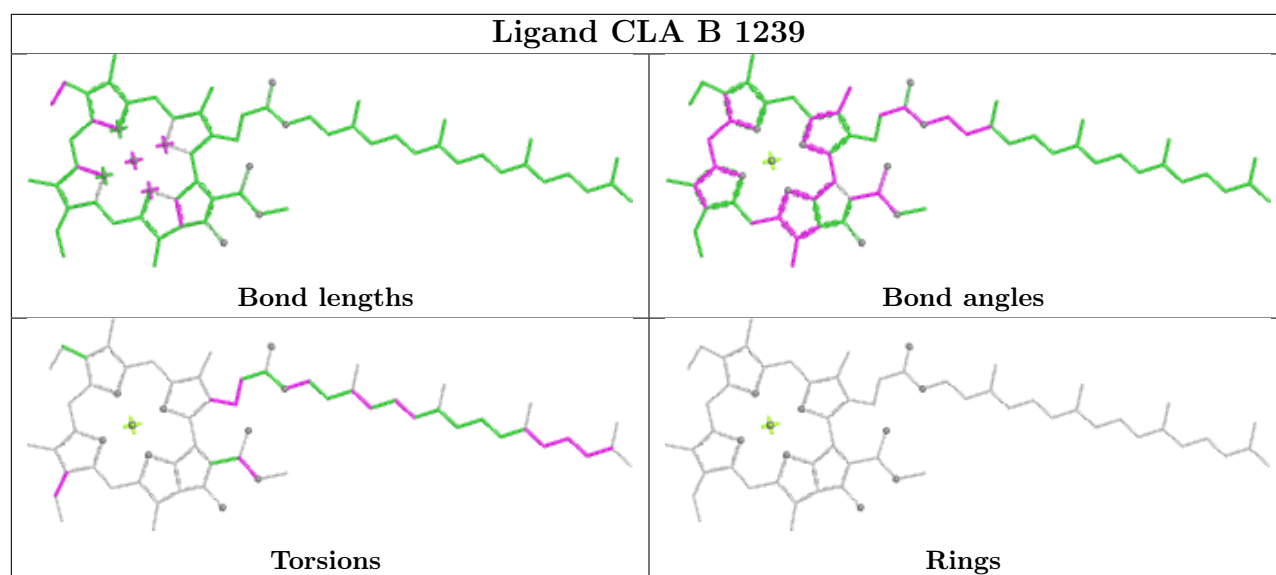


Ligand CLA 6 603

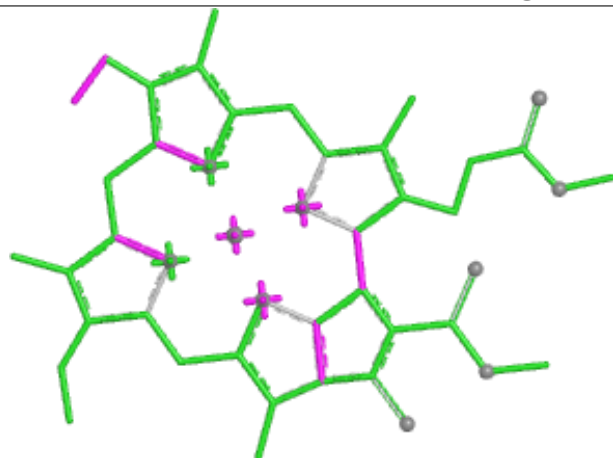


Ligand CLA G 1601

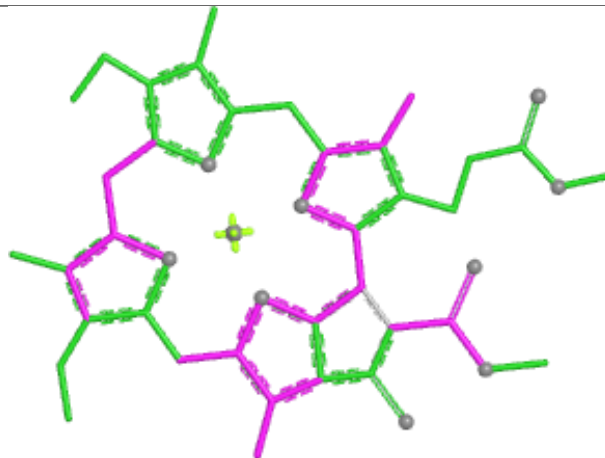




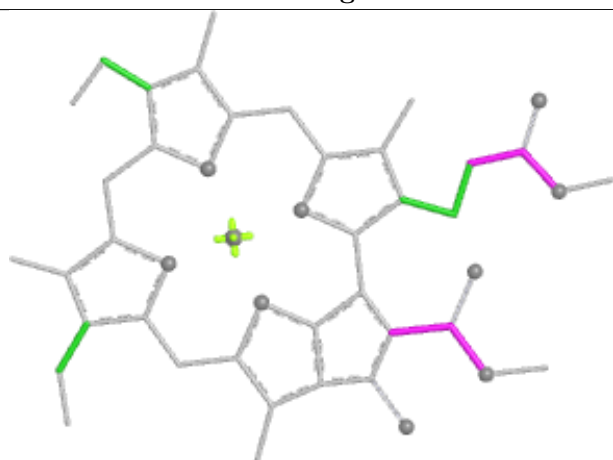
Ligand CLA 3 602



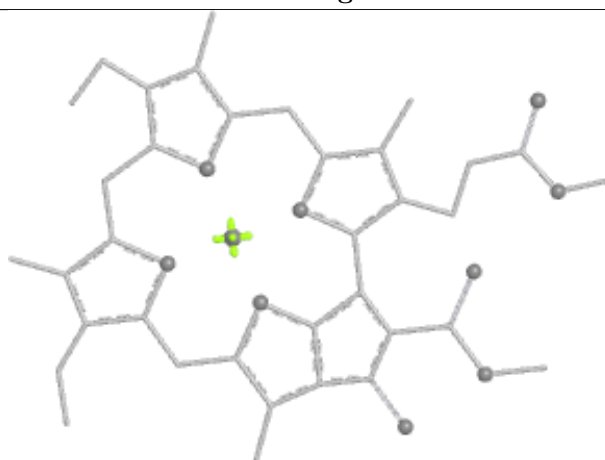
Bond lengths



Bond angles

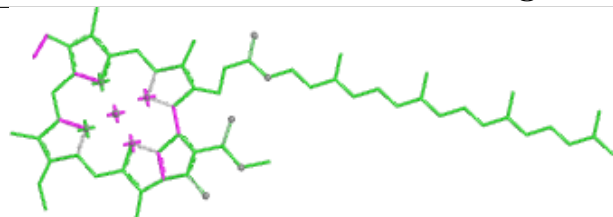


Torsions

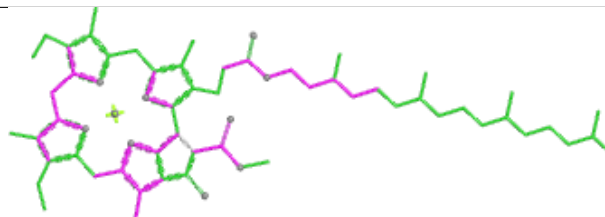


Rings

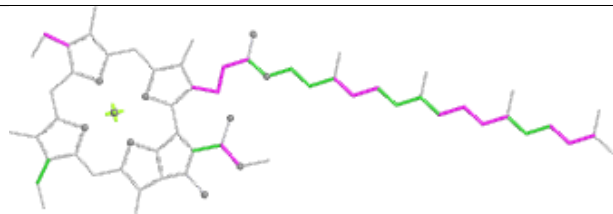
Ligand CLA 1 612



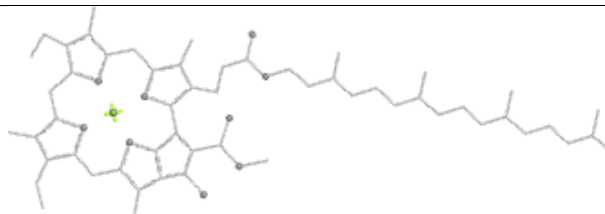
Bond lengths



Bond angles

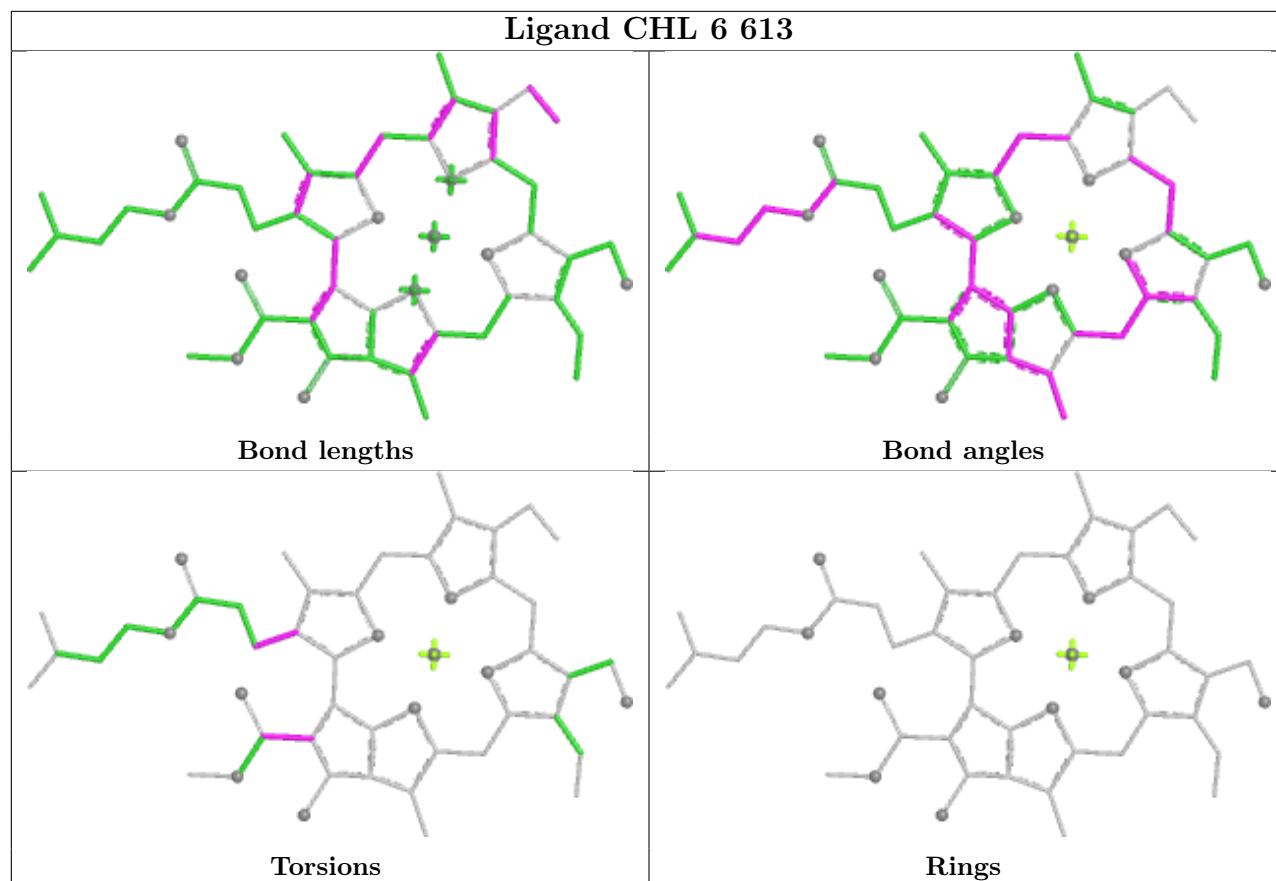


Torsions

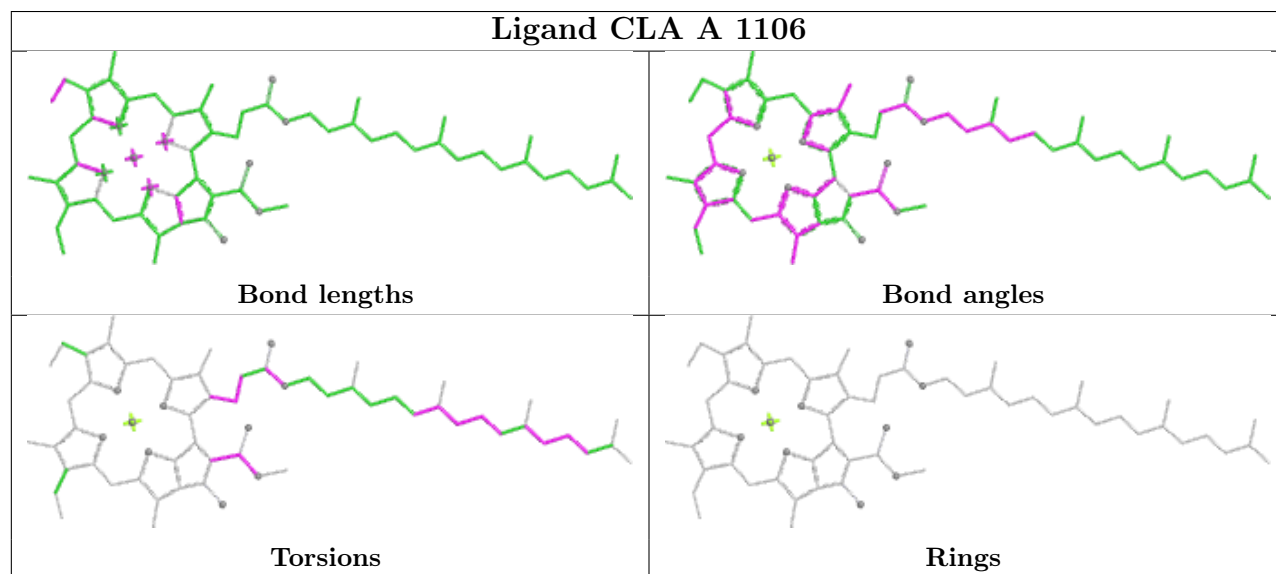


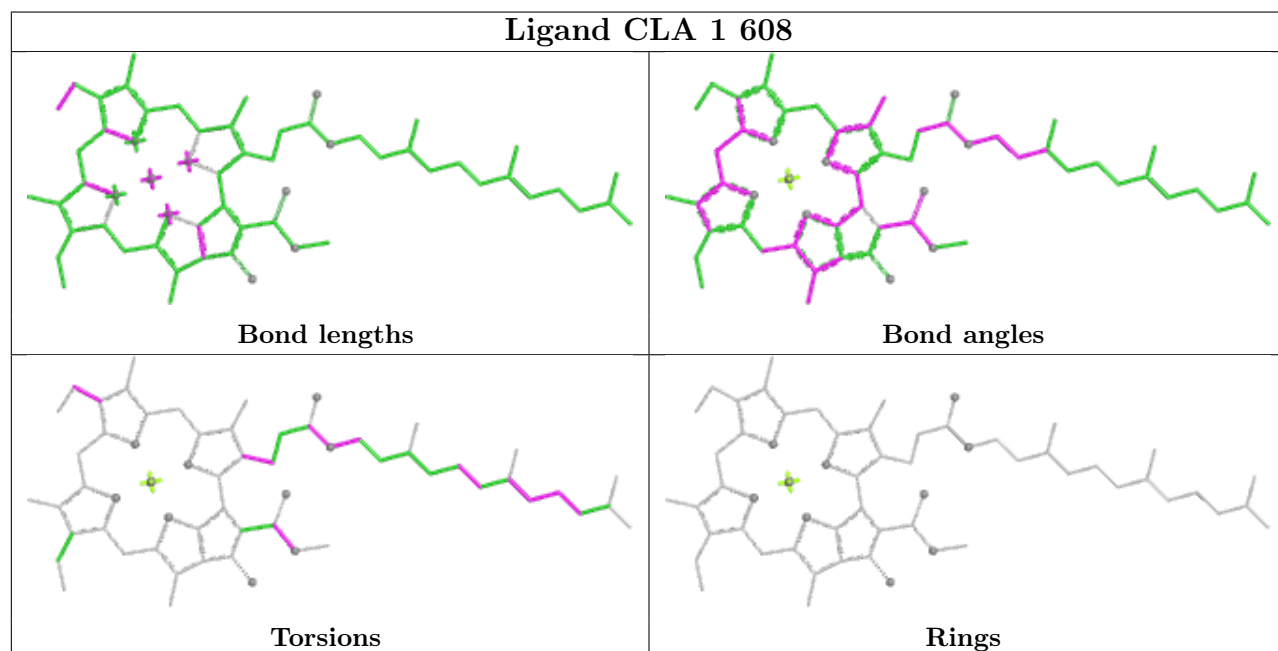
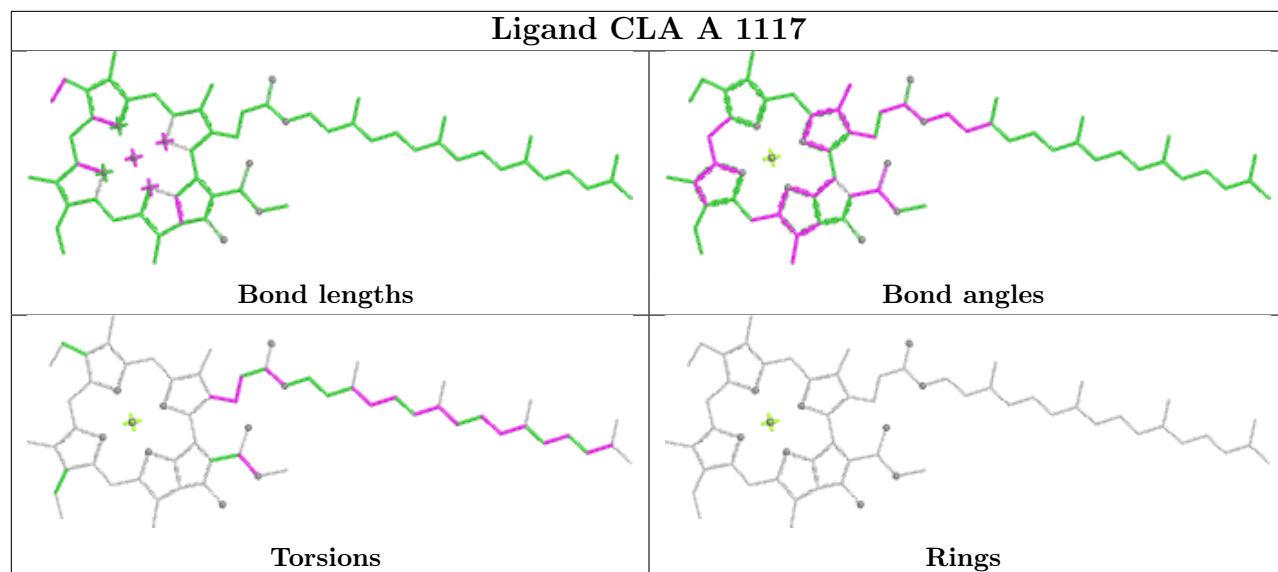
Rings

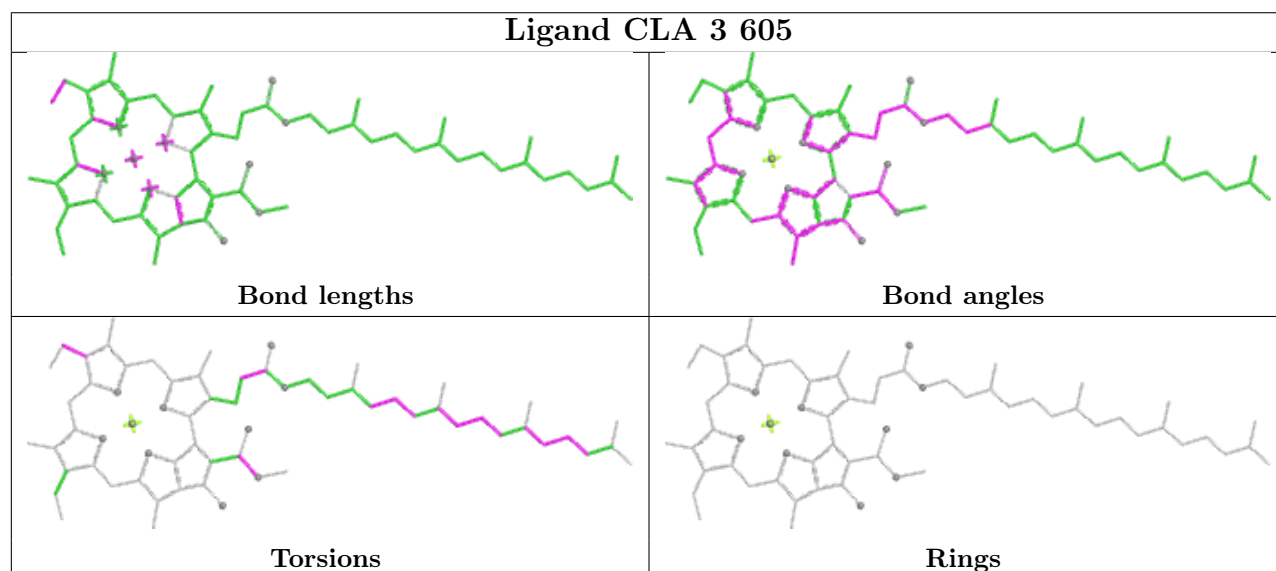
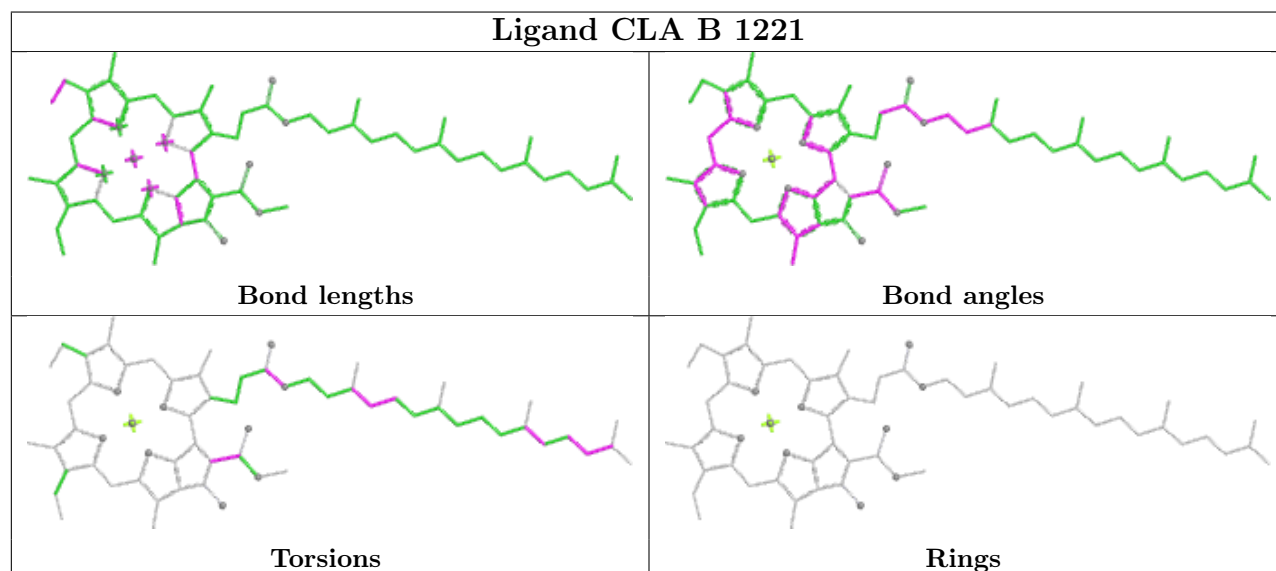
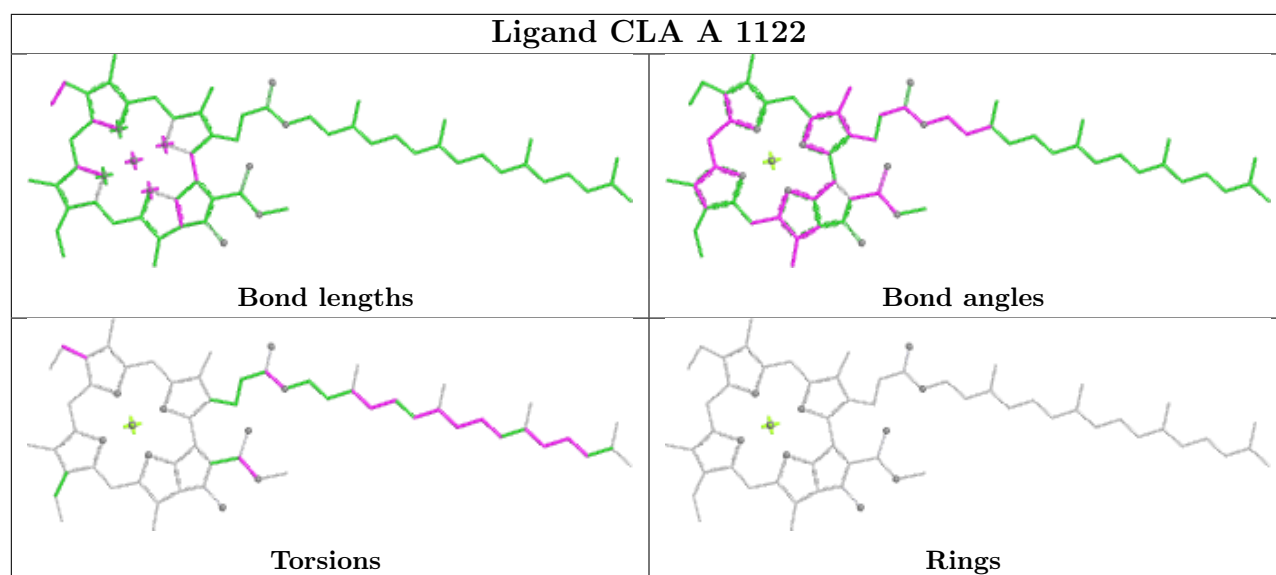
Ligand CHL 6 613

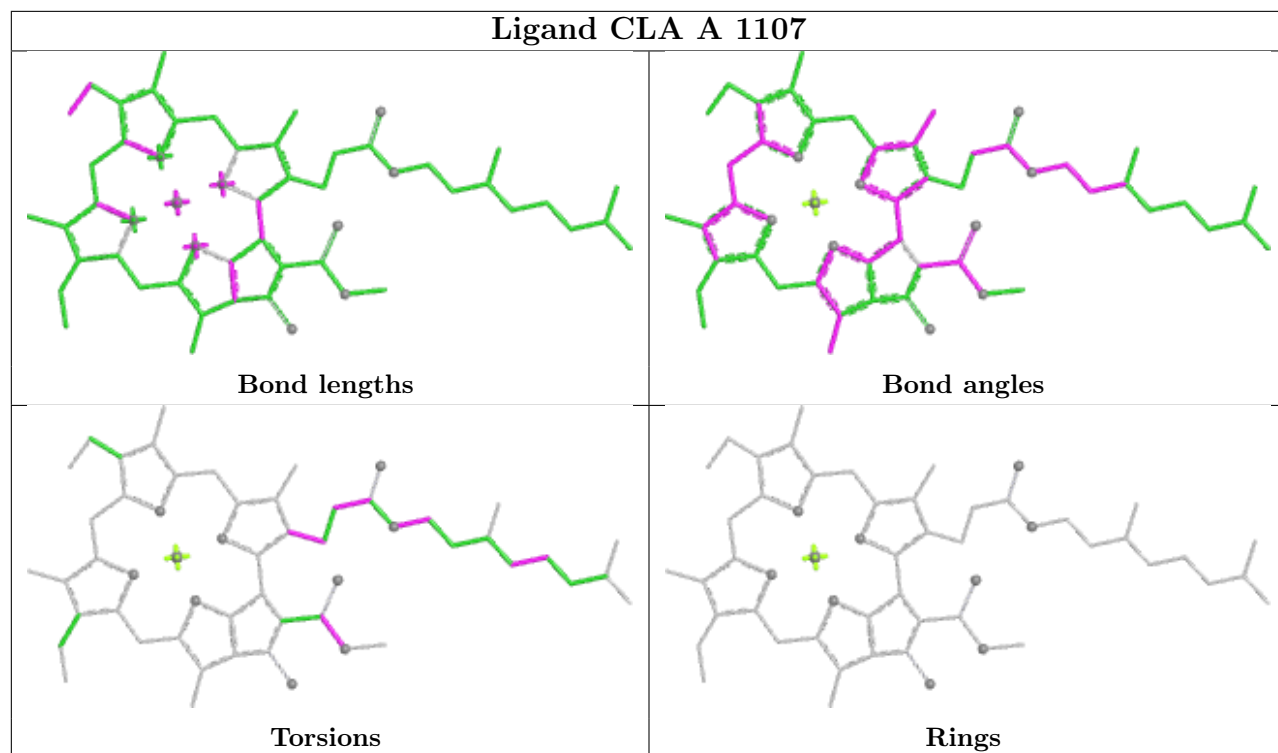


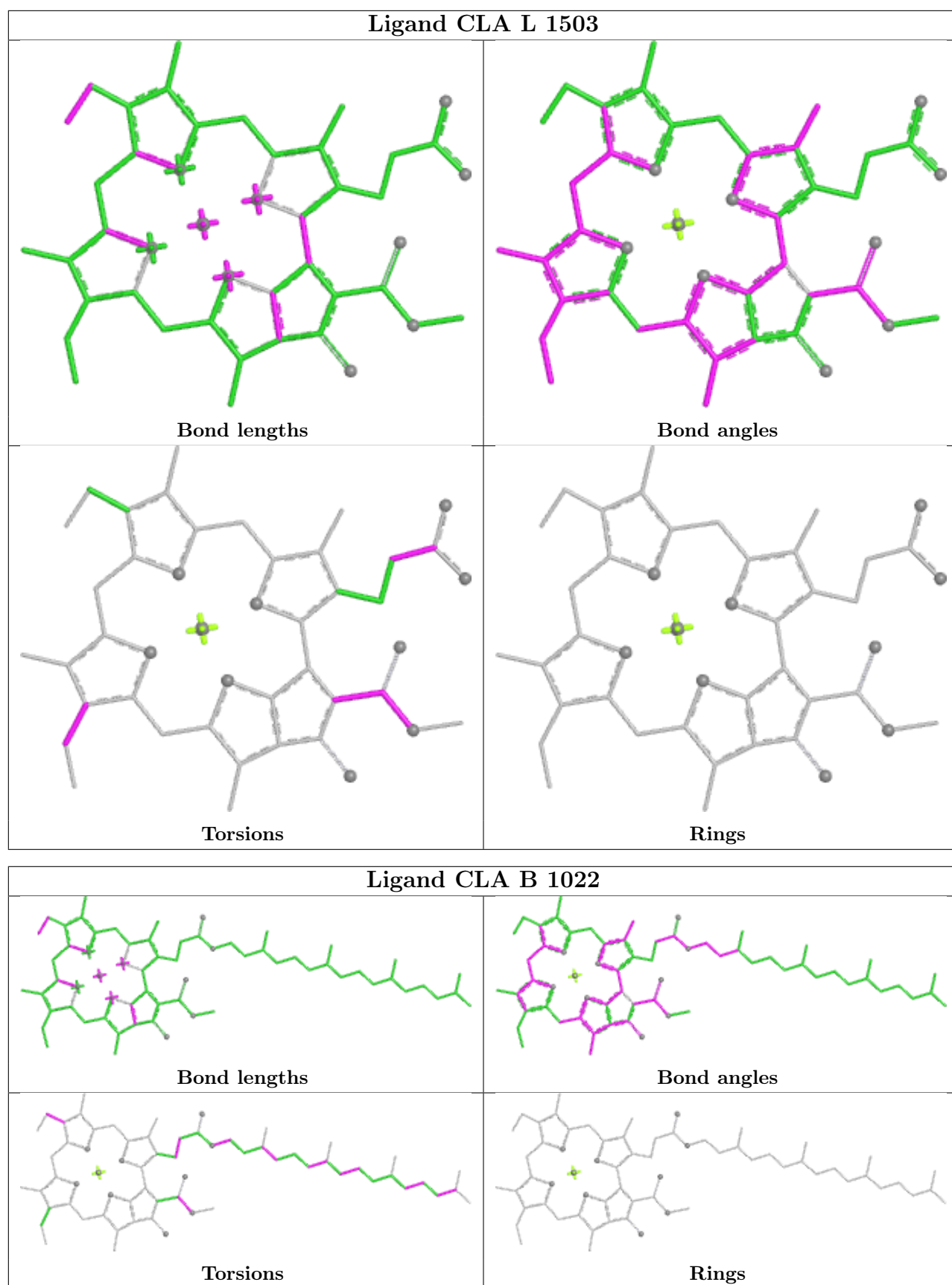
Ligand CLA A 1106

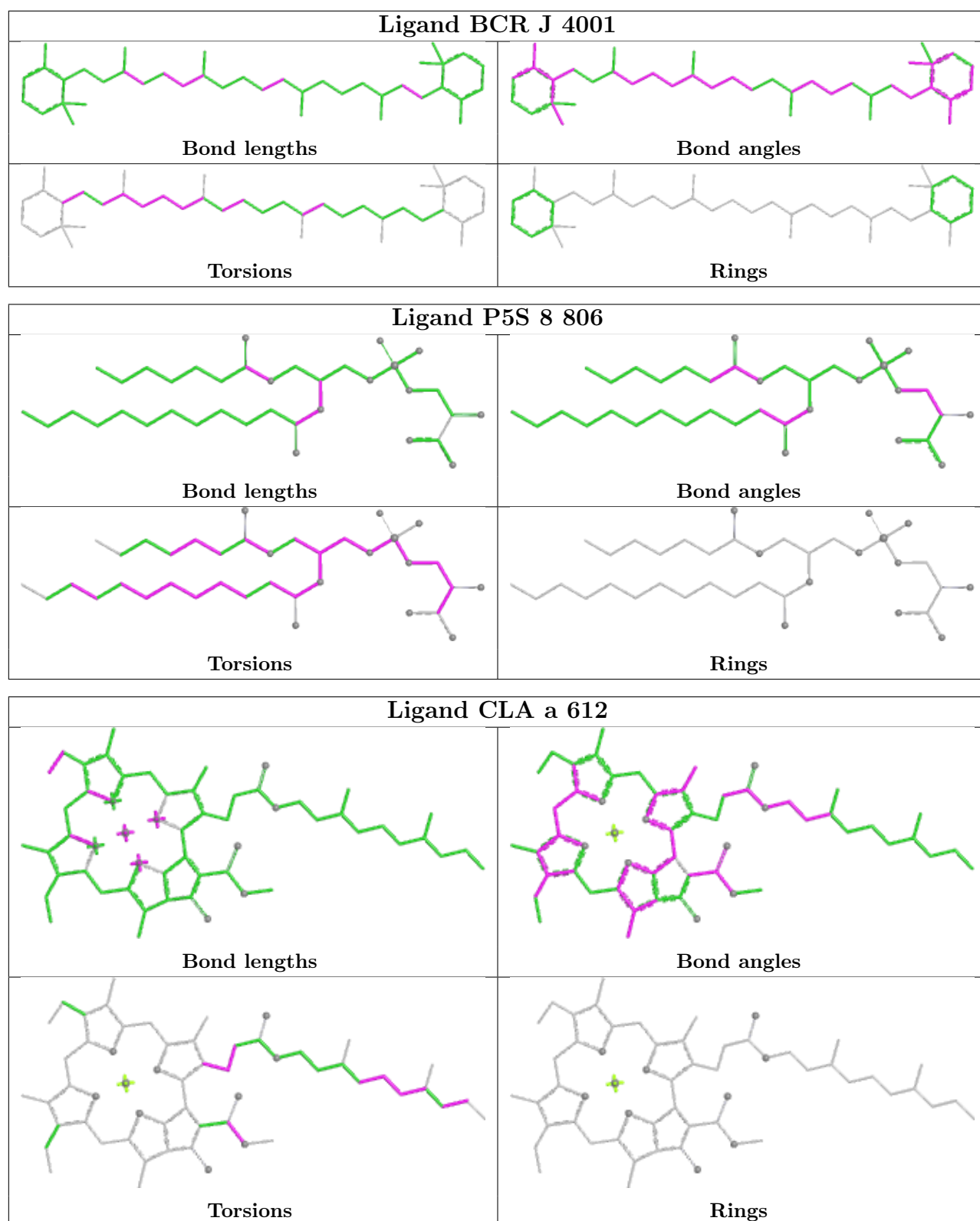


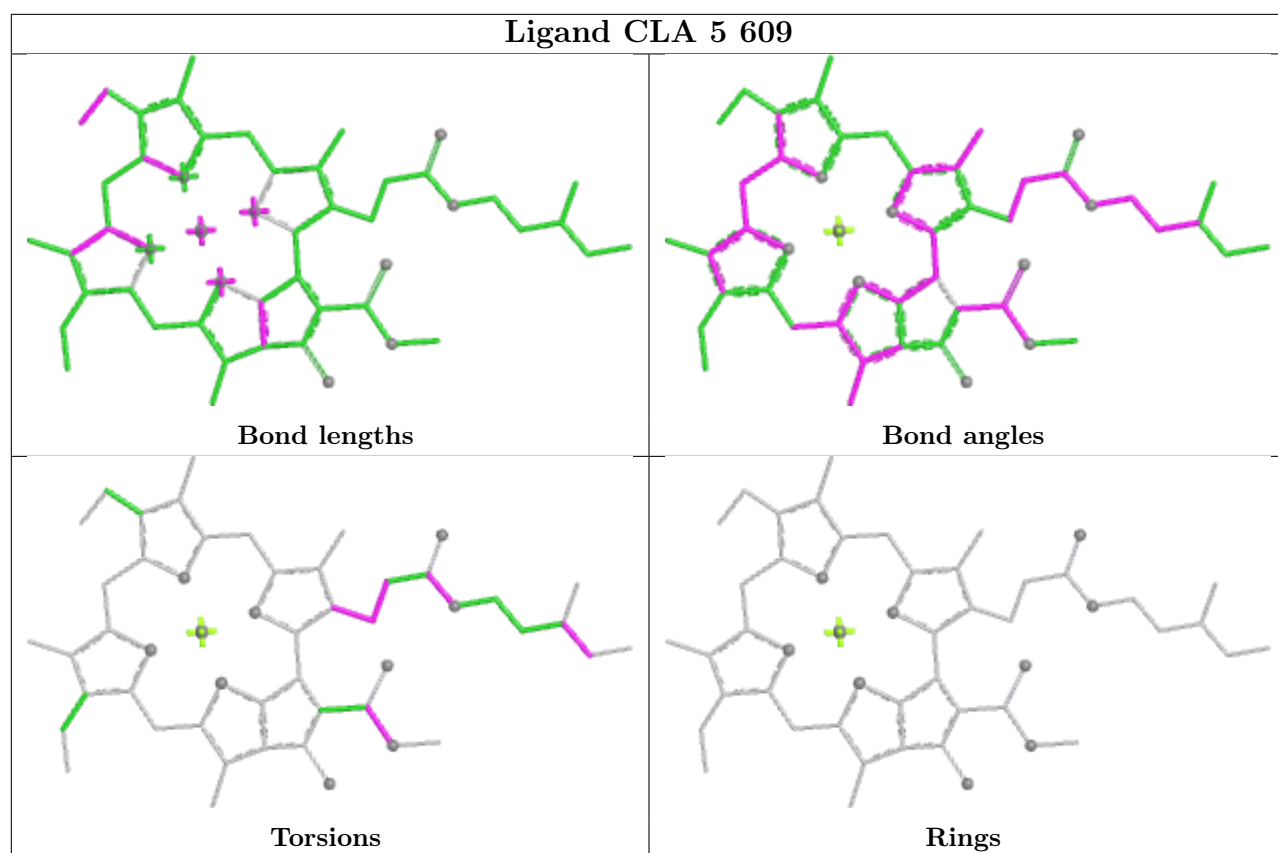


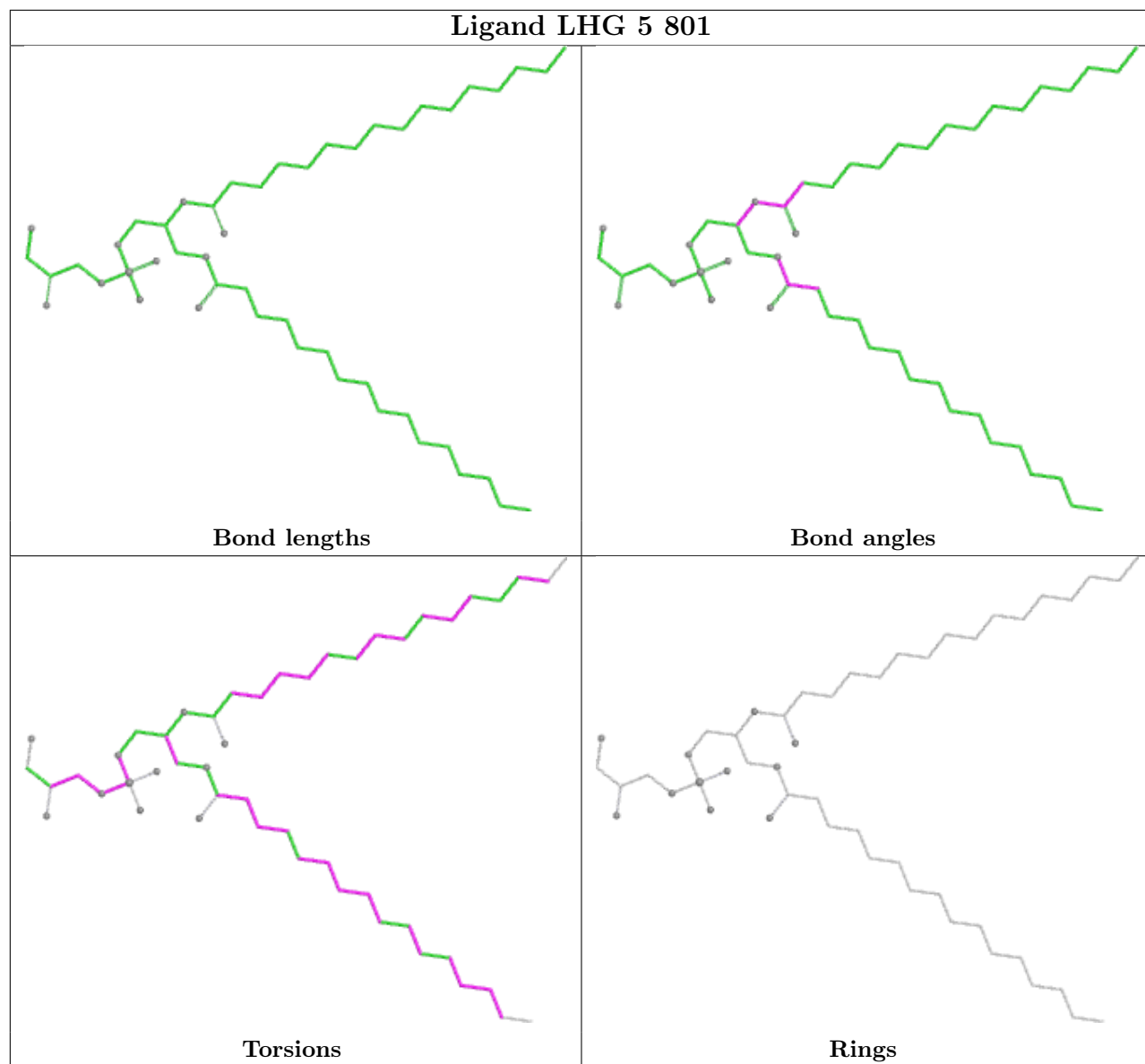


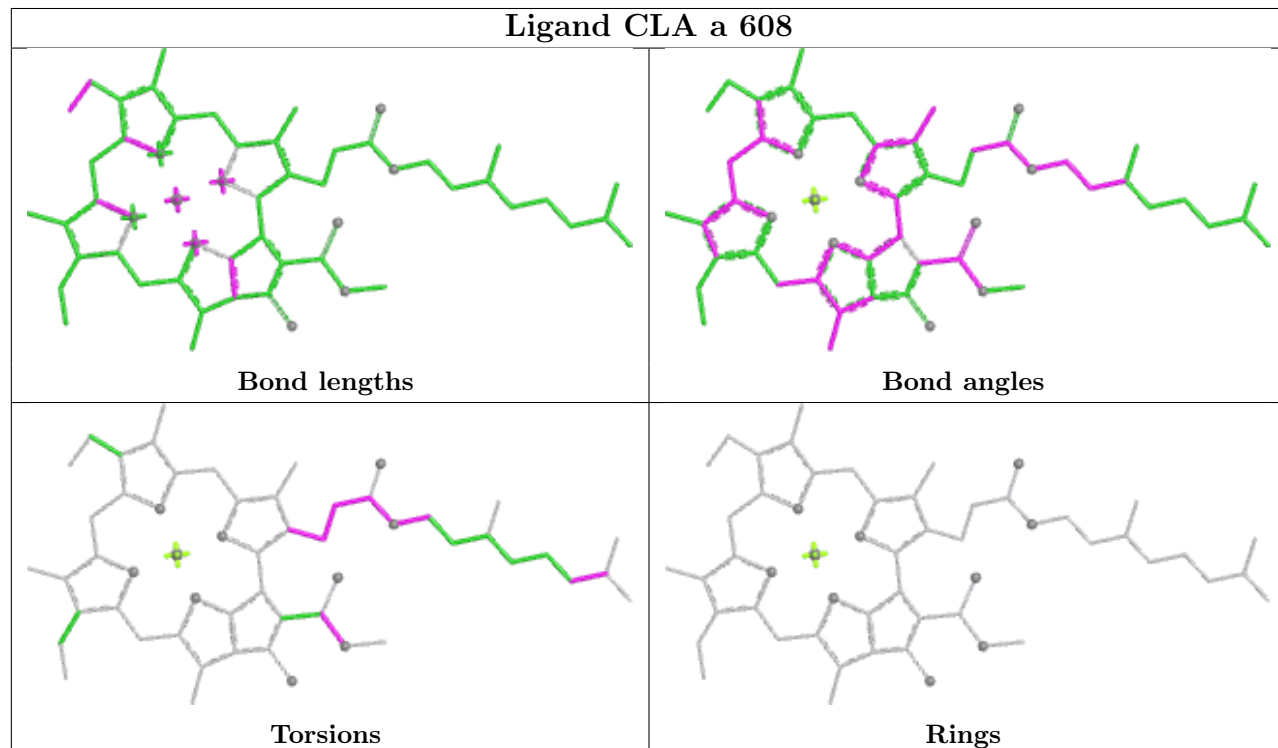
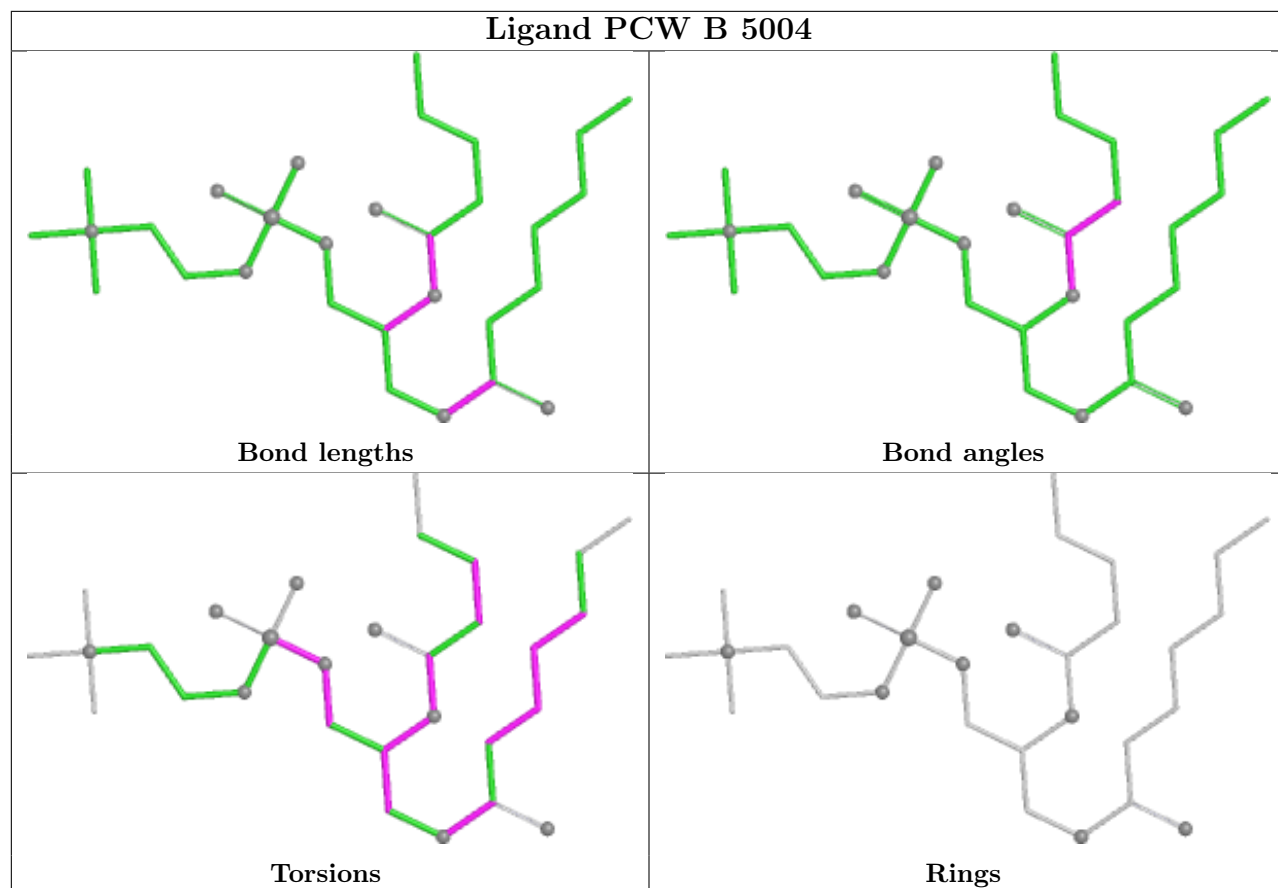


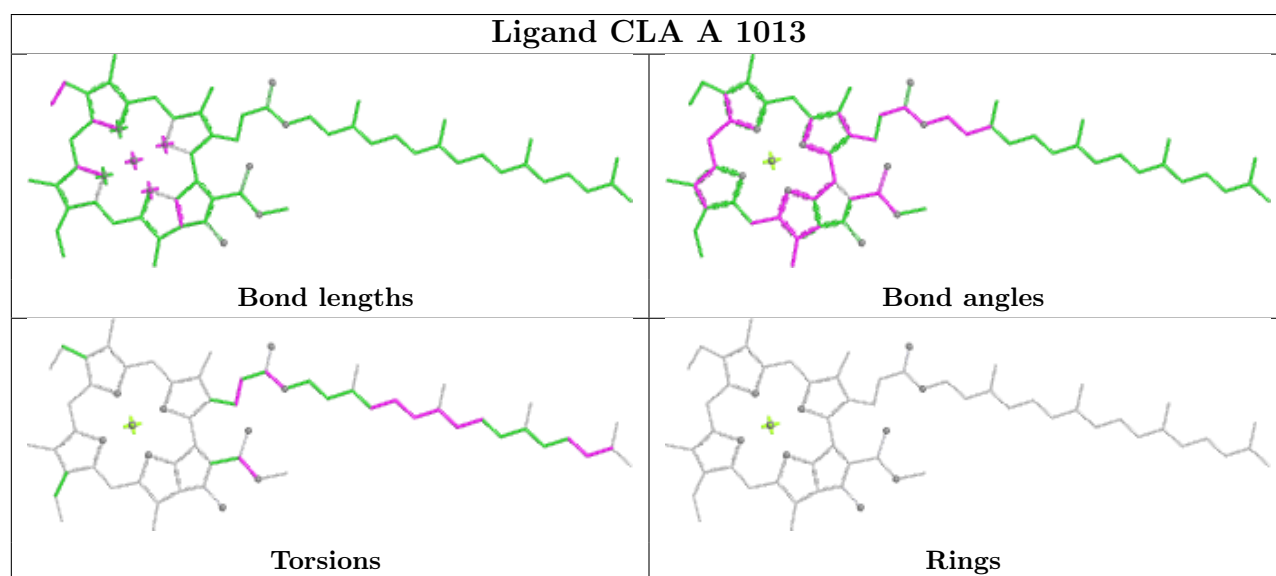
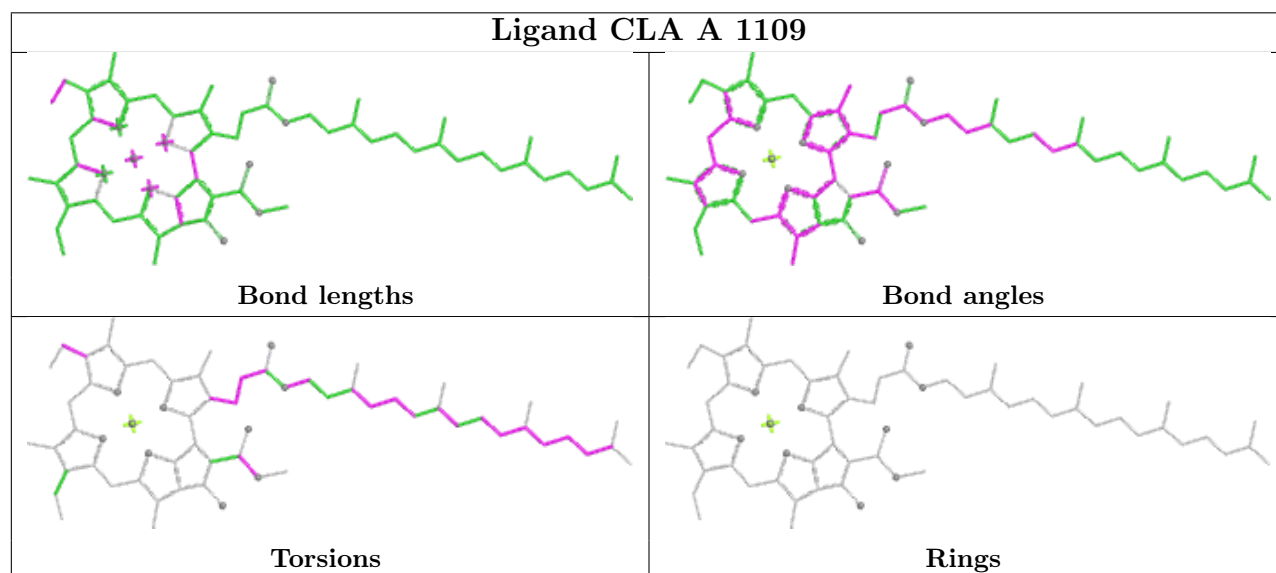
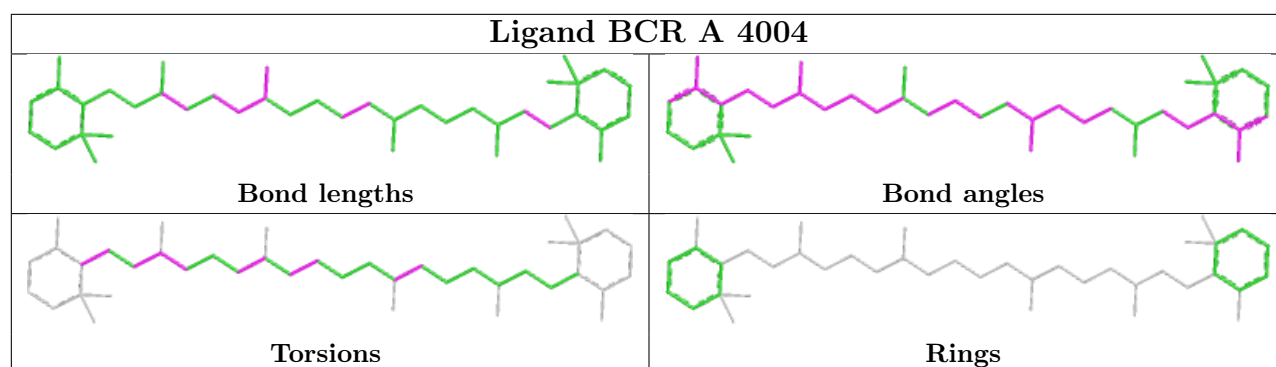


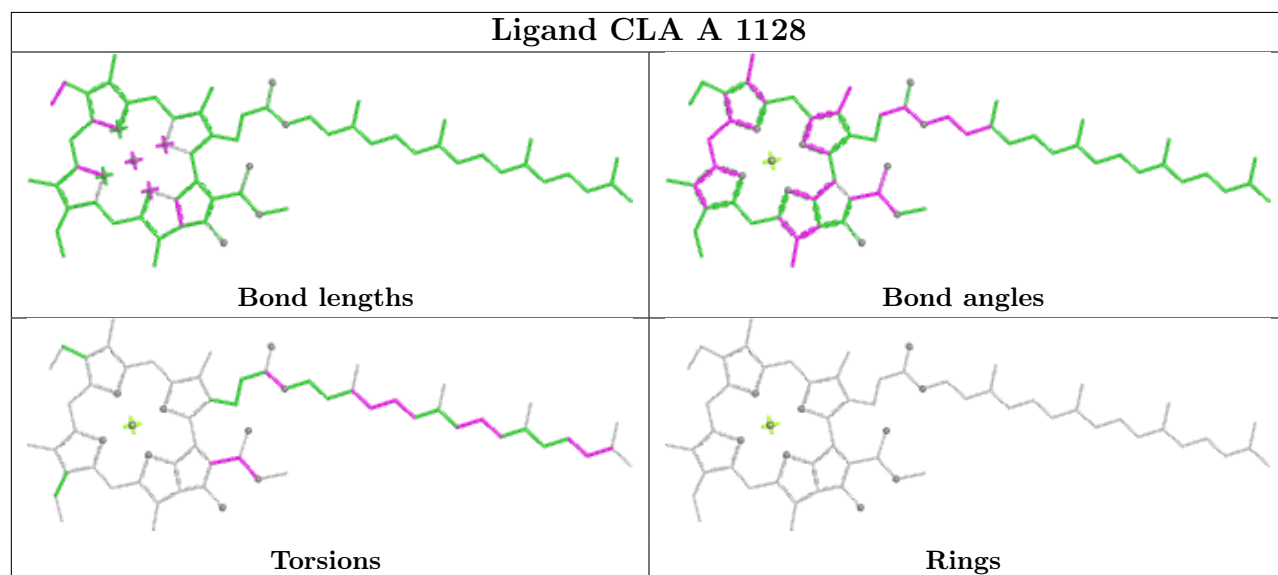
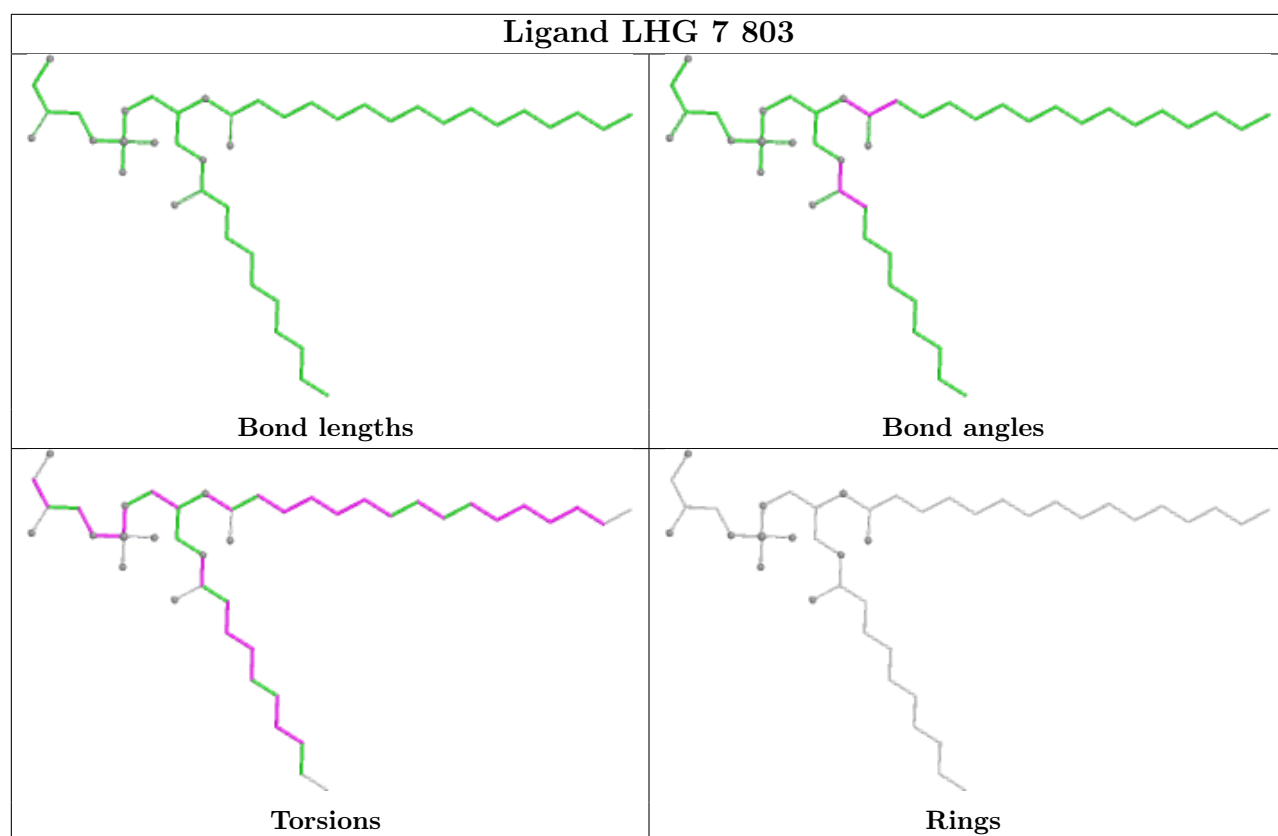


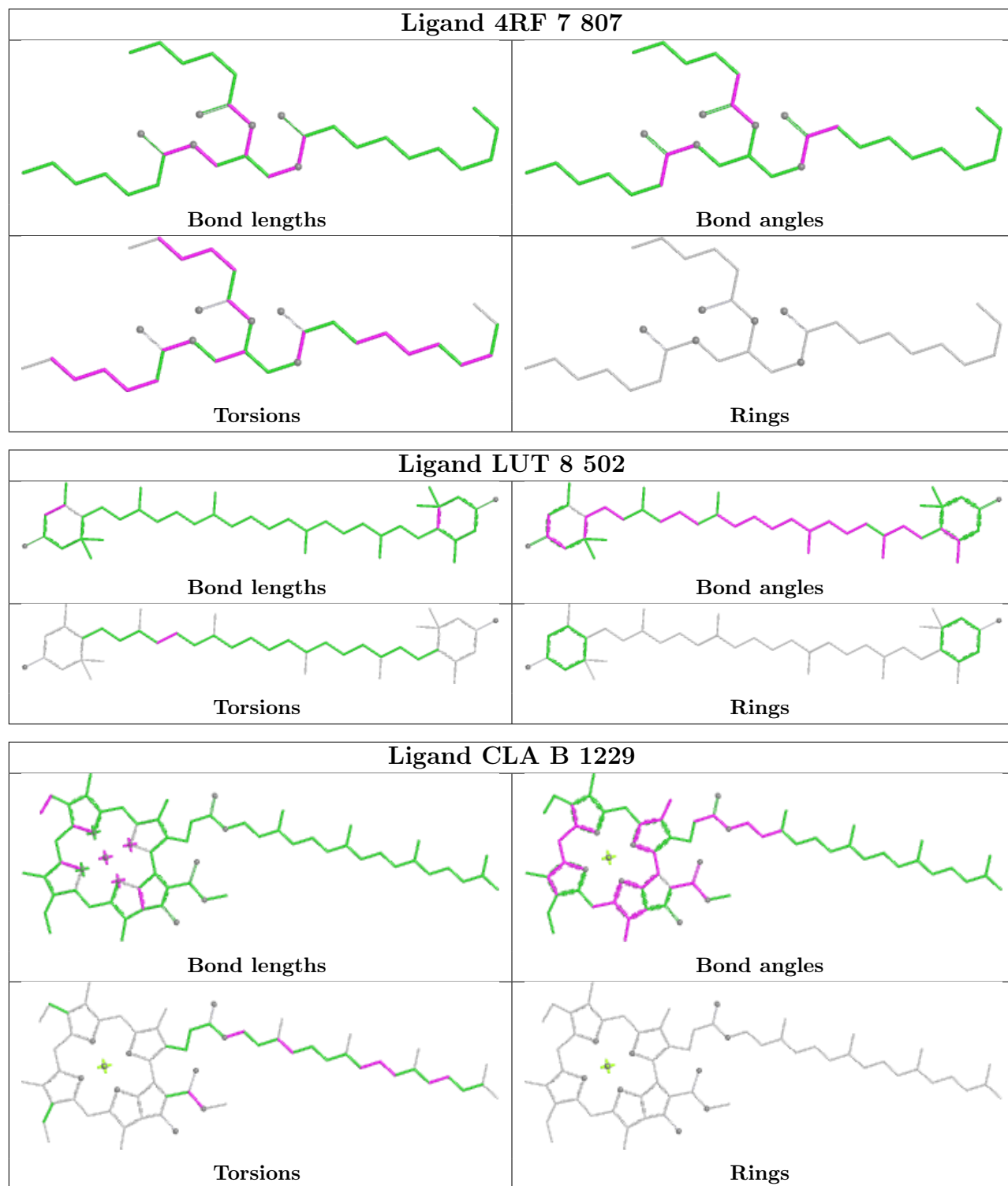


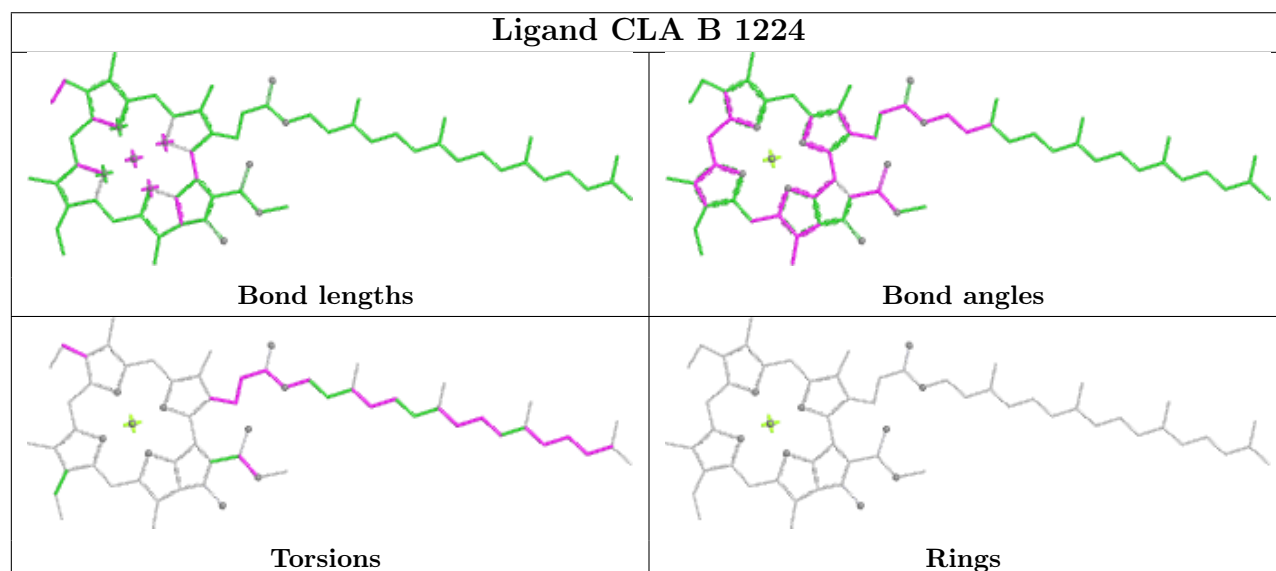
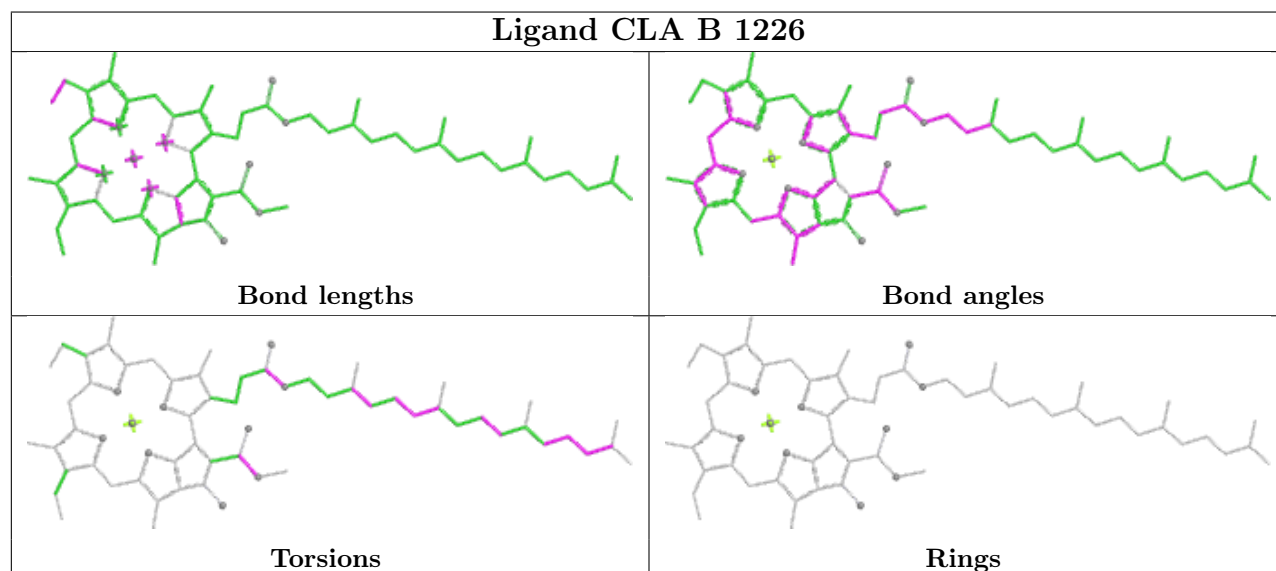
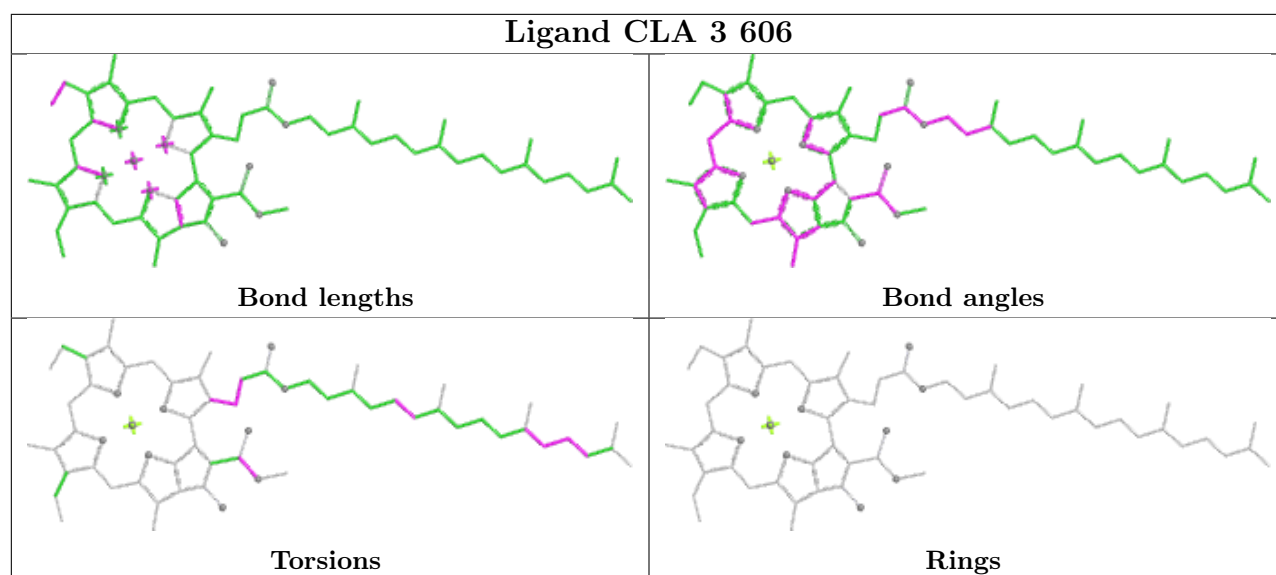


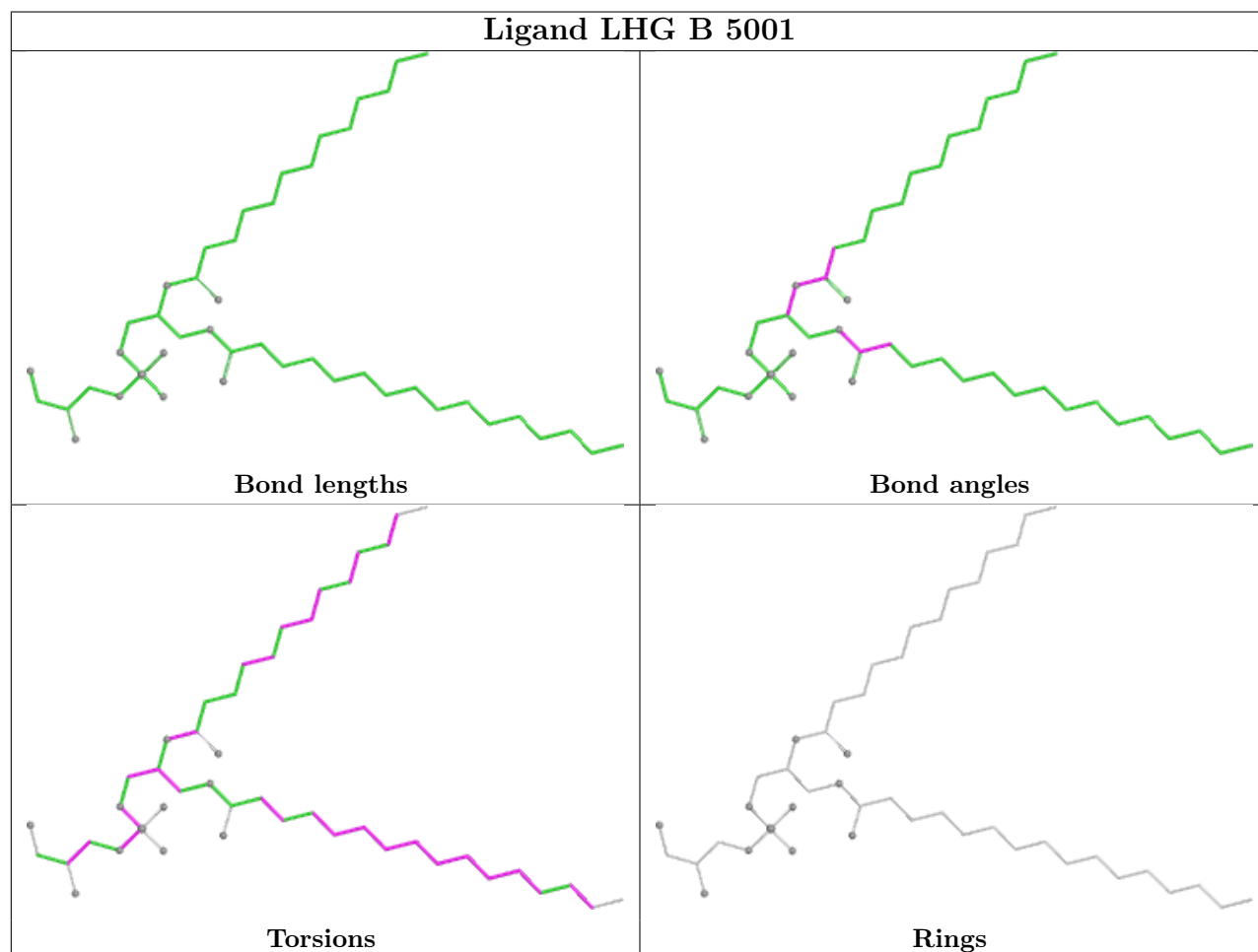
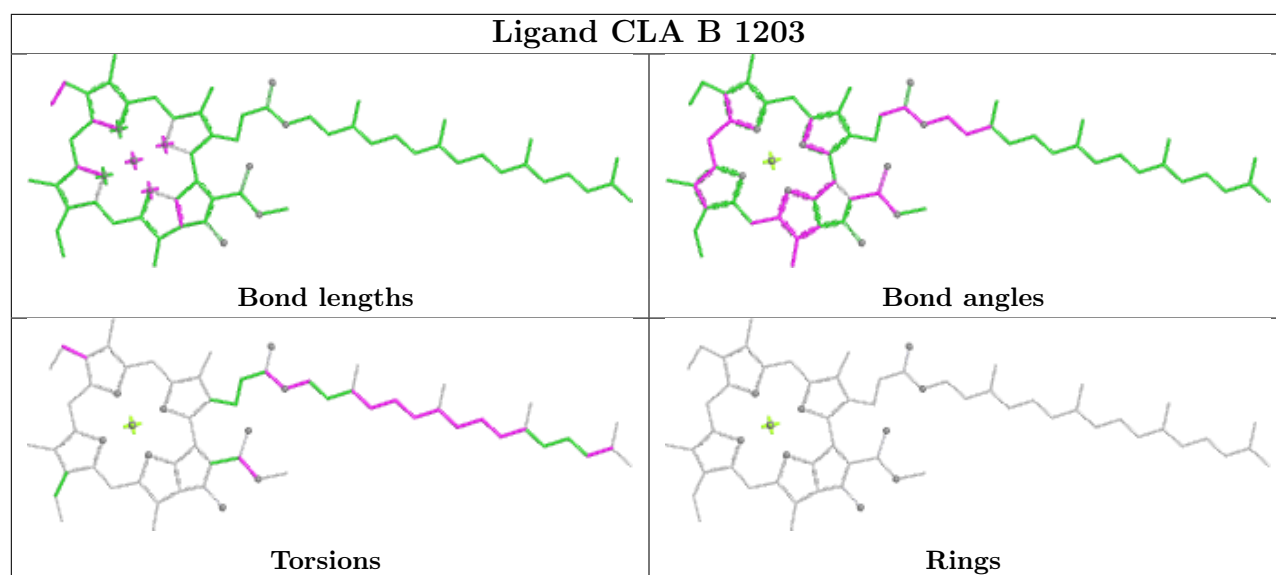


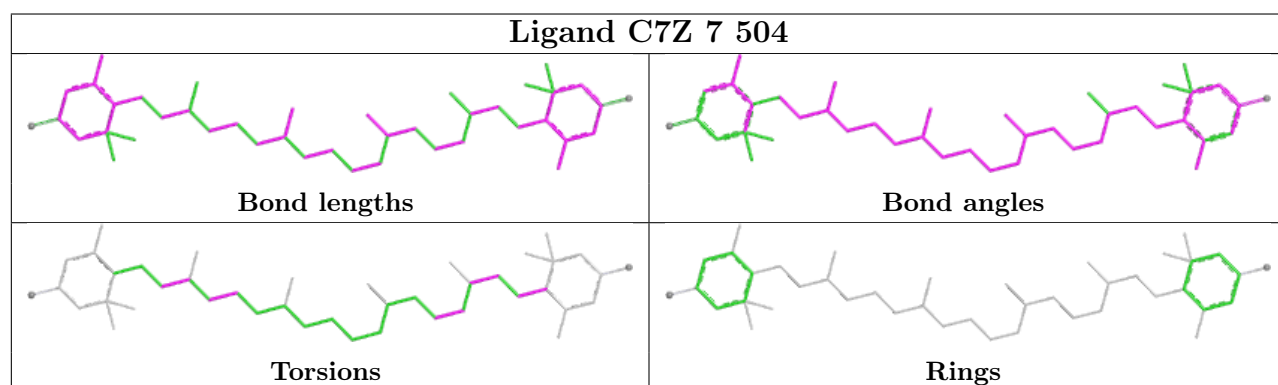
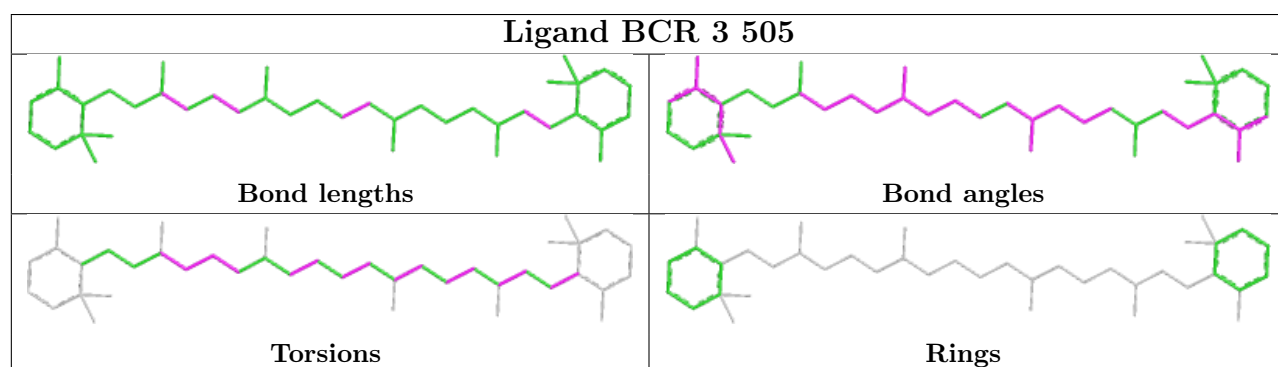
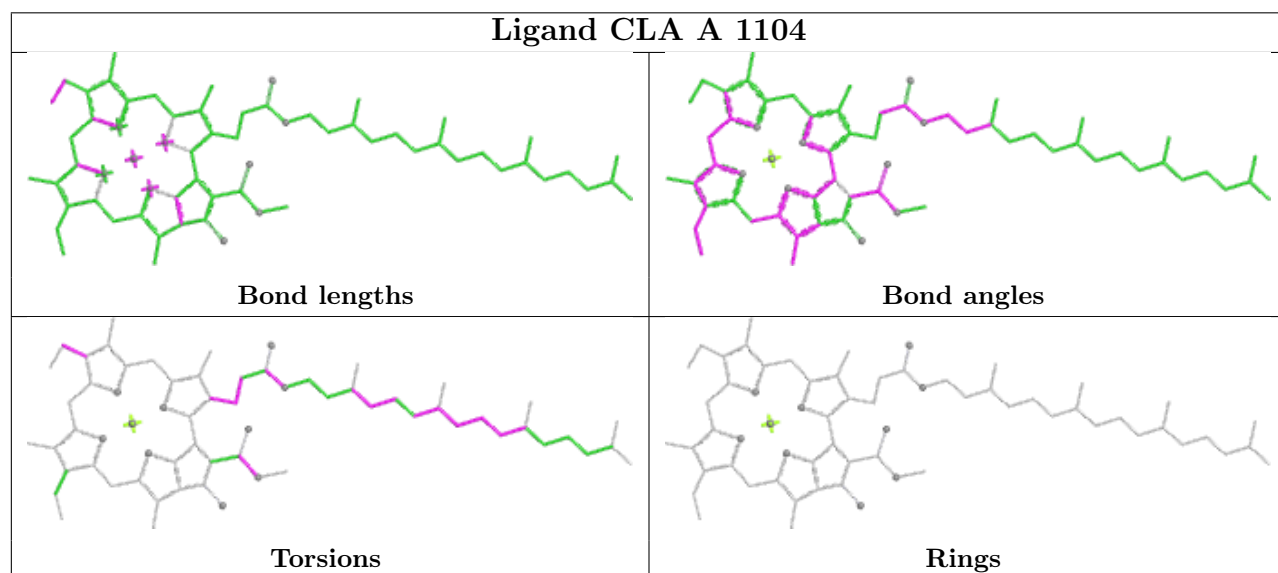
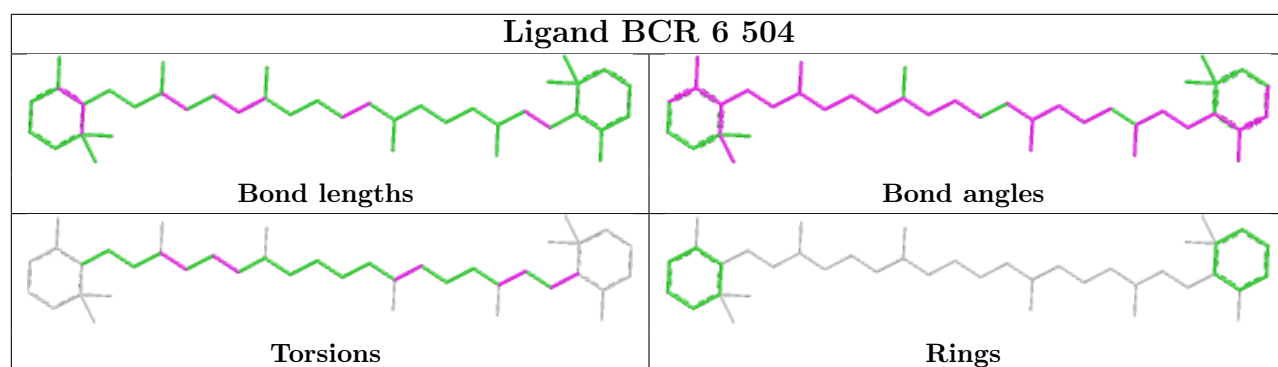




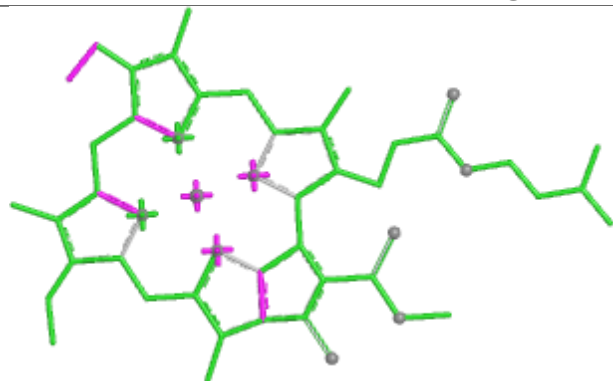




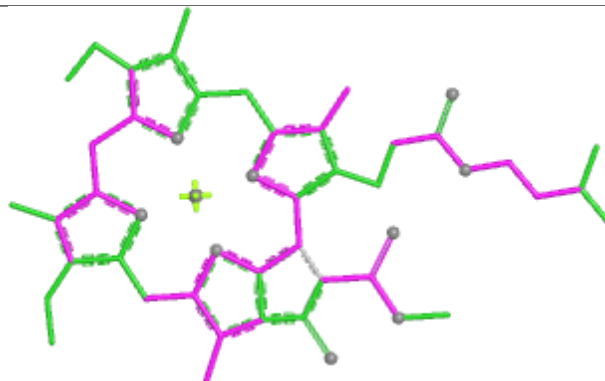




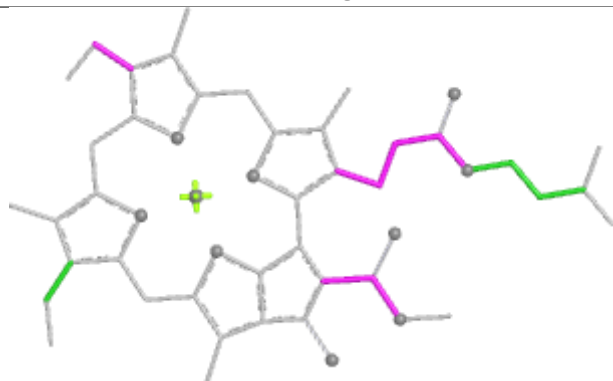
Ligand CLA A 1129



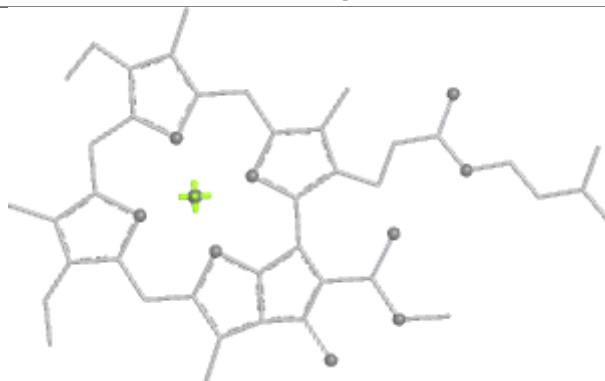
Bond lengths



Bond angles

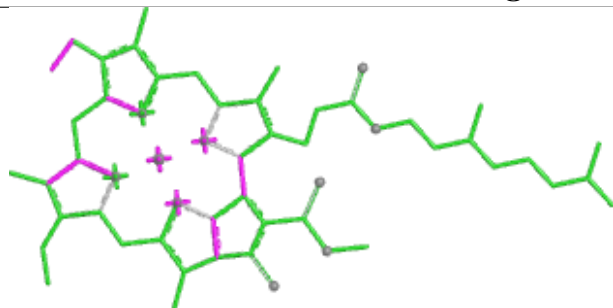


Torsions

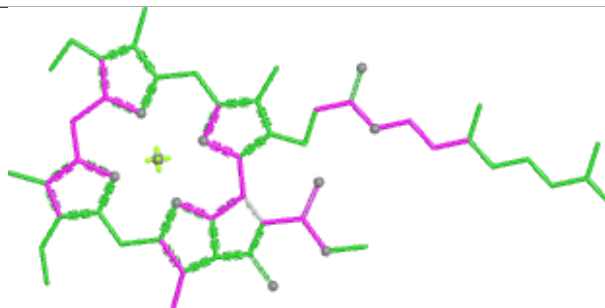


Rings

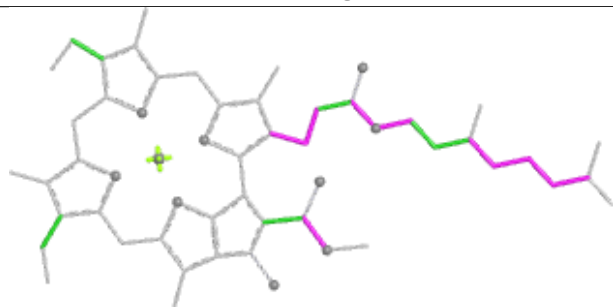
Ligand CLA A 1140



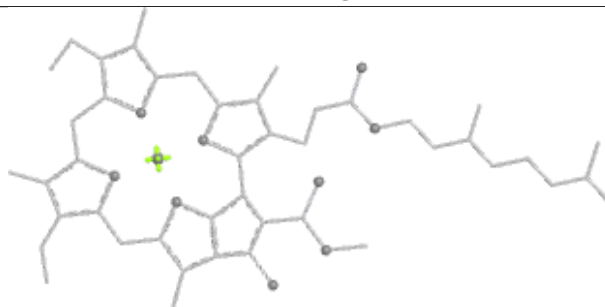
Bond lengths



Bond angles

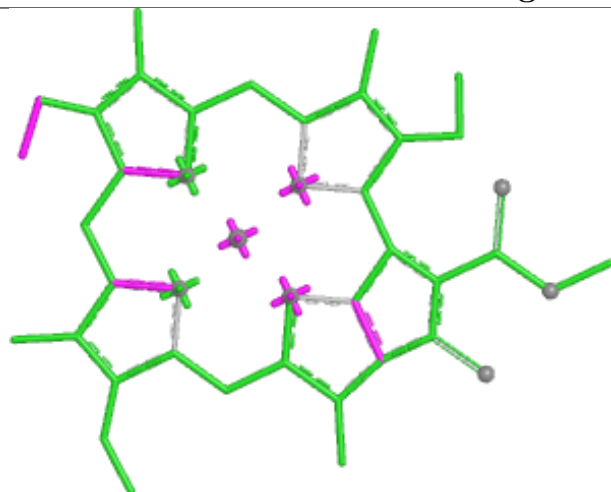


Torsions

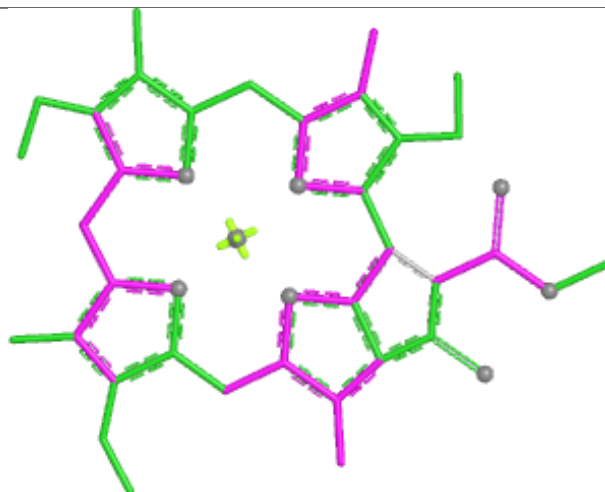


Rings

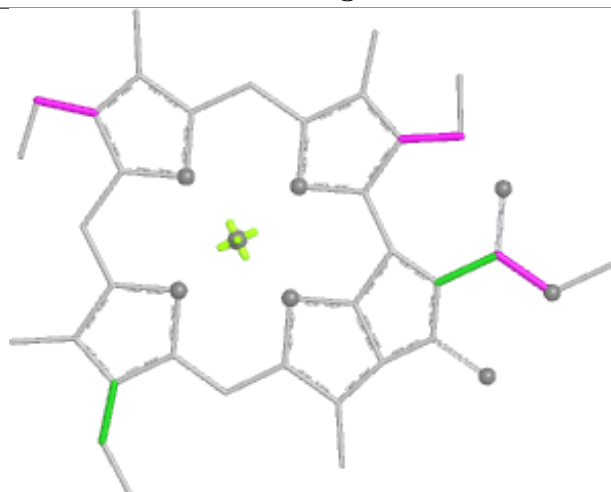
Ligand CLA 7 608



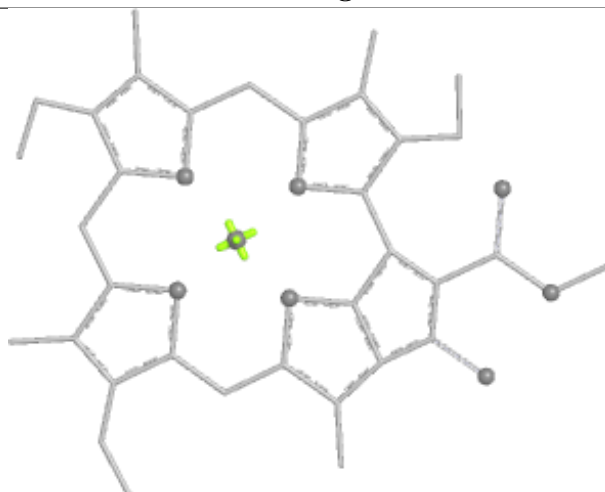
Bond lengths



Bond angles

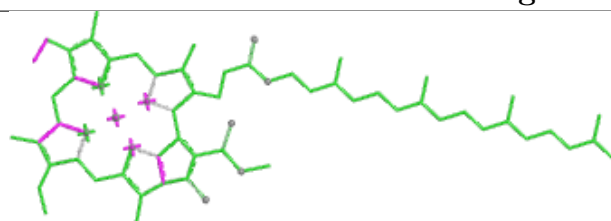


Torsions

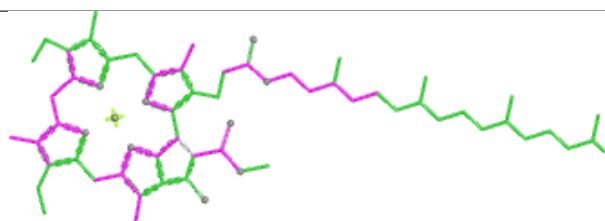


Rings

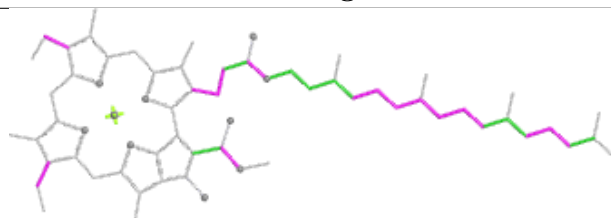
Ligand CLA 1 604



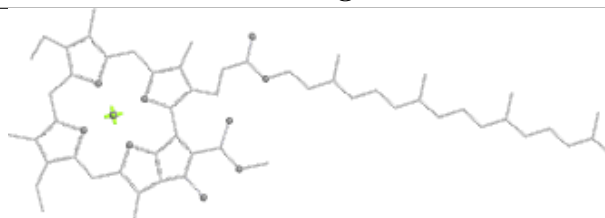
Bond lengths



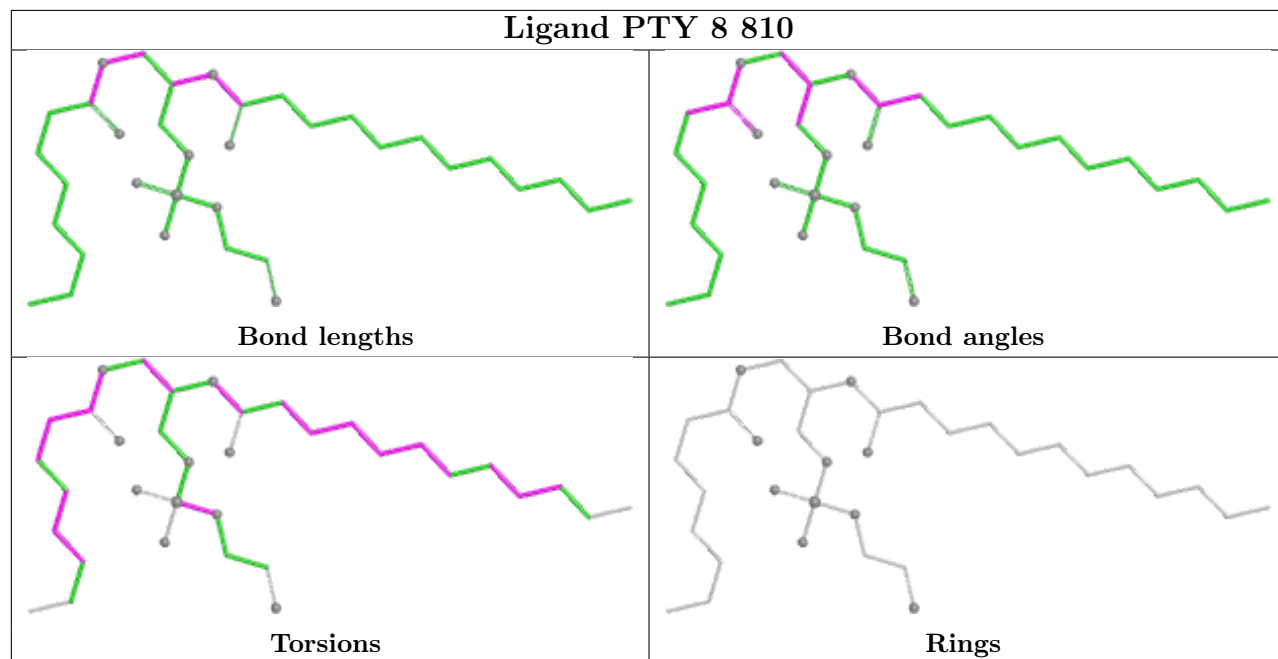
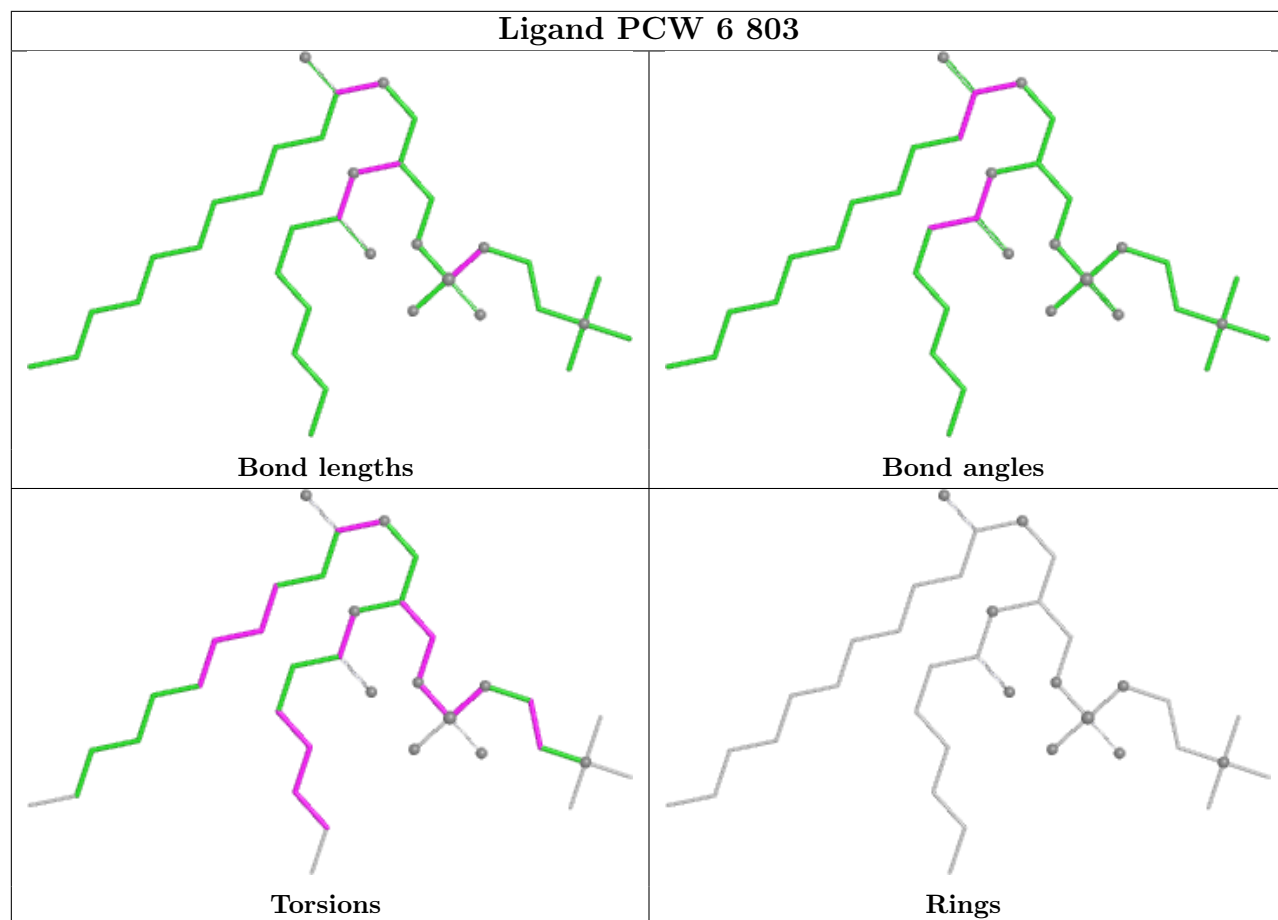
Bond angles



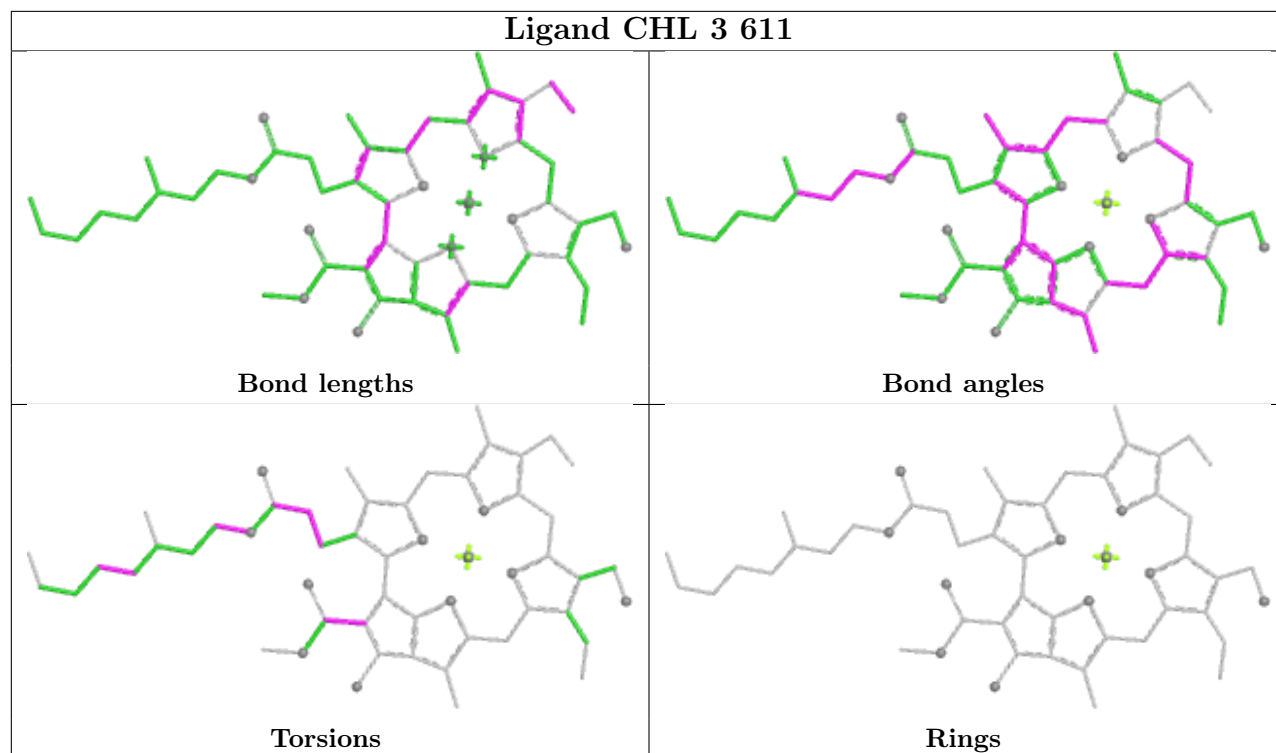
Torsions



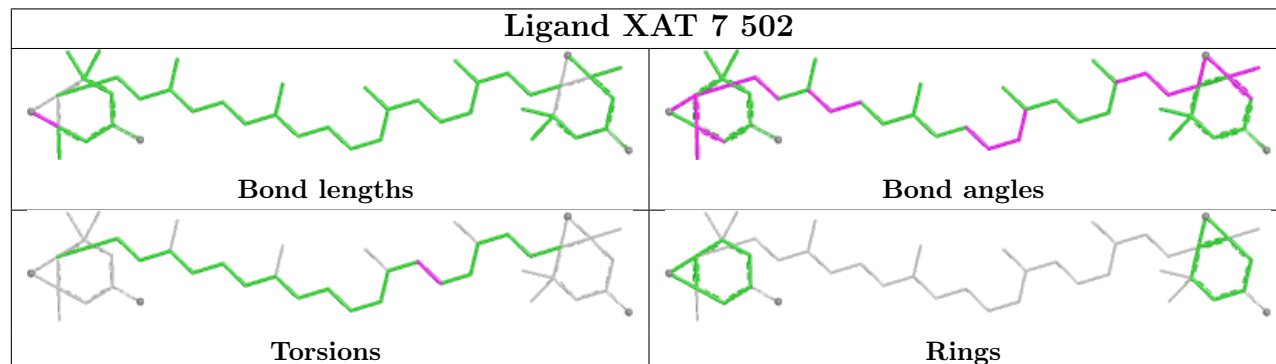
Rings

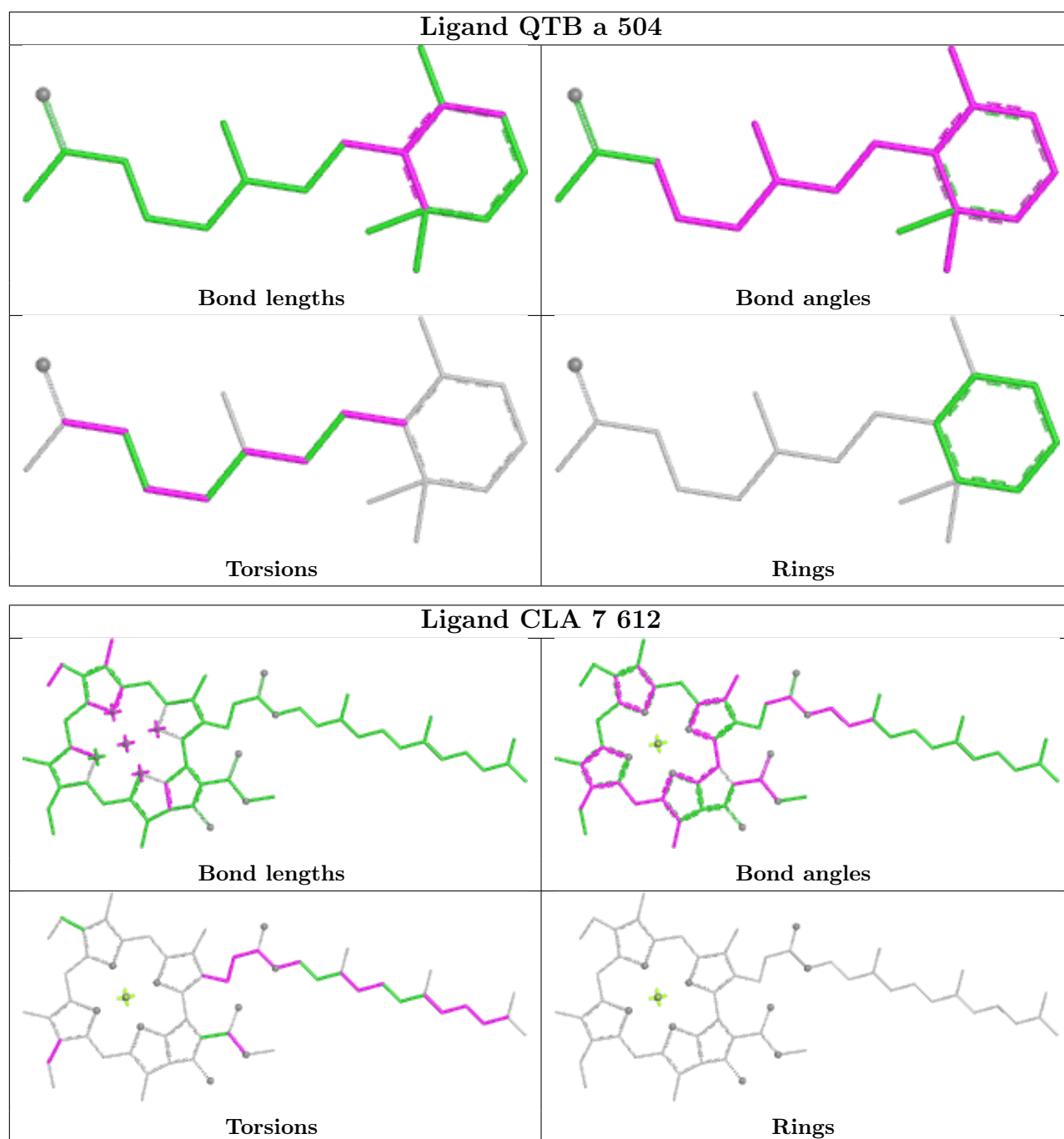


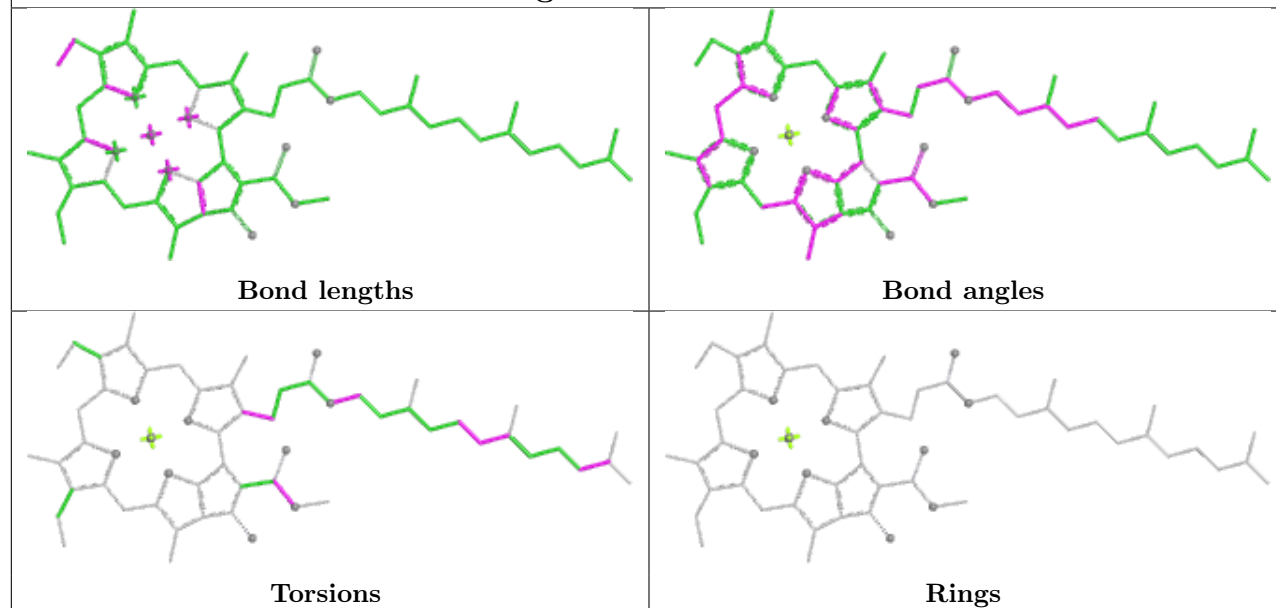
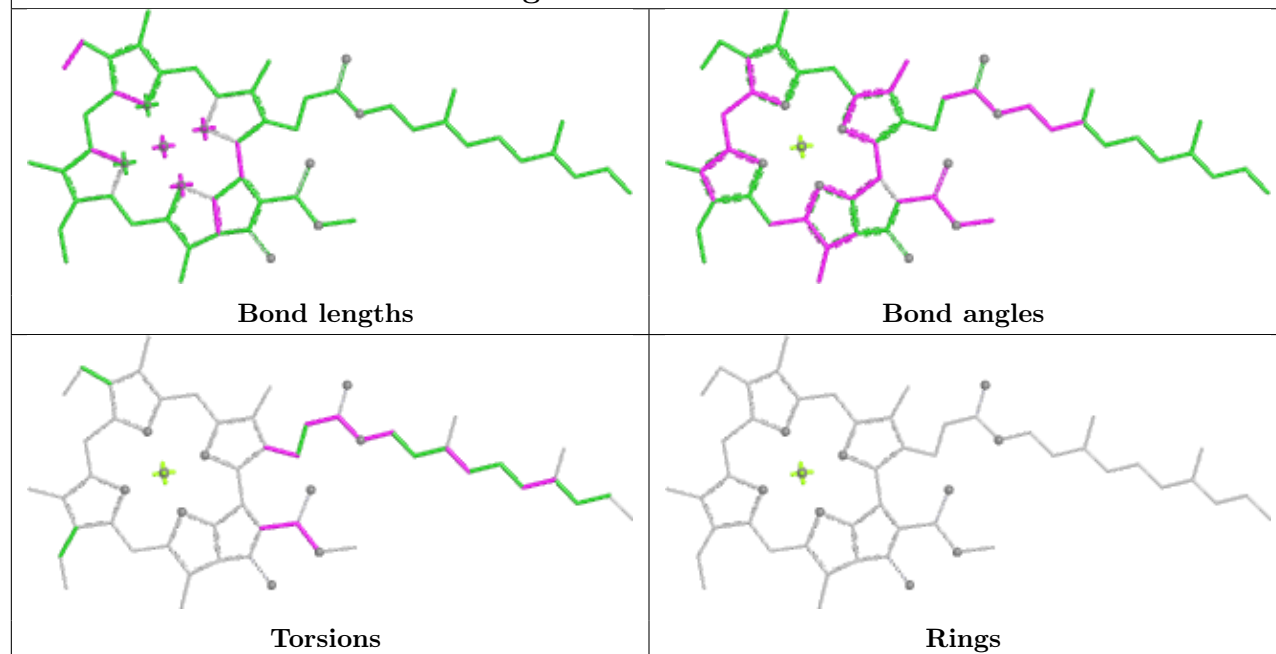
Ligand CHL 3 611



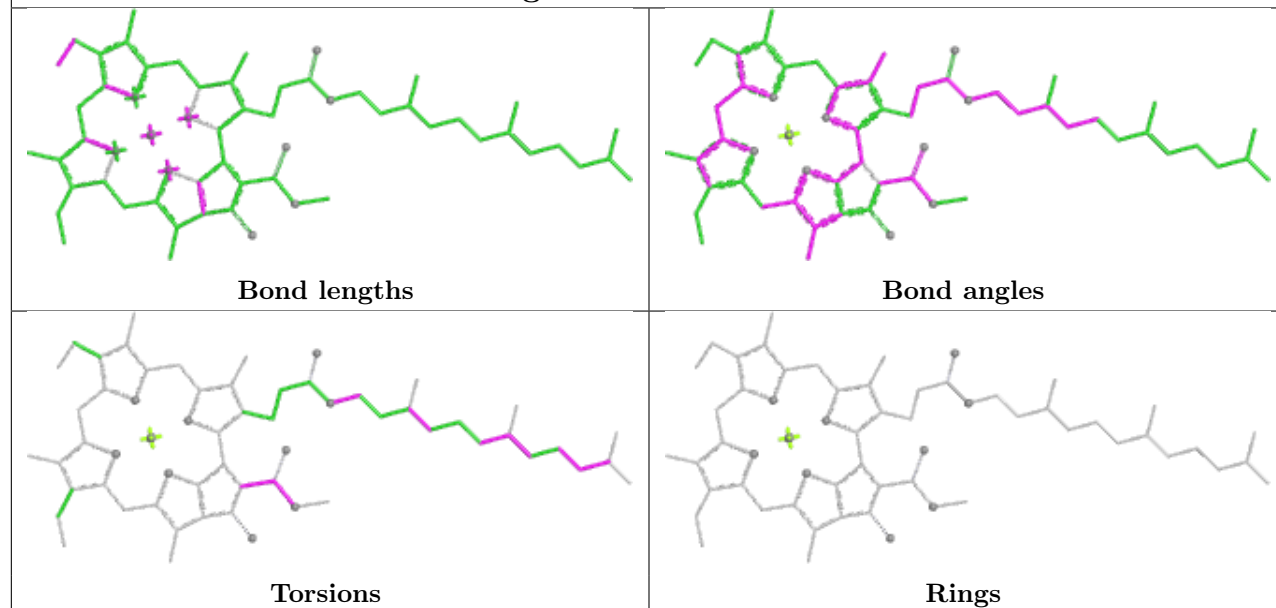
Ligand XAT 7 502



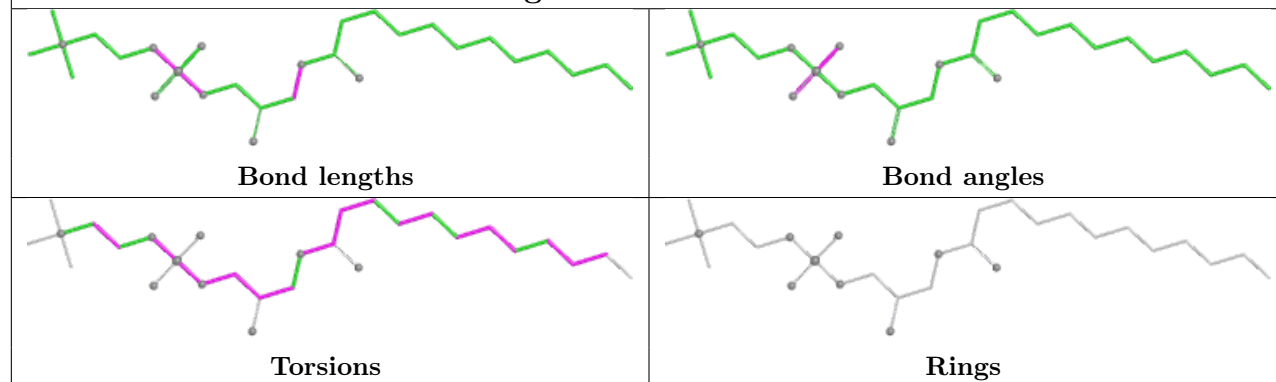


Ligand CLA 1 601**Ligand CLA A 1121**

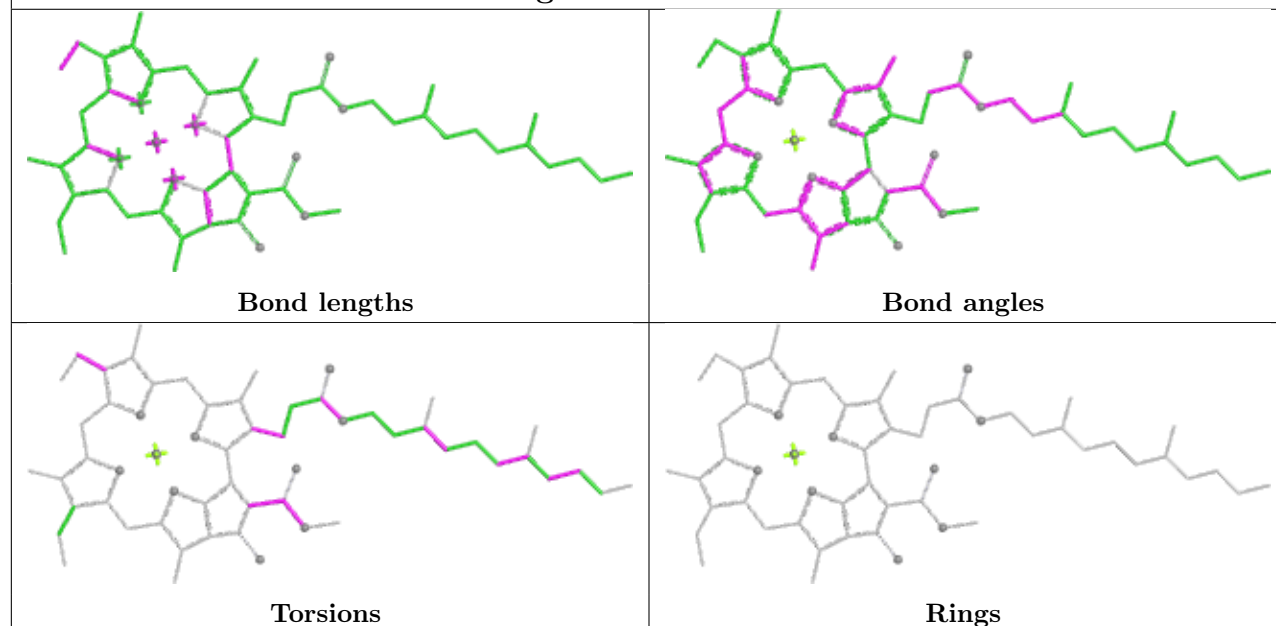
Ligand CLA A 1137

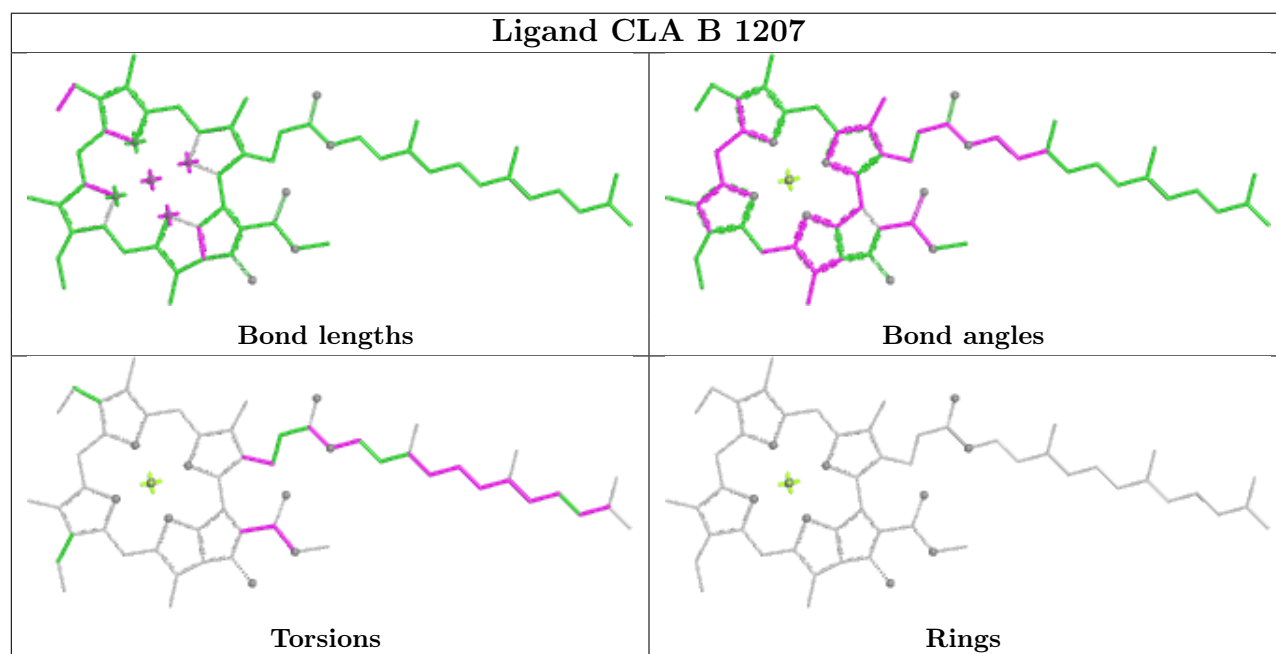
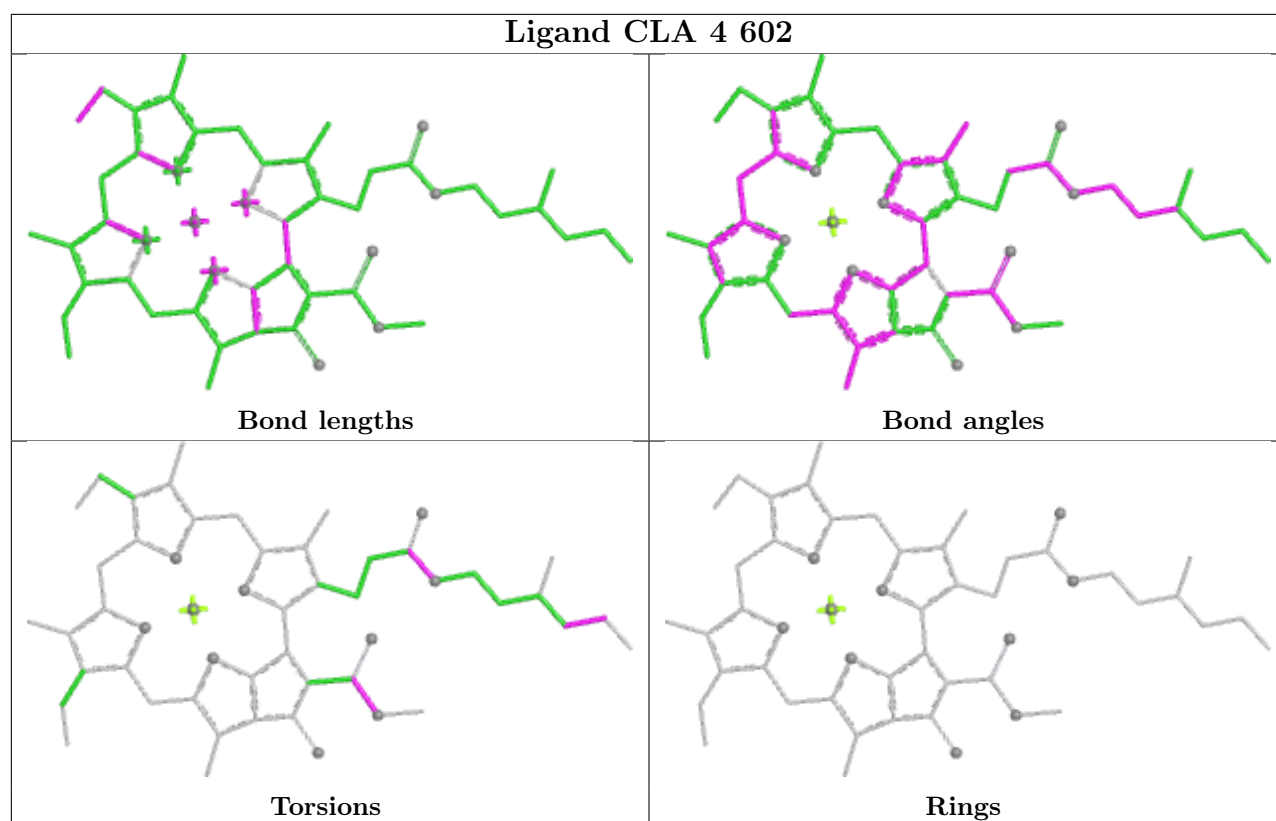


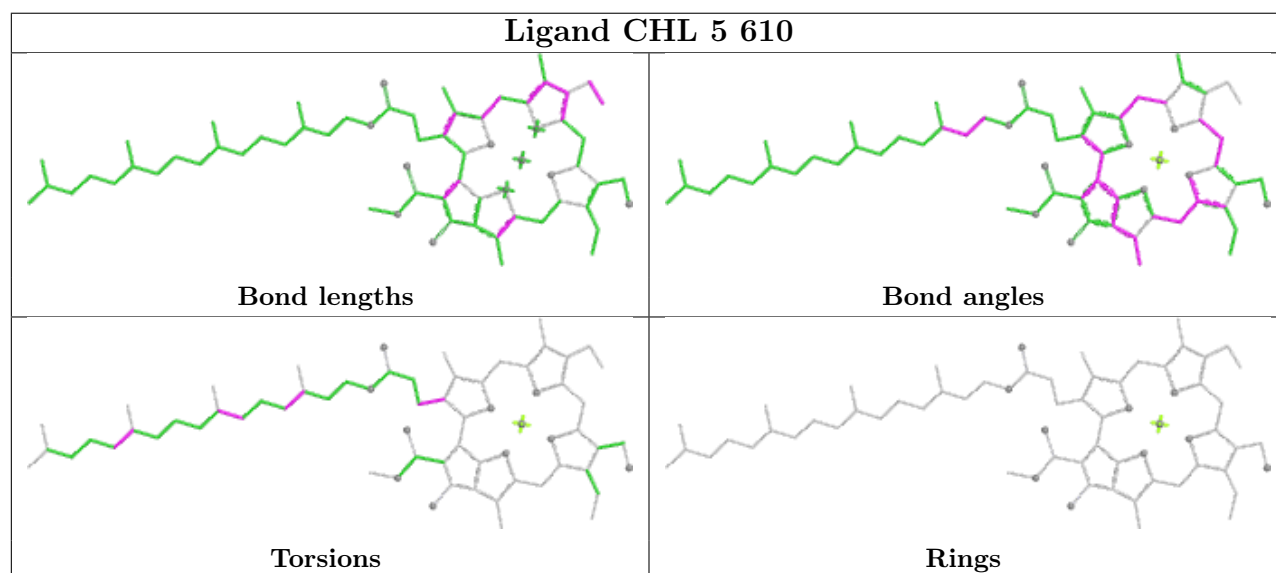
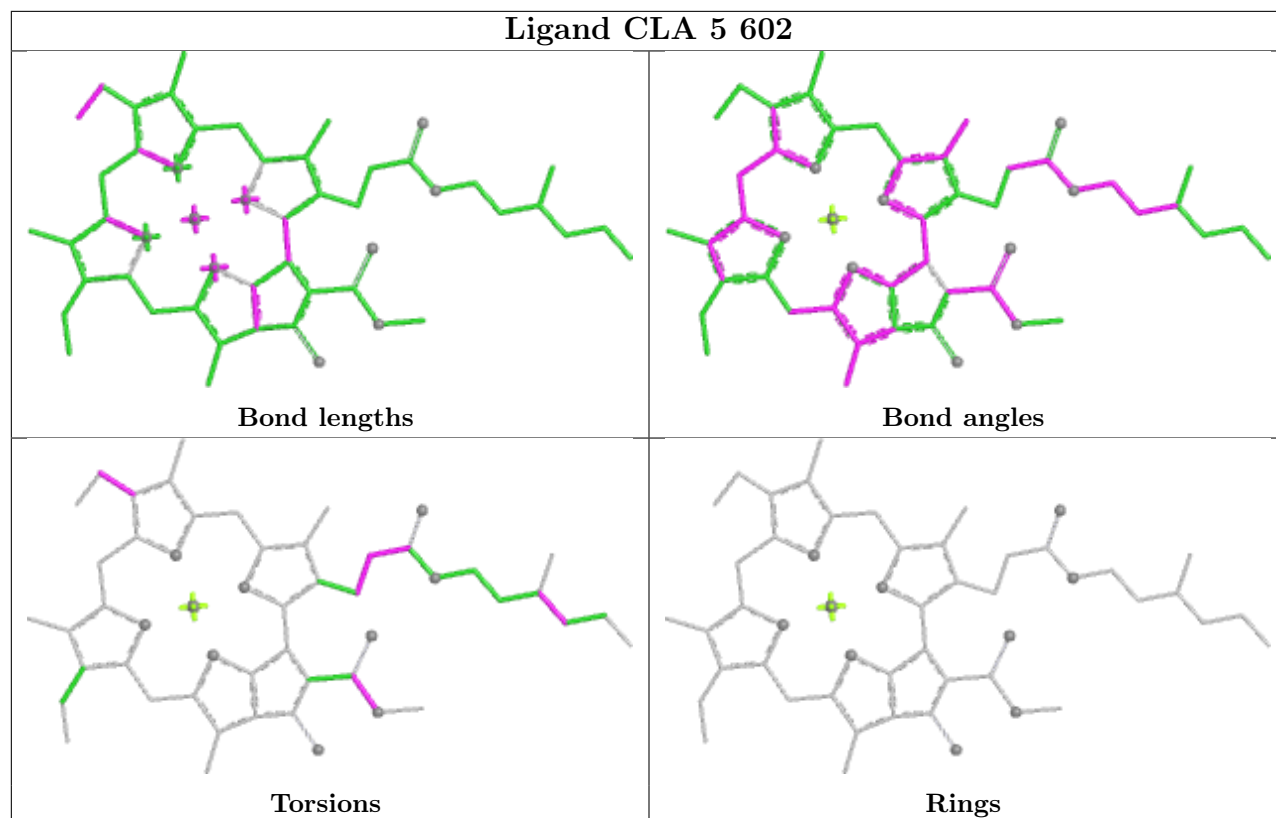
Ligand LAP B 5007



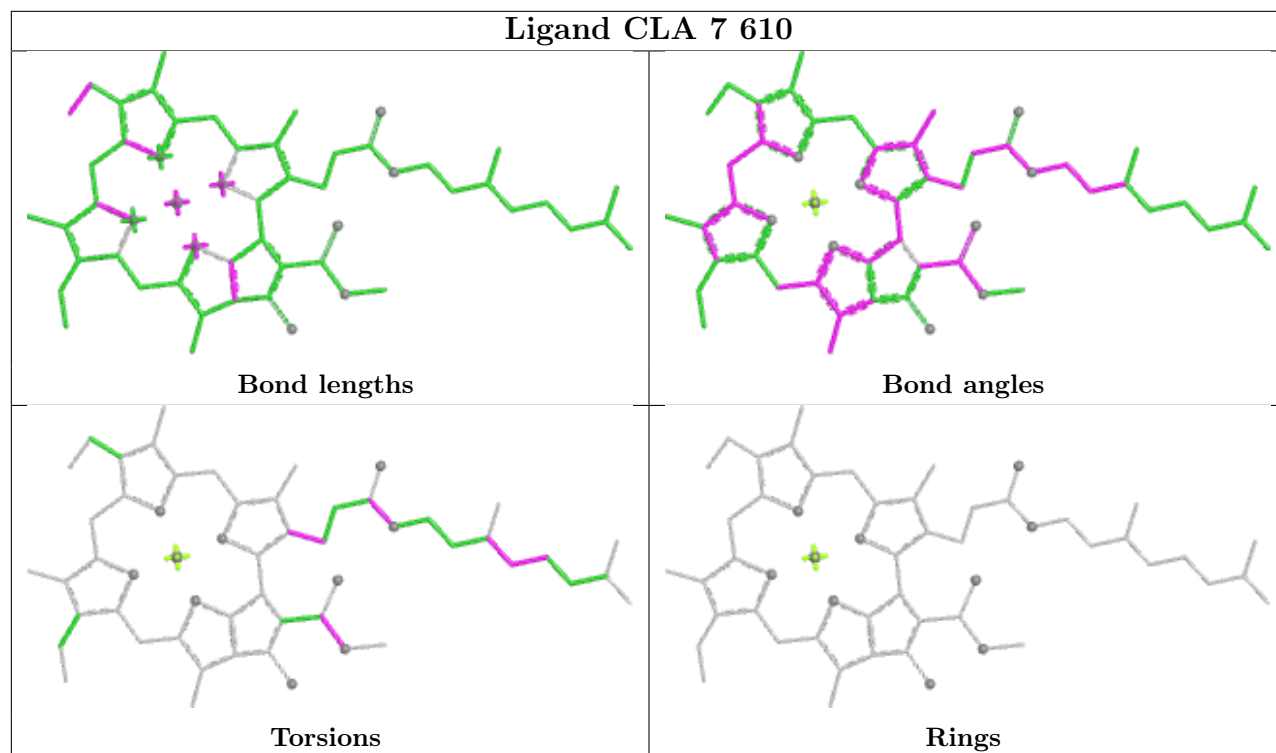
Ligand CLA a 607



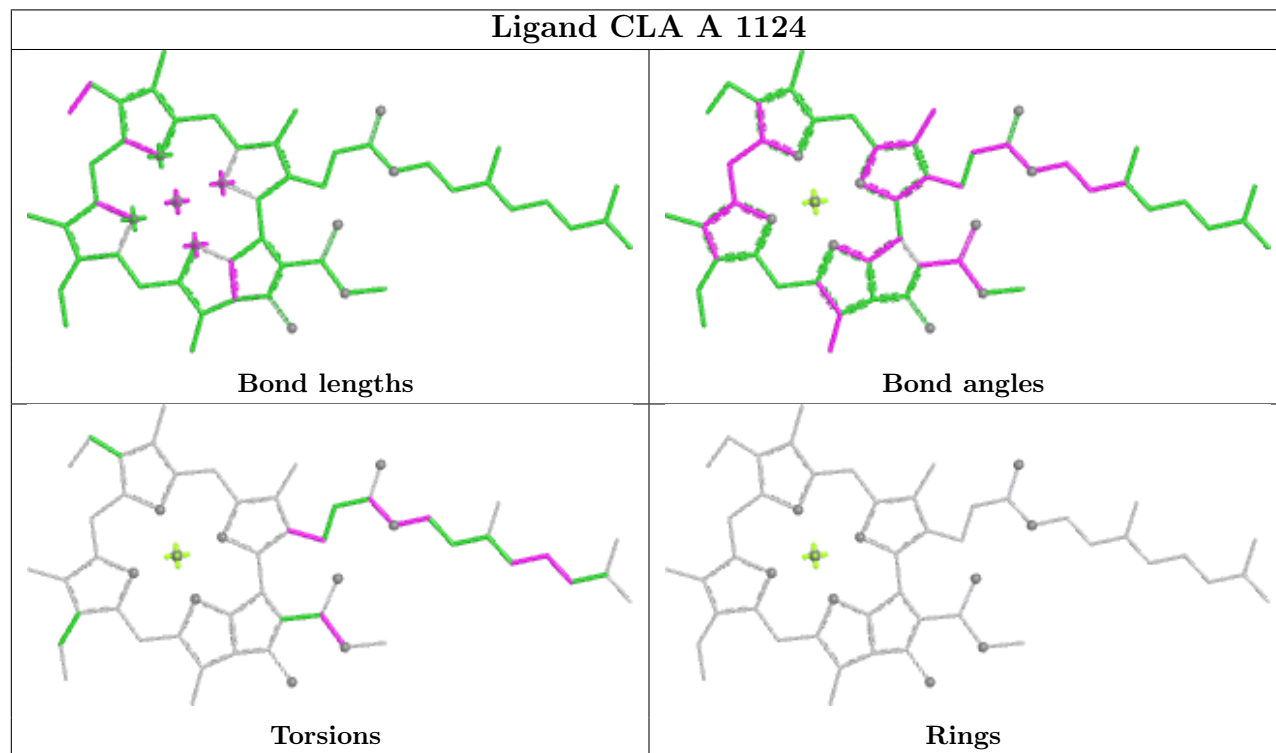


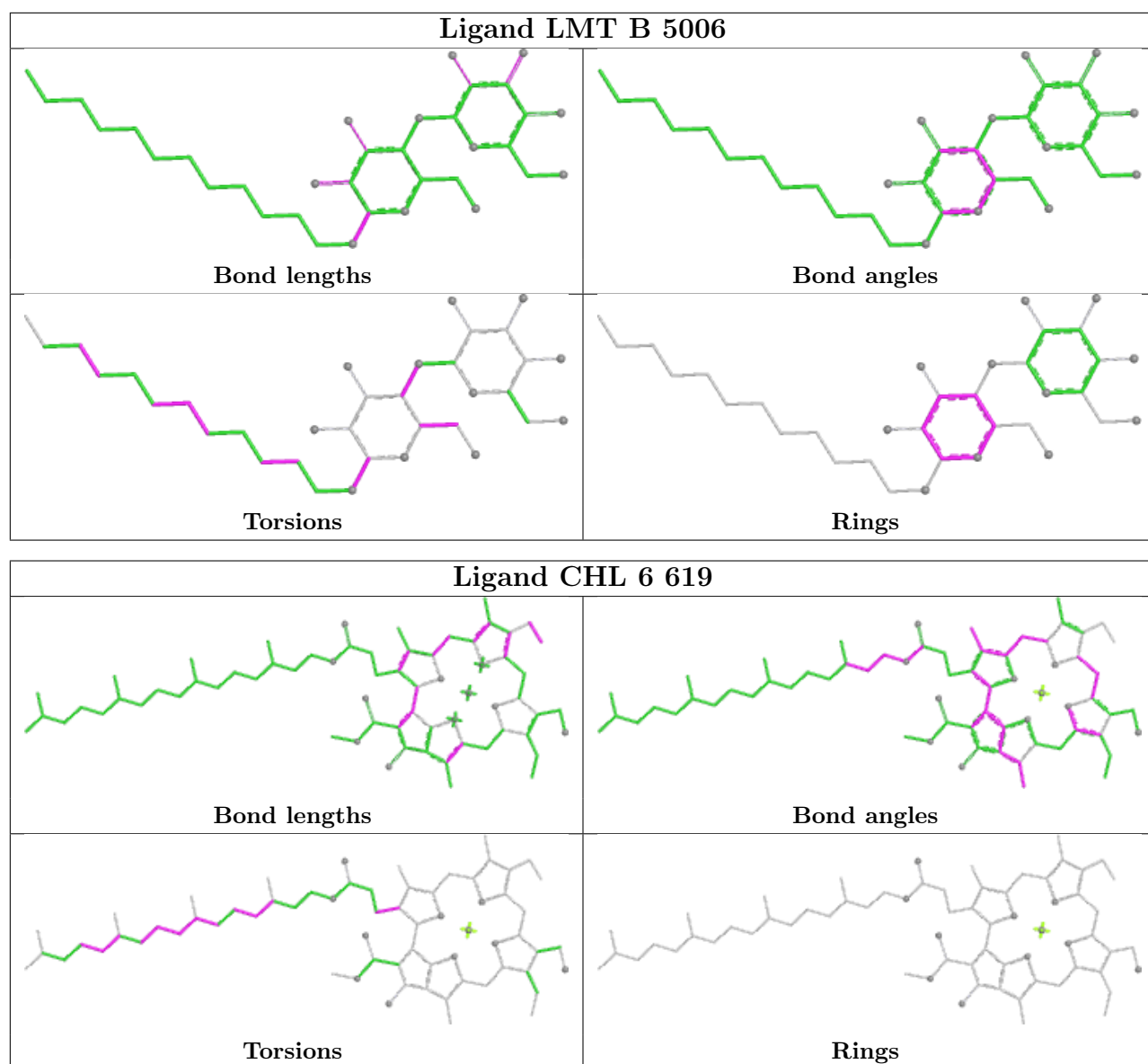


Ligand CLA 7 610

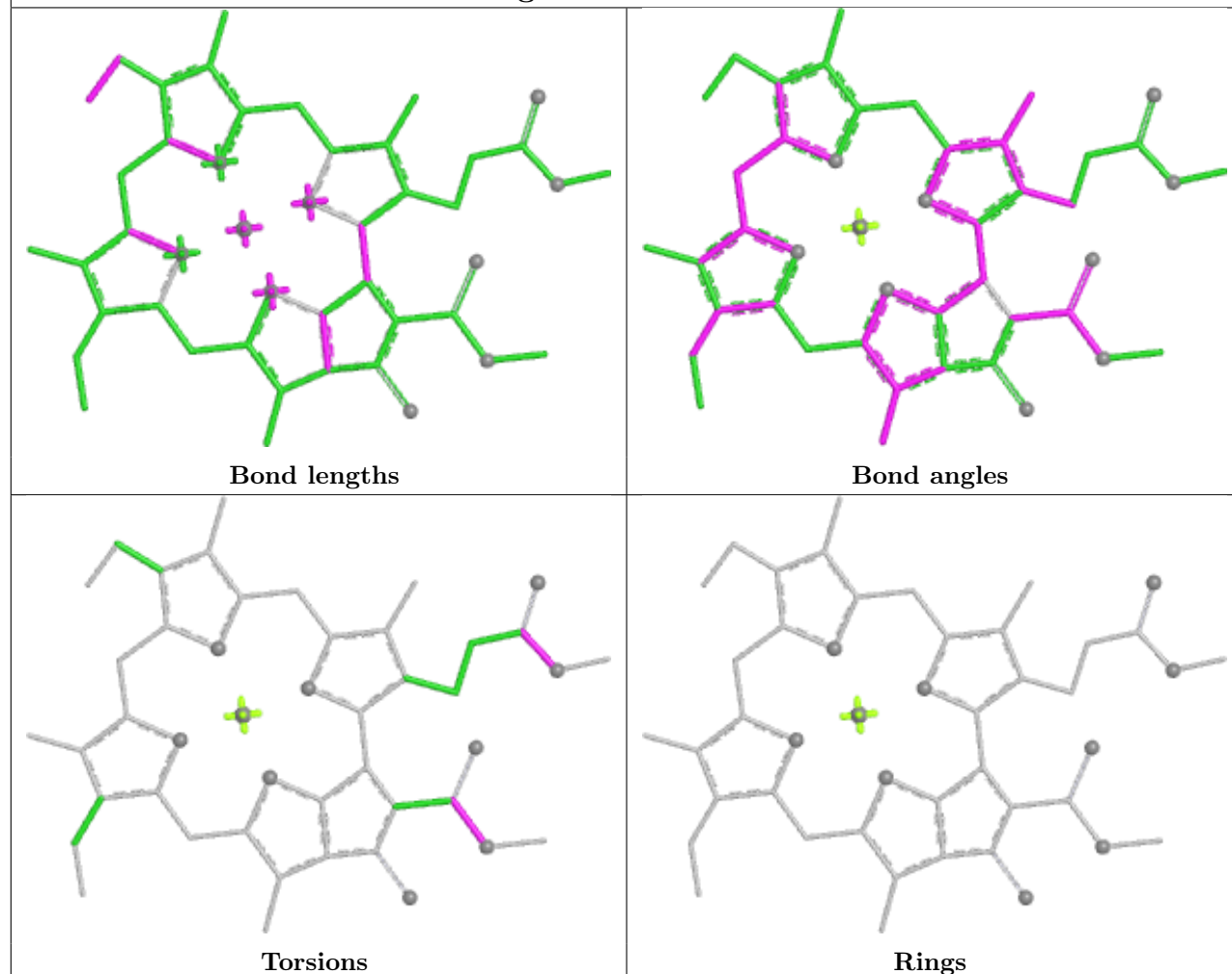


Ligand CLA A 1124

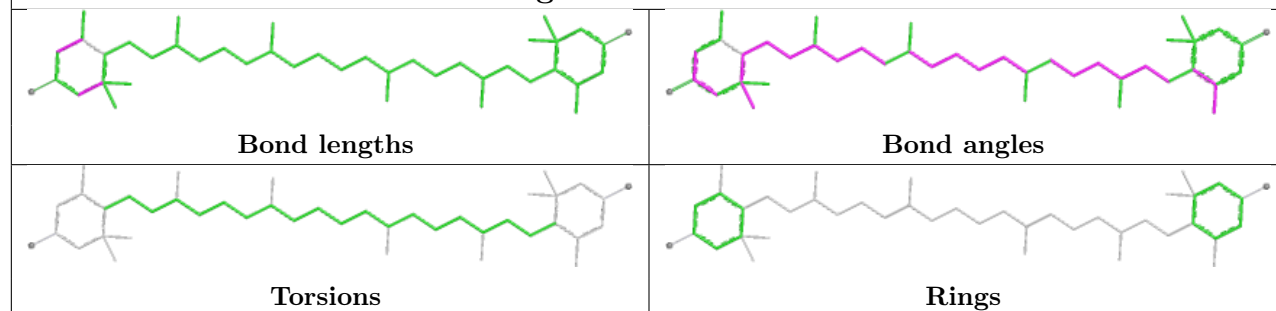


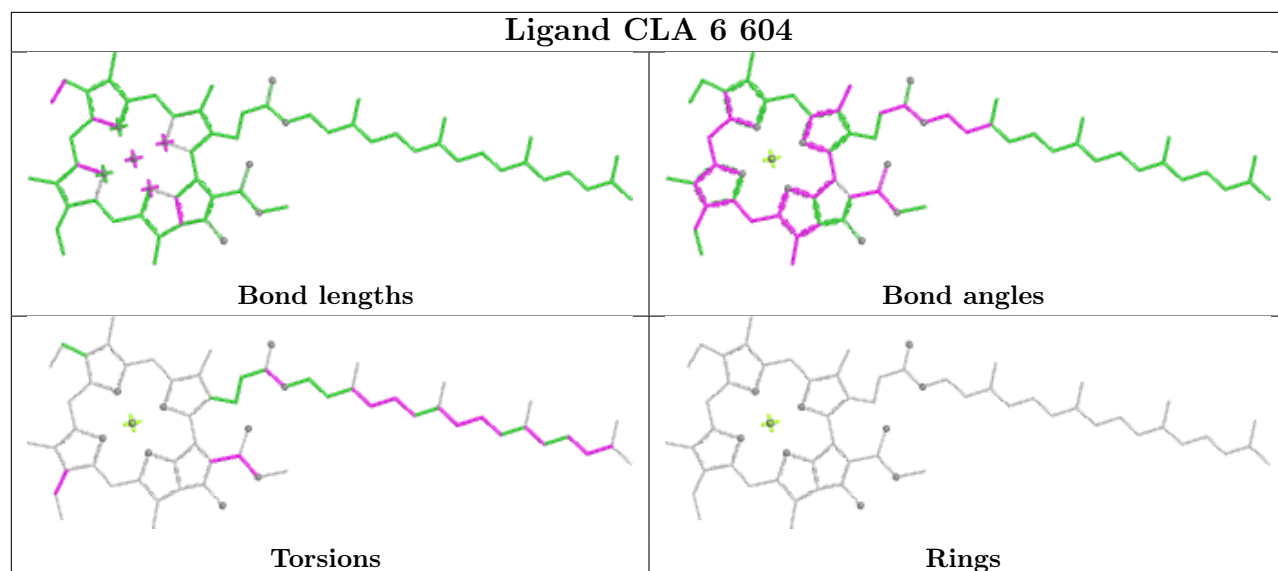
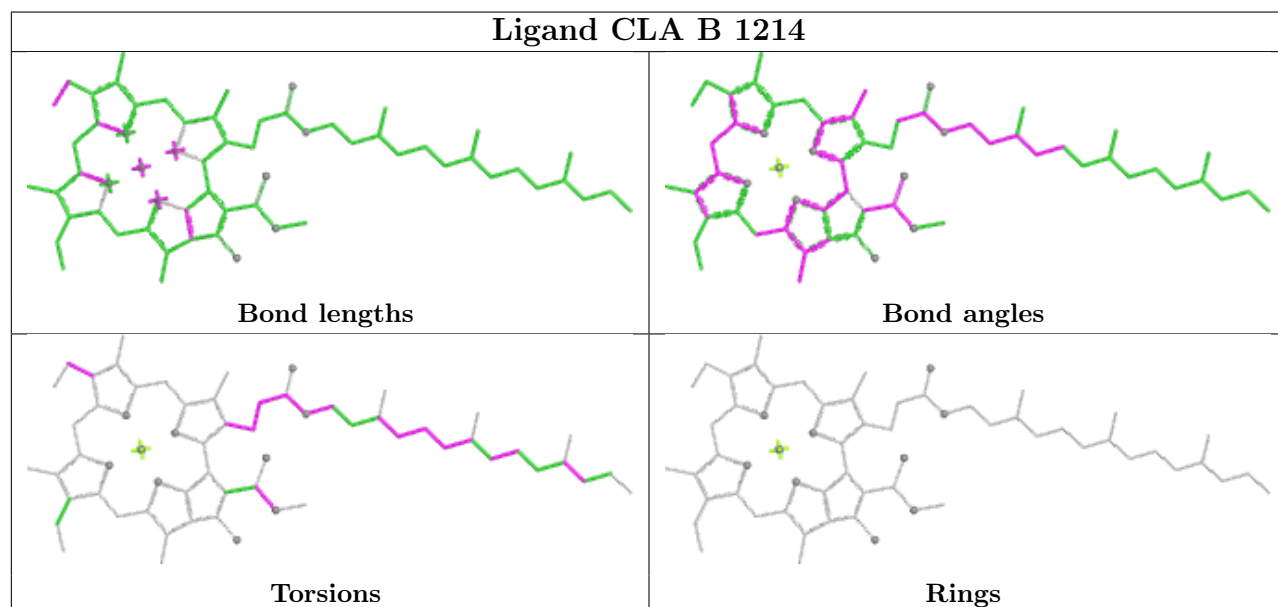
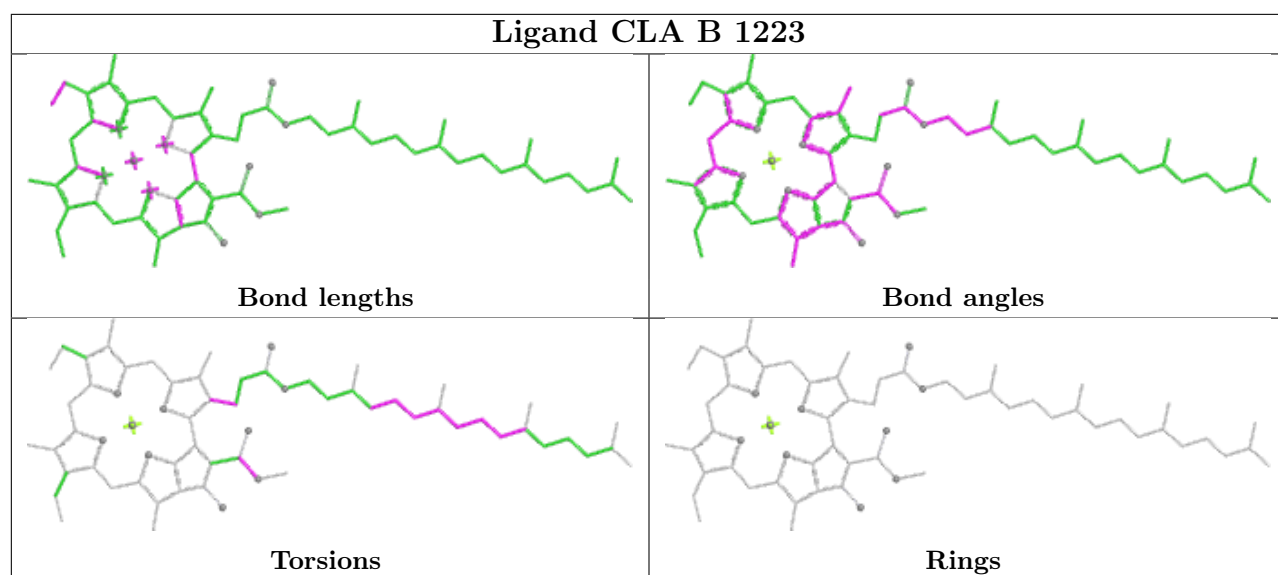


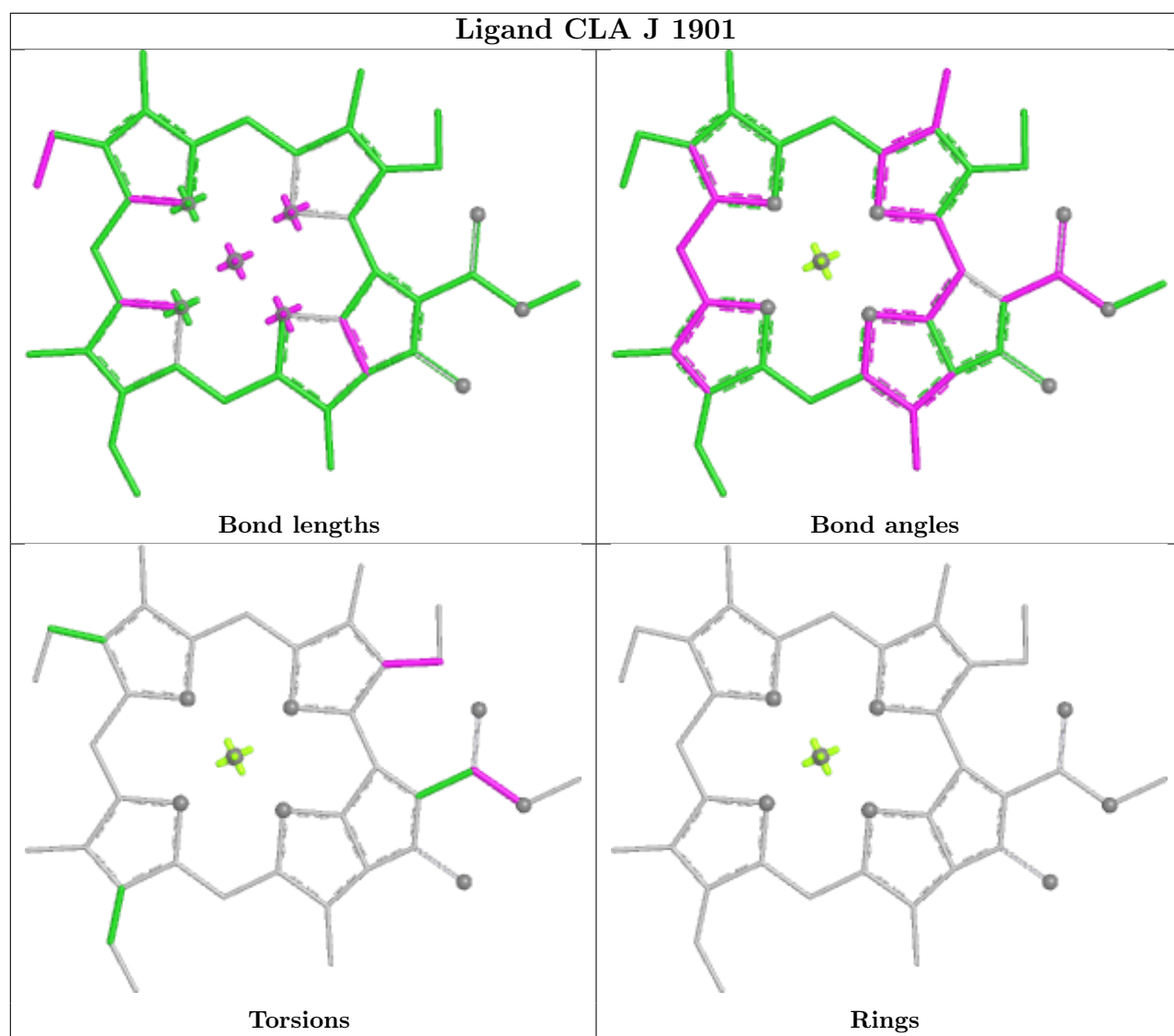
Ligand CLA a 615



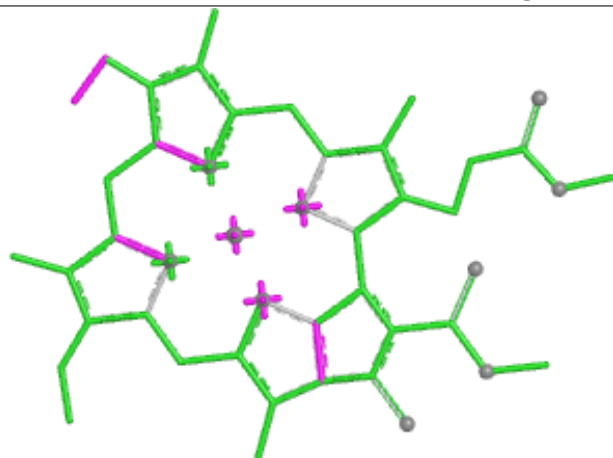
Ligand LUT 8 501



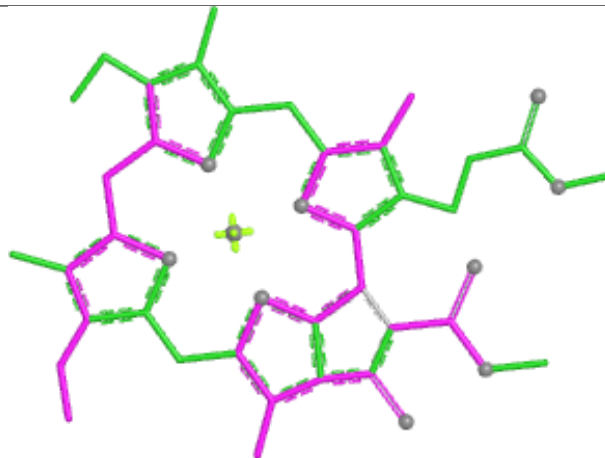




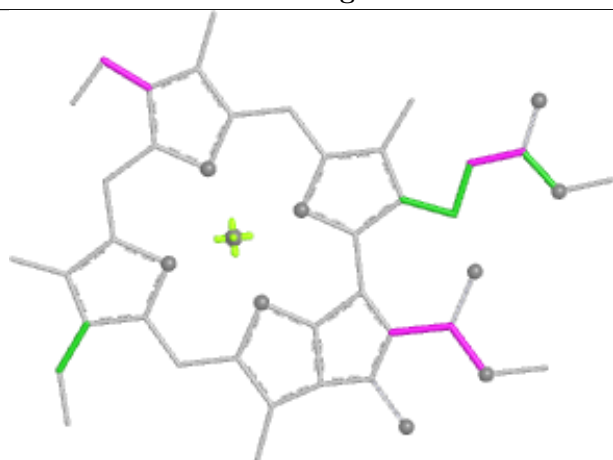
Ligand CLA 5 605



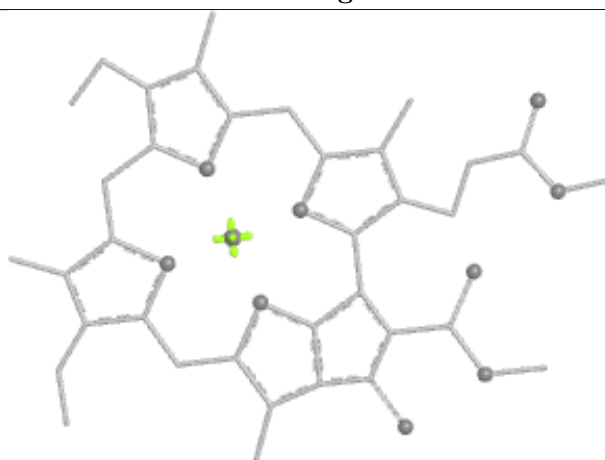
Bond lengths



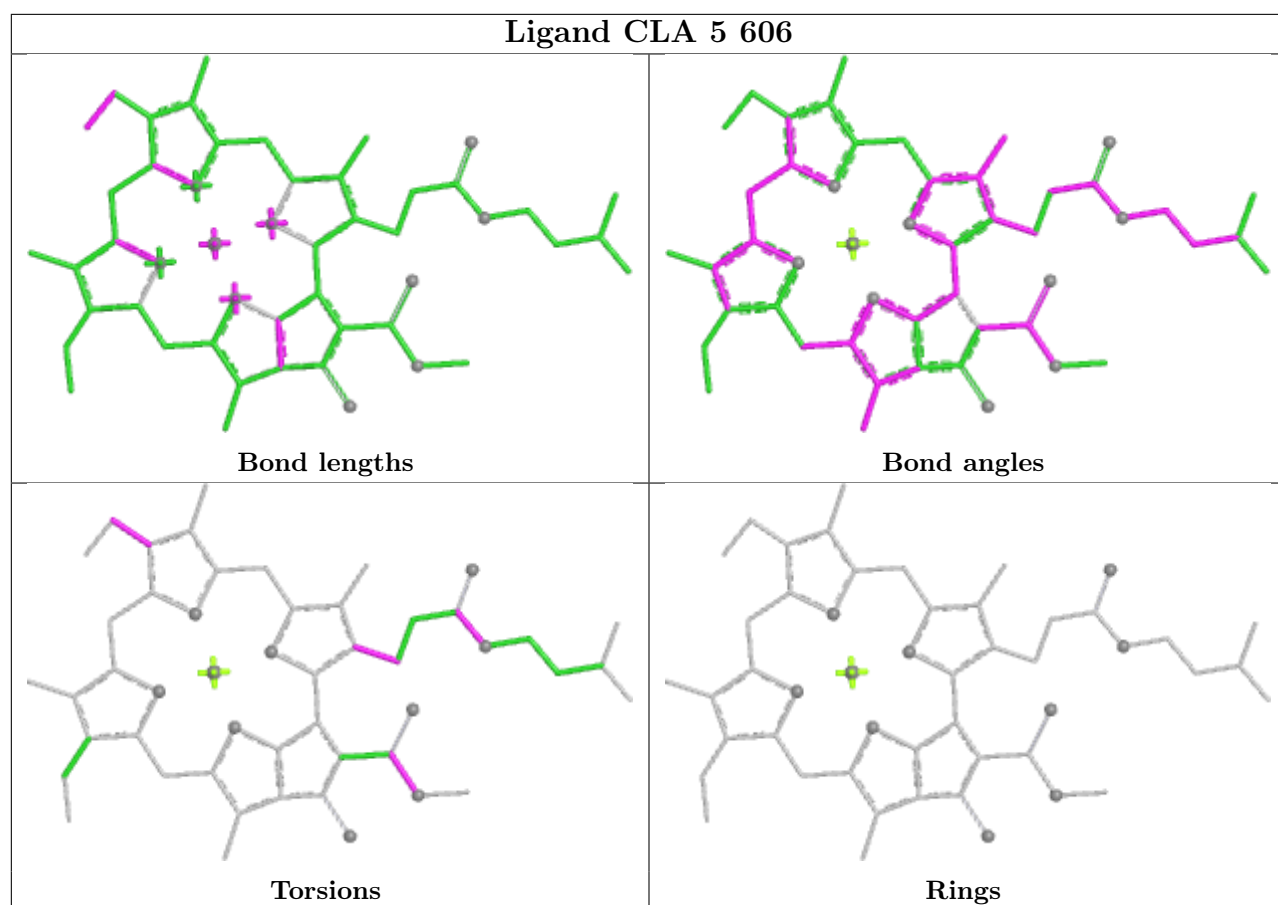
Bond angles



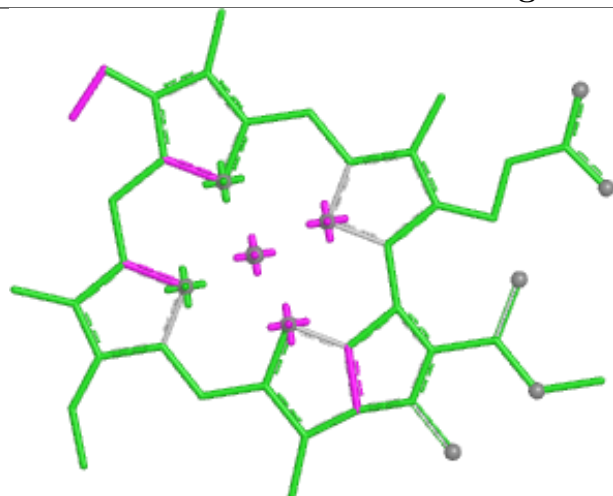
Torsions



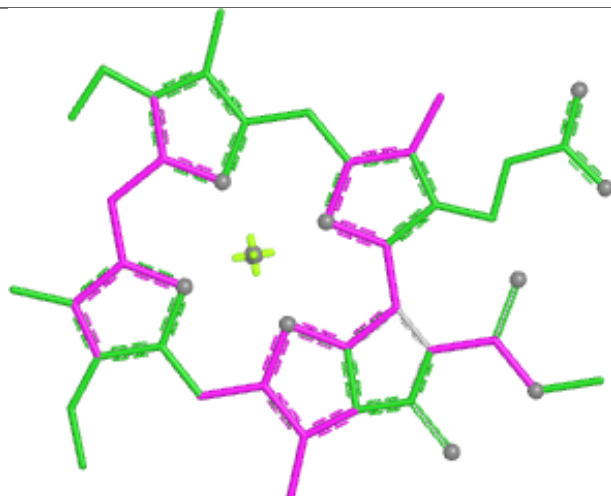
Rings



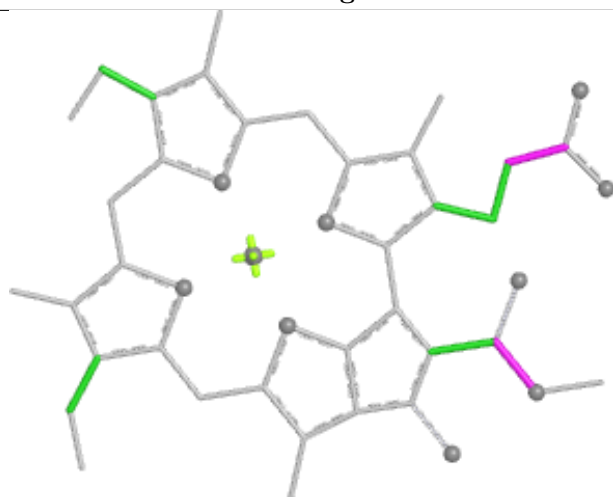
Ligand CLA 8 605



Bond lengths



Bond angles

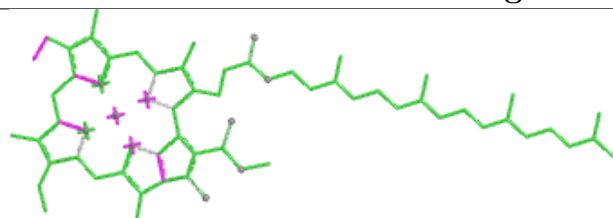


Torsions

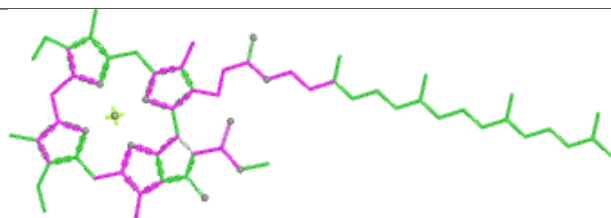


Rings

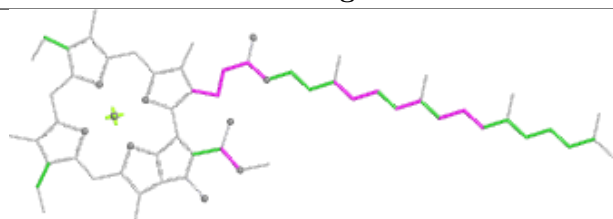
Ligand CLA A 1103



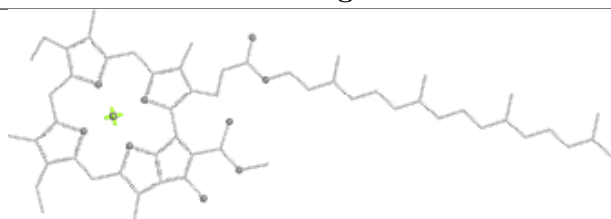
Bond lengths



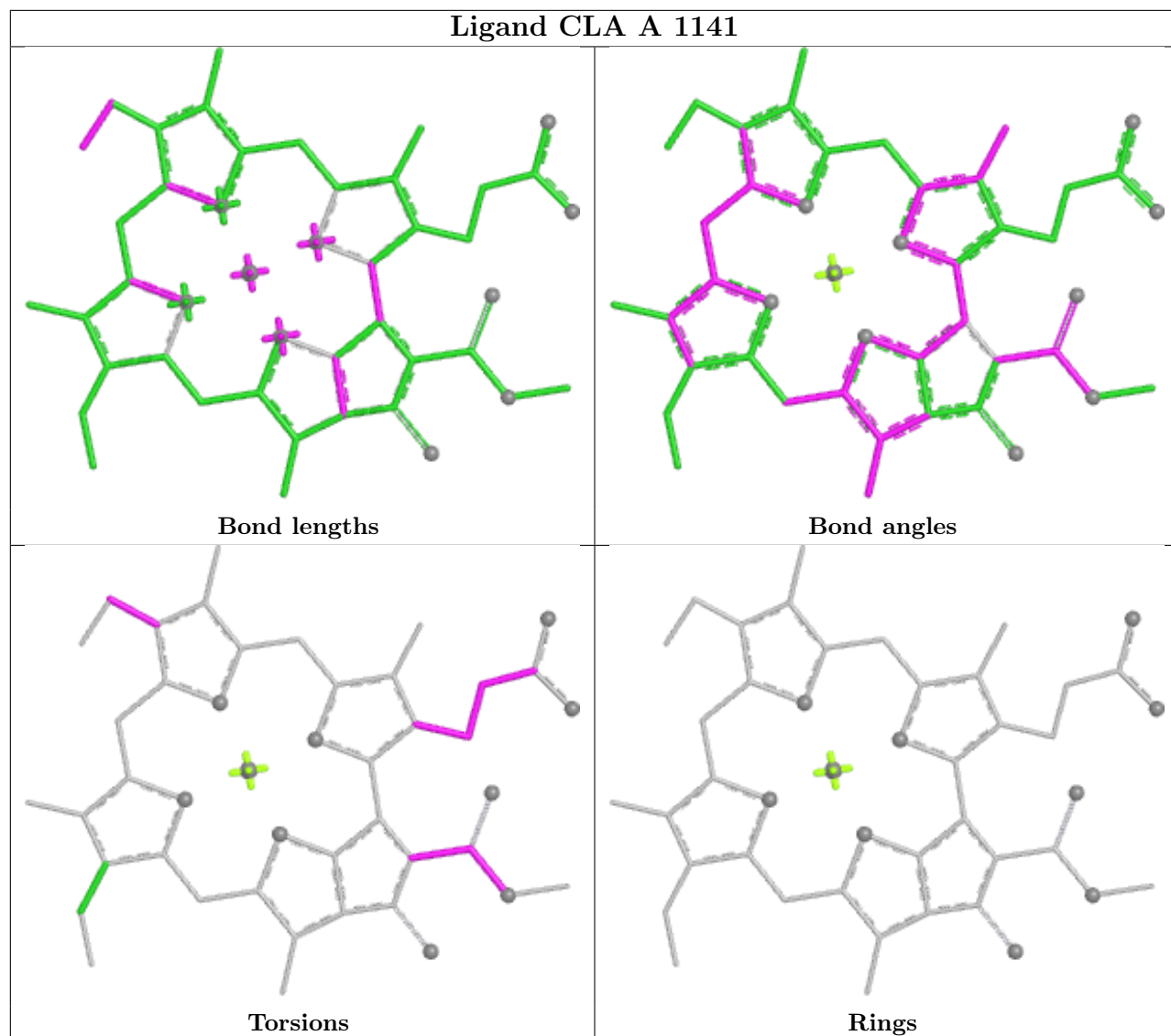
Bond angles

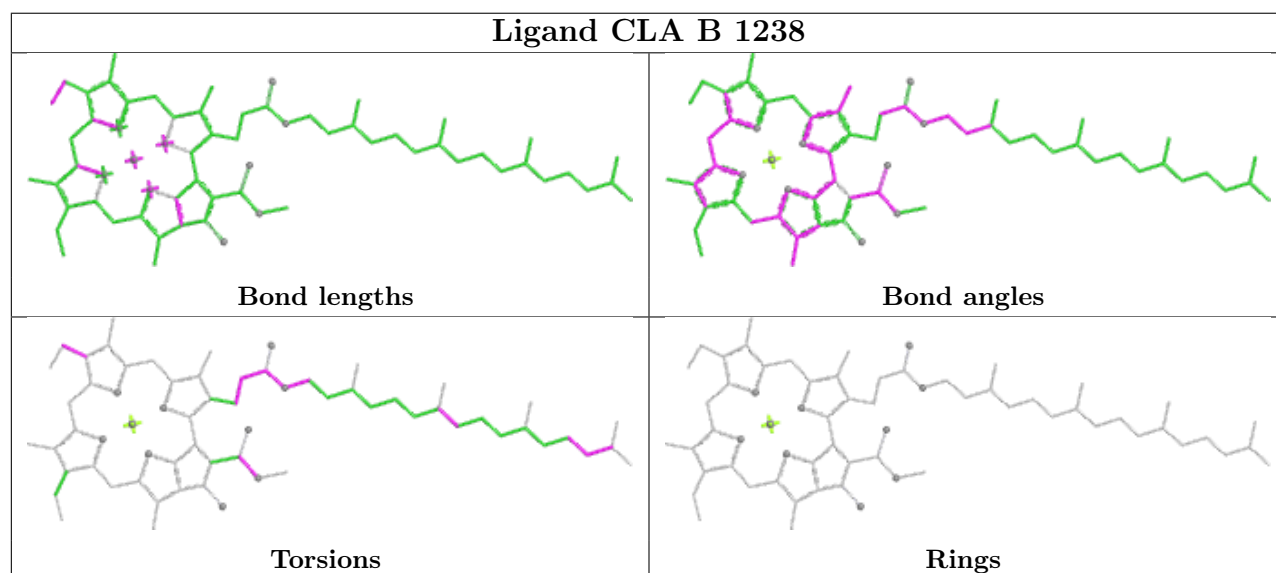
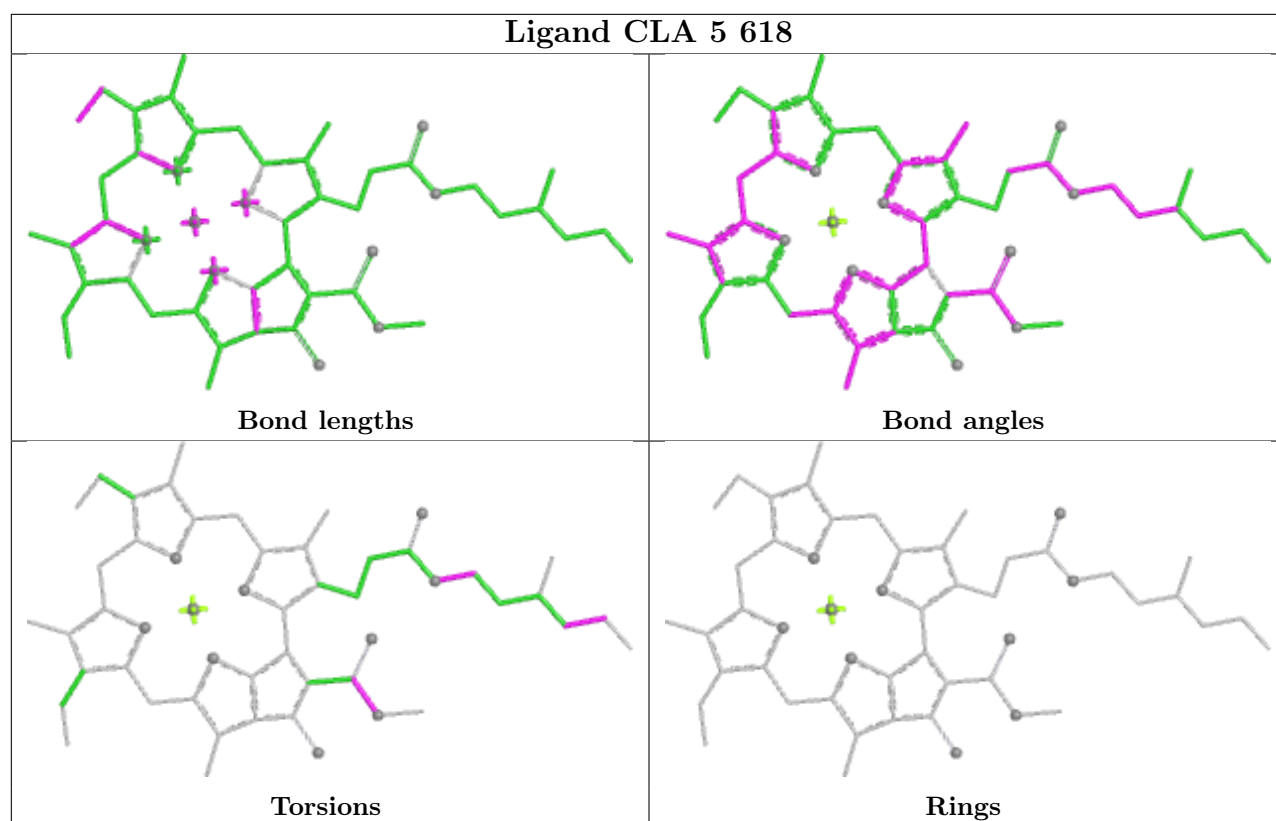


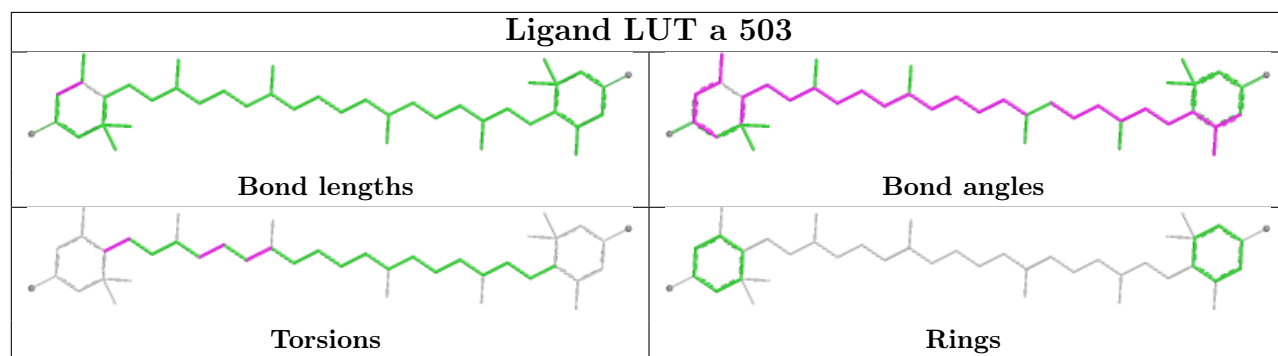
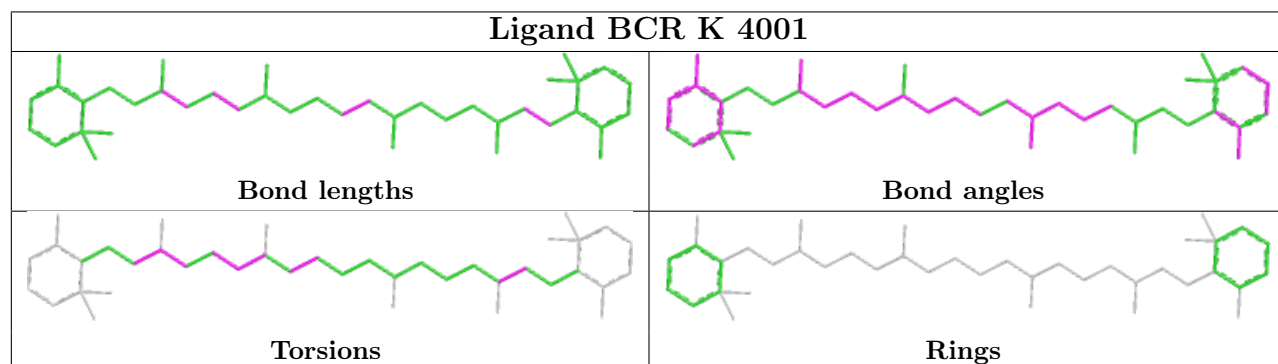
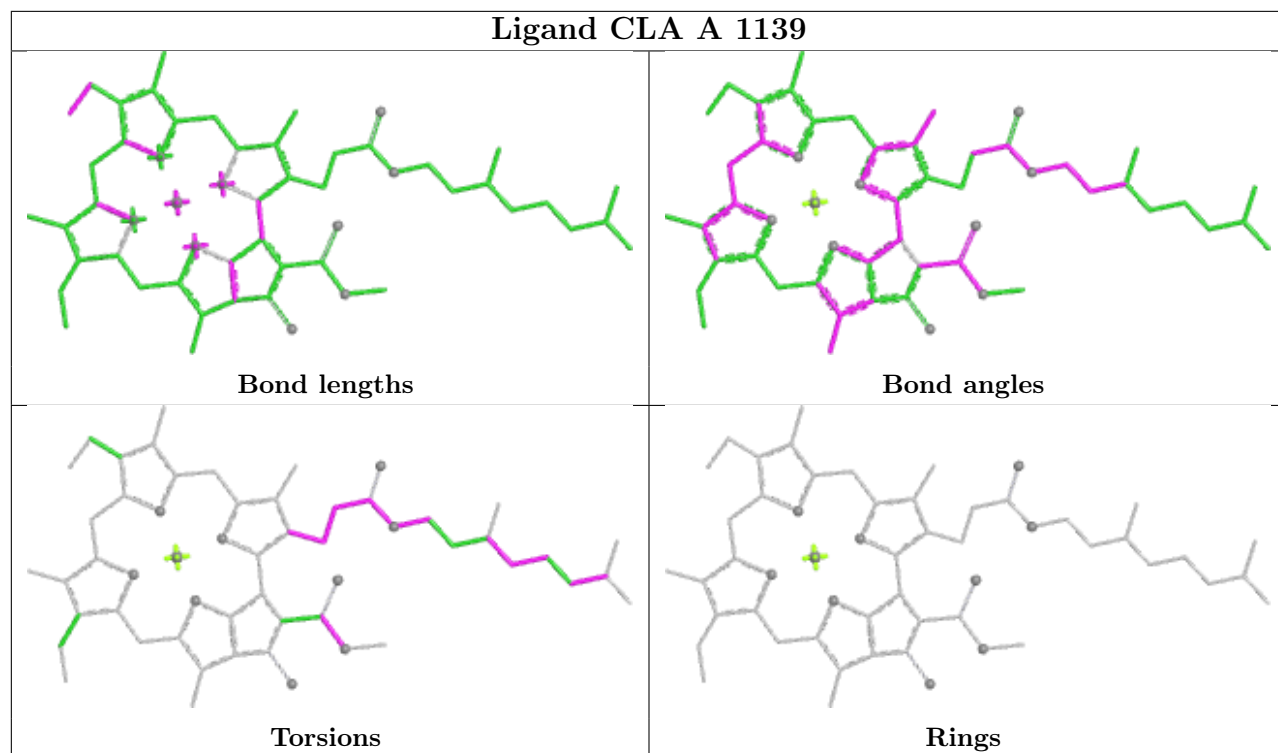
Torsions

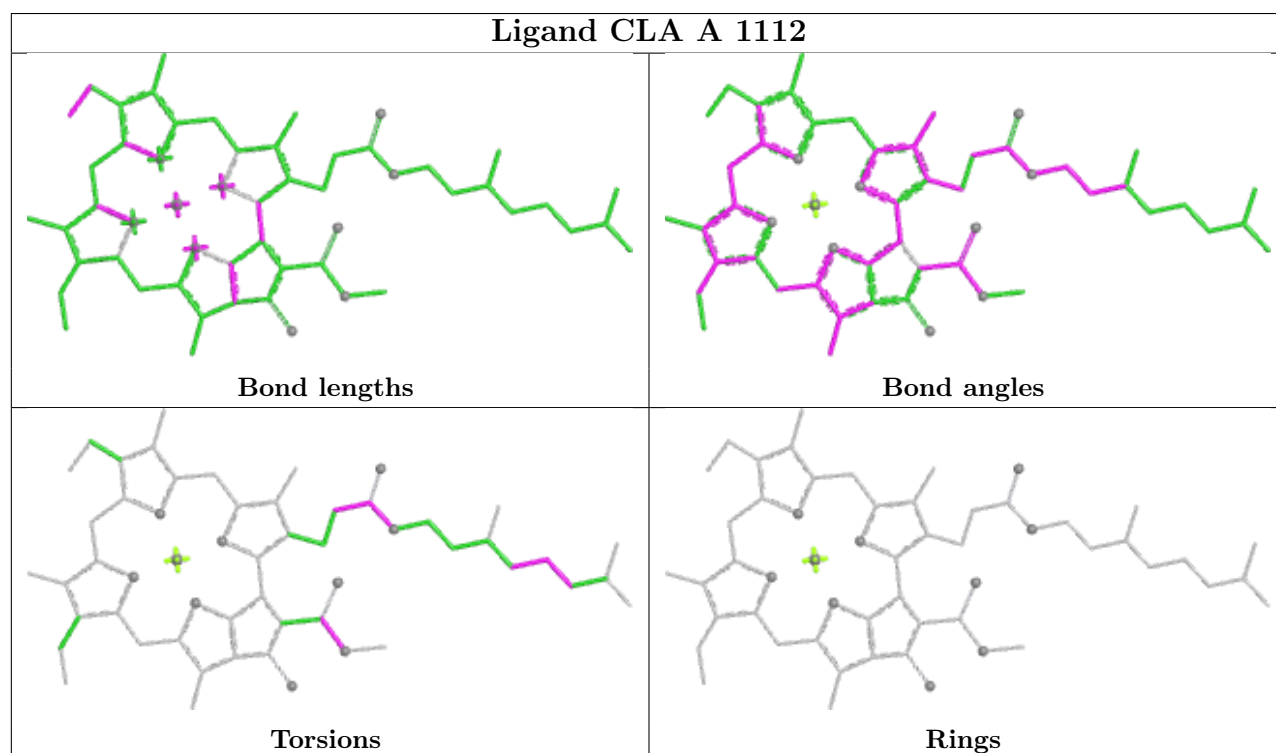
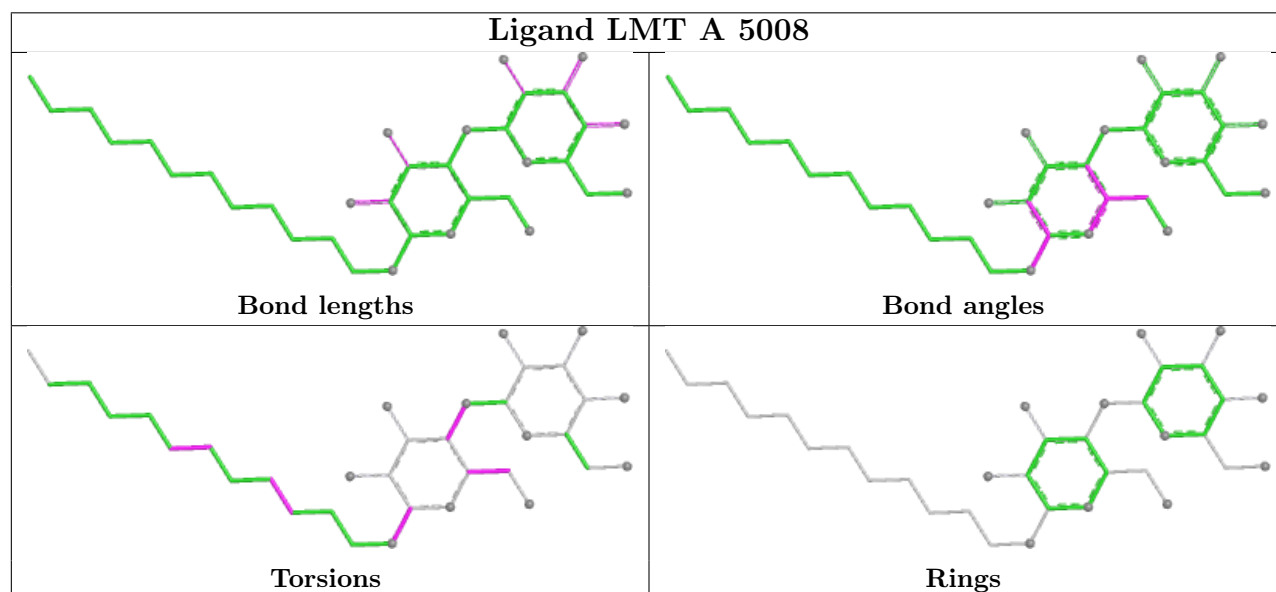
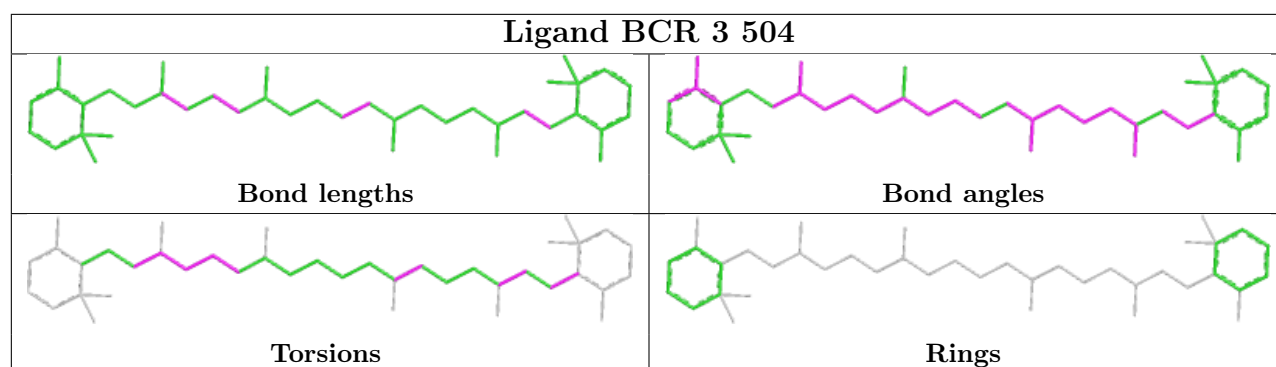


Rings

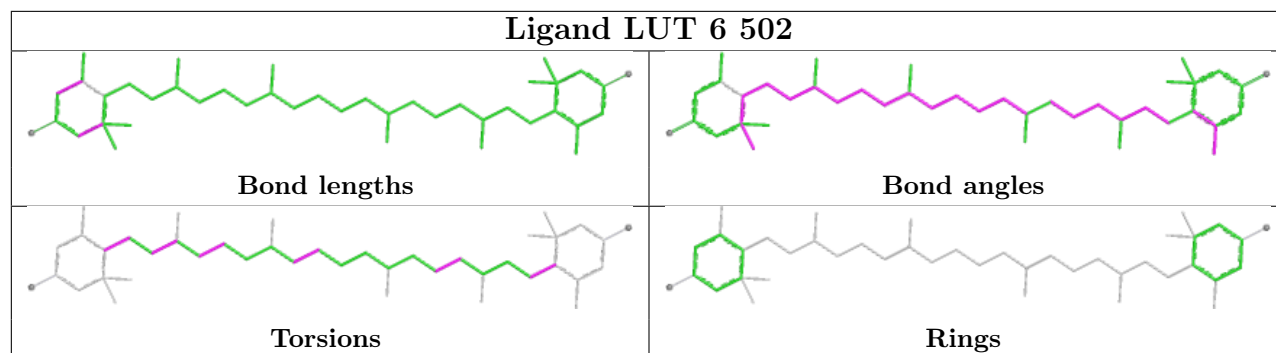




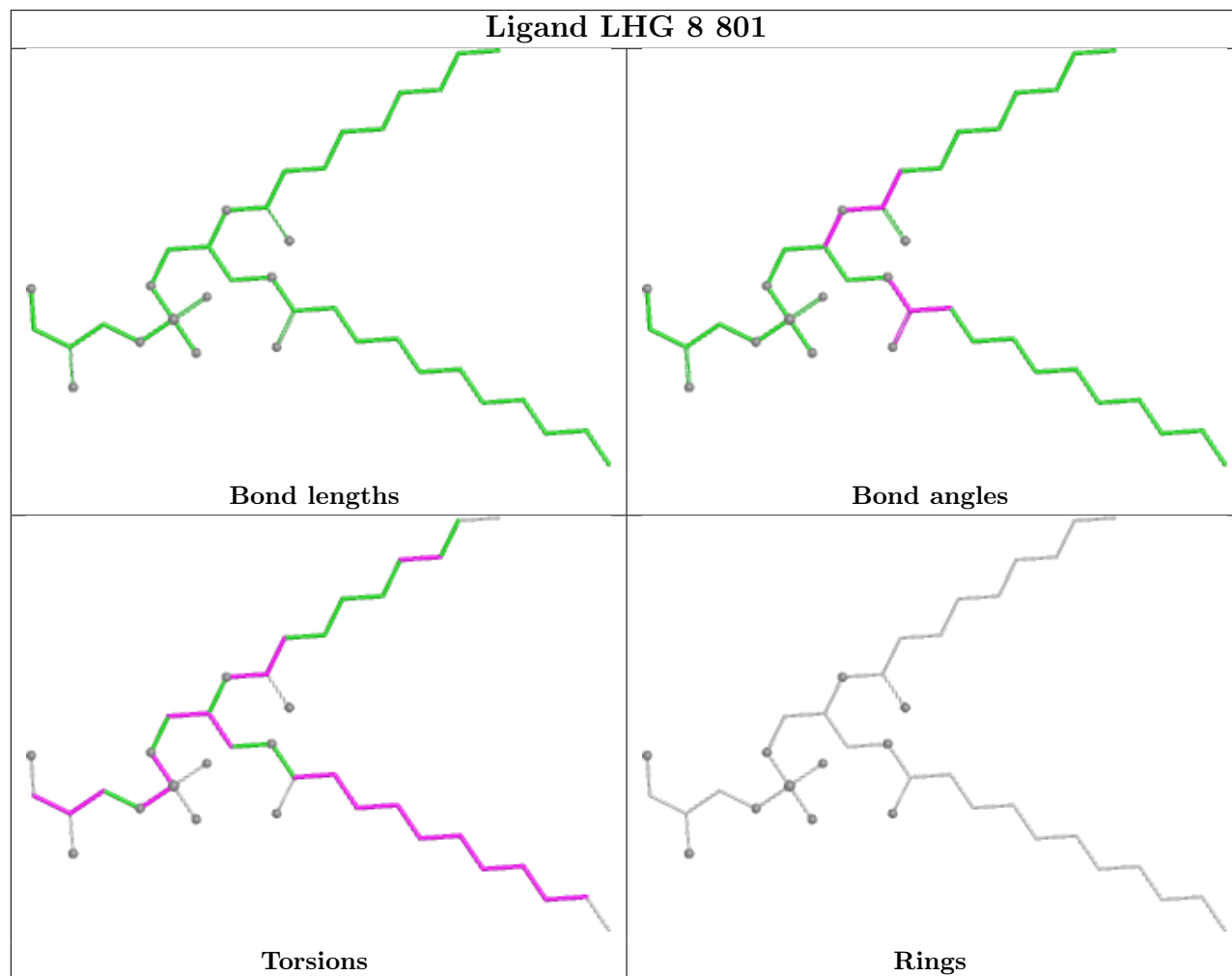




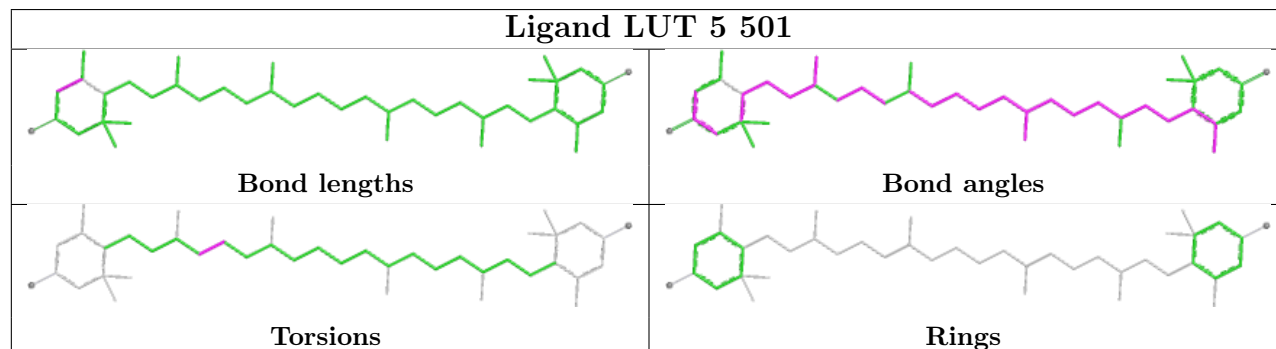
Ligand LUT 6 502

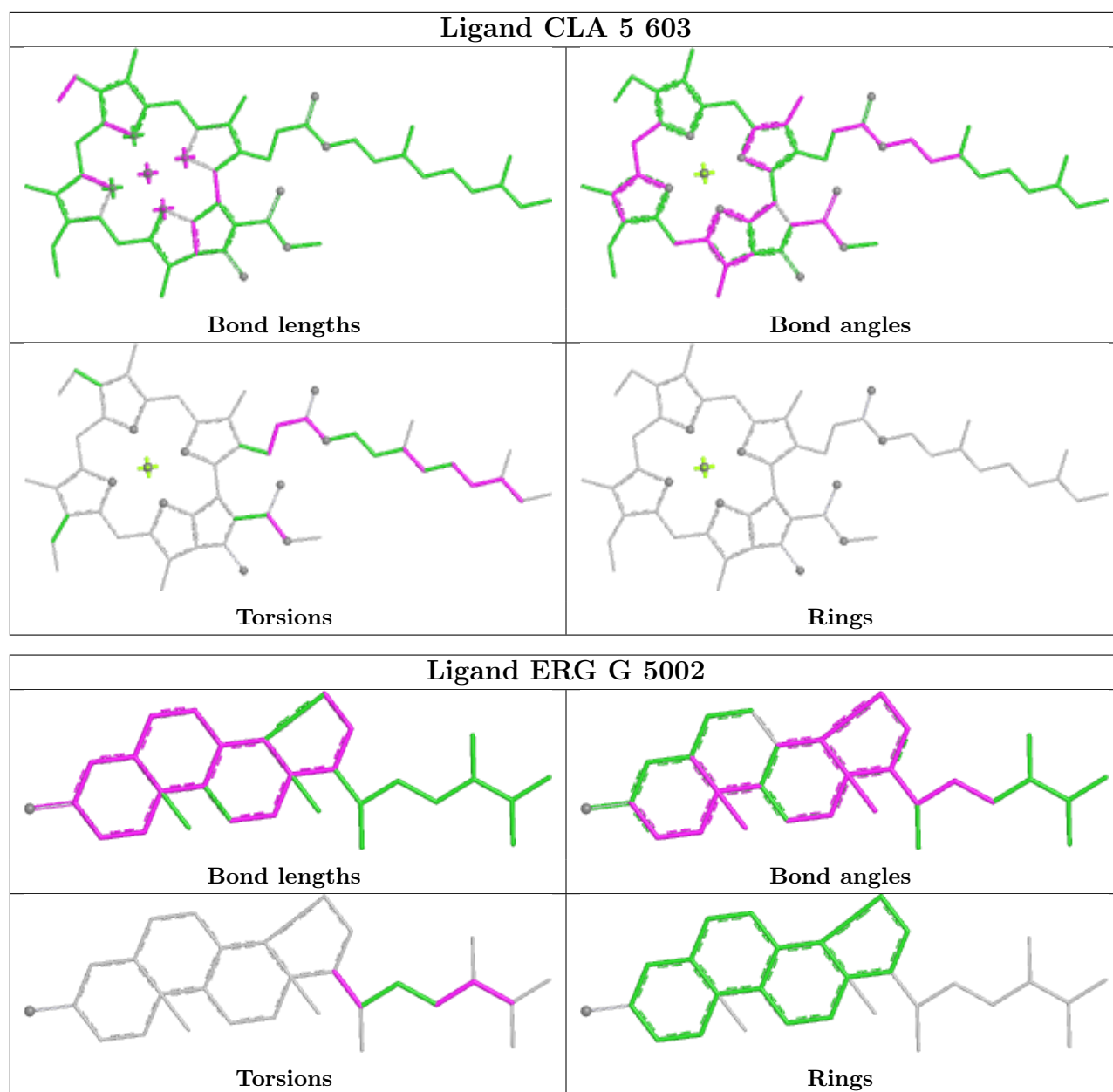


Ligand LHG 8 801

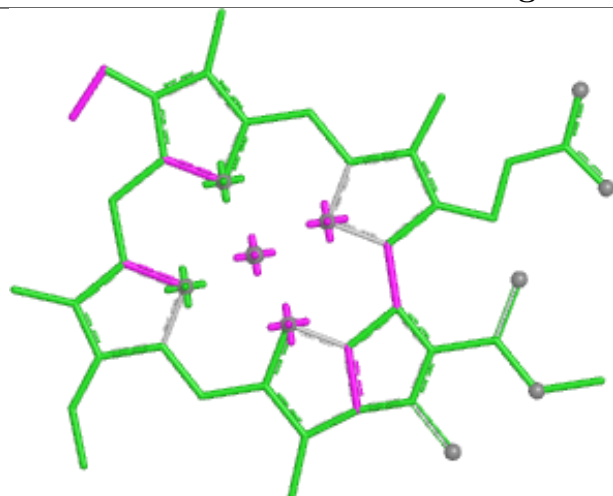


Ligand LUT 5 501

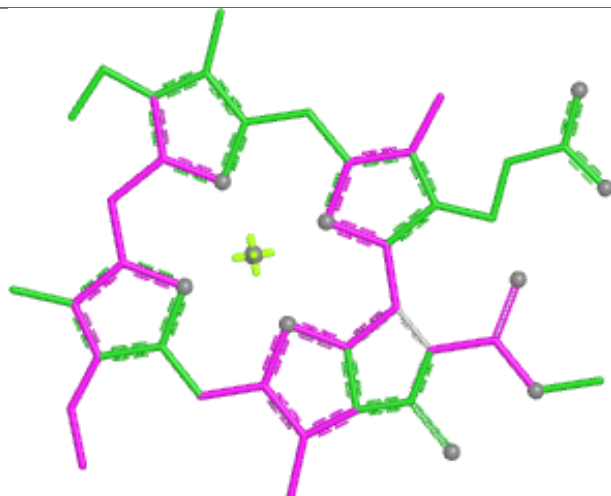




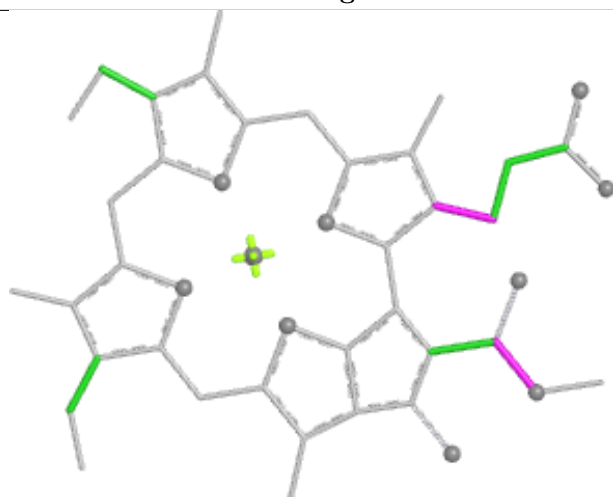
Ligand CLA 6 617



Bond lengths



Bond angles

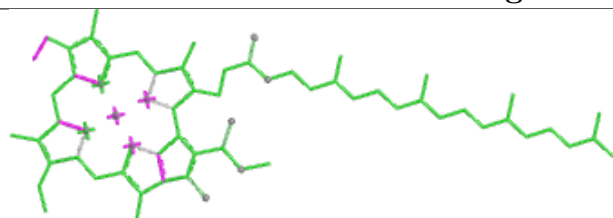


Torsions

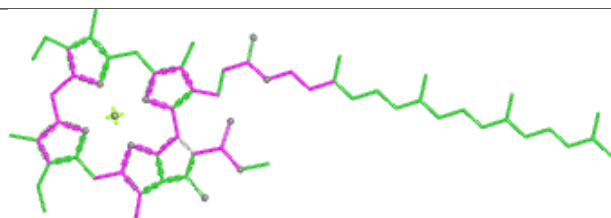


Rings

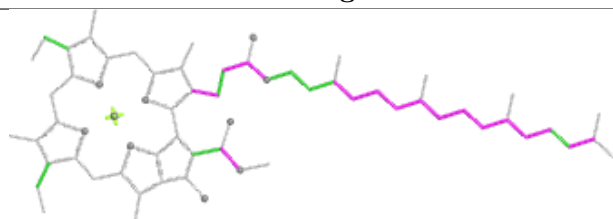
Ligand CLA B 1021



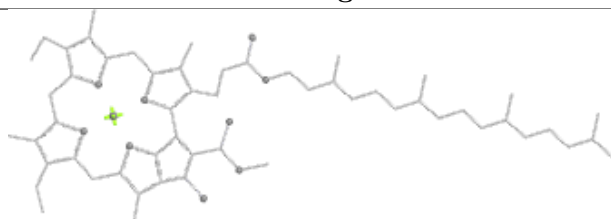
Bond lengths



Bond angles

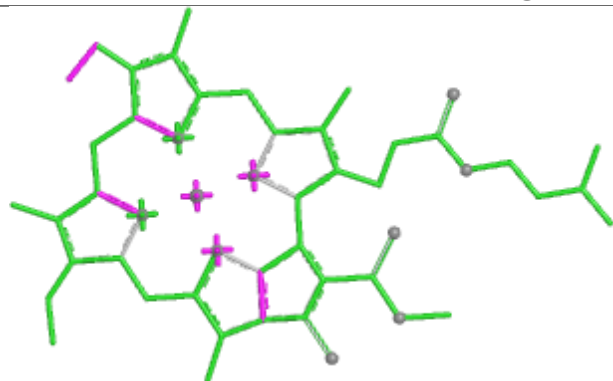


Torsions

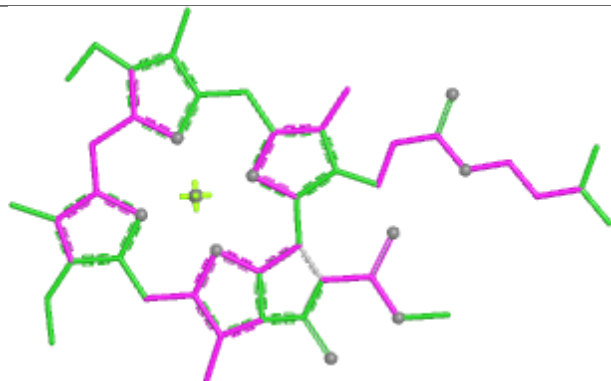


Rings

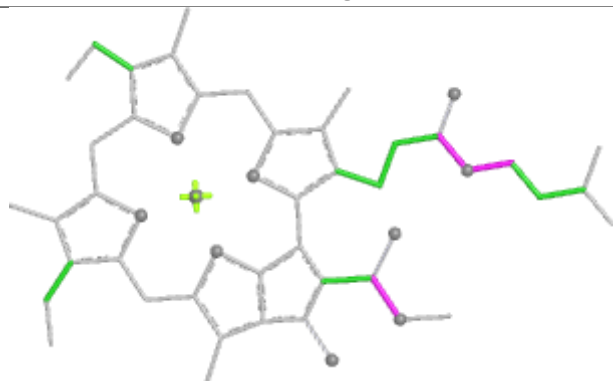
Ligand CLA 8 611



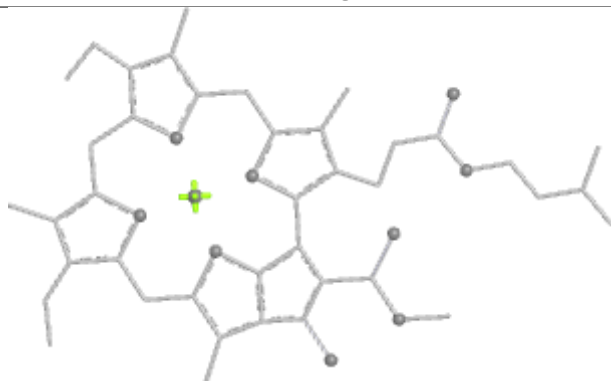
Bond lengths



Bond angles

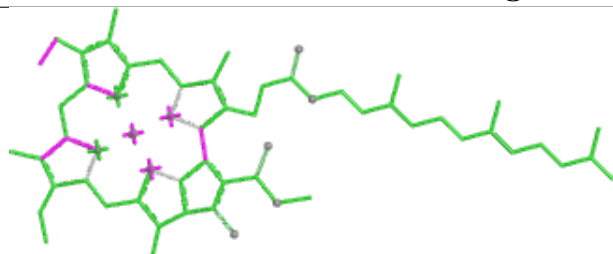


Torsions

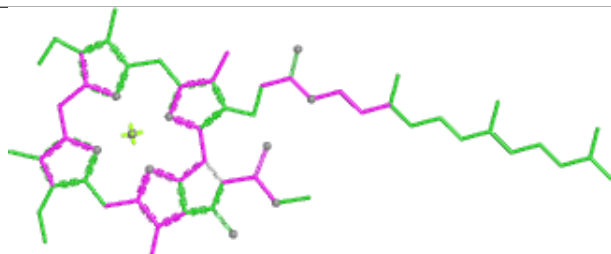


Rings

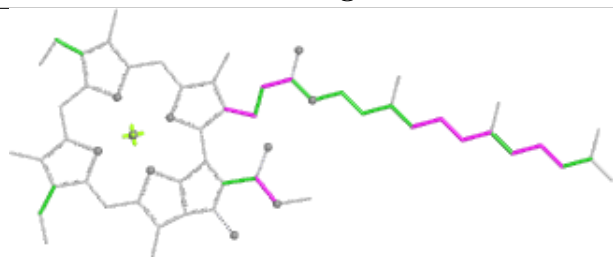
Ligand CLA K 1402



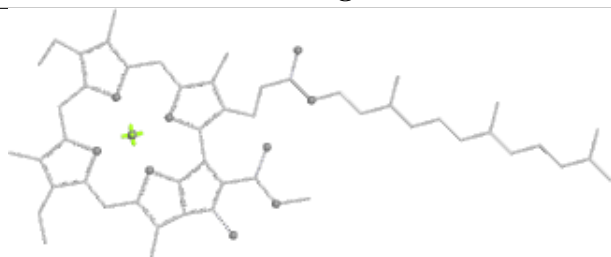
Bond lengths



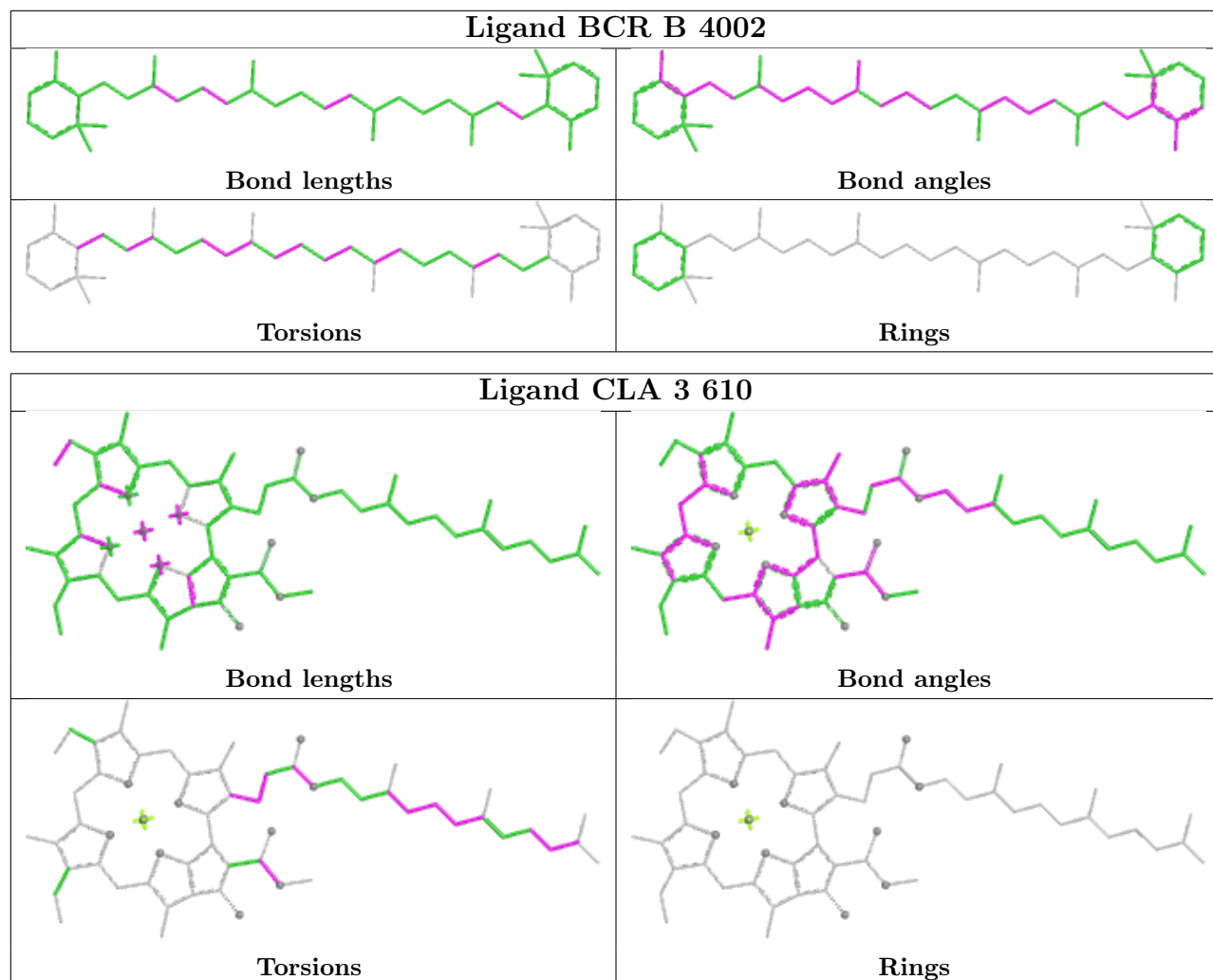
Bond angles



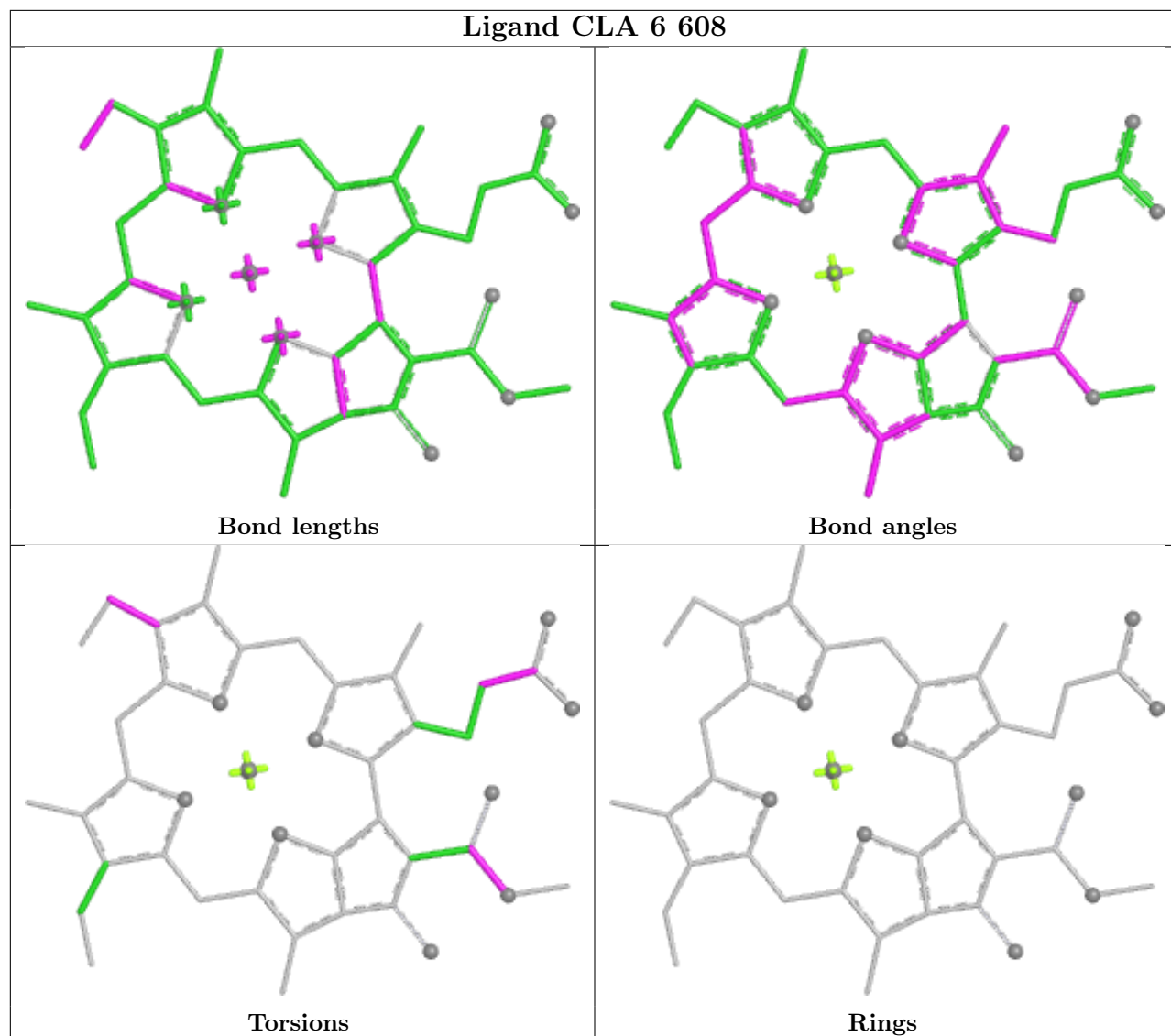
Torsions

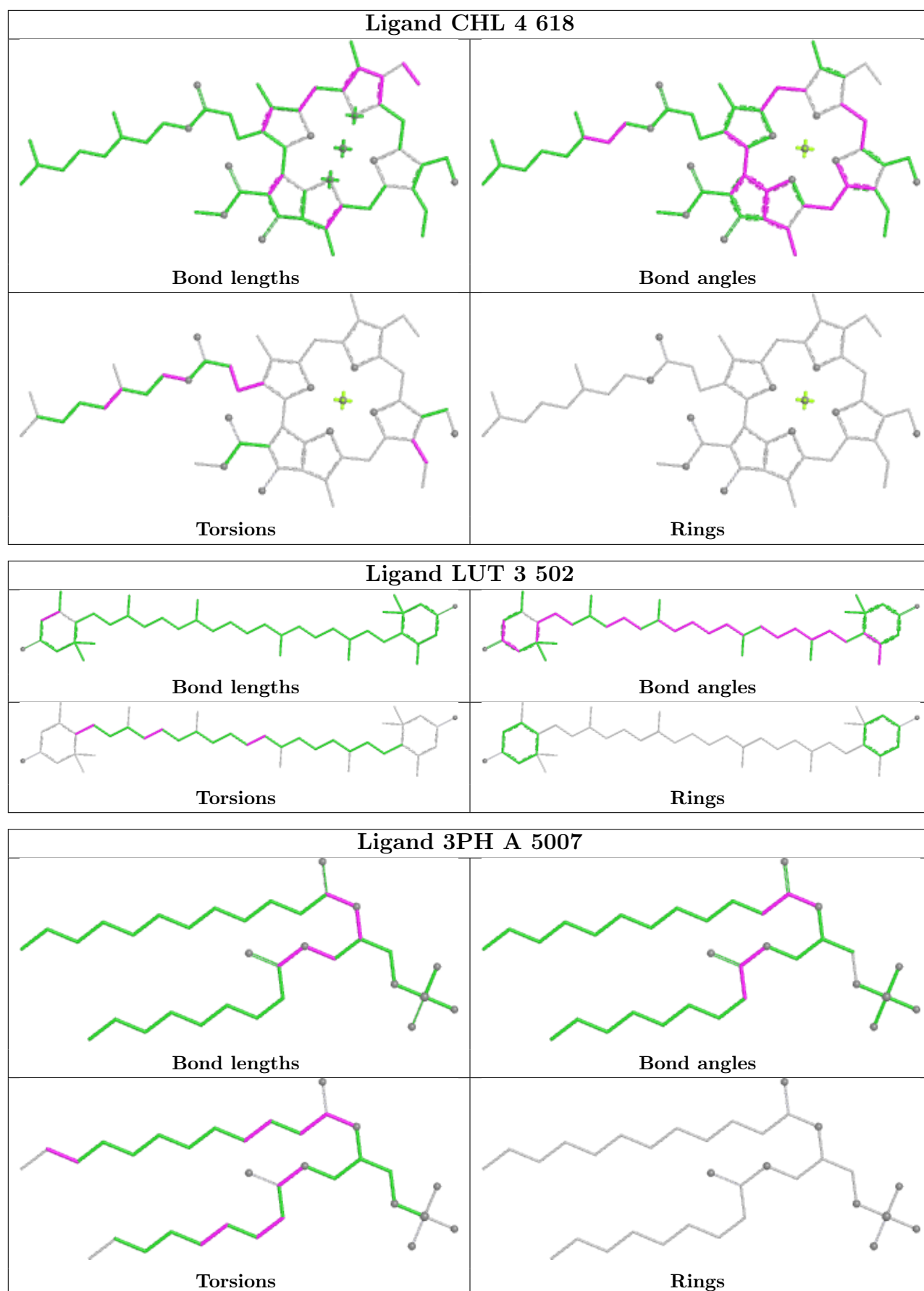


Rings

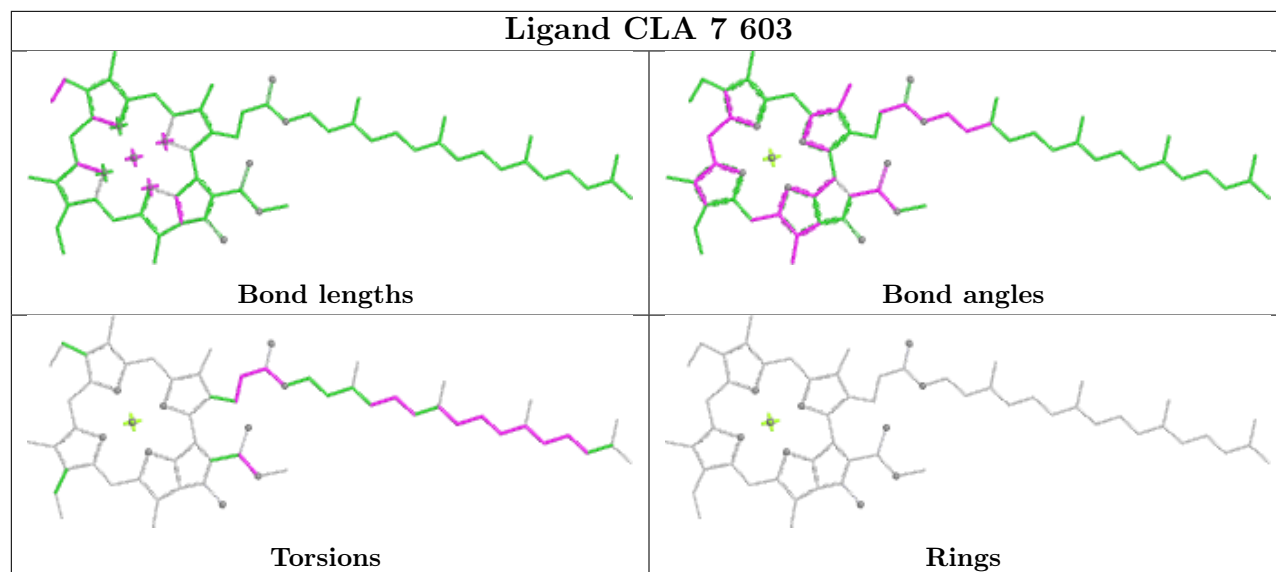


Ligand CLA 6 608

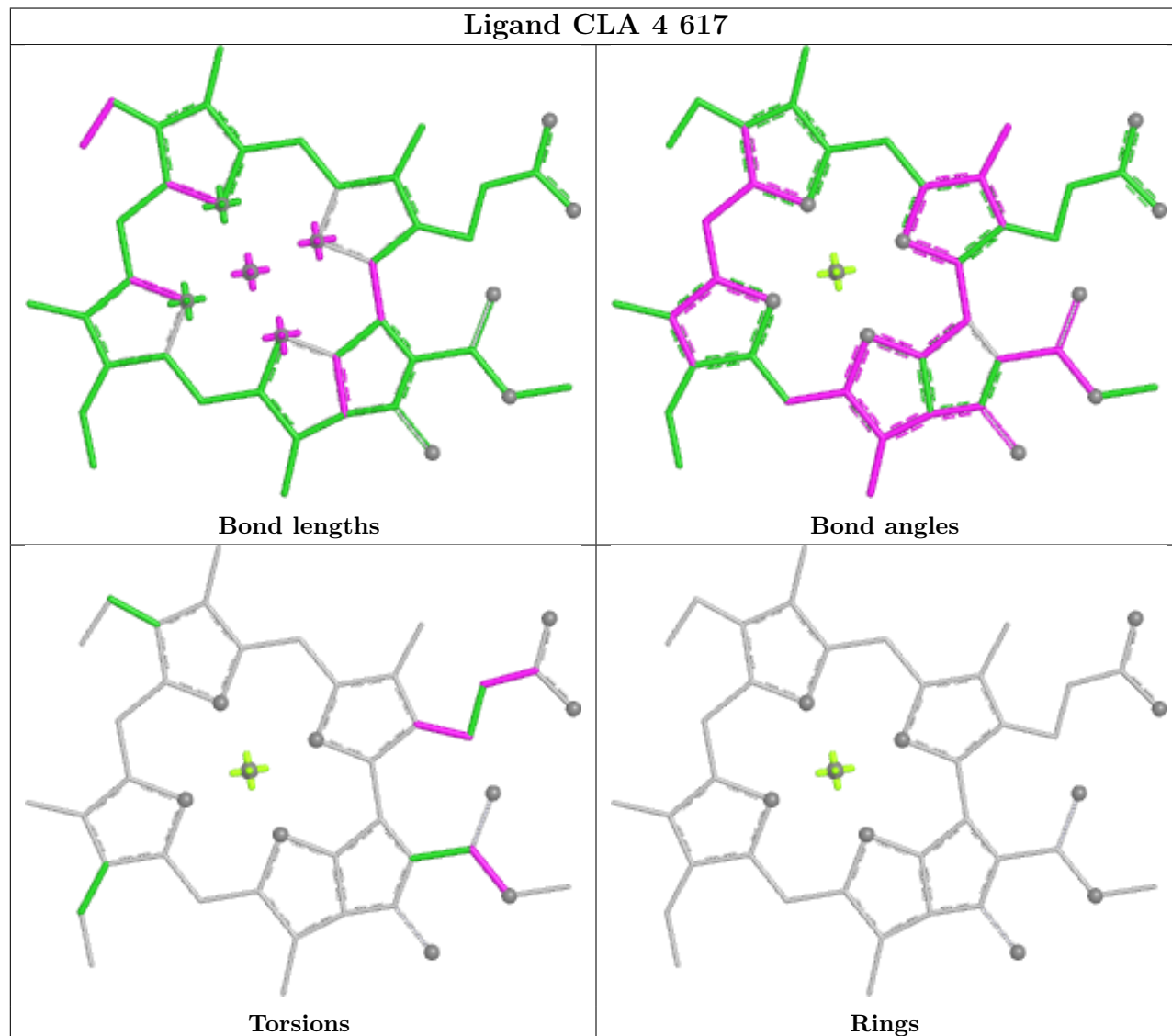




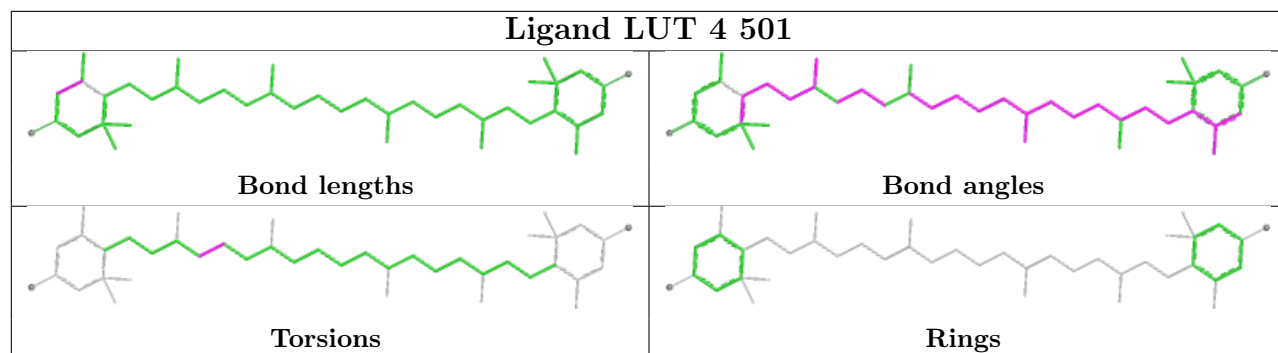
Ligand CLA 7 603



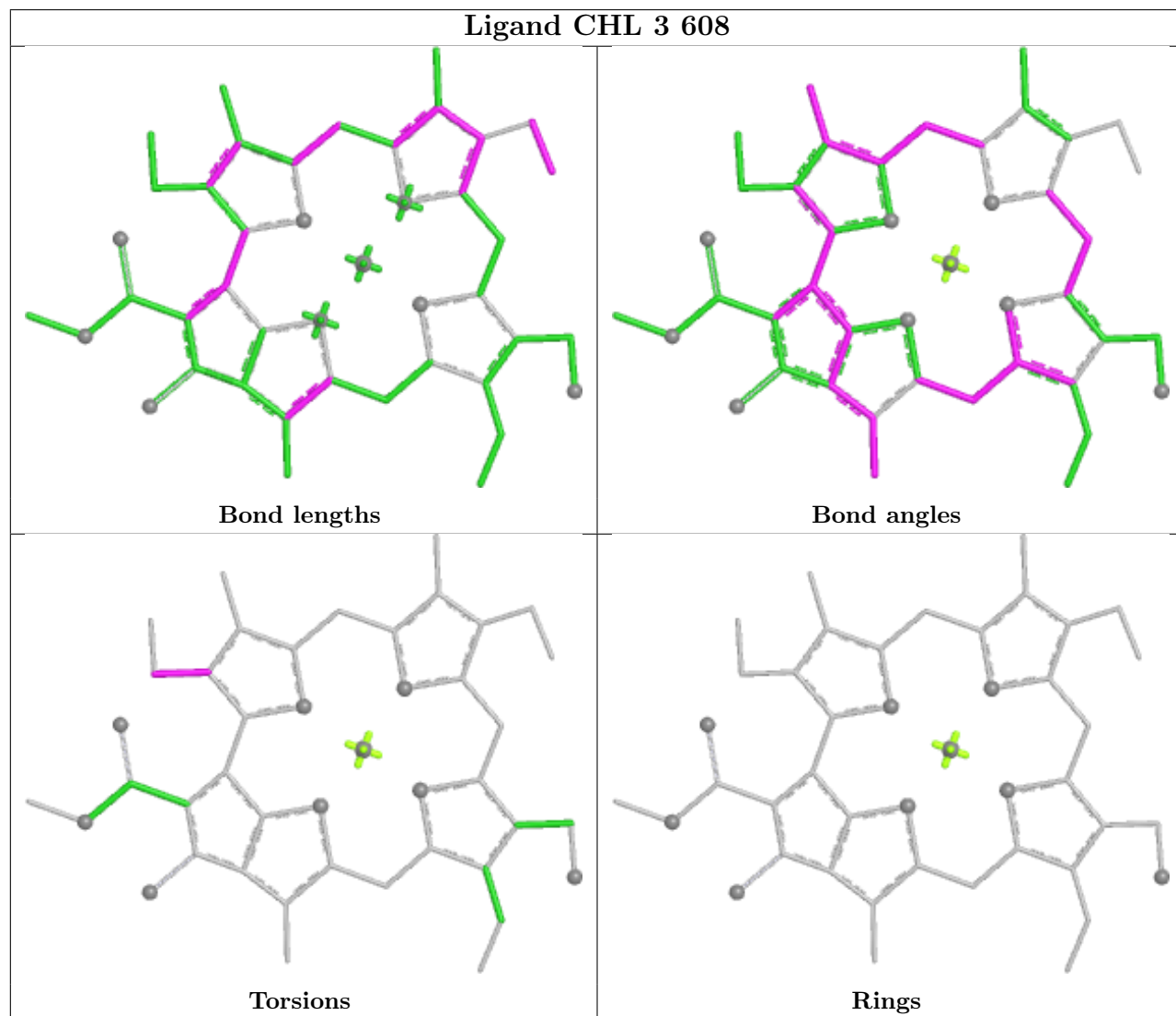
Ligand CLA 4 617

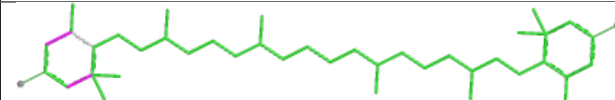
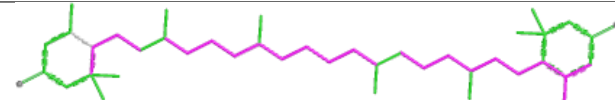
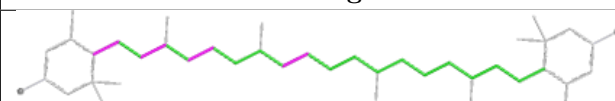
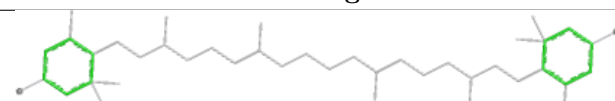


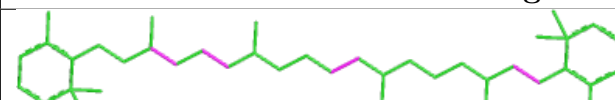
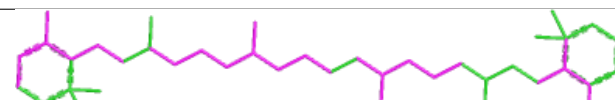
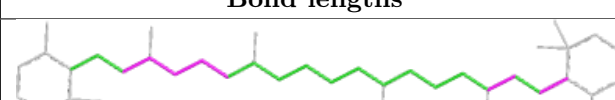
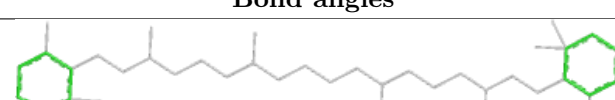
Ligand LUT 4 501

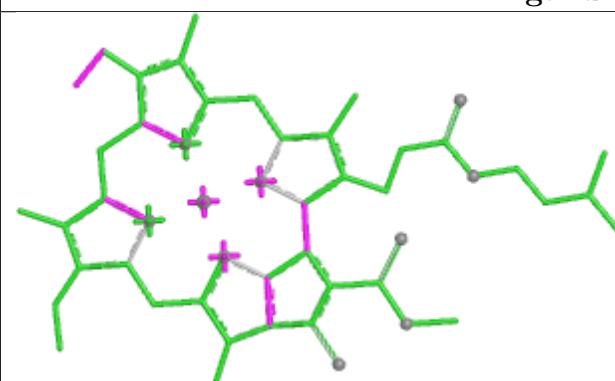
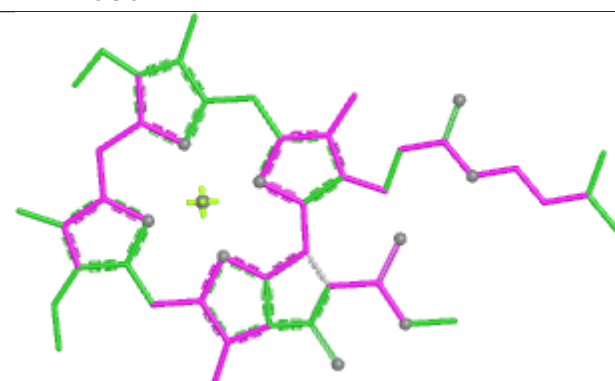
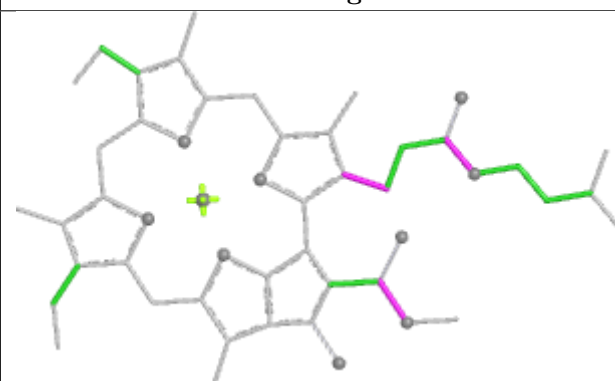
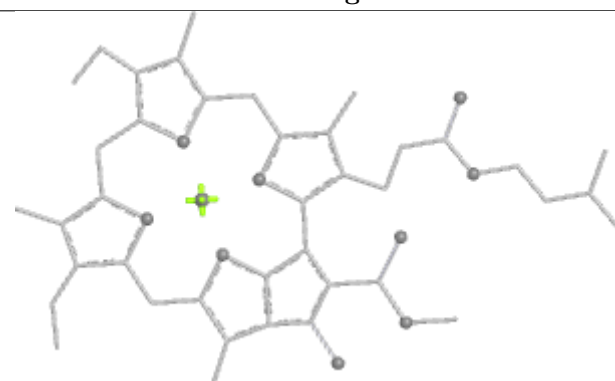


Ligand CHL 3 608

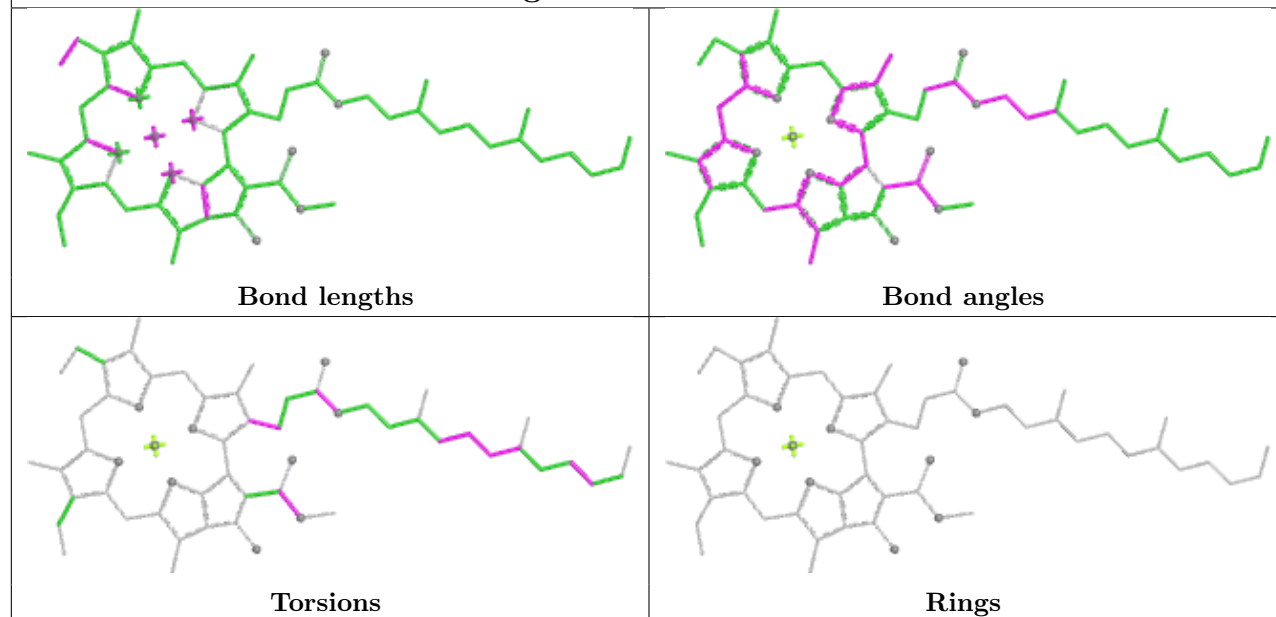


Ligand LUT 7 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

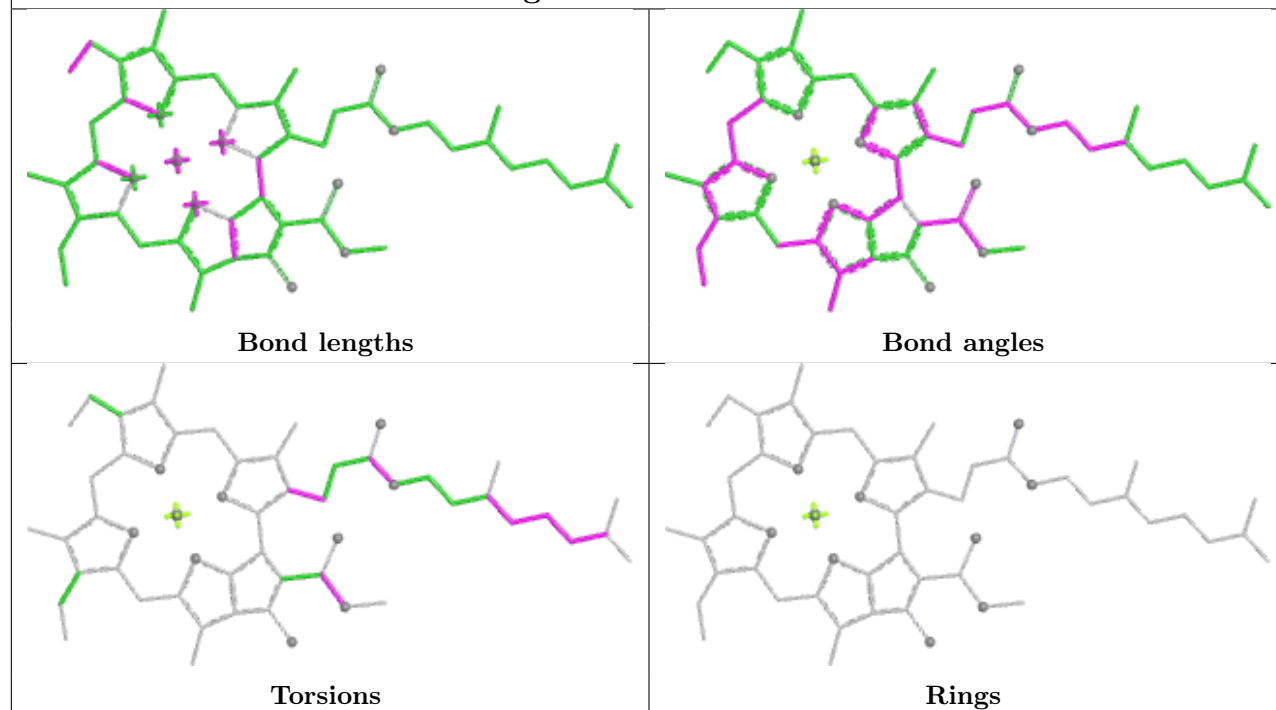
Ligand BCR 8 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

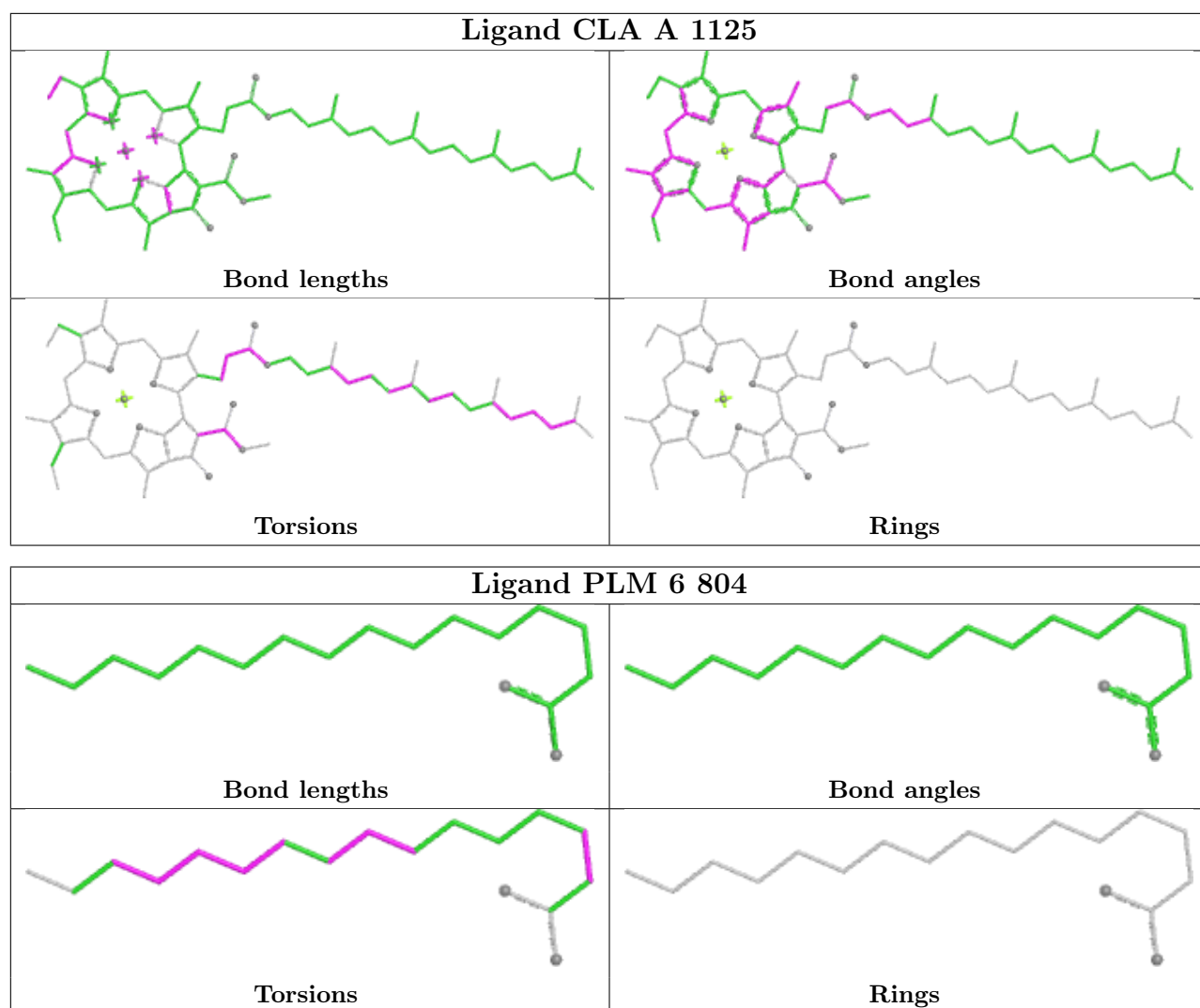
Ligand CLA 4 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

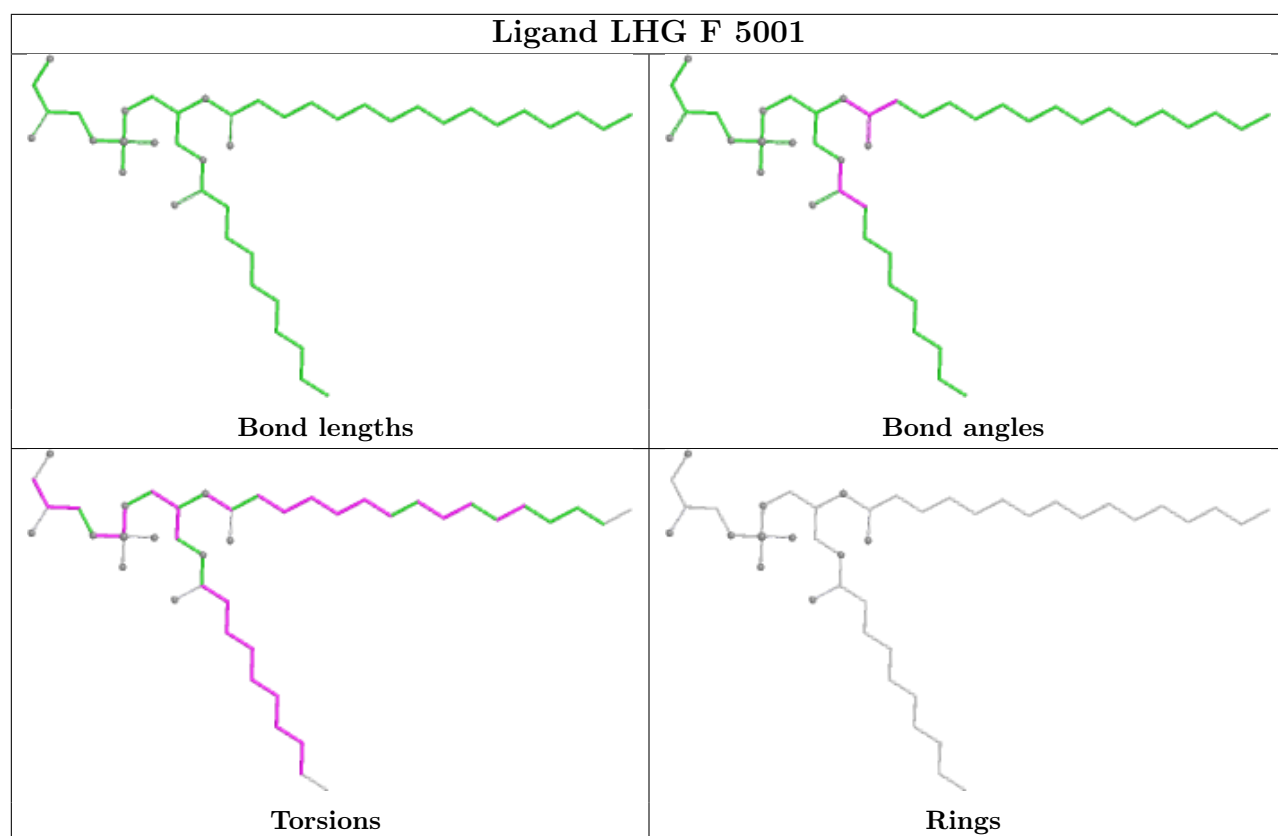
Ligand CLA B 1219



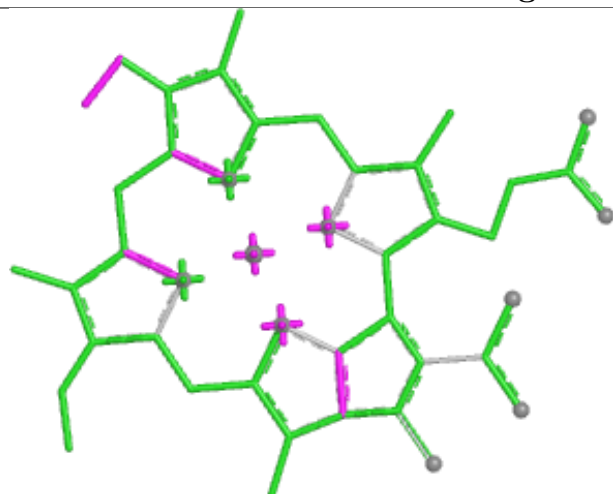
Ligand CLA B 1206



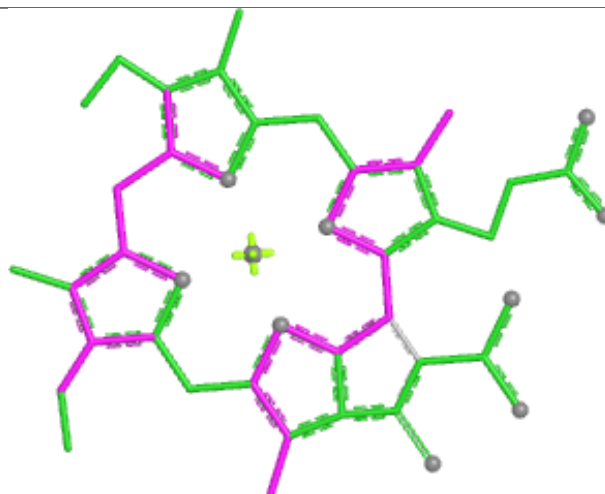




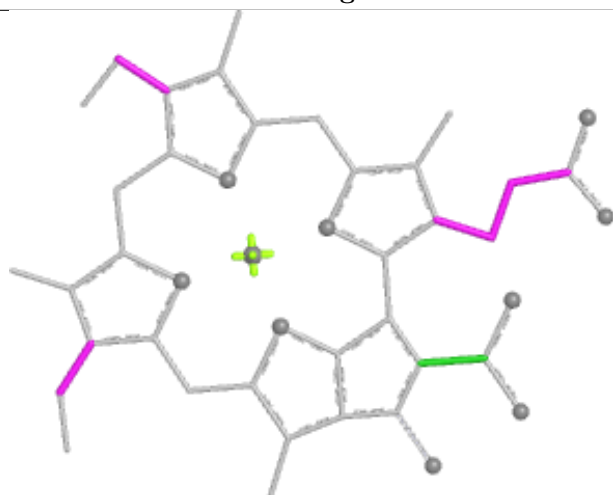
Ligand CLA 7 605



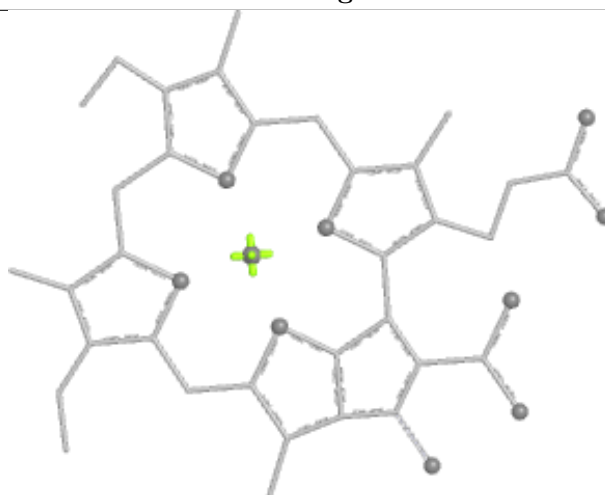
Bond lengths



Bond angles

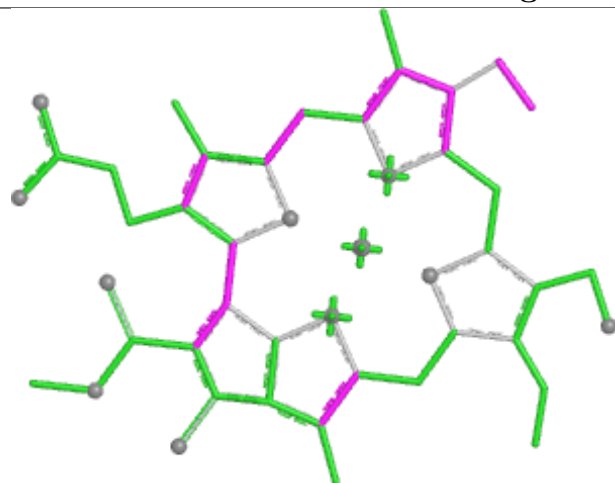


Torsions

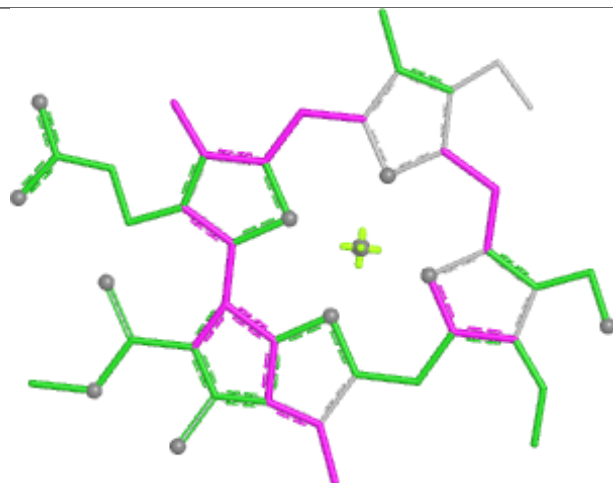


Rings

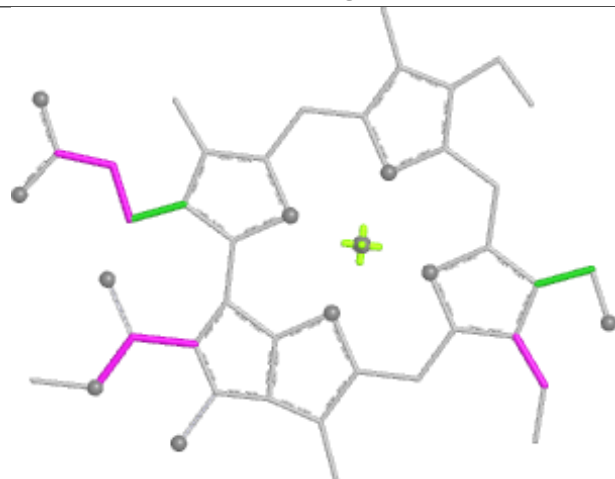
Ligand CHL a 613



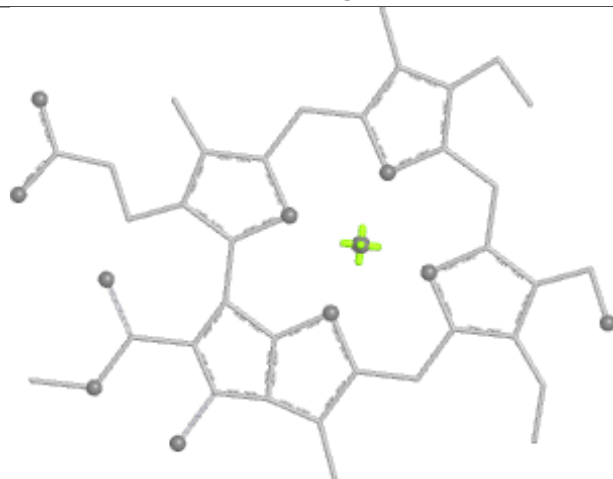
Bond lengths



Bond angles

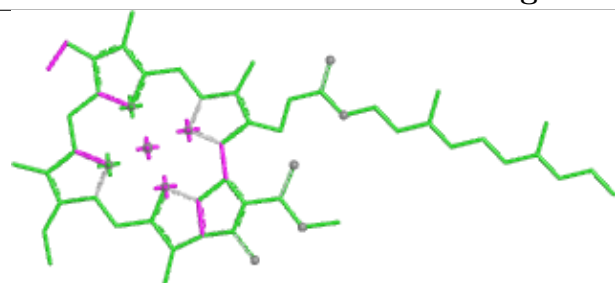


Torsions

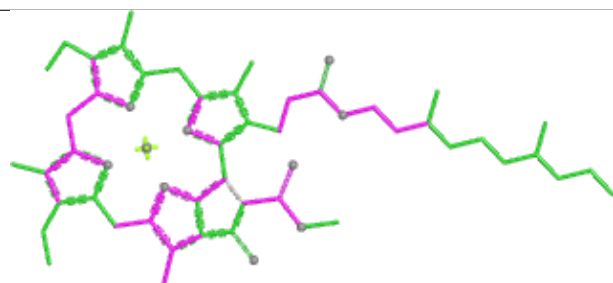


Rings

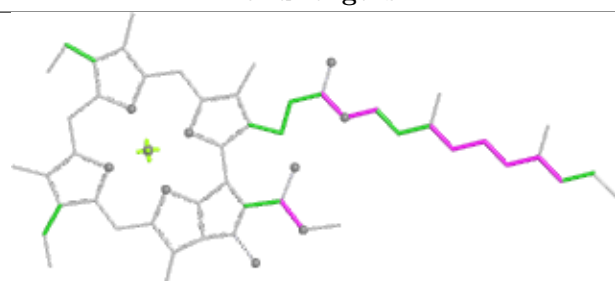
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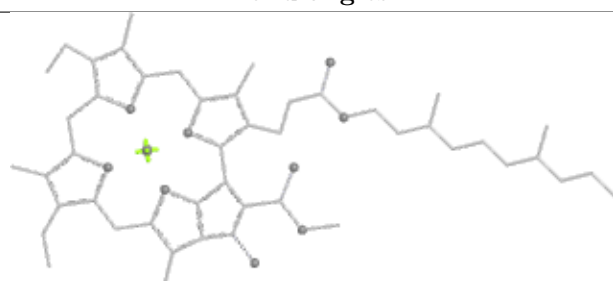
Bond lengths



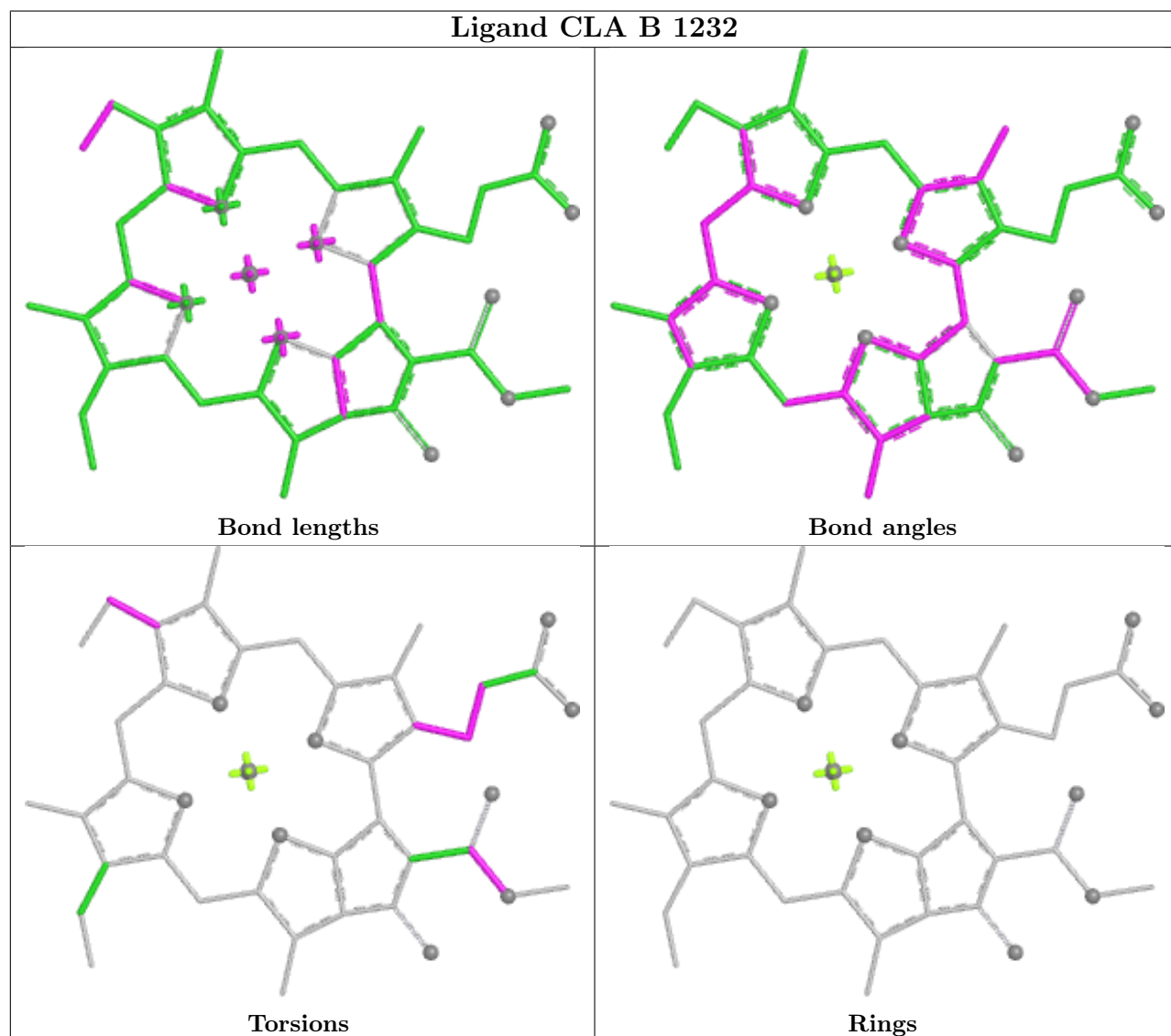
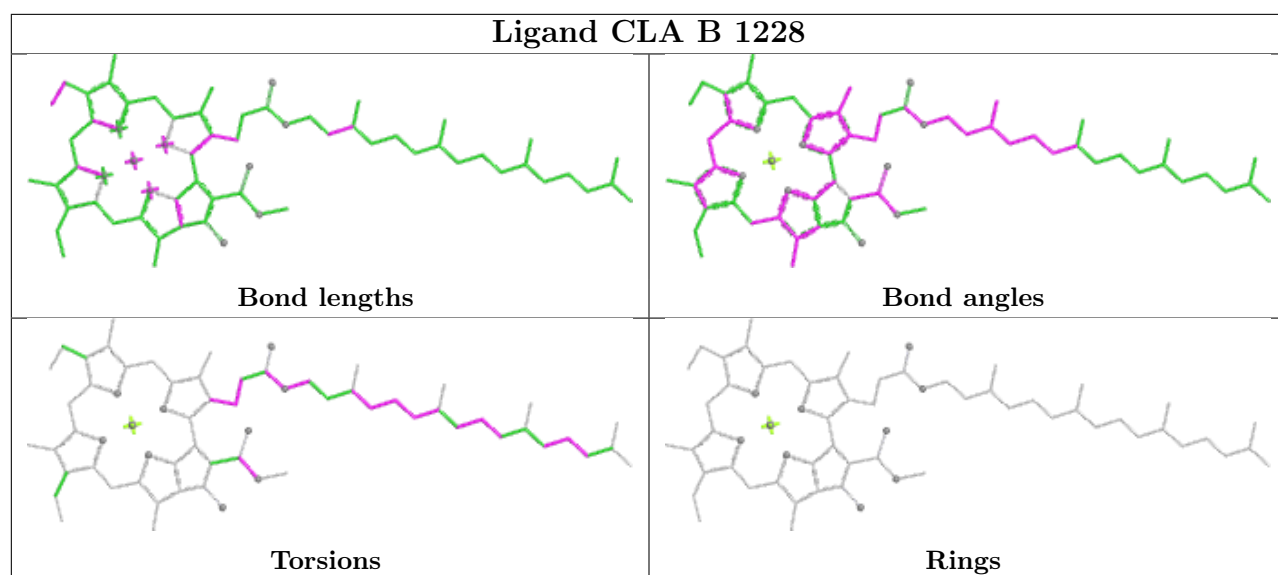
Bond angles



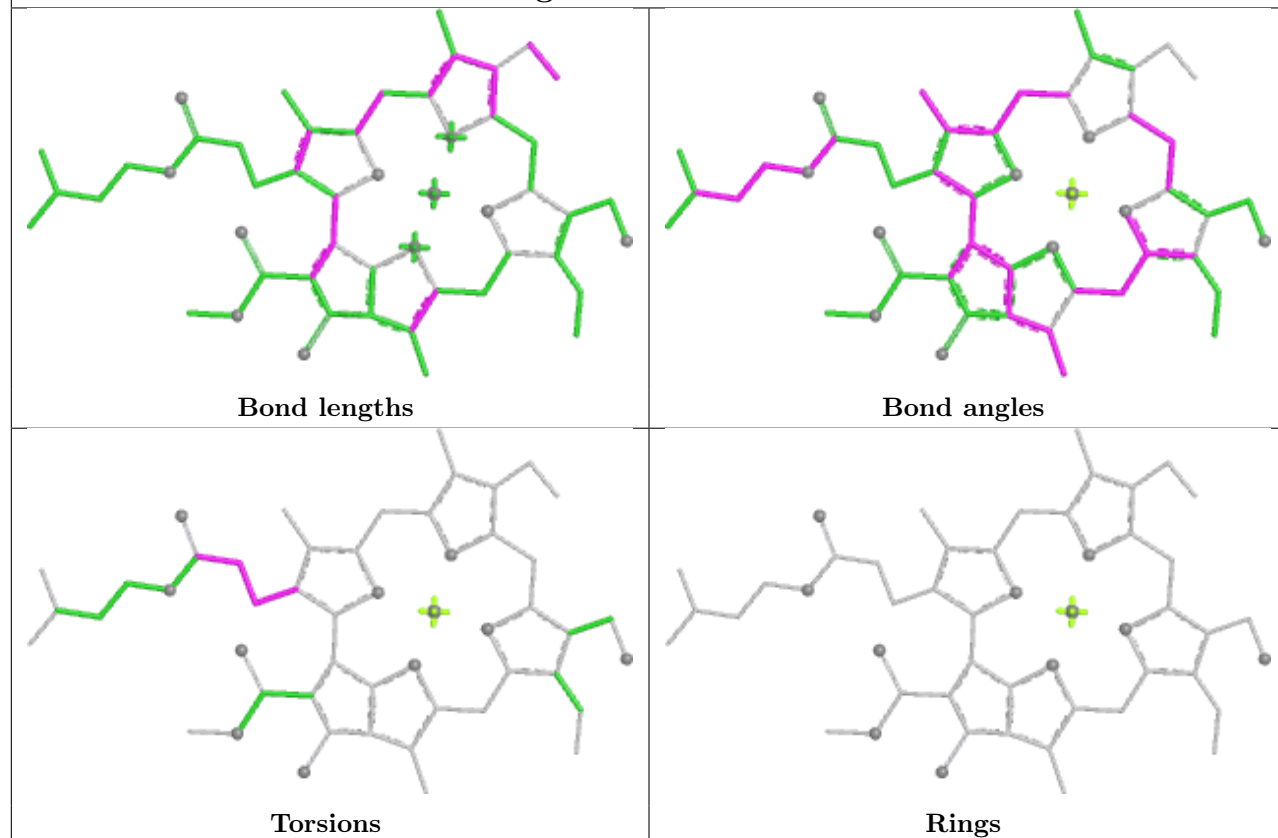
Torsions



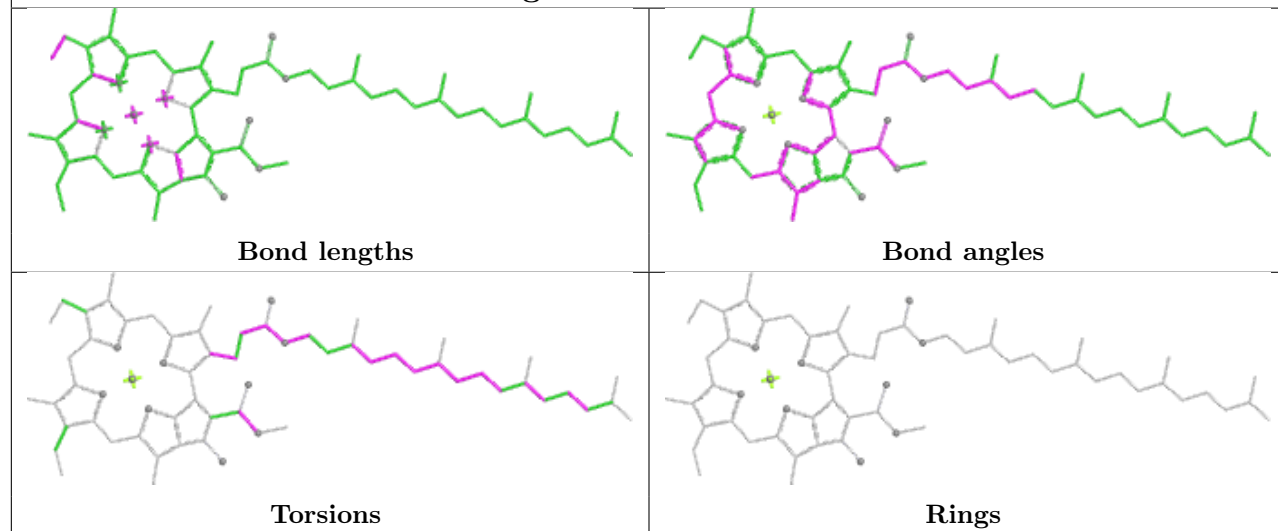
Rings

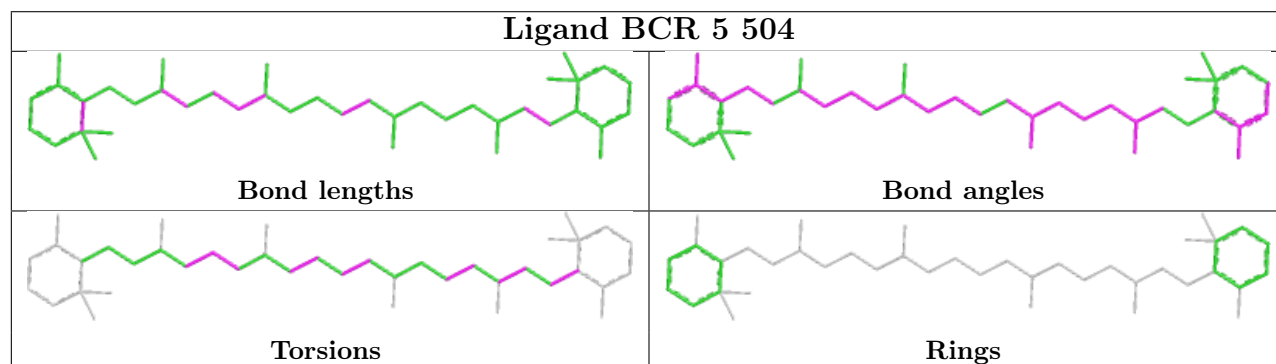
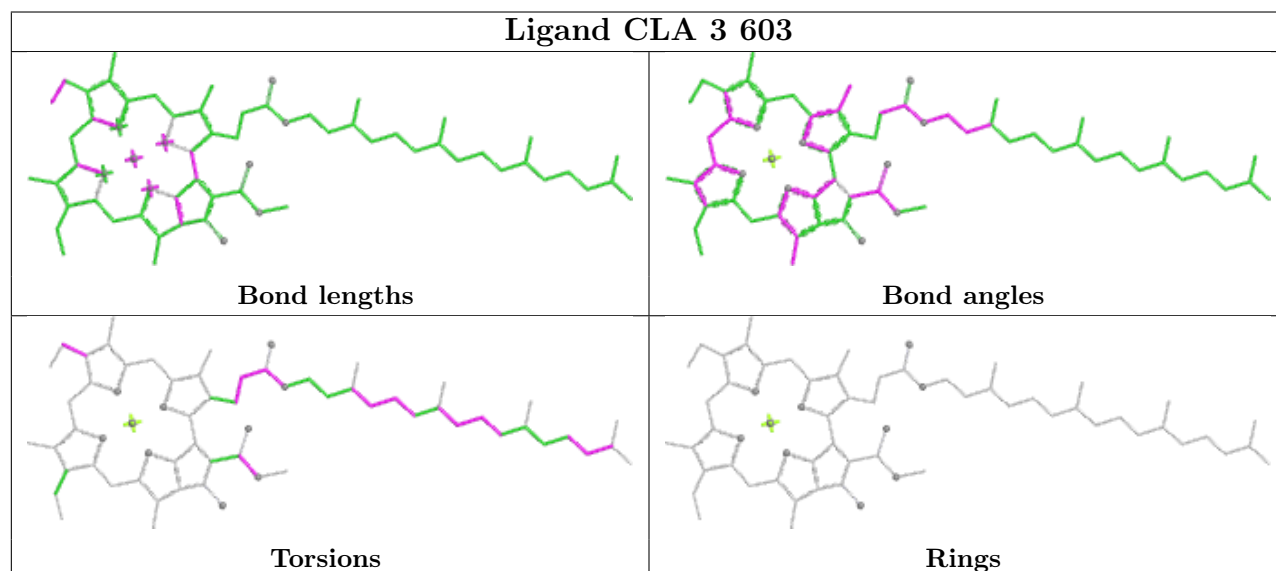
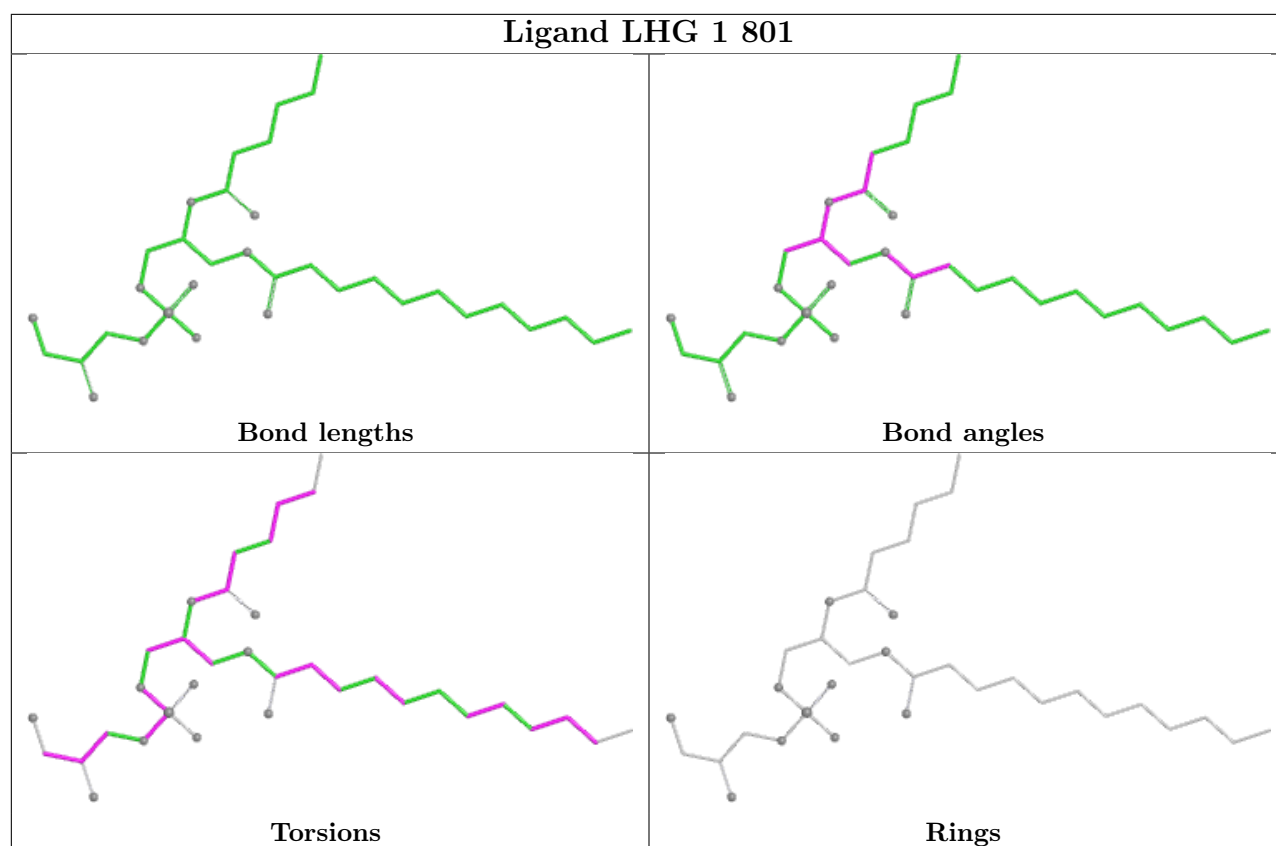


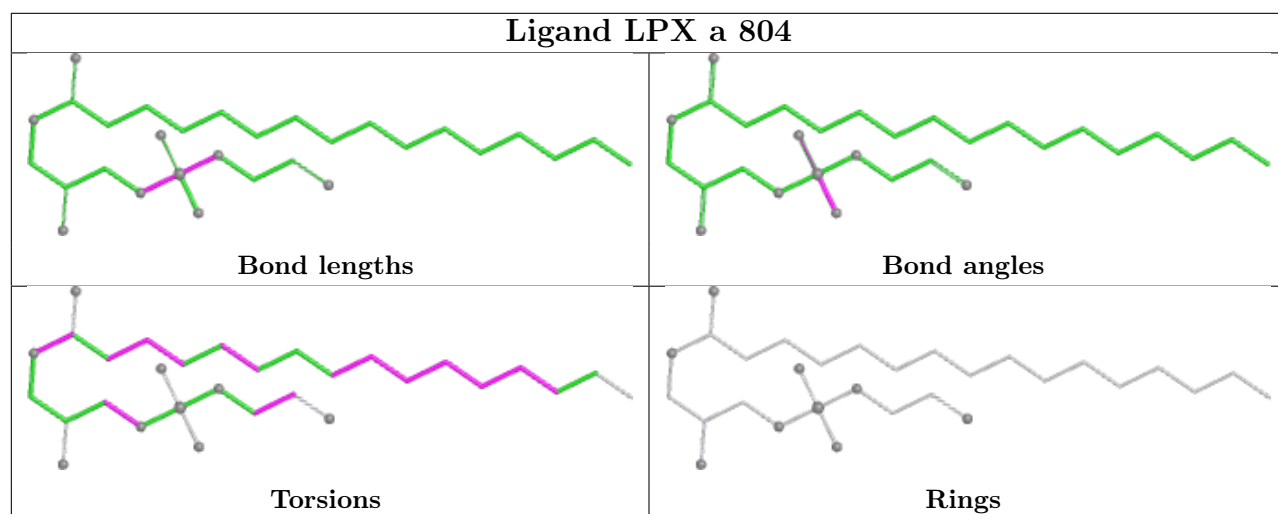
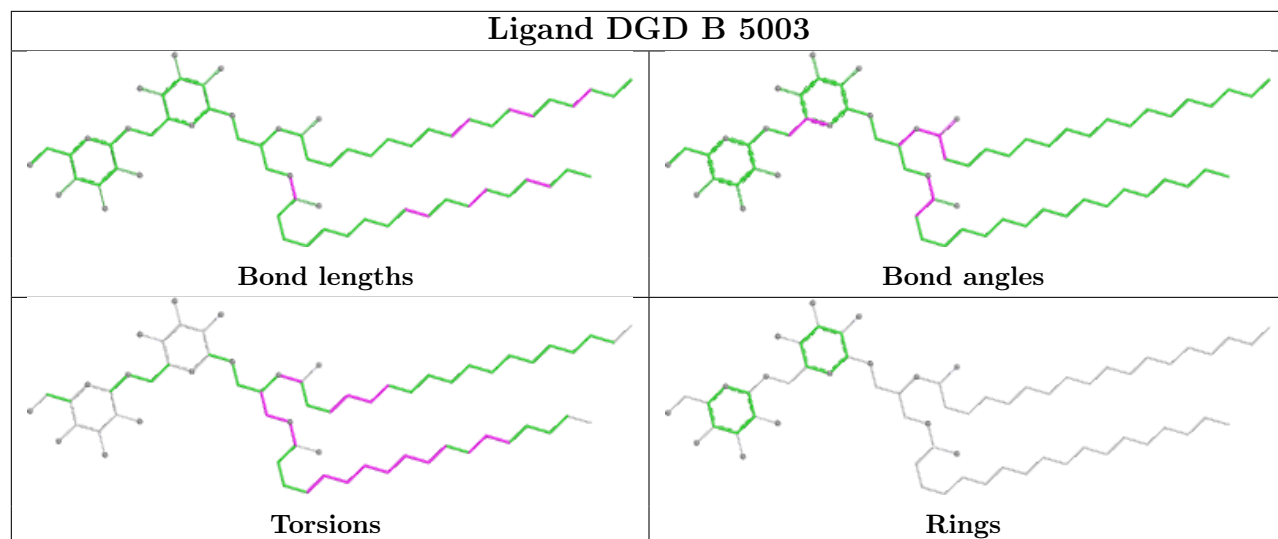
Ligand CHL 5 611



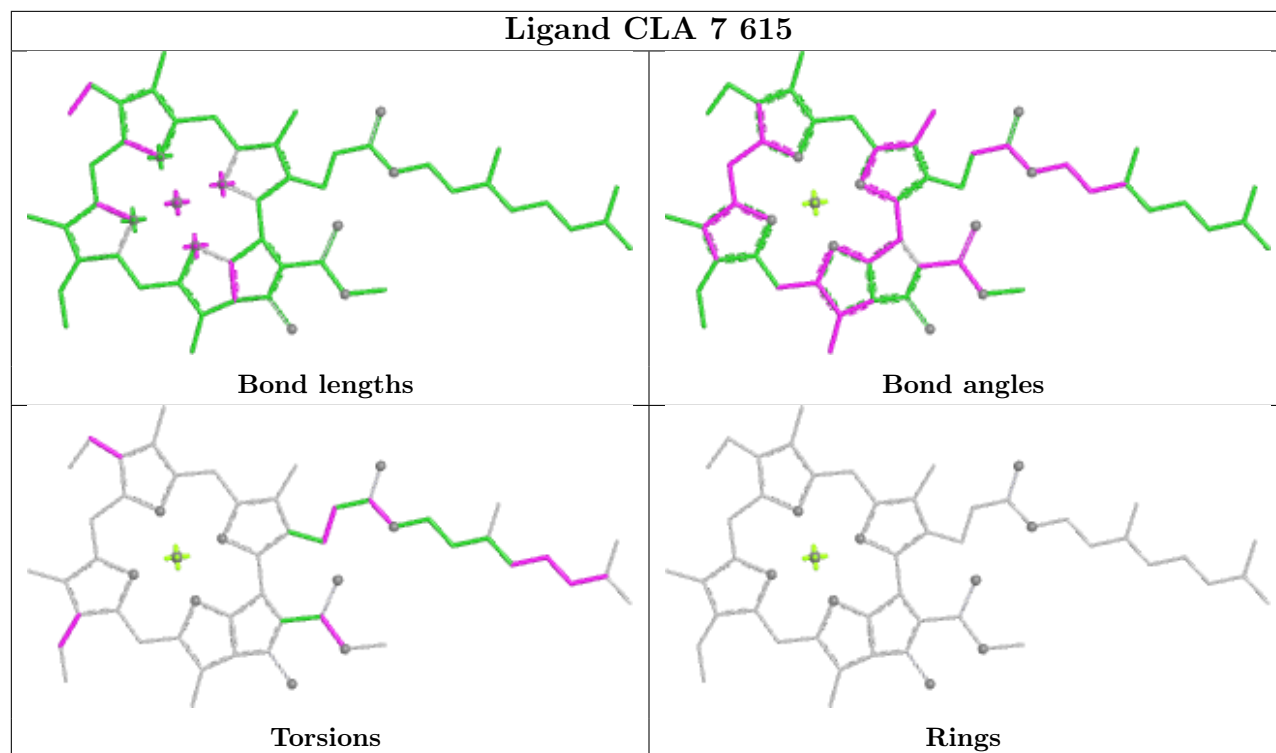
Ligand CLA A 1126



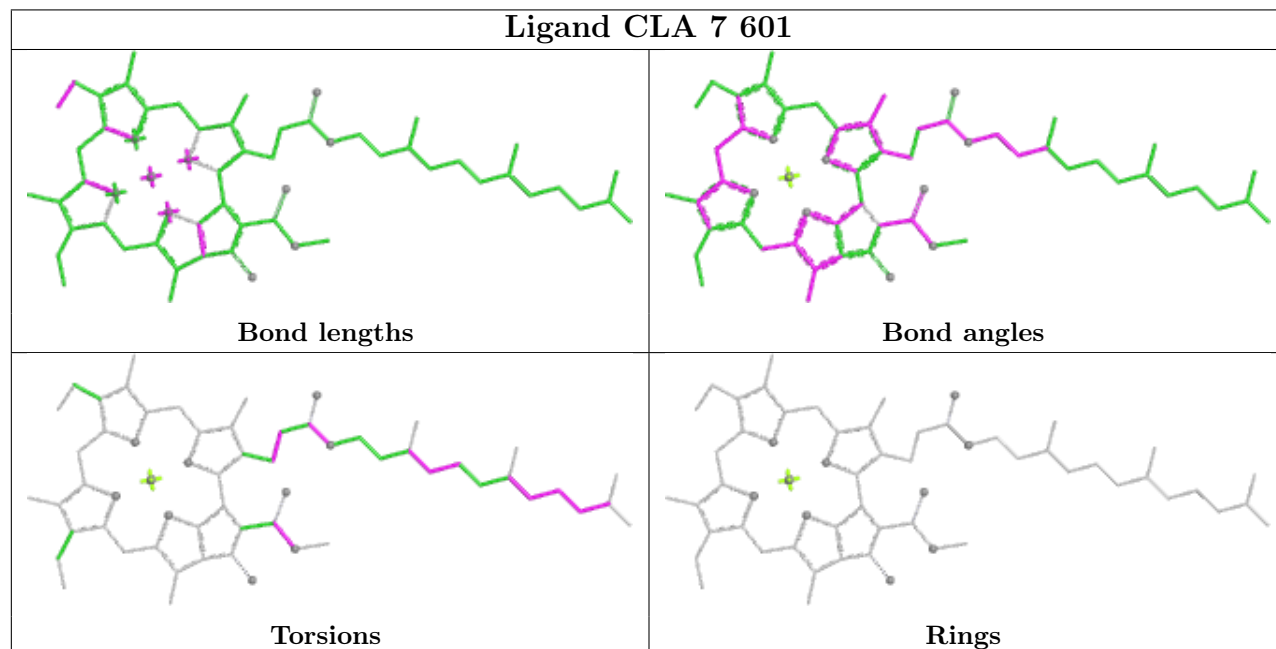




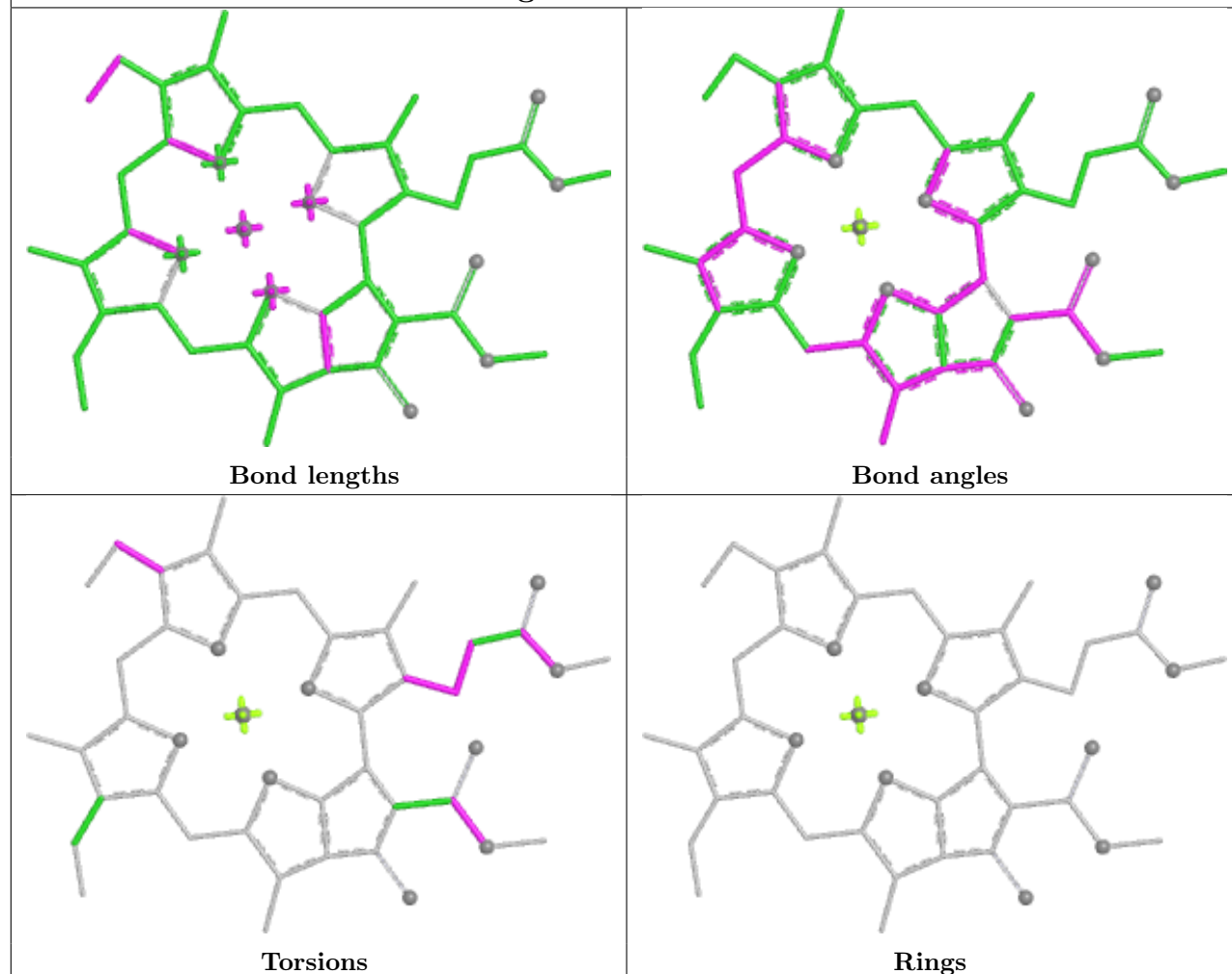
Ligand CLA 7 615



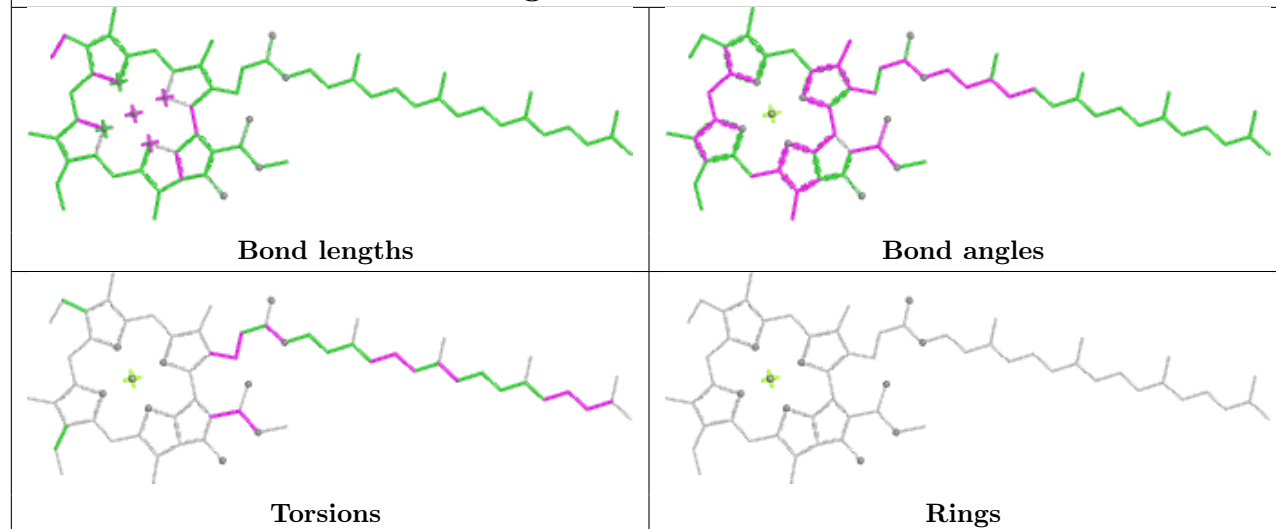
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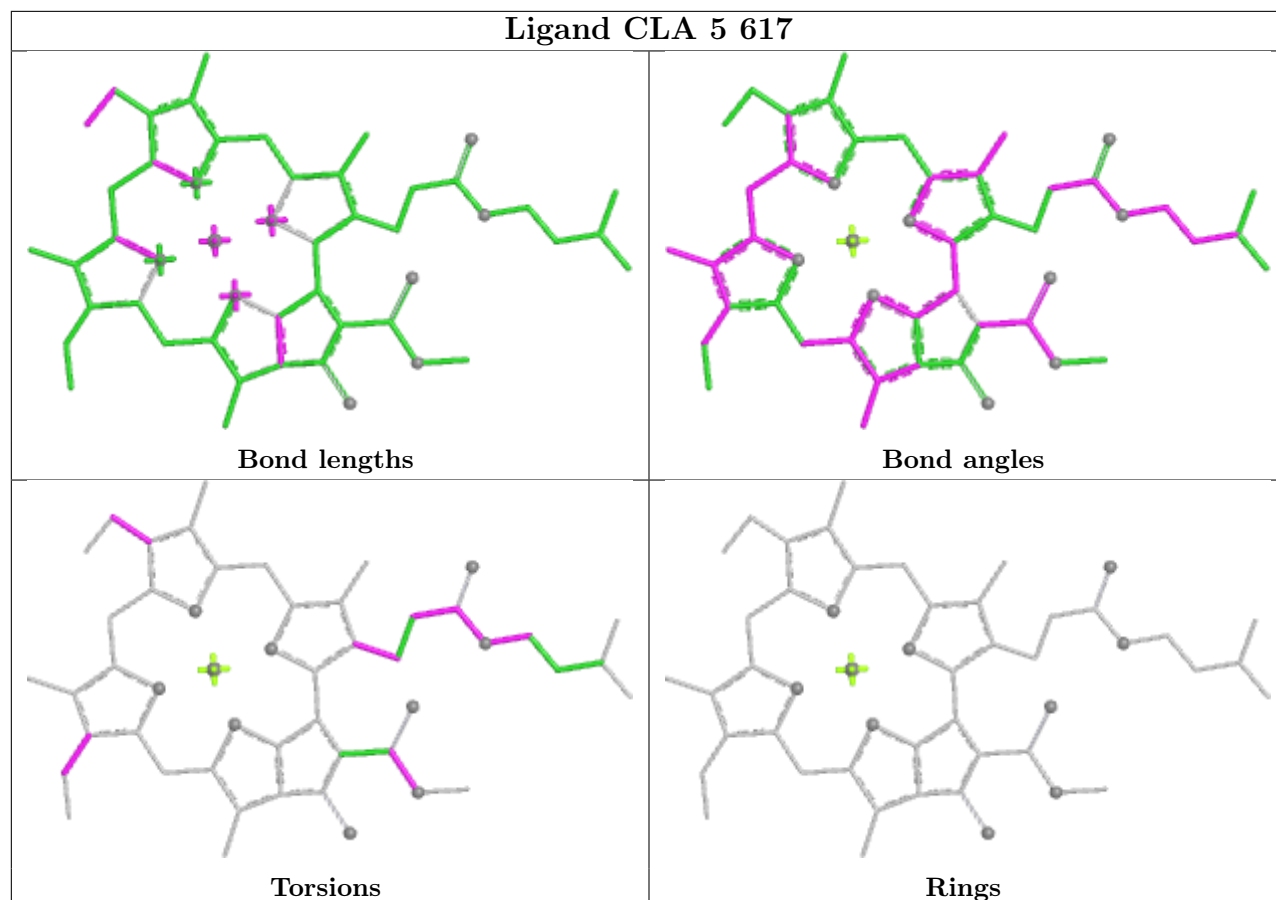
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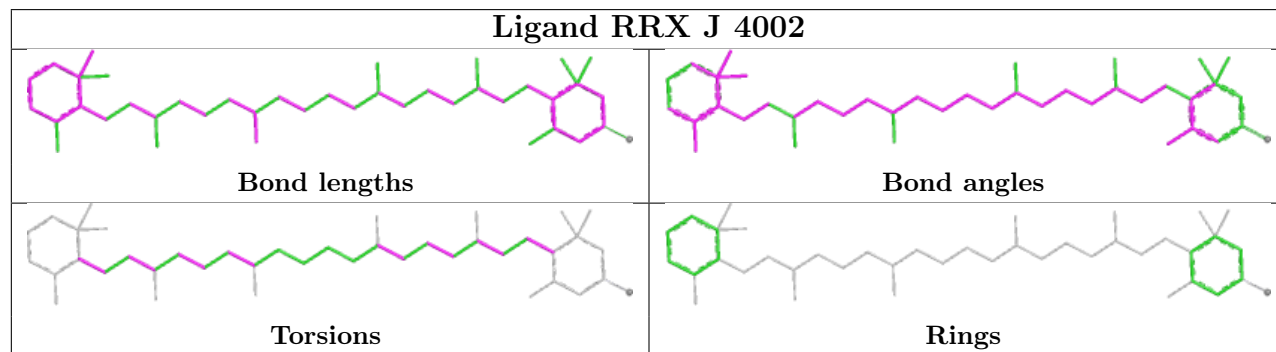
Ligand CLA B 1201



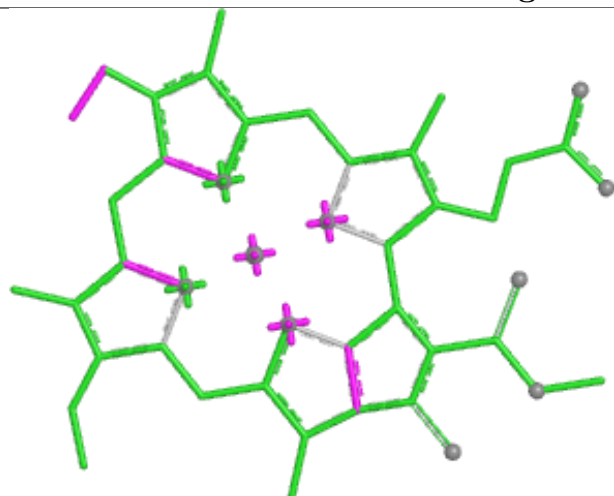
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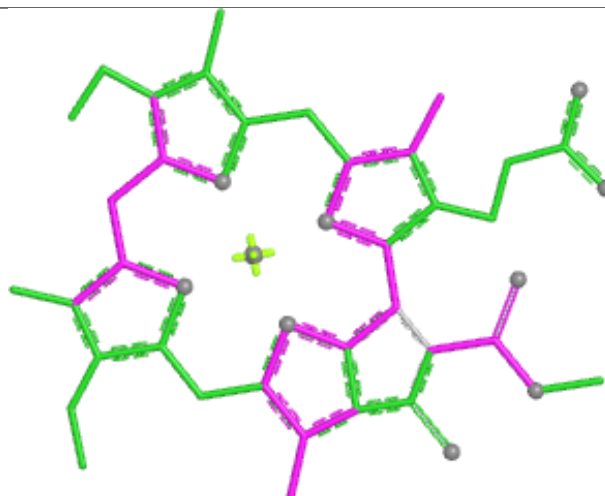
Ligand RRX J 4002



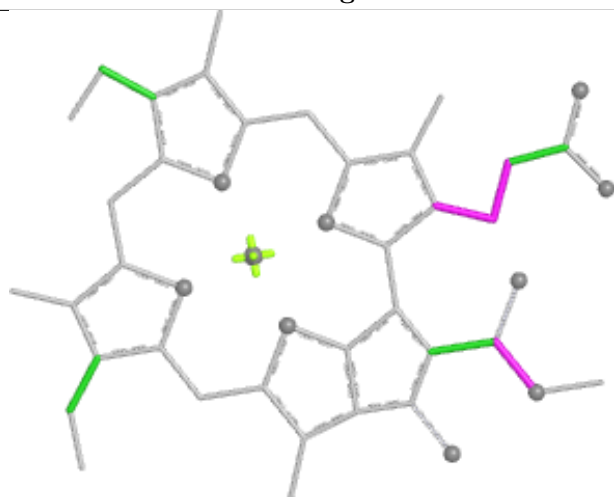
Ligand CLA 1 610



Bond lengths



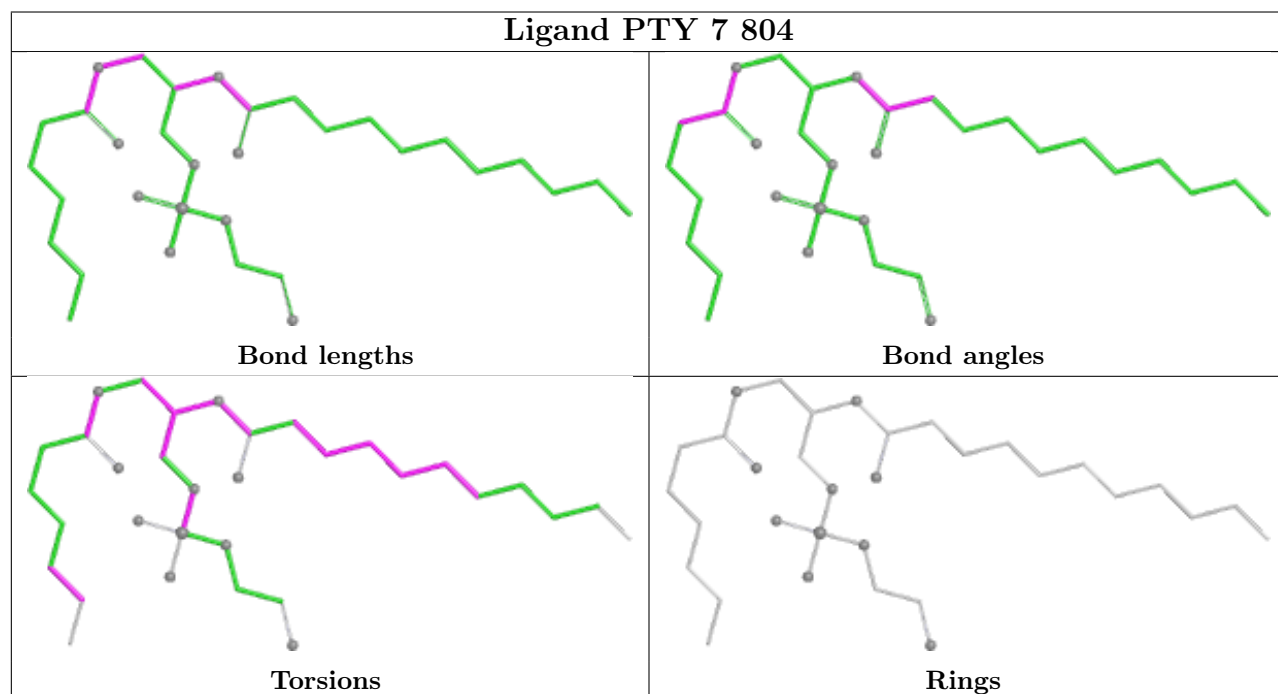
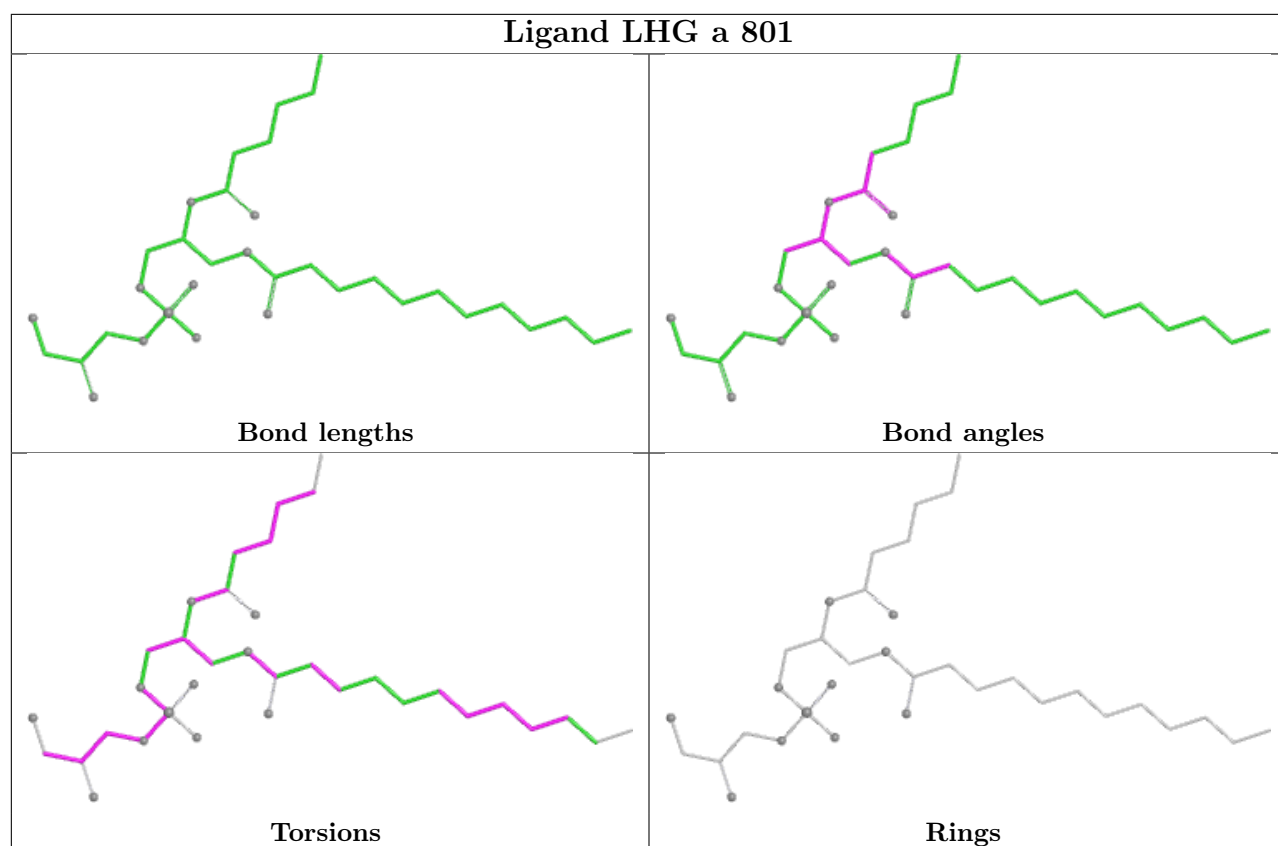
Bond angles

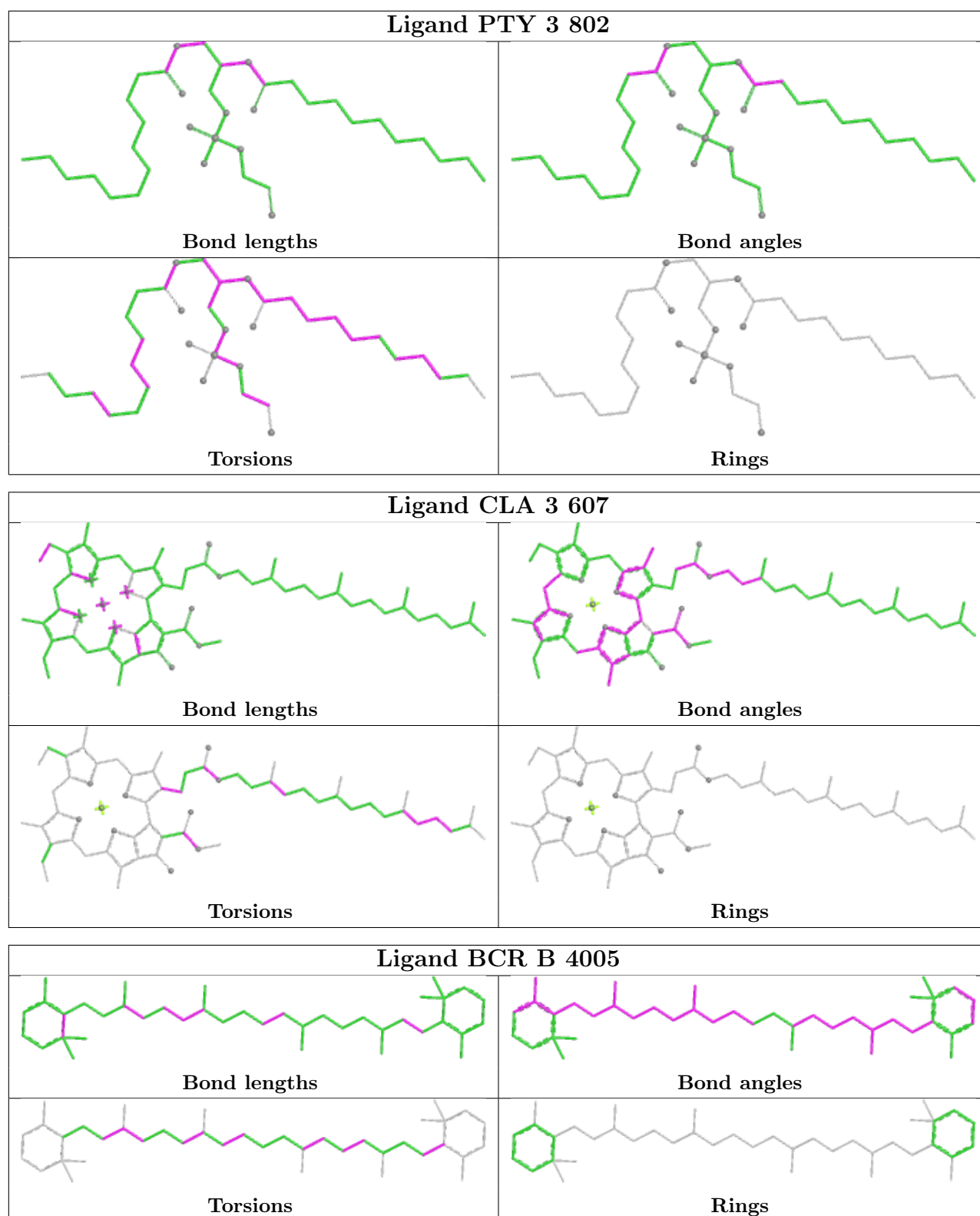


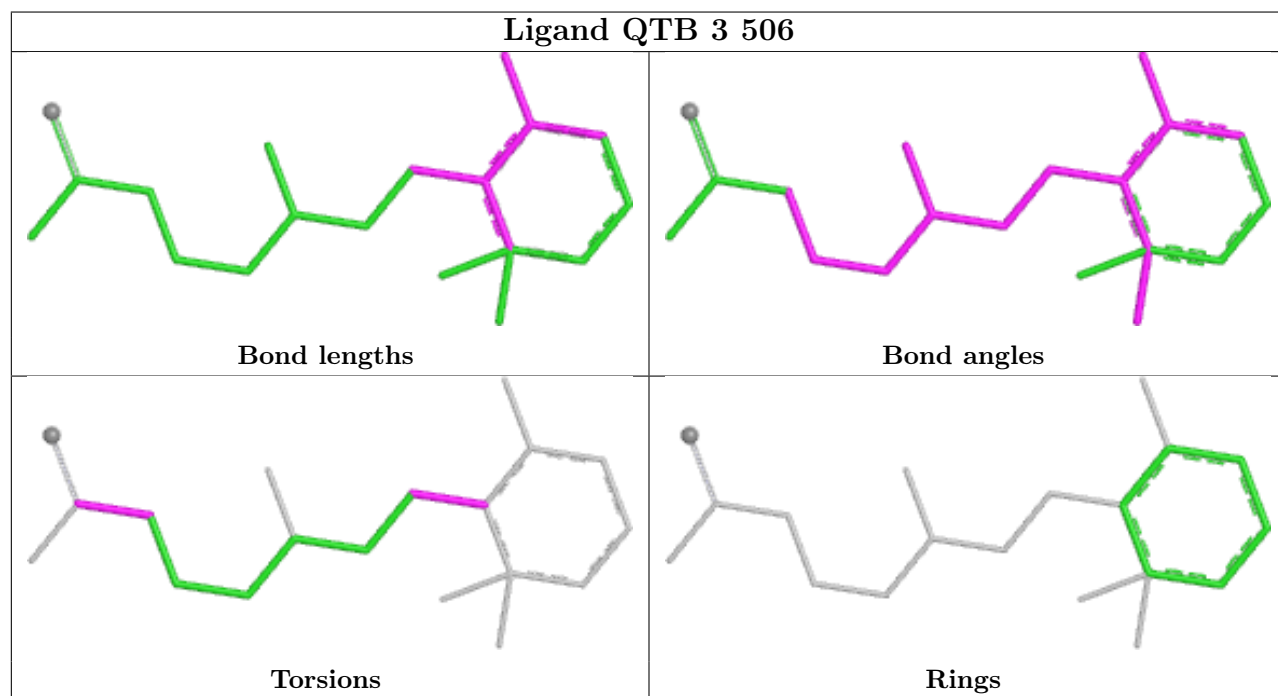
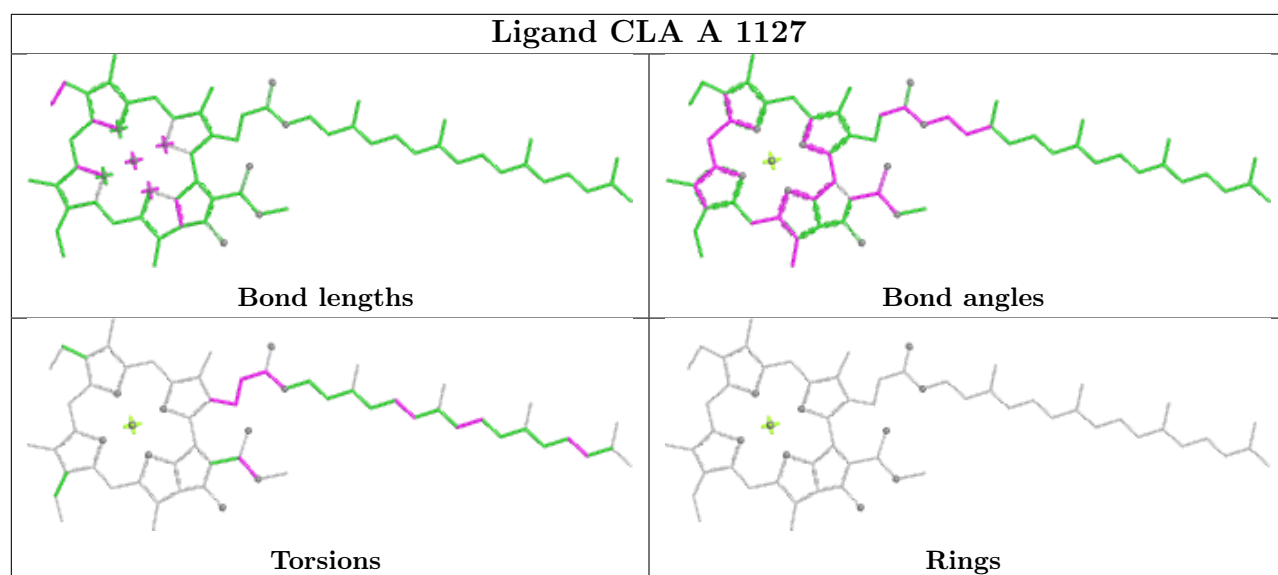
Torsions

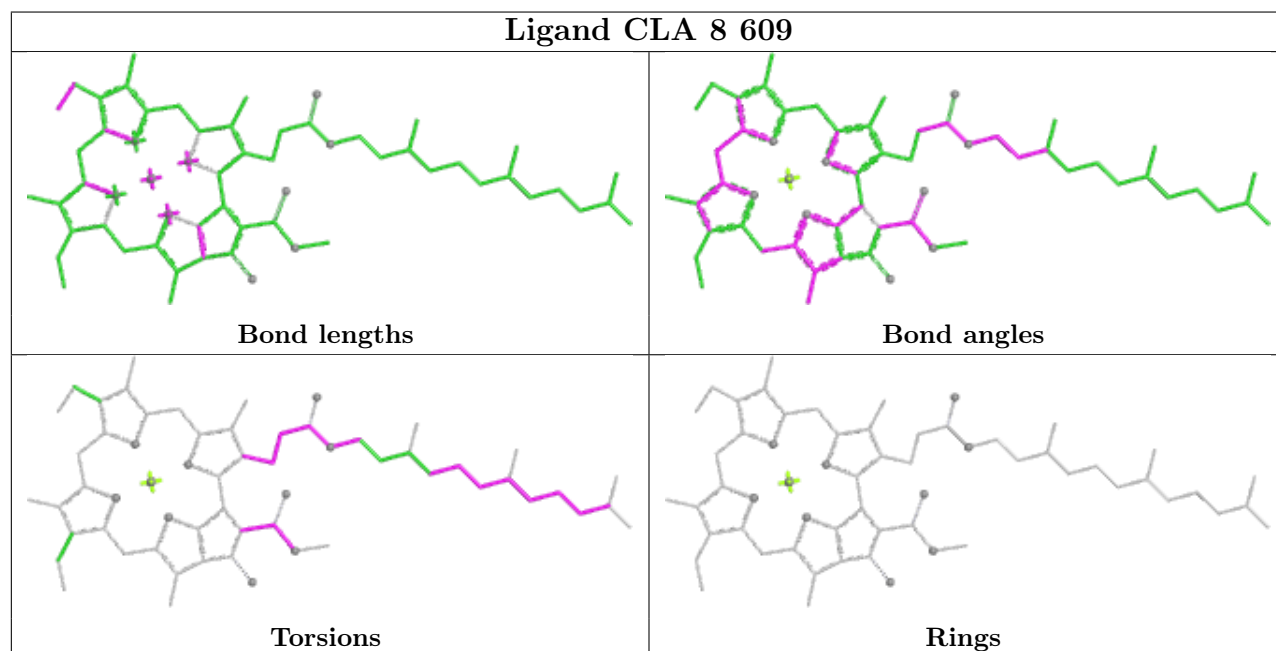
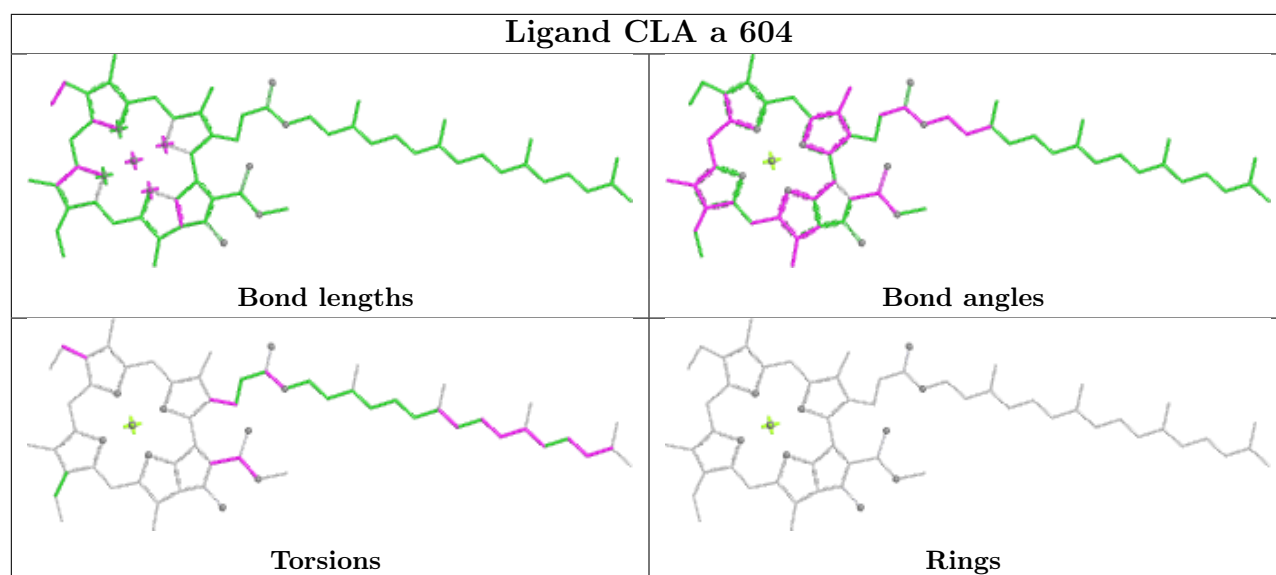


Rings

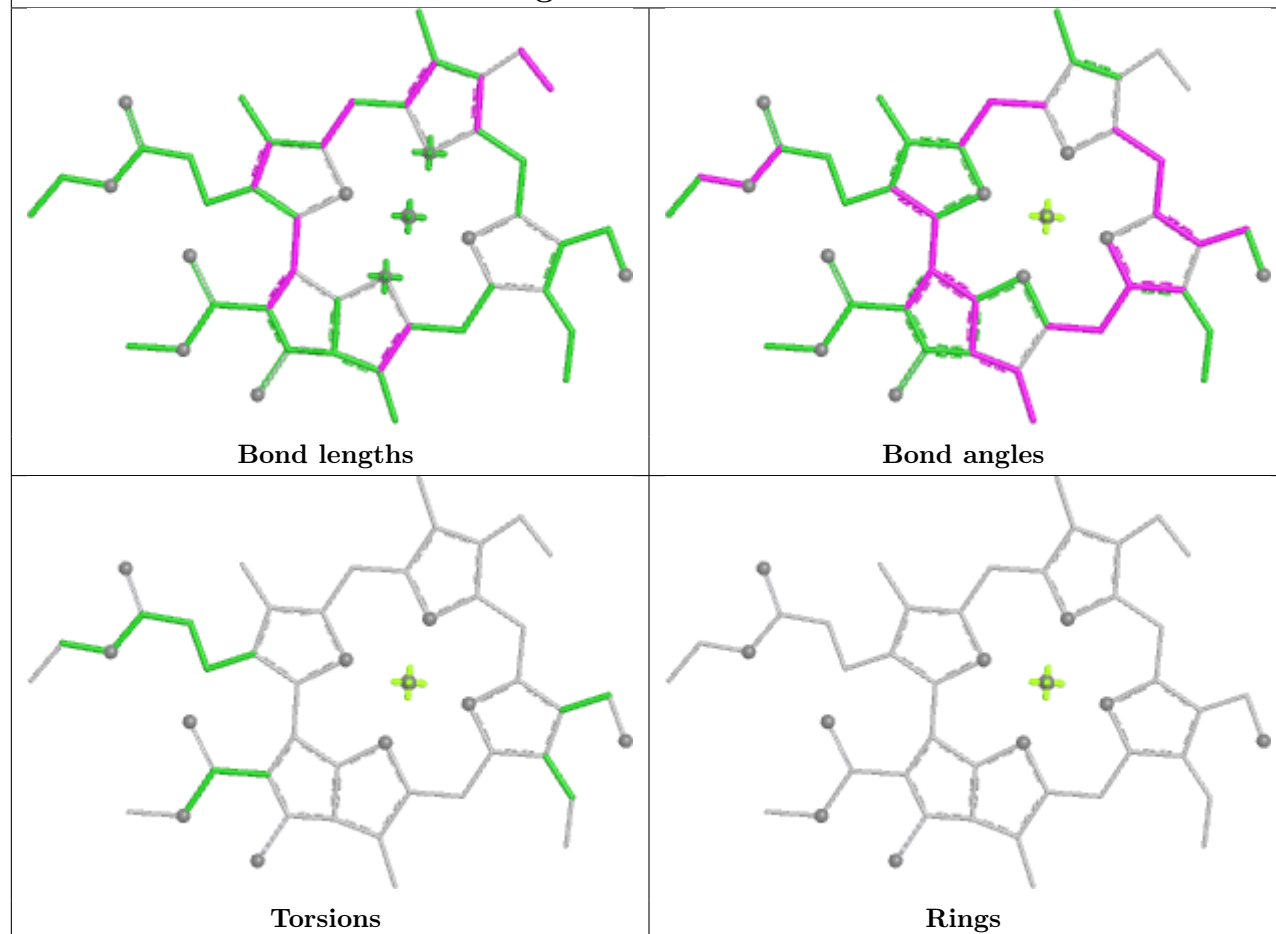




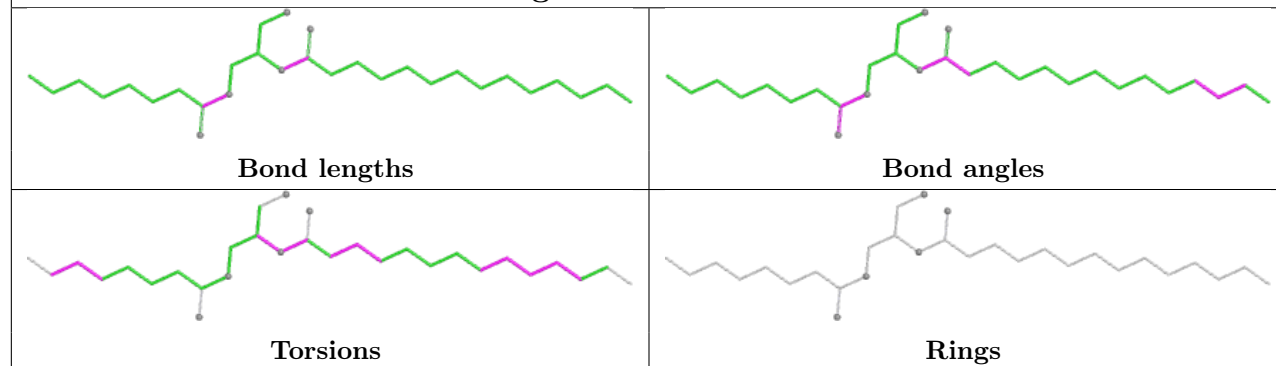




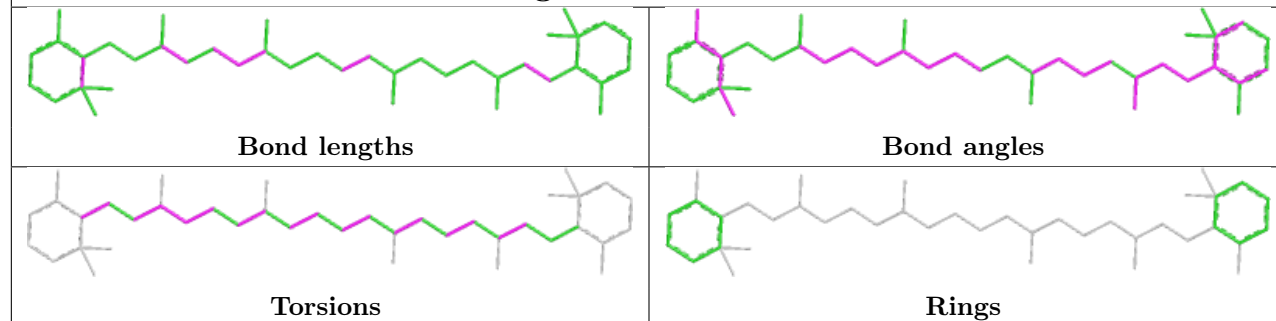
Ligand CHL 1 613



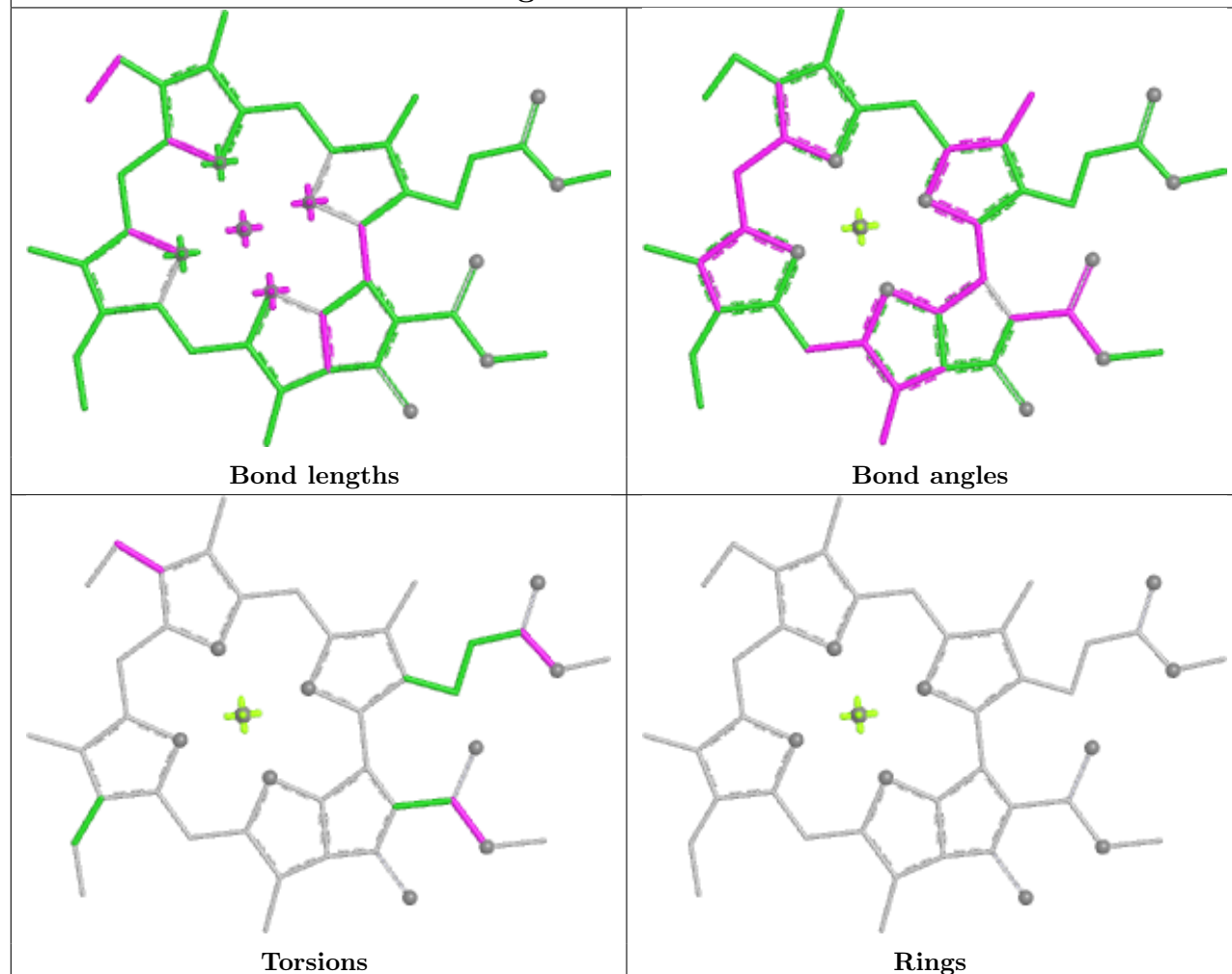
Ligand DGA 8 803



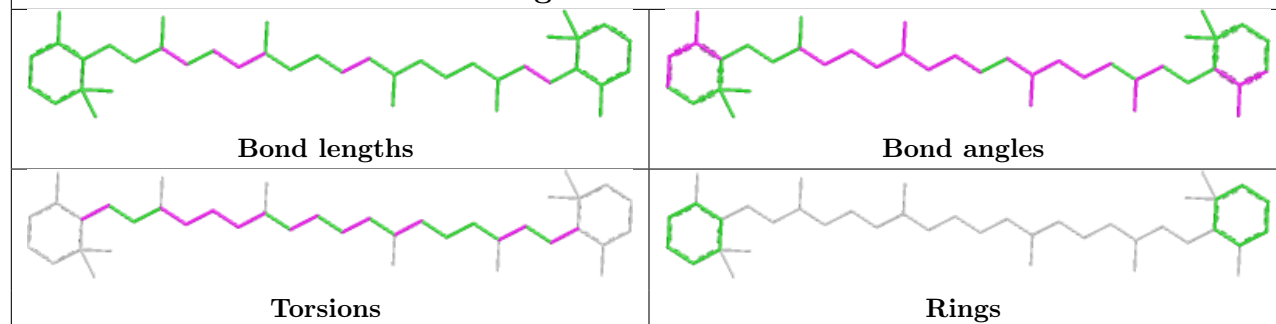
Ligand BCR 7 503



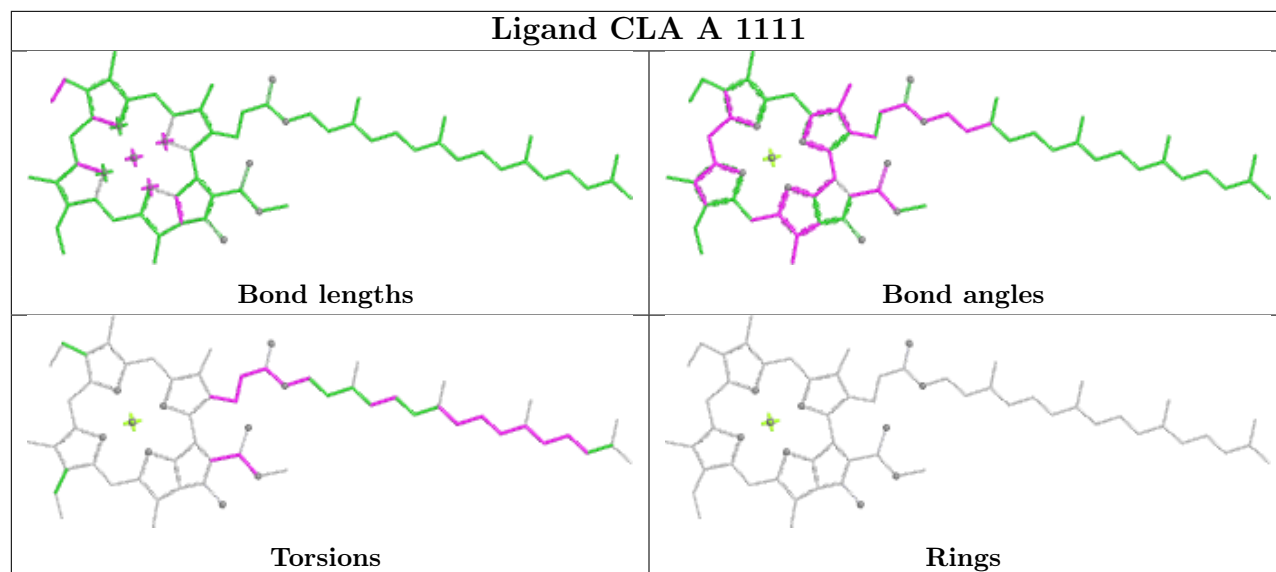
Ligand CLA 5 614



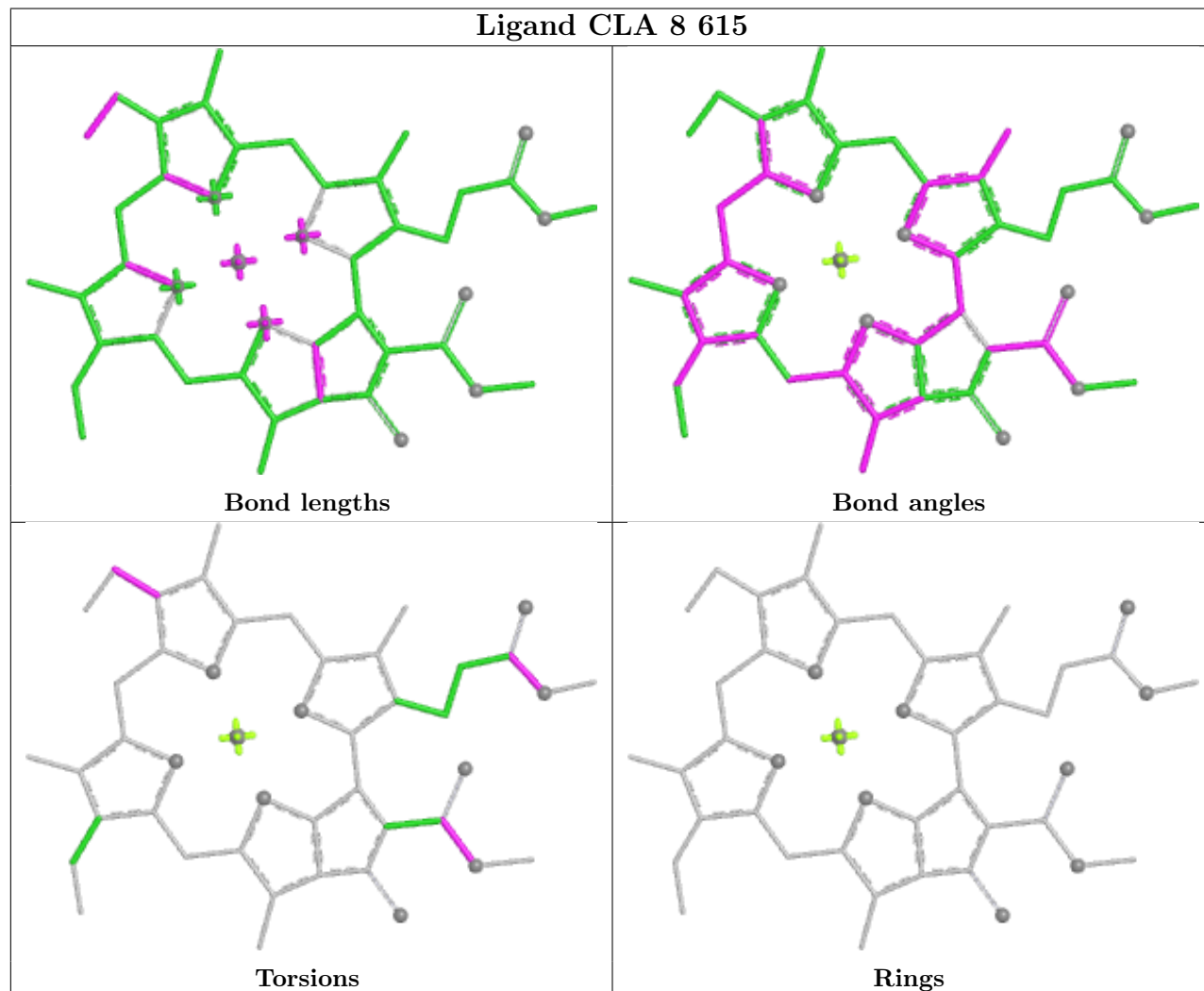
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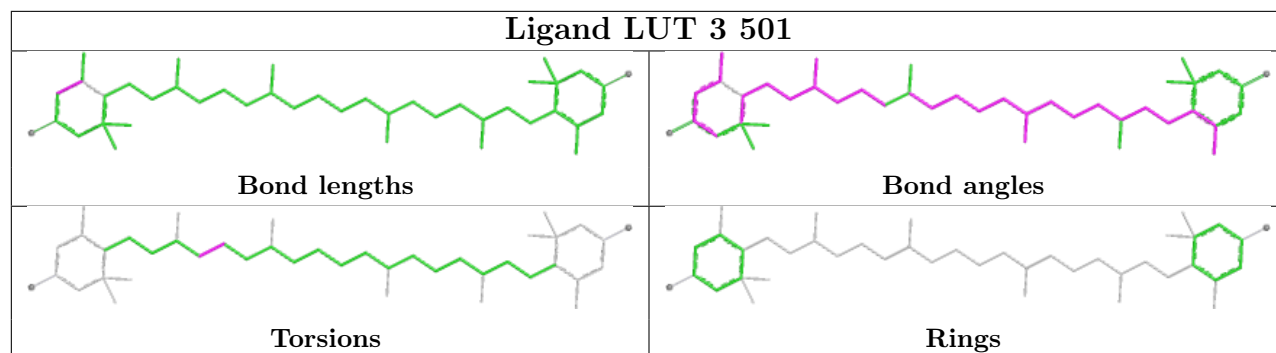
Ligand CLA A 1111



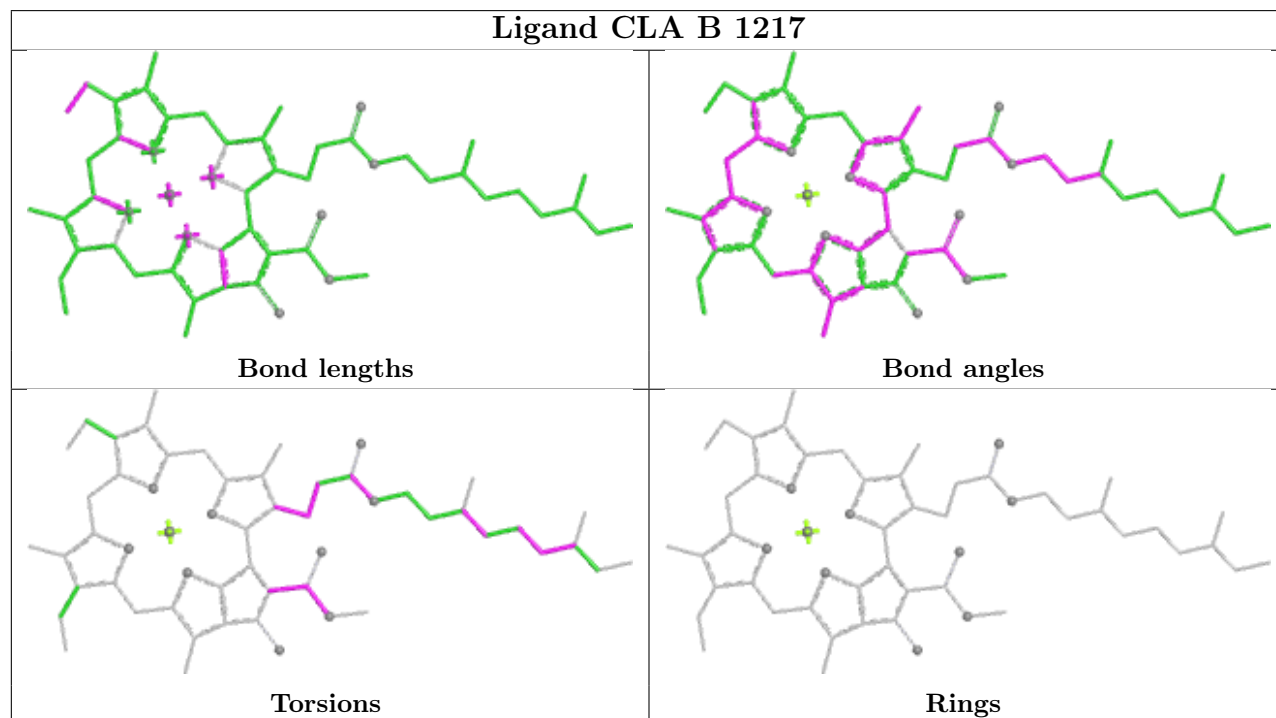
Ligand CLA 8 615



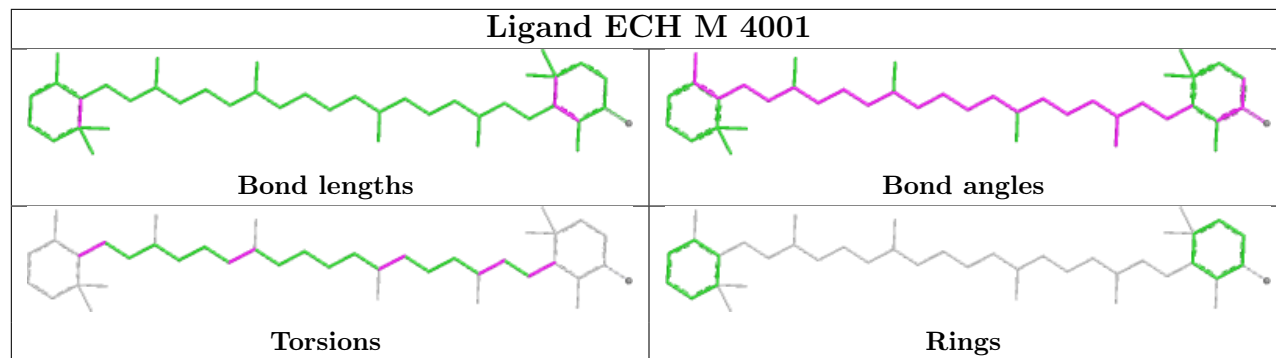
Ligand LUT 3 501

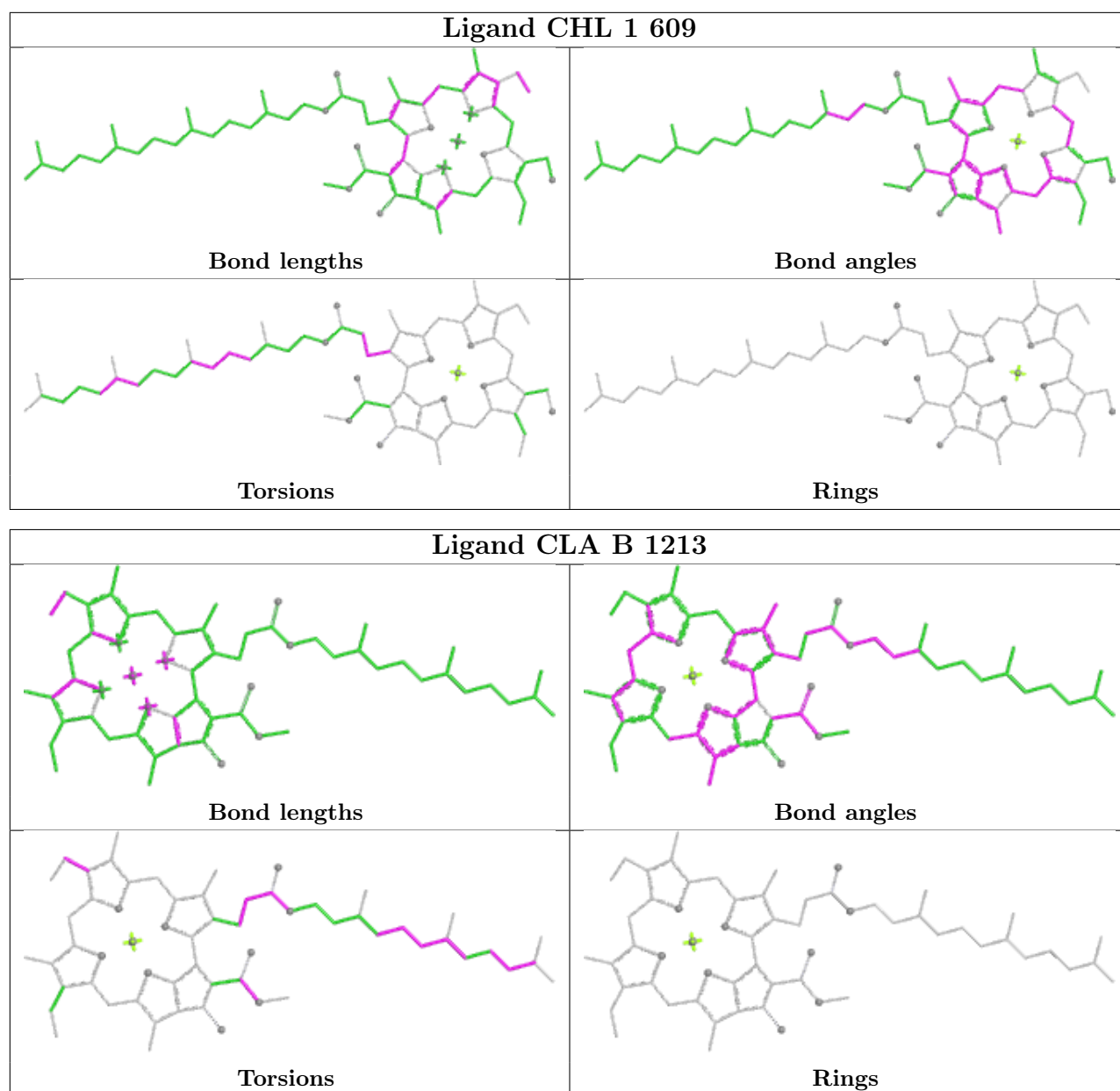


Ligand CLA B 1217

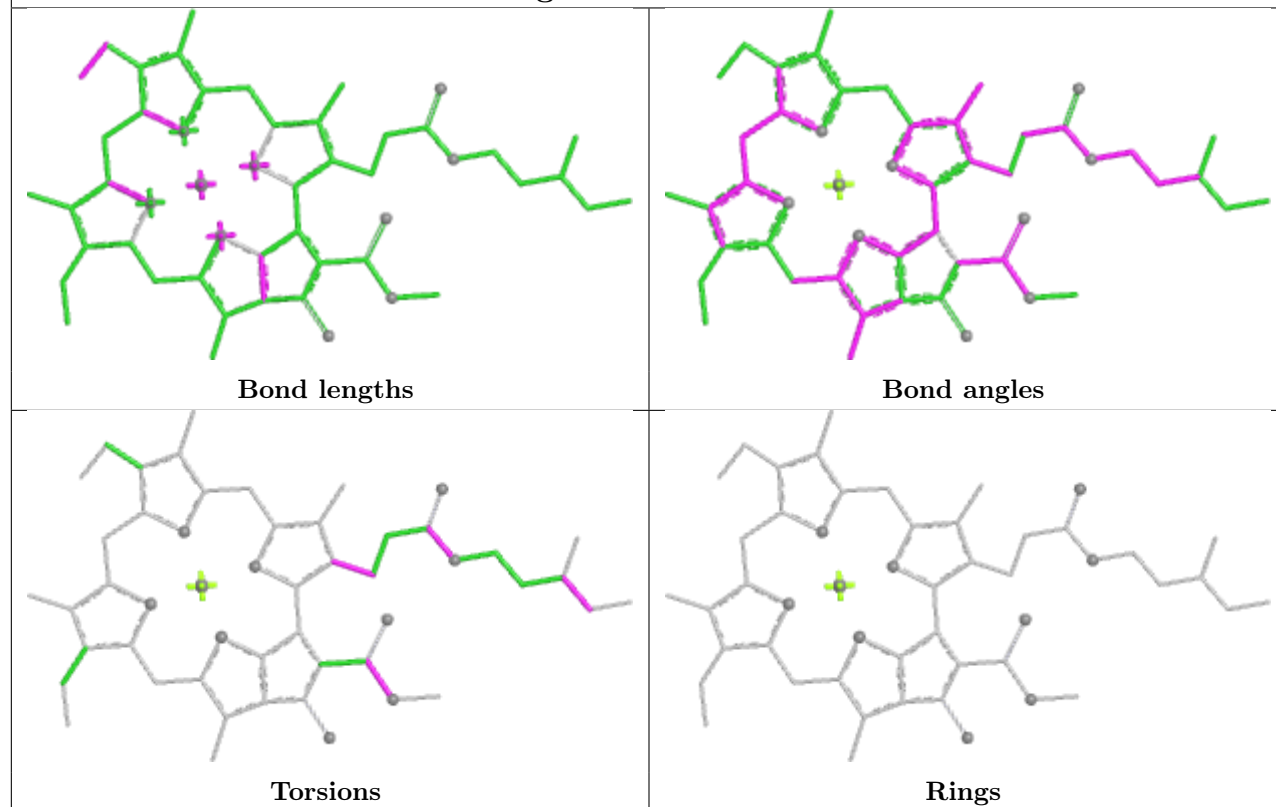


Ligand ECH M 4001

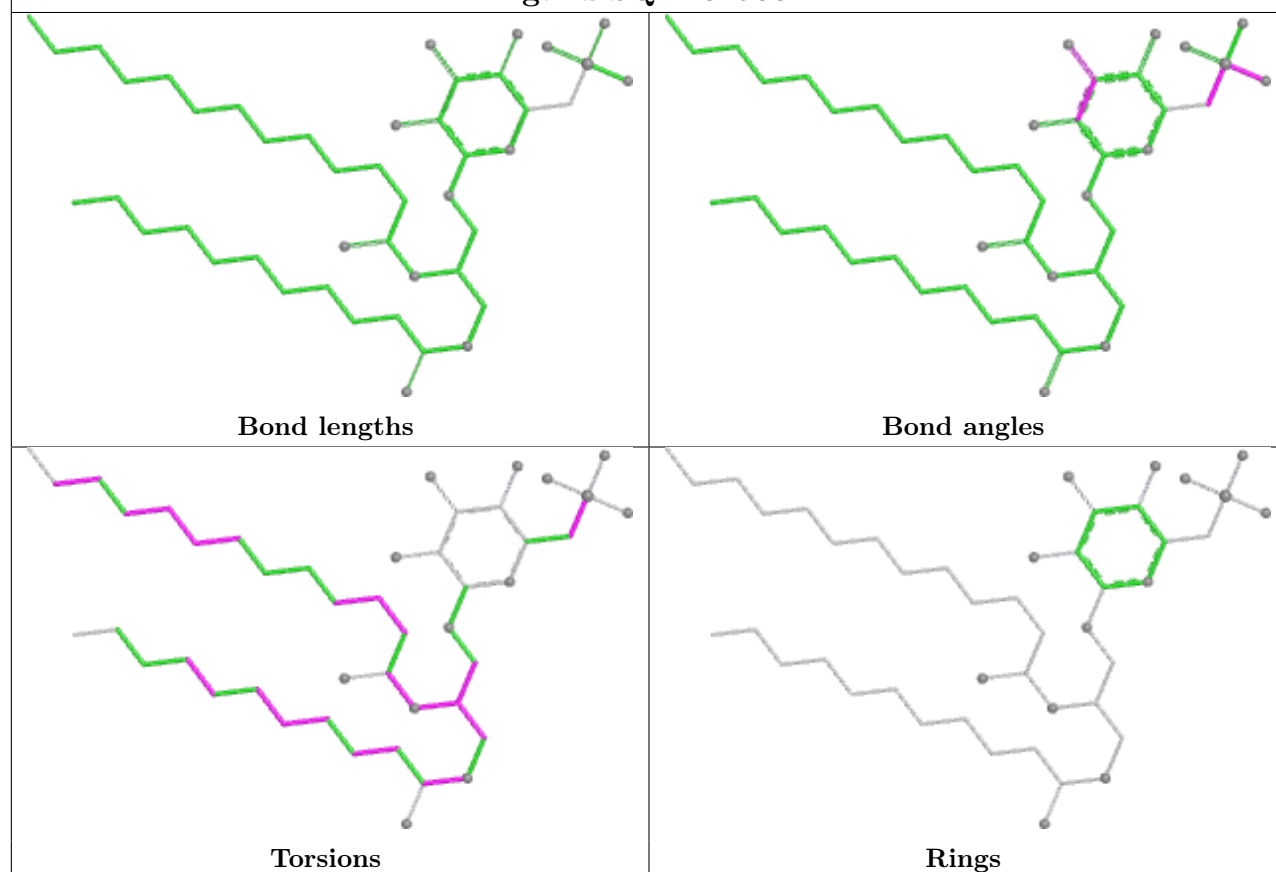


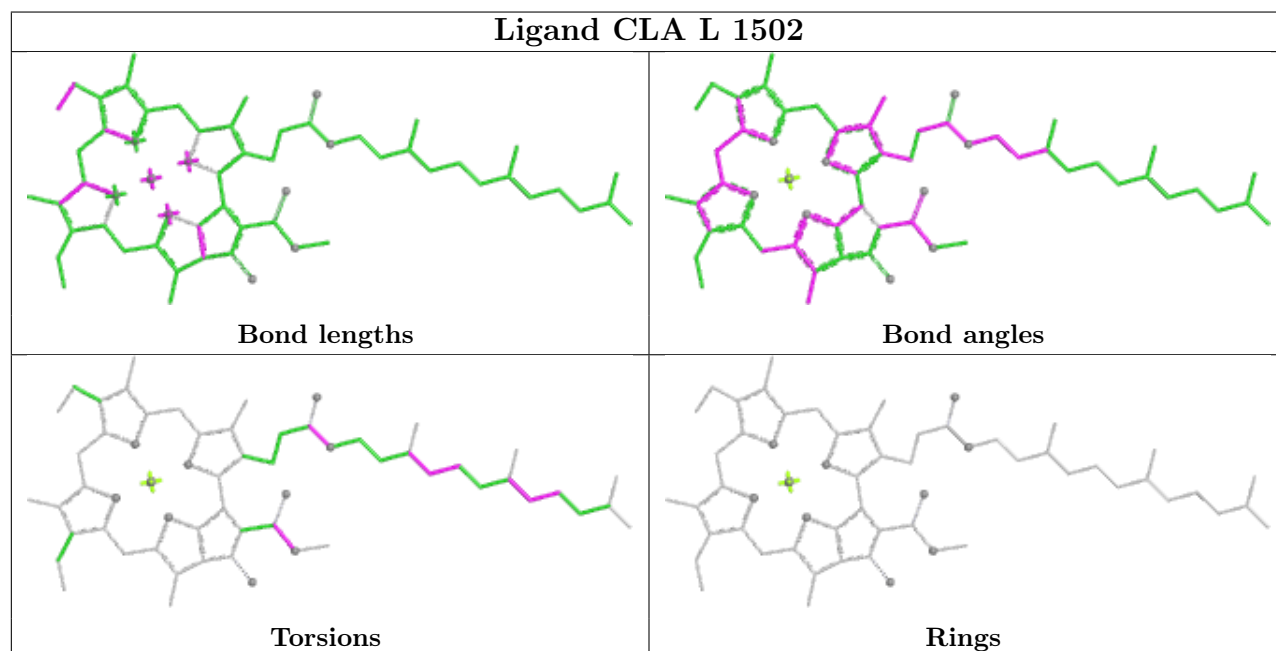
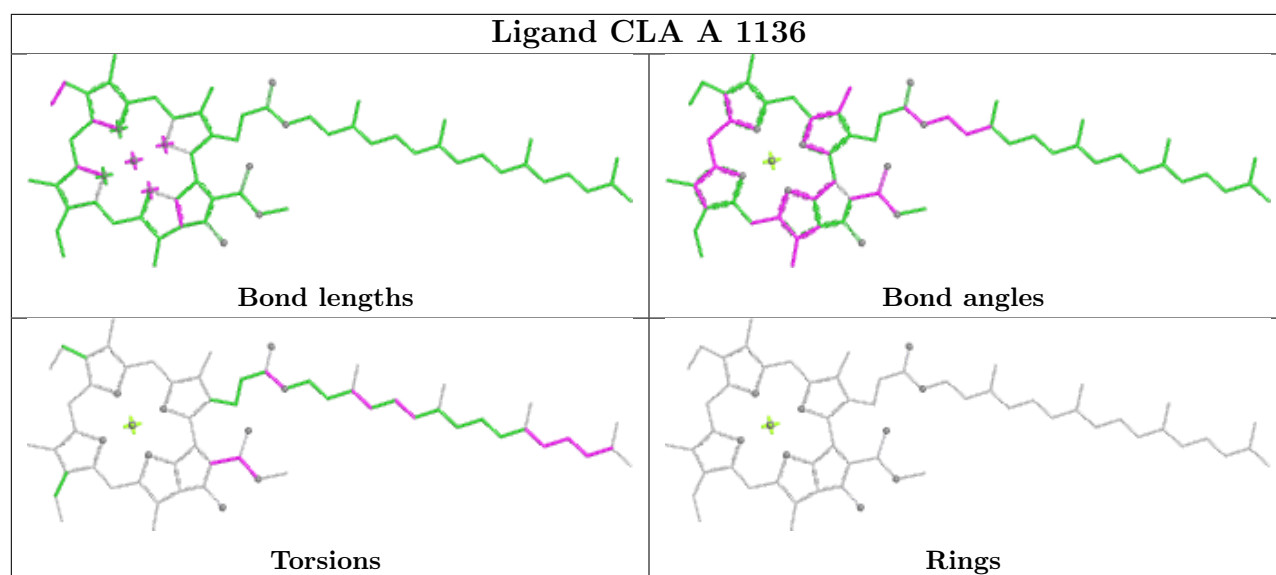


Ligand CLA 4 608

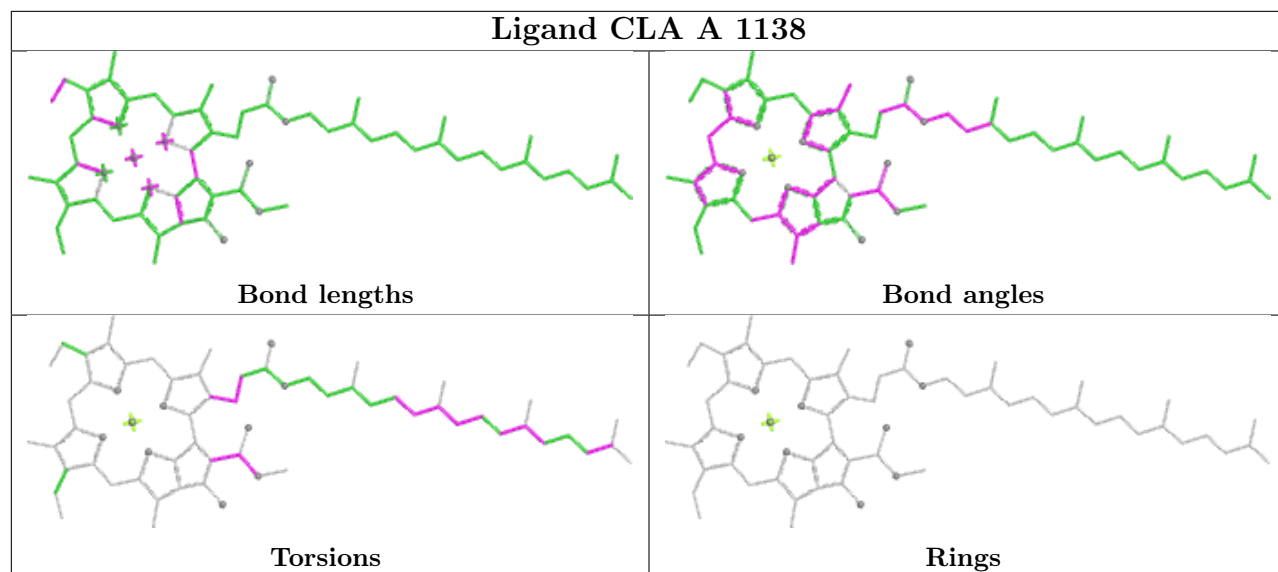


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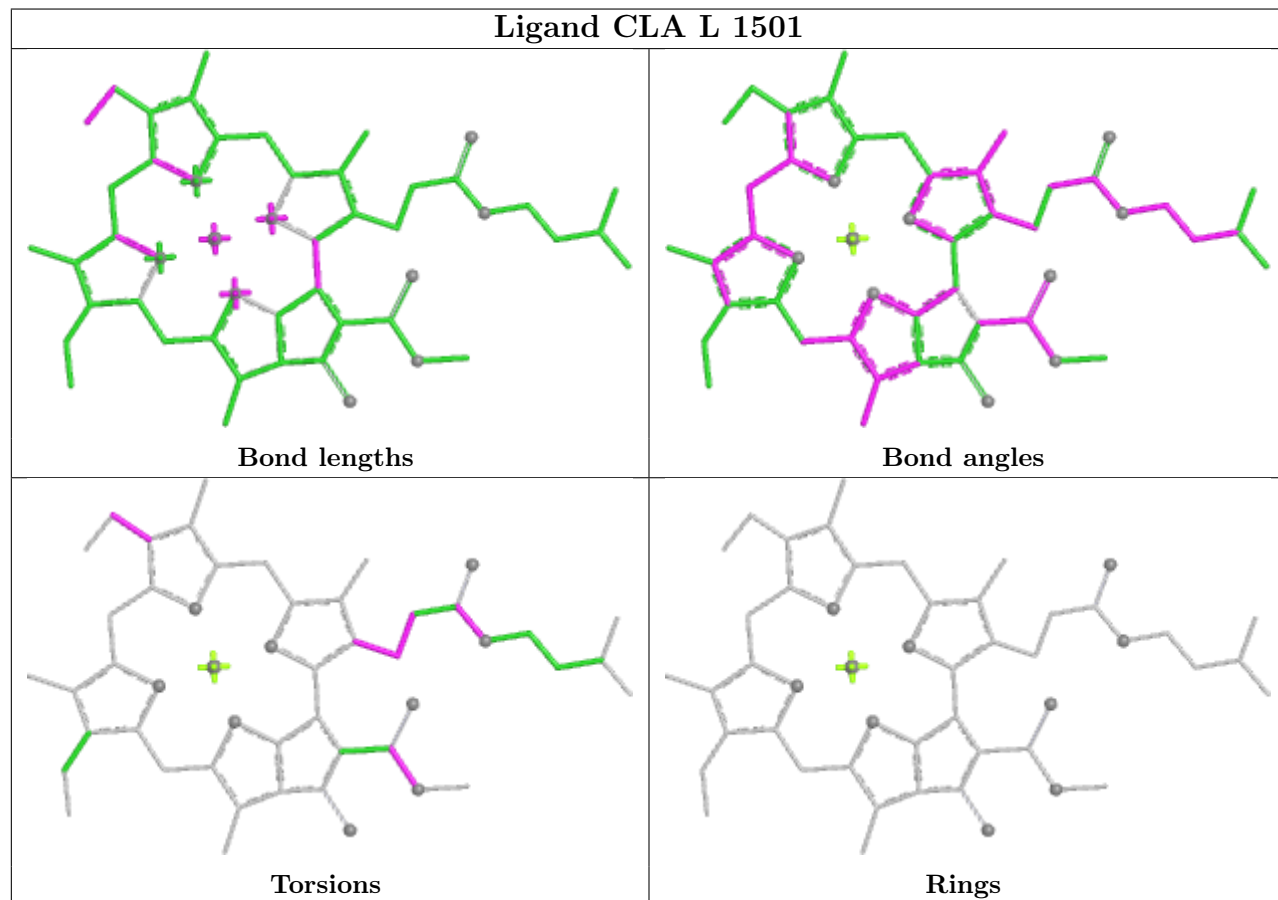




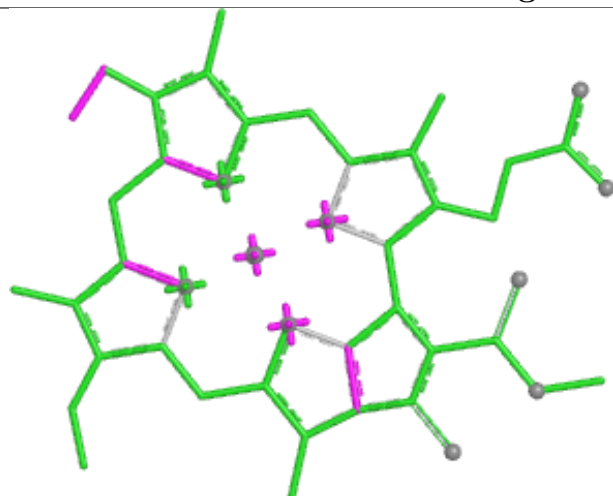
Ligand CLA A 1138



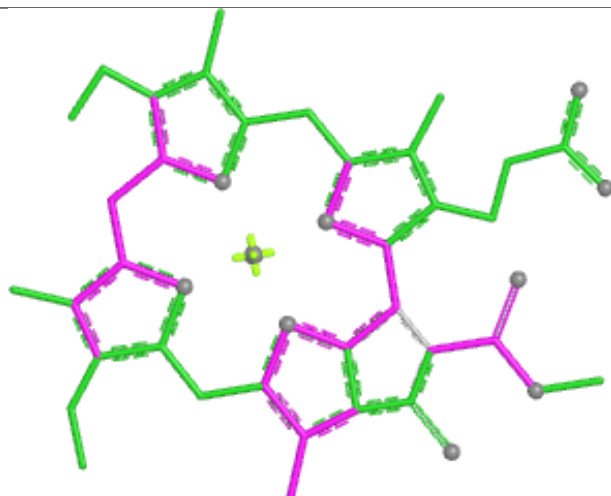
Ligand CLA L 1501



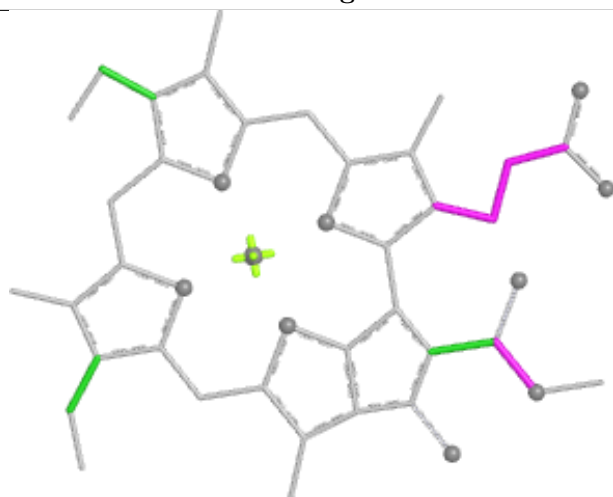
Ligand CLA 1 602



Bond lengths



Bond angles

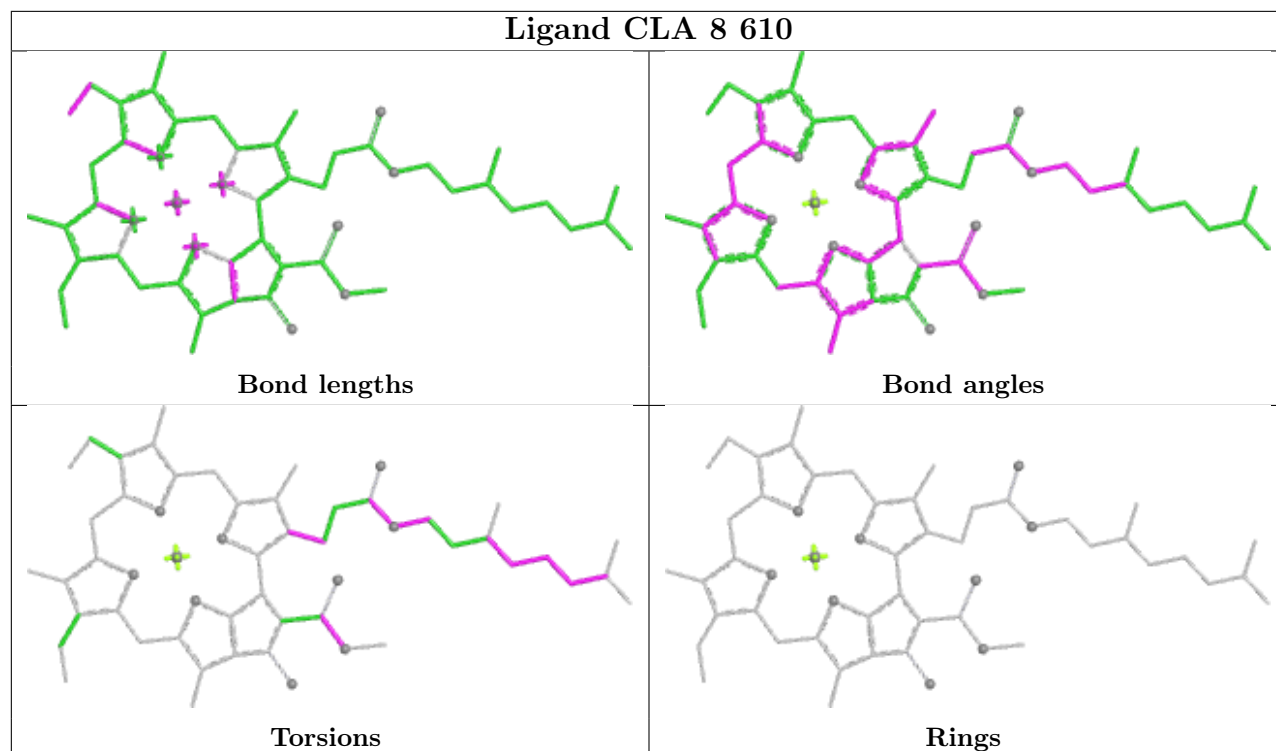


Torsions

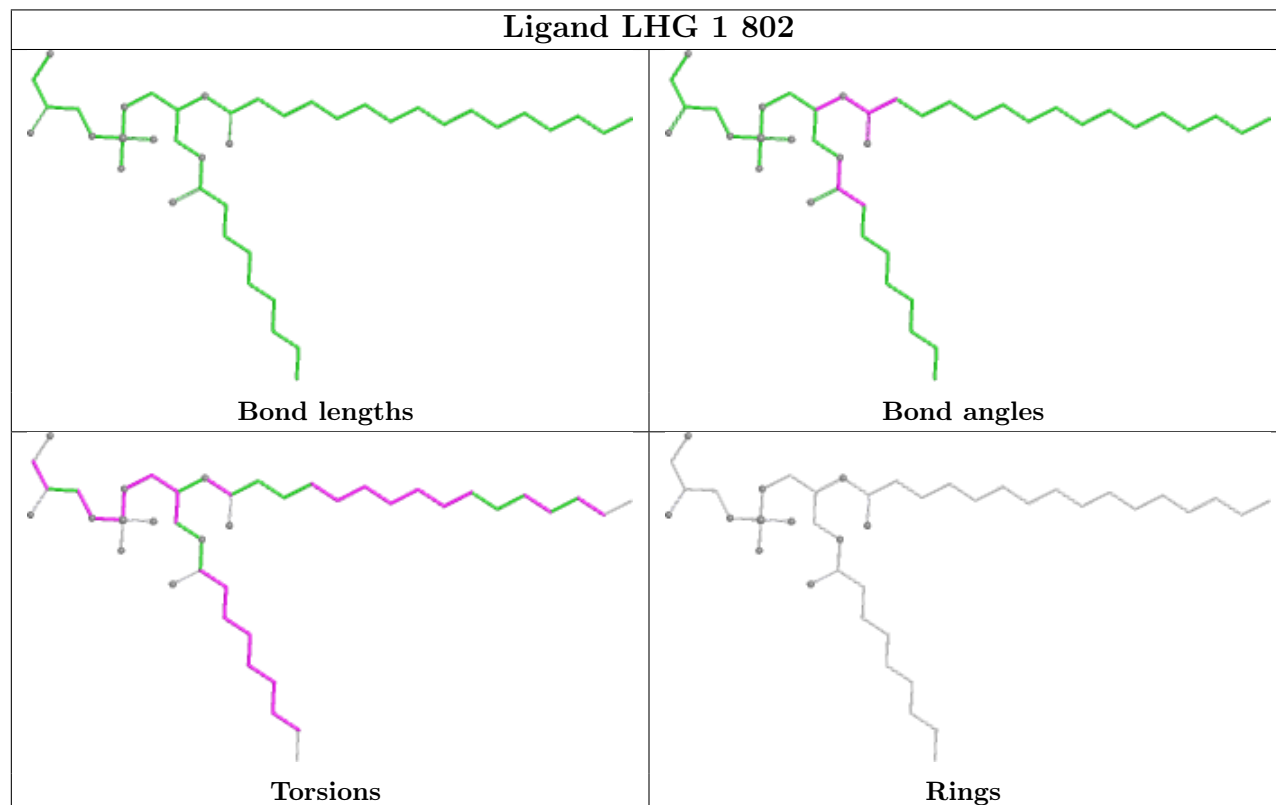


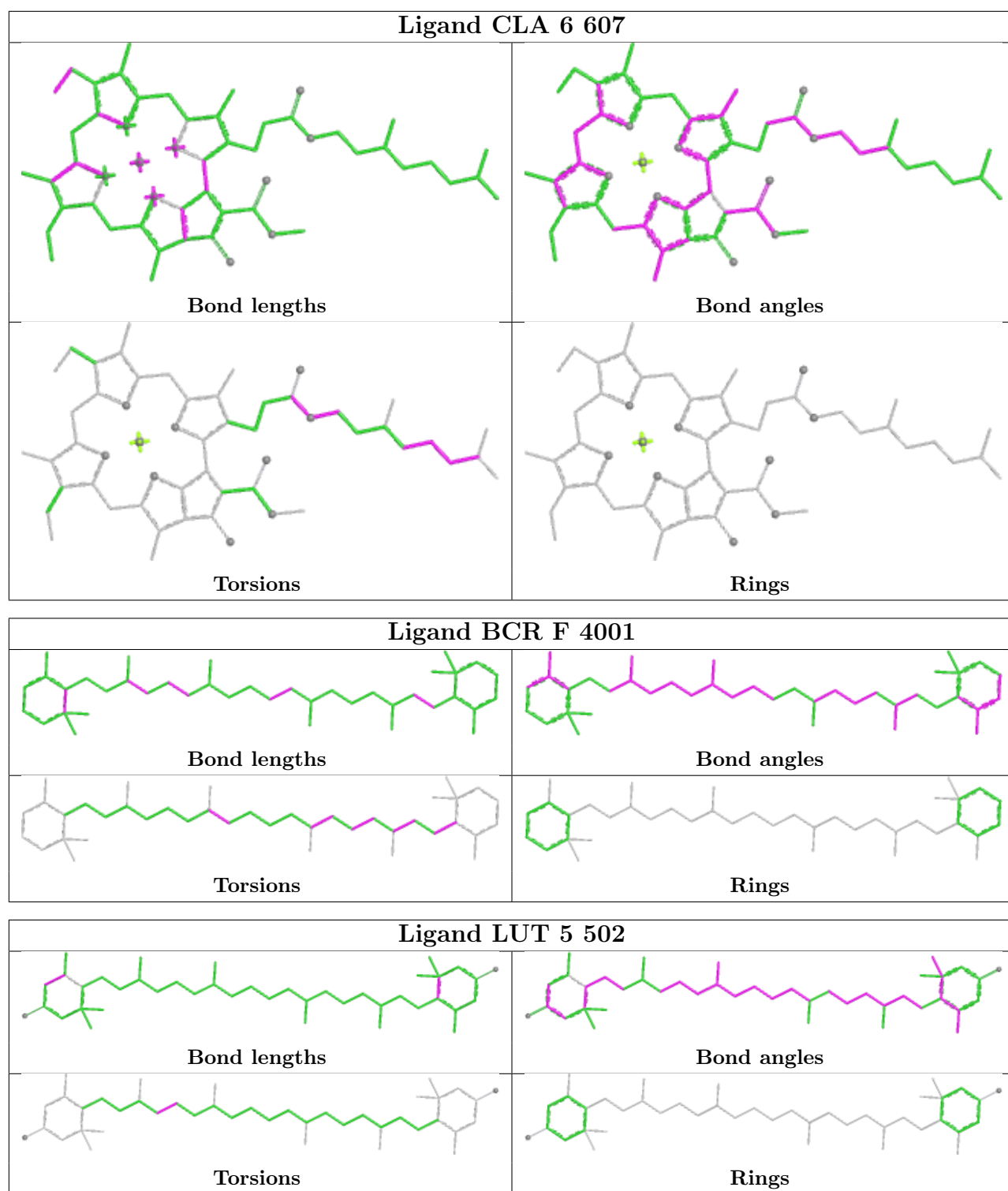
Rings

Ligand CLA 8 610

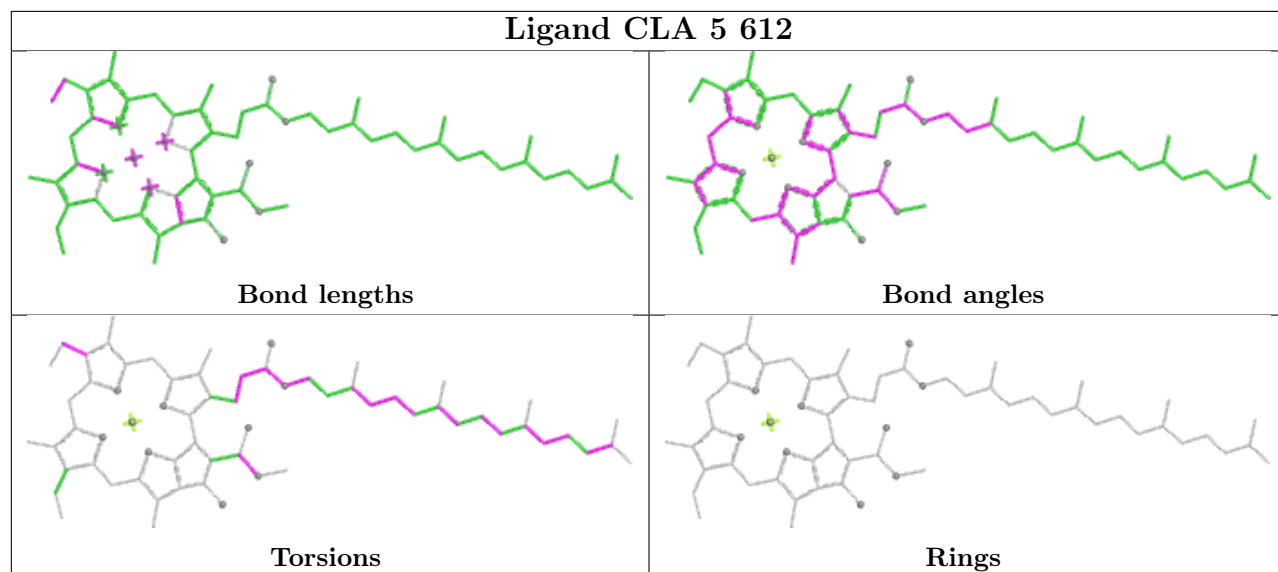


Ligand LHG 1 802

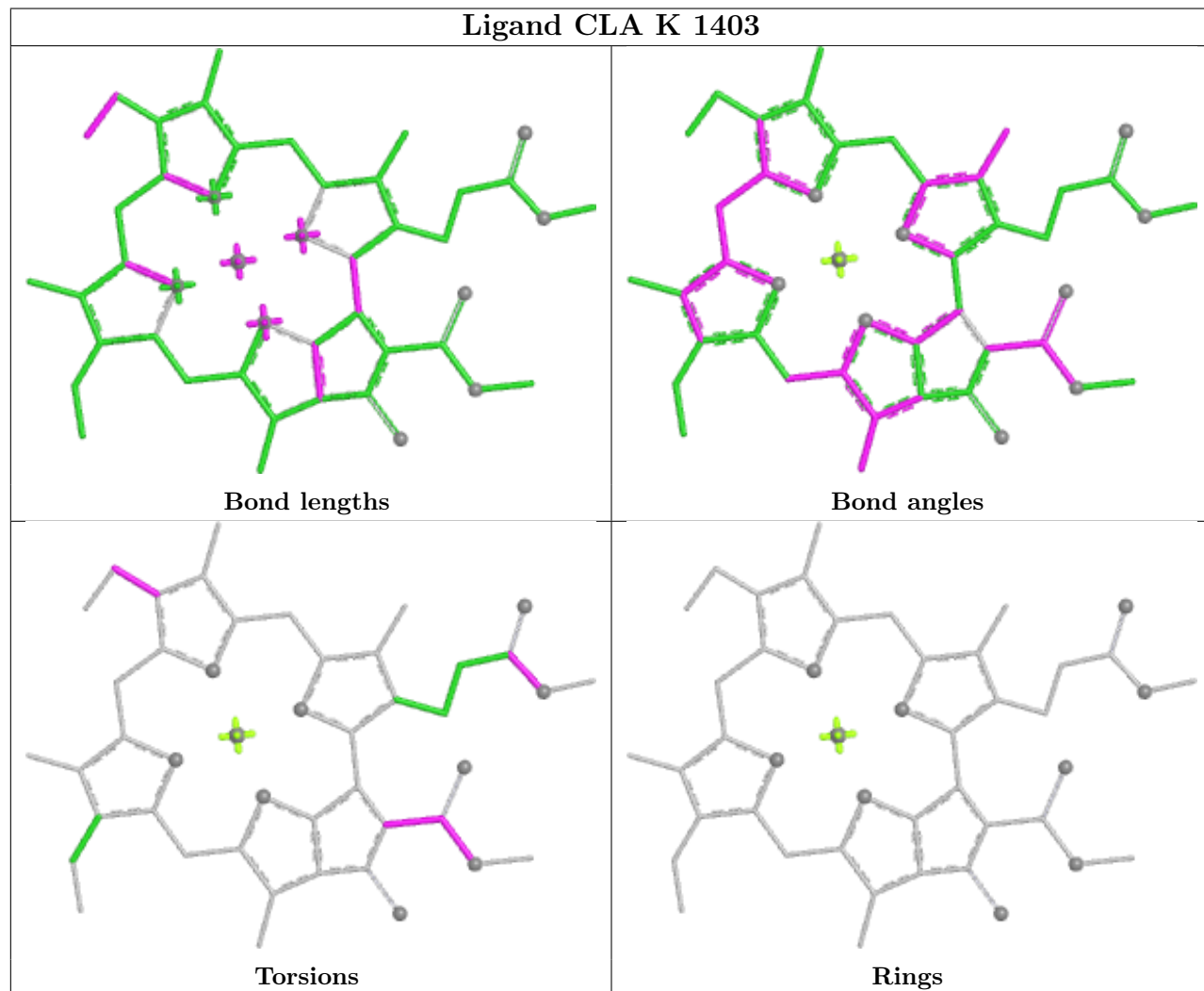


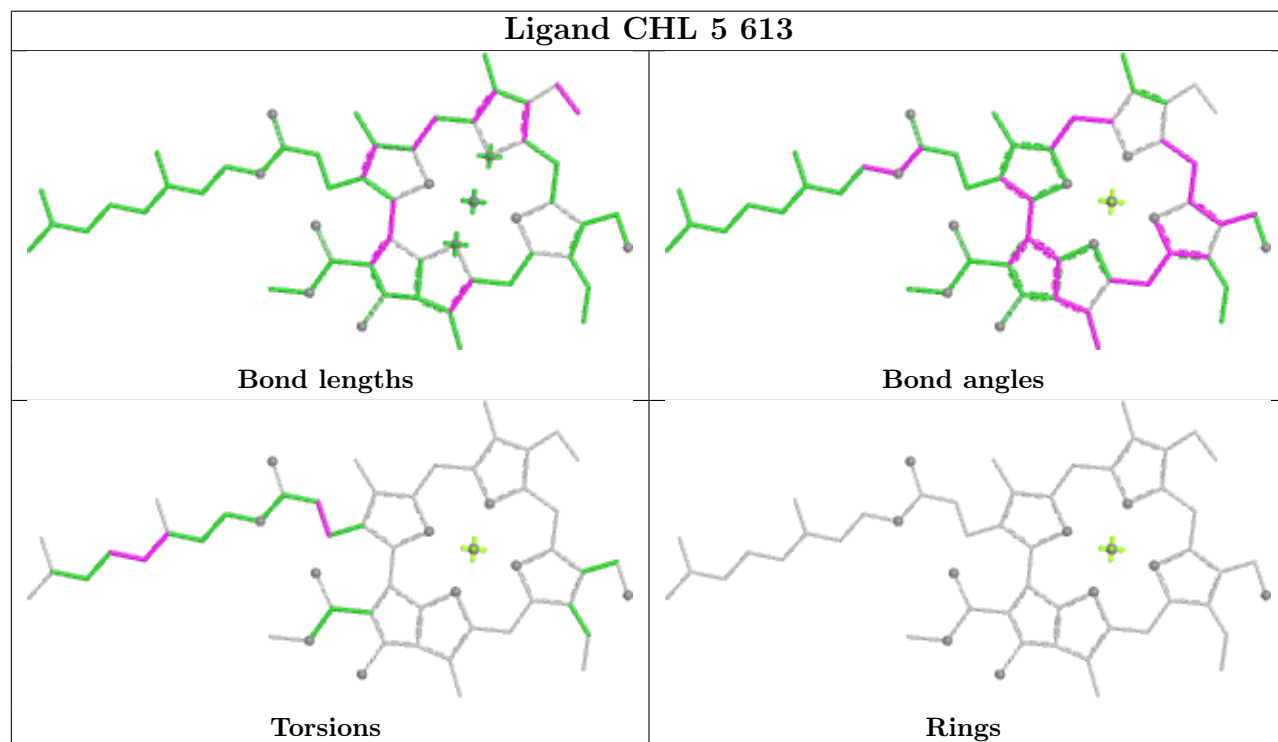
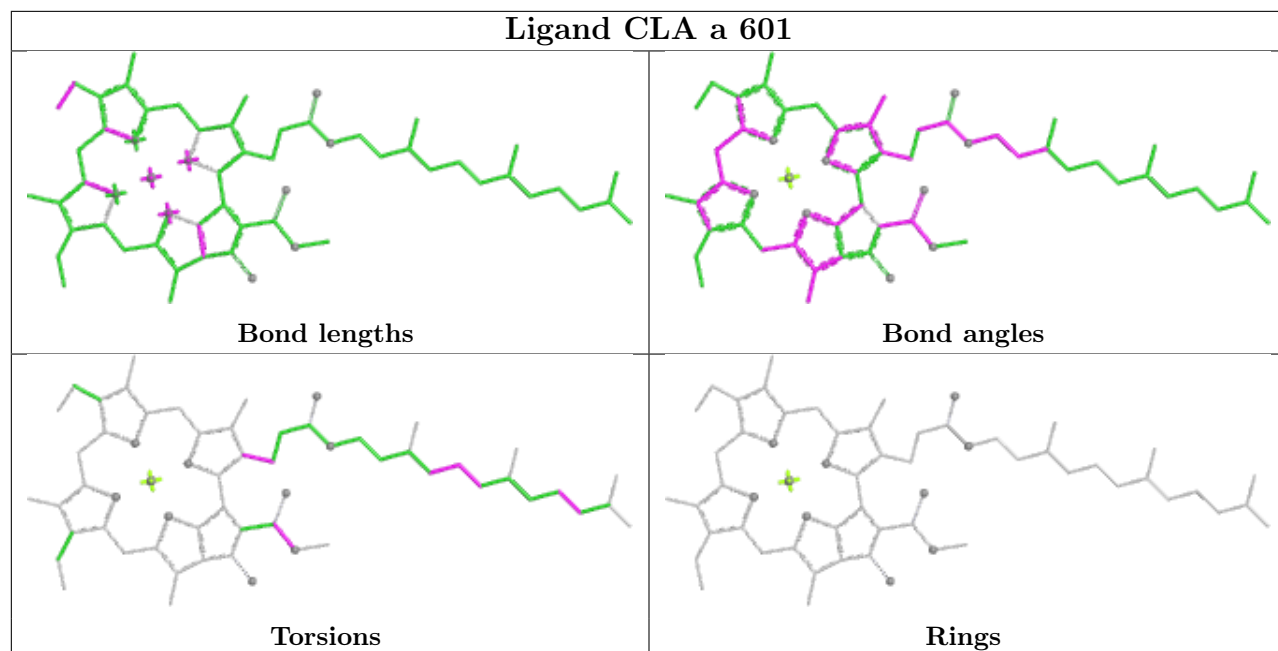


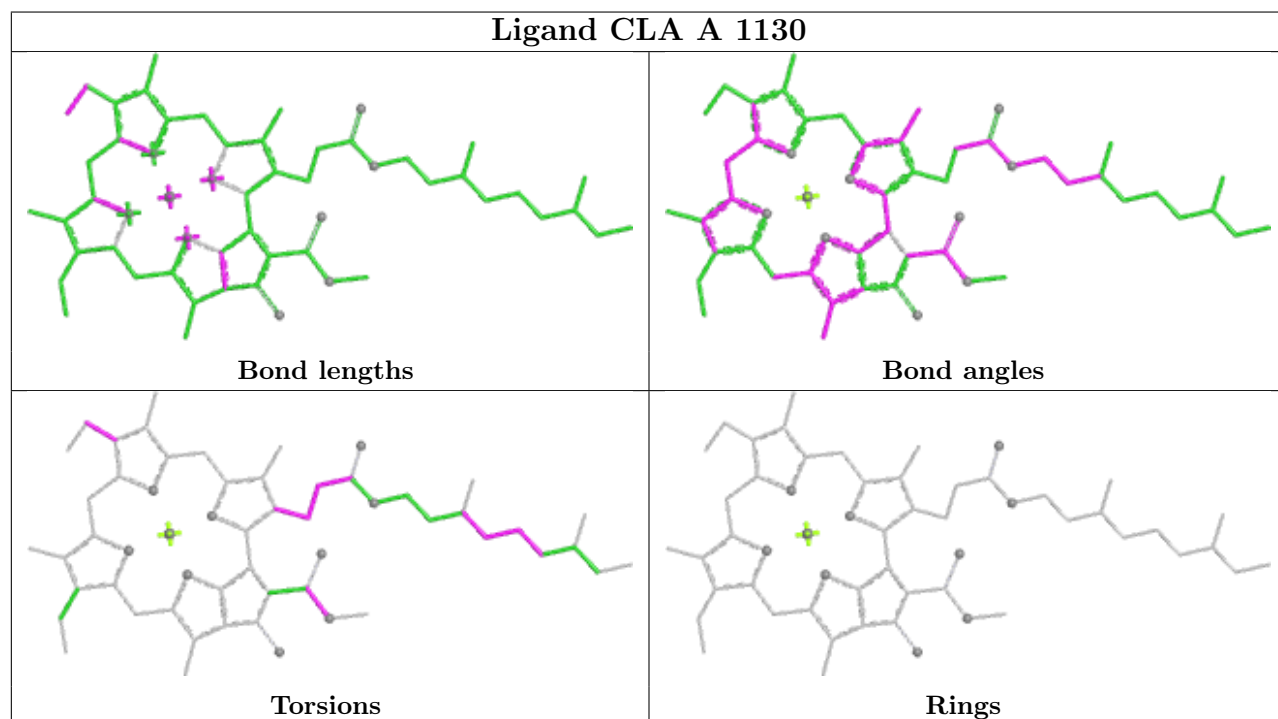
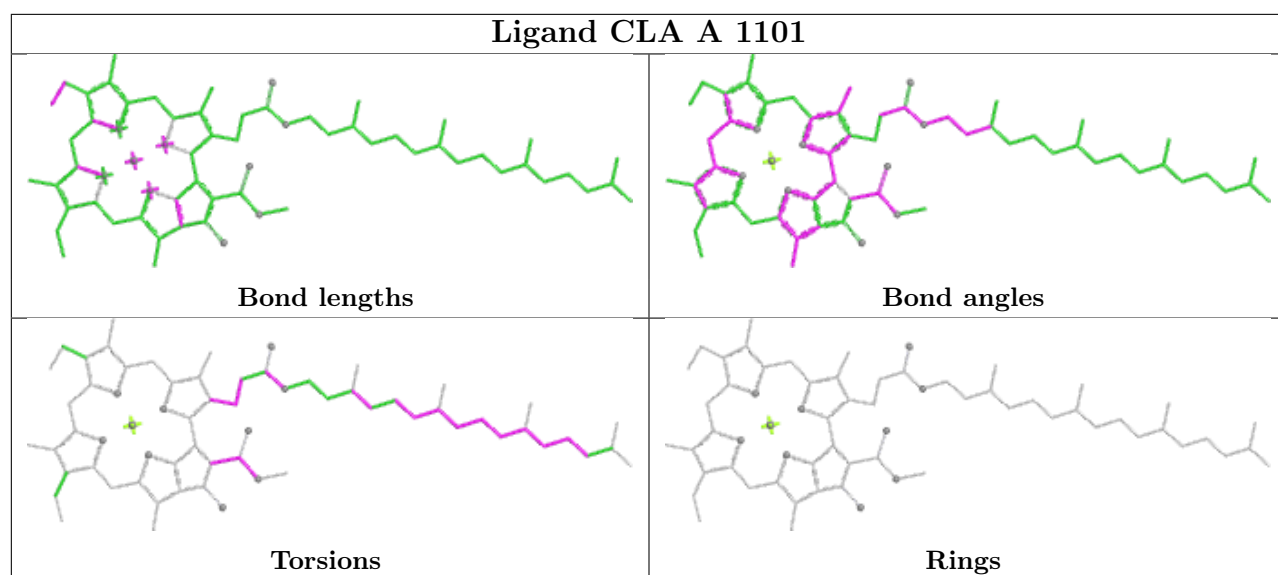
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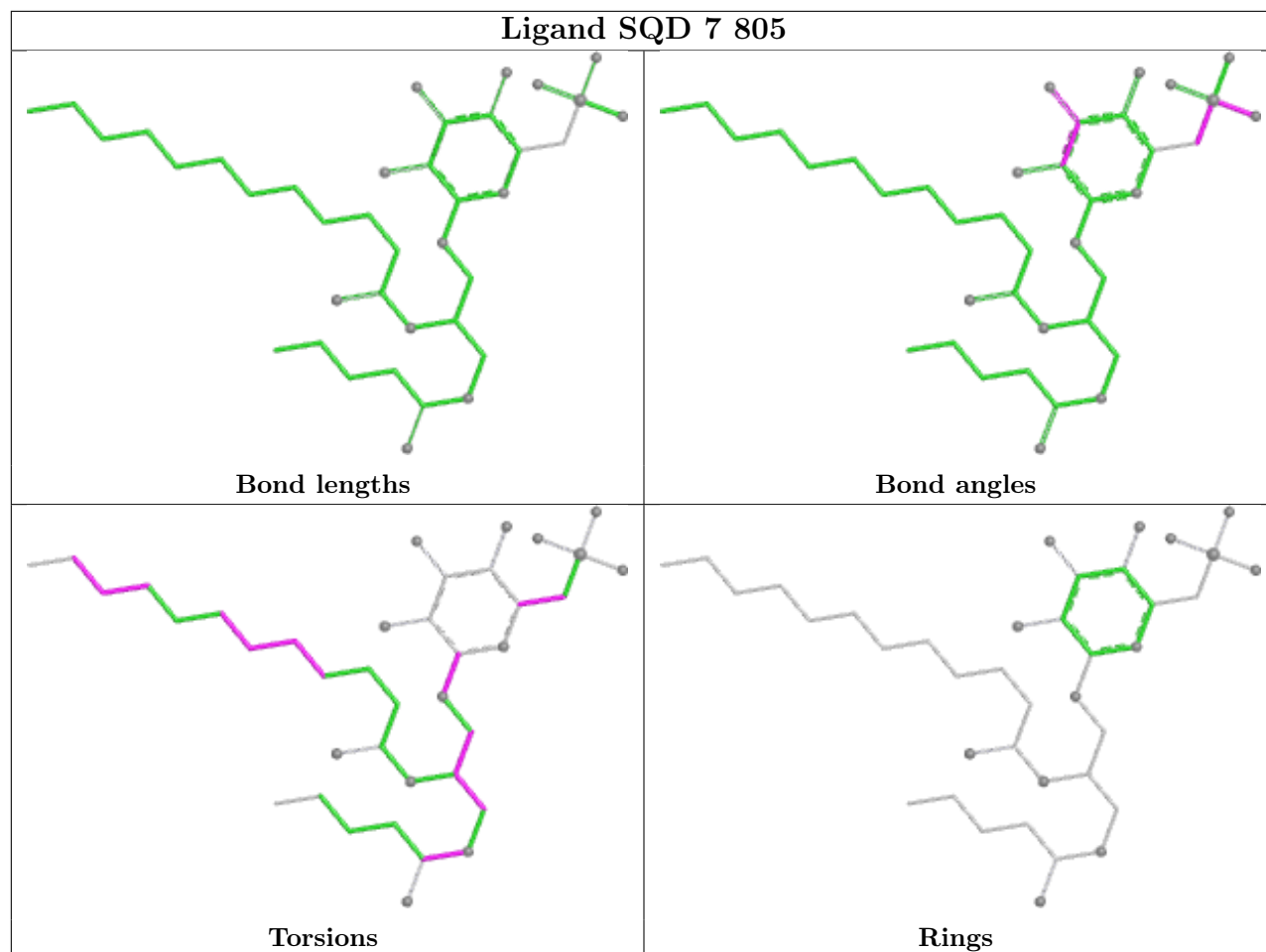
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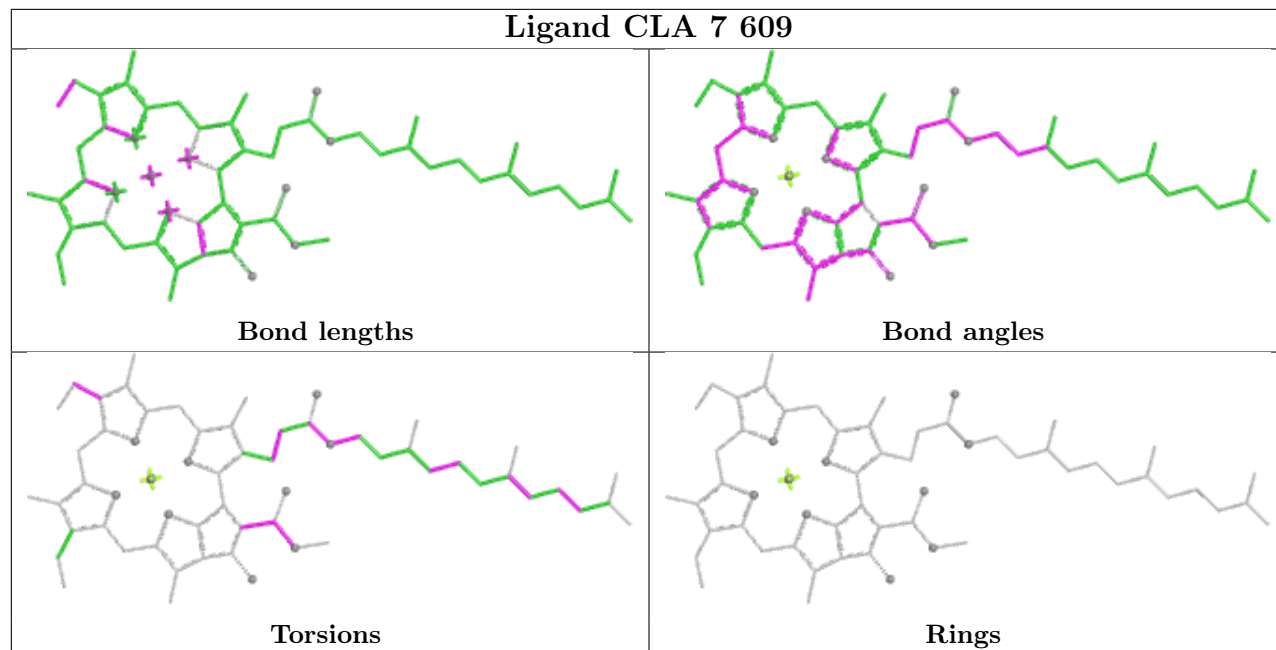


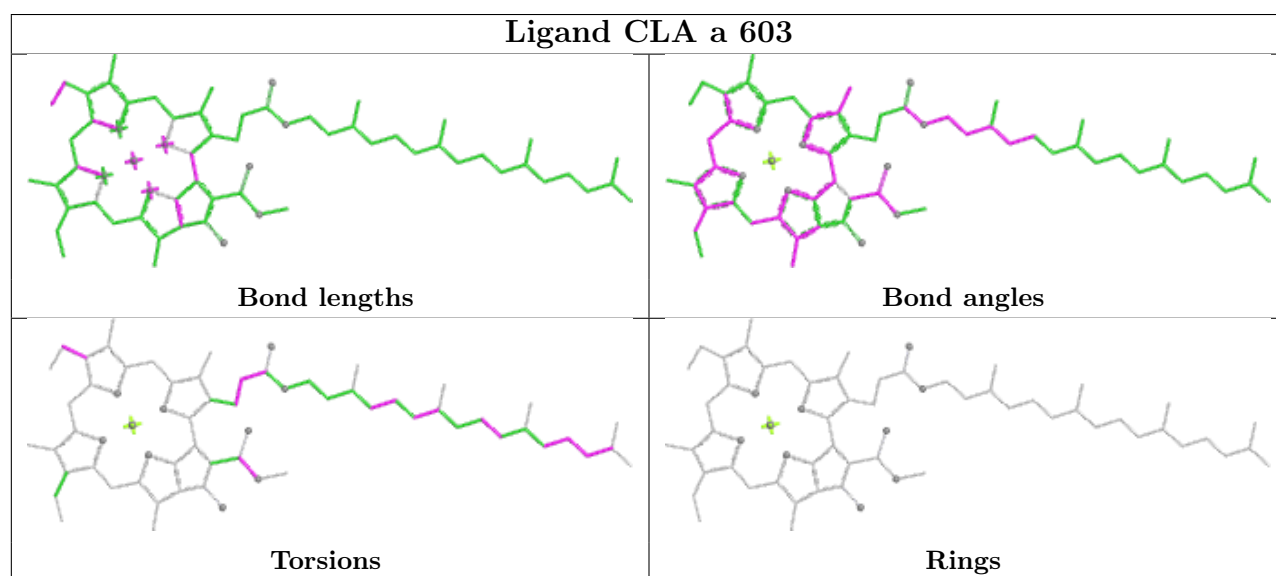
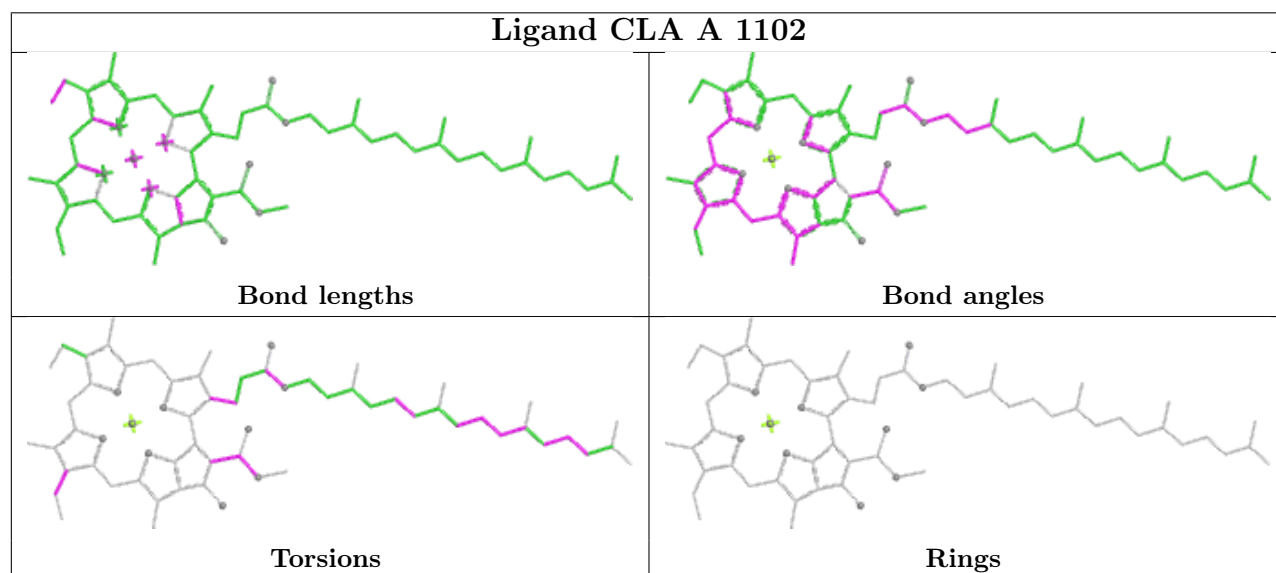
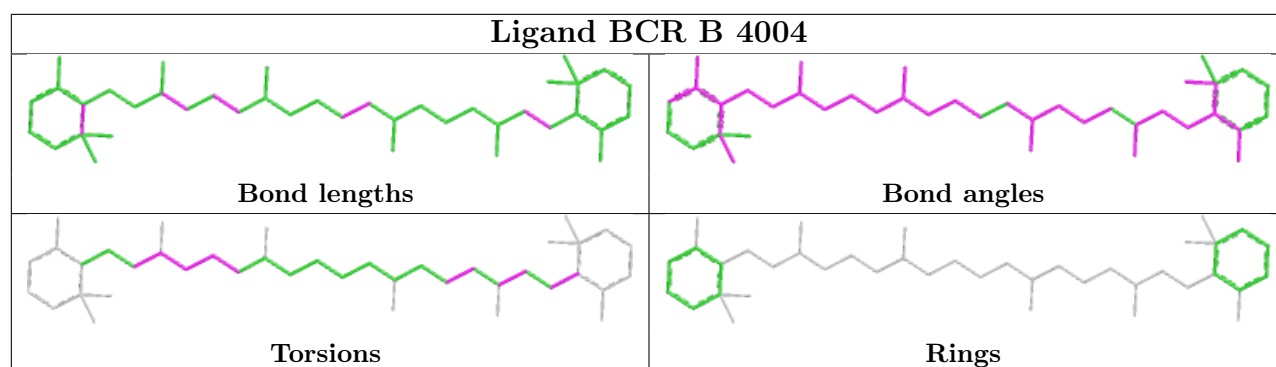


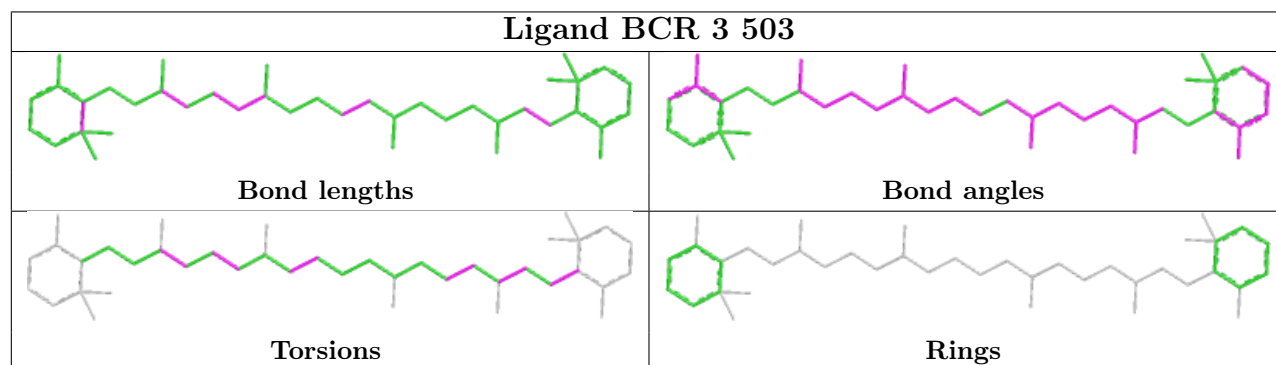
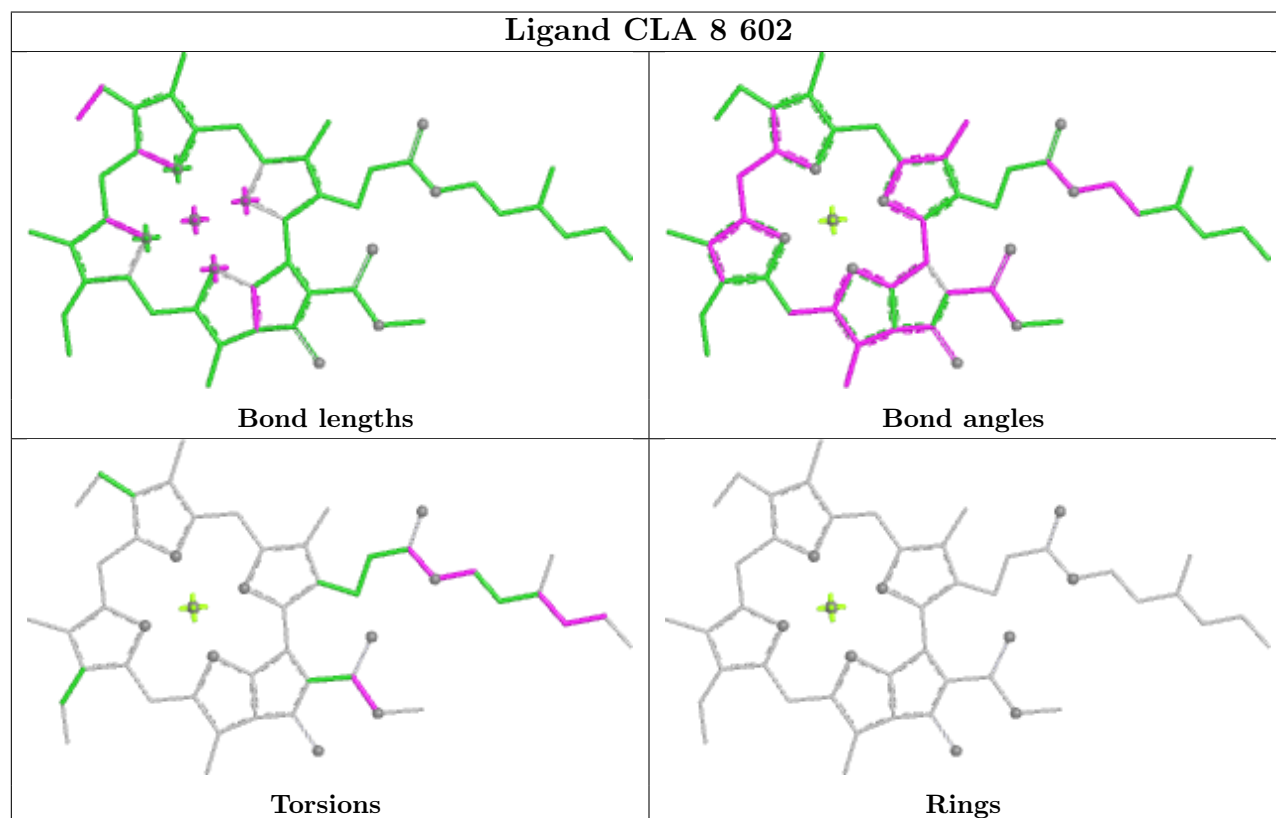
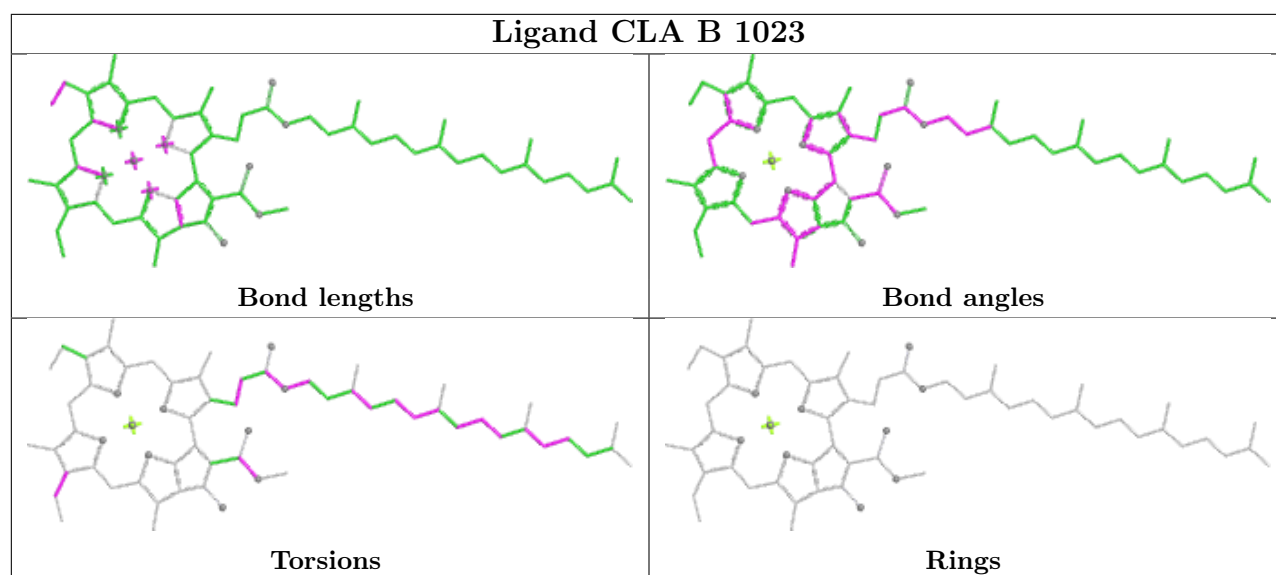
Ligand SQD 7 805

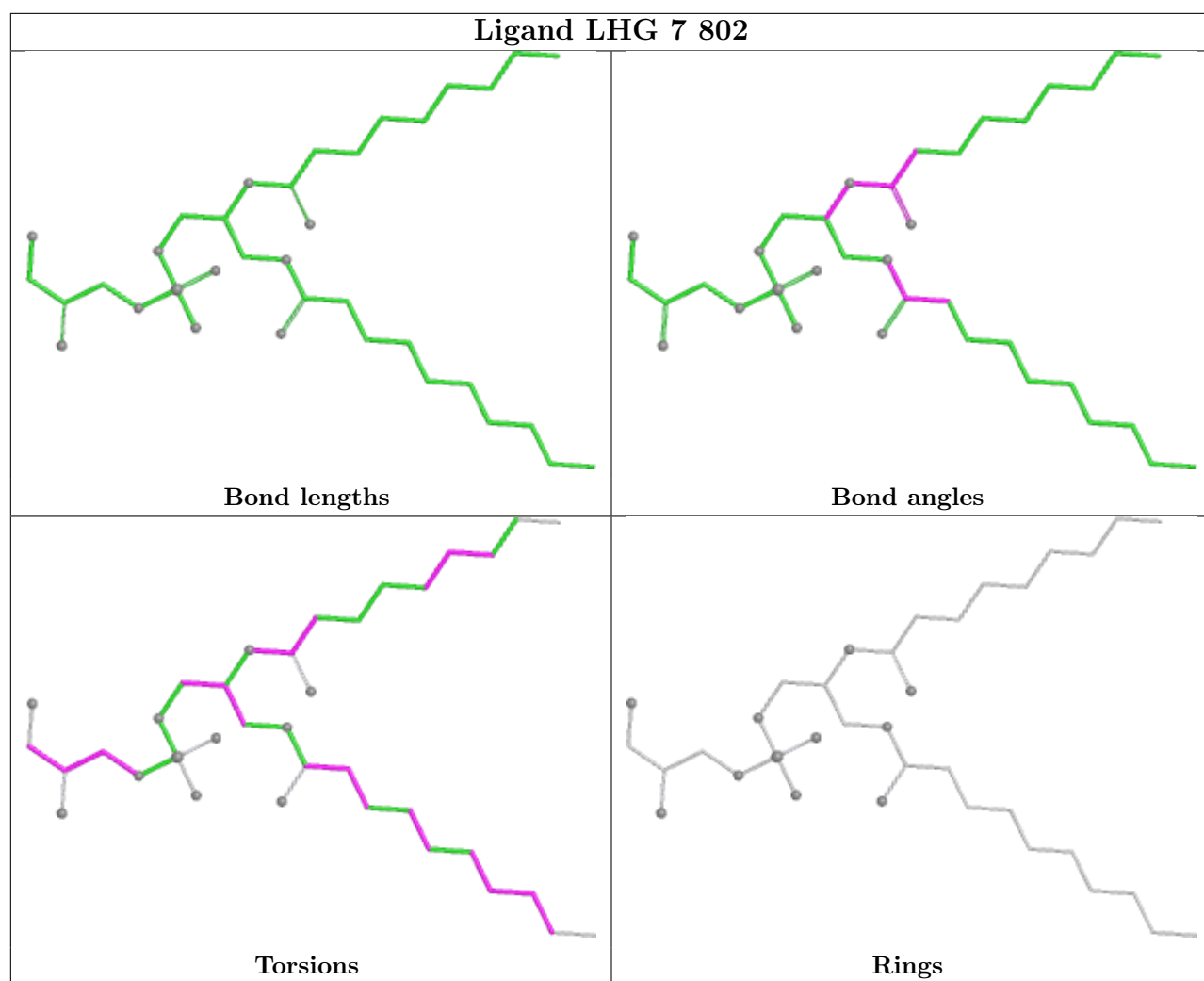


Ligand CLA 7 609

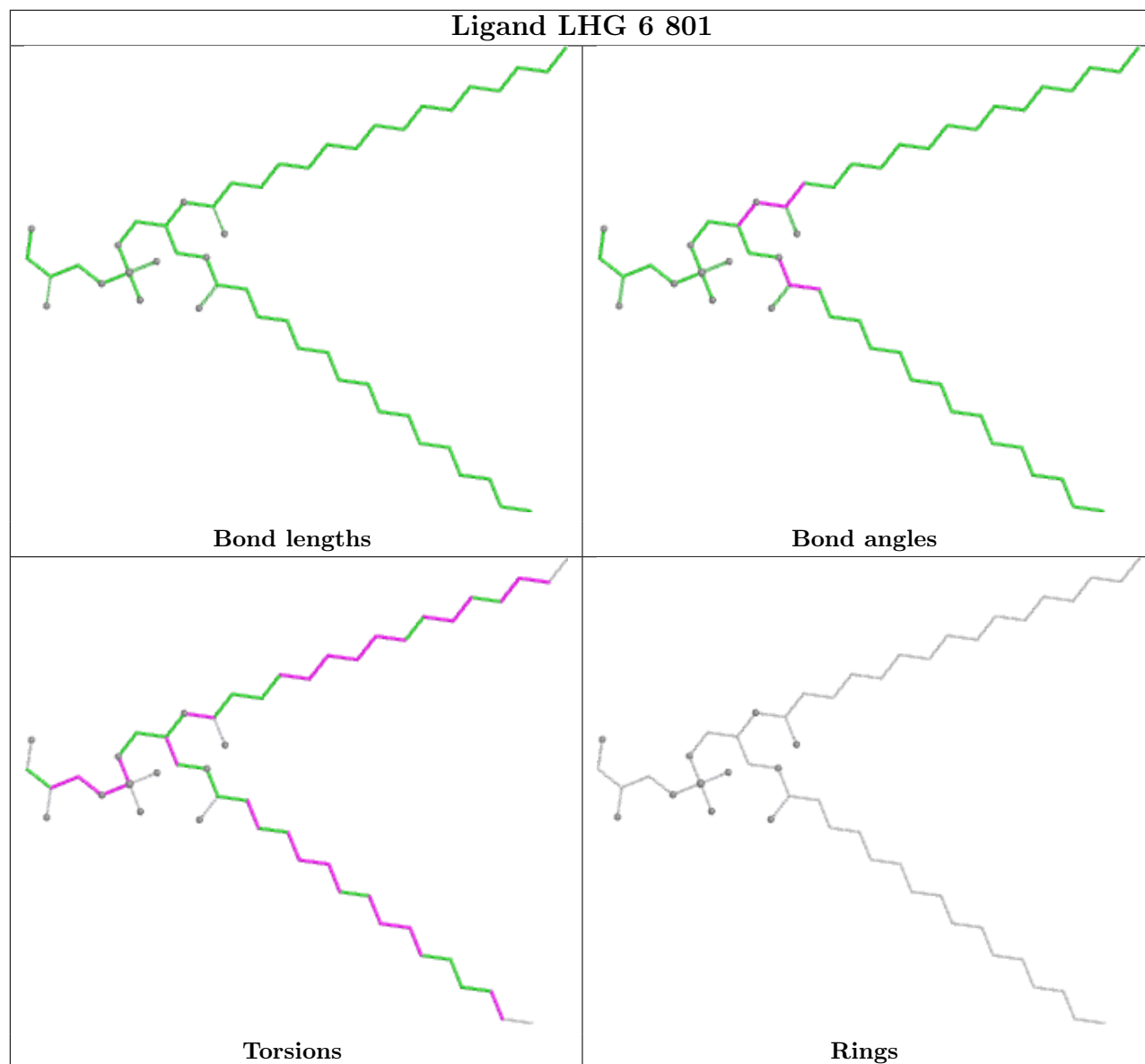




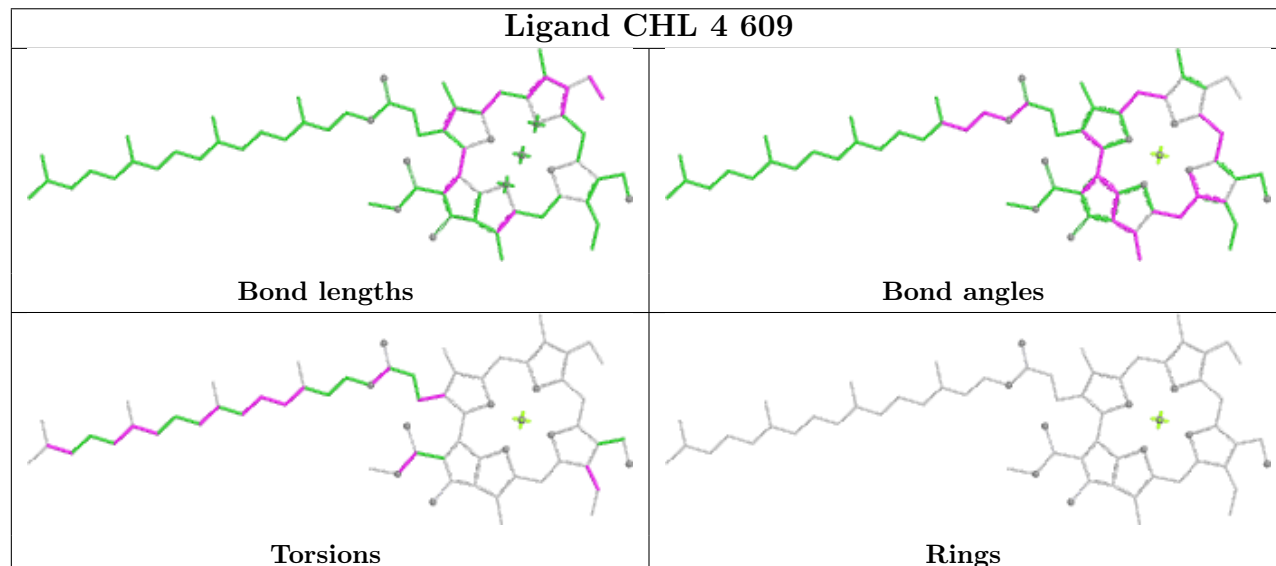


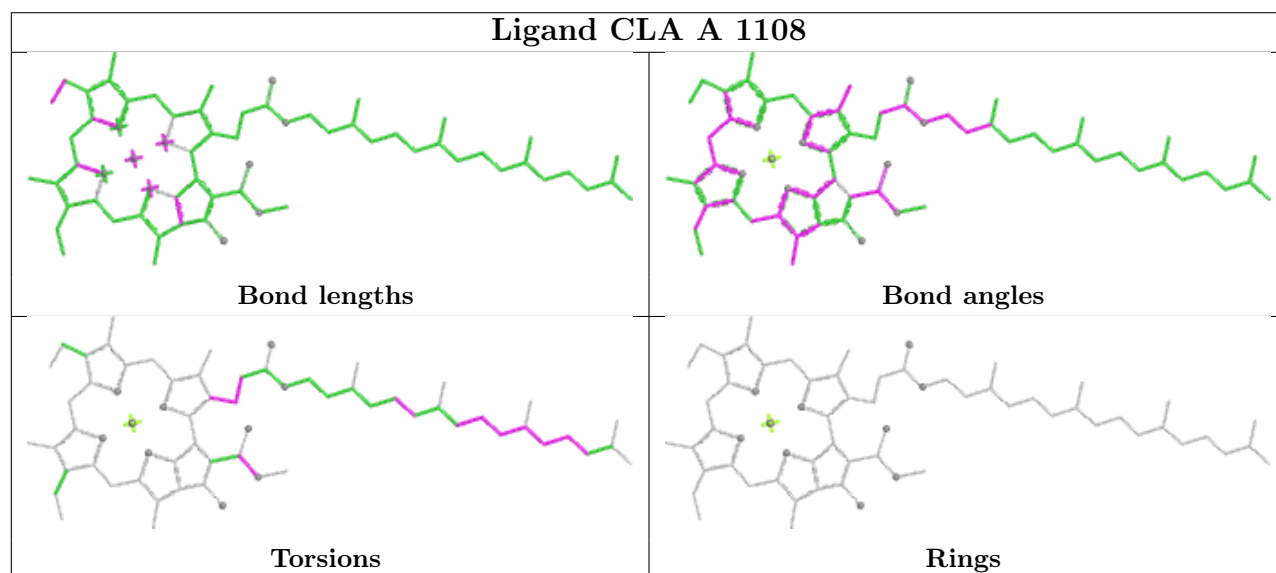
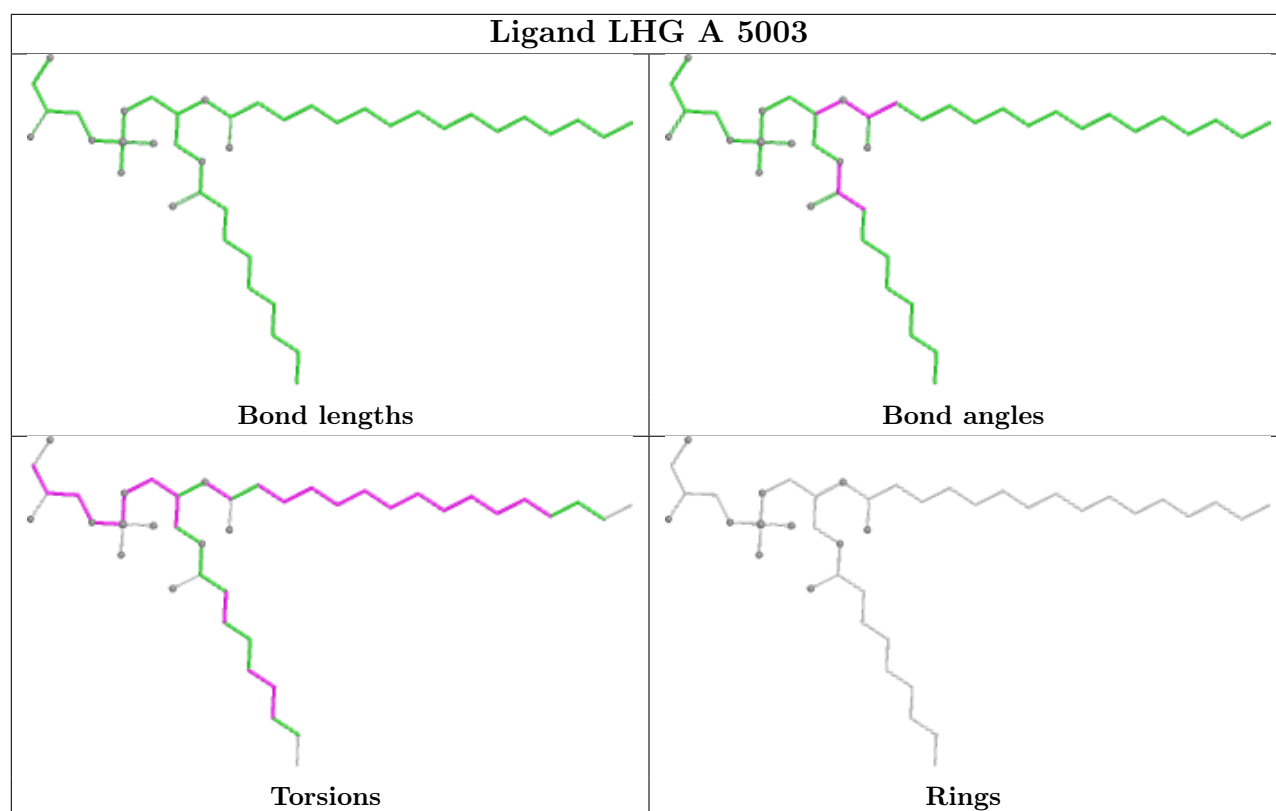


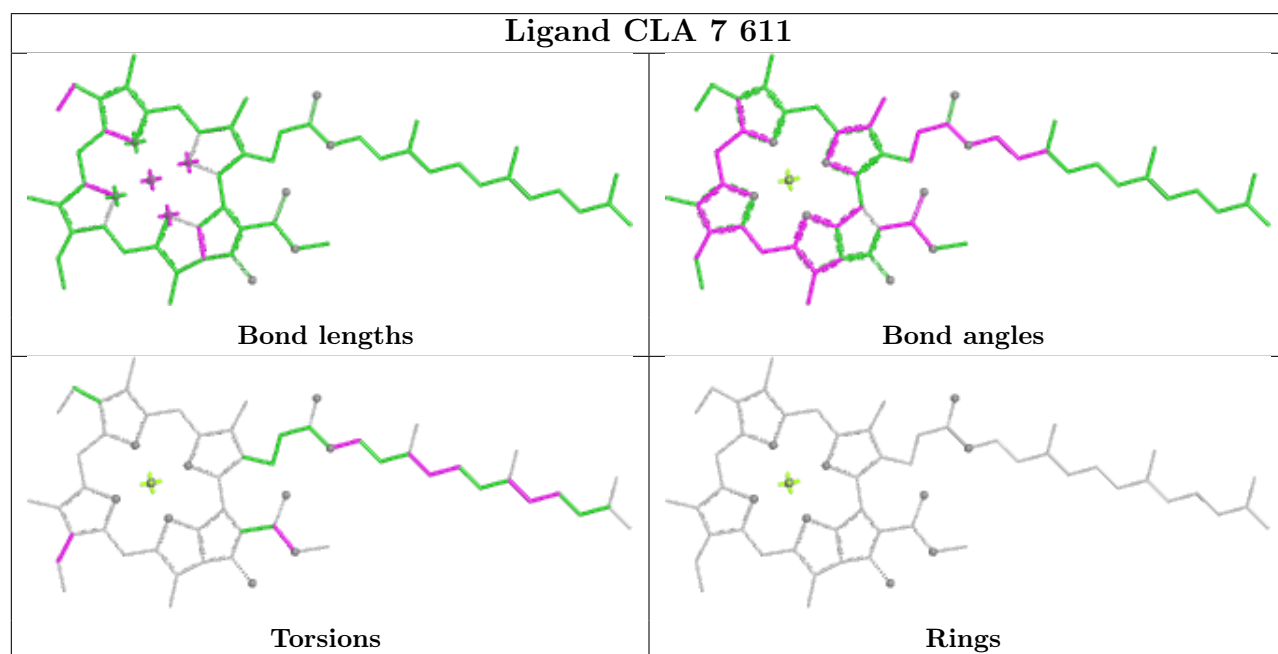
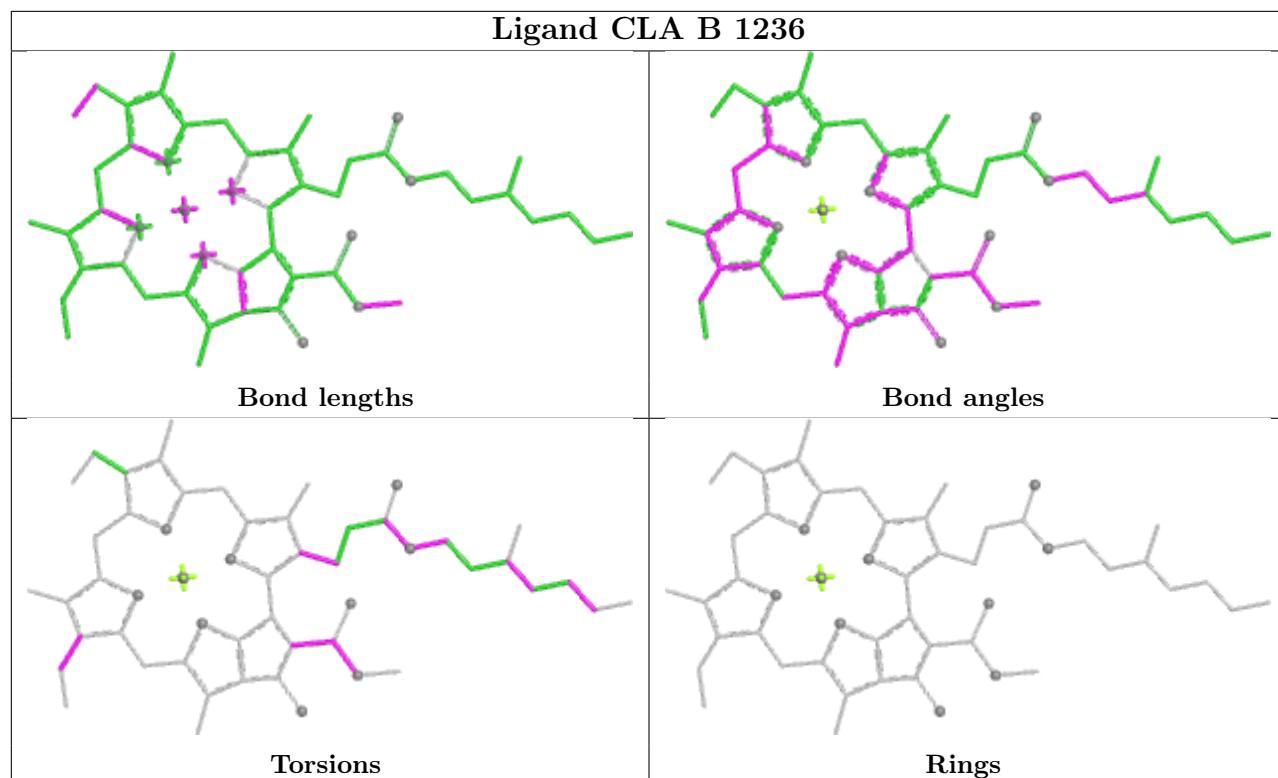
Ligand LHG 6 801

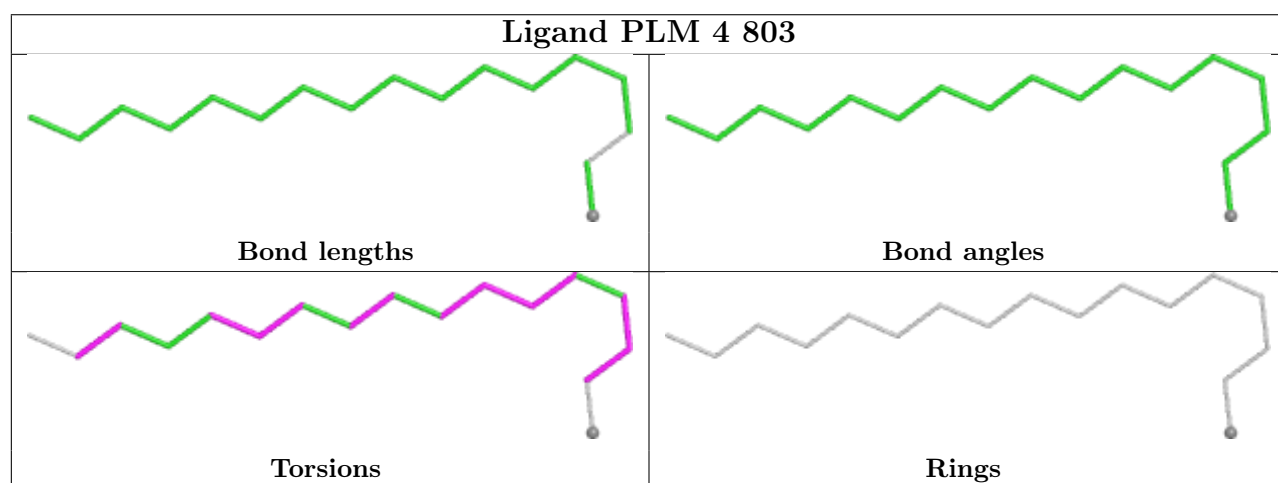
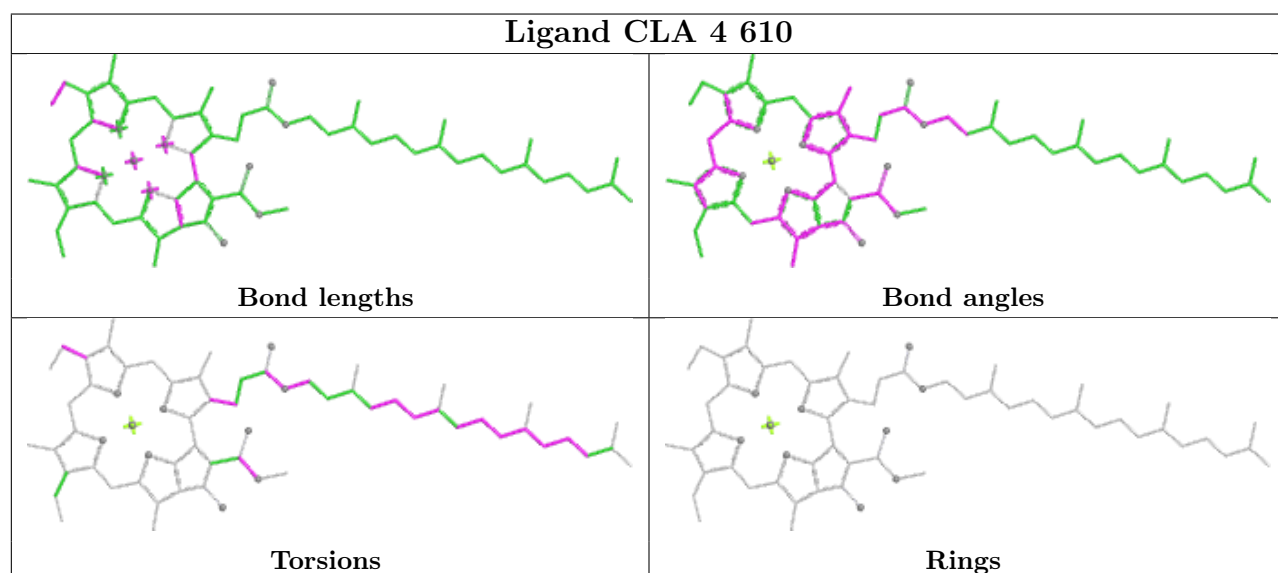
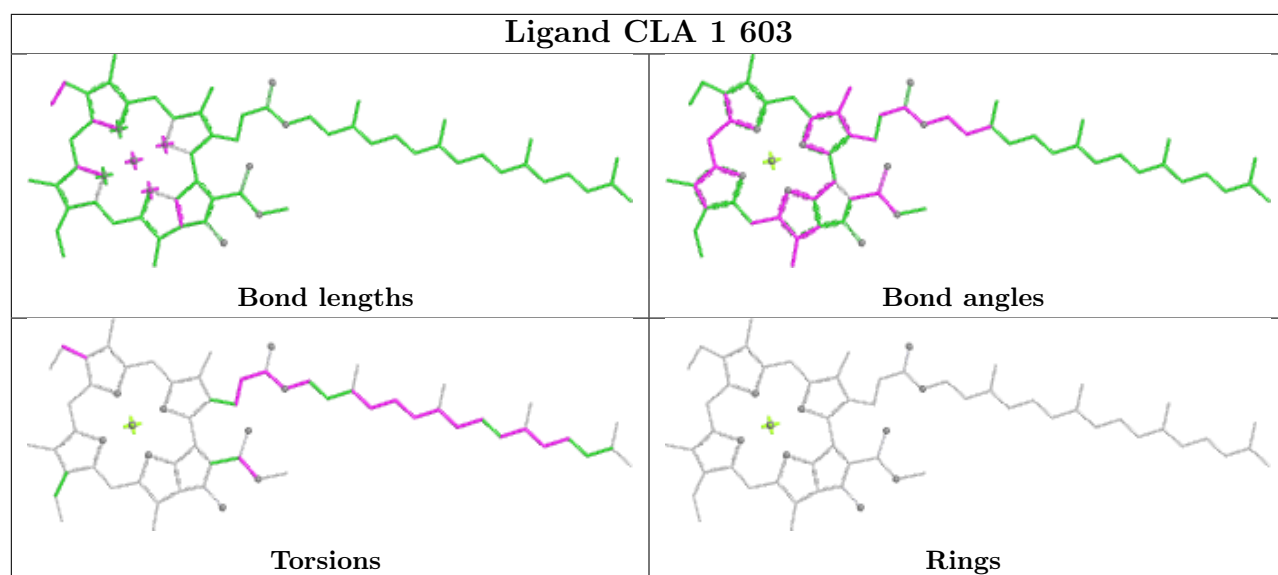


Ligand CHL 4 609

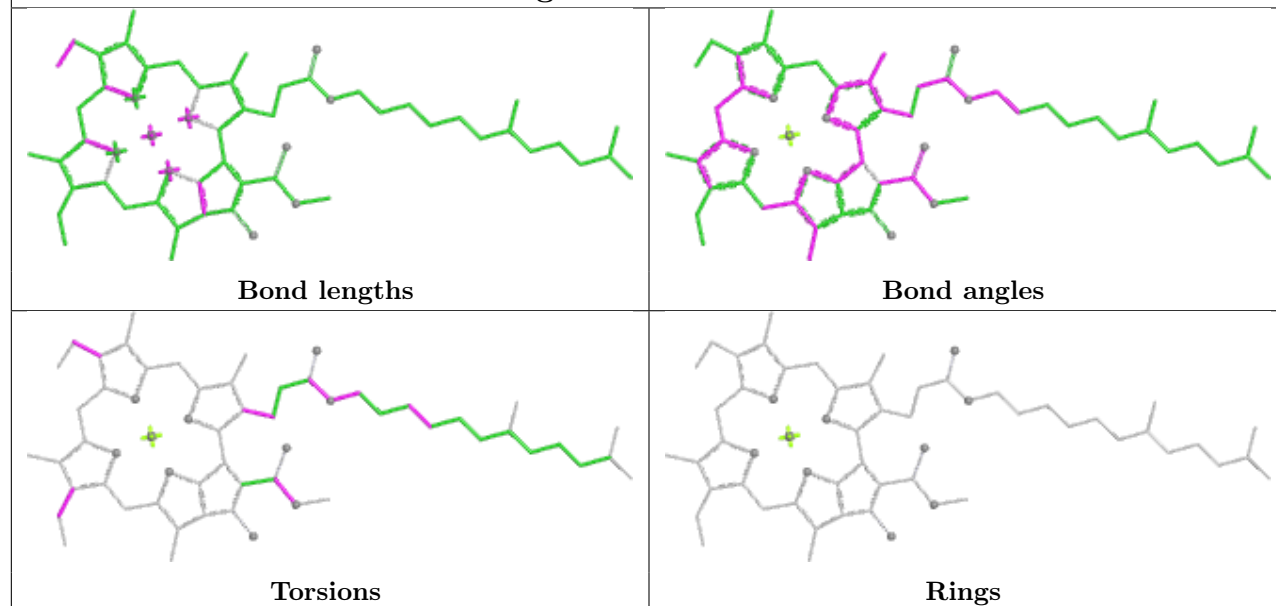




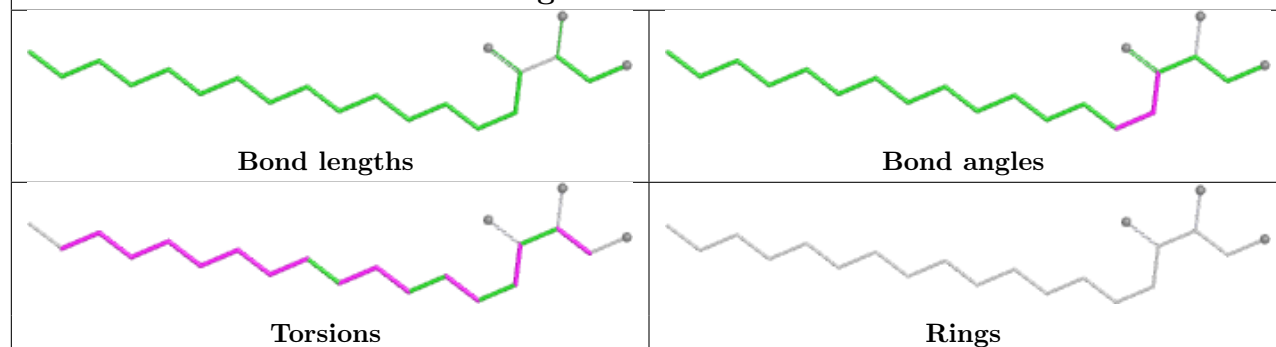




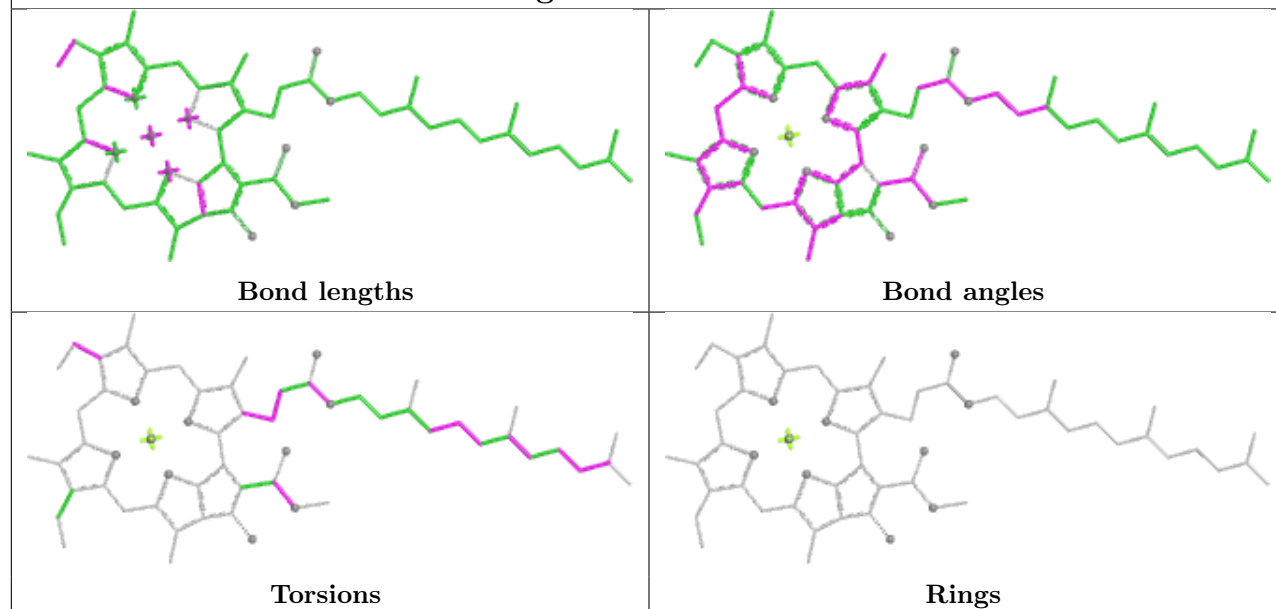
Ligand CLA 7 607



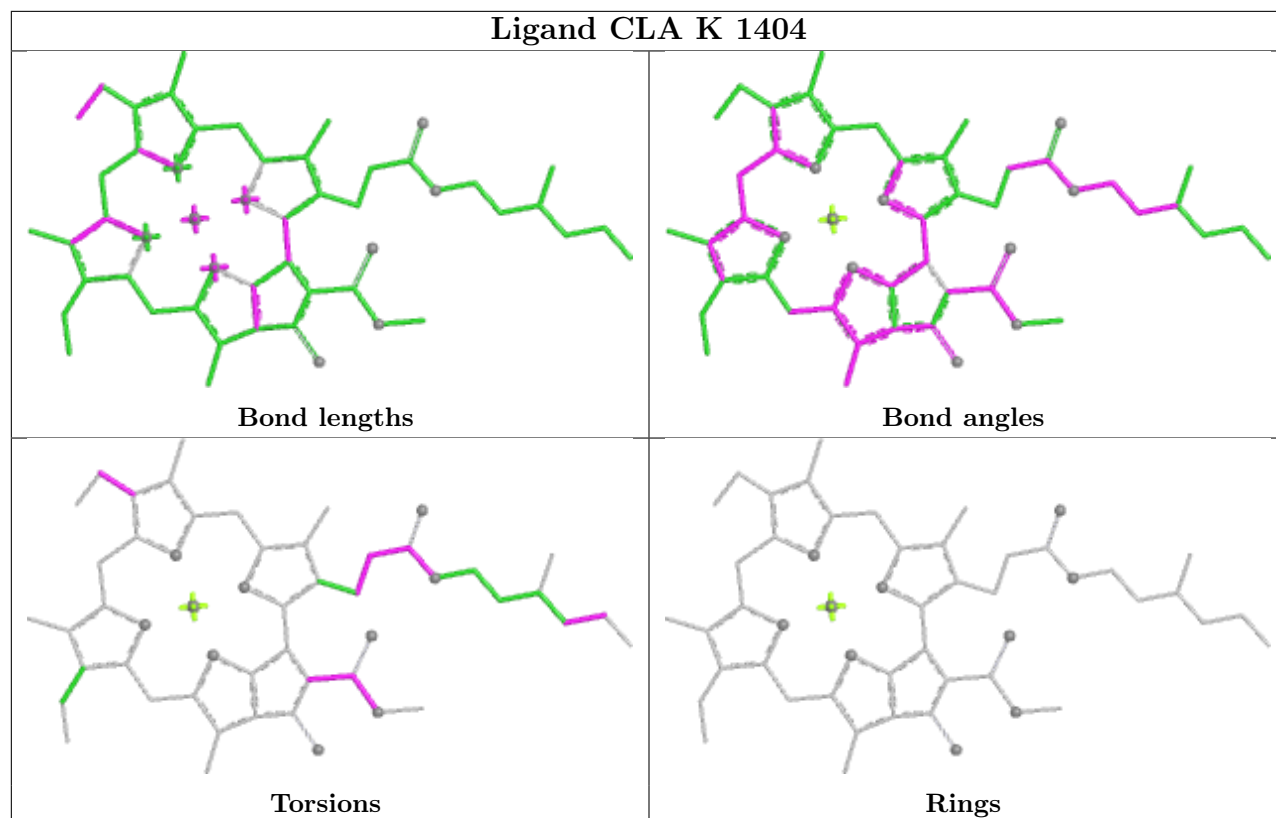
Ligand SPH 6 806



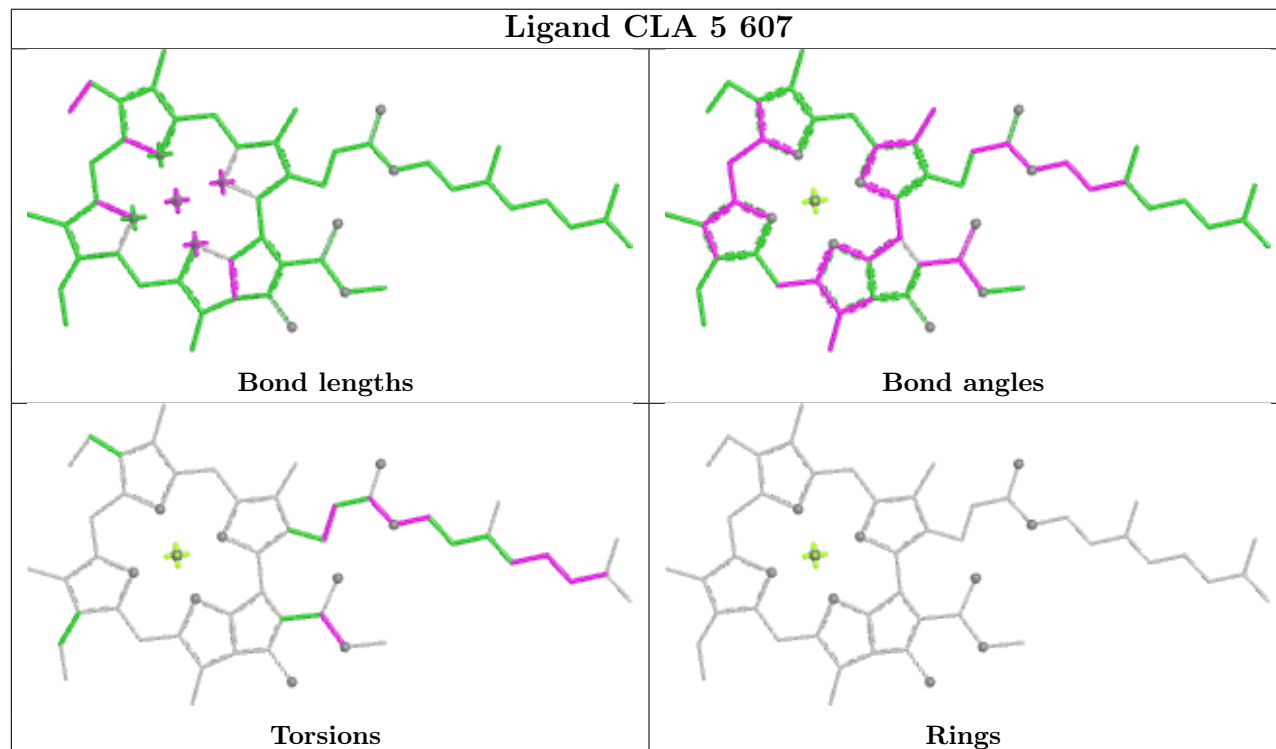
Ligand CLA 8 618



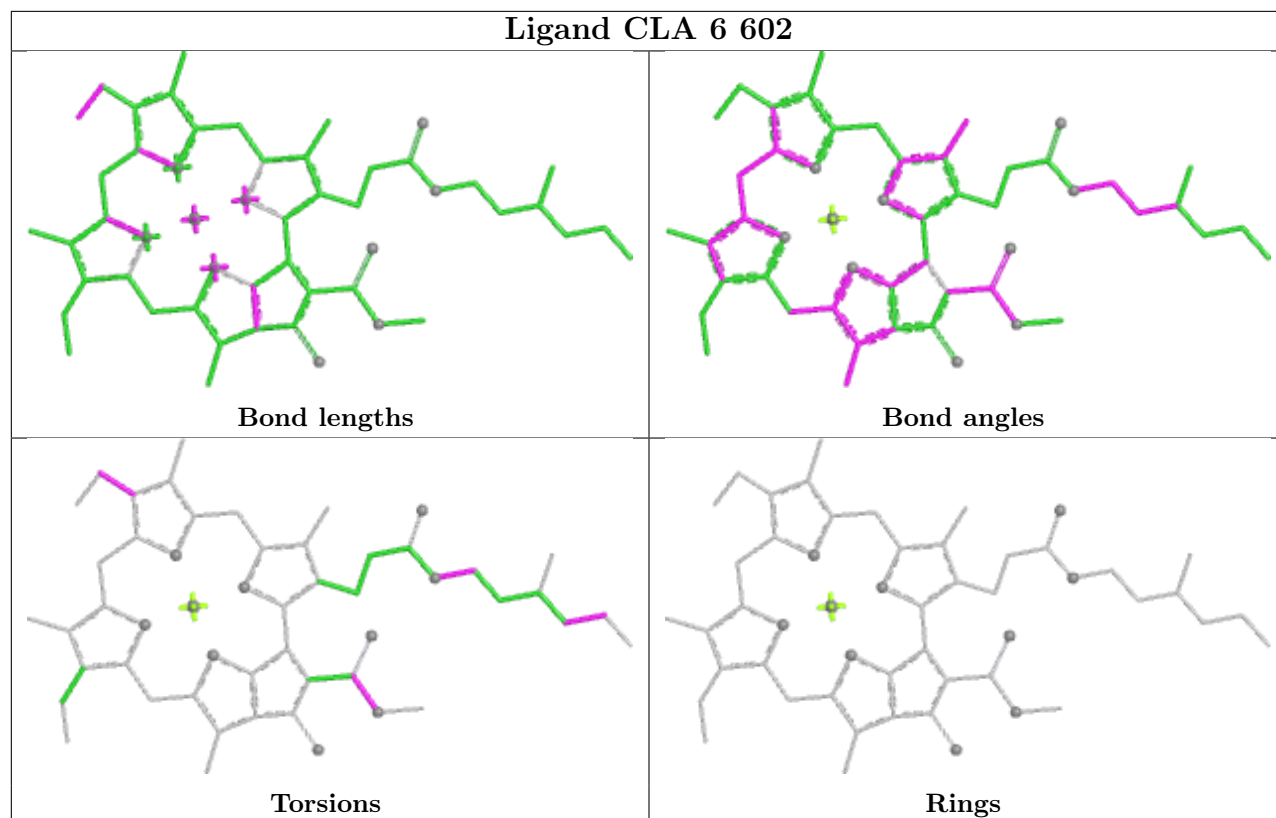
Ligand CLA K 1404



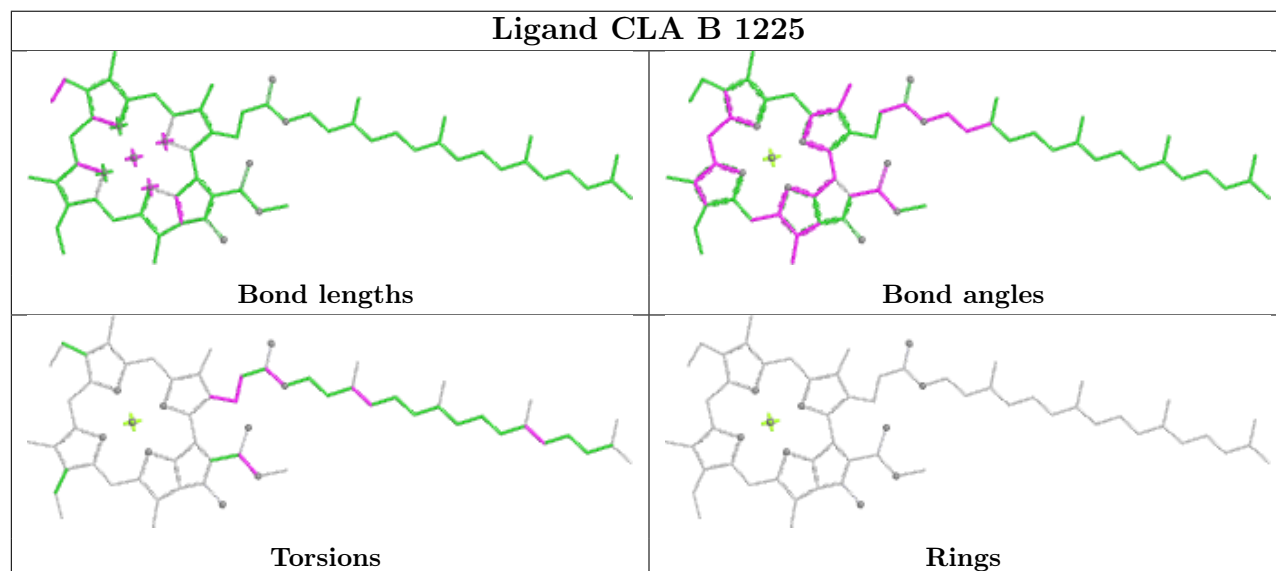
Ligand CLA 5 607

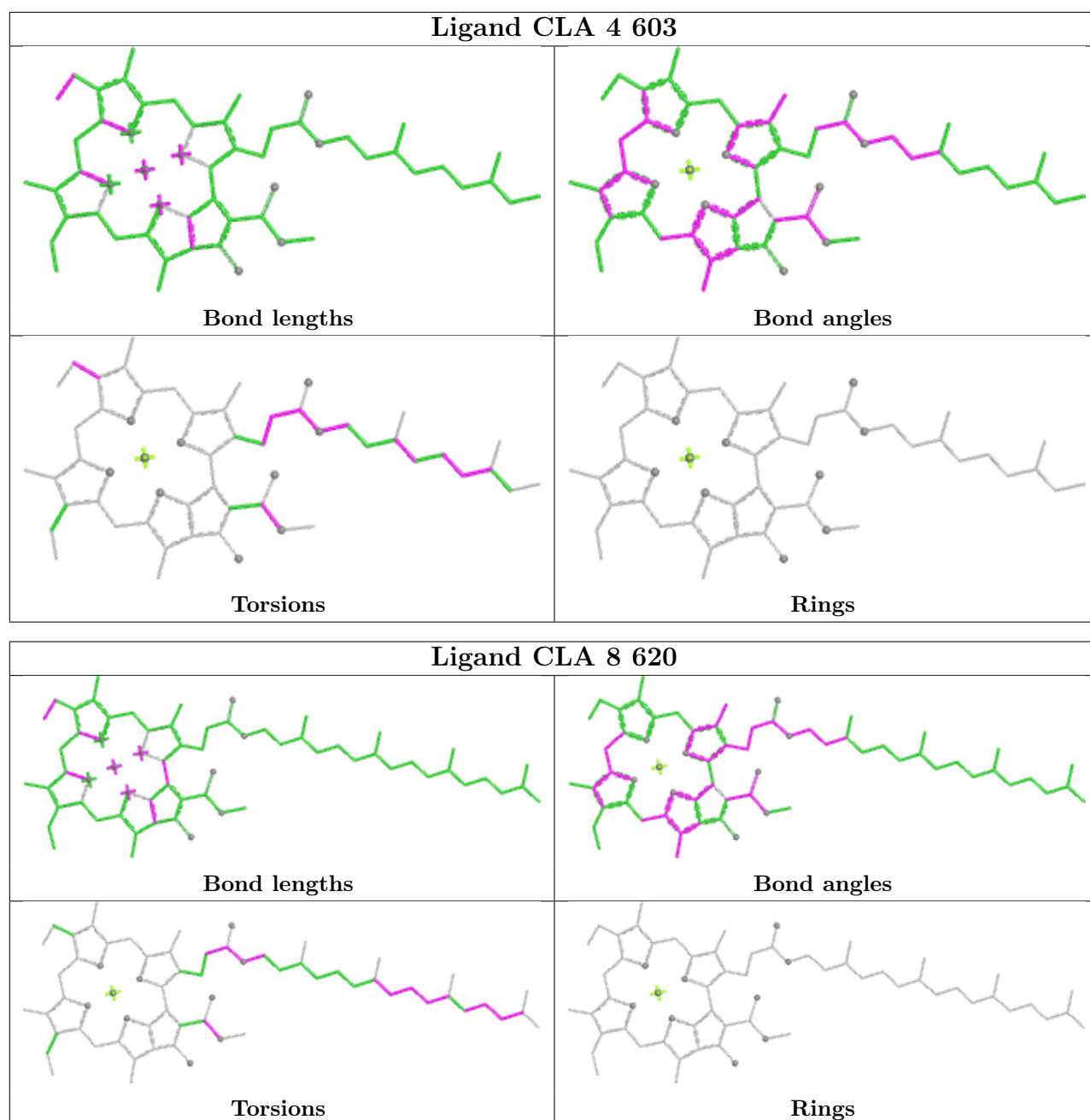


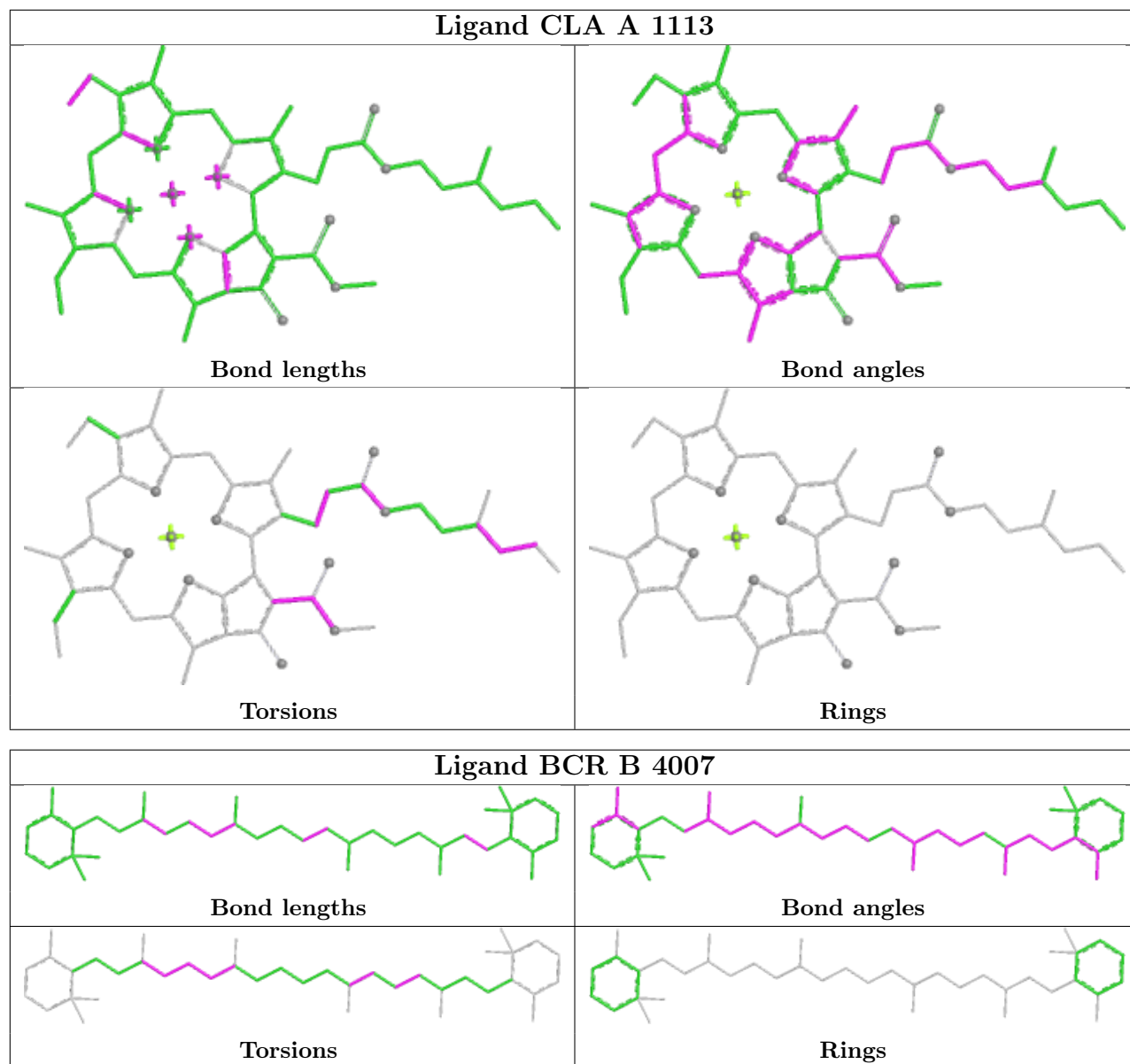
Ligand CLA 6 602



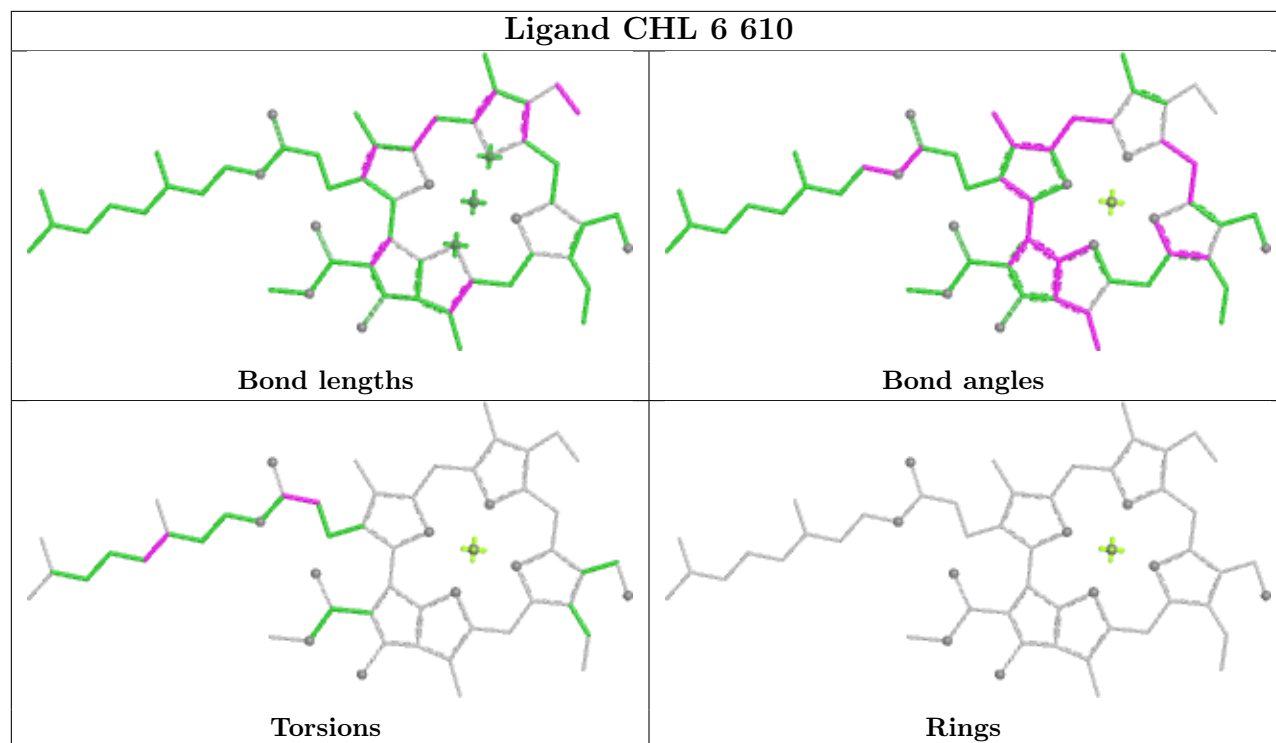
Ligand CLA B 1225



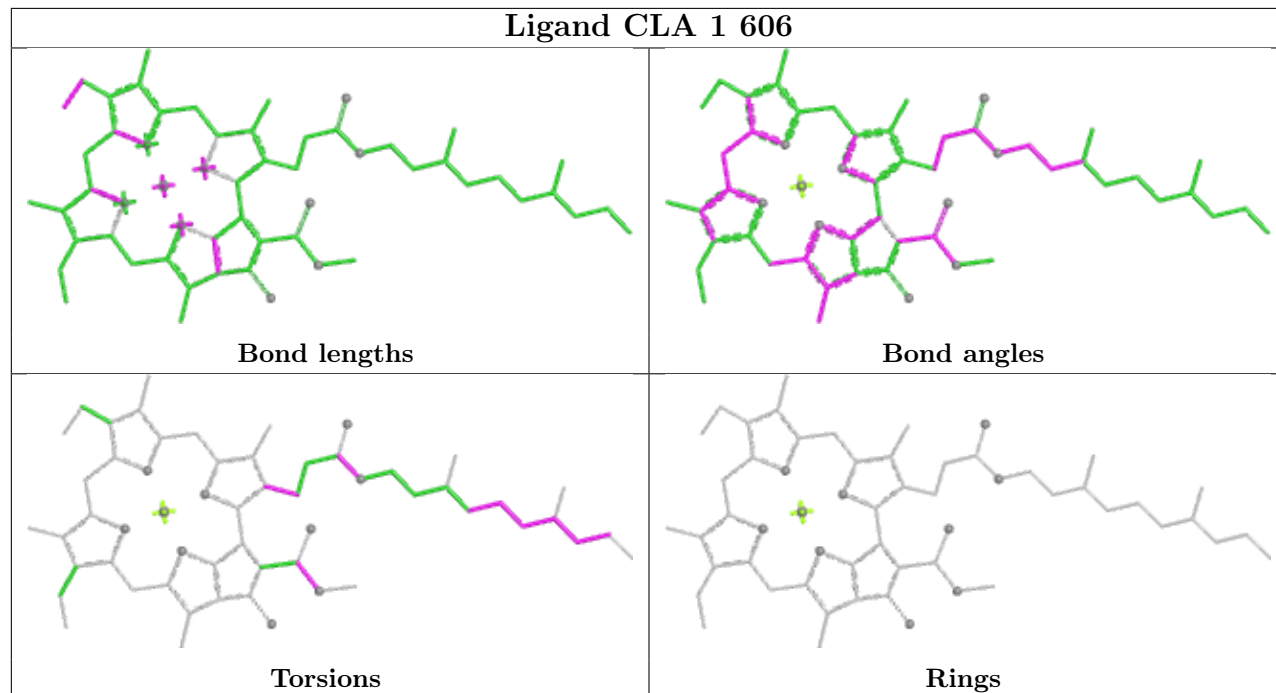


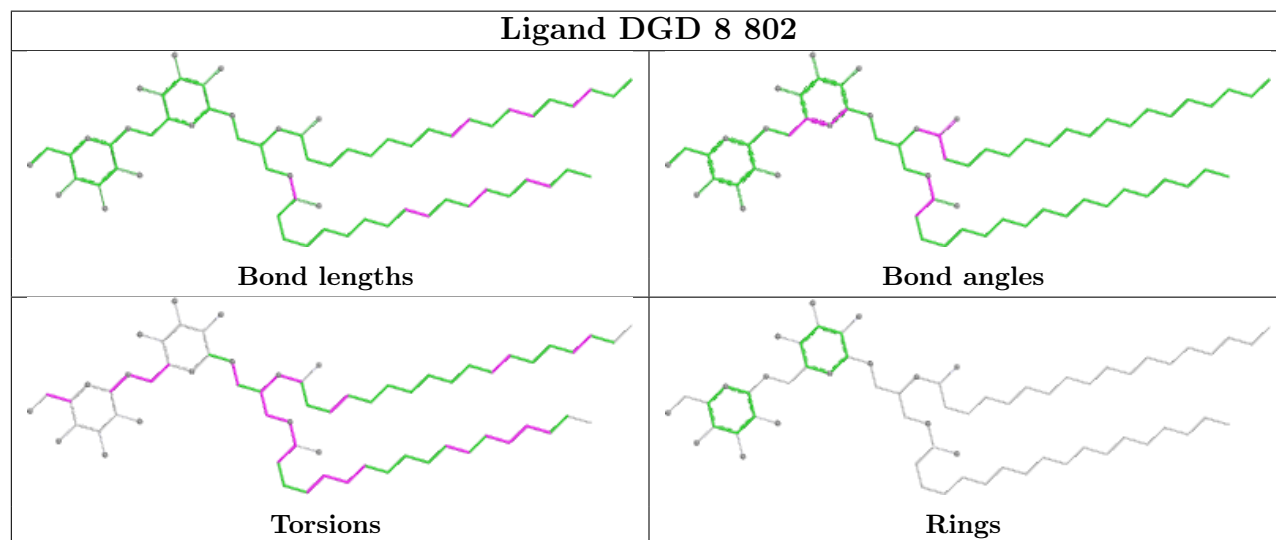
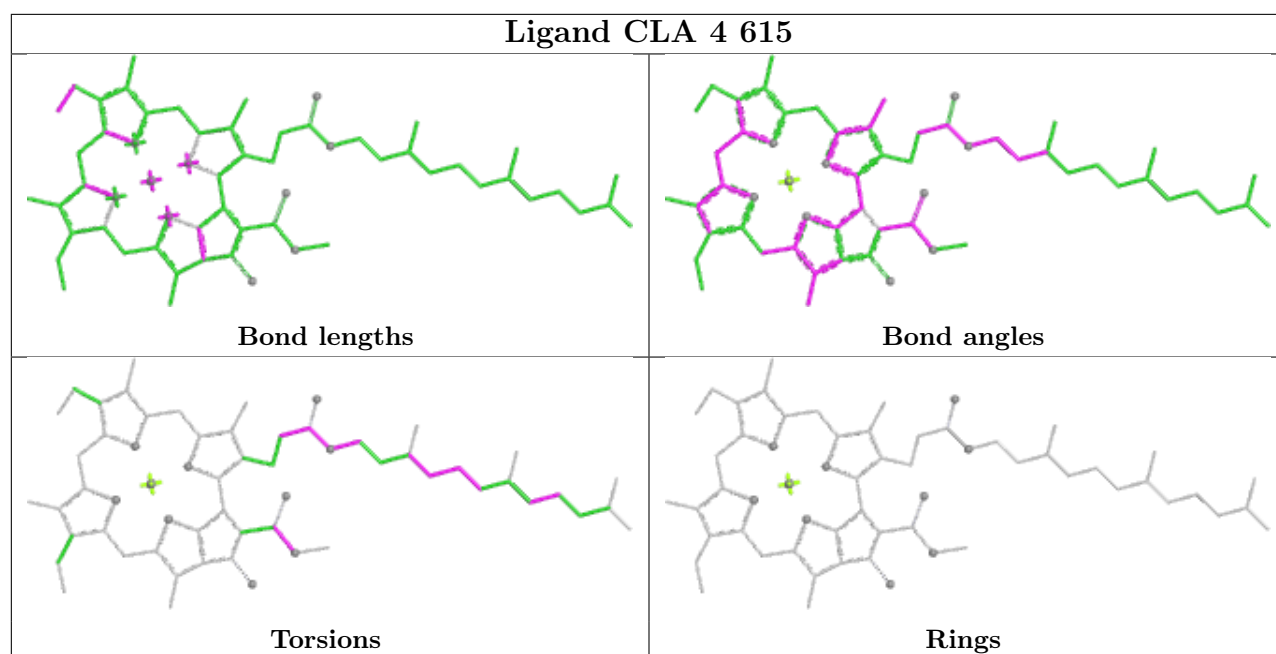


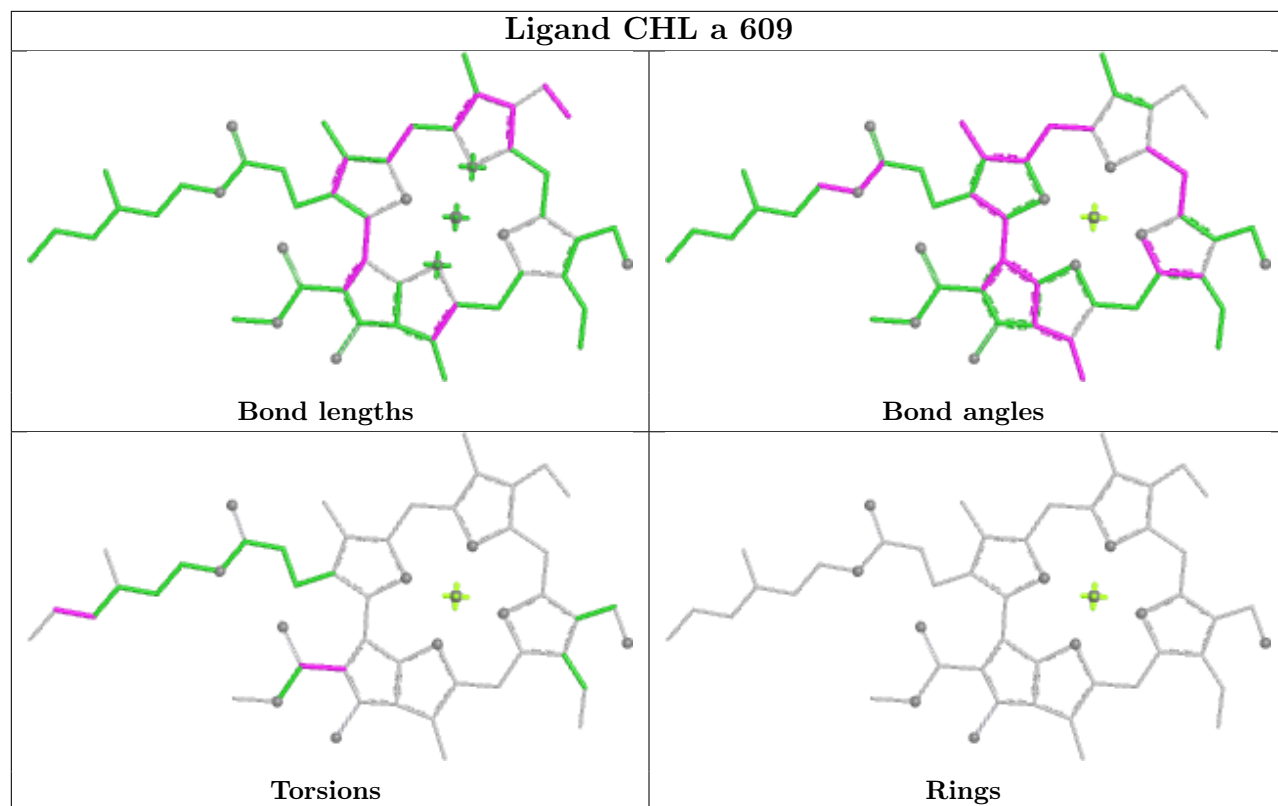
Ligand CHL 6 610



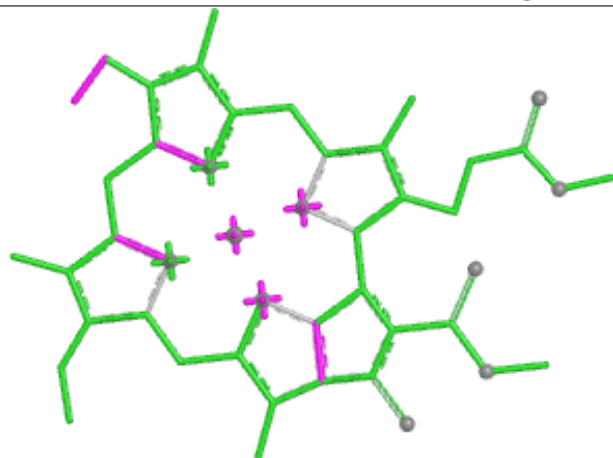
Ligand CLA 1 606



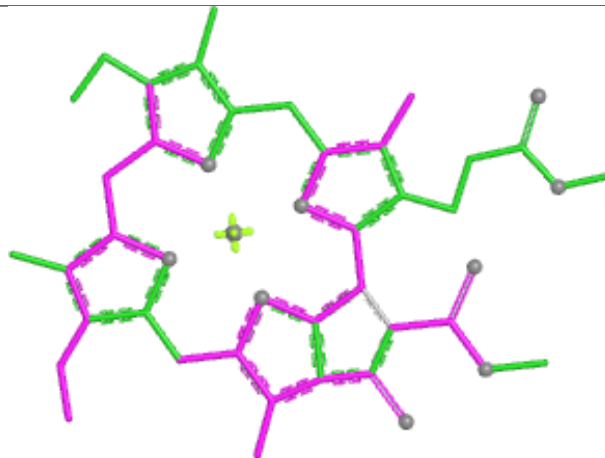




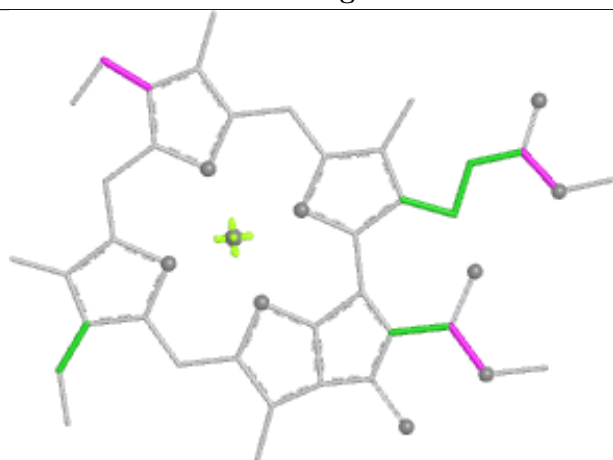
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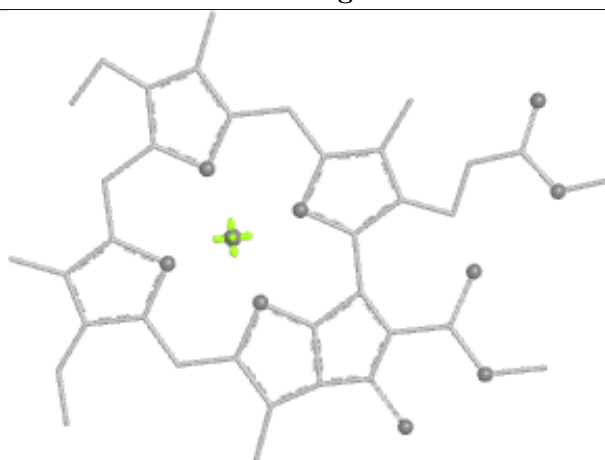
Bond lengths



Bond angles

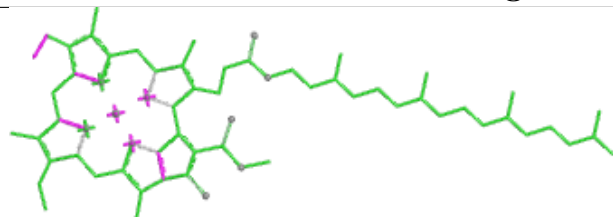


Torsions

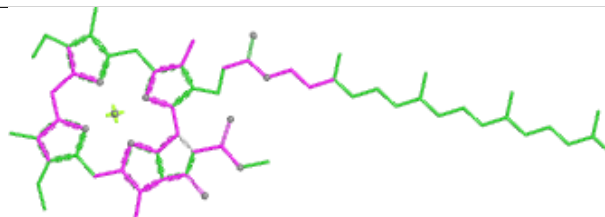


Rings

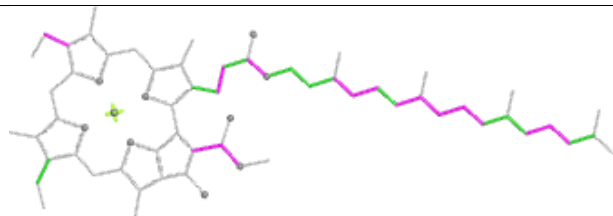
Ligand CLA A 1135



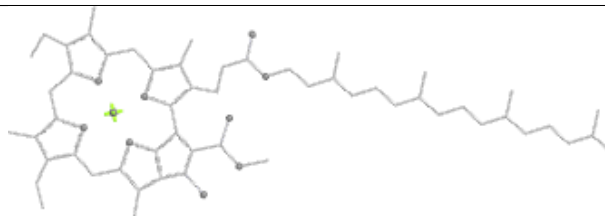
Bond lengths



Bond angles

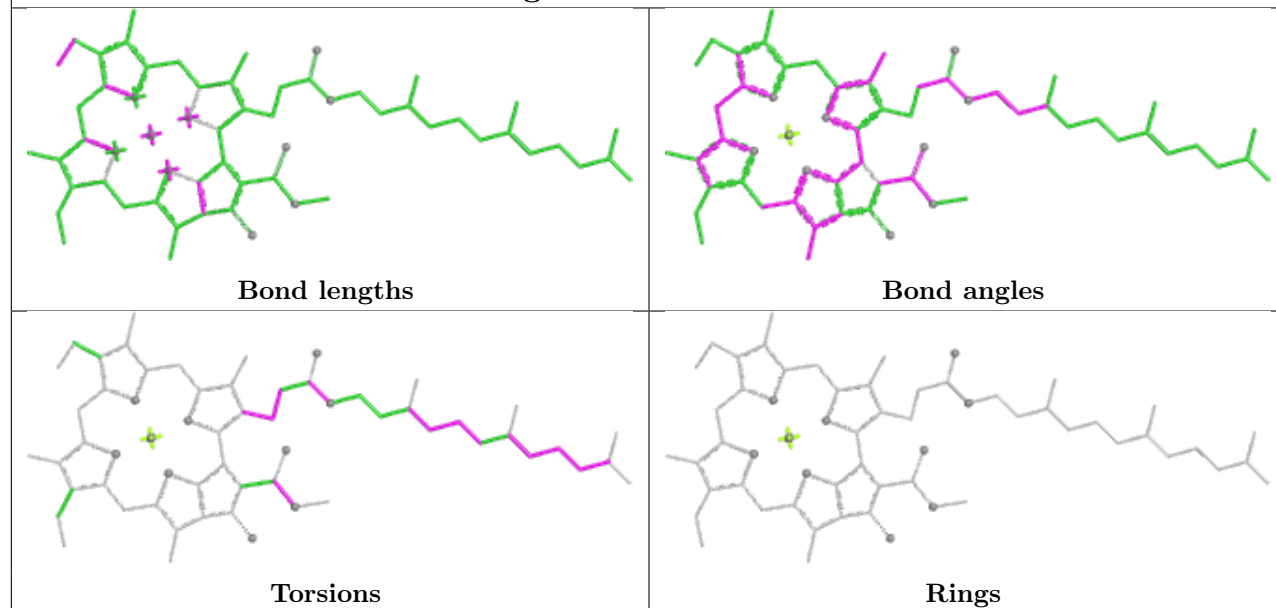


Torsions

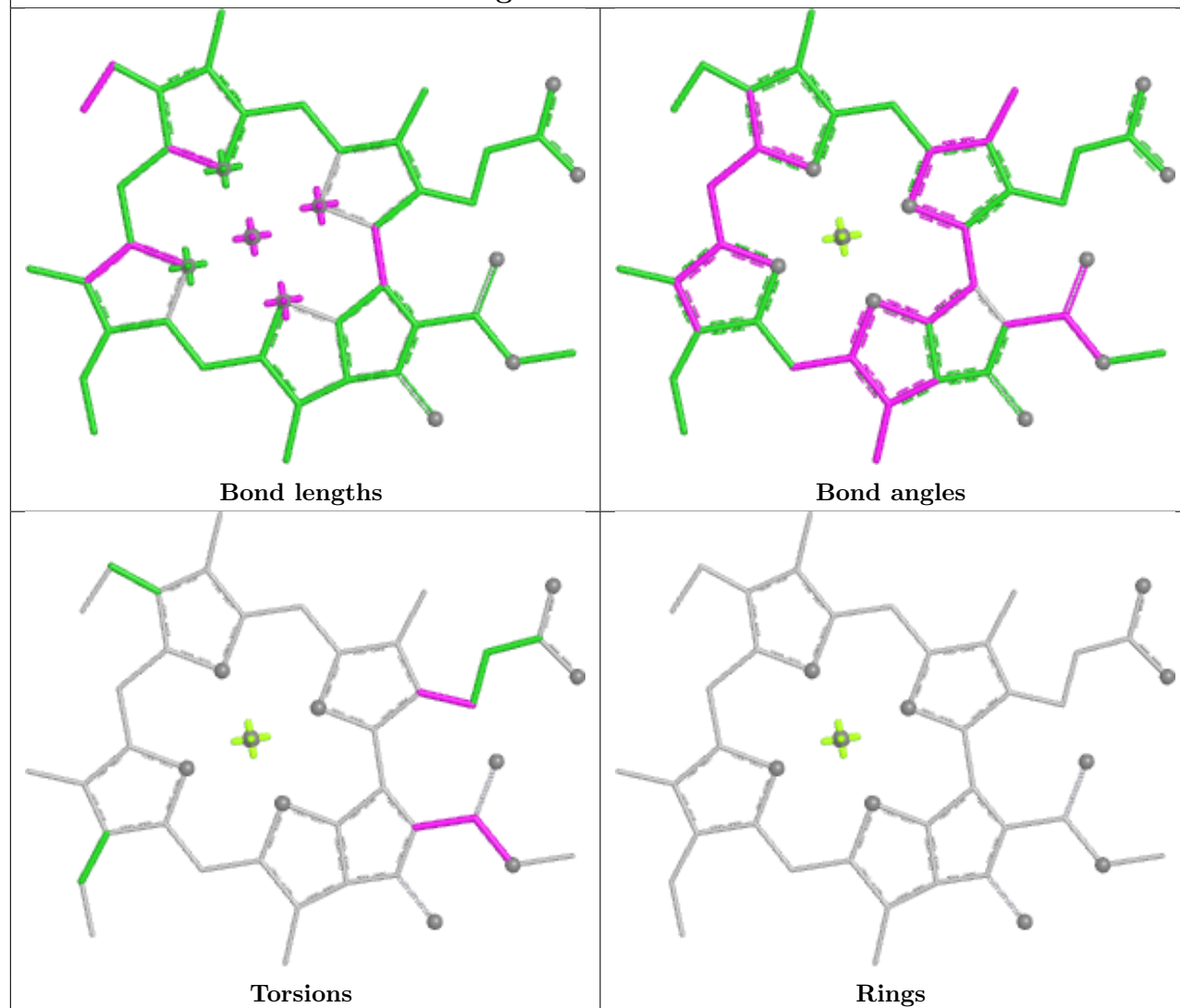


Rings

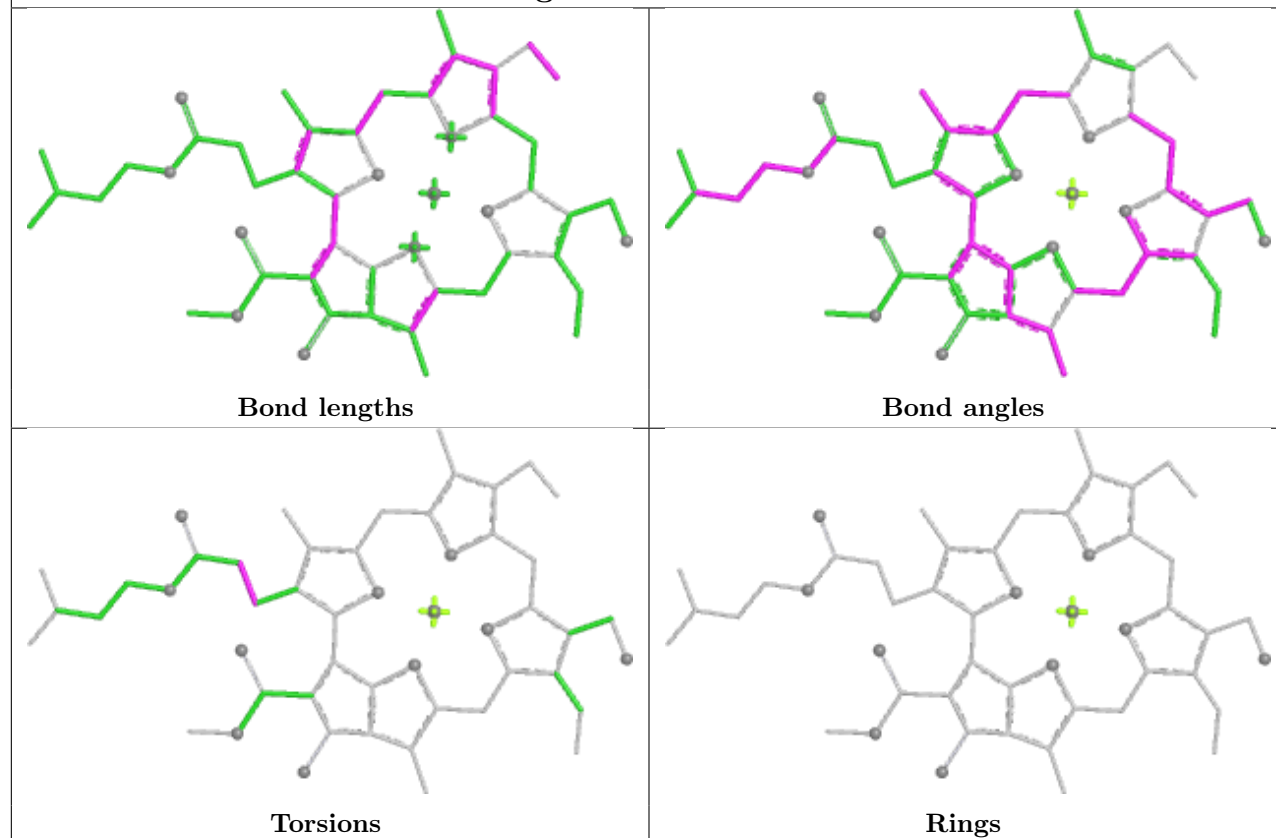
Ligand CLA B 1215



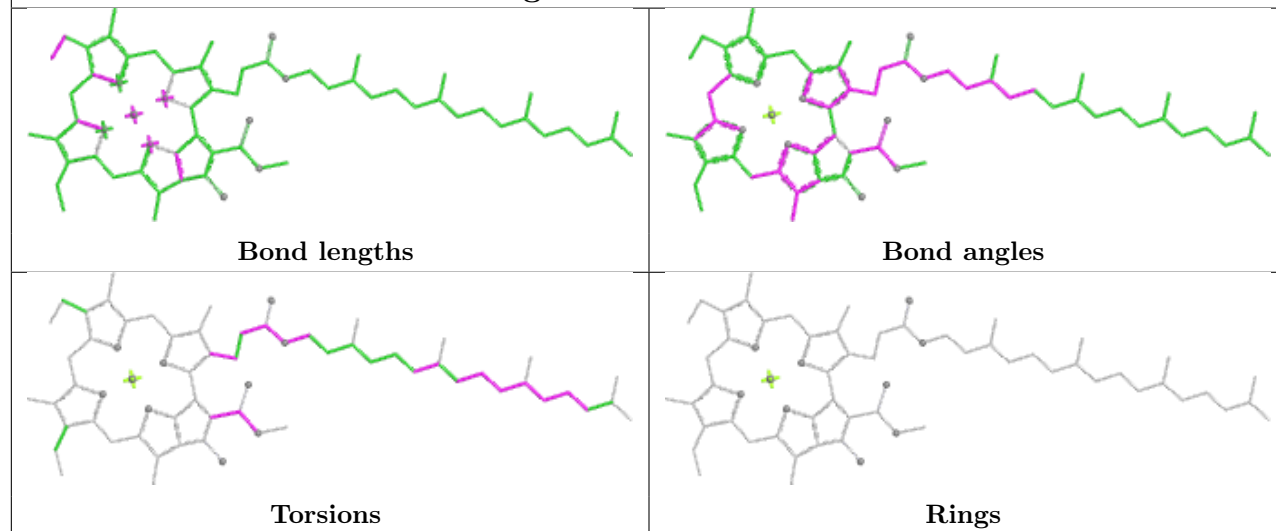
Ligand CLA 5 608

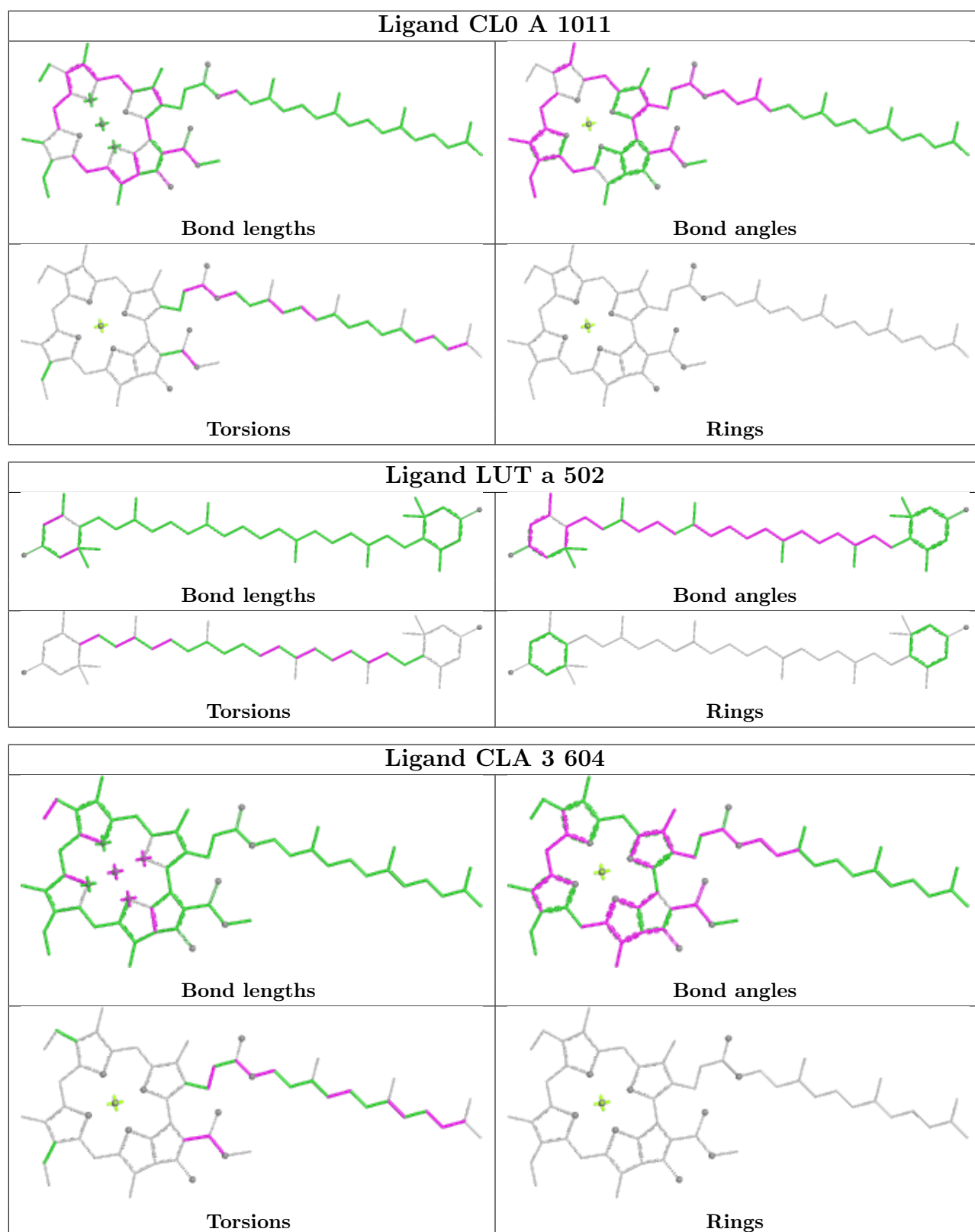


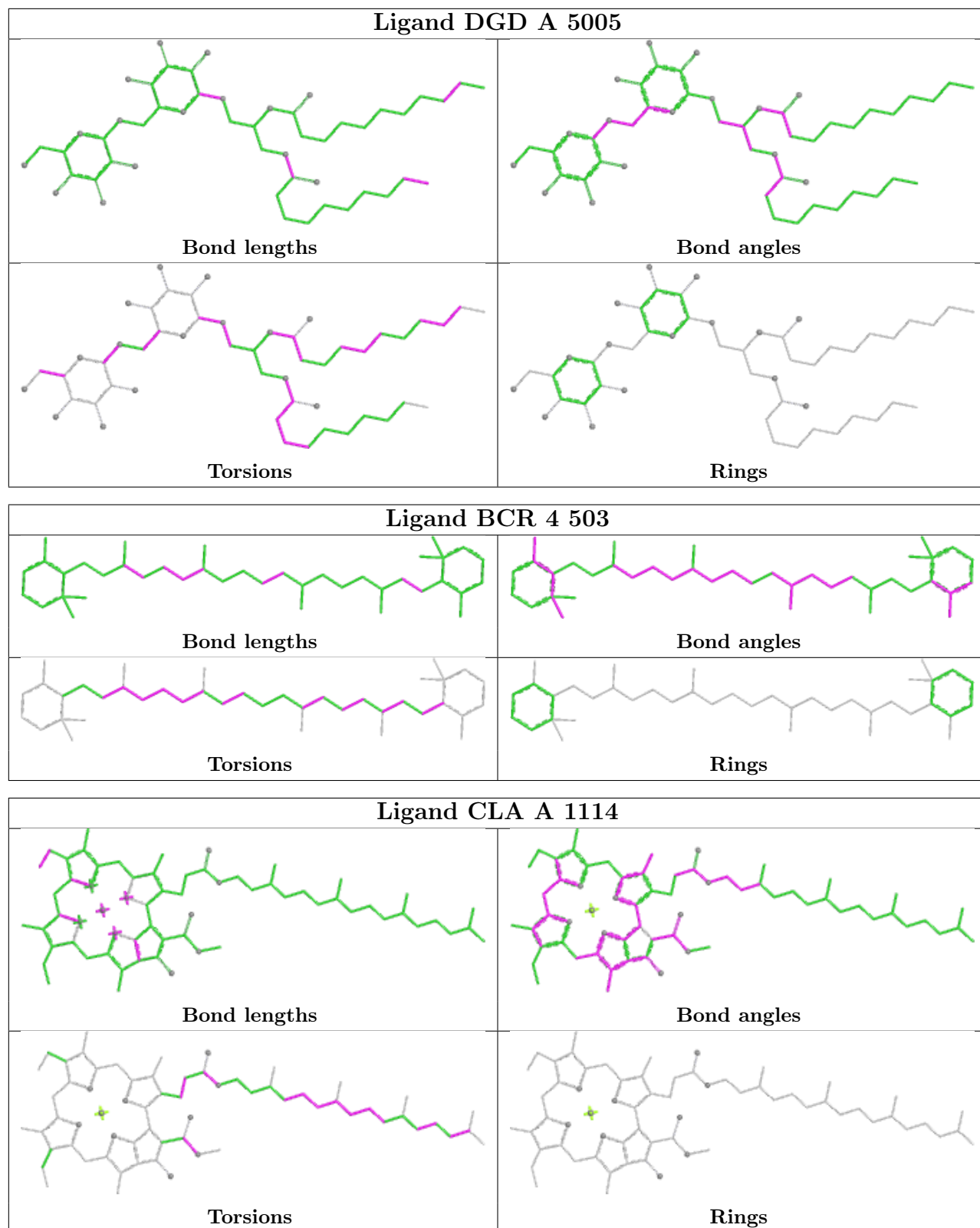
Ligand CHL 8 613



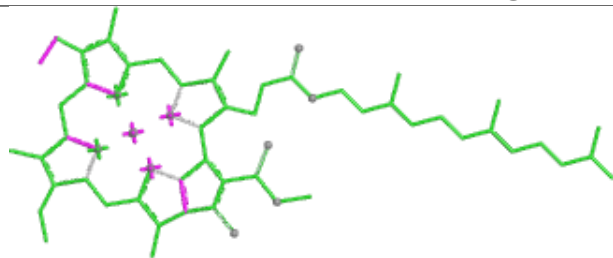
Ligand CLA B 1210



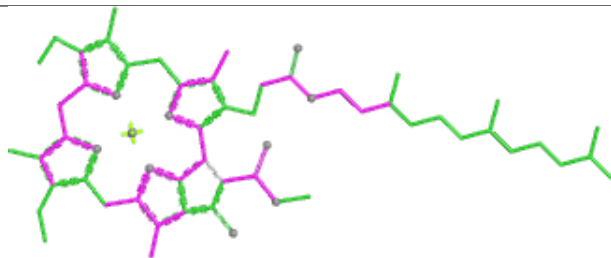




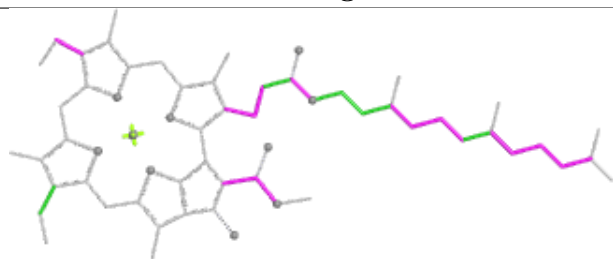
Ligand CLA A 1134



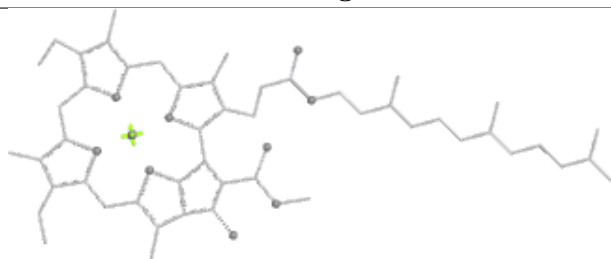
Bond lengths



Bond angles

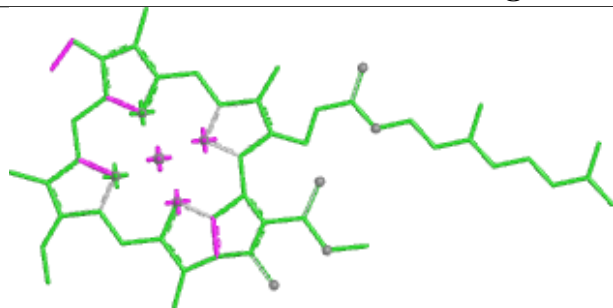


Torsions

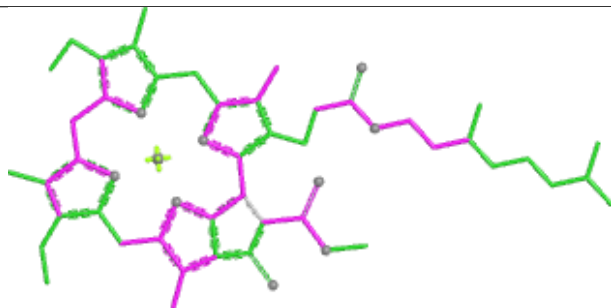


Rings

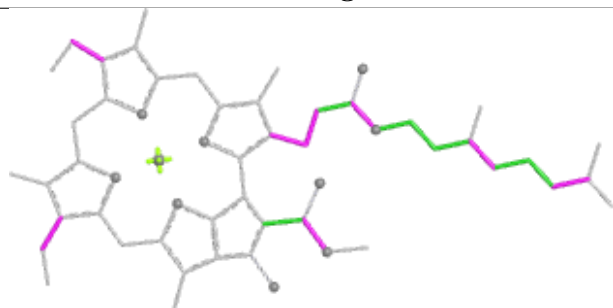
Ligand CLA A 1118



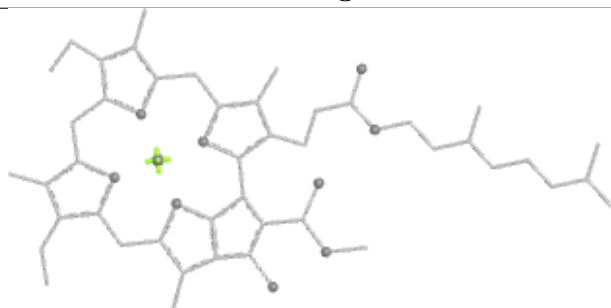
Bond lengths



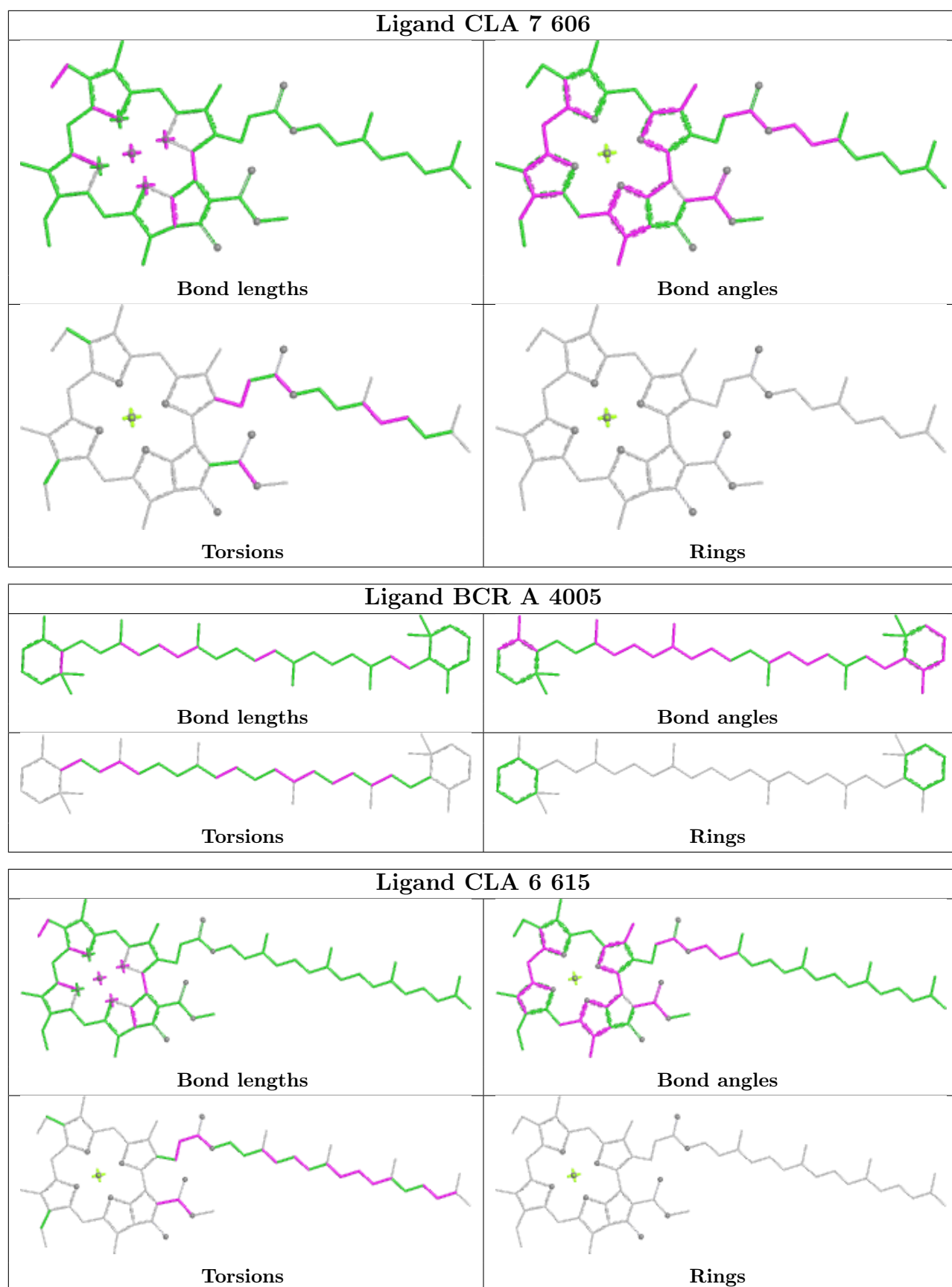
Bond angles

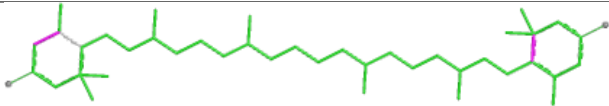
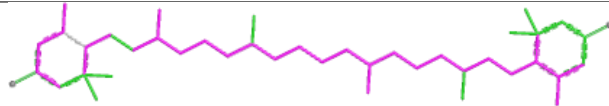
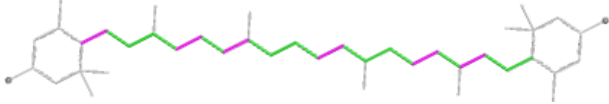
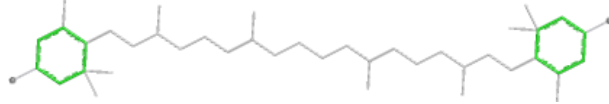


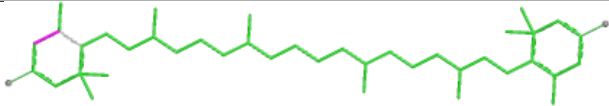
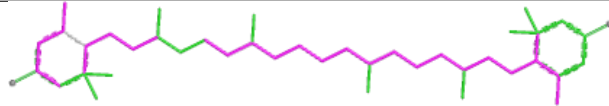
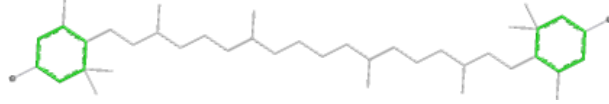
Torsions

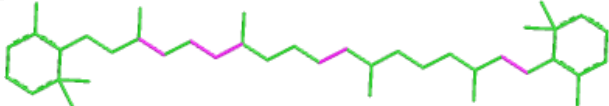
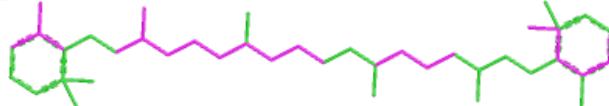
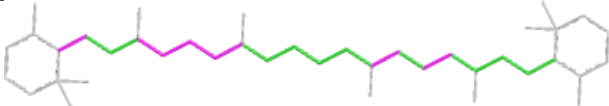
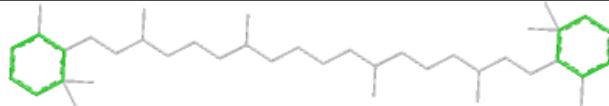


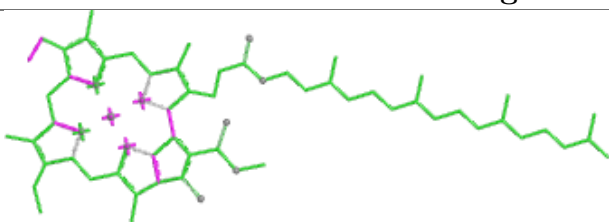
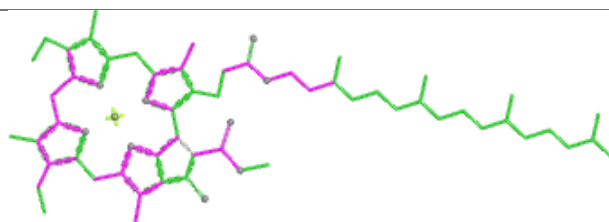
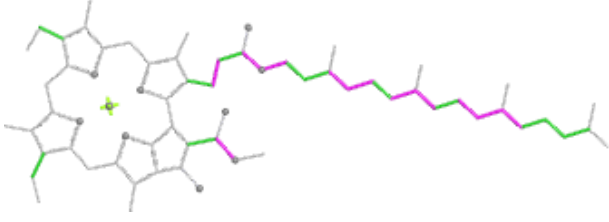
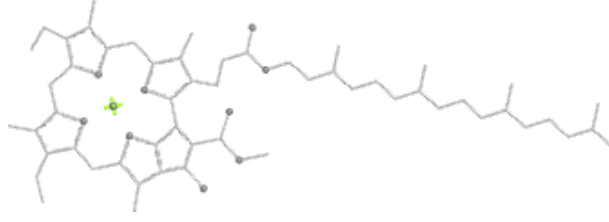
Rings

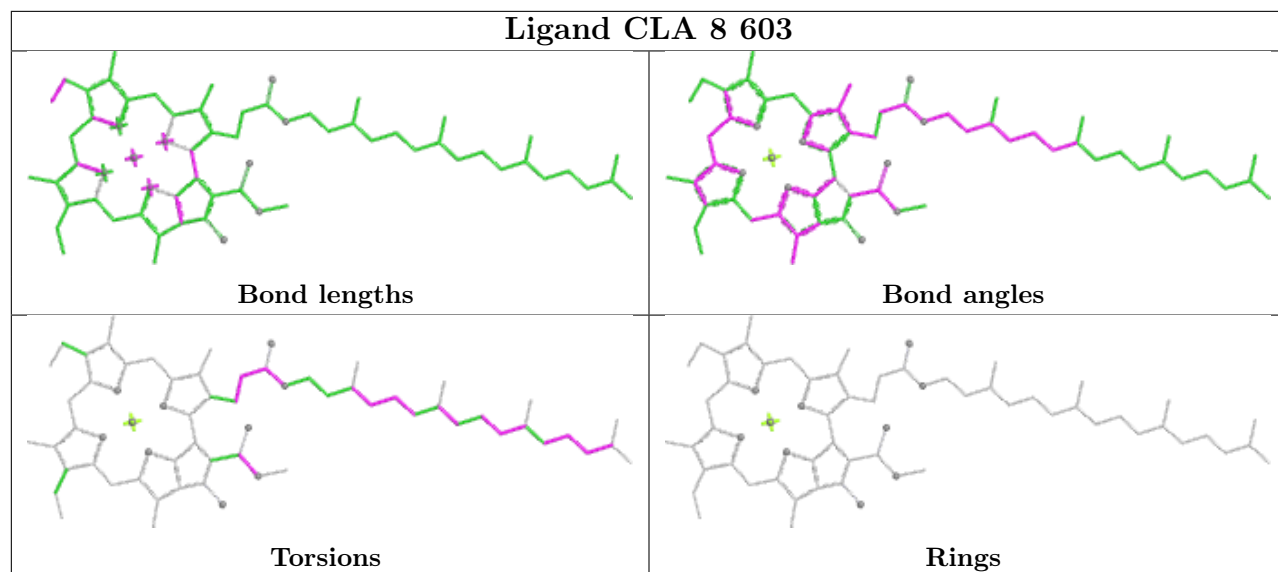
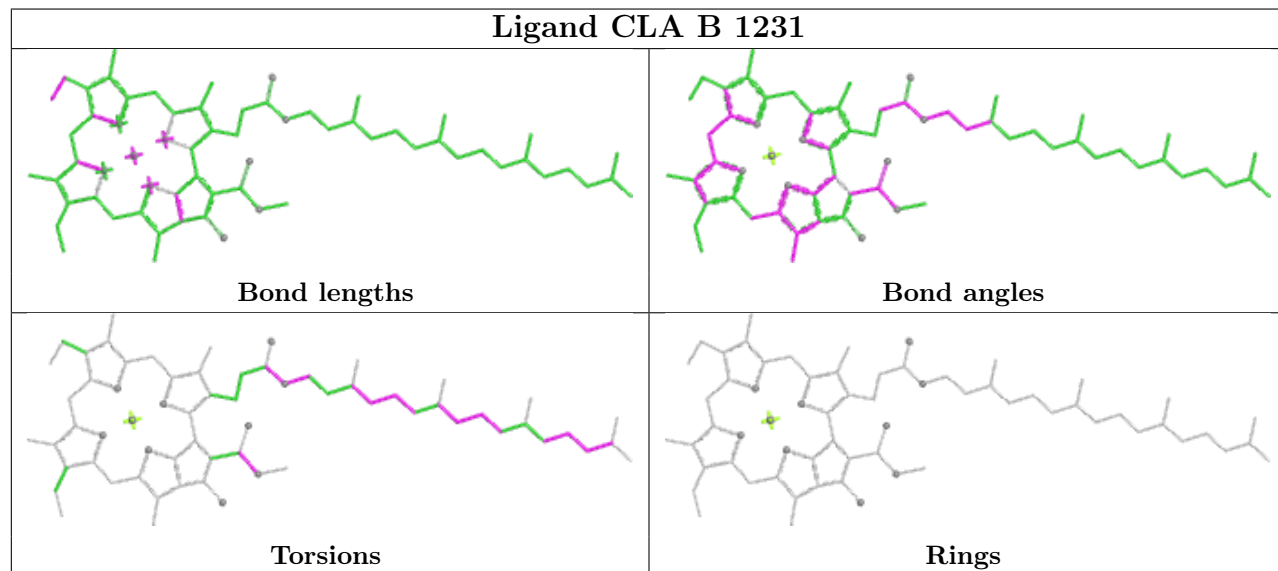


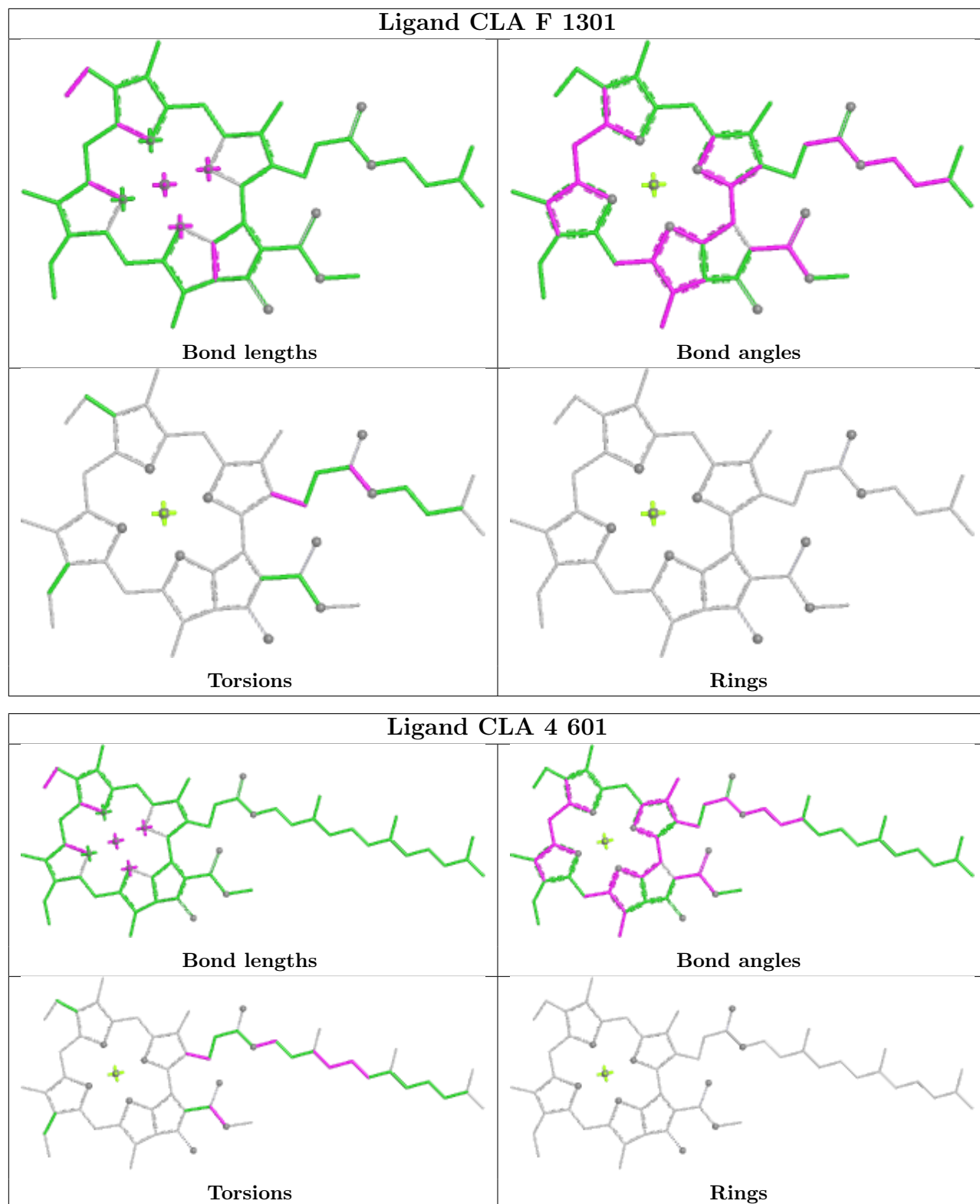
Ligand LUT 5 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 6 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

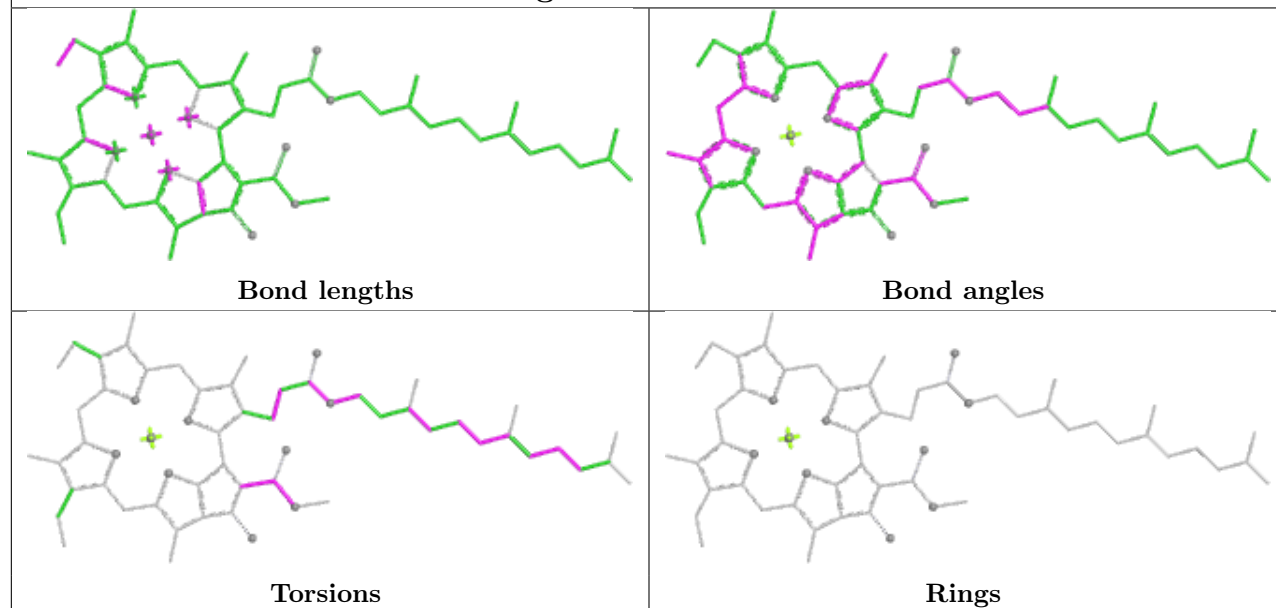
Ligand BCR A 4003	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 1237	
	
Bond lengths	Bond angles
	
Torsions	Rings

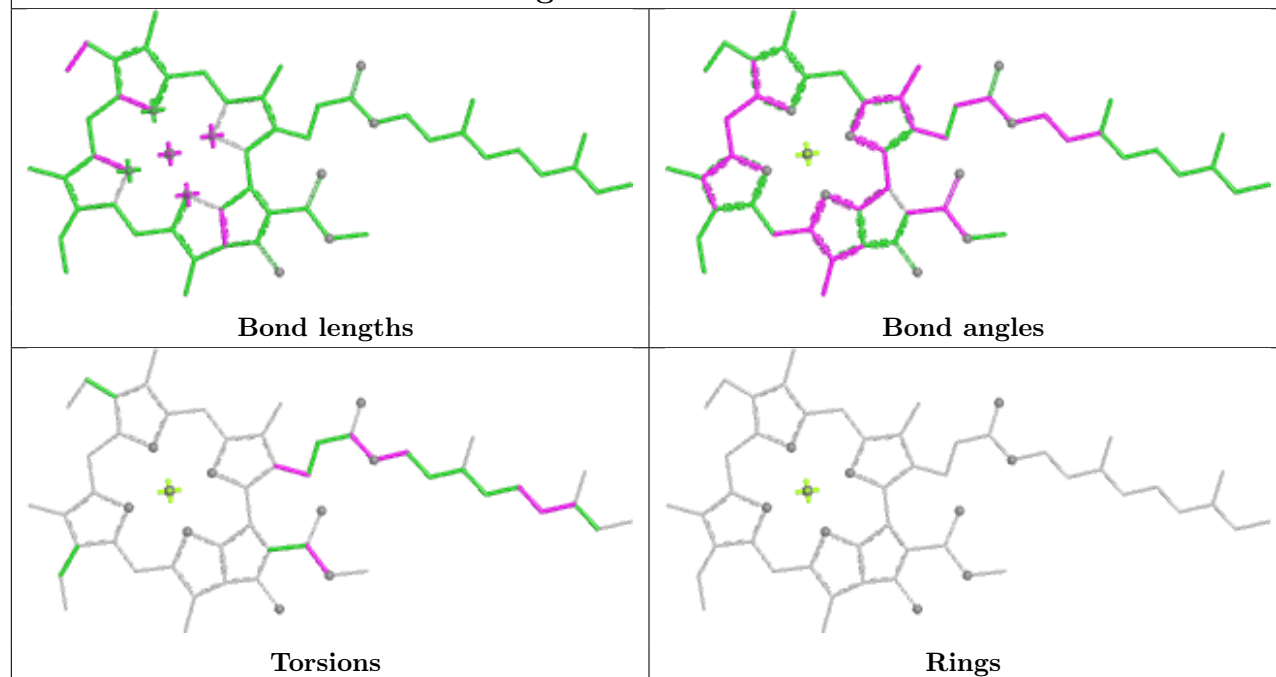
Ligand CLA 8 603**Ligand CLA B 1231**



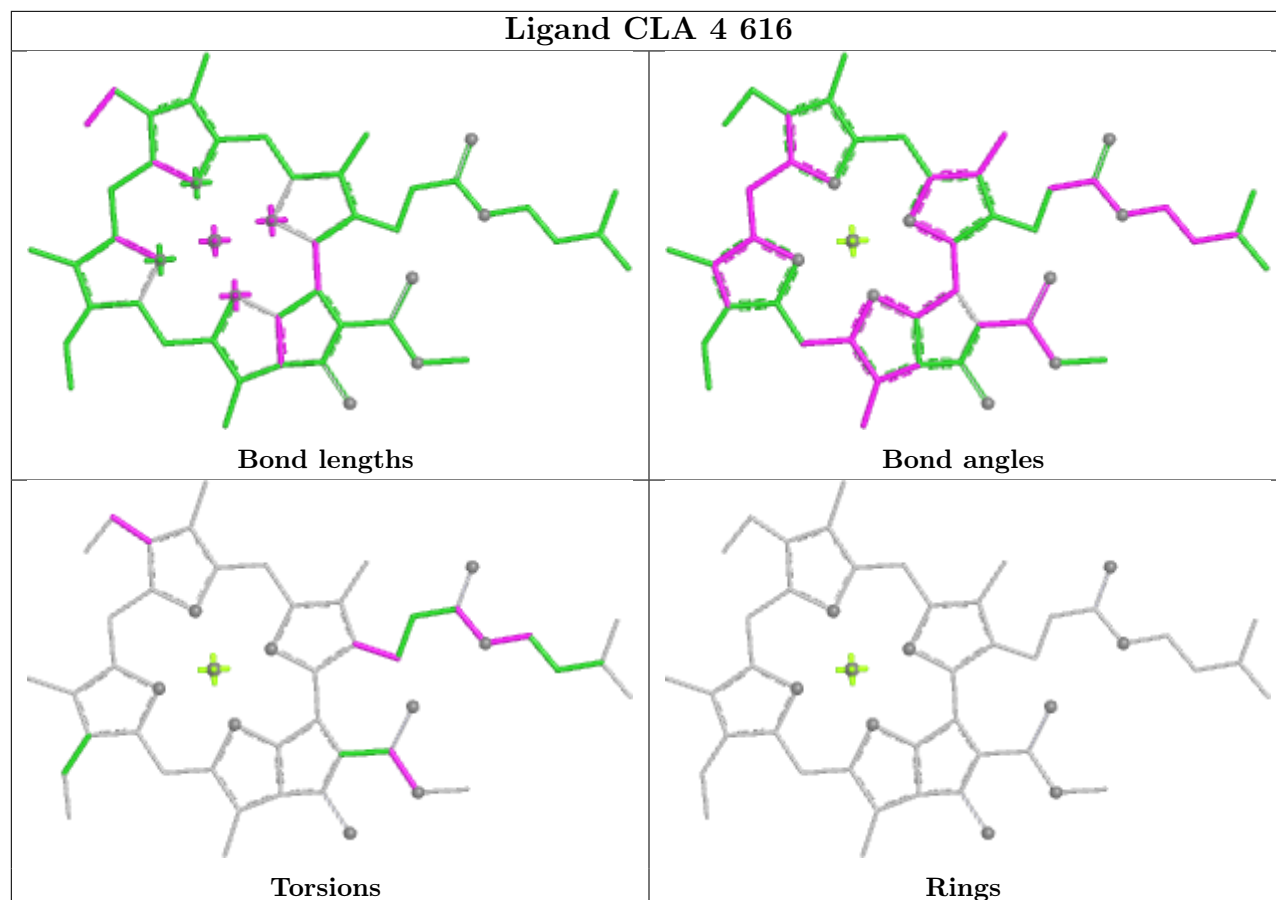
Ligand CLA 4 604



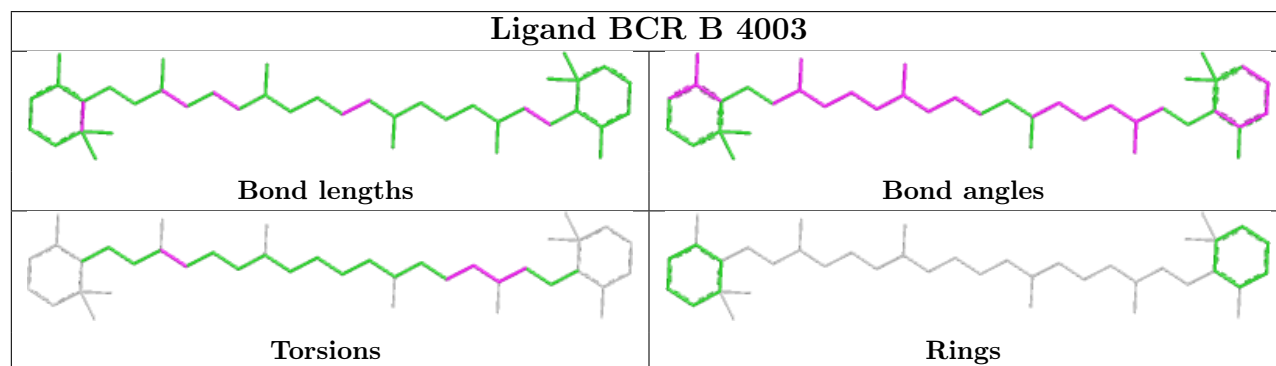
Ligand CLA 4 611



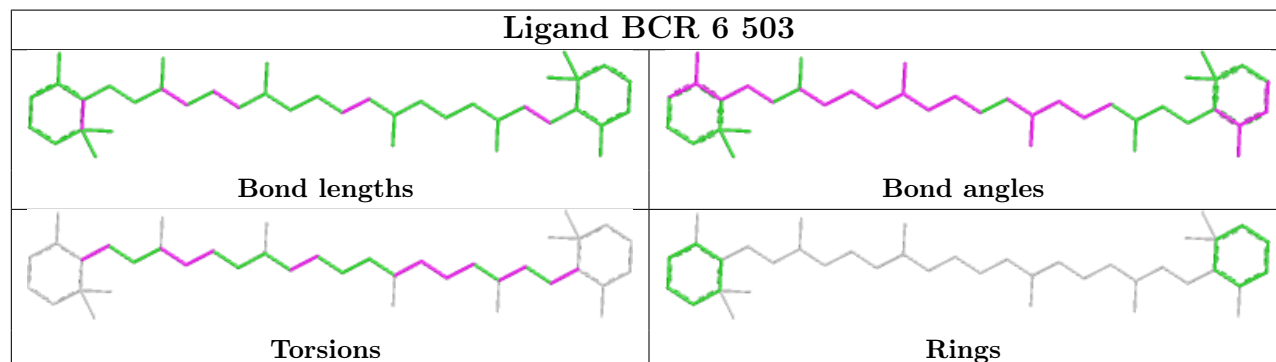
Ligand CLA 4 616

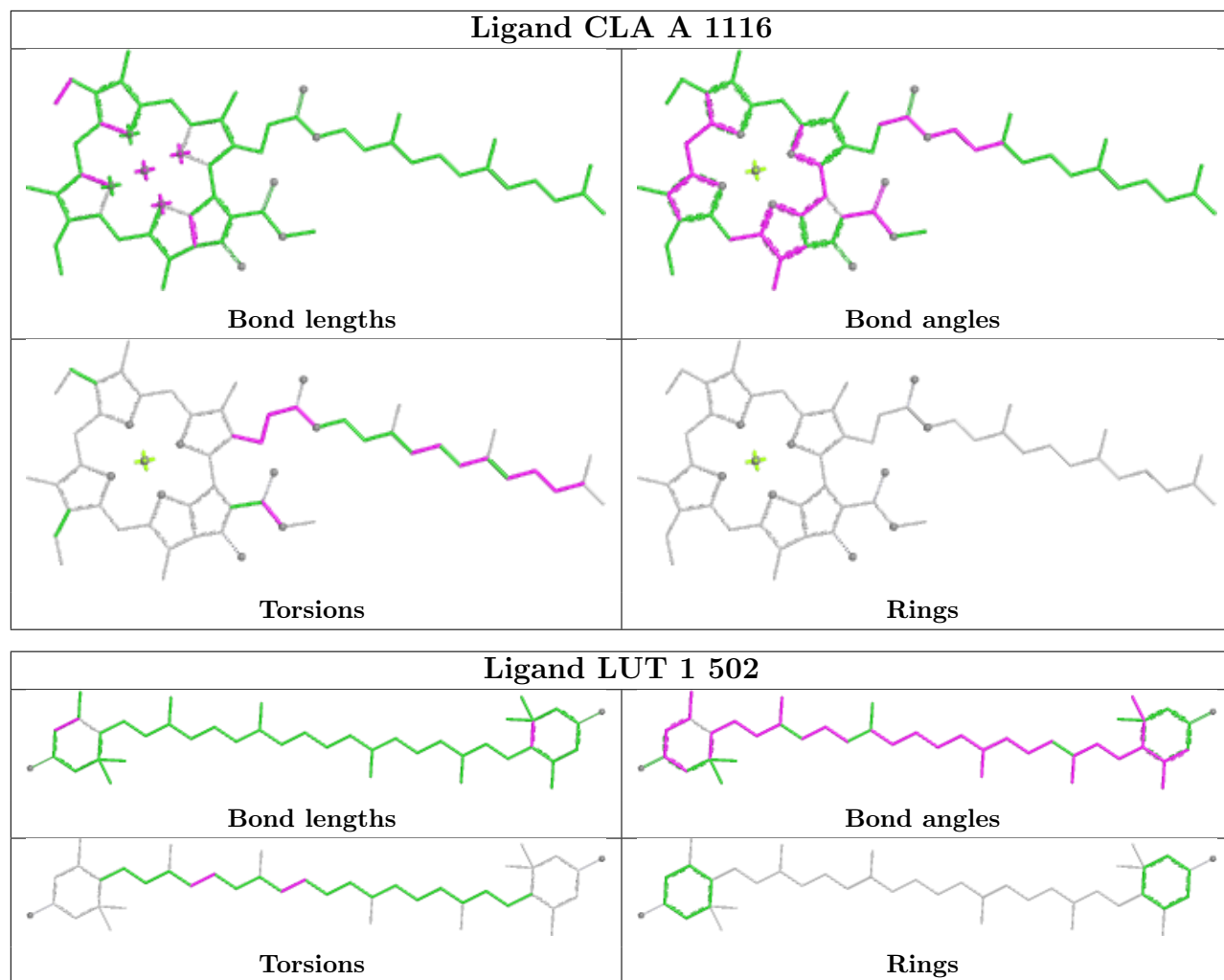


Ligand BCR B 4003

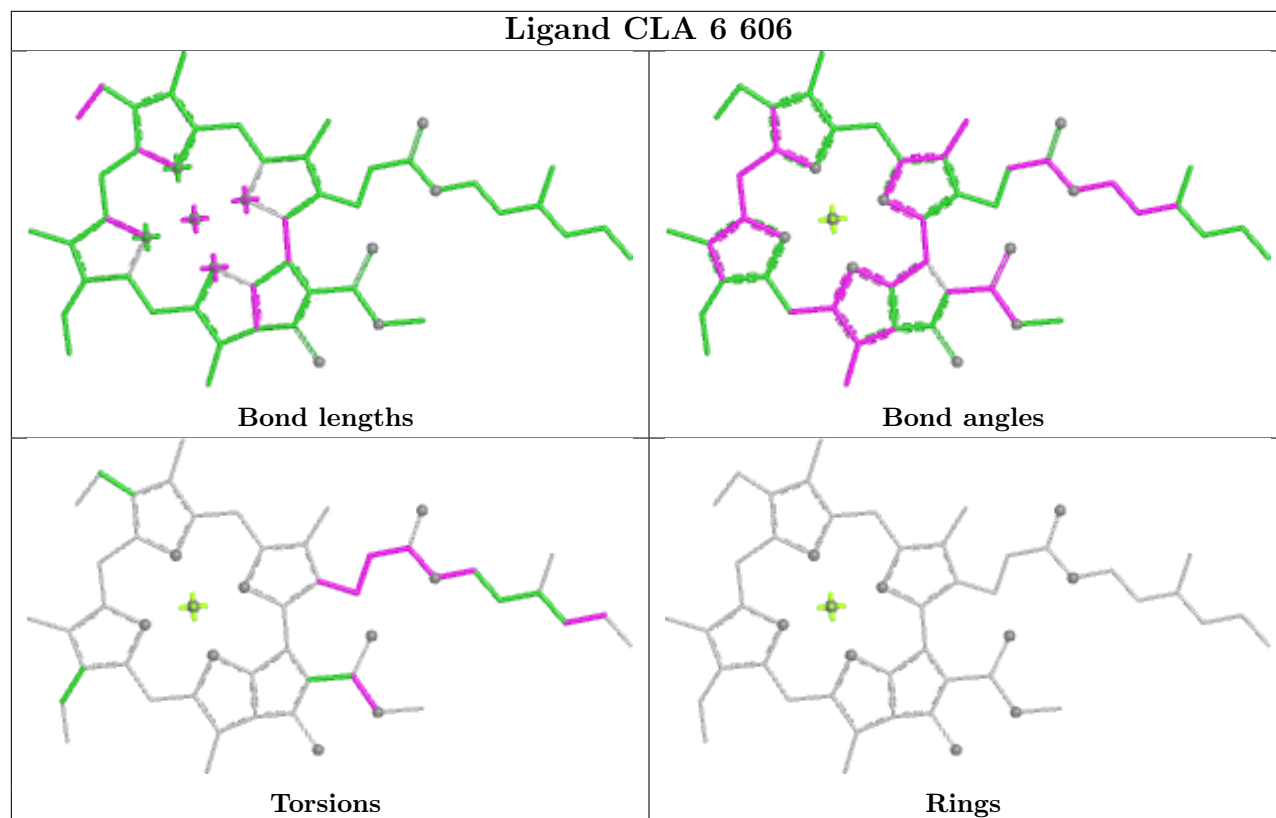


Ligand BCR 6 503

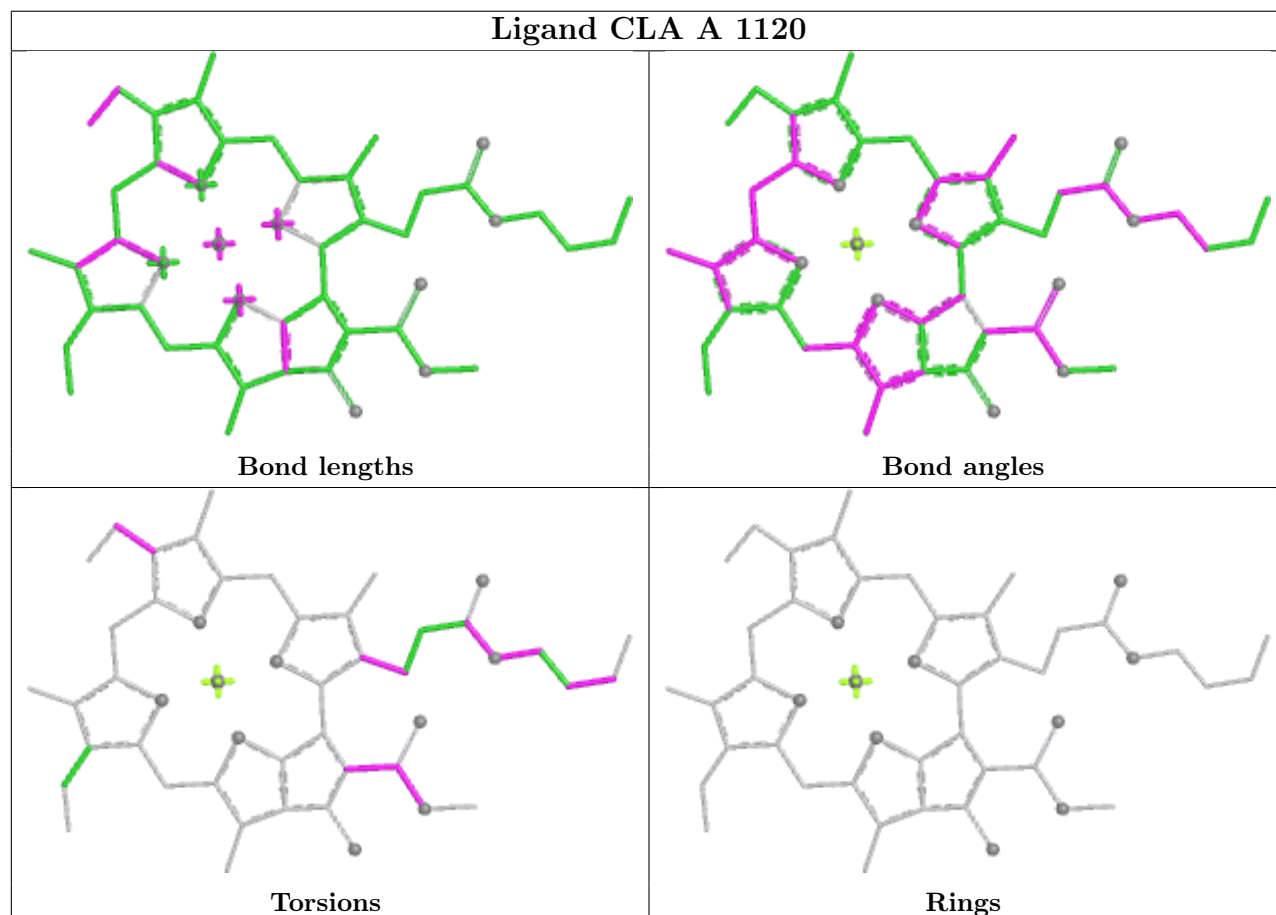


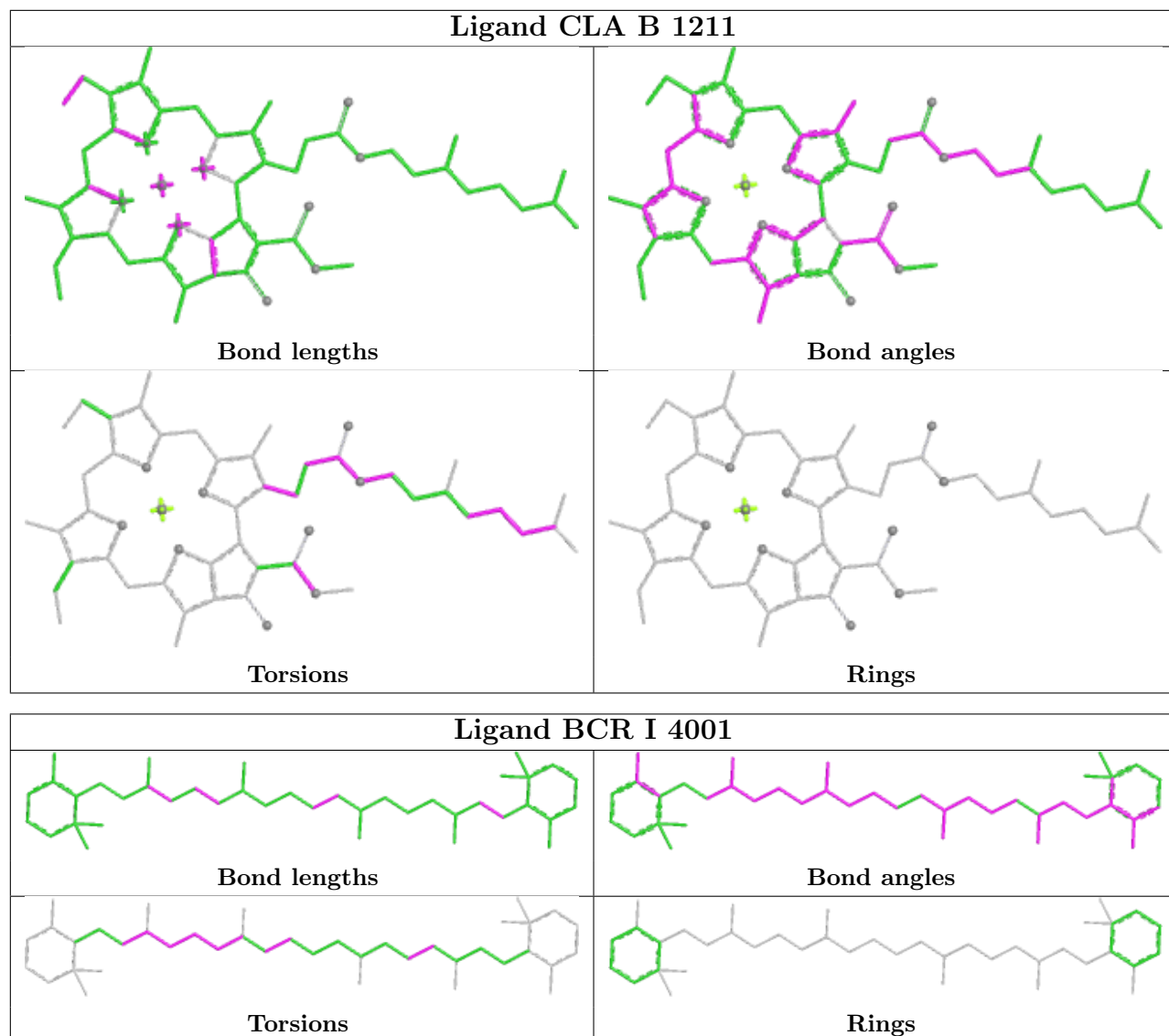


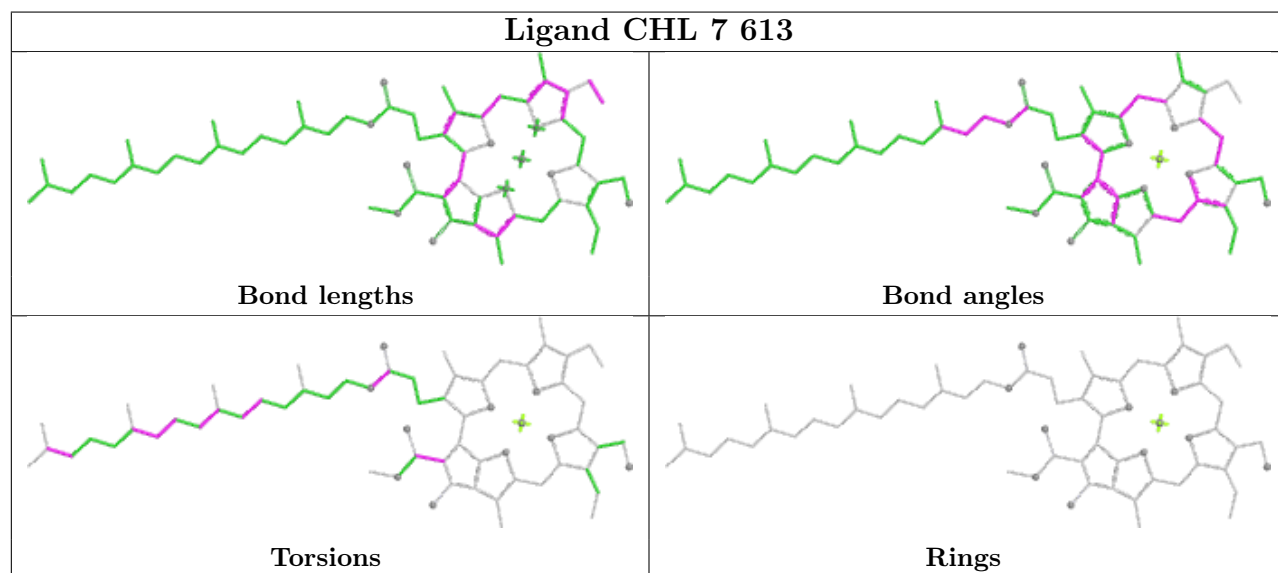
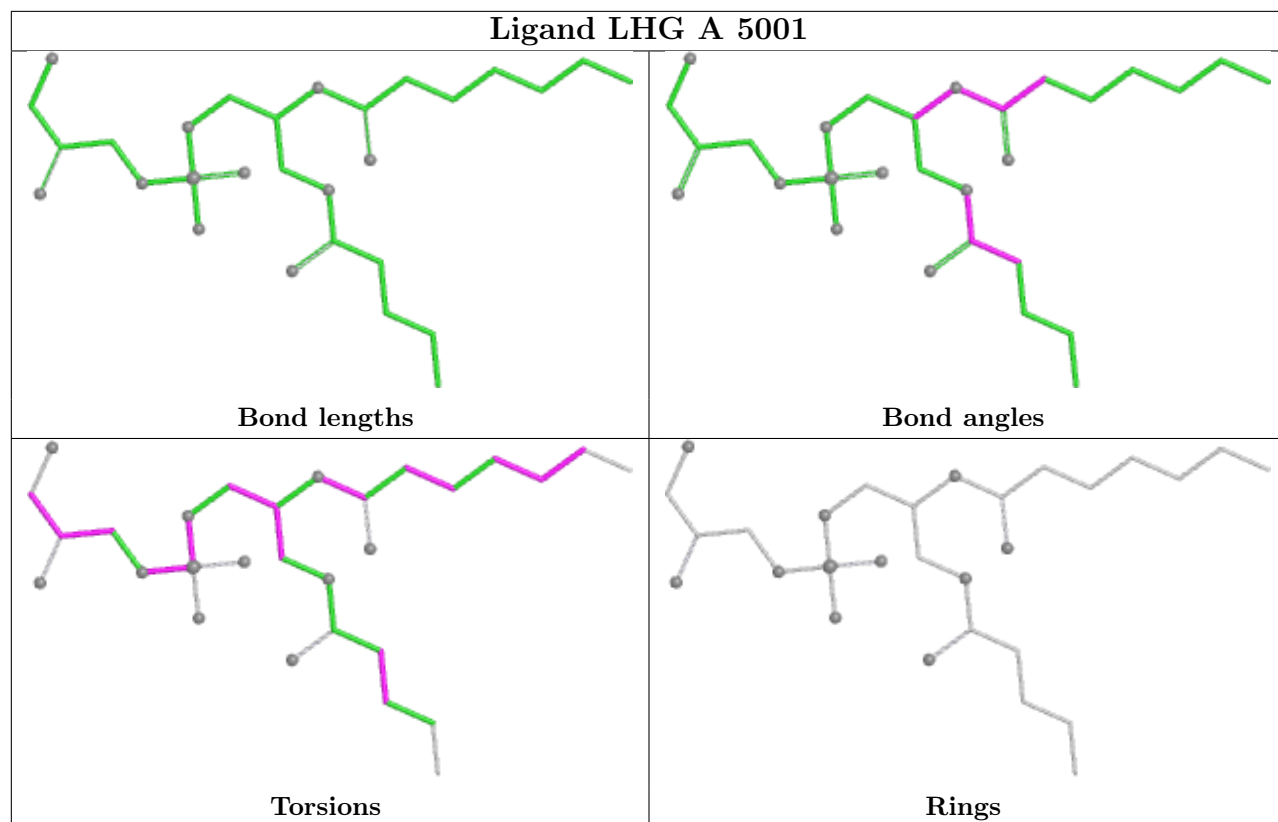
Ligand CLA 6 606

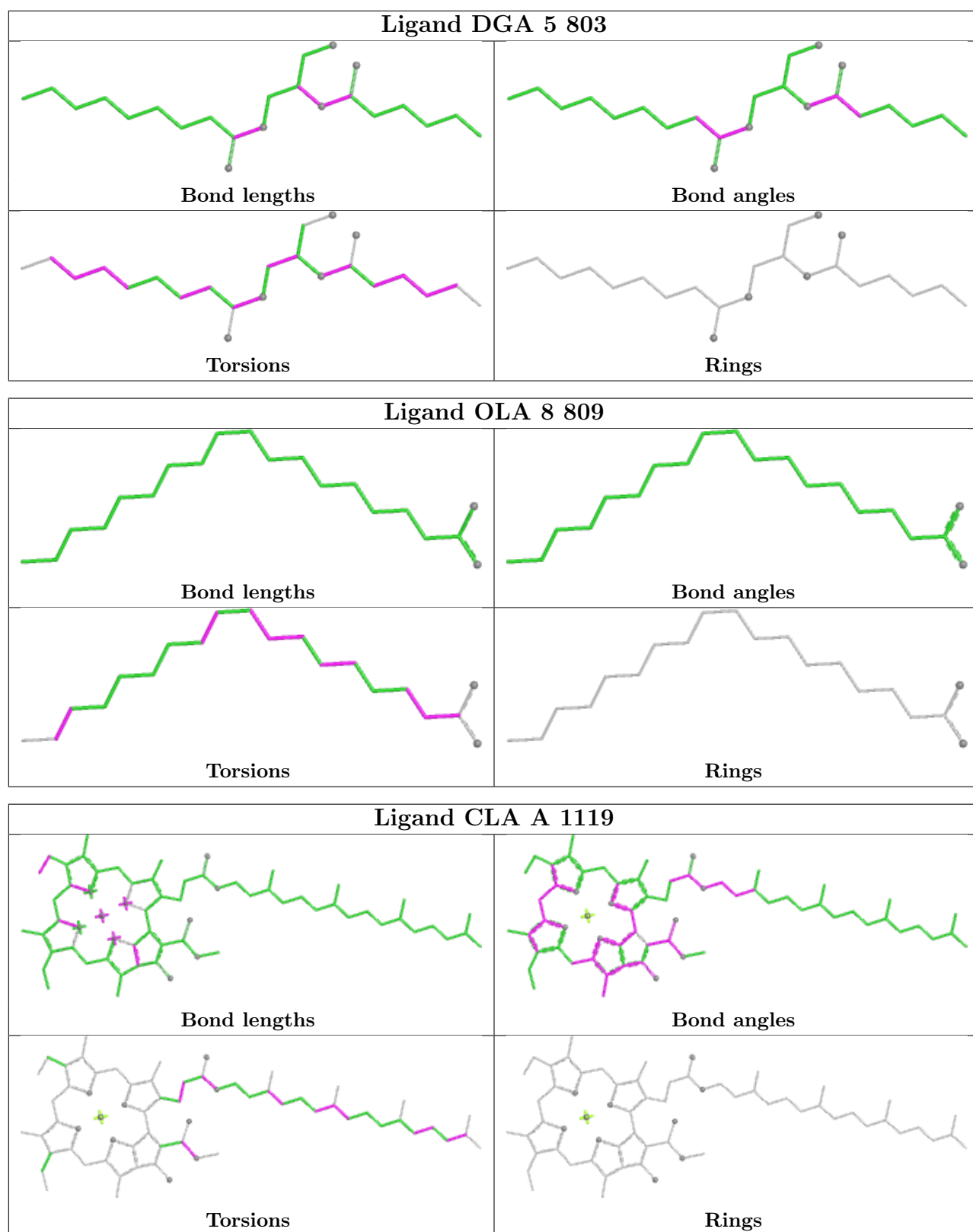


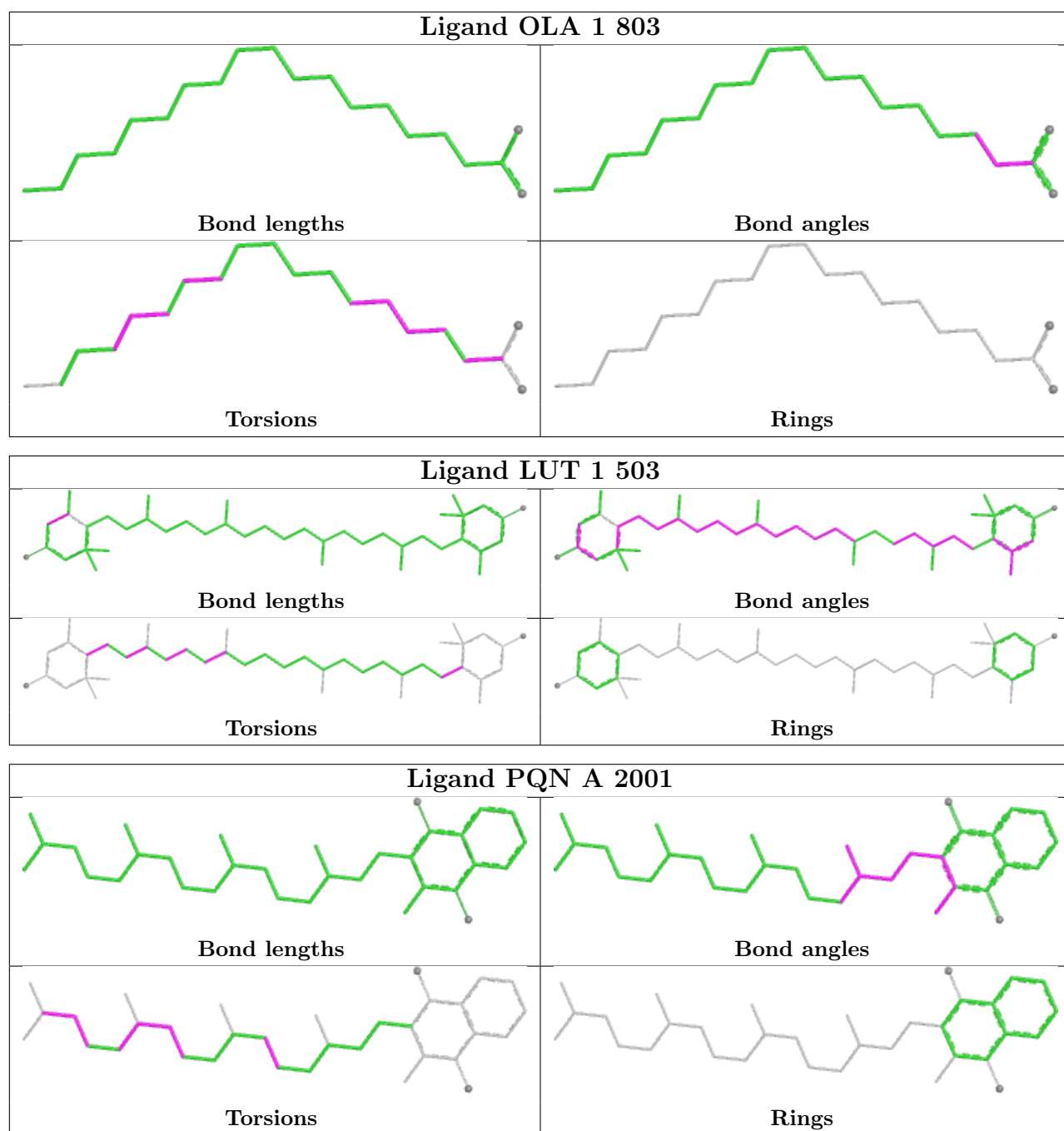
Ligand CLA A 1120



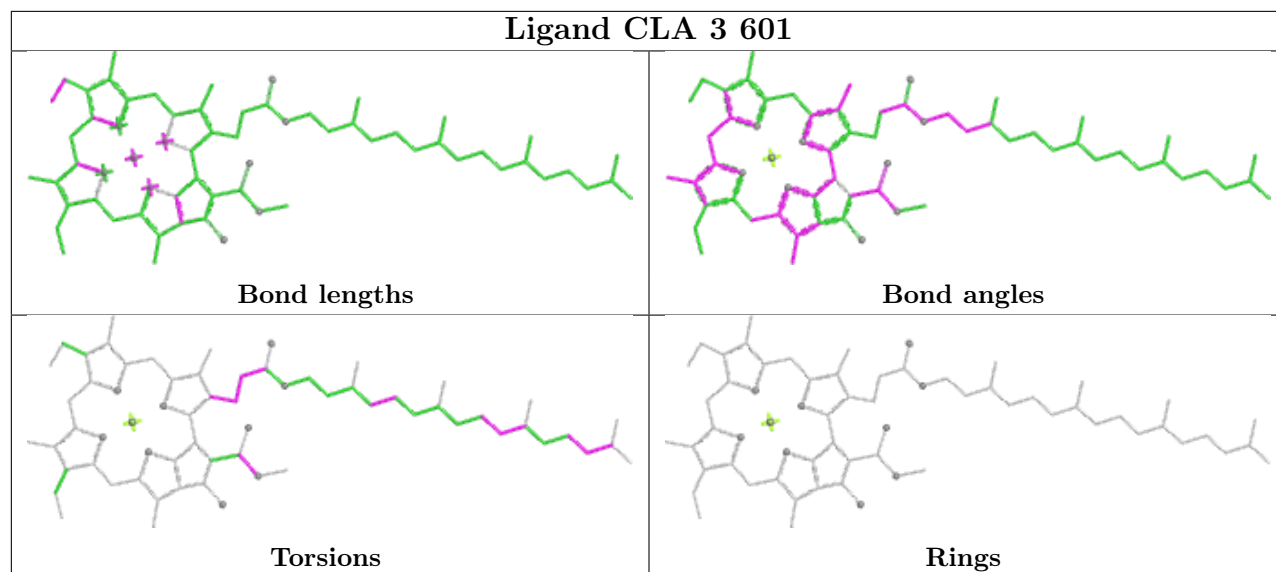




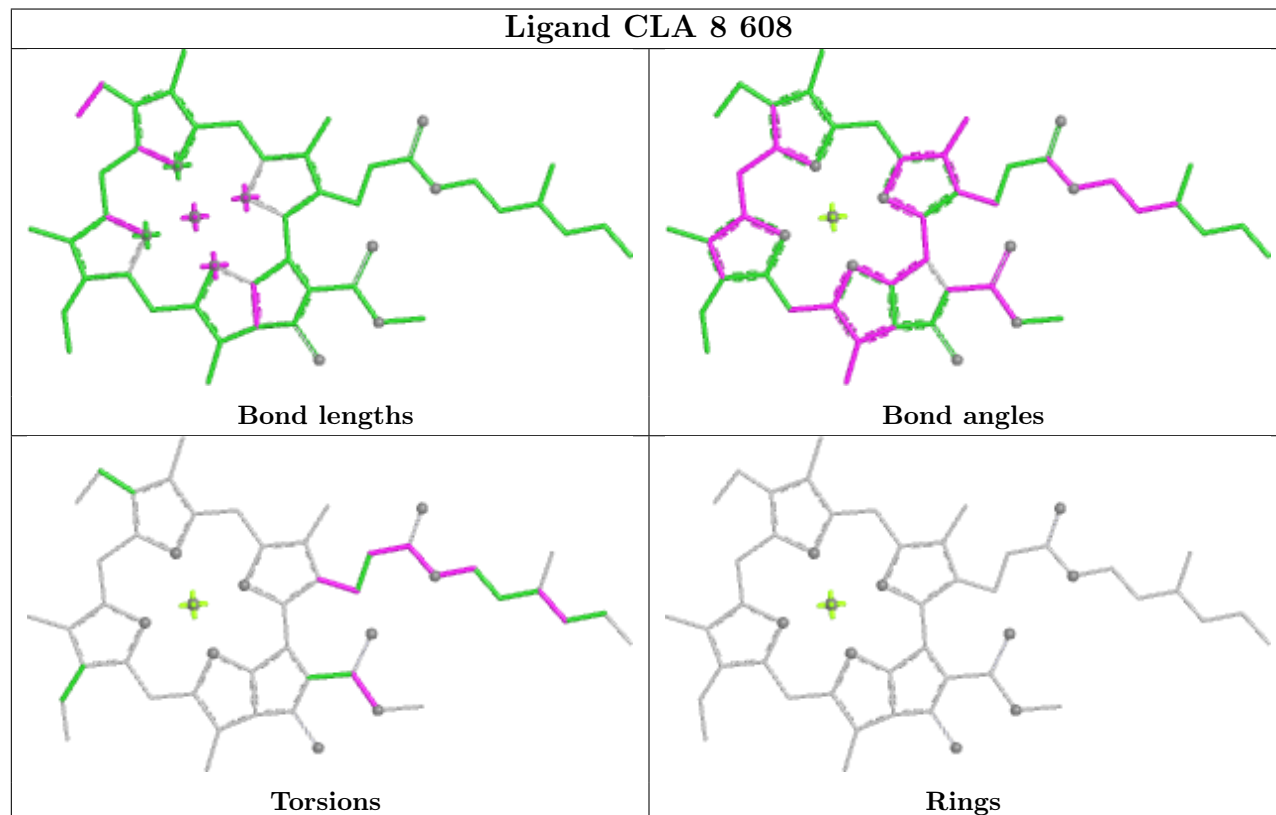




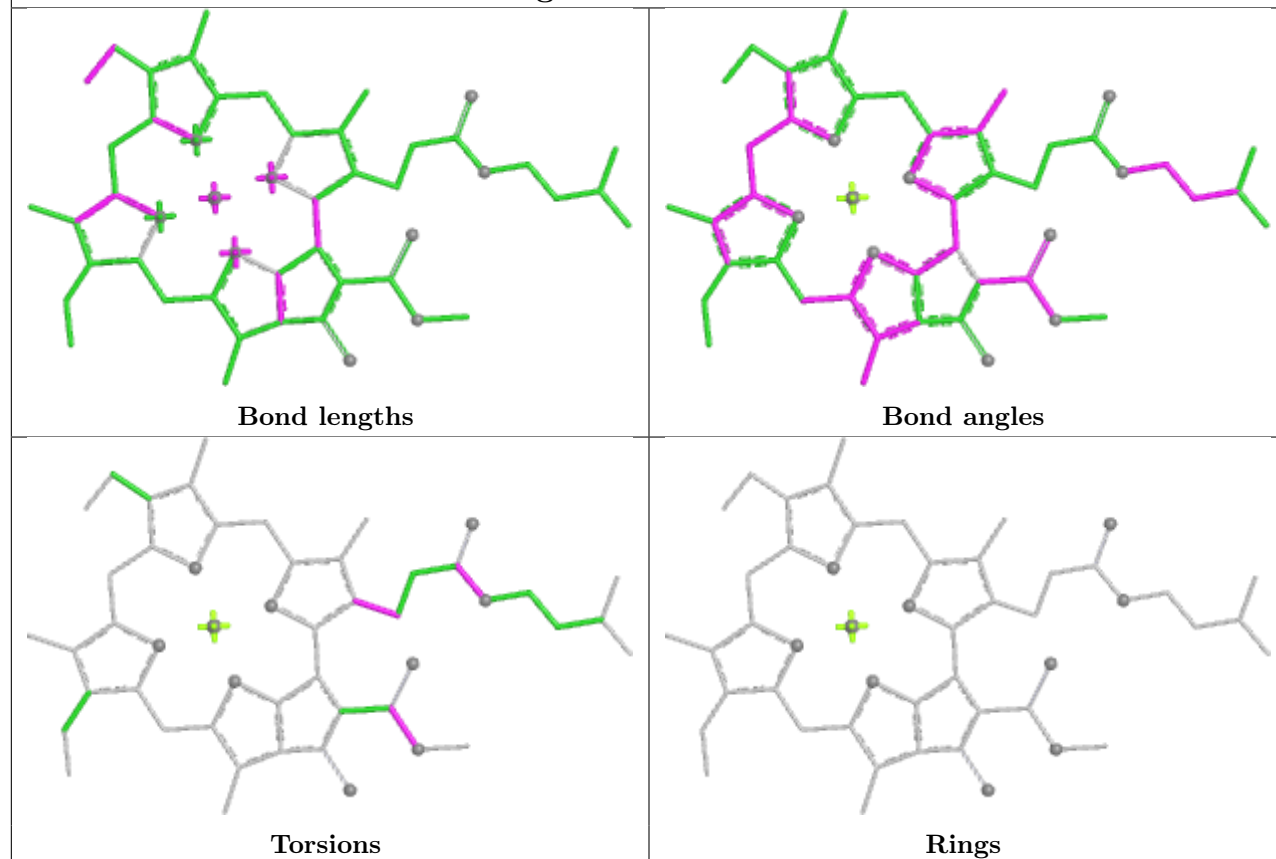
Ligand CLA 3 601



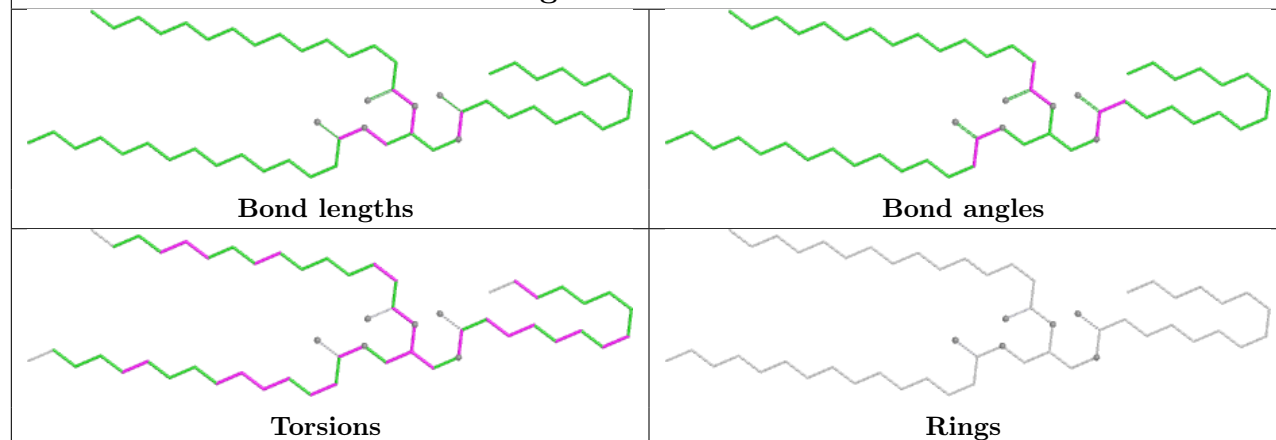
Ligand CLA 8 608

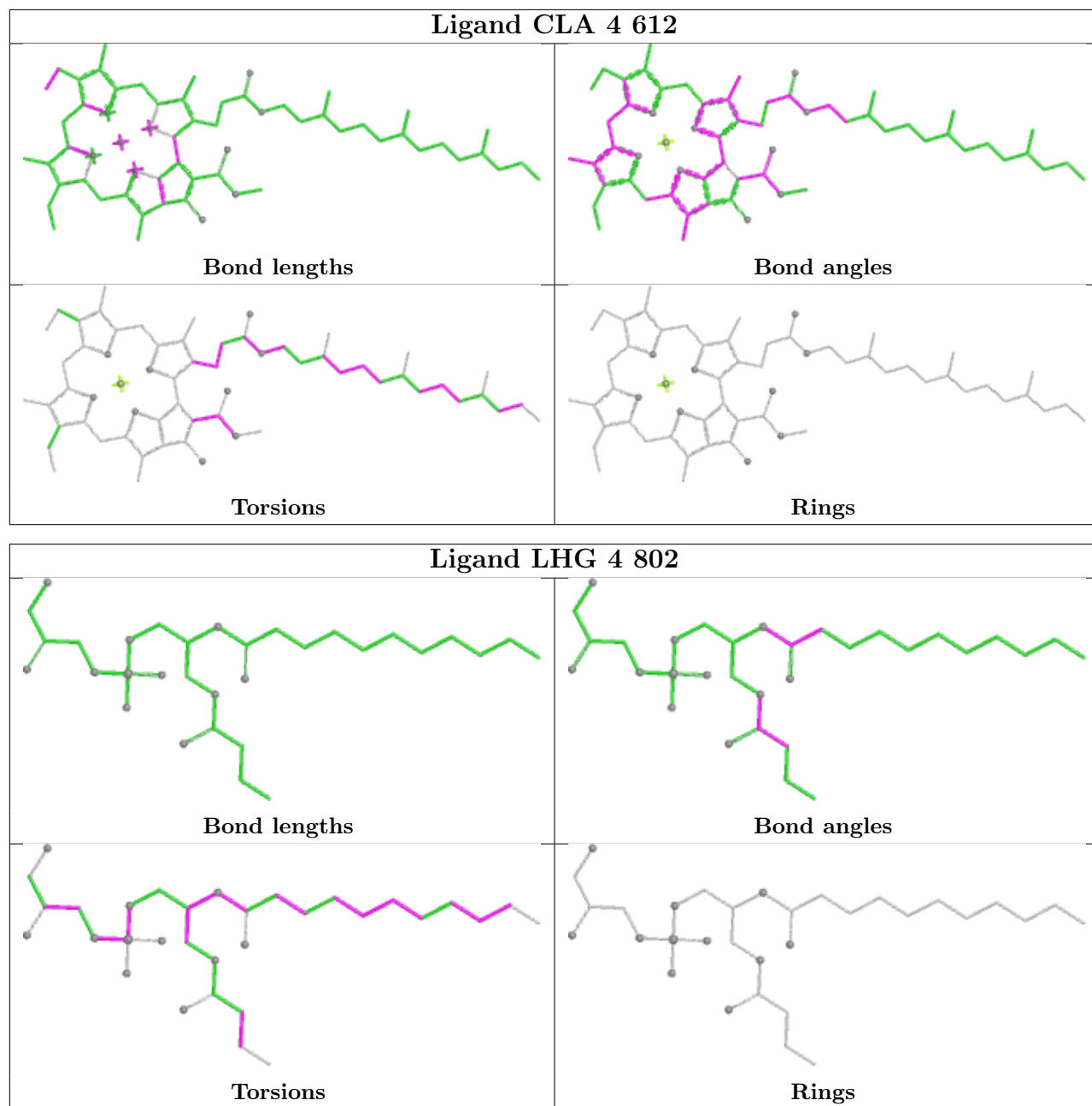


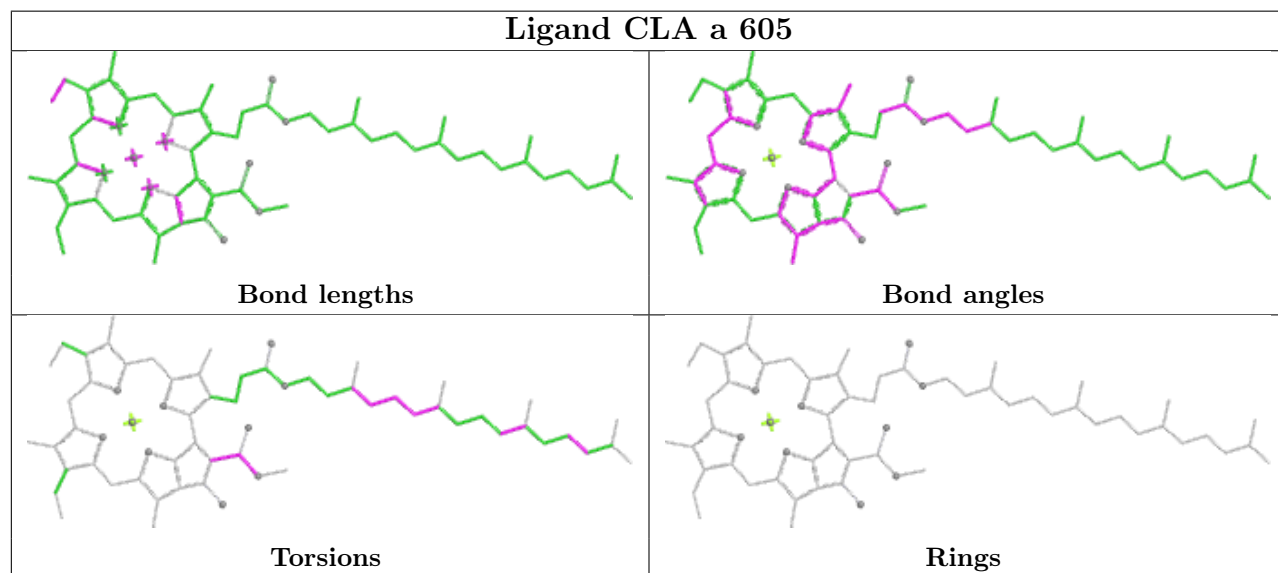
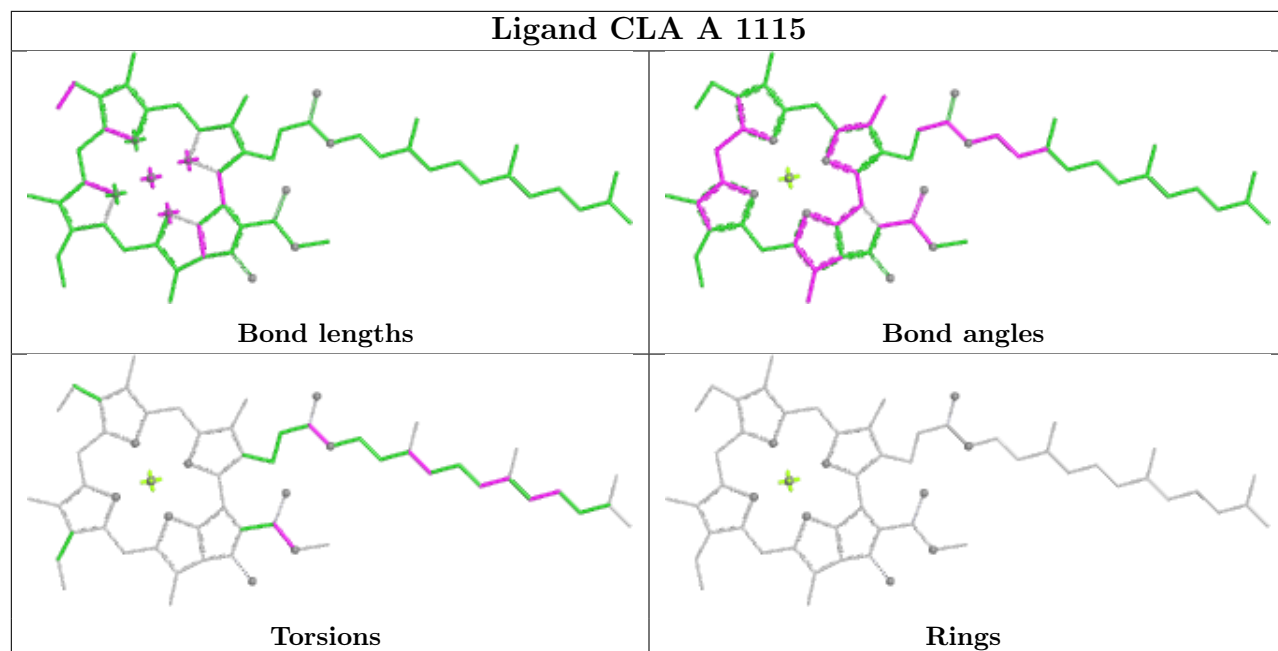
Ligand CLA a 602



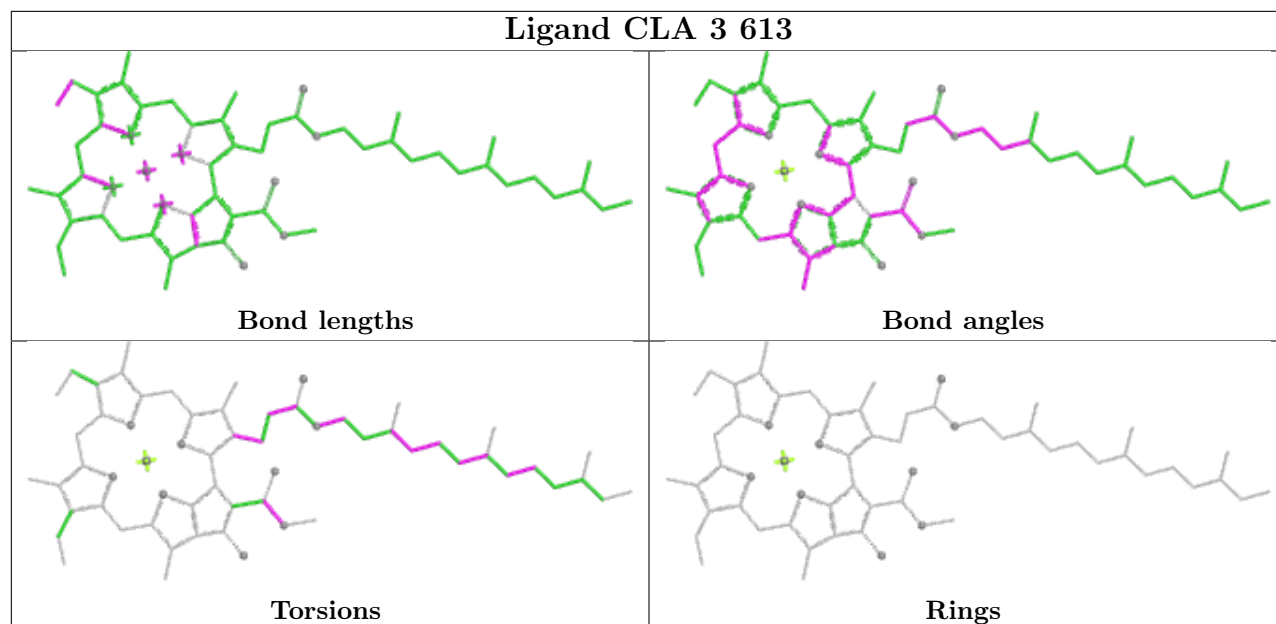
Ligand 4RF 8 808



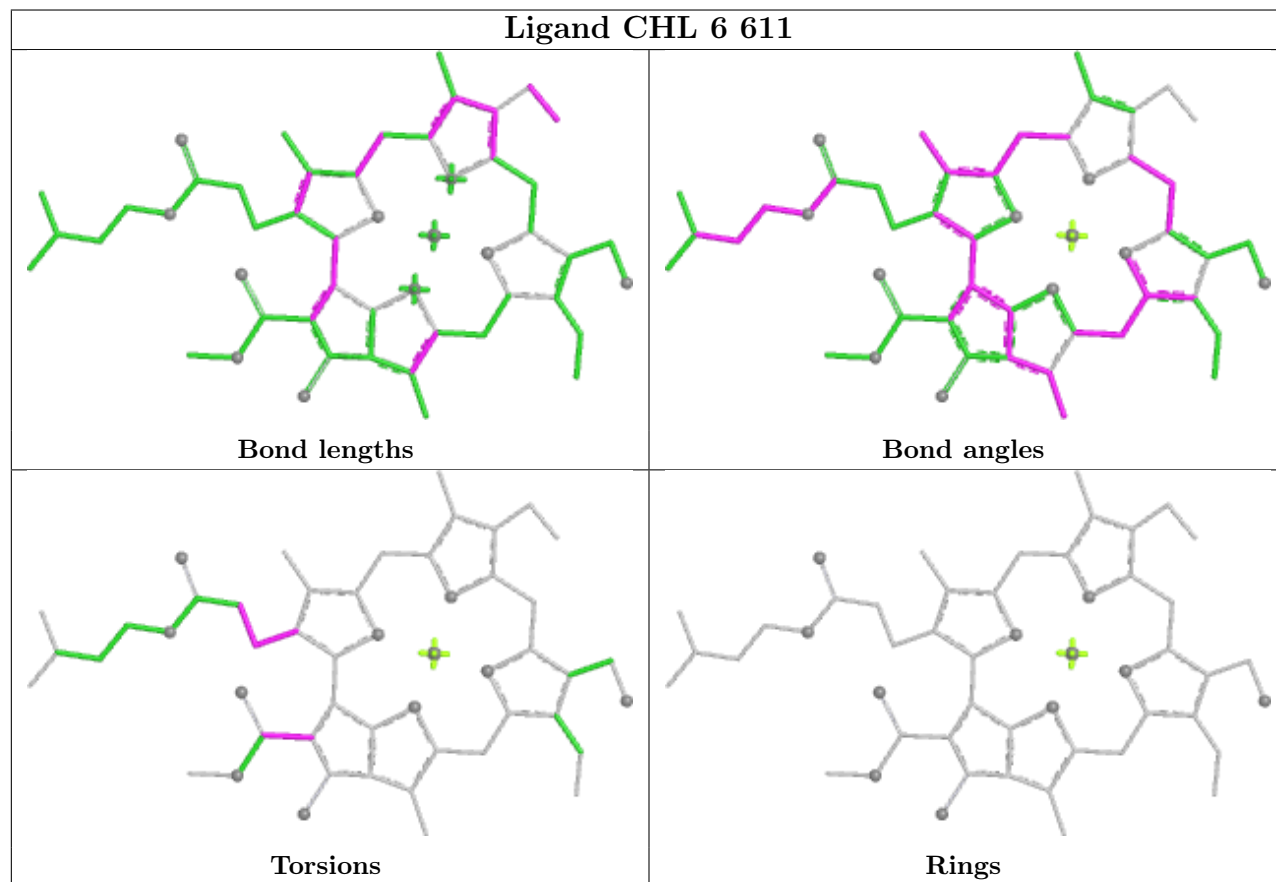


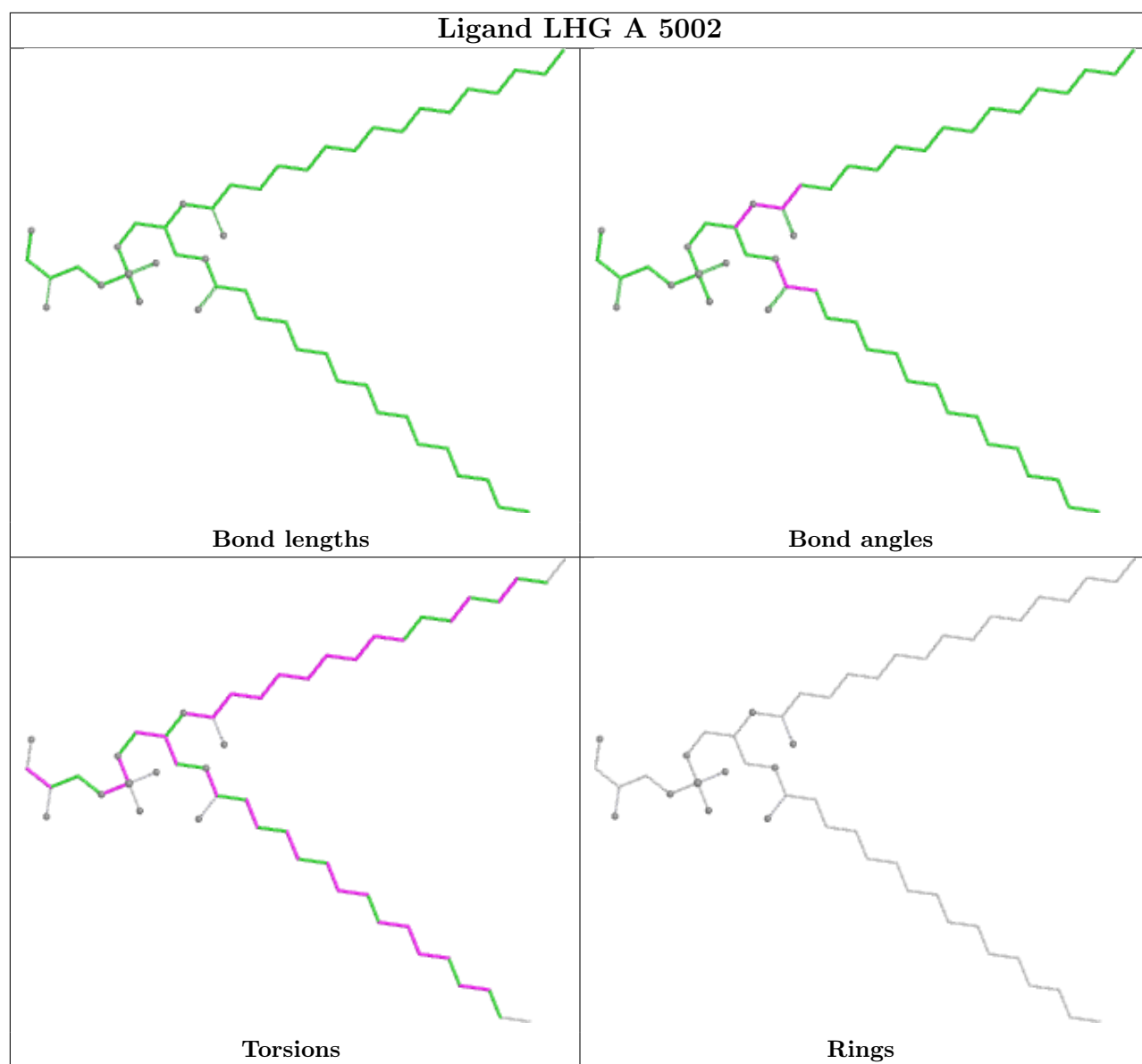


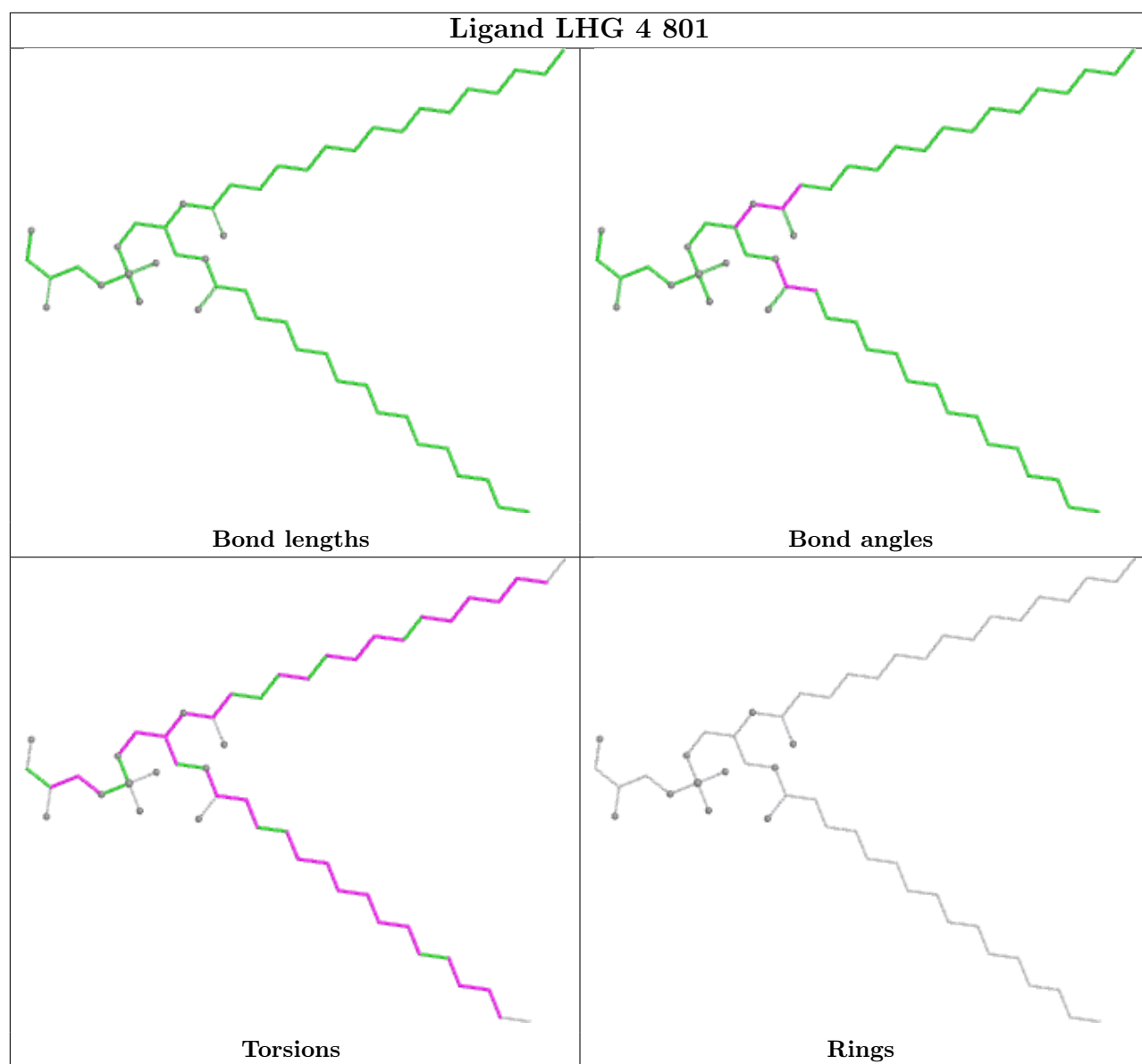
Ligand CLA 3 613



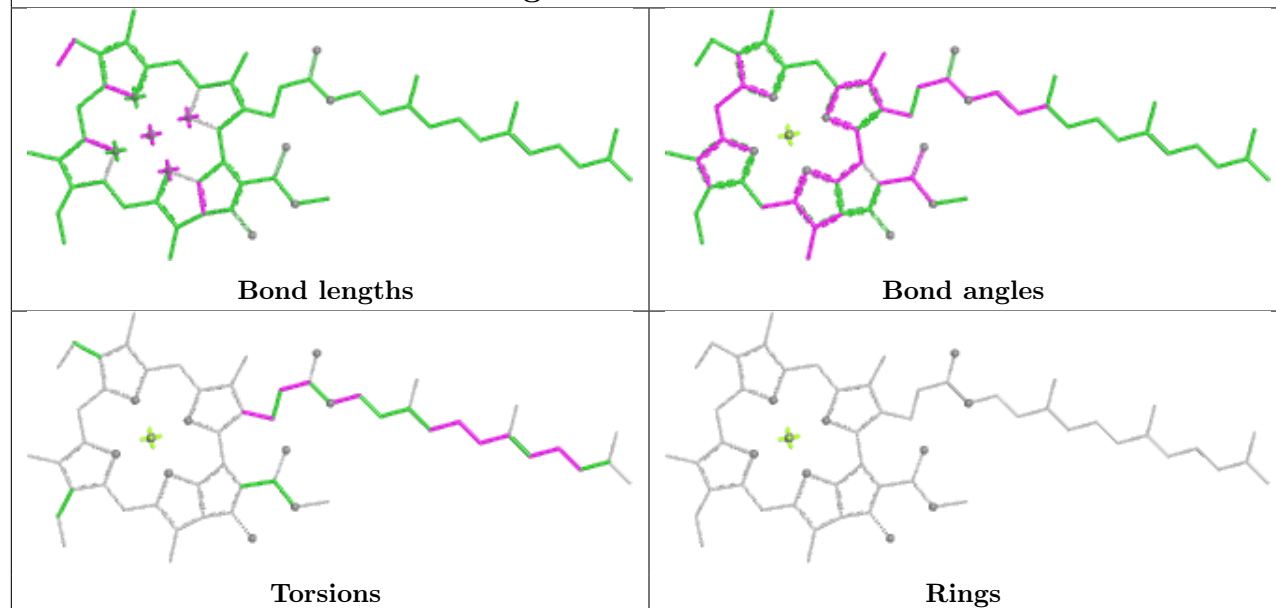
Ligand CHL 6 611



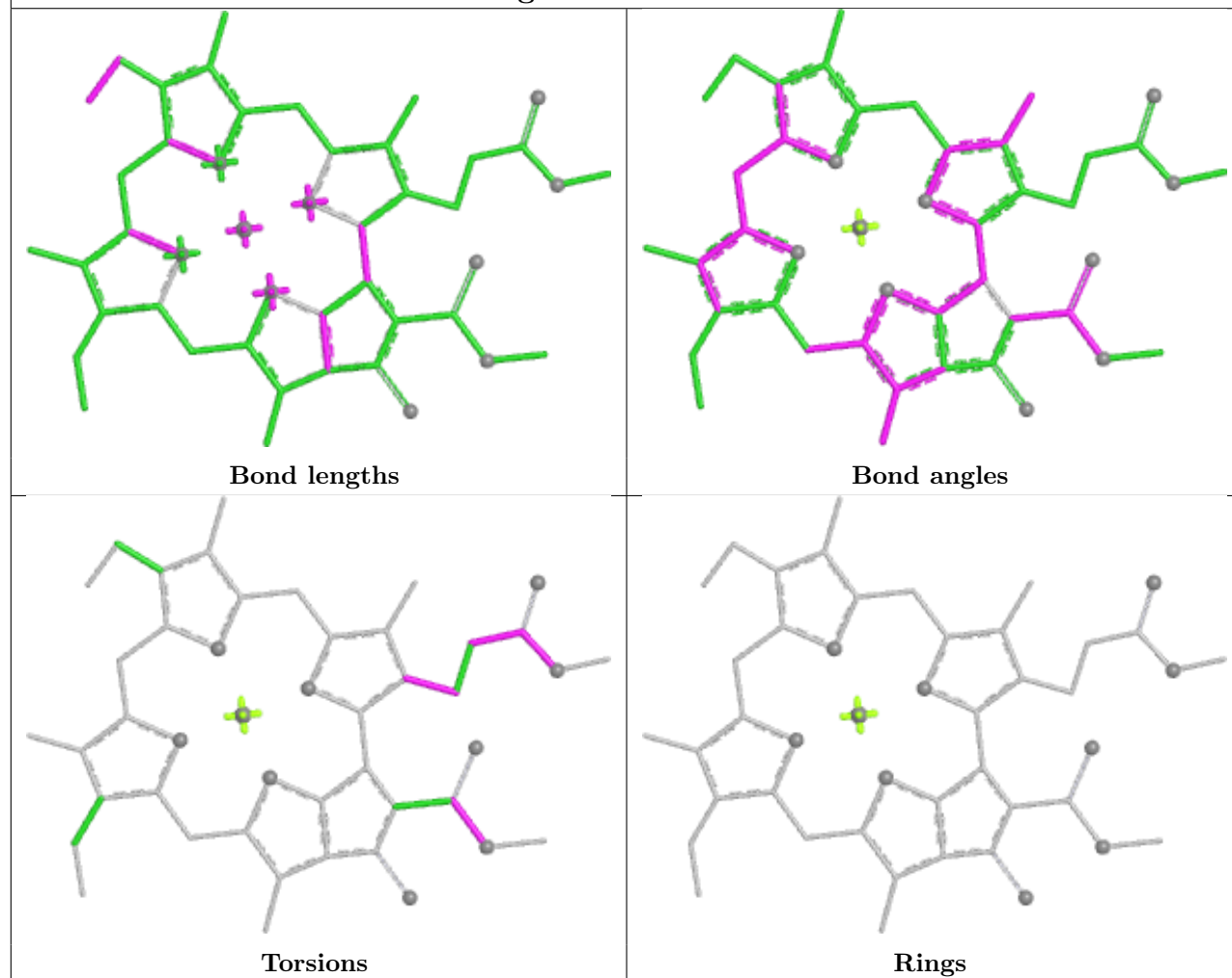


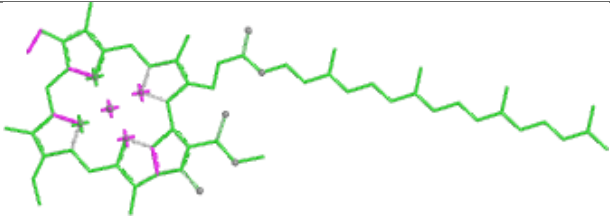
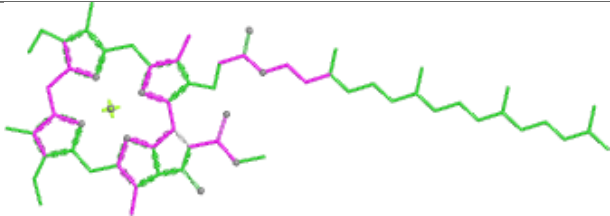
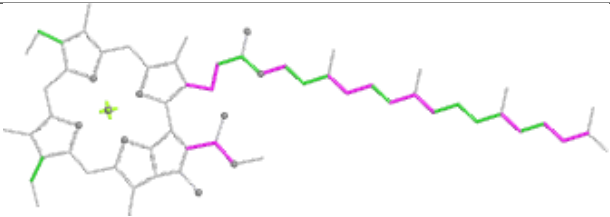
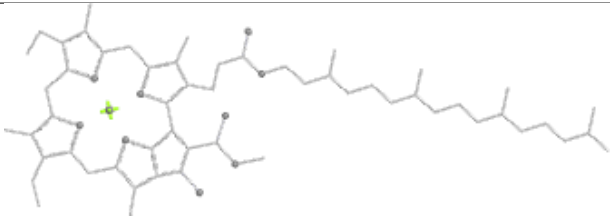
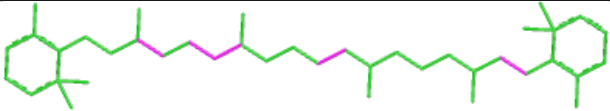
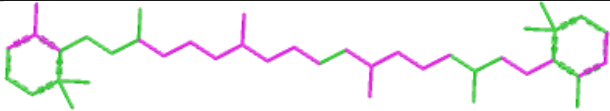
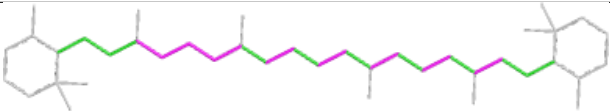
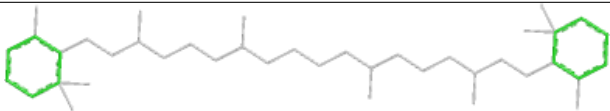


Ligand CLA B 1208

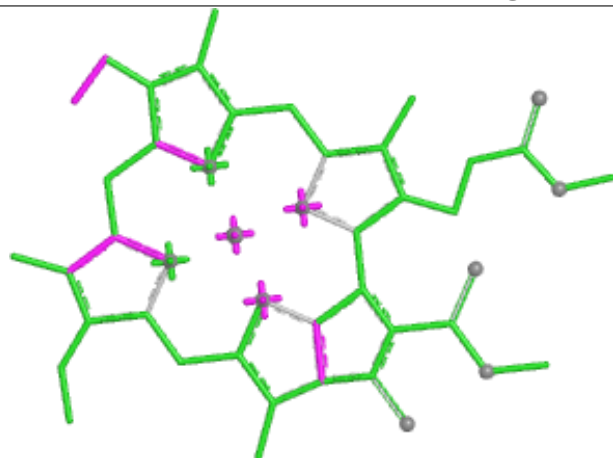


Ligand CLA 6 618

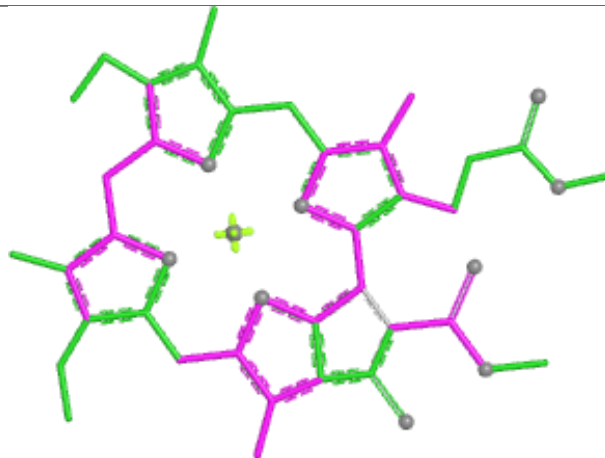


Ligand CLA 6 609	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 4006	
 Bond lengths	 Bond angles
 Torsions	 Rings

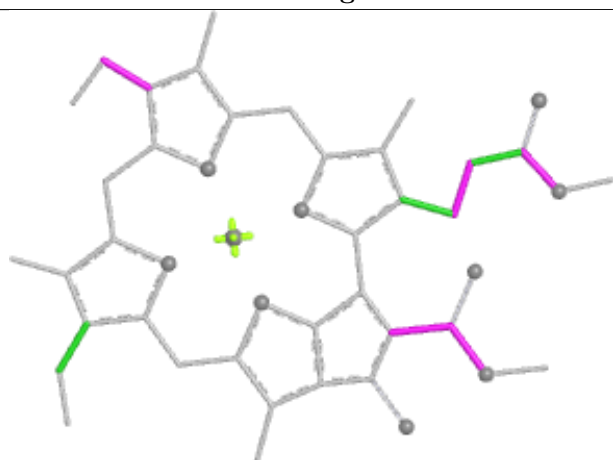
Ligand CLA G 1602



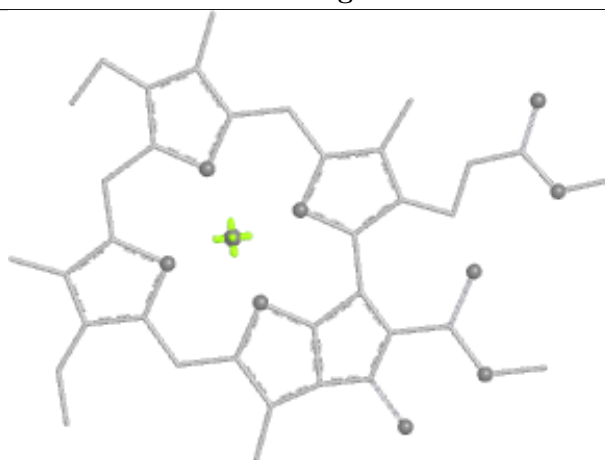
Bond lengths



Bond angles

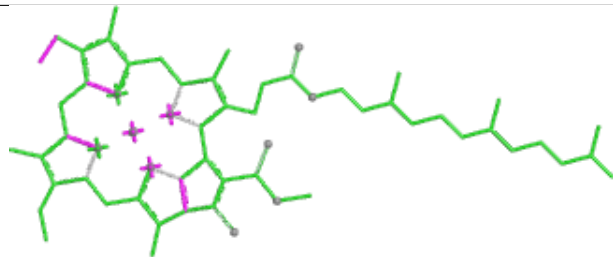


Torsions

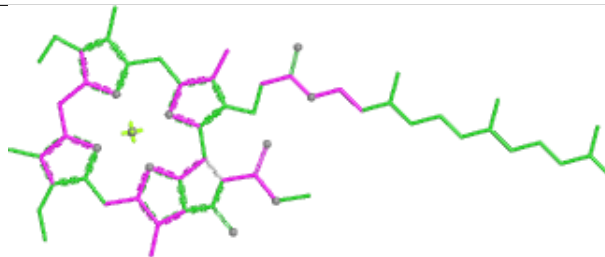


Rings

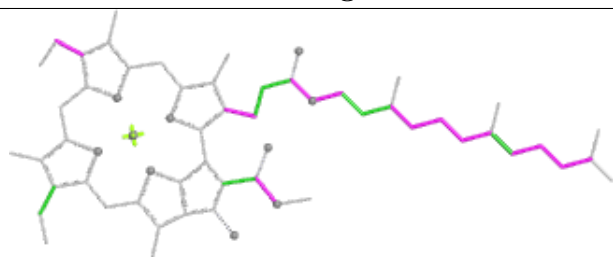
Ligand CLA B 1220



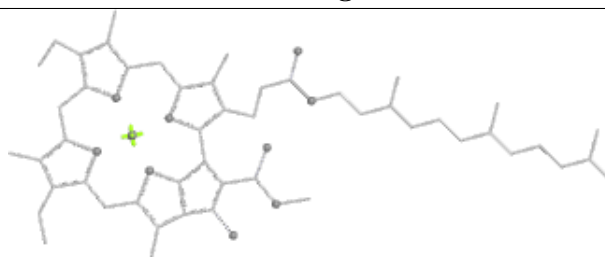
Bond lengths



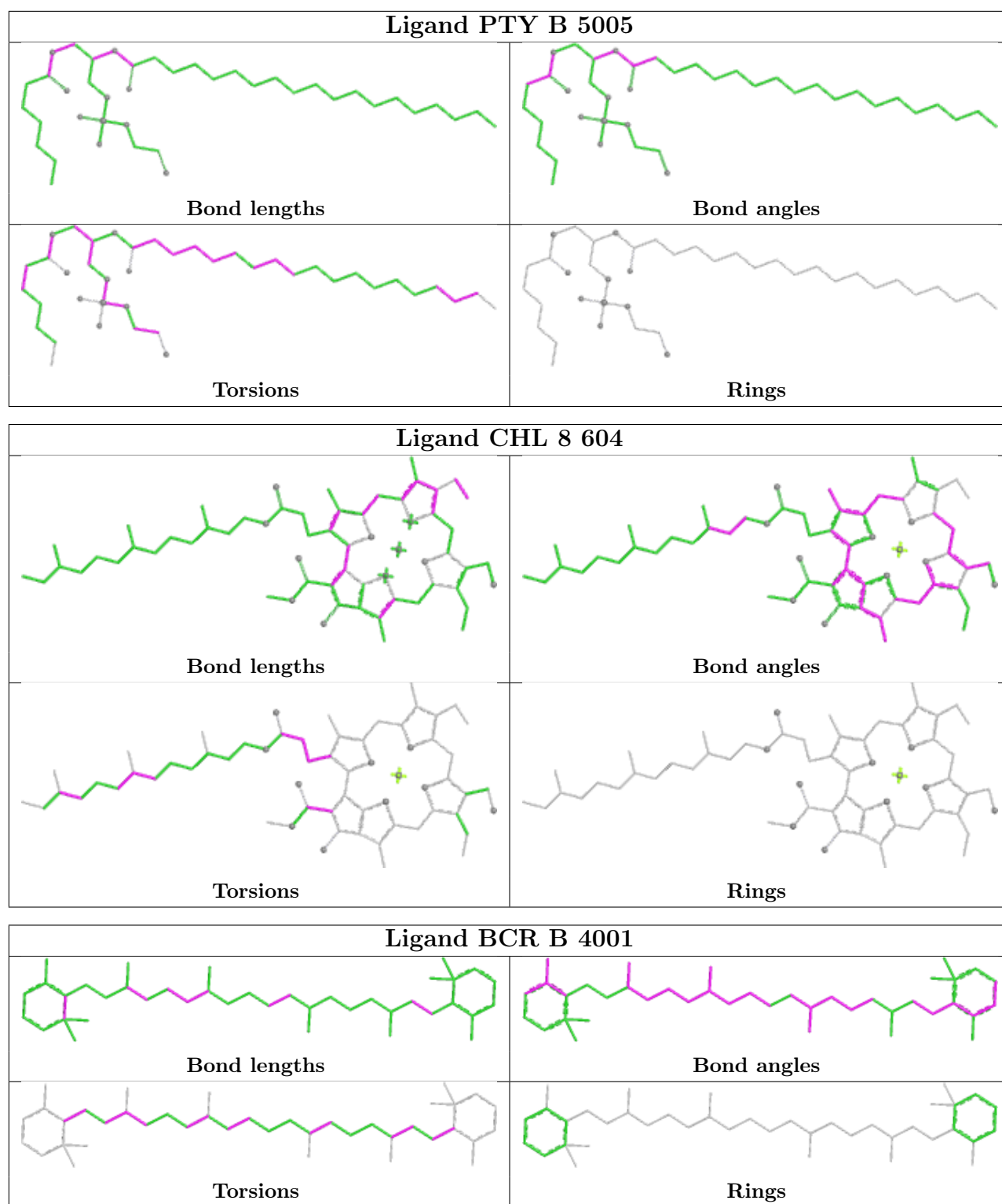
Bond angles

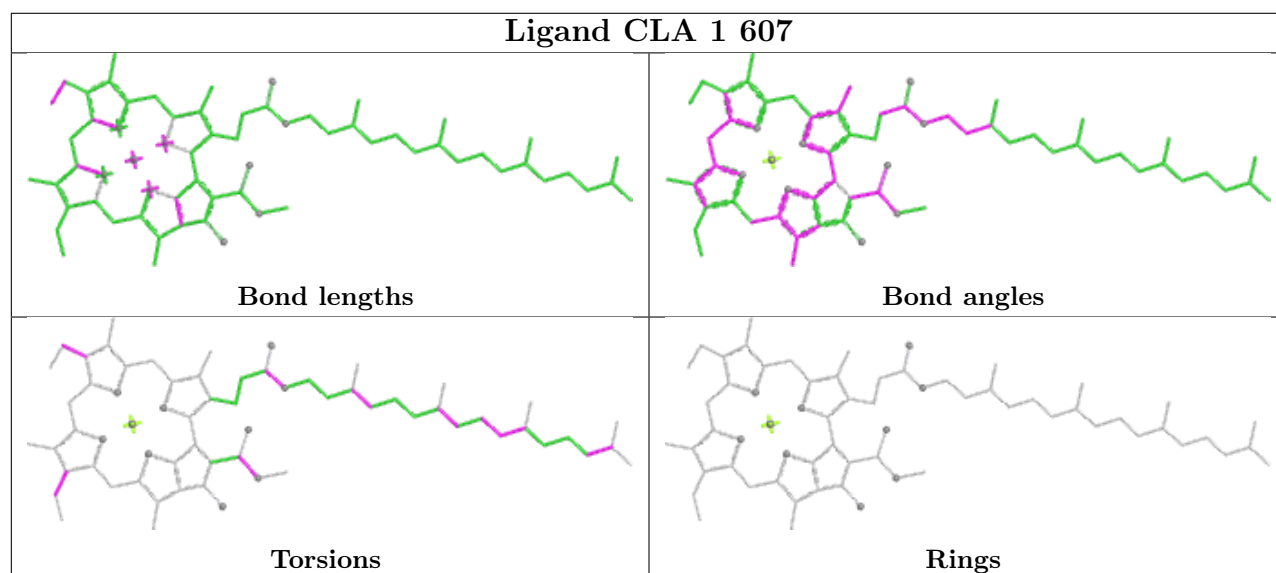
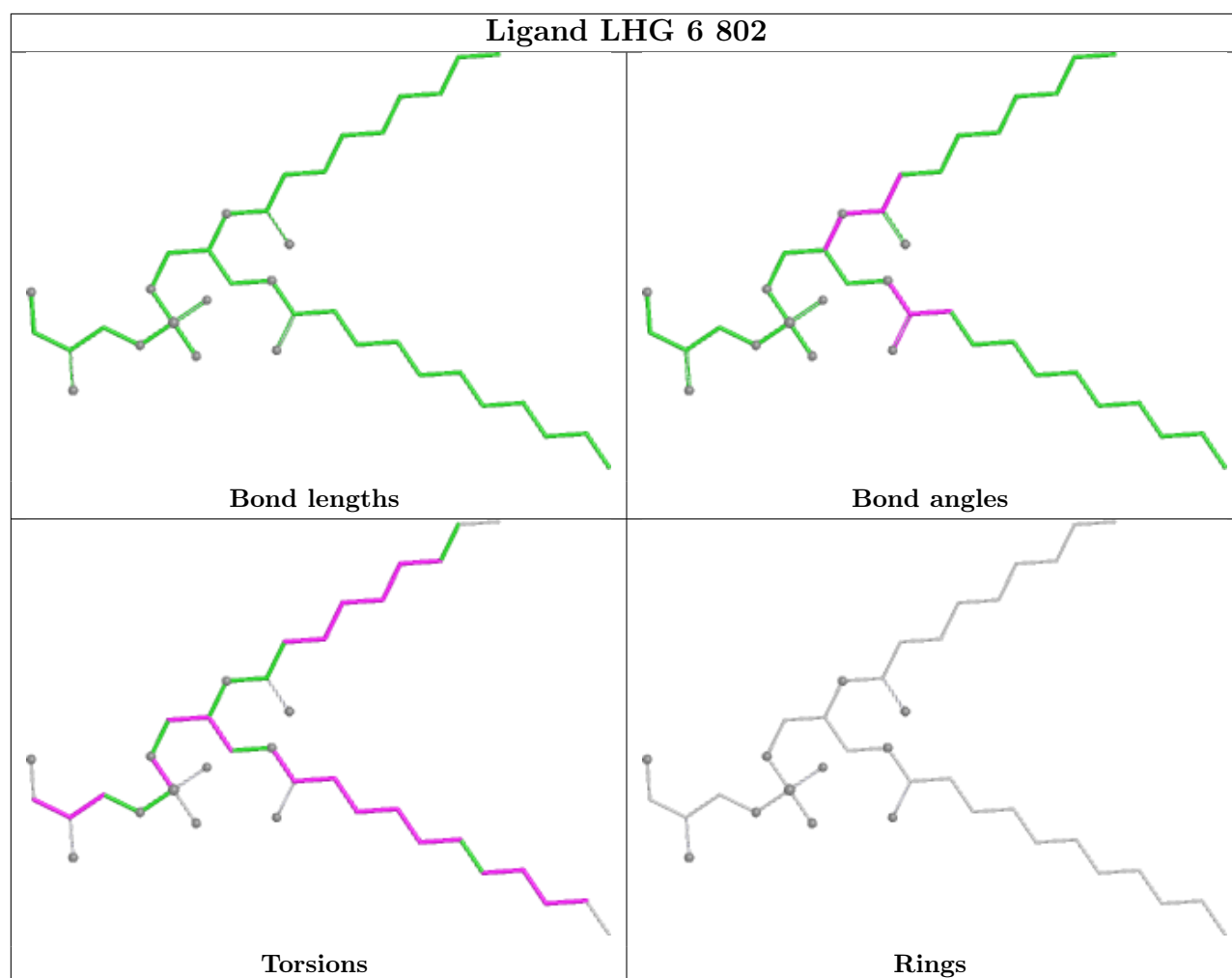


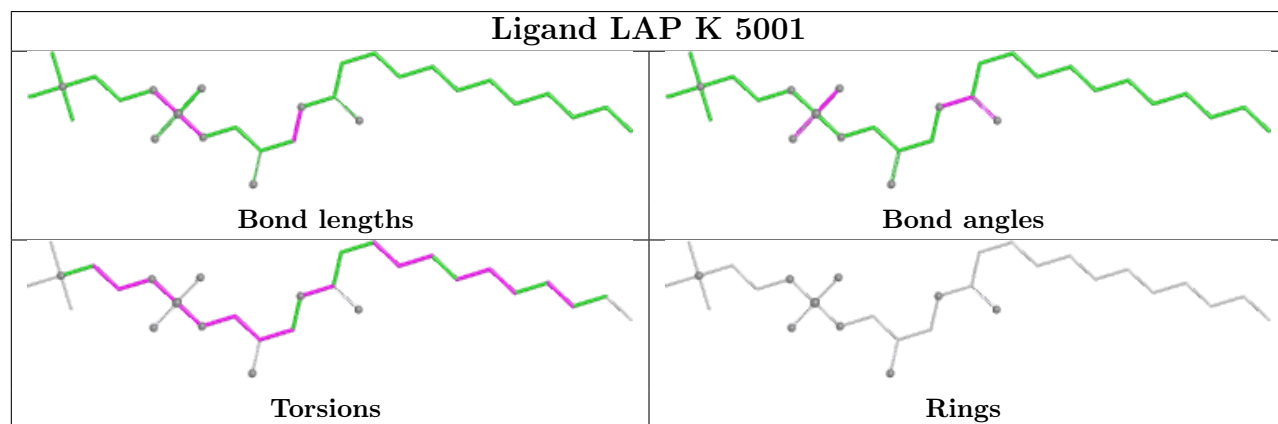
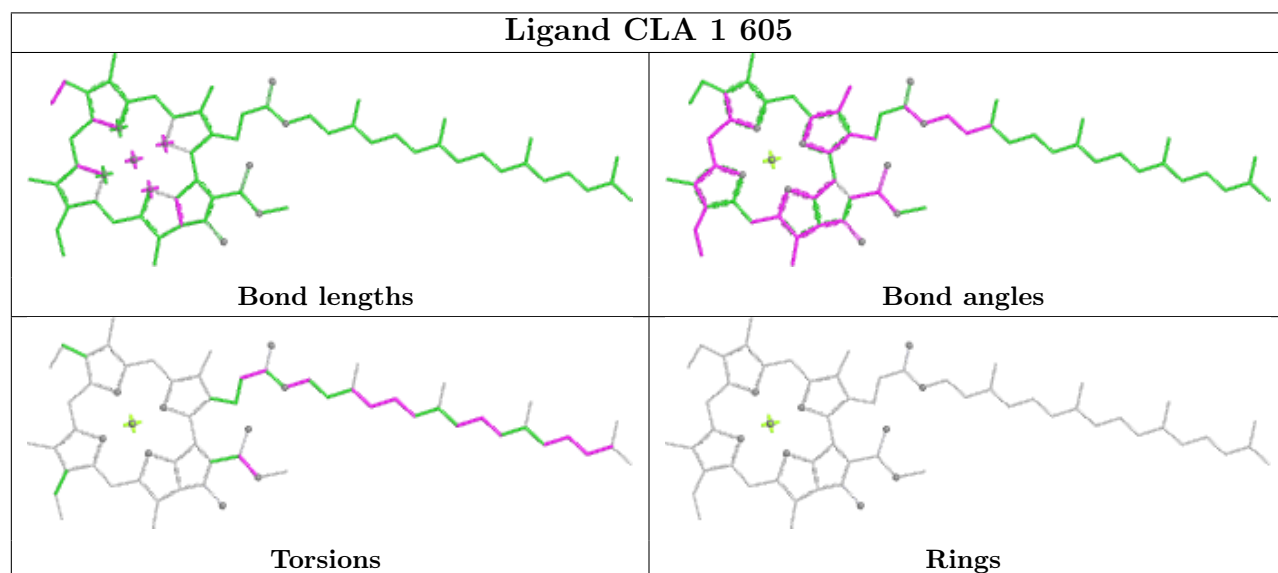
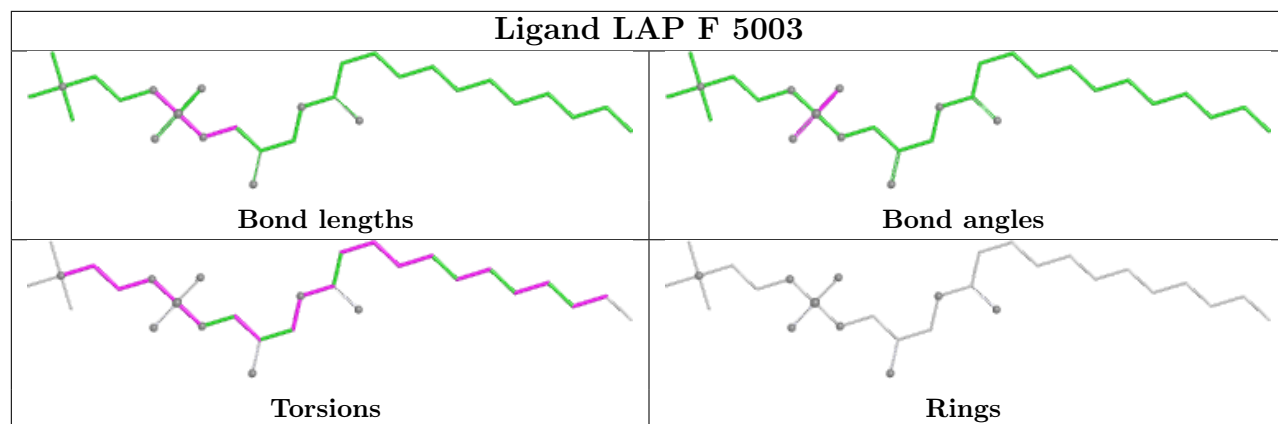
Torsions



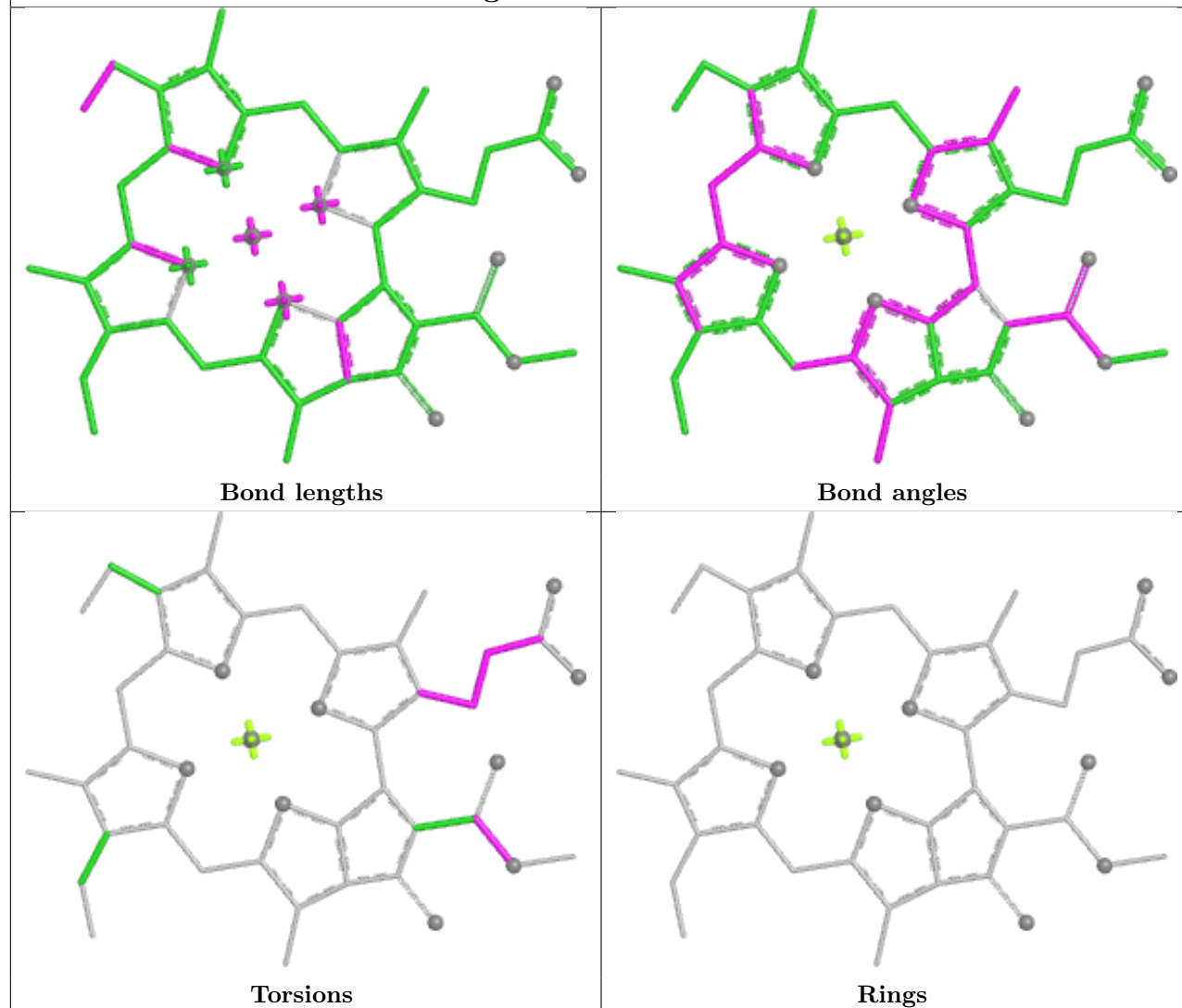
Rings



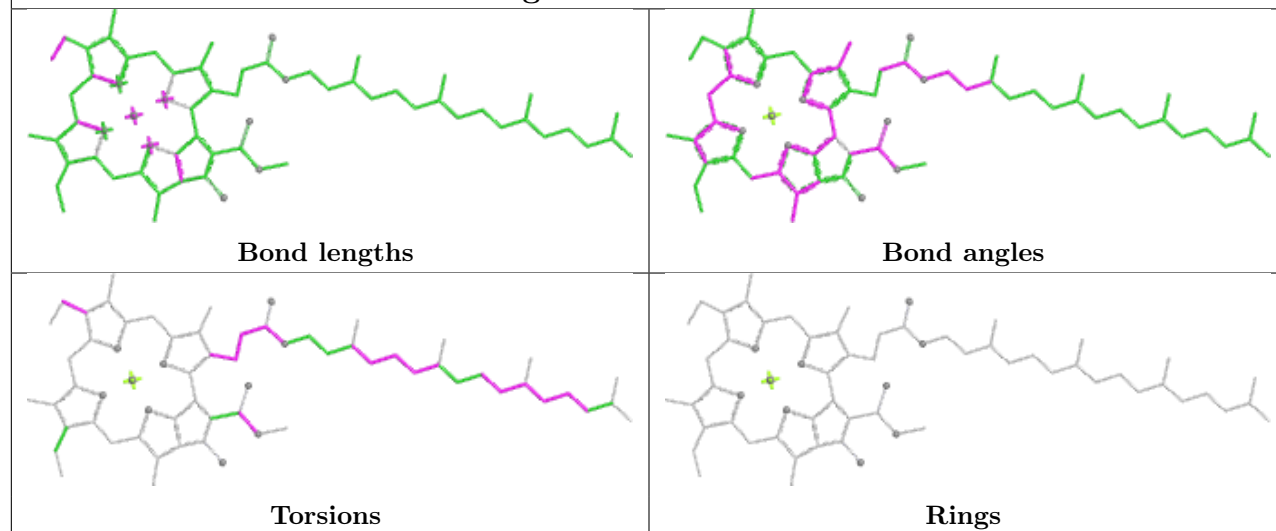


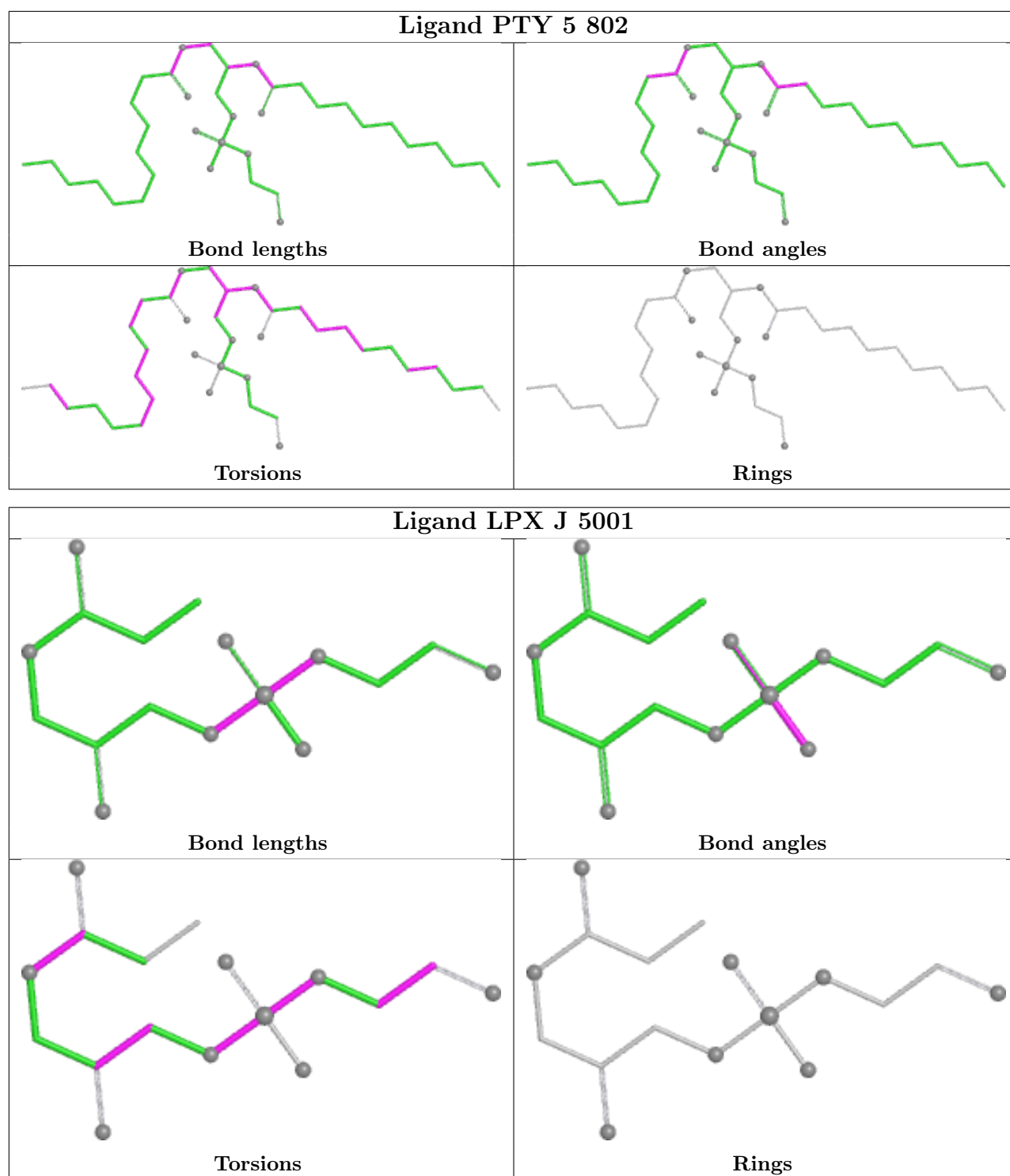


Ligand CLA G 1603



Ligand CLA A 1131





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

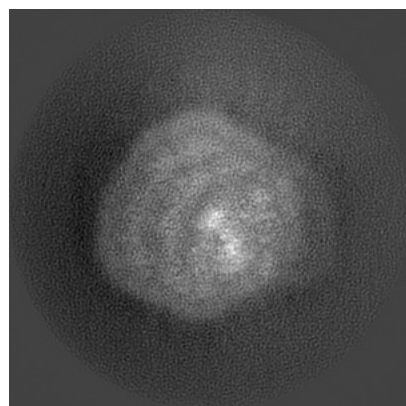
6 Map visualisation [i](#)

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.

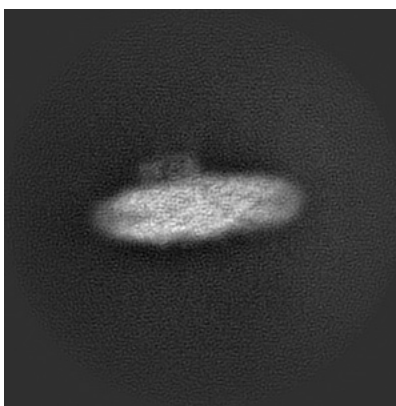
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

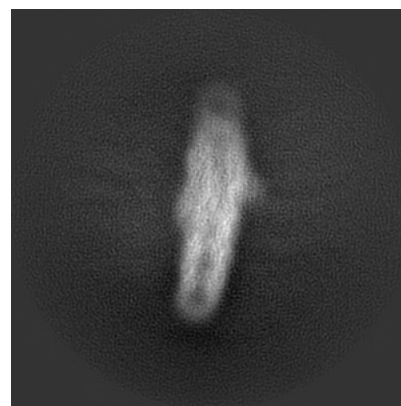
6.1.1 Primary map



X

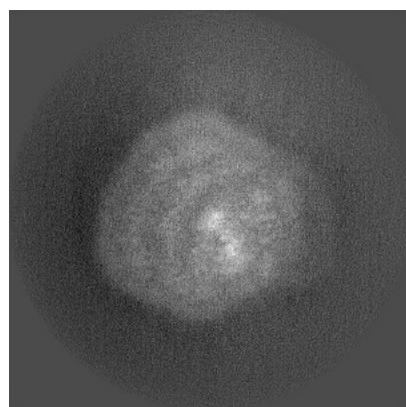


Y

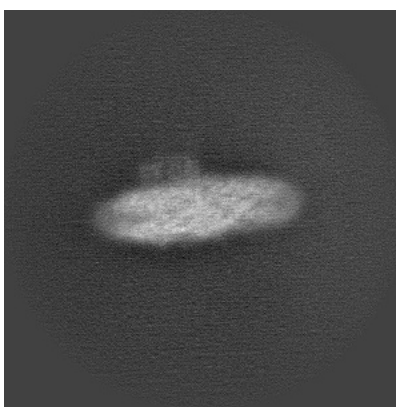


Z

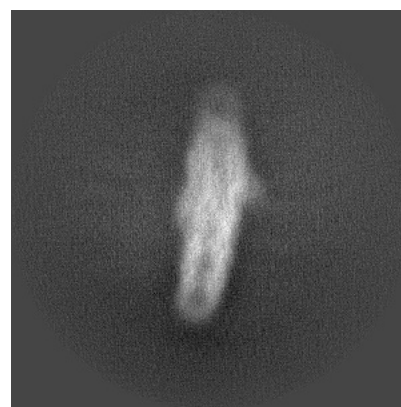
6.1.2 Raw map



X



Y

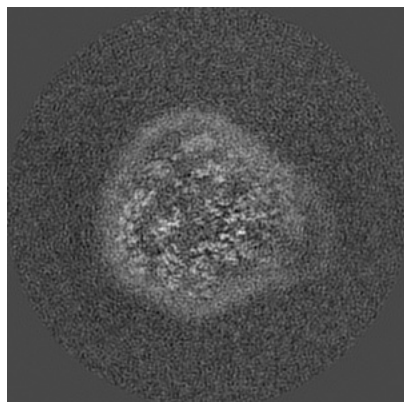


Z

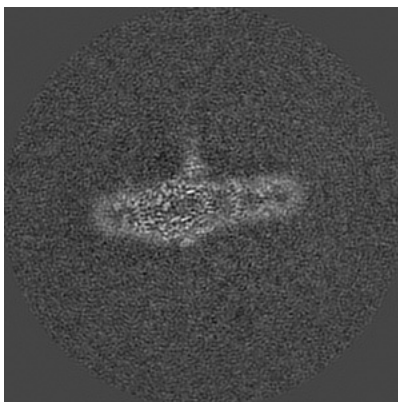
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

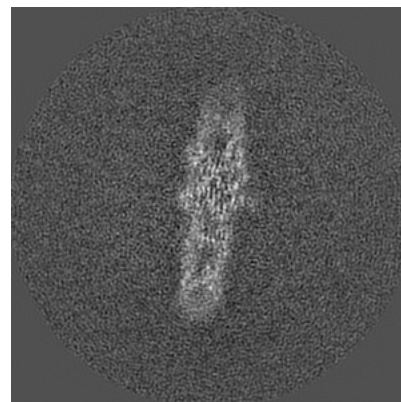
6.2.1 Primary map



X Index: 256

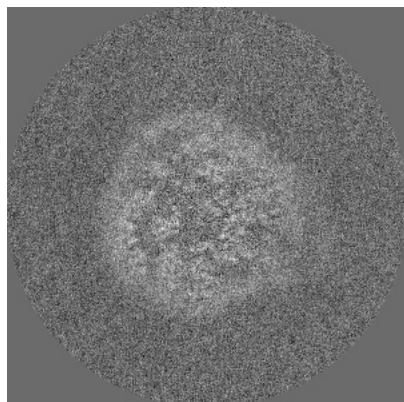


Y Index: 256

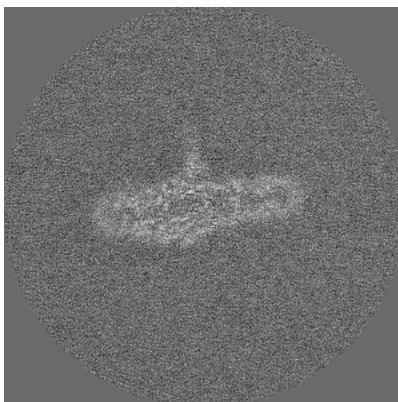


Z Index: 256

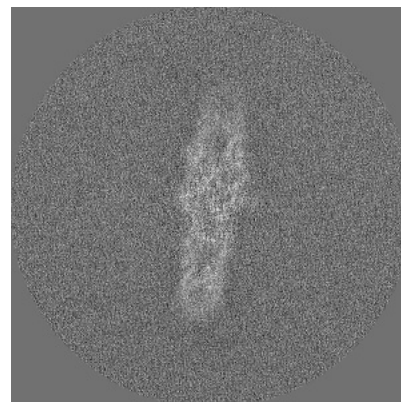
6.2.2 Raw map



X Index: 256



Y Index: 256

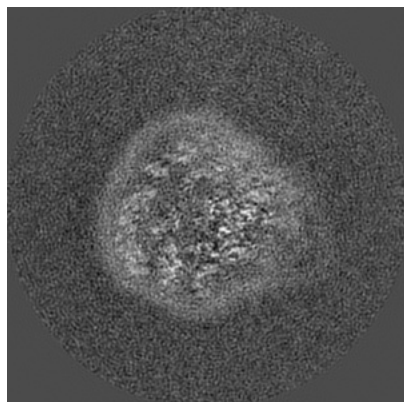


Z Index: 256

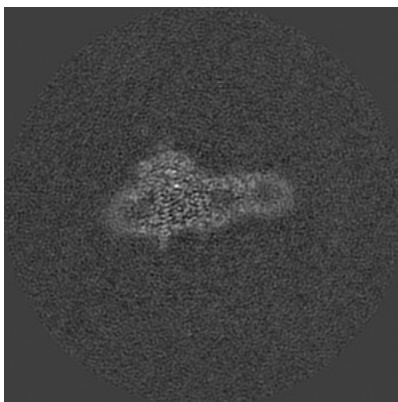
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

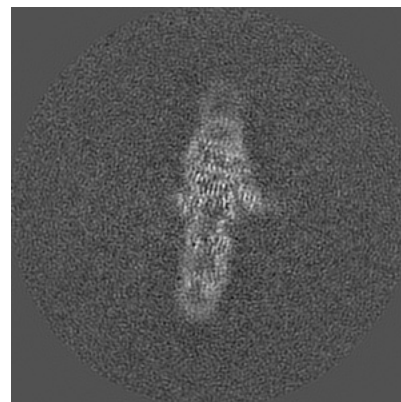
6.3.1 Primary map



X Index: 254

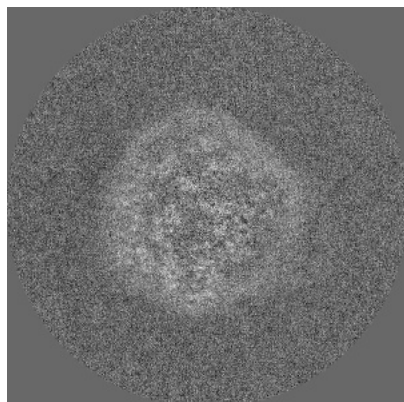


Y Index: 284

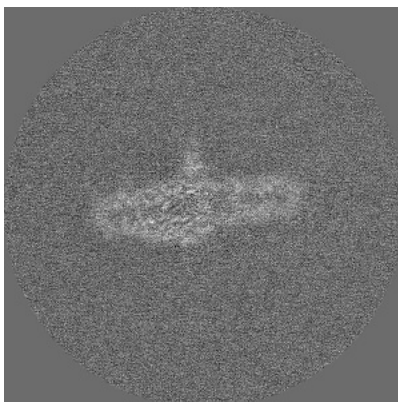


Z Index: 247

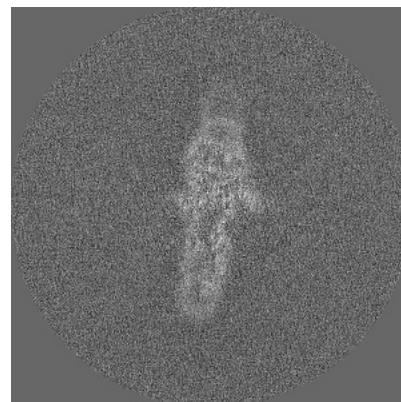
6.3.2 Raw map



X Index: 259



Y Index: 257

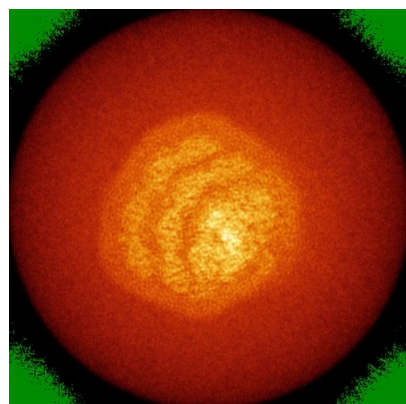


Z Index: 248

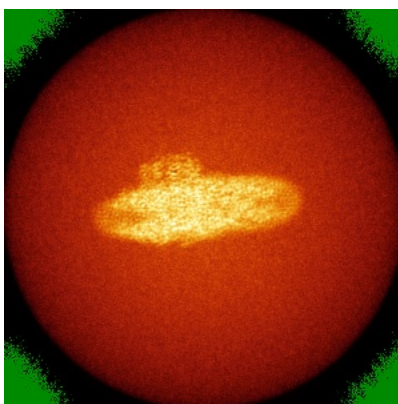
The images above show the largest variance slices of the map in three orthogonal directions.

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

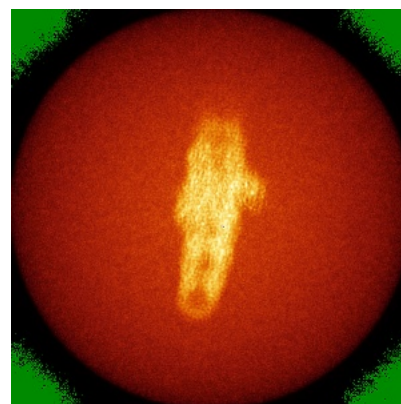
6.4.1 Primary map



X

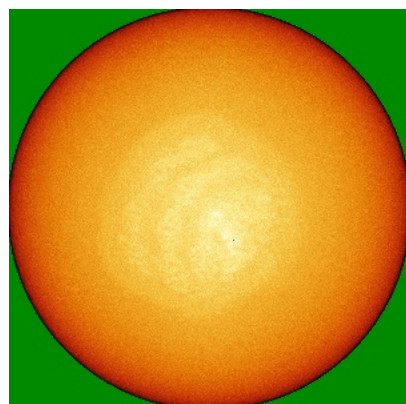


Y

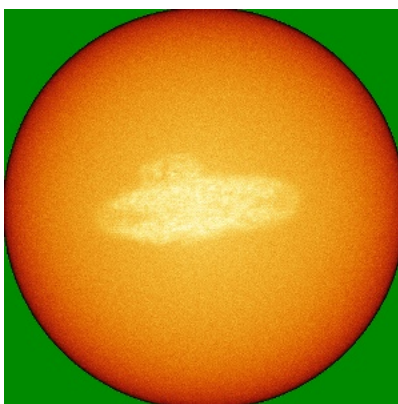


Z

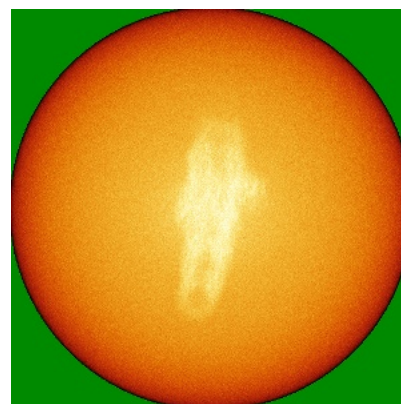
6.4.2 Raw map



X



Y

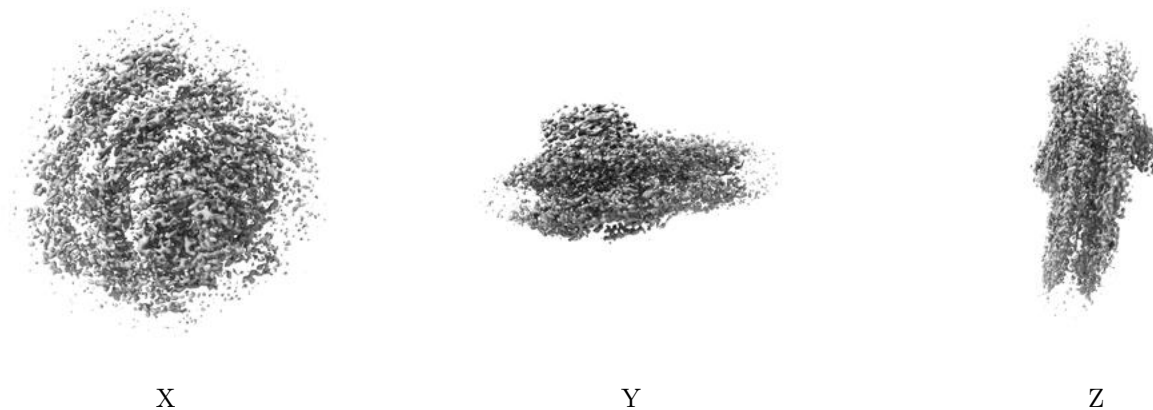


Z

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

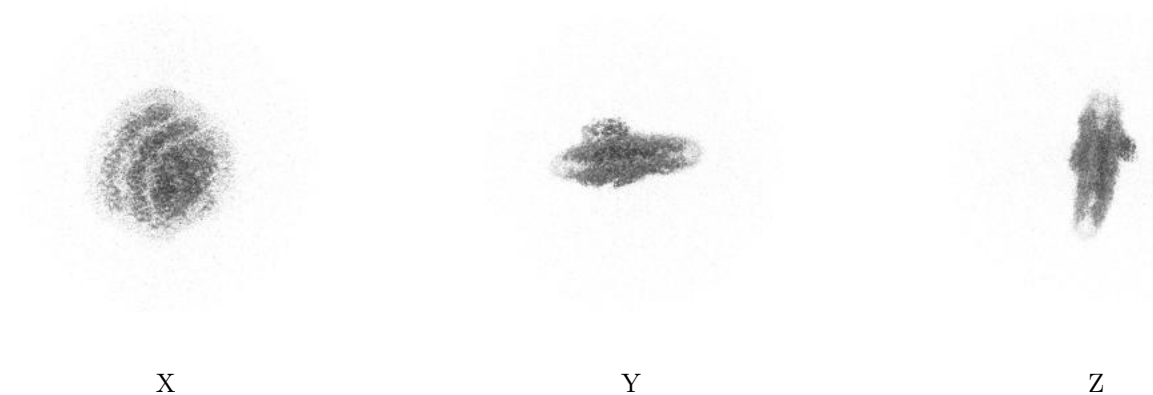
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 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.

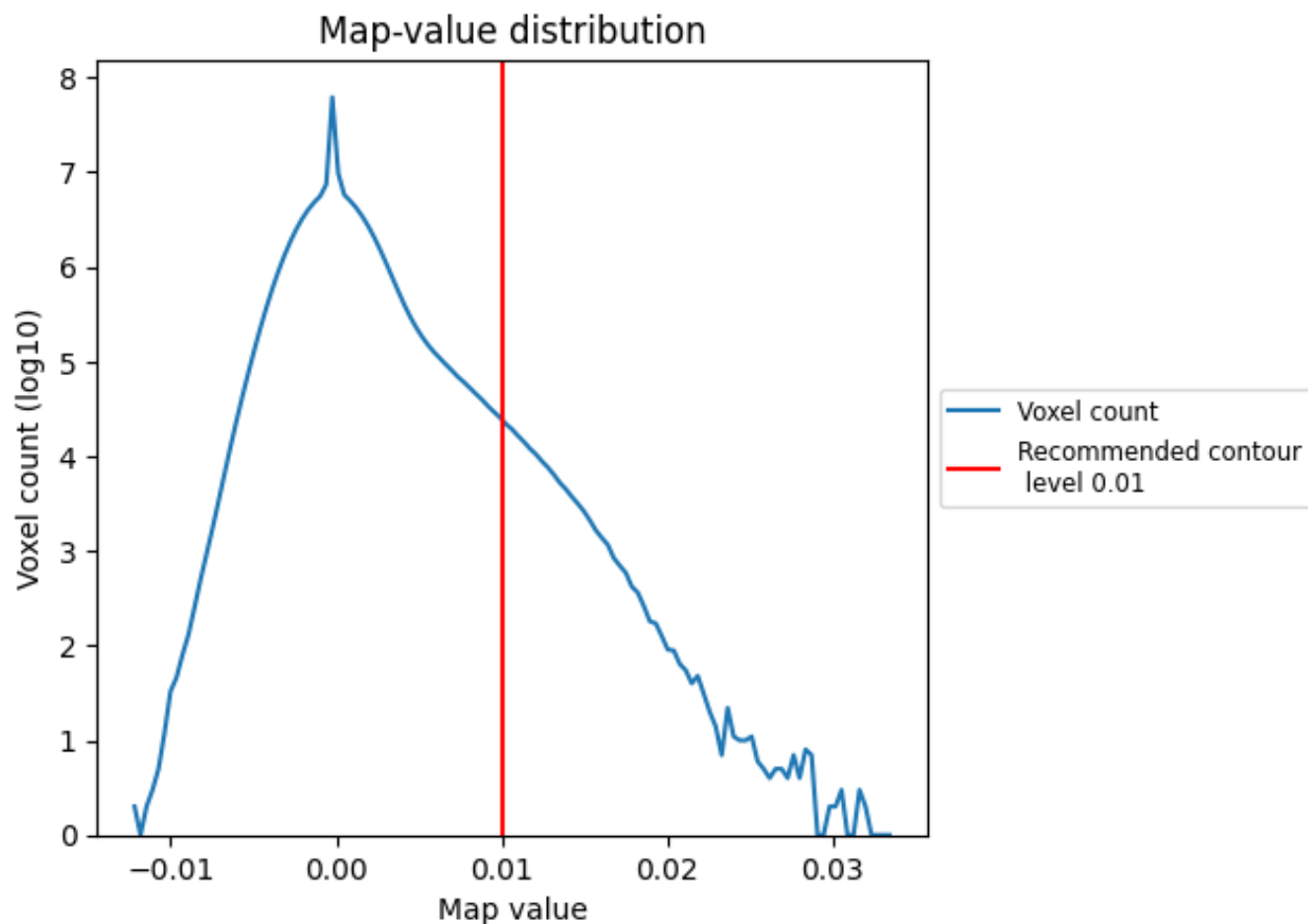
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

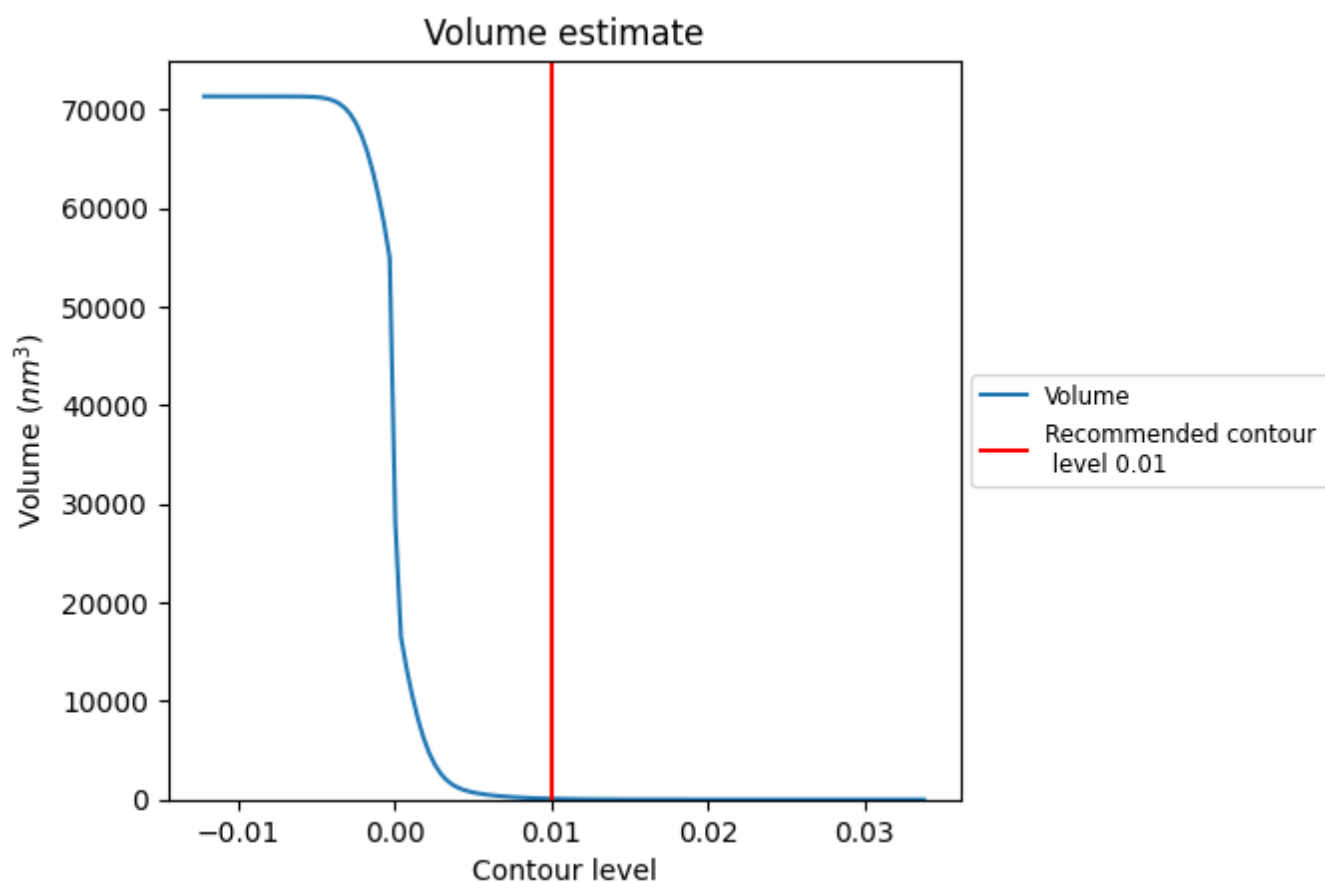
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

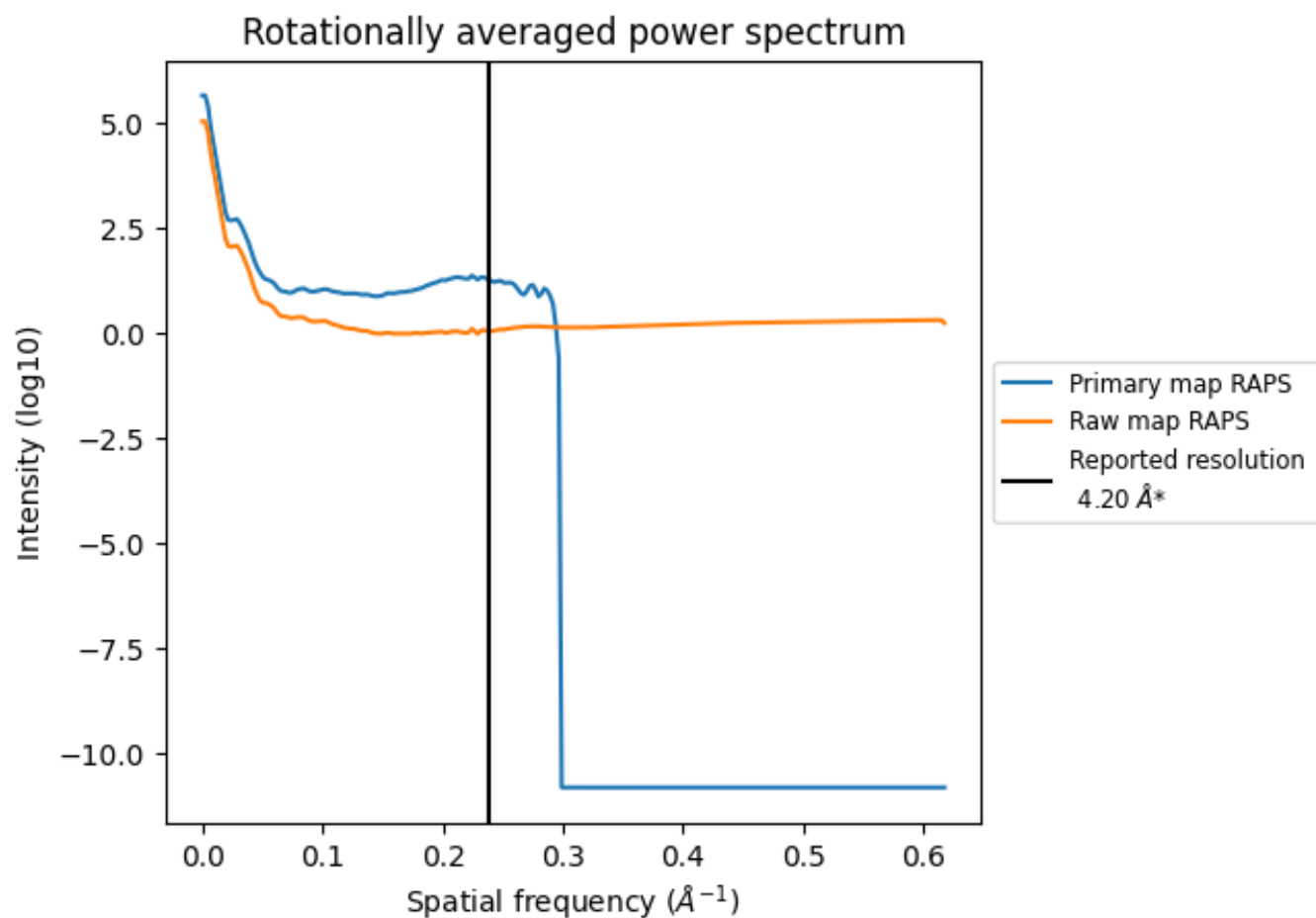
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 ⓘ

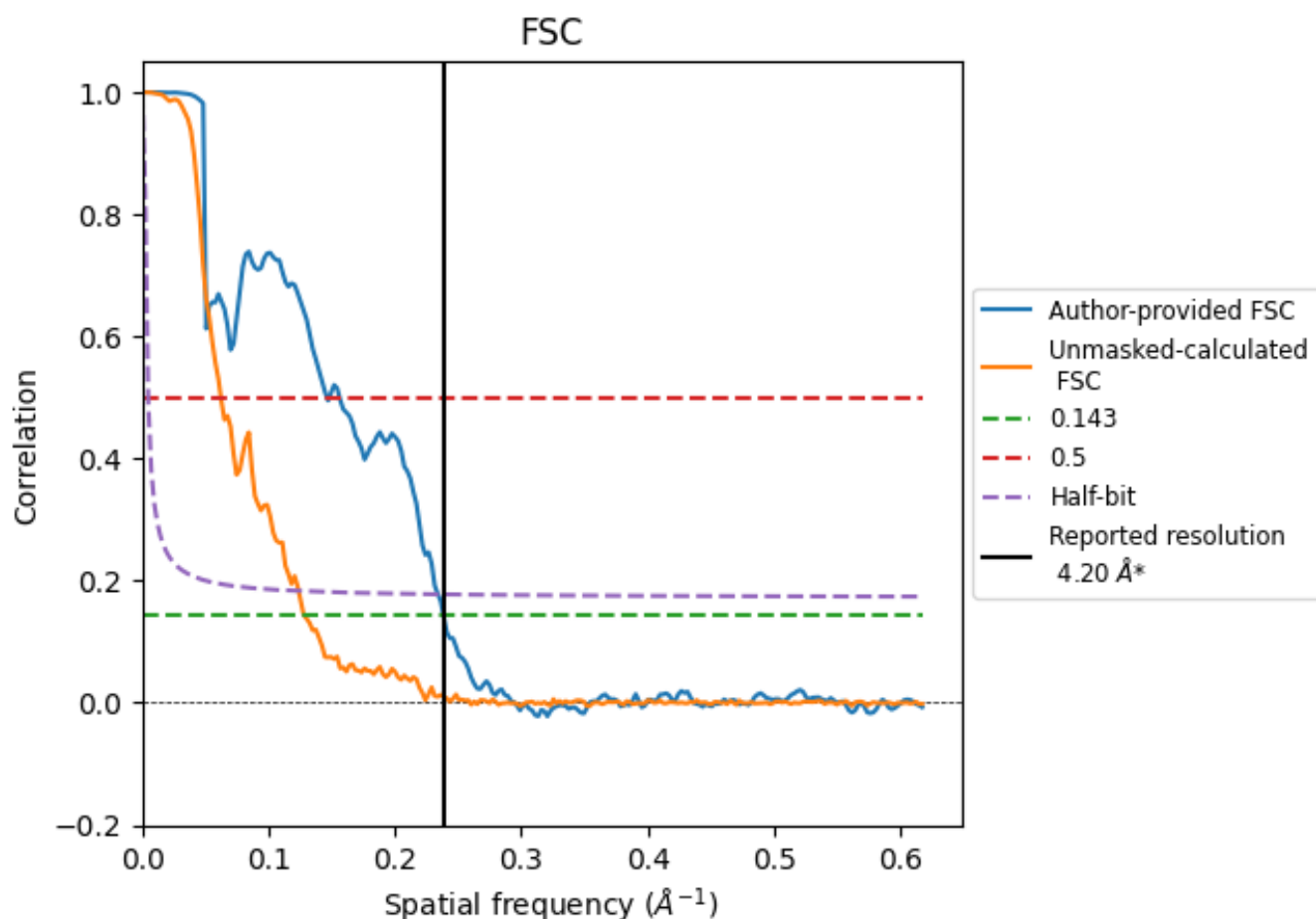


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

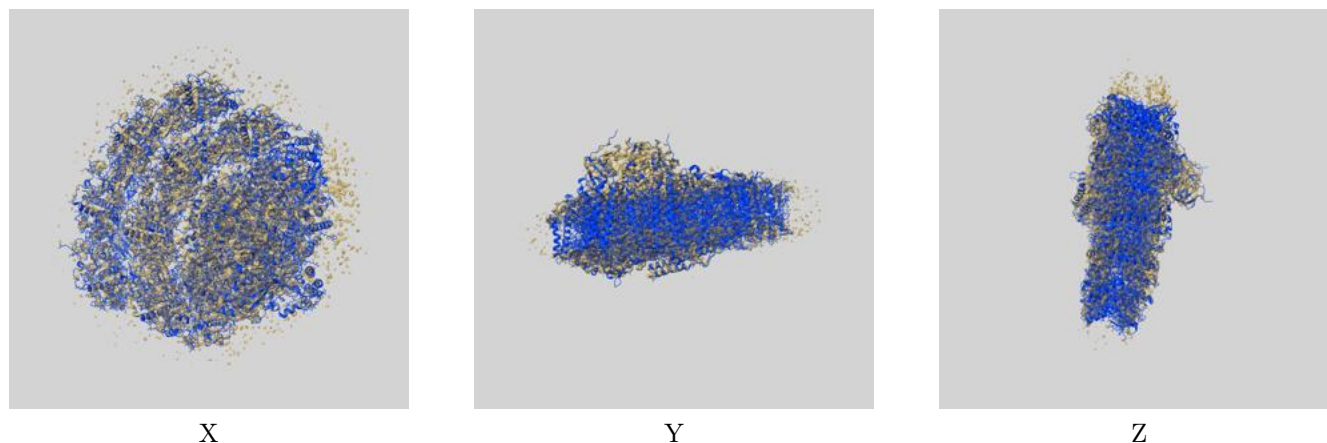
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.19	6.84	4.27
Unmasked-calculated*	7.81	16.08	8.08

*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](#)

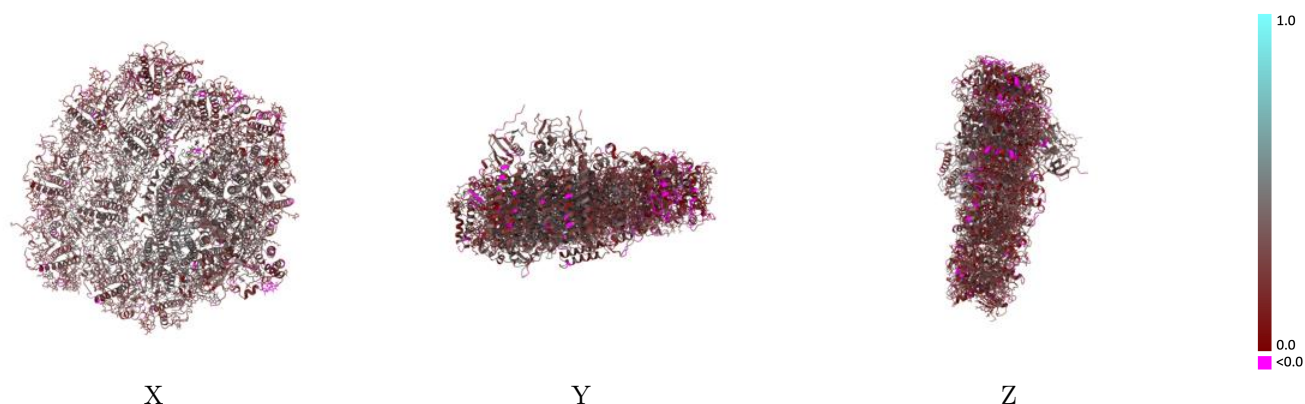
This section contains information regarding the fit between EMDB map EMD-11640 and PDB model 7A4P. Per-residue inclusion information can be found in section [3](#) on page [47](#).

9.1 Map-model overlay [i](#)



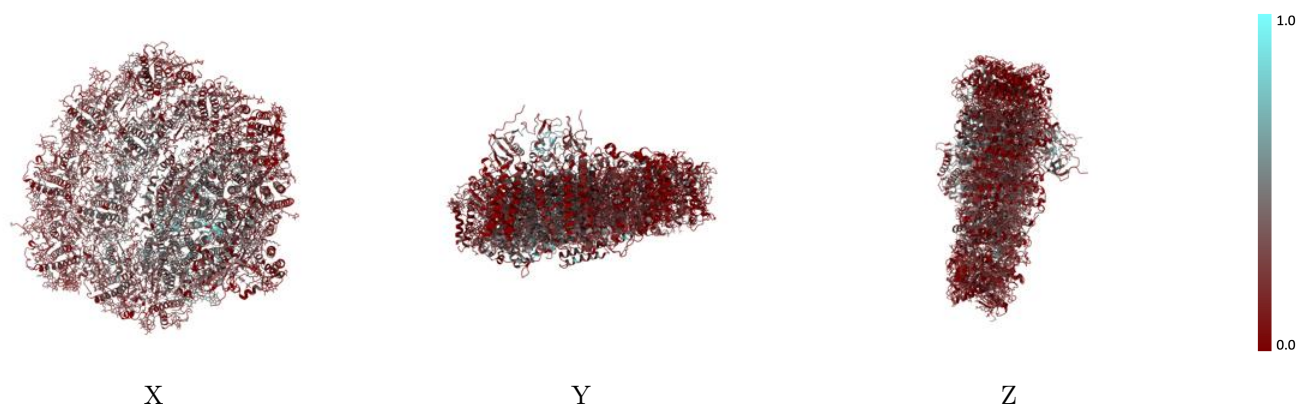
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



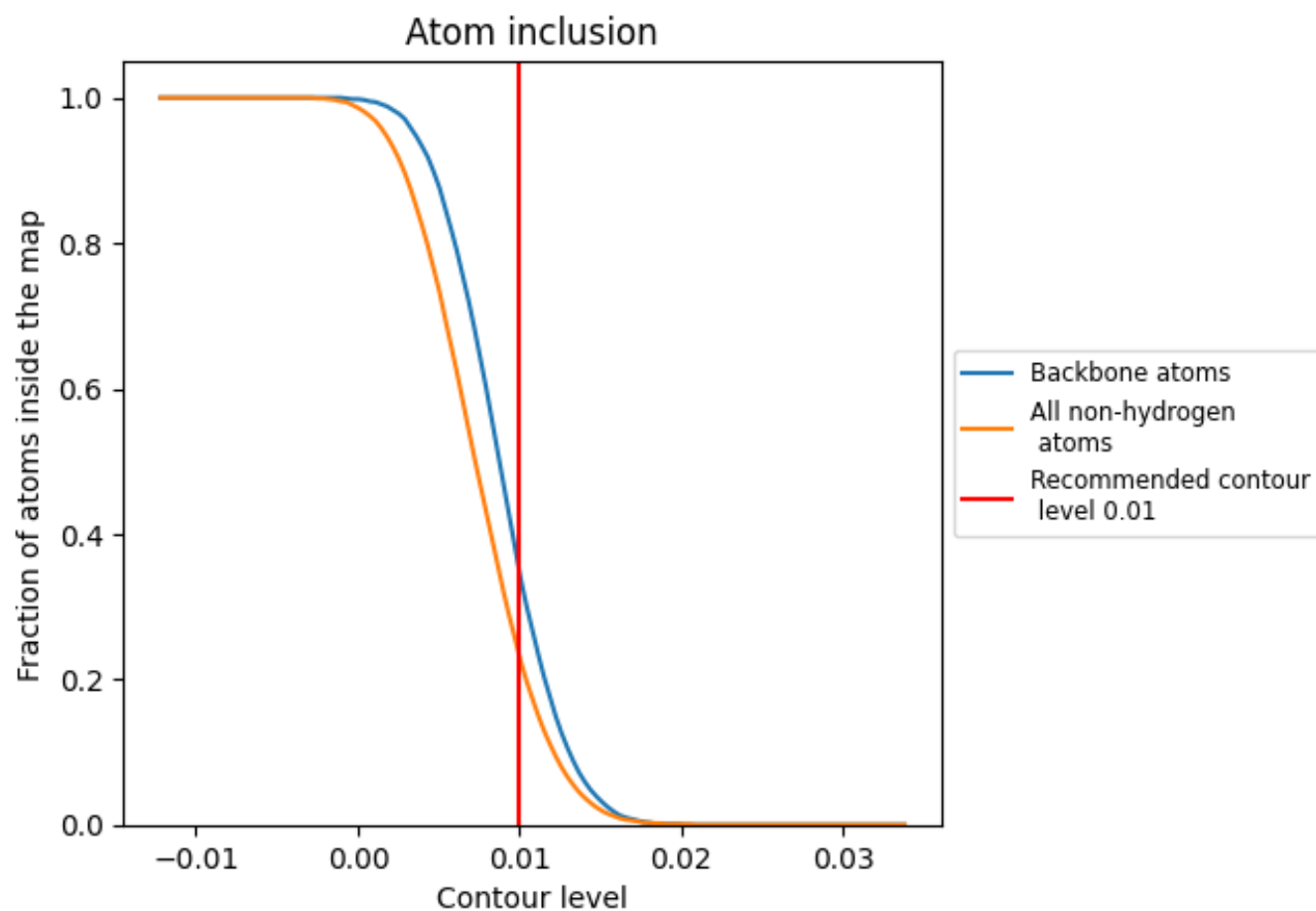
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 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	0.2310	0.2780
1	0.1750	0.2150
3	0.2010	0.2770
4	0.1770	0.2250
5	0.1120	0.2330
6	0.1120	0.2290
7	0.2870	0.2990
8	0.2740	0.2880
A	0.3560	0.3500
B	0.2600	0.3140
C	0.4480	0.3400
D	0.2230	0.2740
E	0.3190	0.2800
F	0.2750	0.2970
G	0.0350	0.1850
I	0.0870	0.2110
J	0.2980	0.3560
K	0.0940	0.2190
L	0.0510	0.1760
M	0.0290	0.1970
a	0.1460	0.1790

